White Paper

GRAND CHALLENGES OF THE FUTURE FOR ENVIRONMENTAL MODELING

Report of the NSF Project (Award # 0630367)
May 2006 - May 2008

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In the Setting of NSF's Environmental Observatories Initiatives

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This *White Paper* has been written solely by the Principal Investigator, who must accordingly assume the customary full responsibility for the views expressed and for any errors and omissions. The overall form of the *Paper* was fashioned initially through an opening Project Workshop held at the University of Arizona, Tucson, Arizona, May 16-17, 2006, and discussions thereafter of the Workshop's outcomes. Design of the Workshop and oversight of subsequent discussion of its outcomes in settling the design of this *White Paper* were the responsibility of an Advisory Committee, whose membership was as follows.

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Grand Challenges of The Future For Environmental Modeling

In the Setting of NSF's Environmental Observatories Initiatives

Foreword

Together with the oncoming environmental cyber-infrastructure,[1] including novel sensors and sensor technologies, the Environmental Observatories (EOs) of the National Science Foundation (NSF) share the collective ambition of bringing unprecedented streams of observations to bear on Environmental Science in the decades to come. Mathematical and computational models are intrinsically generic entities, cutting across specific, disciplinary boundaries, in particular here, those of the Observatories in the Ocean Sciences (ORION), Ecology (NEON), Hydrology and Environmental Engineering (WATERS Network). What new opportunities for research might these EOs bring about for environmental modeling, especially where those opportunities benefit greatly from the cross-cutting, collaborative, integrative style of model building?

This *White Paper* sets out thirteen Grand Challenges of the future for environmental modeling in response to that question. The same grand challenges are also set out in the *Synopsis* of this Paper, which is available as a separate document at www.modeling.uga.edu/EOModels and which can be read as an extended Executive Summary of the present document. Both the *Synopsis* and this *White Paper* introduce and discuss each challenge in the same format: of the context and foundations of — hence, the justification of — why each should have been identified as a challenge in the contemporary research scene; followed by expression of the challenge itself; with then a discussion of some indicative lines of possible responses to the challenge. While composition of this *White Paper* has been prompted by the EO initiatives, our grand challenges have been evolving over the years, and will endure into the future, irrespective of the substantial current commitments to plans for realizing the ambitions of the Observatories. They therefore merit significant consideration as matters for further research in their own right.

Our thirteen challenges span the three domains of:

> ***Science***, predominantly so, and especially in respect of bringing together thinking and research from across the above disciplines, and indeed from beyond them (reaching notably into the biomedical sciences);
>
> ***Policy***, given the vital role of computational models in decision support for environmental stewardship; and
>
> ***Society***, in view of the great, contemporary debate over sustainable development of the biosphere.

Motivated by NSF's EO initiatives, nevertheless, this *White Paper* is concerned to assess how those initiatives, with all their technical innovations in monitoring and sensors, as well as the prospective environmental cyber-infrastructure, have collectively: (i) created entirely novel and unexpected challenges; (ii) accelerated our approach to identifying and defining otherwise less swiftly emerging challenges; or (iii) significantly changed our opportunities for successfully responding to long-standing, recalcitrant challenges of the past several years, if not decades.

[1] The Engineering Research Plan for the WATERS Network defined a cyber-infrastructure in the following terms (WATERS, 2007a): "A cyberenvironment [cyber-infrastructure] is an integrated system for automated collection, storage, retrieval, and analysis of data accessible by multiple parties through a Web portal. It includes various tools for real-time collaboration with other remotely based researchers and provides access to the monitoring information collected by an observatory's field facilities, as well as historical and other relevant data. Analytical (e.g., statistical), modeling, and visualization tools needed to conduct engineering analyses are provided within the system. An operational cyberenvironment also could include control and feedback systems for decision-making and management."

Four recommendations are made. They are intended to be generally indicative of the mix of strategies that might eventually be deployed for developing and implementing specific responses to specific challenges. Especially important in this will be the determined pursuit of more than a superficial appreciation and cultivation of the "people skill-set" required for the conduct of inter-disciplinary research. The recommendations of this *White Paper* are also intended to complement, not duplicate, recommended actions now emerging from the science and education plans of the EOs themselves. There are two recommendations of a more specific nature, however:

(i) The procedures of Observing System Simulation Experiments (OSSEs) should be applied sooner rather than later in designing the Observatories, and certainly *before* their construction; and

(ii) Having now brought together the community associated with this cross-cutting theme of environmental modeling, the fruits of that effort should not be allowed to dissipate through lack of support for its *active* promotion and management in the future.

Passive management, or management "by default", in contrast, will not be a successful strategy for responding to what we are about to express as the grand challenges of the future for environmental modeling.

Preface

How to Use this White Paper

The length of this *White Paper* may be both striking and off-putting to the reader. We offer the following advice, therefore, on how to make the most of the work invested in composing it.

The following *Executive Summary* largely comprises expression of the ***Grand Challenges*** and ***Recommendations*** (exactly as they appear in the main body of the *Paper*). These are linked together with just the minimum of logic necessary to convey an impression of the coherent whole.

A separate *Synopsis*, wherein the logic generating the coherent whole is provided in a more expansive, but nevertheless succint, form, is available for downloading at www.modeling.uga.edu/EOModels.

In the main body of the *White Paper*, we have placed lengthier background, illustrative, or exemplary material in boxes. This material is entirely integral to our justifications for singling out the various ***Challenges***, or to indicating possible lines of responses to them. The purpose of setting such material aside in this manner, however, is to allow the reader to focus on following the overall logic of the *White Paper*, yet in more detail than in the *Synopsis*.

Finally, some words must be offered on the matter of what is understood as a model. Any logical "if"-"then", or like, rule of (mental) reasoning could constitute a *model*. Belief Networks (BNs), for example, are formally organized stacks of such rules, realized in encoded, algorithmic form and manipulated on the computer for deducing outcomes from premises and assumptions. The distinction is a fine and subtle one, however, between where mental reasoning should cease, because of the danger of inconsistent and erroneous reasoning with too many such rules, and computations be commenced with a formal, numerical BN model. It is less subtle in the case of a differential equation as the model. Most, if not all, models would, or should, have begun in this way, through the rules of mental reasoning, before the arrival of differential calculus, or when puzzling for the very first time over how an algal cell grows and divides. In Environmental Science, we have come to equate a model with a set of differential equations, even though it is self evident that other forms of model, such as agent-based models, are now prominent objects of study and manipulation on the computer.

"Model", as used herein, will signal anything that has passed beyond the fine and subtle line of mental reasoning into numerical manipulation on a computer. But while this implies that any form of model along the continuum from BNs to partial differential equations will come within the purview of this *White Paper*, it is acknowledged that models as sets of differential equations are the predominant form of model of concern and discussion. It could be argued, of course, that it should be the purpose of the Environmental Observatories and the environmental cyber-infrastructure to propel the evolution of any model of an environmental system along this continuum towards differential equation forms.

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Executive Summary

MOTIVATION

The National Science Foundation (NSF) is supporting the development of three major Environmental Observatory (EO) initiatives, in the Ocean Sciences, Ecology, and Hydrology-*cum*-Environmental Engineering. Modeling, and the mathematical problems and methods it encompasses, provides a natural language for communication across the various disciplines contributing to the EOs. With this in mind, NSF supported a Workshop in May, 2006, in Tucson, Arizona[2], to begin assessing the views of the environmental modeling community on how it might collectively contribute to the success of the planned EOs. Design of the Workshop and overall design of this *White Paper*, duly informed by the proceedings of the Workshop, were the responsibility of a Committee of sixteen scientists and engineers, chaired by M Bruce Beck of the University of Georgia. The content of the *White Paper* has subsequently been developed from an extensive review of the contemporary literature. The result is a set of ***Grand Challenges*** — their origins, context, and possible lines of enquiry in response to them — for the future of research into Environmental Modeling.

CONTEXT

Environmental models, as we have come to know them over the past half century — as predominantly digital computer realizations of differential-equation solvers — are not going to "go away", no matter how much some members of the Environmental Science community might wish it so (Pilkey and Pilkey-Jarvis, 2007). Great tension between empiricist and theorist is present in the heated contemporary debate over whether climate change influences hurricane intensity and *vice versa* (Mooney, 2007). Such is the stuff indeed of popular fiction (Crichton, 2004). Models are destined to become ever more complex, tending towards Virtual Realities. That progression, however, will not expunge uncertainty. In response to Moorcroft's question (Moorcroft, 2006), we are still some distance, perhaps considerable indeed, from a "predictive science" of the biosphere. And people and policy-makers *will* use models, for good (NRC, 2007) and ill: to shape environmental policy to the likes of their special interests, or repel, oppose, or delay unwanted policy, and in what are called scientifically untenable ways (Pilkey and Pilkey-Jarvis, 2007).

The environment, the biosphere, are just too complex for us to reason through the needs of Policy without models. Yet the more complex the models themselves become, paradoxically the less they may be trusted by the public, and the greater the surprise (to some) when models fail to account for what comes to pass in actuality, as they surely will. Climate models inevitably have incomplete structures and the various alternative models tend to have similar model structures. Consensus can seem stronger and more brightly illuminated than it ought, while significant unknowns and possibilities at the periphery of our understanding and vision are left to lurk in the shadows (Oppenheimer *et al*, 2007).

Some, examining the use of models for forecasting in the domain of Environmental Science, from their perspective in business and econometric forecasting, go so far as to charge this (Green and Armstrong, 2007):

> The forecasts in the [2007 IPCC WG1] Report were not the outcome of scientific procedures. In effect, they were the opinions of scientists transformed by mathematics and obscured by complex writing. Research on forecasting has shown that experts' predictions are not useful in situations involving uncertainty and complexity. We have been unable to identify any scientific forecasts of global warming. Claims that the Earth will get warmer have no more credence than saying that it will get colder.

Models, then, have joined the armory of Policy Foresight and Science, but as a two-edged sword: *Models à la Mode — the Promise and Peril of Integrated Environmental Modeling*, as Clarke entitled his 2004 paper (Clarke, 2004) for the Foresight and Governance Project of the Woodrow Wilson International Center for Scholars (Washington, DC).

[2] Original material for the Workshop can be found at www.modeling.uga.edu/EOModels

THE CHALLENGES

Challenge # 0: Models and the Growth of Knowledge

Neither Environmental Science nor modeling has been the object of sustained enquiry by philosophers of science. If there has been any philosophy of environmental modeling, it has been one of: as computational capacity grows, so larger sets of equations may be solved simultaneously, hence — all else being equal — we shall have models that are ever better approximations of the truth of the matter. We ask, then, as a ***Grand Challenge*** arching over the entirety of this *White Paper*:

> ***How does knowledge grow through the deliberate development, evaluation, and use of a computational model? What, in fact, should be a proper, sound philosophical basis for employing models, by design, in this context of basic scientific discovery; and how can the community of environmental modelers contribute to the construction of these philosophical foundations?***

Challenge # 1: Global Issues of Science

Beyond the customary view of them as formal archives of constituent scientific hypotheses, models can be exploited in a more active manner:

> ***Given the proposed Environmental Observatories (EOs), how can we deliberately design and employ models for the identification of important scientific questions in Environmental Science, with the accompanying potential for basic scientific discovery, in particular, at the interfaces between — and in the interstices amongst — the various disciplines within that Science?***

Such questions of a *global* scientific nature, associated expressly with modeling, are defined *not* in the sense of "extending over the entire globe", but in the sense that they can only be perceived and addressed when a (reasonably complex) model of the multi-disciplinary *whole* has been assembled from the mono-disciplinary, sub-model *parts*.

Challenge # 2: Role of Cyber-infrastructure in Addressing Global Issues

Delving more deeply into the computational mechanics of responding to ***Challenge # 1***:

> ***What kinds of software platforms within the environmental cyber-infrastructure will be necessary for supporting extensive, heuristic experimentation with a model's structure, i.e., in facilitating experimental "rewiring" of its constituent hypotheses and their interconnections in the assembly of the whole, while the inter-disciplinary community of environmental scientists works at formulating and resolving core science questions in the interstices amongst the constituent disciplines?***

How, for example, could the environmental cyber-infrastructure — as the complement of the manual labors of the scientific analyst under ***Challenge # 1*** — increasingly automate coverage of all the gaps amongst the disciplines, so that the potential discovery of significance is not overlooked? At the same time, how could it facilitate discrimination of the singularly key from the plethora of potentially spurious constituent hypotheses of which the multi-disciplinary whole of the model has been composed?

Challenge # 3: Universal Science Issues and Process Mechanisms

We know that variations across scales of observation and simulation are crucial to understanding and stewarding biodiversity and resilience of behavior in environmental systems:

> ***Is there a unifying and uniquely distinctive approach to the use of models in exploring issues of scale, and cross-scale interactions, along each of the three dimensions of (i) time, (ii) space, and (iii) biogeochemistry, where this last manifests itself across scales from molecular biology up to all the chemical and biological species comprising whole ecosystems?***

Challenge # 4: *Universal Science Issues of a Biological Nature*

We may be forgiven for believing we live in a "biological age". All of the "Recommended Immediate Research Investments" of the NRC's 2001 Report on the *Grand Challenges of Environmental Sciences* (NRC, 2001) relate to ecology. Hence:

> ***What breakthroughs are needed in order to develop a more effective and complete paradigm of modeling biological processes — common to the ocean sciences as much as to terrestrial ecology or biological wastewater treatment — across all scales: from molecular biology to whole ecosystems, and including mimicking of the intelligence and metabolism of individuals in a population, their movement through an environment, and their interactions with other individuals, as a function of that intelligence and metabolism?***

What novelty might then be unleashed by turning insights, acquired from working with the Individual Based Models of ecological and social systems, towards study of the predominant physics and differential-equation models of Hydrology and the Ocean Sciences?

Challenge # 5: *Applied Mathematics and Generic, Dynamical Systems Properties*

While there is the scope for significant rewards to be returned from bringing together the various disciplines of the EOs through the devices of modeling, so the community of environmental modelers should be assiduous in ever looking outwards from the confines of their own collective discipline:

> ***Building on the shoulders of the various mathematical theories of catastrophe, chaos, and complexity — but with the ambition to go beyond these — what new insights into the generic and fundamental dynamic properties of the behavior of systems can be obtained from the deliberately orchestrated*** **in situ** ***observation of the behavior of many specific environmental systems and the modeling thereof? In particular, how can the rich experience of elucidating these generic features from studies of whole ecosystems, indeed social-ecological systems, be productively interfaced with exploration of the novel properties of dynamical systems behavior yet to be discovered in the study of cellular metabolism, self-repair, and self-replication? How can coordination of relevant research across all of the Environmental Observatories uniquely accelerate such development? Looking towards*** **Challenge # 12**, ***how can the community of model-builders in the Environmental Sciences best be organized so as to benefit as much as possible from novel developments in modeling in general, as they arise in, for example, the quite disparate disciplines of the biomedical sciences, social sciences, cognitive sciences, artificial intelligence, and artificial life?***

How, in other words, might study of the behavior of *specific* environmental systems contribute to the development of *generic* theories about the behavior of dynamic systems?

Challenge # 6: *Observatory Network Design and Operation*

We know well enough the merits of Observing System Simulation Experiments (OSSEs). Their future use in the design of the EOs constitutes the rare exception of being a specific recommendation of this *White Paper*. But what of the subsequent stages in the life cycles of the Observatories, for which we ask:

> ***Given a mature complex of environmental cyber-infrastructure and sensors, with — crucially — both an ever-alert monitoring and horizon-scanning facility and in-depth capacity for real-time processing of information and production of knowledge, what kinds of novel, model-based computational schemes of adaptive environmental sampling will be needed to enable rapid re-targeting of observing capacity for on-line probing of, and experimentation with, systems behavior?***

The cyber-infrastructure of Mahinthakumar *et al* (2006) — inspired by the emergence of "Dynamic Data Driven Applications Systems" (DDDAS; Darema, 2005), and intended for threat-response in public, potable water supply systems — is one instance of the vision implied in answering such a question.

Challenge # 7: System Identification

This, which is to say, model calibration writ massively more richly, is pivotal in reconciling observation with theory. As a problem it has been long-standing and inadequately treated, and largely, but not entirely so, because of the historic absence of adequate streams of field data. The unresolved, but engaging, tension between empiricists and theorists in Mooney's 2007 popular-science book *Storm World*, provides every reason for why our community should be drawn to this challenge:

> ***Under the expectation of massive expansion in the scope and volume of field observations generated by the Environmental Observatories coupled and integrated with the prospect of equally massive expansion in data processing and scientific visualization enabled by the future environmental cyber-infrastructure, what radically novel procedures and algorithms are needed to rectify the chronic, historical deficit of the past four decades in engaging complex models (VHOMs)[3] systematically and successfully with field data for the purposes of learning and discovery and, thereby, enhancing the growth of environmental knowledge?***

The environmental cyber-infrastructure holds out the promise of supporting the "tinkering paradigm" from ***Challenge # 2,*** of rewiring at will the constituent hypotheses assembled in the model. Scientific visualization and animation of the conceptual structure of the model — not its input or output data fields — can be expected to be a necessary part of realizing this intellectual support.

Challenge # 8: Predictive Science and Uncertainty

Taking a lead from the question that is the title to his paper (Moorcroft, 2006), "How Close Are We To a Predictive Science of the Biosphere?", this *White Paper* enquires:

> ***Recognizing the inevitably flawed and uncertain conceptual foundations of many environmental models — while acknowledging the possibility of natural features of biological acclimation, even evolution, over a longer-term horizon, especially in response to the introduction of invasive species, and the high likelihood of continual adaptation in the behavior of many types of environmental system — how are structural error/uncertainty and structural change in these models to be identified, quantified, rectified, and accounted for (in the propagation of prediction errors and the making of decisions)? What new schemes of generating environmental foresight will be needed to cope with these challenges?***

And to some considerable extent, the rejoinder to Moorcroft's question can be found in Oppenheimer *et al* (2007), who in their turn question the value of premature consensus around climate change assessments, when in truth structural error/uncertainty in models seems both inevitable and to be guarded against.

Challenge # 9: Assimilating Data and Processing Information in Real-time

To be able to conduct the affairs of science and environmental engineering in "real-time" is recognized as a major opportunity for the community of environmental modelers. It is in keeping with the general quickening of the pace of things, as a manifestation of contemporary society. Under the EO initiatives, employing models and signal-processing algorithms in real time has all the thrill of conquering some final technical frontier:

> ***In a world of increasing inter-connectedness and instantaneous communication, environmental vulnerability, and infrastructure systems fragility — subject in all probability to higher-amplitude extreme events, natural disasters, terrorist threats, and the like — how best can the expected innovations in cyber-infrastructure***

[3] Very High Order Models.

and sensors under the Environmental Observatories programs be used in developing models and real-time data-processing and forecasting algorithms: for the on-line detection of faults, failures, anomalies, and the weak signals portending imminent dislocations in system behavior; and for orchestrating/guiding rapid counter-measures for enhancing and resuscitating/reviving damaged system functioning, system survivability, and resilience?

Whereas ***Challenge # 6*** asked how might models be used to inform the deployment and re-deployment of observing capacity in a built, operational EO, ***Challenge # 9*** is now different. The challenge is one of reconstructing coherent, homogeneous fields of variables internal to the model: in particular, from all manner of heterogeneous observing platforms and devices; and, in principle, across the dimensions of time, space, *and* biogeochemistry. In this — as opposed to many of the preceding ***Challenges***, wherein questions of a biological or ecological nature tend to predominate — studies tied to the relevant physical attributes of Hydrology and Oceanography are expected to continue to be in the vanguard of responses.

Challenge # 10: Management and Decision-support

In the measured prose of any report from the National Research Council, we find acknowledgment of a turning away from the prevailing view of models as "truth-generating machines" towards an outlook embracing other perspectives, most notably that of the model as a "tool", such as a hammer or screwdriver, designed to fulfil, in particular, the predictive tasks of supporting regulatory, environmental decision-making (NRC, 2007). In more colorful terms, van der Sluijs (2007) introduces the image of uncertainty as the "monster" at the interface between Science and Policy — monstrous in the sense of confusing what were previously kept strictly separate, i.e., the objectivity of Science and the subjectivity of value systems. This *White Paper* asks, therefore:

Under the prospect of lengthy and costly social negotiation and legal discourse over policy formation, wherein the placing of trust by various stakeholders in the models underpinning that policy is crucial, and where it has come to be recognized that the needs of model evaluation and peer review for conventional research science are different from those of regulatory science, what new methods of evaluating the alternative models designed to fulfil the predictive tasks of policy formation, decision-support, and management for environmental stewardship are urgently needed? How is the uncertainty associated with both the model and the decision-making context to be handled computationally and what new algorithmic and procedural developments will this warrant?

Challenge # 11: The Long View: Towards Sustainability of the Built Environment

Since the greatest debate of our times is the "sustainability debate", with its significant implications for the design and operation of the built infrastructure at the interface between Man and Environment (most conspicuously so at the urban centers of socio-economic activity), how best should the Environmental Observatories be deployed and, more specifically, what kinds of models should be developed in order to promote a better strategic alignment of the study of urban metabolism with that of ecosystem services, all within the web of global biogeochemical cycles? How too, in the widest of possible terms, can innovations in information and communication technologies (ICT) — as realized in the environmental cyber-infrastructure — lead to tangible gains in reducing the unsustainability of current patterns of socio-economic behavior?

It is easy to imagine mathematical programming and optimization to have been made for charting a course towards sustainability of the built environment: find those policies and technologies maximizing the rate of departure from unsustainability, subject to their satisfying the constraints of being {environmentally benign}, {economically feasible}, and {socially legitimate} — the triple bottom line. A fine line indeed separates what of human nature, preferences, and values should be approximated and manipulated by a model and what should rightly remain in the space of public debate and democracy.

A simulated life-time of *your* simulated self with *your* personal/private preferences, undergoing forms of learning and negotiation with other simulated beings over aspirations for less unsustainable futures, is in prospect. Environmental modeling, and those who construct and use models, may increasingly be drawn into the unfamiliar territory of unusual and novel questions of ethics.

Challenge # 12: Community Structure

Looking across the ***Grand Challenges*** now expressed, each calls for investments in changing habits of mind as much as in equipment, computing, specialized field campaigns, and so on. We ask therefore:

> ***What steps can the community of model-builders in the Environmental Sciences take to pre-empt and reduce to a minimum the still readily apparent scope for re-inventing the "wheels" of modeling in contemporary research across the various disciplines of the EOs? How can our community best be organized so as to benefit as much as possible from novel developments in modeling in general, as they arise in, for example, the quite disparate disciplines of the biomedical sciences, social sciences, cognitive sciences, artificial intelligence, and artificial life? More broadly, how should the community of modelers best work with the community of primary field scientists to promote the development of models for basic scientific discovery at the interfaces amongst multiple disciplines? In the light of universal and ever-more urgent calls for profound changes in the manner in which the next generation of scientists and engineers is educated, trained, and formed — all of which calls focus on "inter-disciplinarity" — what special role can models serve in meeting these needs?***

RECOMMENDATIONS

Two general and then two specific recommendations follow.

Recommendation # 1: Within Community Orchestration: Substance **Not** *Form*

Models, as the *lingua franca* for communicating amongst the Ocean Sciences, Ecology, Hydrology, and Environmental Engineering, are integral to our becoming inter-disciplinary.

> ***Having brought a significant proportion of the community together, through a Workshop, and now — by virtue of the literature reviewed herein — this*** **White Paper*****, it would be a missed opportunity not to provide the wherewithal for the continuing active maintenance, development, and scientific prosperity of the modeling community under the EO initiatives.***

Inasmuch as not all of us have the talents for becoming an astronaut or brain surgeon, not everyone is suited to engaging fully and effectively in inter-disciplinary work, including when the object of enquiry is the development and application of models. Substance, as in recognizing and cultivating an appropriate set of "people skills", may be more important than the organizational and administrative form of community orchestration.

Recommendation # 2: Cross-Community Communication: Attaining The Bigger Picture

The mathematical methods of modeling, like the software and algorithms of an environmental cyber-infrastructure, can seem opaque and impenetrable when radical inter-disciplinarity and cross-communication are called for, between the technical expert and the technically lay person, even when seemingly so little as the divide between the field science and the modeling must be bridged. The oft-heard plea to "Let the data speak for themselves" is revealing of the attitudes of other professional scientists towards modeling and modelers.

Given that modeling cannot proceed in a vacuum, detached from reality, case studies and case histories should be prepared and packaged in forms designed to serve the ever-present need of the modeling community to build and maintain fruitful relationships with a variety of other communities — of philosophers, scientists, engineers, scholars, policy-makers, and the public — in developing the beginnings of responses to the Grand Challenges.

Environmental modeling has now a history of at least four decades to look back upon. This is long enough for us to discern the significance — or otherwise — of models: from their role in the philosophy of science and the growth of knowledge, to that in the successive and "jerky" exchanges between Science and Policy, such as those recorded in Dennis (2002) and Schertzer and Lam (2002). The very struggles within our own community, to attain that strategic sense of the "big picture", should facilitate its articulation in a variety of more comprehensible forms for a variety of audiences. It is time to engage in such struggles.

Recommendation # 3: *Models for Design/operation of the EOs*

Given the maturity of Observing System Simulation Experiments (OSSEs), and their obvious potential role in the design of all the Environmental Observatories, investment in the work needed to respond to this facet of Challenge # 6 is recommended. In seeking progress on a variety of fronts, however, such investment should be directed beyond the pragmatic needs of EO design, for example: to furthering the social and professional aspects of bridging any divides between the field-science and model-building communities; and to propelling OSSEs as much as possible beyond the current state of their art.

As generally understood in an OSSE, simulation is based on sets of differential equations as representations of the observed system's behavior. Developing schemes of OSSEs founded upon the Individual Based Models (IBM) typical of Ecology appears to remain as yet an essentially untouched domain of research.

Recommendation # 4: *Training the Next Generation*

Having argued a case in favor of the special role of models, as the **lingua franca** ***of inter-disciplinary research, we recommend investigating the merits of complementary alternatives to vehicles such as NSF's Integrated Graduate Education Research and Training (IGERT) schemes for the purpose of training the next generation of environmental modelers.***

We would not want to pursue any alternative, however, without a systematic prior assessment of how young researchers mature to become leaders of inter-disciplinary thinking.

CONCLUSION

Models need data for their evaluation. Essentially, we wish to know whether the model approximates well enough the behavior of the real thing. Imagining a future with High Volume High Quality (HVHQ) streams of data emanating from the Environmental Observatories is to look beyond a "nonlinear" break with the terms and conditions under which Environmental Modeling has labored in the past. Reconciling Very High Order Models (VHOMs) with the HVHQ data of the EOs, in the workspace of the future environmental cyber-infrastructure attuned to provoking new knowledge, has thus the air of a ***Grand Challenge*** that is *primus inter pares*.

Acknowledgments

As Principal Investigator of the Project (and Workshop) from which this *White Paper* has emerged, I am indebted to many persons. First of all, there are my colleagues on the Advisory Committee, who have long awaited the Project's outcome, which is this *White Paper*. For their patience and assistance, I thank them. It is a pleasure to record my thanks to Hoshin Gupta, Ed Rastetter, David Tarboton, and Chris Shoemaker, in particular. I thank Hoshin Gupta, most especially, for his diligence and the giving of constant encouragement. And I am grateful to Jerry Stedinger for his comments on an earlier draft of this *Paper*. Special thanks are also due to Dr Femi Osidele (SouthWest Research Institute, San Antonio, Texas) and Dr Zhulu Lin (North Dakota State University, Fargo) for their assistance throughout the Project. I am also grateful to all those who participated in the Tucson Workshop, in particular, to Dr Yuqiong Liu and Koray K Yilmaz of the University of Arizona. Together with Drs Osidele and Lin, they acted as Workshop Rapporteurs. On-site logistical support for the Tucson Workshop was graciously given by Rannie Fox.

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It is a rare pleasure too to record here my sincere thanks to Jenny Yearwood, Program Coordinator, University of Georgia, whose administration of this Project during its entire two years — and for all of the work of my office for many years prior to this Project — has afforded me the luxury of focusing on enquiry, research, and writing. I also wish to acknowledge what has been for me a most satisfying, and startling, experience in the graphical design and layout of this *White Paper*. In one 30-minute conversation with J P Bond, Graphics Designer, Warnell School of Forestry and Natural Resources, University of Georgia, I was enabled to express a research agenda I had been coveting — visually, in my mind, if inarticulately so — since about 1996. It is entirely fitting to thank J P for this and for the graphical design and production of this *White Paper*.

Last, I wish to acknowledge the profoundly important privilege it has been for me to occupy the Wheatley-Georgia Research Alliance Chair at the University of Georgia these past 15 years and more. I am just as happy to acknowledge the significant influence on this *Paper* of my continuing involvement with the International Institute for Applied Systems Analysis (IIASA), Laxenburg, Austria.

M B Beck

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April, 2009

PART I:
INTRODUCTION

Chapter 1: Why Models?

What we can all readily appreciate today about the behavior of our environment is its complexity: massive in its extent, yet impressively subtle and almost incomprehensibly intricate in its detail. We can reason with classical pencil and paper about the ramifications of man's actions — disturbances and perturbations of the environment — up to a point. Beyond that, our reasoning over the past 40 years or so has become progressively more reliant on the development and application of computational models.

Indeed, the uniquely distinctive and essential role of a model is to allow us to grapple with such complexity. This is especially true in respect of being utterly systematic in connecting together multiple, constituent hypotheses — each of greater or lesser security — about the behavior of complex systems. While we would not use computational models to reason through elementary problems (except where extremely fast, unerring decisions must be made, as in automated, real-time control), the inner workings of models of complex systems must nevertheless ultimately be comprehended succinctly: by model developers, from a multiplicity of disciplines; by model users; policy makers; and by those scientifically lay parties affected by the decisions guided by models. The irony, then, is that in the end our essential understanding of the environment — albeit duly informed by models — may have to be expressible in just the ordinary terms to which pencil and the proverbial "back of an envelope" naturally confine us.[1]

No-one, of course, is conceiving of the Environmental Observatories (EOs) of the National Science Foundation (NSF) in the *absence* of a significant role for models. This *Paper* addresses therefore the strategic question of what exactly should be the elements of that "significant role": in support of the primary science to be conducted under the auspices of the EOs; in articulating the fruits of that science at the interfaces amongst environmental science, policy, stewardship, and the public; and in promoting substantial advances in the scope, sophistication, and practical relevance of environmental modeling, in particular, across *all* the disciplines of the EOs.

We begin with some prefatory considerations of philosophy and method. These are necessarily neither simple nor readily accessible to a general reader. But they are brief and their tone should not be read as that of the entirety of this *White Paper*.

1.1 Over-arching Challenge: Models and the Growth of Knowledge

We know that models can be used as succinct archives of knowledge, as instruments of prediction in support of making decisions and stewardship of the environment, or as devices for communicating scientific knowledge to a scientifically lay audience. But how, we must ask, might the development and application of models serve the purposes of basic scientific discovery and, therefore, the growth of knowledge? For the EOs are first and foremost science- and research-led programs.

Let us set down, then, an over-arching challenge for this entire *Paper*.

Challenge # 0:

> ***How does knowledge grow through the deliberate development, evaluation, and use of a computational model? What, in fact, should be a proper, sound philosophical basis for employing models, by design, in this context of basic scientific discovery; and how can the community of environmental modelers contribute to the construction of these philosophical foundations?***

[1] The evidence from research on judgement and decision-making still errs towards the essential conclusion from Kahneman *et al* (1982): that a great deal of our reasoning and deciding is based on simple heuristics, which reduce what would otherwise be a process consuming vast computational resources and time in order to arrive at a "normatively correct solution" (Ayton, 2007). Essentially here, all involved parties must — somehow — come to judgements *inter alia* on the quality and reliability of models and their forecasts.

In an article on interactive computing as a teaching aid, MacFarlane (1990) presented a three-element characterization of knowledge. According to the American philosopher Lewis these three elements are (as reported by MacFarlane):

(i) the given data;

(ii) a set of concepts; and

(iii) acts which interpret data in terms of concepts.

While we do not propose to enter here into any deep philosophical treatment of our subject nor suggest that we subscribe solely to Lewis's particular philosophy of science — for those are in fact the subjects of the challenge — we note in passing that he was associated with the American pragmatist school of thought. Rather, these three pillars, and their inter-relationships, will help to structure our introduction of this *Paper* and therefore clarify the roles of modeling within the EOs.

Thus, for example, we can see that the impact of the EOs on the *given data* in this schema should be substantial and profound. Excellence in modeling cannot be achieved in the absence of first-class data for rigorous (whole) model testing and evaluation.

Just as profound, if not more so, should be the impact of the environmental cyber-infrastructure on mechanizing the *set of concepts* in computable form — although we should take care not to confuse the notion of a computational model entirely with the set of concepts or a theory. For models are a secondary science, in the sense of enabling organized assembly and encoding of the distilled knowledge emerging from the primary field sciences. But that distilled knowledge is not indisputable fact. It is an assembly of a host of constituent "atomistic" theoretical elements, each themselves reflecting individual hypotheses quarried from laboratory science or a particular field science, often crafted in disciplinary compartments without the benefit of the entire picture of the whole system necessarily in mind. The environmental systems we observe and study behave as indivisible wholes, however, so that a basic question becomes: when placed together in the organized structure of a computational model, which of the constituent hypotheses are adequate/inadequate, in terms of determining the performance of the whole; and how should the inadequate constituents be removed, modified, and re-introduced in more adequate form? The urgency of this matter can only but grow as mounts the number of constituent hypotheses upon which one wishes to draw (for a description of the real system's behavior).

What will be the implications of these profoundly important advances — in the sensing technologies of the EOs and in the environmental cyber-infrastructure — for Lewis's *acts which interpret data in terms of concepts*? Indeed, how does this interpretation actually come about? How does one, for example, reconcile a large-scale geophysical model of global deglaciation with (reconstructed) relative sea level observations at 392 sites spanning a period of some 15,000 years (Tushingham and Peltier, 1992)? More specifically, which constituents of the very large and very complex assembly of micro-scale theory is at fault when the model fails — as inevitably it does — to match the relatively macroscopic historical observations? Interpretation is a result of juggling with, and sifting through, a unique assortment of disparate facts and figures assembled by the individual, upon which some kind of order is eventually imposed. It is a subjective mental process.

In short, that there will be significant developments in the technical support necessary for engaging the model in a meaningful interpretation of the data, is by no means assured. News of advances in computational capacity is abundant (witness NSF, 2006); news of advances in the technology of instrumentation and remote sensing is commonplace (witness NSF, 2005); news of the *increasing* capacity of the brain to juggle with disparate facts and concepts is non-existent. In this resides arguably the greatest of opportunities to flow from the EOs and the oncoming environmental cyber-infrastructure for the future of environmental modeling — as in responding to what will be expressed subsequently as our grand ***Challenge # 7***.[2]

Lewis, of course, offered up his philosophical views long before computational models were in widespread use. His three-element characterization of how knowledge grows must be re-visited and now re-examined, especially in the light of our own personal experiences as modelers. For why should not those of us working at the "coal face" of modeling environmental systems reflect on how we have gone about our research over the past several decades, thus to contribute to building a contemporary perspective

[2] Throughout this *Paper* grand challenges will be denoted with this typeface.

on the philosophical basis for the role of models in the advance of scientific knowledge? The paper of Beven (2002) is one such exemplar, albeit biased towards the physics of water flows in hydrology, as opposed to the biogeochemistry of ecology. The book by Petersen (2006) is a more substantial, deeper treatment, devoted to the physics and chemistry of climate science. There should be others. This is precisely the intent of our ***Challenge # 0***, along with its appeal to philosophers of science to join us practitioners in responding to it.[3]

One of the most important developments of the past 10-15 years, at least in environmental engineering (water quality modeling), has been the introduction of comprehensive, multivariable, real-time monitoring systems, i.e., systems providing high-frequency sampling of behavior along the three continua (dimensions) of (i) space, (ii) time, and (iii) biogeochemistry (improving capabilities greeted with enthusiasm in, for example, Kirchner *et al*, 2004). Progress outwards from the origin of Figure 1 is intended to encapsulate not only this increasing intensity of sampling — at more points in space, time, and biogeochemistry[4] — but also its extent, as in observing at ever higher sampling frequencies over ever longer (unbroken) periods.

Once was the situation (point A in Figure 1) when little more than temperature, pH, conductivity, or dissolved oxygen concentration were readily measurable at isolated locations in a watershed. Today, automated observing capacity has been projected beyond these more customary physical and chemical segments of the biogeochemical continuum (in aquatic systems) into access to nutrients and macroscopic features of microbiology, for instance, chlorophyll-*a* and indicators of bacterial respirometry. Time-series such as those of Figure 2, therefore, reflect a sampling frequency of once every 15 minutes or so (in a record of over two months in extent), at six spatial locations no more than tens of meters apart, in the "sensor-hostile" environment of a biological wastewater treatment plant — point B in Figure 1, as it were.

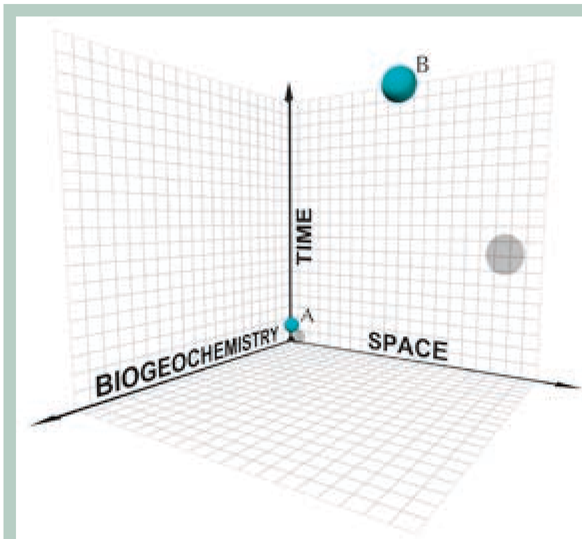


Figure 1
Three-dimensional volume — of time, space, and biogeochemistry — in which to gauge advances in the intensity, extent, and diversity of instrumentation and sensor systems for observing the environment. For the purposes of illustration: (A) where we were 20-25 years ago, say, in respect of monitoring water quality; (B) contemporary capabilities. A similar figure, we note, has come to be known as "Maidment's Data Cube".

Progress such as this, doubtless hard won, has had two significant consequences. First, and in contrast to the preceding, prevailing thrust of modeling, it has become untenable to reject discrepancies between observed and estimated behavior as the result of inadequate data — in particular, in the case of very high-order models (VHOMs).[5] The alternative inference has to be that either the constituent hypotheses drawn from primary science are not correct, or that they are correct, but have not been assembled in the correct organizational (multivariable) manner. Second — as the complement of the classical procedure of designing a laboratory experiment, wherein all variables are in fact kept *in*variant, except those describing the cause and effect of the archetypal single hypothesis relating one to the other — reconciling models with field data (our ***Challenge # 7***) requires and enables, by contrast, the testing of an entire complex of multiple, interacting, elemental experiments, as a whole, as these would be encountered *in situ*. Indeed, the very innovation of the EOs can be expected to move the subject of Environmental Science still further away from a reliance primarily on the classical scientific paradigm of controlled experiments.

[3] And there are those so inclined, for example, Ravetz and Funtowicz (Funtowicz and Ravetz, 1990), Morton (Morton, 1993), and Oreskes (Oreskes *et al*, 1994).

[4] We suppose this continuum to be gauged (loosely) in terms of the following illustrative sequence of sampling points, of increasing size of entity: OH^- ion; enzyme; bacterial cell; zooplankton; fish; and so on.

[5] Where "high order" refers to the numbers of state variables, parameters, and/or rules in the model.

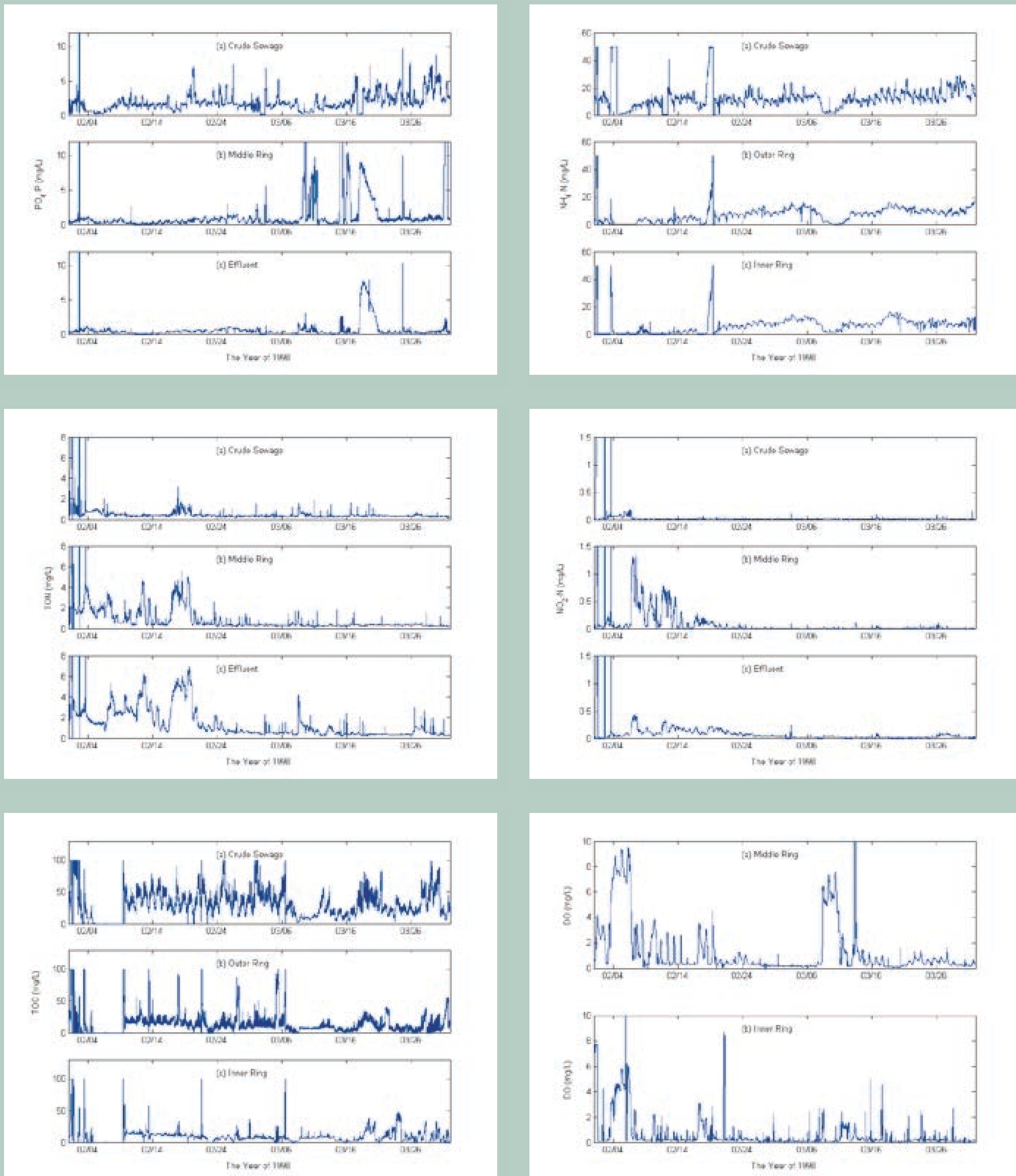


Figure 2
Time-series observations of water quality (orthophosphate-P, ammonia-N, total oxidized nitrogen, nitrate-N, total organic carbon, and dissolved oxygen concentrations) in the biological treatment unit of the Athens, Georgia, Water Pollution Control Facility # 2, during Winter, 1998. These are part of a data base collected through the Environmental Process Control Laboratory, University of Georgia, a mobile platform for real-time monitoring of water quality in various aquatic environments. They are accessible and freely available, along with other like data bases, at www.modeling.uga.edu/gwis.

Lewis's three-element characterization of knowledge growth may therefore no longer suffice for guidance. MacFarlane himself asserted long enough ago that (MacFarlane, 1990):

> Modern scientists and engineers no longer work only in terms of theory and experiment. Their attack on the problems of describing Nature and on creating useful artefacts now has three fronts:
>
> - experiment
> - theory
> - computation
>
> Computation is opening up vast new continents in Popper's World 3.

To build upon this, and thereby to define briefly the contents of Popper's three "Worlds" (Popper, 1972), our philosophically naïve expectations of these three elements should be these:

> *Experiment*: Designed to probe the nature of Popper's World 1, which is the physical world, or world of physical states;
>
> *Theory*: A conjecture drawn from Popper's World 2, that being the mental world, or the world of mental states; and
>
> *Computation*: A conjecture drawn from assimilation of the (unexpected) consequences of computational simulation, i.e., from Popper's World 3, the world of all possible objects of thought, existing outside and independent of any individual. Presumably, this would be especially the case for computationally derived "consequences", which practically could not have been reasoned about in Popper's World 2 (because what is being simulated is simply far too complex for unerring, mental reasoning alone).

Given these, the possibility of *three* kinds of "acts" is opened up:

> *Acts # 1*: The familiar acts of reconciling computation (computational models) — *not* theory itself — with the outcomes of experiments and experimental/observing experience;
>
> *Acts # 2*: Those which Lewis must originally have had in mind, i.e., acts reconciling theory with experiment;
>
> *Acts # 3*: Which enfold the matter of reconciling computational models with theory, where this now (presumably) can work in both ways, i.e., that computational models can be improved so as to mimic theory better (albeit never completely), while theory can be adapted so as to reflect better the consequences of computation — could we say "discoveries" even? — hence to provoke new forms of experimentation.

In other words, understanding — that is, assimilation of material into an appropriate mental structure (or mental model) — may derive increasingly from the *belief* that the virtual computational world (Popper's World 3) has been founded upon true and correctly applied theories at the micro-scale and does not generate broad, macroscopic, qualitative predictions in obvious, absurd discord with whatever can be observed of the real thing in the physical world (Popper's World 1). This would be the embodiment of Acts # 1. In contrast, it seems difficult to credit Acts # 3 with the power to fuel a growth in knowledge through reconciling the computed macro-scale consequences of micro-scale theory with that *self-same* micro-scale theory. After all, the entire notion of founding the growth of knowledge on the classical basis of reconciling the given data with the set of concepts (Acts # 2) rests itself upon maximizing the intellectual "distance" between the two sources of experience of the behavior of the world.

How exactly, then, should we go about assessing the scientific security of the constituent theories assembled in a VHOM? And given the unending nature of the quest, as ever higher-performance computing within the cyber-infrastructure propels these VHOMs towards a variety of virtual realities, what exactly are the *distinctive* challenges of developing and deploying such models over the next 5-10 years? For this should go beyond the challenge of encoding in these virtual realities yet more of the purported micro-scale behavior of the environment, should it not?

The need for our ***Challenge # 0*** to have the strongest possible appeal to philosophers of science should now be obvious, not least so given the puzzles and puzzlements exposed in our conjectures on the roles of models in Popper's three Worlds. Perhaps the nature of Acts # 3 has been incorrectly expressed above, so that this misleadingly suggests self-delusion rather than the wellspring of new questions about basic Environmental Science.

We shall return to these more philosophical considerations on several occasions. First, however, we need to set up a methodological framework for developing and applying environmental models. Having examined briefly how models fit into the broader philosophical picture underpinning the science of the EOs, therefore, our goal now is to introduce a helpful organizing framework for thinking about modeling as a subject in its own right.

1.2 Developing and Applying Models: The {*u*, *M*, *y*} Triplet

Let us assume the scope of model building can be succinctly defined by the triplet of the observed inputs (***u***), model (***M***), and observed outputs (***y***), and that the attaching tasks are those of the mathematical textbook: given two out of the three unknowns, find the third. Thus, in subsequent parts of this *Paper* we shall need to enquire into the nature of the grand challenges associated with the three principal computational and algorithmic questions of:

(i) Given ***u*** and ***y***, find ***M***. This we shall refer to as system identification, i.e., principally Acts #1 of Lewis's pragmatic school of thought on the growth of knowledge, under which falls the task of choosing the contents of ***u*** and ***y*** so as to maximize the "identifiability" of ***M*** — a matter of the design of experiments and sensor networks;

(ii) Given ***M*** and ***u***, find ***y***. The problems of forecasting, and scenario and foresight generation; and

(iii) Given ***M*** and desired, feared, and/or threatened ***y***, find ***u***. The problems of control, management, decision-support, and policy formulation.

From (i) emerges a fourth question, of course, which is:

(iv) How well does ***M*** approximate the real thing, and what are we going to do in respect of the other two questions ((ii) and (iii)) given there is never such a match, i.e., that there is more or less substantial uncertainty to be dealt with?

In large part the ordering of these succinct questions — (i), (ii), and (iii) — reflects the organization of this *White Paper* (set out in Section 1.3 below). But we must note briefly here certain other features of model-building important to its role within the context of the EOs.

Abstracted, as they are, the preceding tasks and questions clearly transcend the confines of study in any single EO. Model-building, in that sense, is generic. Significantly, the process has the power to promote and nurture links across disciplines, something so self-evidently vital in almost all contemporary discussions of how we ought to be organizing scientific enquiry and educating and training the next generation of scientists (for example, NRC, 2001, 2004; NSF, 2006).

But a moment's thought is needed to appreciate how terrestrial ecology interacts with the hydrology and aquatic ecology of a watershed and the built environments of cities, and they in turn with estuarine and coastal ecosystems, hence the open oceans. In this "whole" system, significant elements of all the EOs are encompassed. Consider, then, the image of a model — for that whole — as the vessel into which the contributions from all of those relevant disciplines must be poured in a consistent and compatible manner. The systematic character of model-building, together with the discipline imposed by the formal algorithmic and mathematical logic of the models themselves, can at the least assist in eliminating daft ideas — constituent hypotheses from different disciplines that do not mesh logically together — sooner rather than later. From the demands of such consistency derives the metaphor of models affording us a *lingua franca* for communicating across disciplines. And in this, it is the process (of model building) that may be as important as the product (the model itself), if not more so.

There is something less obvious, but equally as important, about the generic role of computational model-building as a cross-cutting exercise. Inasmuch as this can support links amongst scientific disciplines, so it can be turned to illuminating gaps in our knowledge in the interstices amongst disciplines. It is not at all self-evident, however, whether and how the capacities of all three EOs should be orchestrated collectively — through the development of models — in order to support studies at the intersections amongst issues such as biodiversity, invasive species, pathogen adaptation, ecosystems, and climate change, for example.

1.3 Organization: Science, Policy, and Society

Oriented thus towards Science, models might best be viewed as archives of hypotheses about the nature of an environmental system's behavior, with the word "archive" suggesting a degree of consolidation and agreement regarding the hypotheses chosen for archiving. Thinking of models designed (expressly) as vehicles for the discovery of our ignorance evokes something of a complementary idea: that the model can fulfil the task of detecting anomalous or previously undetected features in the system's behavior. Guided by such revealed anomalies, models may be deployed as experimental facilities — as generators of novel hypotheses — within which to speculate about possible explanations of these anomalies, as well as to prompt questions of an essentially scientific nature at the interstices between the disciplines of the EOs. In assembling our review, we have paid special attention to connections across the vastly different scales of molecular biology and Earth Systems Analysis. And in keeping with the times, we have been especially concerned to create the future potential to elucidate novel, general ideas about dynamical systems behavior, at the intersection of such superficially diverse disciplines as the biomedical sciences, ecology, social sciences, cognitive sciences, artificial intelligence, and artificial life. All these are tracked across ***Challenges # 1*** through ***# 8*** in Chapter 2 of Part II of this *White Paper*.[6]

It is *not* our view, not surprisingly, that the development and application of models should follow in the wake of any of the EOs coming to fruition, without their design and construction having been informed by current research in environmental modeling. Inasmuch as one of the greatest of our challenges relates to the role of models in reconciling theory with observation, equally so models can be used to design experiments, and to redeploy field observing equipment as contingencies arise. Much, nevertheless, is expected of models. A significant portion of Chapter 2 of the *Paper* is devoted, therefore, to the culmination of this expectation (in ***Challenge # 8***): of environmental science becoming a "predictive science"; and of how such a science must deal with uncertainty.

[6] Each ***Challenge*** is presented in an identical manner. First its context, foundations, and justification in the contemporary research scene are set out as preamble; the ***Challenge*** is then expressed; and thereafter possible lines of response to the ***Challenge*** are indicated.

As Science starts to be turned towards the needs of Policy and practice, so our *White Paper* travels over the challenges of assimilating data. These will be data fully anticipated to be heading towards analysts and the environmental cyber-infrastructure in ever greater volumes at ever higher speeds, calling thus for their assimilation in the ever shorter-term, even in real-time. ***Challenge # 9*** merits its own chapter, therefore: Chapter 3 on Science and Engineering in "Real Time".

Chapter 4 of Part II covers the final triplet of ***Challenges # 10*** through ***# 12***. These are in turn Policy- and community-oriented. They depart from the focus on the "here and now" of Chapter 3 towards the use of models for exploring longer-term futures in support of decision-making, management, and environmental stewardship. Sustainability, and herein the development and deployment of associated environmental models, is clearly an issue embedded in the huge complexities of the interfaces amongst Science, Policy, and Society (***Challenge # 11***). Our discussion of it precedes our closing challenge (***Challenge # 12***), which appropriately we turn back on to our own community: how shall we begin to think of organizing our habits of work, and of educating and training our successors, in order to respond to all of the above grand challenges?

Part III of the *White Paper* is devoted to our Recommendations (Chapter 5) and Conclusions (Chapter 6).

PART II:
THE CHALLENGES

Chapter 2: Science

2.1 Global Issues of Science

By *global* science questions associated with modeling, we mean issues defined *not* in the sense of "extending over the entire globe", but defined in the sense that they can only be perceived and addressed when a (reasonably complex) model of the whole has been assembled. In thinking about the growth of knowledge, our over-arching ***Challenge # 0*** (in Chapter 1.1), the significance and number of these issues look set to mount. We assert that the primary field sciences cannot as readily — as model-building and the use of models — illuminate and articulate these questions, challenges, and properties emerging from the joined-up thinking typical of our attempts at attaining the "big picture".

Challenge # 1:

> ***Given the proposed Environmental Observatories (EOs), how can we deliberately design and employ models for the identification of important scientific questions in Environmental Science, with the accompanying potential for basic scientific discovery, in particular, at the interfaces between — and in the interstices amongst — the various disciplines within that Science?***

Significant recent reports and surveys by the National Science Foundation (NSF) and National Research Council (NRC), amongst others, speak of the growing prominence of models and modeling in basic, scientific discovery. Here, for instance, is how a report from a blue-ribbon panel on *Simulation-Based Engineering Science* put it — echoing MacFarlane's earlier remarks (NSF, 2006):

> Computer simulation represents an extension of theoretical science in that it is based on mathematical models. Such models attempt to characterize the physical predictions or consequences of scientific theories. Simulation can be much more, however. For example, it can be used to explore new theories and to design new experiments to test these theories.

Further echoes can be found reverberating around a recent review paper on the role of individual-based models (IBMs) in integrating up from the micro-scale of an individual organism to the macro-scale of whole ecosystems (Grimm *et al*, 2005):

> This approach may change our whole notion of scientific theory, which until now has been based on the theories of physics. Theories of complex systems may never be reducible to simple analytical equations, but are more likely to be sets of conceptually simple mechanisms (e.g., Darwinian natural selection) that produce different dynamics and outcomes in different contexts. POM [Pattern-Oriented Modeling] thus may lead us to an algorithmic, rather than analytical approach to theory.

In a special supplement to the journal *Nature* (published on the threshold of the new millennium in December, 1999), Schellnhuber contributed a paper entitled "'Earth System' Analysis and the Second Copernican Revolution" (Schellnhuber, 1999). Its synopsis runs as follows:

> Optical magnification instruments once brought about the Copernican revolution that put the Earth in its correct astrophysical context. Sophisticated information-compression techniques including simulation modelling are now ushering in a second 'Copernican' revolution.

Schellnhuber goes on to make a particular point of the role of models — of an intermediate complexity (neither over-simplified nor overly sophisticated), drawn from the subject of Earth Systems Analysis — in articulating his vision of this second Copernican revolution (Schellnhuber, 1999). We must conclude that he has basic, core, curiosity-driven scientific discovery in mind, for in a subsequent paper (Schellnhuber *et al*, 2005) we find this:

> [D]iscovery of maximum reduction in stratospheric ozone came as a total surprise. This phenomenon was not predicted by

> "traditional" science; it occurred in a section of the atmosphere furthest from the regions of CFC releases to the atmosphere and where ozone loss was thought to be impossible. The Earth System science expected to emerge from the second Copernican Revolution will have to do better by predicting at least the possibility of future "ozone holes" — that is, major disruptions of some planetary modes of operation.

When Moorcroft asks "How close are we to a predictive science of the biosphere?", he proceeds to define computational models as providing the foundations of scientific understanding (Moorcroft, 2006):

> [L]ike many areas of climate change science, but unlike most areas of ecology, *understanding* of biosphere-atmosphere interactions *fundamentally* relies on the predictions of large, *complex models* whose parameters are too difficult to measure and that make predictions at scales far larger than we are typically able to make measurements. [Emphasis added]

Yet nowhere in any of these papers is a sound philosophical case made for articulating the role of computational models in basic discovery and the growth of scientific knowledge, hence precisely our ***Challenge # 0***.

Responding to ***Challenge # 1*** rests significantly on the way in which the community of environmental modelers can likewise respond to ***Challenge # 0***, but not entirely so. Some basic scientific problems and questions, perhaps many, will reside as yet undisclosed in the interstices between the disciplines contributing to the EOs.

Working at the Interstices

Take, for example, the broad subject area of coastal ocean dynamics and ecosystems, one of seven research themes and opportunities of strategic importance in the Ocean Observatories Initiative (ORION Executive Steering Committee, 2005). Suppose our interest is in understanding the occurrence of harmful algal blooms (HABs) of the *Phaeocystis* species and their many distorting and unwelcome effects (Veldhuis and Wassmann, 2005). What disparate blocks of knowledge might have to be pushed up against each other in full pursuit of this interest? What heterogeneous, mono-disciplinary sub-models might have to be poured in a consistent manner into the holds of our metaphorical vessel of the model of the multi-disciplinary whole? How can the practicalities of this be employed in supporting the creativity of both asking novel, basic scientific questions and of wringing the elegance of a more coherent theoretical whole out of the incoherent parts?

From a global perspective, and therefore certainly at a *macroscopic scale*, transport of materials and organisms (such as larvae) across the coastal ocean margin exerts a dominant control over major, global chemical cycles, most obviously so at the interface between the terrestrial and oceanic realms (ORION Executive Steering Committee, 2005). Significant material transfers are also occurring, however, across the interface between atmosphere and ocean, including the invasion of CO_2; and the resulting acidification may interfere with biogenic calcification, possibly associated with organisms linked through an ecosystem to the *Phaeocystis* algal species.

At an intermediate scale — let us say, *meso-scale* — one (if not several) blocks of knowledge regarding the hydrodynamics of the coastal margin will have to be brought together: on stratification, as a function of freshwater inputs, including from groundwater through the coastal ocean bed; on ocean fronts, and specific filaments and jets thereof, whose movement and meandering across the margin may be guided by specific bottom topography; and on regimes of sediment erosion, transport, and deposition. These factors influence the occurrence of hypoxia events (another block of knowledge), which in turn influence marine biogeochemical processes, such as the removal of biologically available nitrogen through denitrification. Such factors also induce patchworks of unique habitats (yet another block of knowledge) capable of dominating the structure and behavior of these same biogeochemical processes (ORION Executive Steering Committee, 2005).

Coming down to a literally *microscopic scale*, without losing sight of entire ecosystems at the meso-scale, still other blocks of possibly ill–fitting knowledge must be dove-tailed into the whole: on the physiological, behavioral, and morphological characteristics of individual species. Understanding polymorphism amongst the six currently identified *Phaeocystis* species of algae, manifested as free-living single-cell species, as opposed to gelatinous, colonial species, is crucial. For it affects variously the efficiency of cell/colony growth; virus penetration of cells and therefore their mortality; escape from ingestion by predators; exudation of predator-repellent chemicals; and the scavenging of bacteria and viruses from the water column, as particulate fragments are generated during disintegration of the colonies (Veldhuis and Wassmann, 2005).

Alternatively, turning the course of this argument landward, as it were, Box 1 examines the possible gaps existing at various scales and amongst the many constituent disciplines and models germane to studies in uncoupling the nutrient and water metabolisms of cities.

For problems such as these, do we have a model, or a suite of models, capable of addressing the functioning of such complex systems spanning so many different disciplines and scales and, most importantly, illuminating thereby interesting, novel, *basic* scientific questions at the interstices amongst these disciplines and scales?

As the sceptic would say, "there is nothing new under the sun", of course. After all, Integrated Assessment Models (IAMs) have been available for some time now (Risbey *et al*, 1996; Schröter *et al*, 2005; Letcher *et al*, 2007), as have multi-media (air-water-soil) models (Efroymson and Murphy, 2001; Babendreier and Castleton, 2005), while Bayesian (or Belief) Networks can also be seen as a systematic framework for pinning together constituent knowledge bases and sub-models of quite eclectic origins (Borsuk *et al*, 2004). All, however, are turned *not* to the purpose of generating new hypotheses, but to that of answering questions of policy and decision-making: of discriminating reliably between those hazardous waste streams that could safely be released to the environment and those that could not (Babendreier and Castleton, 2005); of the vulnerability of supplies of ecosystem services across Europe in the face of climate change (Schröter *et al*, 2005); or of determining a Total Maximum Daily Load (TMDL) of nitrogen discharges in order to subdue the extent of eutrophication in an estuary (Borsuk *et al*, 2004).

To many readers of this *Paper* at least one of the gaps in the above (and in Box 1) will not seem as such at all and will doubtless have been the subject of some investigation, possibly with the use of a computational model. This is not the point. Rather, the question is whether and how the growing potential and scope of environmental modeling, underpinned by the expected advances in environmental cyber-infrastucture and sensors, can be used *deliberately* to arrange and manipulate cross-disciplinary knowledge in a way that provokes or prompts the kind of basic scientific questioning that Schellnhuber and colleagues expect of the second Copernican revolution — and more readily so than would otherwise be the case.

When a model is constructed, certain pieces of the primary science bases are presumed known and included in explicit mathematical form, to which we shall refer as the {presumed known}. This implies a complement, of that which is acknowledged as not known — the {acknowledged unknown} — and therefore not included in the model's structure, except typically under the lumped, and largely conceptual, stochastic processes customarily referred to as the system and/or observation noises. This, then, is part of the challenge. What methods are available, or are conceivable, for systematic probing and exploration of the {acknowledged unknown}, in particular, those portions of it associated with the *interfaces* between disciplinary sub-models?

The conventional view of models as archives for passively consolidating the "known" must be complemented by the view of models as vehicles for actively probing the "unknown". That is exactly what is called for in ***Challenge # 1***.

We recognize full well, nevertheless, that the occurrence of important insights and the formation of profound questions cannot be reduced to formal logic alone in any deliberate design and deployment of models, since this occurrence is almost always a strong function of what we acknowledge as "serendipity". When the procedure of Regionalized Sensitivity Analysis (RSA) was first proposed (Young *et al*, 1978), it was described as a computational, model-based scheme for hypothesis generation — suggestive indeed of things to be sought in the {acknowledged unknown}. In practice, it is better understood as a scheme for discriminating key from redundant hypotheses, where the skill of the analyst resides in carefully assembling in the {presumed known} as many such candidate hypotheses as may be thought remotely relevant to the issues at hand, albeit under gross uncertainty.

Our challenge still stands, therefore, although with now an inkling of one possible avenue for developing a response to it; yet an avenue capable of fully exploiting the future cyber-infrastructure and the VHOMs

BOX 1

Uncoupling the Nutrient and Water Metabolisms of Cities

Problems Across The Scales

At one scale (the city) food and water enter the city in separate flows; under the modern sewage treatment paradigm of the Global North, they exit the city comprehensively mixed and destined for the aquatic environment. Those nutrients entrained into the water efflux should not be headed for the aquatic environment. How can this be halted, by what adaptations and re-engineering of the city's water infrastructure? How does mass collective human metabolism influence the fluxes of nutrients through the city, including the entrainment of pharmaceutical residues and pathogens, as a function of nutritional requirements, dietary preferences, and public health considerations?

At another, larger scale (the watershed) the city and its water infrastructure, constituting Integrated Urban Water Management (IUWM), are embedded within schemes of Integrated Water Resources Management (IWRM) across the watershed, and the practices of both (IUWM and IWRM) interact — for ill, or good — with the provision of the region's ecological services.

At yet another scale (the globe) 70-80% of Man's appropriation of the Earth's freshwater has to do with the production of food; vast quantities of water, as much as significant amounts of nutrients, are "burned up" in the process. In the global production, transport, trading, and consumption of foodstuffs, these constituents embodied in the food participate in a global cycling of materials, largely "virtual" in the case of water (Allan, 2003; SIWI-IWMI, 2004), literal in the case of the nutrients. Looked at globally, the quality of agricultural soils in food-producing parts of the world is being stressed, if not degraded, while eutrophication is occurring in the coastal ecosystems "downstream" of the cities in food importing countries (Grote *et al*, 2005), with possibly wider consequences for harmful algal blooms (HABs) and the evolution of marine ecosystems more generally (Jackson *et al*, 2001).

At still another scale (the local, and the very personal) to what extent would a re-plumbing of households in the Global North — to accommodate the broad-scale substitution of urine-separating devices for current toilet designs — allow us to uncouple the water and nutrient fluxes in the metabolism of a city? Would such a technological "solution" be sufficiently socially legitimate? And how might we judge the sustainability of this infrastructure change over the span of generations?

Interstices and Models

There are significant gaps amongst the disciplines and models that might be assembled to address such a "mess" of a problem with its many questions, as we shall see later (***Challenge # 11***).

First, it is not common to link analyses of the urban water infrastructure of potable water supply upstream of the household to those of the wastewater infrastructure downstream thereof, and little or no accompanying systematic account is taken of the role of collective human agency within a household (such as dietary preferences and health-care status) in connecting the two.

BOX 1

Second, we do not know how to assess individual items of technology, such as the urine-separating device, or even the entire web of technologies comprising water infrastructure, on the basis of their roles in the interaction between the city's metabolism and global material cycles (notably the N cycle) — yet we can see this would be hard to achieve without a complex model.

Third and likewise, we do not have any clear, quantitative expression of the relationship between the urban water and nutrient metabolisms and the ecosystem services deriving from the surrounding watershed.

Fourth, but a few pioneering studies have examined the interactions between groundwater and urban water infrastructure, let alone the feedbacks between groundwater extraction, water tables, city land subsidence, and vulnerability to flooding (Howard and Gelo, 2003).

Fifth, and last, we have only recently begun to conceive of the microbial ecosystems of biological wastewater treatment as microcosms for studies in generating novel, generic insights into the behavior of dynamical systems — such as metabolism, self-repair, self-replication, and their relationship with the notion of ecological resilience — and infrastructure design.

enabled within it. For merely integrating the various blocks of knowledge, such as those apparent in Box 1, or in the example of coastal ocean dynamics and ecosystems, is not a trivial technical matter. For instance, in developing supporting computational work for the scenarios element of the recently completed Millennium Ecosystem Assessment (Carpenter and Folke, 2006; www.MAweb.org), an inability to link the models from the disparate components comprising the necessary inter-disciplinary synthesis was indeed an insuperable, technical barrier to progress.[7] Removing this kind of barrier presents us thus with a challenge in itself, and one closely bound to innovations in the environmental cyber-infrastructure.

[7] Schröter *et al* (2005) confirm this, albeit indirectly. Their work amounts essentially to a bundle of climate and societal scenarios acting as input forcing functions for a collection of more or less complex, but *independent*, sector models.

2.2 Role of Cyber-infrastructure in Addressing Global Issues

The NSF Blue-ribbon Panel on Cyberinfrastructure held out this promise (NSF, 2003):

> [A] new age has dawned in scientific and engineering research, pushed by continuing progress in computing, information, and communication technology, and pulled by the expanding complexity, scope, and scale of today's challenges. The capacity of this technology has crossed thresholds that now make possible a comprehensive "cyberinfrastructure" on which to build new types of scientific and engineering knowledge environments and organizations to pursue research in new ways and with increased efficiency.

For our present purposes, the Engineering Research Plan for the WATERS Network defines a cyber-infrastructure in the following terms (WATERS, 2007a):

> A cyberenvironment [cyber-infrastructure] is an integrated system for automated collection, storage, retrieval, and analysis of data accessible by multiple parties through a Web portal. It includes various tools for real-time collaboration with other remotely based researchers and provides access to the monitoring information collected by an observatory's field facilities, as well as historical and other relevant data. Analytical (e.g., statistical), modeling, and visualization tools needed to conduct engineering analyses are provided within the system. An operational cyberenvironment also could include control and feedback systems for decision-making and management.

Seamless integration and consistency of functions should be of the essence.

Models and an Environmental Cyber-infrastructure

At the May (2006) Workshop in Tucson, Arizona, a substantial amount of time was devoted to assessing the role of the cyber-infrastructure in enhancing the functions of models, in particular, in the context of the

EOs. Inasmuch as a snapshot can be taken of such a rapidly evolving field, our conclusions were broadly as follows.

First, the cyber-infrastructure would support:

(i) Integration of the heterogeneous data bases and data streams, from all manner of sensing platforms (satellite, buoy, flux tower, and so on) and devices (mobile, DNA micro-array, and so forth) far better than previously, and more completely, into a coherent, transparent whole comprising (yet to be) standardized components.

Nowhere more so are data heterogeneous than in Ecology, argue Jones *et al* (2006). In a refreshingly candid survey, they note that: (a) current spreadsheets do not provide the tools to promote good data management; (b) the alternative of data warehouses may well not succeed, since no reward system is in place for recognizing contributions made by sharing data — indeed, the absence of an appropriate system of rewards is "[p]erhaps the most pervasive cultural factor stalling access to digital data"; (c) retirement, career changes, and death of the original investigator can have a dramatic impact on the availability of metadata — information used to document and interpret data — and therefore the utility of the data themselves; and (d) the prevalent model for funding of scientific research overlooks the need for long-term preservation of data, the costs of which data curation are substantial ($10M per annum, even in best of circumstances, for the National Center for Biotechnology Information). Their conclusion is thus inevitable (Jones *et al*, 2006):

> It is false economy, and poor scientific practice, not to ensure that the data are present and useful to all users in the future.

It is no surprise that substantial resources are being devoted to addressing this widespread concern. The Consortium of Universities for the Advancement of Hydrologic Science, Inc (CUAHSI), supported by NSF, has been developing a Hydrologic Information System (HIS), presently at the stage where Horsburgh *et al* (2009) have announced their standard method of publishing environmental and water resources point observations data as providing:

> [A] framework in which data of different types and from disparate sources can be integrated, while overcoming syntactic and semantic heterogeneity in the data from each source.

Second, the cyber-infrastructure would likewise enable:

(ii) Integration, more complete and far better than before, of what would otherwise become heterogeneous sub-models, with differing terminologies and units, differing spatial, temporal, and biogeochemical resolutions, differing process mechanisms and, more fundamentally, differing conceptual foundations. As our work is drawn on by the need and ambition to encapsulate ever more of "the expanding complexity, scope, and scale of today's challenges" (NSF, 2003) in model assemblies of the whole, the challenge of overcoming such conceptual heterogeneity must be addressed (as already sufficiently apparent in the preceding Challenge # 1).

Drawn on by policy imperatives in the European Union (its Water Framework Directive), the Open Modelling Interface and Environment (OpenMI) has the ambition of facilitating migration of existing models (and the development of future models) to a new standard of software. Model inter-operability would be increased and accessibility and reusability improved thereby (Rizzoli and Argent, 2006). The 2008 Catalog of software manufacturer The DHI Group promotes MIKE 11 and MIKE SHE as "OpenMI™ Compliant" amongst its comprehensive range of products for simulating urban, water resources, and marine environments. The scientific visualization of DHI Group's MIKE Animator, quite inadequately sampled in Figure 3, is indicative of the immense technical sophistication of such software. Drawn on by the same European Directive, but inducing innovations at a more basic, scientific level, the PIREN-Seine study (France) broke new ground, as far as we can tell, in placing the formerly incompatible sub-models of the watershed, watershed headwaters, main-stream channels, estuary, and coastal zone on a single, consistent biogeochemical basis (Billen *et al*, 2007b; Even *et al*, 2007a).

Third, an environmental cyber-infrastructure should:

(iii) Enable the two, data (from (i) above) and theory (from (ii) above), to be brought to each other more smoothly and from any source.

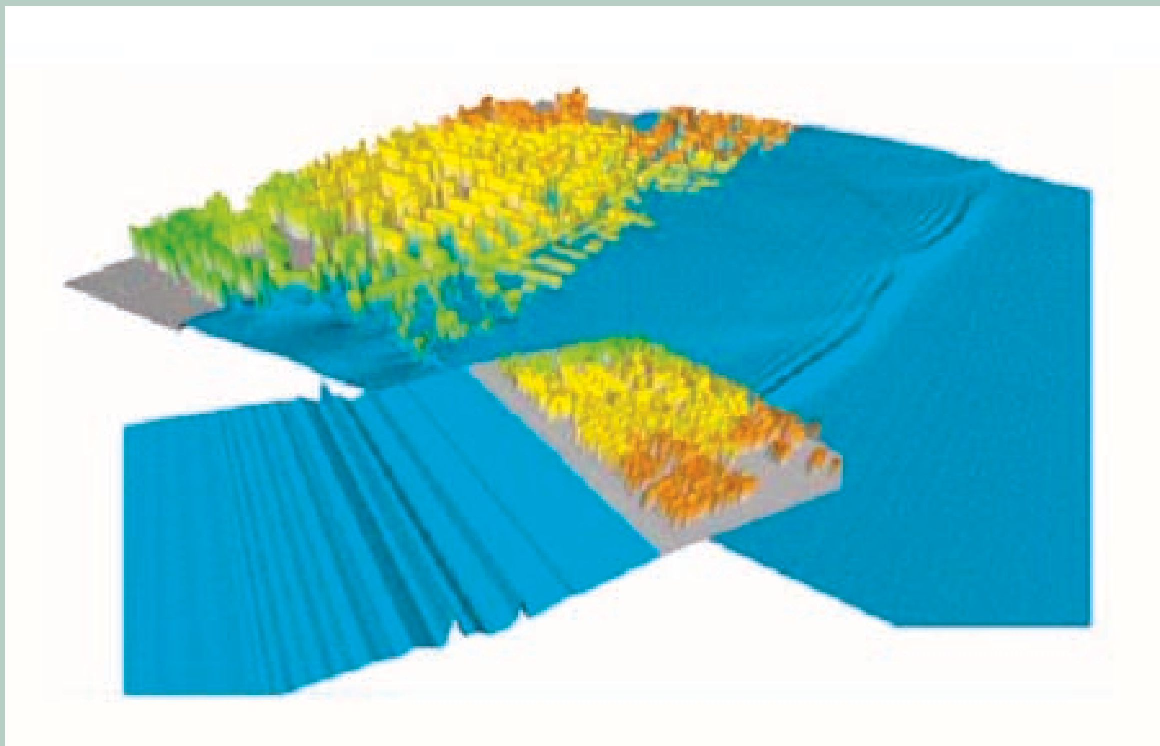


Figure 3
Image used to advertize capabilities for scientific visualization of model outcomes through DHI Group's MIKE Animator software (reprinted with permission from the 2008 DHI Group Catalog).

As we shall see later (***Challenge # 9***), data assimilation is to (iii) what semantics and ontologies are to (i), in terms of curbing heterogeneity (Jones *et al*, 2006).[8]

Last, but emphatically by no means least, the cyber-infrastructure must:

(iv) Facilitate less disjointed community collaboration — in principle, given the differing "languages" (jargon) and cultures of the myriad disciplines keying into the EOs — amongst more individuals in a more widely shared (virtual) workspace.

We can see how even the fine detail of an integrated system for publishing environmental observations data (Horsburgh *et al*, 2009) contributes measurably to this.

The potential role of models, as the systematic *lingua franca* of a good deal of inter-disciplinary collaboration, is obvious in this last element (iv) of the vision. Looking ahead therefore to what will be expressed as one of the greatest challenges we face (***Challenge # 7***), we can imagine the archetypal Statistician interpreting the data, using the artful visualizations of the self-organizing maps of data-mining, and gifted with the superbly trained eye for spotting the unexpected and uncommon correlation, or the intriguing nonlinear anomaly between data and model. But s/he is almost certain to be insufficiently grounded in the domain knowledge of the Marine Ecologist, who can proffer the hypothetical conjectures on why the correlation or curious anomaly is occurring. How might the two, one on a boat at sea, the other in a city office, tinker with one and the same scientific visualization of the model's structure, at the

[8] "Semantic integration involves clarifying data content in ways that are similar to controlled vocabularies, but using more powerful formal structures known as ontologies", according to Jones *et al* (2006), who define "semantics" as enabling computers to interact powerfully and appropriately using familiar and meaningful concepts for humans, and "ontologies" as formal models of knowledge in a particular subject area useful in making inferences about data.

same time, on their own respective computer screens? ***Serving Science***

Such a vision of the role of the environmental cyber-infrastructure is beyond our reach, for the moment. The thrust of current research is towards realizing two primary facilities: first, assimilating data into a model, because this very process embodies the goal of rendering integrated and homogeneous what would otherwise be heterogeneous and disjoint (McLaughlin, 2002; Williams *et al*, 2005; Lermusiaux *et al*, 2006a); and fore-, hind-, and now-casting with very large models in *real time*, because we have in prospect the wherewithal of peta-scale computing so to do.

At bottom, however, such applications accept the prior conceptual model structure as given, not to be questioned. Our next challenge is therefore this:

Challenge # 2:

> ***What kinds of software platforms within the environmental cyber-infrastructure will be necessary for supporting extensive, heuristic experimentation with a model's structure, i.e., in facilitating experimental "rewiring" of its constituent hypotheses and their interconnections in the assembly of the whole, while the inter-disciplinary community of environmental scientists works at formulating and resolving core science questions in the interstices amongst the constituent disciplines?***

Given the inexorable expansion in coverage of the continua of time, space, and biogeochemistry — to include the ever smaller, the ever larger, and more of what is in between those expanding boundaries — what are the scientific milestones in what can seem an otherwise rather mechanistic, somewhat routine process of "technology-push"? What, in this same vernacular, is the scientific, demand-side pull? For the issue is not so much one of merely employing peta-scale computing, because it has become readily available, but of clarifying how exactly that technical advance changes the questions we can ask of science, and hope to answer. What kinds of scientific visualization of models, not currently met by the likes of Figure 3, will facilitate the freedom of endless questioning and creative dialog, as we have just imagined between our archetypal Statistician and Marine Ecologist?

The *automated* "computational thinking" (NSF, 2007) of the anticipated environmental cyber-infrastructure should be to the present ***Challenge*** what the "*manual*" thinking of the systems scientist was to the preceding ***Challenge # 1*** — in working to spot and craft core, basic scientific questions at the interstices amongst the discipline-specific sub-blocks of a composite model. The one — unerring, systematic (here) — should complement, if not provoke more, of the other — the serendipitous (there, under ***Challenge # 1***). As called for in the current NSF Program Solicitation for new research on "Cyber-Enabled Discovery and Innovation (CDI)" (NSF, 2007)[9]:

> Ambitious CDI projects in this area [From Data to Knowledge] will allow investigators to confirm the expected and reveal the unexpected in multiple science or engineering domains.
>
> [C]omputational thinking ... promises paradigm-shifting advances in more than one field of science and engineering

For instance, in a recent (2006) internal report from CUAHSI entitled High Performance Computing for Hydrological Sciences (CUAHSI, 2006), it is apparent how attaining the goal of substantially greater computational refinement enables a better appreciation of some basic questions of science. In this case, computational refinement amounted to finer spatial grids and smaller time steps for integration of the relevant sets of differential equations, within coupled groundwater, surface water, land-surface, and meso-scale atmosphere models. The questions of science better then to be addressed were those of how spatially distributed feedbacks from the land surface influence weather events and the climate system. Preliminary results with such models (Chow *et al*, 2006) indicate the sensitivity of convective storm generation and precipitation events to soil moisture fields. This in turn prompts the more precisely targeted scientific question of what might be the quantitative impact of antecedent such fields on precipitation.

Advances likewise in ever more refined computational realizations of interactions at the ocean-atmosphere interface have enabled the question of whether climate change is affecting hurricane intensity to be accompanied now by the equally hotly debated

[9] With echoes therein of Popper's three Worlds and ***Challenge # 0.***

complementary question of whether hurricanes have a significant role in affecting climate (Emanuel, 2005; Mooney, 2007).

It remains to be seen, however, what other such basic questions of science might be unearthed: first, were these works grounded in differential-equation models to be confronted with the rather different conceptual and computational frameworks of (spatial) pattern-process analyses of landscape ecology (Schröder, 2006; hence, the IBMs of Grimm *et al*, 2005); and second, were the demands of cross-scale temporal considerations (minutes to decades) to be imposed upon them, as they must in the terrestrial biosphere models of Moorcroft (2006). Not yet apparent either is the extent to which the OpenMI or other software protocols (Rizzoli and Argent, 2006) would bridge with ease the heterogeneity of these computational frameworks and scales, thus to accelerate liberation of the all-important core scientific questions.

Other instances can be found of this kind of convergence amongst domains of enquiry previously largely separated, where the act of synthesis has itself been enabled by the inexorable refinement and expansion in computational coverage of the continua of time, space, and biogeochemistry. In their study of the design and operation of fish passage systems in the Pacific Northwest of the USA, Goodwin *et al* (2006) have brought together: (i) a contemporary computational fluid dynamics (CFD) model to generate a hydrodynamic field; (ii) an interpolation scheme to convert this field from an Eulerian mesh to a Lagrangian framework; within which, (iii) an agent-based model of a salmon — a virtual fish (or Numerical Fish Surrogate; NFS) — determines movement of that individual in response to abiotic stimuli in its computed environment, such as water motions and physical barriers (a biological guidance structure, a trash-boom, and so on).

Several points are salient about this work. First, it was the culmination of an idea first proposed nearly two decades previously. Second, it benefitted no doubt from advances in sensor technology over that period, specifically in respect of acoustic-tagging of fish for observing their navigation through a body of water. Third, suggestive of what has been called the scientific demand-pull above, it looks towards a future in which, for the purposes of "decoding" patterns of movement of individual salmon, as they put it (Goodwin *et al*, 2006):

> We believe new emerging methods such as large eddy simulation (LES) CFD modeling may be needed to more accurately resolve eddy formation and turbulence production at spatio-temporal scales important to fish behavior.

"Decoding" is an opaque, if not tentative, word for using a model at the interstices amongst disciplines in order to shape and address questions of basic, scientific discovery. Much less hesitant is the work of Ruardij *et al* (2005), as we now relate.

Models and Hypotheses at the Interstices: the Case of **Phaeocystis** *Revisited*

What essentially causes the alga *Phaeocystis* to prosper as a "harmful algal bloom" in marine ecosystems? Amidst all the physical, chemical, and biological factors that could be relevant to answering this practically important question, as already recounted in respect of ***Challenge # 1*** (Chapter 2.1), much may pivot on understanding the occurrence of polymorphism amongst the six currently identified *Phaeocystis* species (Veldhuis and Wassmann, 2005).

On the one hand, from the context of examining the system *in situ*, derives a fairly complex model: an assembly of candidate, constituent hypotheses pinned together as a composite conjecture on what should happen as a whole in the uncontrolled "mess" of the field (Ruardij *et al*, 2005). Sensitivity analyses of this model, designed to provoke the discovery of "new science", corroborate in part one elemental hypothesis — while discrediting an alternative — about virus penetration of a colony-forming species of *Phaeocystis*. Hence follows either the prosperity of the colonial form or its demise (Ruardij *et al*, 2005). This is what they say of the outcomes of their "Hypothesis testing by [model] sensitivity analysis" (Ruardij *et al*, 2005):

> [W]e indicated that a reduced encounter rate between virus particles and colony spheres is adequate to explain the low rate of infection of embedded colonial cells. The suggested impermeable skin of the colonies is an unnecessary *Deus ex machina* for protection against virus. [emphasis added]

On the other hand, from the context of investigations *in vitro*, under the exquisitely controlled conditions of the laboratory, wherein careful scrutiny of a single, elementary hypothesis can proceed unimpeded, the evidence is that polymorphism can occur at different times in one and the same *single* species of the prey alga, namely, *Phaeocystis globosa*. It arises through (defensive) adaptation triggered by differing chemical signals in the proximity of differing forms of predator, each with substantially different eating habits (Long *et al*, 2007).

Taken side by side, the chemical signaling hypothesis has fallen through an inter-disciplinary gap in the composite conjecture of the model, whose study pointed instead towards further exploration of a viral-infection hypothesis. The provisional validity of the chemical-cue hypothesis, however, built on the foundations of artificially isolated laboratory investigations, demands exhaustive further testing — through the model — in the quite different setting of the approximated mess of multiple, interacting, ongoing hypothetical experiments that *is* the behavior of a field system *in situ*.

With the prospect of the automated, computational thinking of a cyber-infrastructure, to accompany the thinking we shall always be doing for ourselves, our essential challenge is this. How might alternative designs of a model, organized and deployed within the environmental cyber-infrastructure, enhance the speed and efficiency of both pinpointing the potential questions provoking core scientific discovery and covering the gaps through which they might evade detection — and all as a complement of the much more familiar analyses of laboratory science?

What other such milestones, across the fields of the EOs, ought to be attainable 5-10 years' hence, as grand scientific challenges associated expressly and uniquely distinctively with modeling?

2.3 Universal Science Issues and Process Mechanisms

The mechanics of fluid motion or the kinetics of microbial metabolism and growth do not recognize the borders we place around our disciplines. Such issues of scientific enquiry and their attaching process mechanisms are *universal*, in the sense that they present themselves in largely identical form, in developing and constructing models, within each of the domains of the three Environmental Observatories (EOs). These matters could be fully addressed within the confines of a single EO.

But how, we must ask, might their study be diminished in the absence of collaboration across the EOs? Or, put the other way around, what might be the added value of coordinating enquiry into these subjects, without restriction to any single EO, around the focus of models, with the intent of (again) serving the purpose of basic, curiosity-driven scientific discovery? And which subjects, in particular, might be those where models fulfil a role not substitutable by other forms of enquiry, which role itself is likely to be substantially enhanced by the advent of an impressively better environmental cyber-infrastructure?

A "Tyranny of Scales"

While ***Challenge # 1*** dealt with cultivating research at the interstices amongst a variety of disciplines, equally significant issues of handling computational representation at a variety of scales were hardly ever out of focus — witness the case of *Phaeocystis* and the challenge of "Uncoupling the Nutrient and Water Metabolisms of Cities" set out in Box 1 of Chapter 2.1. These matters of scale surfaced just as palpably in the foregoing discussion of ***Challenge # 2*** (Chapter 2.2); and they will here be brought to occupy center-stage.

Hydrologists have long been familiar with the problem of how to accommodate issues of scale in their models (Blöschl and Sivapalan, 1995). And scale itself has a number of facets to it, ranging from dependence on spatial scale of the mechanisms of contaminant dispersion in a moving fluid (Pang and Hunt, 2003), to upscaling and downscaling of the fluxes of water, heat, and carbon (C) through the soil-plant-atmosphere continuum (Anderson *et al*, 2003), and on up to the perspective of Earth Systems Analysis in Moorcroft (2006).

Challenge # 3:

Is there a unifying and uniquely distinctive approach to the use of models in exploring issues of scale, and cross-scale interactions, along each of the three dimensions of (i) time, (ii) space, and (iii) biogeochemistry, where this last manifests itself across scales from molecular biology up to all the chemical and biological species comprising whole ecosystems?

We are drawn on by the widening scope and increasing depths of our needs and ambitions to comprehend the world about us, seeking especially for this understanding to span vastly different scales of enquiry and analysis. Where the Blue-ribbon Panel on Cyberinfrastructure (NSF, 2003) saw in this the enormous promise of our conducting science and engineering studies in quite novel ways, so the Blue-ribbon Committee on *Simulation-based Engineering Science* feared the "tyranny of scales" (NSF, 2006). Scale is identified as the first of its six core issues, where "core" signals an issue common to the "challenges, barriers, and requirements for research breakthroughs" of all five of the societal benefits expected to flow from an investment by NSF in SBES.[10]

So great indeed appears the challenge that the Report talks in headline terms of "The Tyranny of Scales: The Challenge of Multiscale Modeling and Simulation". It proceeds to observe that (NSF, 2006):

> Virtually all simulation methods known at the beginning of the twenty-first century were valid only for limited ranges of spatial and temporal scales. Those conventional methods, however, cannot cope with physical phenomena operating across large ranges of scale — 12 orders of magnitude in time scales, such as in the modeling of protein folding, or 10 orders of magnitude in spatial scales, such as in the design of advanced materials. At those ranges, the power of the tyranny of scales renders useless virtually all conventional methods. Confounding matters further, the principal physics governing events often changes with scale, so that the models themselves must change in structure as the ramifications of events pass from one scale to another.

It is in this sense that hydrologists acknowledge that the mathematical structure of the description of the mechanisms of contaminant dispersion changes significantly with spatial scale.

The language of the NSF Report is robust, if not florid. It leaves us in no doubt:

> In many ways, all that we know about the physical universe and about the design and functioning of engineering systems has been partitioned according to categories of scale. ... Today, we are attempting technological advances that cannot tolerate any view of nature that partitions phenomena into neat categories of scale. ... The tyranny of scales will not be defeated simply by building bigger and faster computers. Instead, we will have to revamp the fundamental ways we conceive of scientific and engineering methodologies, long the mainstays of human progress.

Not surprisingly, the Report finds on this topic that (NSF, 2006):

> Formidable obstacles remain in linking highly disparate length and time scales and in bringing together the disciplines involved in researching simulation methods. These issues are common to many SBES applications. Fundamental discoveries will be needed to surmount these obstacles.

We shall see more than enough evidence later of such "highly disparate length and time scales" in the science and engineering of the EOs.

Cross-scale Interactions: Space, Time, Process-Mechanism, and Pattern

Ecologists well appreciate the challenges of addressing cross-scale interactions, expressed succinctly here by Levin (2000) in a paper on "Multiple Scales and the Maintenance of Biodiversity":

> Pattern and diversity arise through positive feedbacks on short time scales and local spatial scales and are stabilized by negative feedbacks on longer time scales and broader spatial scales.

[10] These being in medicine, homeland security, energy and the environment, materials, and industrial and defense applications.

Important dynamical properties of ecosystems, specifically resilience and regime changes, are a function of the subtle — and, as yet, not well elaborated — interplay amongst system state variables with very different characteristic time-constants (Carpenter and Folke, 2006). Sudden shifts in regime, signaled by high-amplitude, fast, transient responses in some state variables, can be triggered by almost imperceptible changes over time in other (slowly changing) state variables. For example (Carpenter and Folke, 2006):

> By operating at different spatial and temporal scales, competition among grazers is minimized and the robustness over a wider range of environmental conditions is enhanced.

Put another way around, turning the balance in our thinking somewhat away from variations of process mechanisms along the continuum of temporal scales towards variations along the spatial continuum and the emergence of patterns, we have (Grimm *et al*, 2005):

> Ideally, the patterns used to design a model occur at different spatial and temporal scales and different hierarchical levels, because the key to understanding complex systems often lies in understanding how processes on different scales and hierarchical levels are bound to each other.

Or yet again, there is this, more obviously indicative of reining in the computational tyranny of scales (Goodwin *et al*, 2006):

> The resulting ELAM [Eulerian-Lagrangian-agent model] framework is well suited for describing large-scale patterns in hydrodynamics and water quality as well as much smaller scales at which individual fish make movement decisions. This ability of ELAM models to simultaneously handle dynamics at multiple scales allows them to realistically represent fish movements within aquatic systems.

In systems of environmental engineering and the built infrastructure, where it might well be highly desirable to see notions of ecological resilience incorporated into the design of such infrastructures, it is now readily apparent that understanding the occurrence of faults and failures, i.e., fast transient excursions from "desired" performance (and their management), is unlikely to proceed far without conceiving of the system's behavior in terms of (spectral) frequency distributions and responses — a framework in which all temporal scales of behavior are succinctly embraced (Beck, 2005a).[11] Cross-scale interaction would there be expressed as a slow, incremental accumulation of technologies over the decades and centuries, "locking in" to a macroscopic form (or pattern) of infrastructure increasingly vulnerable to fast, transient losses of desired functions over hours and minutes; hence today the challenges of Box 1 in Chapter 2.1.

In short, and to paraphrase a part of Levin's (2000) synthesis, the essential questions of cross-scale interactions — manifest inseparably across the space and time continua — are these: what processes-mechanisms produce pattern in space-time; and, more pragmatically, what cross-scale interactions amongst a host of processes-mechanisms produce biodiversity? If we were to acquire understanding in answering these questions, we would have insights into the stewardship of biodiversity.

What ***Challenge # 3*** calls for, then, are responses to this kind of question: will our overcoming the "tyranny of scales" — in modeling and computational terms, that is — afford us the possibility of coming up with new, core scientific insights into Levin's synthesis of the "problem of multiple scales", and uniquely and more swiftly so than without the development of models.

[11] But see also Kirchner *et al* (2004) in a related sense.

2.4 Universal Science Issues of a Biological Nature

In the abstracted setting of Figure 1, drawn for the purposes of gauging advances in our capacity for observing the environment, the third dimension of biogeochemistry appears on an equal, conceptual footing with those of space and time. This obliged us to think there in terms of sampling, sensors, and instrumentation ranging from very small biogeochemical targets (dissolved chemical solutes) to the very large (whales), and to conceive of the intensity of consistent sampling in space-time of the species/individuals within that (bounded) biogeochemical range. Our discussion of scale in the foregoing (***Challenge # 3***) articulates well some of the issues in employing models in addressing, for example, cross-scale interactions amongst species/individuals on the space-time plane (of Figure 1). By comparison, it leaves unattended the challenges of cross-scale interactions along the biogeochemical dimension. For these, in more familiar, less abstract terms, are nothing more than the common subjects of enquiry in Molecular Biology, Ecology, the Biosphere, and Earth System Science.

Bringing together these disciplines of such vastly different space-time scales into very close proximity — literally, within the span of a single breath, if the relevant part of the foregoing sentence were to be spoken aloud — motivates our next challenge:

Challenge # 4:

> ***What breakthroughs are needed in order to develop a more effective and complete paradigm of modeling biological processes — common to the ocean sciences as much as to terrestrial ecology or biological wastewater treatment — across all scales: from molecular biology to whole ecosystems, and including mimicking of the intelligence and metabolism of individuals in a population, their movement through an environment, and their interactions with other individuals, as a function of that intelligence and metabolism?***

We live in a "biological age", in which appeal to the human organism and to the biological attributes of evolved nature as the metaphor for the epitome of good design has come to stand alongside the clockwork mechanism of a former century. All of the "Recommended Immediate Research Investments" of the NRC's 2001 Report on the *Grand Challenges of Environmental Sciences* (NRC, 2001) relate to ecology: from biological diversity and ecosystem functioning, through infectious disease and the environment, to ecosystem functioning and ecosystem services in respect of land-use dynamics, and on even to the need for hydrologic forecasting to include considerations of the ecological consequences of hydrologic events and behavior. The Report calls for, *inter alia* (NRC, 2001):

> New techniques and capacity for nonlinear dynamic modeling ... that integrate information from the genome to the ecosystem

and

> New methods developed to forecast blooms of toxic algae, incorporating both remote and on-site monitoring of population dynamics and toxin production.

In response, and as evidence of another kind — of the current hegemony of matters biological — we find this (Grimm *et al*, 2005):

> Ecology, in the past 30 years, has produced as many individual-based models as all other disciplines together have produced agent-based models ...

Frontiers Across the Disciplinary Domains of the Environmental Observatories

Let us put aside considerations of time and space, therefore, to focus on interactions and integration across scales along the continuum of biogeochemistry (as we are here using that expression), thus to enquire: in what state do we find the modeling of environmental systems and the biota therein, as the platform on which then to begin to construct illustrative responses to ***Challenge # 4***?

The majority of such models, from the microbial ecosystems of biological wastewater treatment (Henze *et al*, 1999) to ocean ecosystems (for example, Baretta *et al*, 1995; Woods, 2005; Dippner, 2006;), rarely, if ever, ascend further up the (aquatic) foodweb than some generic, predatory fish "aggregate", nor descend further than varieties of mutations of some species within phytoplankton, at the very base of the living part of the foodweb, or their infection by a "virus" state variable (Ruardij *et al*, 2005). Exceptions to this are the policy-oriented multi-media models underpinning assessments of human and ecological risks from exposure to hazardous substances, whose computations must necessarily reach into effects on a host of organisms, such as earthworms, bald eagles, large-mouth bass, and white-tailed deer, amongst others (Efroymson and Murphy, 2001), and, of course, humans, who merit discrimination amongst five age groups (Babendreier and Castleton, 2005).

Scanning more broadly the frontiers of contemporary research across the various domains of aquatic and terrestrial ecosystems, we find the boundaries of the lowermost levels to which the biogeochemical continuum has been resolved in computational models described by the following salients:

(i) an account of the penetration of a phytoplankton cell by a virus and subsequent lysis of the cell with the release of more viruses (Ruardij *et al*, 2005);

(ii) recourse to appreciating the manner in which a fish detects accelerations and gravitation through the otolith of its inner ear, in order to account for how, through a computational, game-theoretic approximation, various data streams are processed by that fish as it then determines its next move (Goodwin *et al*, 2006);

(iii) similarly, an appreciation of the neurobiology of the brain, thus the locus of spatial memory in a network of hippocampus place cells, in order to simulate the migration of elk, as boundedly rational agents (Bennett and Tang, 2006); and, more generally

(iv) making an individual animal's strategy for foraging through its environment depend upon a state variable quantifying that individual's energy reserves, where such individuals make choices over time "to maximize their probability of surviving to, and having energy reserves for, future reproduction" (Railsback, 2001).

Marked out thus, we can observe how these frontiers of environmental modeling have yet to make in-roads into the simulation of neural control of animal locomotion, such as a lamprey (Ijspeert and Kodjabachian, 1999) or salamander (Ijspeert, 2001).

Neither, as far as we are aware, has the coverage of any environmental model yet been refined down to the (very) small scales of the fields of computational systems biology and computational toxicology, which account for the impacts of chemicals — for good or ill — on the biological macro-molecules and signaling networks within an individual cell, within a tissue, within an organ, within an organism (Andersen *et al*, 2005).

For example, Figure 4 (from *The MathWorks News & Notes*, June, 2007) is indicative of what we might find in those fields. It could easily be mistaken for a representation of the interactions amongst the multiple biogeochemical species in a model of a marine ecosystem, cast well above the scale of an individual organism. The "sampling span" of the biogeochemical continuum in even the WPB virtual marine ecosystem of Woods (2005), with its underlying ambition of placing elucidation of the laws of Biology on the same footing as those as of Chemistry and Physics, does not begin to approach the intensity and refinement of Figure 4. For all the branches and nodes of Figure 4 would not collectively rise to the significance of just a *single* state variable in the WPB model (Woods, 2005). The entirety of their effect would have to be relegated to a "parameterized", probably invariant, model coefficient. Figure 4, if not complex enough in its own microscopic context, is described in a matter-of-fact manner as merely a "small section of a biological system", albeit a part of "the world's most complex dynamic systems" (as trumpeted on the cover for that issue of *The MathWorks News & Notes*).

Elsewhere, one or two isolated studies make the great intellectual and computational leap across very widely separated scales: from global climate to the genomes of host plants and their pathogens, at least in principle (and seemingly in response to the NRC's Report on *Grand Challenges in Environmental Sciences*; Garrett *et al*, 2006); and from particle-tracking across the Caribbean Sea using an oceanographic model, to prediction of the genetic patterns resulting from long-distance dispersal of larvae from populations of the staghorn coral (Galindo *et al*, 2006).

No study with an environmental model, however, has yet availed itself of any interim outcomes of the Human Physiome Project, whose ambition is to generate a model of the human body, from the genome upwards (Hunter and Borg, 2003), across events spanning from

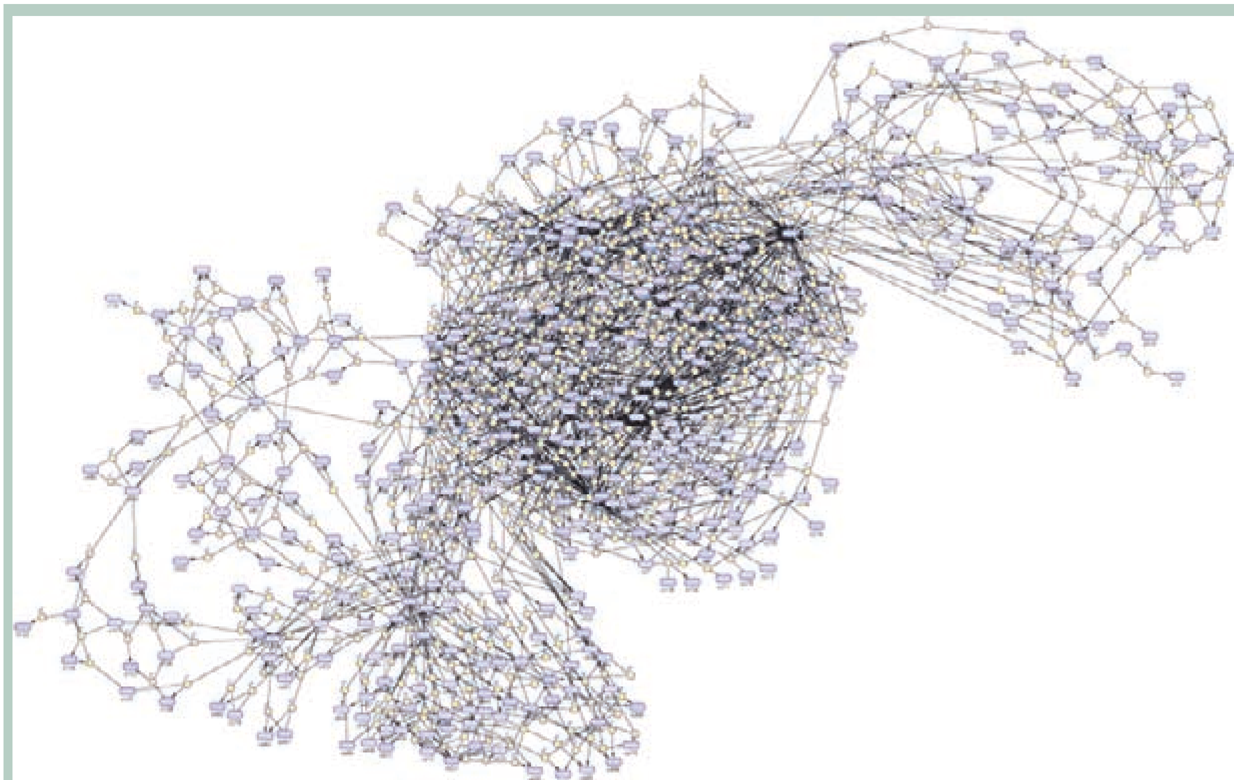


Figure 4
A model of a "small section of a biological system", albeit a part of the "world's most complex dynamic systems", from the cover of *The MathWorks News & Notes*, June, 2007.

10^{-6} to 10^{+9} seconds, disparate enough in the terms of the "tyranny of scales" referred to in the NSF Report on *Simulation-Based Engineering Science* (NSF, 2006).

One wonders, then, how long it will be before these burgeoning forms of computational technology-push are incorporated more fully into the mainstream of environmental models. More importantly, however, we should wonder to what purpose of what core scientific demand-pull are they to be put, and contingent upon what innovations in sensor technologies across the EOs (NSF, 2005)? What manner of data, we should ask, would have to be acquired by the Observatories to evaluate and revise a model as complex as that of Figure 4 (a question to be left to ***Challenge # 7***)?

On the Threshold of a Breakthrough?

What unites the disciplines contributing to the EOs — the Ocean Sciences, Ecology, Environmental Engineering and Hydrology — is their shared enquiry into the nature of the biogeochemistry in their respective domains, in particular, issues towards the biological and organismal end of that continuum. The distinction of ***Challenge # 4***, and therefore its differentiation from the foregoing ***Challenge # 3***, is its call to go beyond the historical use of crude, lumpish "biomass" as the epitome of the state of a population of organisms. The "individual" is instead of growing importance: its metabolism, at various more refined scales of representation; its motion through a geochemical space; and its interactions with other biological individuals, both alike and different from itself.

That growing importance will be seen to permeate many of the subsequent challenges of this *White Paper*, not least that which follows (***Challenge # 5***). Some of these are revealed in the sweep of the following sequence of indicative challenges, scaling up from the smallest of cellular details to an earth systems perspective and then scaling back down to behavior within the cell.

From the Human Physiome project (Hunter and Borg, 2003), therefore,

> through applications of the mathematical theory of adaptive dynamics in respect of understanding speciation and evolution (Dieckmann and Metz, 2006);
>
> traveling over the regional-scale biogeochemistry of the Seine-Paris watershed (Billen *et al*, 2007a);
>
> on up to Moorcroft's (2006) question of "How close are we to a predictive science of the biosphere?";
>
> and then from within that perspective of Earth Systems Science, across to the Millennium Ecosystem Assessment (Carpenter and Folke, 2006);
>
> Kremen's (2005) tabulation of the associated (global) ecosystem services;
>
> in which she calls expressly for the design of new such services, all the way back down at the scale of the (engineered) microbial ecosystems of wastewater treatment and the work of Graham and Smith (2004);
>
> who, in turn, call expressly upon the development and application of models for such a purpose (Saikaly and Oerther, 2004);
>
> which models have long stood on the verge of characterizing the state of the system below the level of the individual (generic) cell of a given species, which, as we know well, is already being achieved elsewhere (outside the disciplines of the EOs), in models of the metabolic maps and systems of enzyme-catalyzed reactions within bacterial cells (Alvarez-Vasquez *et al*, 2005; Voit *et al*, 2006);

we find — from across all these particular lines of enquiry, spanning such a huge range of scales — a tumultuous ferment of inter-related ideas. And for the moment, and more so than in the common thread of fluid mechanics running through the EOs, this intellectual ferment conveys hints of a nonlinear dislocation in problem-solving, somewhat different from the "linearity" of expecting that our models will continue to cover more things, in more detail.

From enquiry with the global-scale models of Earth Systems Analysis (Schellnhuber, 1999; Schellnhuber *et al*, 2005), based on sets of differential-equations, to the local-scale of individual-based models (IBMs) of fish and elk (Grimm *et al*, 2005; Schweitzer (2003)), to the NSF's Blue Ribbon Committee on Simulation-Based Engineering Science (NSF, 2006) and its CDI Program (NSF, 2007), the strong suggestion is of change being afoot — something *universal* — in the way we engage the development and application of models in scientific investigation.

2.5 Applied Mathematics and Generic, Dynamical Systems Properties

Three decades on from the seminal publications of Holling (1978) and Casti (1979) on applications of the mathematical theory of catastrophe; two decades on from Sir James Lighthill's apology for the predominant determinism of applied mathematics having misled the public, in the face of the growing appreciation of mathematically chaotic behavior in systems (Lighthill, 1986); and a decade on from the emergence and diffusion of complexity theory into the study of environmental systems (for example, Levin, 1998), what today is the legacy of these theoretical developments?

It is, we submit, primarily the dynamical feature of *resilience* in the behavior of systems, in particular, ecosystems. The course of its development is signaled through the benchmarks of Holling (1973, 1986), up to the milestone of Peterson *et al* (1998), on "Ecological Resilience, Biodiversity, and Scale". Its extension to "systems" more generally is expressed in Gunderson and Holling (2002). Its further codification, with corroborating empirical evidence is reported in Folke *et al* (2004). And some of its other manifestations are encapsulated in what we have already quoted from Levin's (2000) work on "Multiple Scales and the Maintenance of Biodiversity" (in Chapter 2.3, in response to ***Challenge # 3***).

Both Holling and Levin appreciate full well the benefits of "systems thinking" and models, as the means to cut across disciplines in the process of intellectual distillation and synthesis. Here is what Levin has to say of this, in the context of discussing self-organization in ecological systems (Levin, 2005):

> It is a common exercise in evolutionary theory to posit assumptions about interactions, and then to use the general approaches of dynamical systems theory to explore what the consequences of those assumptions would be were they valid.

And here, writing on the role of game theory in identifying properties of the dynamic behavior of social systems, he gives succinct expression to the following principle (Levin, 2006):

> Build models of the dynamics of systems given particular behavioral rules, and then explore the adaptive dynamics by allowing mutations and introductions of rare novel behaviors.

These are modes of scientific enquiry pivoting on hypothetical experimentation with computational *models* and directed towards extraction of the essence of an insight into a *generic, dynamical systems property*. They are also modes of enquiry redolent of the discussion of Popper's three Worlds under our overarching ***Challenge # 0*** (Chapter 1.1).

From all the immensely rich complexity of dynamic behavior we find about us, we seek to discern and then extract from study in one domain (Ecology, say) an essential insight about a fundamental attribute of that behavior, such as ecological resilience, and transfer it to the study of some quite other domain — and with handsome rewards. While there has been, and will continue to be, great beneficial scope for transferring the ideas of resilience from one domain to another, we ask: is the time now ripe for something more; something creatively different from that earlier extract of essential insight from Ecology; time for something novel to emerge from studies in a domain quite other than Ecology; and how, in particular, can environmental models and the EOs contribute to extraction of that novelty, if at all? For our concern must be with how the *particular* subject of environmental modeling might contribute in the future to advancing the *general* implications and insights of dynamical systems theory.

There is considerable merit, then, in seeking deliberately to push the responses to the foregoing ***Challenges # 3*** and ***# 4*** towards the goal of our next challenge, thus to communicate into yet broader domains the generic, scientific and mathematical insights deriving from the specifics of the Environmental Science of the EOs.

Challenge # 5:

> ***Building on the shoulders of the various mathematical theories of catastrophe, chaos, and complexity — but with the ambition to go beyond these — what new insights into the generic and fundamental dynamic properties of the behavior of systems can be obtained from the deliberately orchestrated* in situ *observation of the behavior of many specific environmental systems and the modeling thereof? In particular, how can the rich experience of elucidating these generic features from studies of whole ecosystems, indeed social-ecological systems, be productively interfaced with exploration***

of the novel properties of dynamical systems behavior yet to be discovered in the study of cellular metabolism, self-repair, and self-replication? How can coordination of relevant research across all of the Environmental Observatories uniquely accelerate such development? Looking towards* Challenge # 12*, how can the community of model-builders in the Environmental Sciences best be organized so as to benefit as much as possible from novel developments in modeling in general, as they arise in, for example, the quite disparate disciplines of the biomedical sciences, social sciences, cognitive sciences, artificial intelligence, and artificial life?

The challenge is in large part that of drawing communities productively together.

Cross-fertilization: From Environmental to Biomedical Science

At a conceptual level, and in the archetypal mold of systems thinking — wherein generic insights into problem-solution couples from one field can be transferred to a second field whose problems lack solutions — we should be keenly interested in aligning the potential insights into the dynamical properties of metabolism-repair-replication within a biological cell (at the micro-scale) with those of resilience, at the macro-scale of whole ecosystems (Peterson *et al*, 1998). After all, resilience is about the self-organized maintenance of function in the presence of disturbance, even high-amplitude disturbance, just as much as is self-repair in a cell. Alternatively, such eliding of metaphors from biology and ecology can be driven in rather different directions, across to "cities of resilience", as a blueprint for urban planning, notably in the context of one of NSF's urban-centered (Baltimore, Maryland) Long-Term Ecological Research (LTER) projects (Pickett *et al*, 2004).

We, in Environmental Science, have learned much from the study of ecological systems. Now, it might be said, the opportunity is to learn from studies in Biomedical Science. For it is in that domain where the functions of metabolism, repair, replication, and so forth actually operate and are, therefore, most naturally cast for closer study — study targeted, that is, at discerning (and extracting) key, generic properties of dynamical systems behavior.

What theoretical advance might eventually be expressed from this muddling of ecology, cellular biology, and cities? Consider this, then. The seminal notion of ecological resilience has been elaborated further as entailing the following (from Peterson *et al*, 1998):

> ... [E]cological resilience is generated by diverse, but overlapping, function within a scale and by apparently redundant species that operate at different scales, thereby reinforcing function across scales.
>
> The combination of a diversity of ecological function at specific scales and the replication of function across a diversity of scales produces resilient ecological function.

What principles for re-designing the dynamic performance of a city's water infrastructure could we derive from these, through merely substituting the word "species" by "unit process technology"?[12] Furthermore, let us recall the multiplicity of "scales" apparent in the illustration of "Uncoupling the Nutrient and Water Metabolisms of Cities" in Box 1 in Chapter 2.1. Mixing now our domain metaphors (from Ecology and Biomedical Science): how could any such principles of design be employed to compensate for the ills of the city's metabolism, including in respect of subliminal (self-organized) damage-limitation and the initiation of self-repair in the face of disturbance and threat (Beck, 2005a)?

Cross-fertilization: From Environmental to Social Science

To reiterate, many of the insights we have acquired over the past 30-40 years about the dynamic behavior of systems, in general, have been insights about the behavior of ecological systems, in particular. Such growth in knowledge, however, has been drawn largely from the perspective of populations of species (phytoplankton, zooplankton, budworms) viewed broadly and crudely as "biomasses". The behavior of individual organisms within any biomass was customarily not singled out for simulation: neither in respect of that individual navigating through its

[12] In asking this question, we acknowledge both the essential differences between "engineering resilience" and "ecological resilience" (as discussed in Holling, 1996) and the fact that the latter has itself yet to be incorporated into the design of these technological systems of water infrastructure (Beck, 2005a).

environment, while negotiating with other individuals (in its, or another, biomass); nor in respect of the dynamically changing state of an individual, either in terms of its metabolism (at a sub-cellular level) or its intelligence and perception of its surroundings.

In short, the frontier stands now at the desire and need to understand and simulate the sentient individual organism within its ecosystem, i.e., its environment containing individuals from its own and other species. The difference is subtle, but highly significant. The complement of driving the insights of resilience into the more microscopic details below the crudeness of simple biomass is that of learning from peering outwards and upwards to the larger society in which that biomass participates. Whereas opportunity lies in the study of problems in biomedical systems, so too does it lie in tapping into the domain of modeling in the Social Sciences.

Steeped in the conceptual framework of resilience, Hawes and Reed (2006) are embarking on seizing that opportunity, with their ambitious agenda for the computational study of that dynamical systems property, notably in agricultural and terrestrial ecosystems:

> Though there are many models of system change and resilience in ecology, and many applications of computational techniques to ecological systems, there are few that unite the two disciplines, placing ecological interactions at the heart of new computational algorithms. The project for which this work forms a part aims to take ecological approaches to system function, and individual-based modelling in particular, as a starting point for development of a massively scaled multi-agent system that uses inter-agent communication to model the flow of energy through the system.

The significance of what we here would call the imminent environmental cyber-infrastructure has not escaped their notice (Hawes and Reed, 2006):

> The system implementation and resilience analysis protocol will first be validated by comparison with existing ecological data, before then being applied to new problems of larger, more complex ecosystems, and thence to similar problems of large scale distributed and Grid computing. In this way, we aim to develop a practical theory of resilience which can be reused in the design of artificial complex systems in eScience and e-commerce domains.

It is but a short step from agency in these terrestrial and agricultural systems of Hawes and Reed (2006) to the metaphor of an "animal grazing in its pasture", offered by Rees and Wackernagel (1996) for conceiving of a city's ecological footprint. With the connection to the city thus established, a further small step will take us to transcribing the notion of the "sentient organism in the ecosystem" to that of the "{city and its infrastructure} in the {watershed}". Paris, given the accumulating restoration of the past several decades (Billen *et al*, 2007a), could well be conceived of as the "bull" in the "china shop" of the Seine watershed — a metaphor provoking yet further steps towards conceptions of what cities could become (Crutzen *et al*, 2007).

Models, we already know, have been developed for simulating how elk and fish navigate through their environments (Bennett and Tang, 2006; Goodwin *et al*, 2006), with recourse in their construction to anthropocentric notions such as a "game-theoretic approximation" and "boundedly rational agents" (Chapter 2.4 and the foregoing ***Challenge # 4***).

Yet another step outwards and away from mere biomass as state variable in a model brings us to the intense, current interest in deploying the models of computational game theory in order to understand how cooperation amongst individuals arises in a community (for example, Dieckmann and Metz, 2005; Levin, 2006; or Ohtsuki and Iwasa, 2006). Indeed, this interest may not only be intense, but urgent. In his Kyoto Prize Laureate Lecture (November, 2005), entitled "Learning to Live in a Global Commons: Socioeconomic Challenges for a Sustainable Environment", Levin gives us yet another insight into the cross-disciplinary nature of systems thinking (Levin, 2006):

> The great challenge then is to understand when and how cooperation has evolved in biological systems, and what lessons we can derive from these insights for how to achieve cooperation in dealing with our future environment.

Finally, beyond the rudimentary psychology of Ohtsuki and Iwasa's (2006) search for the theoretical underpinnings of cooperation, another step can be notched up, in our path towards Social Science. It would bring us to the work of Janssen and Carpenter (1999) in simulating the interaction between the environment and human agents, each imbued with varying cultural outlooks on the Man-Environment relationship and capacities for learning (from each other, and from economic and environmental data). Few, if any, computational environmental studies have yet gone further.

Synthesis (Culmination): Nurturing Classical "Systems Thinking"

When contemplating the behavior of individuals in herds, flocks, swarms, communities, or societies, it has become natural to think of simulation in terms of agent-based models, or the IBMs of Grimm *et al* (2005). Our hopes for this are not small (Levin, 2005):

> The literature is too diverse and fast moving to allow an adequate review here; suffice it to say that the development of agent-based approaches to understanding all aspects of biospheric organization, from proteomics to nutrient cycling to civilizations, is one of the most active and exciting areas of research, crossing disciplines and yielding new insights into the workings of the world.

"Systems thinking" and synthesis flow in other ways as well. The following — on extracting generic insights into adaptive dynamics in systems and then mobilizing them across various disciplinary domains of enquiry — is a classic expression thereof (Levin, 2006):

> Moving from the ecological to the social or economic situation simply completes the loop — these are ideas that had their origins in economics, were adapted and modified for biology, and now find new application in their original setting.

We shall encounter later (in respect of ***Challenge # 12***) the telling significance of this in responding to the community-oriented issues of our current ***Challenge # 5***.

The essence of ***Challenge # 5***, however, lies not so much in advancing the sophistication of IBM computational platforms, but in developing and implementing programs of research designed to reveal new insights into general dynamical systems properties (from the study of those environmental systems within the purviews of the EOs).

We presume there must be alternatives to the pursuit of IBMs alone, since nonlinear differential equations and classical calculus are clearly still predominant in so many other areas, at scales both above and below that of an individual organism. They are used in the very small, to study metabolic maps (systems) of enzyme-catalyzed reactions within bacterial cells (Alvarez-Vasquez *et al*, 2005; Voit *et al*, 2006) (exemplified by Figure 4). And they are as much the basis of models literally of global behavior (Kohring, 2006), whose concern is to find (and avoid) chaotic behavior in Sanderson's elementary model of global demographic, economic, and environmental interactions (Wonderland; Sanderson, 1994).

But what could these two schools of thought generate, in response to our challenge, when pursued in tandem: the classical nonlinear dynamical analyses associated with control theory, on the one hand,[13] and the IBMs of Grimm *et al* (2005), Levin (2005), and Hawes and Reed (2006), amongst many others, on the other hand?

Tending in an encouraging direction from the one side is Casti's (2002) advocacy of "biologizing control theory", with its intellectual foundations set in the mathematical analysis of autopoietic systems — defined as those that are "capable of self-maintenance owing to a process of components self-generation from within", which "generalizes the definition of life" according to Bitbol and Luisi (2004). Such systems, it appears, are not "Turing computable", however (Luisi, 2003). The pragmatic challenges of our needs for the oncoming environmental cyber-infrastructure, such as those of software protocols for bridging the heterogeneity of computational frameworks (for example, that of OpenMI arising under ***Challenge # 2*** in Chapter 2.2), would seem to pale into insignificance in comparison to that challenge.

[13] Which analyses have struggled to find proper and effective expression in ecology (Loehle, 2006), albeit less so in the metabolism of cells, where Voit *et al* (2005) are now able to characterize a feedforward switching mechanism in bacterial glycolysis and lactate production.

2.6 Observatory Network Design and Operation

Let us recognize a fact. This *White Paper* would not have been written, nor would there have been any Workshop in Tucson on "Grand Challenges of the Future for Environmental Modeling", were there to have been no Environmental Observatory initiatives in the first place. Grand issues in science provoke equally grand programs of observation, to the outcomes of which — data streams — developments in computational modeling will be tailored. In terms of large expenditures of funds, the logic is unlikely to run the other way, although in places our ***Challenge # 1*** urges that it should, as in prompting basic enquiry at the interstices amongst disciplines. Others have ventured further (Dennis *et al*, 2002). They recommend that priorities for developing novel sensing devices should be contingent upon those barriers to theoretical progress identified in unraveling the complexities of atmospheric chemistry when assembled and simulated in a large-scale computational model.

Nothing in the strength of this generally forward flowing logic from field observation to model, however, precludes the effective use of models in the design of observing programs and, therefore, parts of the Observatories themselves. As we turn now to this topic and embark on the next sequence of challenges (***Challenges # 6*** through ***# 9***), we shall pick up our organizing triplet $\{\boldsymbol{u}, \boldsymbol{M}, \boldsymbol{y}\}$ from Chapter 1.2 — of the observed inputs ($\boldsymbol{u}$), model ($\boldsymbol{M}$), and observed outputs ($\boldsymbol{y}$) — and put it to work, to ask in various textbook ways: given two out of the three unknowns, find the third.

An Immediate Need for Models: Observing System Simulation Experiments

No experimental design, or design of an EO, can proceed technically in the absence of a model, albeit a mental model. Our focus herein is on computational, mathematical models ($\boldsymbol{M}$) and their role in both the design and operation of observatory monitoring and sensor networks. The work of Wu *et al* (2005) is indicative of this focus. In their case, complex groundwater flow and contaminant transport models are used to generate a cost-effective sampling strategy intended for management of a contaminant plume. Clearly, in so very many cases across all facets of the EOs, our $\boldsymbol{M}$ are self-evidently much more sophisticated than mere mental models. There are, therefore, many instances in which computational models should be (and are) employed in the designs of the EOs, before they are put in place.

Observing System Simulation Experiments (OSSEs) have a long history, originating in meteorology and climatology, where over 20 years ago Arnold and Dey (1986) found the subject already sufficiently mature to warrant a survey of its "past, present and future". Almost as mature are their applications in oceanography (for example, Raicich, 2006). The proposal of Krajewski *et al* (2006) for a Remote Sensing Observatory (RSO), as a CUAHSI-inspired form of hydrological EO, cites OSSEs as the means of estimating the "impact of planned future observing systems and determining requirements or gaps to help guide priorities for unplanned future observing systems". OSSEs in Environmental Engineering, directed expressly at operational management under all manner of observing network and sensor failures, incorporate the simulated dynamics of not only the observed entity but also of the sensing instruments themselves (Rosen *et al*, 2008).

In our cryptic notation, presuming a model $\boldsymbol{M}$ and given an input, forcing-function sequence $\boldsymbol{u}$, some hypothetical bundle of data $[\boldsymbol{u},\boldsymbol{y}]^0$ can be generated, as though "complete" observations of the real system, error-corrupted or not, resolved down to some fine spatial and temporal scale (if not biogeochemical scale). The goal of the OSSE is to find that "incomplete", i.e., sampled, more coarsely-scaled combination of measured variables $[\boldsymbol{u}',\boldsymbol{y}']^S$ that optimizes some function of monitoring cost and/or measure of confidence (uncertainty) in the recovery of estimates of $[\boldsymbol{u},\boldsymbol{y}]^0$ from $[\boldsymbol{u}',\boldsymbol{y}']^S$.[14] In the context of the OSSE, the model serves the purpose of identifying an appropriate sampling strategy for yielding data about the state of nature, as encapsulated in $[\boldsymbol{u},\boldsymbol{y}]$. These data will then serve the purpose of various scientific questions, *not* necessarily the goal of expressing anything further about a computational model, including that ($\boldsymbol{M}$) employed in the OSSE itself.

Across the spectrum of disciplines, the most insistent plea emerging from the Tucson Workshop was for the systematic application of procedures such as

[14] Here $\boldsymbol{u}'$ and $\boldsymbol{y}'$ denote vectors of observed system inputs and outputs of, in principle, different (smaller) orders and different elements from those of $\boldsymbol{u}$ and $\boldsymbol{y}$; superscript S denotes the fact that observations are taken at discrete points in space and instants in time, such that they are not literally continuous at some sufficiently fine-grained scale, denoted by superscript 0.

OSSEs in the design of each EO, *before* it is fully constructed — as currently intended in Phase II of the WATERS Network EO (WATERS, 2008). OSSEs are not new. Their maturity indeed strengthens the case for their further use, for contemporary Observatory network design, more so than network operation. And doubtless, their computational scope and sophistication will continue to grow.

Experimental Design for Model Identifiability

The archetypal problem of experimental design expressed in Chapter 1.2, of choosing the contents of $\boldsymbol{u}$ and $\boldsymbol{y}$ so as to maximize the "identifiability" of $\boldsymbol{M}$, has intrinsic merit in the context of *modeling for its own sake*. As opposed to design for stewardship of a contaminated area of land (Wu *et al*, 2005), it is a design for learning, if not discovery: of progressing from a prior model ($\boldsymbol{M}_{prior}$) to an improved posterior model ($\boldsymbol{M}_{posterior}$) of how the observed piece of nature behaves.

Interest in formally solving this problem began in earnest in the 1970s, primarily in terms of finding uniquely "best" or minimally uncertain estimates of the model parameters appearing in $\boldsymbol{M}$, i.e., a "well identified" model. Input perturbation (experimental) design was being studied as a subject of optimization, to serve the needs of the then burgeoning schemes of adaptive, real-time (on-line) control in engineered systems. Today, wherever the nonlinear Michelis-Menten or Monod kinetics of growth of microbial organisms appears in a model — in wastewater treatment (Petersen *et al*, 2001; Brun *et al*, 2002; Stigter *et al*, 2006), river water quality and lake ecology (Brun *et al*, 2001; Omlin *et al*, 2001) or oceanography (Raick *et al*, 2006) — some detailed account of the problem of (a lack of) model identifiability is given.

In fact, the problem of a lack of model identifiability is nigh on ubiquitous: it permeates the present ***Challenge # 6***, in attempts at minimizing, suppressing, or circumventing it; similarly ***Challenge # 7***, where the key goal is to cope with it and quantify its associated uncertainties; as much as in ***Challenge # 8***, which calls for robust forecasts in the face of it. The thread of uncertainty connects the three (Beck, 1987): experimental design for the pre-emptive reduction of model uncertainty (***Challenge # 6***); identifying the model in spite of all the uncertainties — and enumerating them and their loci in the model (***Challenge # 7***); and accounting for the consequences of those residual uncertainties, as they propagate forward in any forecasts generated with the model (***Challenge # 8***). There is no shortage, then, of discussion elsewhere of the issue of a lack of model identifiability, conspicuously so in the literature of Hydrology. This *Paper* will be no exception, although the burden of the attaching discussion will be deferred until expression of ***Challenge # 7*** in Chapter 2.7.

Sustained thus for nearly three decades now, the design of optimal, probing inputs ($\boldsymbol{u}$) is culminating in what can only but be described as "systematization" on an almost industrial scale, as befits the contemporary scene in biotechnology more generally (Lindner and Hitzmann, 2006):

> Combinatorial chemistry will create new enzymes, whose kinetic parameters have to be elucidated efficiently. High-throughput techniques are applied here for target finding. By using such an experimental design approach in this area, the additional effort will be rewarded by a higher precision in parameter estimation, producing more reliable results in target finding.

The work of Lindner and Hitzmann (2006) examines the optimal allocation of finite observing and perturbation capacities, in principle (in theory). That of Petersen *et al* (2001) deals with the same, but in the practical design and operation of instruments to be placed in the harsh, rugged environment of microbial growth in biological wastewater treatment. To their work has been added the significant refinement of adaptive specification of input (feeding) perturbations as learning proceeds on-line in respect of the (model of the) behavior of the system (Stigter *et al*, 2006). We stand, therefore, on the verge of having very "smart" instruments: on-line respirometers, i.e., microcosms of the prototype system, wherein identification of the model of that instrument, $\boldsymbol{M}^I$ (with superscript I denoting instrument), is being performed in a "self-aware" and "self-optimizing" manner in real-time. The smart instrument performs these functions, moreover, in the service ultimately of progressing from a prior model, $\boldsymbol{M}_{prior}$, to an improved posterior model, $\boldsymbol{M}_{posterior}$, of the environmental system itself (*not* the instrument).

Unlike the fed-batch reactor in a respirometric instrument, or even the engineered unit processes of wastewater treatment, larger-scale, field hydrology cannot benefit in general from deliberate manipulation of the inputs to the system ($\boldsymbol{u}$). It does enjoy the significantly perturbing events of precipitation, nevertheless. In a somewhat restricted sub-domain, where knowledge is required of the particular paths of water flow through a watershed (Vaché and McDonnell, 2006) — for example, because of the different chemical signatures attaching to each path (as in the response of streams to inputs of acidic precipitation) — the role of natural tracers in concert with happenstance precipitation sequences has been expressly studied from the perspective of model identifiability and experimental design (Beck *et al*, 1990). Given a model of the watershed (***M***) and observations of stream flow and tracer concentrations, the question was, in essence: what kind of precipitation event at the right time in the right sequence of events (or absence of events) would reveal more about the behavior of the system, and more clearly, with less uncertainty attaching to the posterior estimates of the model's parameters?

Adaptive Sampling and Observatory Operations

From experience of the natural environment, we note the potential opportunity of contingencies. From the well controlled, constructed environments of biotechnically engineered systems, derives access to smart instruments and a rich supply of detailed theoretical studies of experimental design. Benefitting from both, our next challenge assumes this textbook form. Given ***M***, and given the revelation that current observations (***u*** with ***y***) from an operational EO are inconsistent with that ***M***, how should observing capacity (***u***, ***y***) be redeployed?

Expressed less cryptically, we have this.

Challenge # 6:

> ***Given a mature complex of environmental cyber-infrastructure and sensors, with — crucially — both an ever-alert monitoring and horizon-scanning facility and in-depth capacity for real-time processing of information and production of knowledge, what kinds of novel, model-based computational schemes of adaptive environmental sampling will be needed to enable rapid re-targeting of observing capacity for on-line probing of, and experimentation with, systems behavior?***

According to Darema (2005) the phrase "Dynamic Data Driven Applications Systems" (DDDAS) entered the lexicon of discussions of cyber-infrastructure some time in early 2000. It is only because of the advent of Grid computing and the prospect of an environmental cyber-infrastructure that we are able to contemplate responding to the above challenge. And by far the most interesting facet of the envisaged environmental cyber-infrastructure is the presumption of its scope for two-way communications: that somehow the implemented, but planned, observing functions of the EOs are sensitized to detecting an anomaly and invested with sufficient "intelligence" for redeploying observing capacity to re-focus on that peculiarity, in an instant, in real-time.

Figure 5 is one instance of such a vision, taken from the work of Mahinthakumar *et al* (2006) on threat-response in public, potable water supply systems. The purpose of this ever-alert cyber-infrastructure and DDDAS, continually primed and poised to detect an "incident", is to address questions such as these (Mahinthakumar *et al*, 2006):

> Where is the source of contamination? When and for how long did this contamination occur? Where should additional hydraulic or water quality measurements be taken to pinpoint the source more accurately? What is the current and near future extent of contamination? What response action should be taken to minimize the impact of the contamination event? What would be the impact on consumers by these actions?

Its features are not greatly dissimilar from the DDDAS of Flikkema *et al* (2006), which seeks to control a poised, ever-alert network of smart wireless sensors in order to improve (ultimately) the prediction of biodiversity and carbon accumulation in terrestrial ecosystems. The case-specific questions of Mahinthakumar *et al*, (2006), if solved by the cyber-infrastructure in a more automated manner, would begin to articulate some of the ideas of subliminal damage limitation and self-repair expressed earlier in the same domain of metropolitan water infrastructure (with reference to Box 1 of Chapter 2.1, under ***Challenge # 3*** and, in particular, ***Challenge # 5***; Beck, 2005a).

We shall exploit these more generic features of Figure 5 in outlining indicative responses to ***Challenge # 6***.

Consider this. When operating in a normal, routine mode, suppose the Observatory is gathering in data

$[\boldsymbol{u},\boldsymbol{y}]^S$ at some coarse level of resolving power relative to $[\boldsymbol{u},\boldsymbol{y}]^0$ (as previously defined) and with a model of the environmental system that is invariant with time, $\boldsymbol{M}$. In the frame of Figure 5, $\boldsymbol{M}$ will be embedded in the "simulation engine"; $[\boldsymbol{u},\boldsymbol{y}]^S$ are what pass into the "adaptive wireless data receptor and controller" from the sensors; while $[\boldsymbol{u},\boldsymbol{y}]^0$ constitutes the universe of all that could be happening in the environment surrounding the cyber-infrastructure.

Let us further assume that at some point in space-time, $P(t,\boldsymbol{s})$, something in the "gap" between $[\boldsymbol{u},\boldsymbol{y}]^S$ and $[\boldsymbol{u},\boldsymbol{y}]^0$ — something conceptually originating in the {acknowledged unknown} — impinges upon the behavior of the system, including a spontaneous opportunity for better or different learning about the nature of the observed system. Alternatively, suppose something occurring within the data stream $[\boldsymbol{u},\boldsymbol{y}]^S$ is significantly not consistent with $\boldsymbol{M}$, i.e., not consistent with the {presumed known}. Or we could imagine an incident where what the cyber-infrastructure perceives through $[\boldsymbol{u},\boldsymbol{y}]^S$ as anomalous, originates in neither the {presumed known} nor the {acknowledged unknown}. Instead of the event originating in the environment of the cyber-infrastructure, $[\boldsymbol{u},\boldsymbol{y}]^S$ is corrupted as a consequence of faults and failures in the sensor network, such as within the "static water quality sensor network" of Figure 5. Or there again, all three types of event could occur as an entangled, compound incident. In short, the event has propagated into the core of the cyber-infrastructure, triggering the kinds of questions already listed above (Mahinthakumar *et al*, 2006).

At this point in our thought experiment, the essential question of ***Challenge # 6*** is as follows: how should the finite observing capacity be re-deployed, away from the previous regime $[\boldsymbol{u},\boldsymbol{y};t^-]^S$ towards $[\boldsymbol{u}',\boldsymbol{y}';t^+]^S$ where t^- marks time before t and t^+ marks time after t, the moment of the event. What signals are to pass back out of the enabling cyber-infrastructure of Figure 5, from

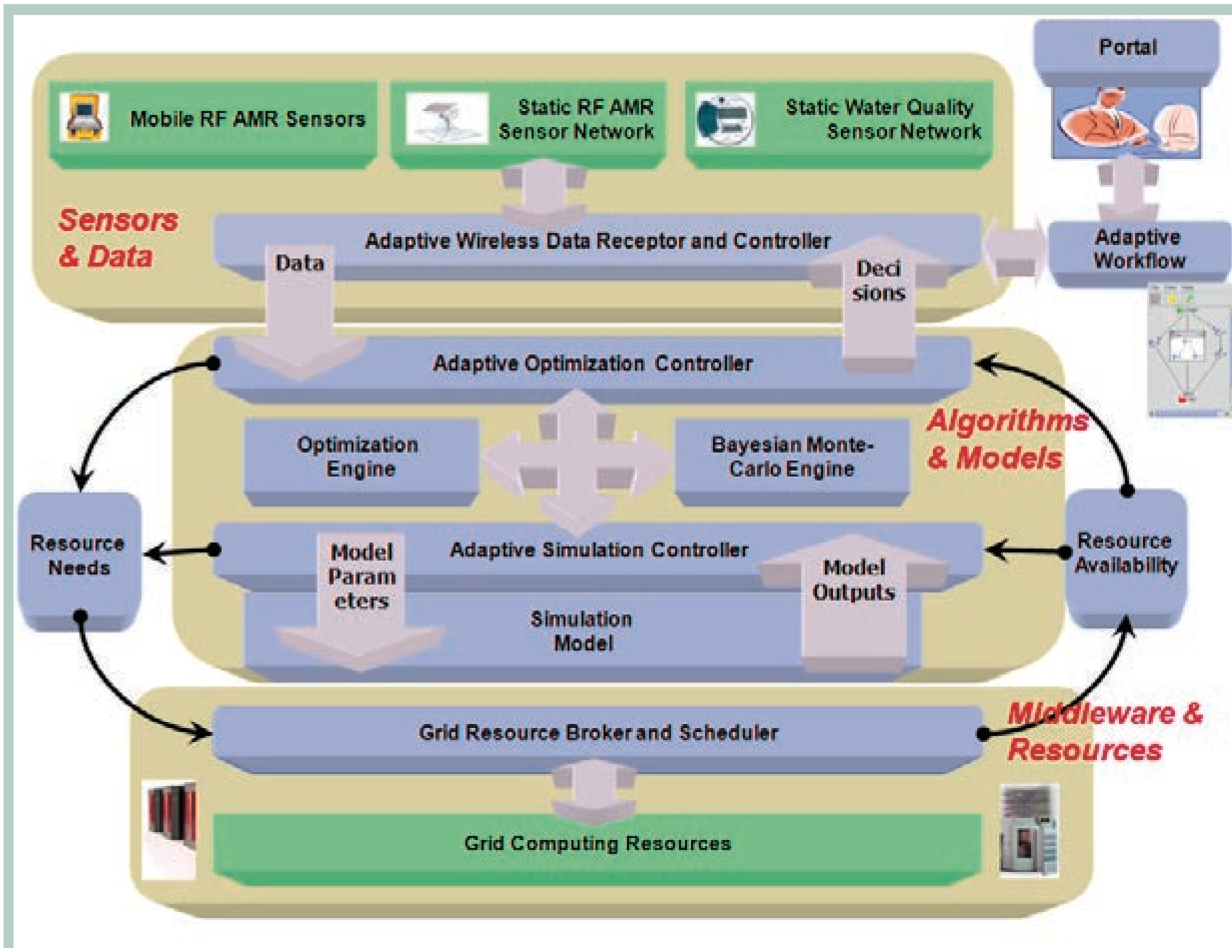


Figure 5
Schematic vision of a Dynamic Data Driven Applications System (DDDAS) for threat response in public, potable water supply systems (Mahinthakumar *et al*, 2006; reprinted with permission).

the "adaptive wireless data receptor and controller" block, to the sensors in the field? This, of course, implies an answer to the prior question, of detecting the occurrence of the event in the first place and then diagnosing the nature of its several possible components.

At the heart of contemporary work on fault detection and environmental vulnerability in a real-time network for monitoring water quality in the Lagoon of Venice (Ciavatta *et al*, 2004), resides the notion of a model of time-varying structure ($\boldsymbol{M}(t)$) as the means to solve such problems. In other words, there can be "structural change" in the behavior of a system. $\boldsymbol{M}$ is not invariant but evolving with time, from $\boldsymbol{M}(t^-)$ to $\boldsymbol{M}'(t^+)$, a matter of considerable significance below in expressing ***Challenge # 7*** (Beck, 2002; 2005b). Cast in the cyber-infrastructure of Figure 5, this would be tantamount to the "adaptive simulation controller" managing an *adaptive* model, with the flow of "model parameters" between controller and "simulation engine" reversed, if anything. For it is the reconstructed temporal variations in these parameters — their drifts, jumps, oscillations, and so forth, estimated recursively in real time (t) — that offer uniquely defining insights into the nature of the event. Hence, a particular re-deployment of the sensor network's observing capacity can be determined; and that is the essential output from the cyber-infrastructure in this instance.[15]

Hints of such adaptive capacity, in the performance of the cyber-infrastructure, as much as through "structural change" in an adaptive model, can be found in Lermusiaux *et al* (2006a), who write as follows of "adaptive sampling" and "adaptive modeling" in the context of ocean research:

> Adaptive sampling forecasts the observing paths that minimize uncertainties, optimizes the sampling of dynamical hot spots and maintains overall coverage. Adaptive modeling selects the physical or biological parameterizations that give the best model-data fit.[16]

They proceed to qualify their definition of "adaptive sampling" as (Lermusiaux *et al*, 2006a):

> The path, locations and other properties of observing platforms and sensors can be optimized and adapted in real-time, so as to respond to the ocean variability and its uncertainties.

and elsewhere as (Lermusiaux *et al*, 2006b):

> [A]daptive sampling estimates the types and locations of the observations that are most needed.
>
> [A]daptive modeling identifies the model properties that need most improvements.

Erasing Boundaries Between System, Sensor, Cyber-infrastructure, and Model

The distinctiveness of the approaching environmental cyber-infrastructure is its promise of a seamless integration of communications: from point of sensing in the environment to the computer screen in front of the analyst; and back, in the reverse direction, from keyboard/touch-screen to the object of scrutiny *in situ*. Anticipating this operational, real-time Observatory facility, science planning for the WATERS EO envisages a continual two-way re-allocation of resources across the cyber-infrastructure to track, for example, any incipient and then unfolding anomaly in the occurrence of a coastal hypoxia event (WATERS, 2007a, 2008).

Where exactly the intelligence of the computational model is to be vested, along the communications bus between office desktop and sensor in the rough of the field (as, for example, in Figure 5), is becoming now a matter of rather free and thought-provoking interpretation. Environmental engineering, for example, is taking such interpretation to considerable sophistication, in particular, in wastewater systems engineering, with its interest in the operational control of microbial ecosystems. As we have seen (Petersen *et al*, 2001; Stigter *et al*, 2006), a model ($\boldsymbol{M}^I$) may become integral to the sensing device, as in the microcosm of an in-line respirometer, whose deliberate mechanical functions, of aeration, mixing, and quiescence, are

[15] Using indeed the same algorithms of recursive estimation undergirding the adaptive, experimental control/probing of Stigter *et al* (2006); and broadly consistent, therefore, with the Bayesian algorithmic setting of Figure 5 (Mahinthakumar *et al*, 2006), likewise too that of Flikkema *et al* (2006).

[16] This may, however, suggest an instance of a number of alternative, time-invariant, candidate, model structures $\boldsymbol{M}_i$, $i = 1, \ldots, n$, with evolving probabilities assigned at succeeding points in time (t) in order to describe the structure most likely to reflect observed behavior at that time — something of significance in ***Challenge # 8***.

geared to maximizing the identifiability of the model of the observed system itself (***M***) (Vanrolleghem *et al*, 1996). In the cyber-infrastructure of Figure 5, $\boldsymbol{M}^{I}$ would be embedded in the sensor block "static water quality sensor network", while ***M*** is lodged in the "simulation engine".

There is a certain complementarity. Just as the model ($\boldsymbol{M}^{I}$) can be embedded in the (real) sensor, so the behavior of the (virtual) sensor can be incorporated within the model (***M***) of the whole — simulation, in effect, of the cyber-infrastructure *and* the observed environmental system (Rosen *et al*, 2008).

Stepping back from the clutter of the technical detail, while noting the potential for our thinking to be blinkered by the focus of this *Paper* on the role of *modeling* in the EOs, three further vital questions follow: can the essential adaptation in re-directing observing capacity (in an instant; at a moment's notice) be implemented without a computational model (***M***); how should the value added in conducting the adaptation with a model be maximized; and can a model be expressly designed with such maximization in mind?

2.7 System Identification

We all want the model to approximate the real thing in some demonstrable manner, for reasons of scientific enquiry or for some other purpose, such as making a prediction in association with determining a course of future actions of environmental stewardship. Indeed, the extent to which the model can be reconciled with past observed behavior is a measure of the extent to which we might judge the primary science to be provisionally corroborated. At the same time, the map of uncertainty attaching to the posterior model's conceptual structure and its constituent mechanisms, after this process of system identification, will have significant consequences for any exercises in forecasting and investigating possible future patterns of behavior (Beck, 1987). In this sense, the second and third of our textbook problems from Chapter 1.2, i.e., "given ***u*** and ***y*** find ***M***" (system identification) and "given ***M*** and ***u*** find ***y***" (forecasting and foresight generation) are intimately inter-related. Both, however, are sufficiently substantial to merit their own respective ***Challenges***, and will therefore be treated in separate chapters.

For a *Paper* on grand challenges for environmental modeling (***M***) — arising expressly from initiatives (the Environmental Observatories) designed to provide access to unprecedented streams of data [***u***,***y***] — there is arguably no greater challenge than that of responding to the novelty unleashed thereby in those "acts" of Lewis, "which interpret data in terms of concepts", i.e., system identification. This is model calibration writ immensely more richly. And because the richer, more philosophical facets of system identification can so often be obscured by the straightforward pragmatism of model calibration, there is considerable intricacy and deeper subtlety now to be conveyed. Much of the supporting detail of the narrative surrounding this next ***Challenge*** has therefore been placed in Boxes 2 and 3. From that detail, however, emerges an important emphasis on scientific visualization as part of a preliminary program of research for responding to the ***Challenge***.

History: Algorithms for Model Calibration

Inasmuch as the 1960s were a time of "youthful exuberance" in the development of environmental simulation, so did great expectations surround the outward dispersal of the computational methods of Statistics, Operations Research, and Control Theory, from aerospace engineering into environmental science and, for present purposes, into the topic of model calibration (Beck, 2002).[17] The prior, rudimentary practice of trial and error — of trying out different values for the model's parameters (**α**) until the "curve" of the estimated outputs would match satisfactorily (in some sense) the "dots" of the observed output data — was to be supplanted by the more systematic, objective procedures of mathematical programming, optimization, mathematical filtering theory, and the like. The modernism of "automatic calibration", detached from subjective manipulation, was to supercede the craft-skill of "calibration by hand". It did not. The two co-exist fruitfully today, notwithstanding the supposed academic inferiority of the latter.

Such difficulties in applying the computational algorithms of model parameter estimation and system identification are not surprising. For we have already examined in some depth model-based procedures of experimental design, for overcoming a lack of model identifiability (in Chapter 2.6 in respect of the foregoing ***Challenge # 6***). To recall, a lack of identifiability is defined technically as the inability to locate a set of values for the model's parameters that are self-evidently superior to the myriad of all other candidate sets of values in generating a uniquely best match between the model and the data. Attempting to overcome a lack of model identifiability matters philosophically — in the growth of secure knowledge — because this implies a determined attempt at expunging ambiguity in interpretation*s* of Lewis's "data" and at reducing to a singularity an otherwise plurality in his plausible "sets of concepts".

These difficulties of a lack of model identifiability arose not because of the inadequacies of the algorithms themselves, but as a result of the growing complexity (and nonlinearities) of the models, on the one hand, and of the nature of the data, on the other — their sparseness across the space-time-biogeochemical continua and their uncertainties. Whereas calibration by hand may never have shed light on such difficulties of model identifiability, automatic calibration revealed them very early on and all too consistently since. They may seem esoteric difficulties, of concern only to Science. Yet they matter to the public, since Mooney fully intends scientifically-lay members thereof to read his (2007) popular account of "*Storm World — Hurricanes, Politics, and the Battle Over Global Warming*" (Mooney, 2007). His account (literally) personifies what we shall describe below as the matter of model structure identification.

One of the most significant algorithmic developments in the 1970s was thus a retreat from the expectations of automatic calibration to a procedure of hypothesis screening, known familiarly today as a Regionalized Sensitivity Analysis (RSA; Hornberger and Spear, 1981). Our discussion has already alighted on this, in Chapter 2.1 (***Challenge # 1***). RSA was tailored to the needs of evaluating the model-encoded science base in those very many situations with but sparse, quantitative data supplemented by the qualitative, subjective, experience of the system's apparent behavior, as gathered informally by scientists working in the field. Its goal was to answer the question: under the gross uncertainties of system behavior observed as such, which more or less speculative constituent hypotheses in the model are key — and which redundant — to discriminating whether the model generates behavior akin (or not) to that observed experience.

This conceptual and algorithmic break with the expected trend was in due course reflected back onto the study of more conventional, less-sparse, data situations (Hornberger *et al*, 1985; Keesman and van Straten, 1990); adapted to incorporate some of the more subjective elements of interpreting matches of model performance with observed data (Wheater *et al*, 1986); and re-combined conceptually with the mainstream of those algorithms of automatic calibration that had evolved in the meantime (Gupta *et al*, 1998); thus to be found in its current realization under the label of a "dynamic identifiability" method (Wagener *et al*, 2003; with further embellishments in Choi and Beven, 2007).

Across those four decades, algorithmic notions of how to attain the optimum — here of estimates of the parameters **α** within the structure of the model ***M*** — had progressed towards computational exploitation of the biological notions of genetics and evolution, combining therein principles of intelligent adaptation and randomized experimentation, as, for example, in the algorithmic innovation of Duan *et al* (1993) and its successors. Significantly, things seem almost to have come full circle, driven by the changing and expanding capacity for observation, perhaps most tellingly conveyed in the increasing refinement, intensity, and extensiveness, of sampling along the space-time-biogeochemical continua already alluded to in

[17] A topic — of whether to calibrate a model or not — that remains controversial, or at least one in which different, opposed schools of thought continue to prosper: witness the current views of the recently published NRC document on evaluating models used in the regulatory decision-making process (NRC, 2007; pp 124-126).

Chapter 2.2 (for instance, Kirchner *et al*, 2004). Accordingly, the original impulse towards what is now the vast field of automated model calibration in its more customary forms may well be enjoying a renaissance, typified by the contemporary works of Mugunthan *et al* (2005) and Moore and Doherty (2006), both notably in respect of models described as "computationally expensive", i.e., VHOMs.

Given this history — and it is the history of the persistent deficit in engaging VHOMs with field data in a context of discovery and learning — our next ***Challenge*** is expressed as follows.

Challenge # 7:

> ***Under the expectation of massive expansion in the scope and volume of field observations generated by the Environmental Observatories, coupled and integrated with the prospect of equally massive expansion in data processing and scientific visualization enabled by the future environmental cyber-infrastructure, what radically novel procedures and algorithms are needed to rectify the chronic, historical deficit of the past four decades in engaging complex models (VHOMs) systematically and successfully with field data for the purposes of* learning and discovery *and, thereby, enhancing the growth of environmental knowledge?***

This is redolent of the over-arching challenge for this entire *White Paper* (***Challenge # 0***).

Likewise, we should be reminded of Lewis's pragmatist approach to the growth of knowledge, in particular, the pivotal element in his schema: of "acts which interpret data in terms of concepts". ***Challenge # 7*** is both more specific in its intent and central in the convergence and potential exploitation of the two principal innovations anticipated with the advent of the EOs. On the one hand, there is the cyber-infrastructure, which continues to extend the ambition of complex models beyond even VHOMs to the ever-receding horizon of virtual realities — the ultimate computational mechanizations of Lewis's sets of concepts. On the other, a qualitatively more comprehensive suite of observing technologies is to be developed and installed (NSF, 2005), yielding what we shall refer to as high volume high quality (HVHQ) data. ***Challenge # 7*** is essentially about the algorithms, procedures, and support-software required to maximize the benefits from these two innovations, taken *inseparably* together.

Should anything be said of responses to ***Challenge # 7*** in respect of charting the future course of algorithms of mathematical programming, albeit those focused on the needs of calibrating environmental models? This, we confess, is beyond the scope of this *White Paper*. We shall merely presume that progress along that avenue will indeed be fruitful and unfold in ways continuing to benefit our systematic attempts at reconciling VHOMs with HVHQ data. Most notably, we should welcome the targeting of such developments at the estimation of very high-order vectors of model parameters ($\boldsymbol{\alpha}$) in addressing a generic problem we shall now call *model structure identification*.

Model Structure Identification: The Problem

There is another reason for the occurrence of a lack of model identifiability, not widely acknowledged until recently, which therefore, by reflection, extends the opportunity of significant novelty in future research.

A fixed model structure ($\boldsymbol{M}$) populated by invariant parameters ($\boldsymbol{\alpha}$), or logical rules (as in IBMs), is a very strong presumption. The structure of a model is defined by the input, state, and output variables chosen to characterize the behavior of the modeled system, the logic of the inter-connections amongst all these variables, and the particular mathematical forms and rules of the various assumed interactions. To say that a model suffers from structural error/uncertainty, or conceptual error, is to indicate error or uncertainty in any one of these facets. For example, and most simply, we might judge that, except for an incorrect mathematical form for the interaction between two variables, all else about the model's structure is correct. More profoundly, however, our view might be that significant and manifest attributes of the system's behavior appear to attach to (unknown) variables entirely omitted from the model.

In introducing the notion of models as devices for hypothesis generation and screening in response to ***Challenge # 1*** — and putting the same to work again in the preceding Chapter 2.6, in respect of diagnosing the nature of incidents impinging upon the ever-alert cyber-infrastructure (***Challenge # 6***) — we made use of the following dichotomy. When a model is constructed, certain pieces of the primary science bases are presumed known and included in explicit mathematical form, i.e., the {presumed known}. Its complement, that which is acknowledged as not known, i.e., the {acknowledged unknown}, is therefore not included in the model's structure, by definition — except typically under the lumped, and largely conceptual, stochastic processes customarily referred to as the system and/or observation noises. In the light of this distinction, the foregoing reference to structural "error/uncertainty" is not a matter of being pedantic. For there are important differences between discovering that the {presumed known} is in fact in *error* and discovering that something of significance, *not* arising from pure chance, resides in the *uncertainty* of the {acknowledged unknown}. This we recognize from ***Challenge # 6***.

To presume such structural error/uncertainty is negligibly small is therefore a strong assumption, especially the greater the coverage in the model of the non-physical quantities along the biogeochemical continuum. Relaxing this assumption, therefore, to proceed from a prior structure for the model, $\boldsymbol{M}_{prior}$, to an improved posterior model, $\boldsymbol{M}_{posterior}$ — and, crucially, by reference to a set of field data — we refer to as model structure identification. The work of Spitz *et al* (2001), on calibrating an ecosystem model for the upper, mixed layer of the ocean to the Bermuda Atlantic Time Series (BATS) observations, turns out to be exemplary in this sense. In their advance from an $\boldsymbol{M}_{prior}$ to an $\boldsymbol{M}_{posterior}$, a new state variable is introduced (meso-zooplankton biomass); the forms of the interactions amongst three states (dissolved organic matter; bacterial biomass; and ammonium) are re-structured to provide an improved account of the microbial loop; and the ratio of chlorophyll-*a* to carbon in phytoplankton biomass — seemingly an *invariant* model parameter — is re-expressed as a function of two state *variables* (Spitz *et al*, 2001).

Responding to the Problem: Conceiving of Model Parameters Not as Constants

A key to solving the problem of model structure identification is the idea that the parameters in a model may vary with time and space. Conceiving of parameters ($\boldsymbol{\alpha}$) in a model as entities changing with time — the notion that they might not actually be "constants" — and applying this outlook within the context of model structure identification, date back at least to the late 1960s (Young, 1978; Beck, 2002), if not earlier (Young, 1984). The logic of why structural error/uncertainty in a model, which is axiomatic, implies the need to conceive of model parameters as capable in principle of variations in time, is an argument of rather more recent origin (Beck, 2002, 2005b), and will not be rehearsed herein. Likewise, algorithmic frameworks enabling computation of estimates of model parameters varying across time (and space), such as recursive estimation, Regionalized Sensitivity Analysis (RSA), and conventional optimization, are merely summarized and briefly illustrated in Box 2.

Ultimately, progress in acquiring knowledge of any system's behavior is gauged by the extent to which the goal of a model populated by parameters that are indeed demonstrably constants, is achieved. Or, in the case of the IBMs of Ecology, similar progress will be evident when it can be concluded that constituent rules of individual behavior are invariably appropriate for all individuals for the entire extent and period of simulation (Grimm *et al*, 2005; Railsback, 2001). Suffice it to say that being able to estimate values for a model's parameters that change with time and space is therefore indicative of that goal not having been attained (strictly speaking, the goal is essentially ever-receding). This is informative evidence of: (i) the fact that the model's structure contains flawed constituent hypotheses or suffers from significant omissions; and (ii) the manner in which those flaws might be rectified and omissions filled, as a part of the search for invariance in the model's parameters and rules, hence provisional stability (or security) in the bits of the science base encoded in the model.

A Broader Context in Which to Deploy the Algorithms

There are higher levels, other than that of the basic, core algorithms of estimation, at which to build a coherent response to the problems of model structure identification embedded in ***Challenge # 7***. Our expectation is of novelty arising precisely from such a greater breadth of perspective, with its scope for orchestrating a greater variety of approaches to problem-solving.

We begin by noting how our discussion hitherto has been dominated by one particular view of environmental models: that they are based on differential equations with the customary algebraic expression of the constituent hypotheses of which such models are composed. The role of models more typical of those labeled as originating in Statistics, such as the transfer functions of time-series analysis (Young, 1998) or wavelet analysis (Kumar and Foufoula-Georgiou,

Algorithmic Frameworks for Reconstructing Parameters Not as Constants

Discerning the significance of the problem of model structure identification, and of the role of estimating parameters that change with time and space in solving that problem, can be approached from several algorithmic points of departure.

Filtering Theory

The most obvious, from the 1960s onwards, has been the availability of mathematical filtering theory and recursive algorithms for state-parameter estimation. These were designed precisely for the purpose of estimating quantities sequentially, at each successive, discrete, observing point in time-space, $(t_i, \mathbf{s}_j)$, for i = 1, 2, ..., n_i and j = 1, 2, ..., n_j. And their availability as solutions can fairly be said to have prompted conception and characterization of the (self-styled) problem of model structure identification in the first place (Beck and Young, 1976). The current incarnation of these algorithms of recursive estimation and filtering theory can be found in Lin and Beck (2007a), from which we take the following illustration of how reconstructing time-varying estimates of a model's parameters, i.e., $\hat{\boldsymbol{\alpha}}(t)$, can be trained on the problem of model structure identification.

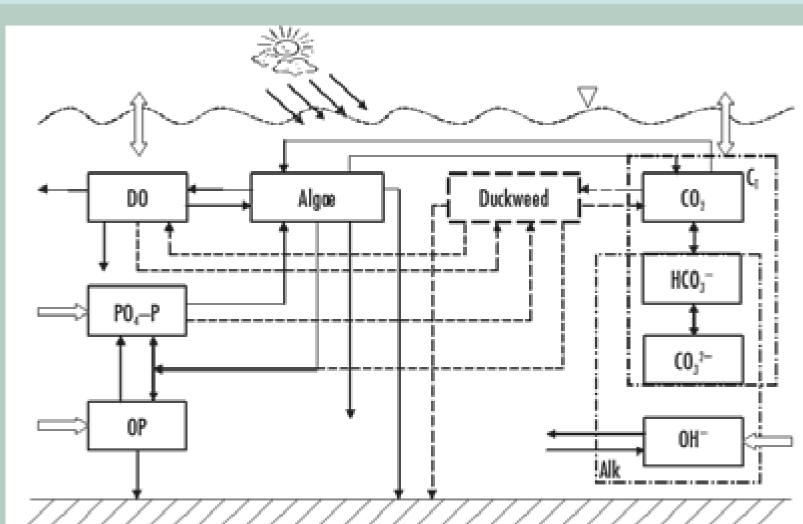


Figure B2.1
Typical block diagram for an *a posteriori* model structure ($M_{posterior}$) of nutrient, algal, and duckweed dynamics in a manipulated aquaculture pond: blocks represent state variables (x); model parameters ($\boldsymbol{\alpha}$) will typically be associated with the mathematical expressions describing interactions among the state variables (lines/arrows in the diagram). Reprinted with permission from Lin and Beck (2007a).

We have access to HVHQ data such as those of Figure 2 in Chapter 1 (for wastewater treatment), although here with reference to the behavior of a manipulated aquaculture pond, a posterior conceptual model of which is shown in Figure B2.1. Figure B2.2 demonstrates the performance of this model. The result can be thought of as but a "snapshot" in the ongoing process of reconciling a succession of evolving candidate model structures with a portion of the HVHQ data. At this particular juncture, the most significant element of the posterior structure of Figure B2.1 is its incorporation of an account of the dynamics of duckweed and alkalinity-related features, omitted from the immediately previous prior model structure and provisionally determined as prime candidates for inclusion.

When reconciliation of that prior candidate model structure (M_{prior}) with the field data was attempted — en route subsequently to the posterior structure ($M_{posterior}$) of Figure B2.1 — that "act" (*sensu* Lewis) yielded the parameter estimates of Figures B2.3 and B2.4. These attach respectively to the {presumed

BOX 2

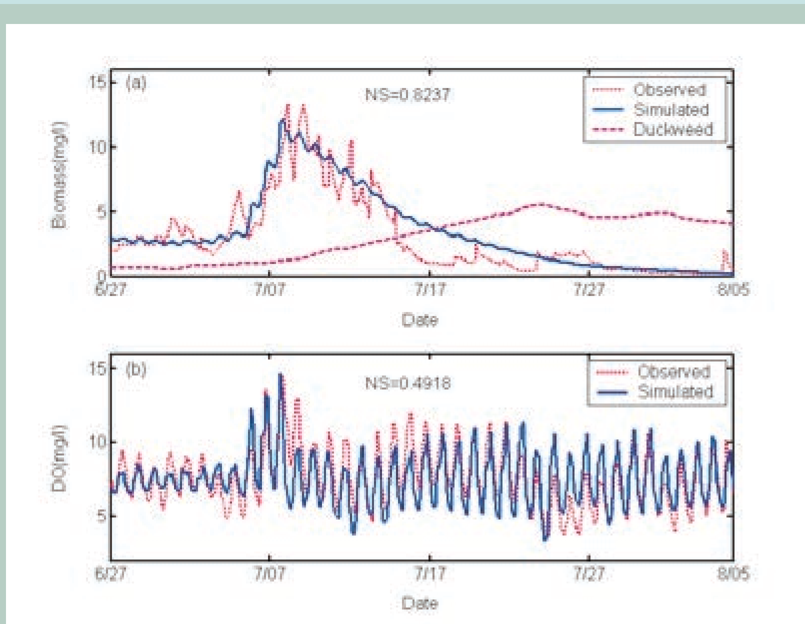


Figure B2.2
Match of behavior of posterior model structure ($M_{posterior}$) with field observations of (a) algal biomass (chlorophyl-a) concentration and (b) dissolved oxygen concentration (DO). The reconstructed (unobserved) state variable for duckweed biomass is shown as the dashed, magenta line in (a). Reprinted with permission from Lin and Beck (2007a).

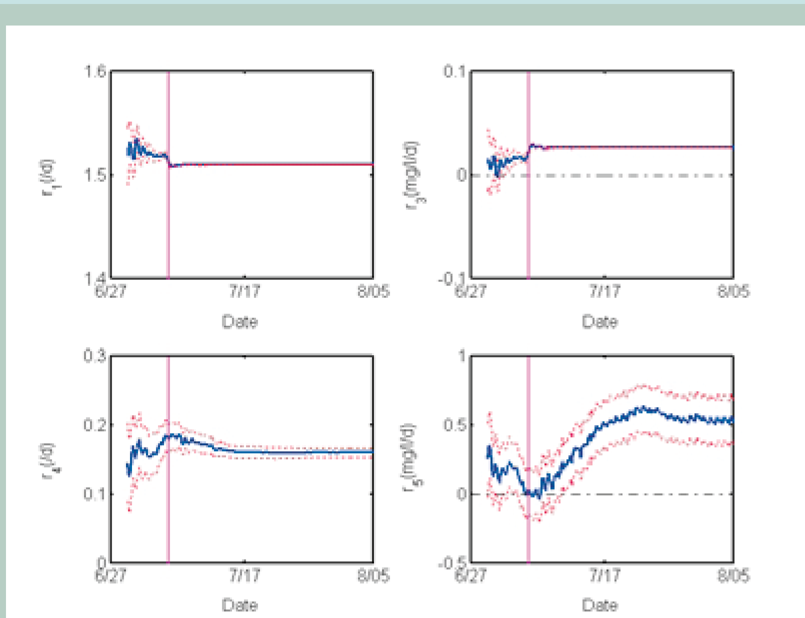


Figure B2.3
Estimates from a Recursive Prediction Error (RPE) algorithm for parameters logically attaching to the {presumed known} of the prior model structure (M_{prior}). Reprinted with permission from Lin and Beck (2007a).

known} and {acknowledged unknown} divisions of the relevant (prior) knowledge base. The estimates derive from a Recursive Prediction Error (RPE) algorithm (Lin and Beck, 2007a). For present purposes, all that needs to be said of these results is merely this: the trajectories of the reconstructed parameter estimates vary, both in terms of departure from their initial values and over extended intervals (in some cases), yet not in an utterly random manner incapable of sustaining any further interpretation. Such interpretation is genuinely a struggle. It is neither trivial nor aimless, in spite of such a simple prior model structure and a rich base of hypothetical knowledge surrounding possible forms of the posterior model, albeit rarely directed at description of the dynamics of duckweed (promotion of whose growth was not part of the deliberations in designing the experimental manipulation of the pond system).

The evidence of Figures B2.3 and B2.4 is a part — and an important part — of what must be fed into the expression of Figure B2.1 from diagnosis of the failure of the prior model. Above all, the availability of such kinds of evidence on parametric variations (or invariance) should accelerate arrival of the moment at

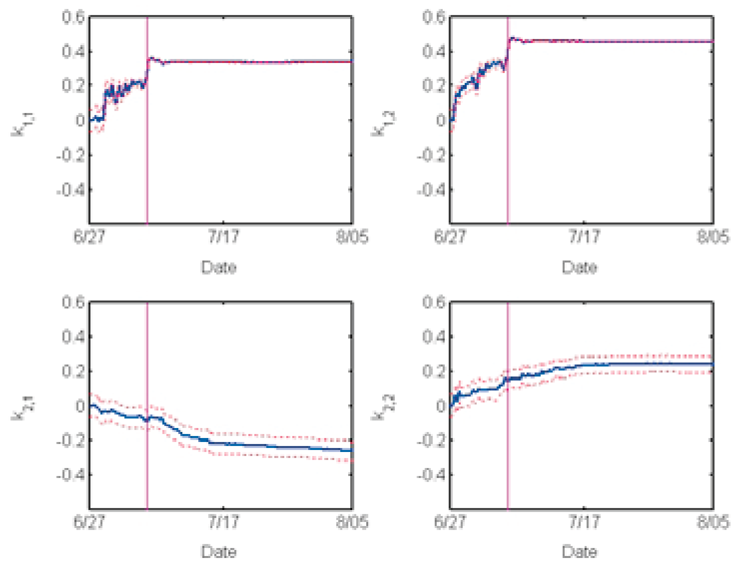


Figure B2.4
Estimates from a Recursive Prediction Error (RPE) algorithm for parameters logically attaching to the {acknowledged unknown} of the prior model structure (M_{prior}). Reprinted with permission from Lin and Beck (2007a).

which the serendipitous thought occurs in the dialog between Statistician and Marine Ecologist, as we have caricatured it in our discussion of ***Challenge # 2*** (regarding the role of the cyber-infrastructure in facilitating basic scientific discovery). It is as though the structure underlying the behavior captured in the data is as that encapsulated broadly in the posterior structure, but demonstrably not so relative to that of the prior structure, some of whose constituent members — hypotheses, embedded in which are parameters — are shown as failing in the attempt to reconcile that prior structure with the data.

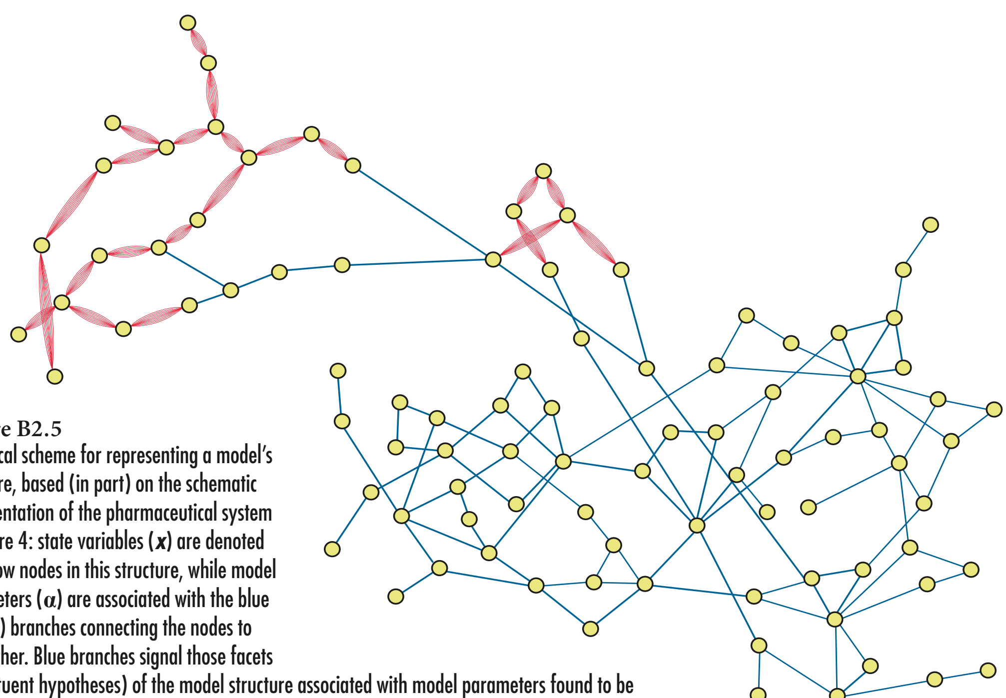


Figure B2.5
Graphical scheme for representing a model's structure, based (in part) on the schematic representation of the pharmaceutical system of Figure 4: state variables (***x***) are denoted as yellow nodes in this structure, while model parameters (**α**) are associated with the blue (or red) branches connecting the nodes to each other. Blue branches signal those facets (constituent hypotheses) of the model structure associated with model parameters found to be invariant and, therefore, robust and reliable in the face of the given test against field observations. Conversely, red branches indicate significant, non-random variability in what are presumed to be (ideally) constants and, accordingly, failure of the model structure, in specific, constituent parts.

BOX 2

To assist, even accelerate, the laborious process of proceeding from an obviously inadequate prior model structure (M_{prior}) to a less inadequate posterior structure ($M_{posterior}$), what we should need, in general, is something such as that of Figure B2.5. Coloring of the branches in this visualization of the essential concept of model structure is quite deliberate: blue for invariant parameter estimates and therefore provisionally secure constituent parameters; red for deformation over time, as the given constituent members (hypotheses) of the structure buckle (fail). We know in principle how the RPE algorithm could generate these colors and their changes with time, which obviously would require some form of animated scientific visualization.

Regionalized Sensitivity Analysis and Dynamic Identifiability

From an algorithmic point of departure quite different from that of filtering theory, and faced with the recalcitrant problem of a lack of identifiability in calibrating hydrological models, Wheater *et al* (1986) sought yet another route to its obviation.

Specific segments, blocks, or windows in the empirical hydrological record are especially informative (information-rich) with respect to identifying the values of particular model parameters. Thus, instead of seeking to choose uniquely best, invariant, singular values for all of the parameters across the entirety of the empirical record, i.e., for all (observed) time, it could be more beneficial to search for uniquely best, invariant, singular values for some of the parameters for some segments of the record, i.e., for some of the time. Thus was opened up the possibility — not exploited at the time — of the parameters desirably having different values at different times.

In a benchmark paper, and likewise faced with an inevitable lack of model identifiability, Gupta *et al* (1998) came to the view that further progress in model calibration would only be achieved through radical changes of perspective. They proposed that algorithms of parameter estimation should henceforth be assigned the task of seeking to minimize structural error in the model at all (discrete) points in time. Further, under a Pareto perspective on the attaching optimality, if this meant different "best" values for the model's parameters at different instants in time, so be it. They too had thereby opened up the prospect of entertaining parameters desirably having different values at different times (Gupta *et al*, 1998).

From an amalgam, in effect, of these ideas of Wheater *et al* (1986) and Gupta *et al* (1998), within the algorithmic framework of Regionalized Sensitivity Analysis (RSA), has emerged the dynamic identifiability procedure of Wagener *et al* (2003). We know that such procedures can succeed when put to work on the problems of model structure identification illustrated above in respect of recursive estimation and interpretation of data from a manipulated aquaculture pond (Chen and Beck, 2002).

Classical Optimization

Entertaining the possibility that a prior candidate model structure (M_{prior}) is actually populated with parameters that vary over a segment of discretized time-space implies a very high order for

BOX 2

that model's parameter vector, i.e., $\boldsymbol{\alpha}(t_i, \boldsymbol{s}_j)$. In particular, the more are the number of points in time and/or volumes in space to which the model (VHOMs) and field observations (HVHQ data) refer, i.e., n_i and n_j are large, so the order of $\boldsymbol{\alpha}(t_i, \boldsymbol{s}_j)$ may, in principle, become very large. Thus derives the considerable significance of having today (and in the future, more so) effective algorithms of mathematical programming, for example, that of Moore and Doherty (2006), for estimating values of very high-order parameter vectors in computationally expensive models. Given such freedom, the essential point is not to match simulated and observed behavior at any cost, such as chaotic variability and utter absurdity in the resulting estimates of all the many elements of $\boldsymbol{\alpha}(t_i, \boldsymbol{s}_j)$. Rather, recalling the kinds of evidence unearthed in Figures B2.3 and B2.4 above, it is to employ the available algorithms to interpret the variability in $\boldsymbol{\alpha}(t_i, \boldsymbol{s}_j)$ in order to modify the structure of the model, hence to arrive at the conclusion of a posterior model ($M_{posterior}$) in which no such variability in the parameters of that final structure can be demonstrated as significant. In short, the prior status of substantial variability in $\boldsymbol{\alpha}(t_i, \boldsymbol{s}_j)$ is systematically reduced to an essentially invariant vector $\boldsymbol{\alpha}$ (in $M_{posterior}$).

1997; Dohan and Whitfield, 1997; Whitfield and Dohan, 1997; Schröder and Seppelt, 2006), and data mining (White *et al*, 2005), has been barely apparent.

Similarly, little mention has been made of the framework of agent-based and individual-based models (IBMs; Grimm *et al*, 2005), essentially because matters of system identification have not been prominent in studies of field observations with such models. But let us recall our discussion elaborating upon Popper's three Worlds as an extension of Lewis's philosophy on the growth of knowledge (our over-arching ***Challenge # 0***). At the very beginning of this *Paper* (in Chapter 1.1), this was expressed:

> [U]nderstanding — that is, assimilation of material into an appropriate mental structure (or mental model) — may derive increasingly from the *belief* that the virtual computational world (Popper's World 3) has been founded upon true and correctly applied theories at the micro-scale and does not generate broad, macroscopic, qualitative predictions in obvious, absurd discord with whatever can be observed of the real thing in the physical world (Popper's World 1).

Our present ***Challenge # 7*** entails quintessentially this question: What should we do if there is such obvious, absurd discord? IBMs naturally embrace this tension between constituent rules cast at the micro-scale of an individual in a species and collective, macroscopic pattern, as Railsback (2001) notes. What then should be the systematic procedure for demonstrating inadequacy of a constituent rule, and unequivocally so; and how should that rule be revised and re-expressed in moving from a prior to a posterior candidate IBM in less absurd discord with the observed pattern of behavior in the field?

The more effective amongst the many possible responses to ***Challenge # 7***, therefore, will be those benefitting from pooling the experience of these hitherto largely separate sub-disciplines and their respective algorithmic heritages, and promoting their cross-fertilization in the future. Such a view is indeed adumbrated in Clark and Gelfand (2006).

Departing in that direction, therefore, consider the following. The "acts" of system identification have conventionally been articulated within just the space of the system's and model's outputs, $\boldsymbol{y}$, where the curve should be seen to pass through the dots. In this space, we know that the familiar theory-based models tacitly dominant in our discussion of discovery and learning can readily be found to suffer from a lack of model identifiability. Unambiguous interpretation of the data is not possible. The data-based models of Statistics, the antithesis thereof, are derived directly from the "data", deliberately with no prejudices about the "set of concepts" that might in due course explain the data. They are well identified, using presumed objective methods of statistical inference. Yet customarily they are believed incapable of supporting a satisfactory theoretical interpretation of the observed behavior they demonstrably replicate.

That conventional perception is changing, driven on the one side by the ideas of "data-based *mechanistic* modeling" of Young (1998) and Young and Ratto (2008). The essence of the dynamic behavior of the identified realizations of these models can frequently be encapsulated in simple macro-parameters ($\boldsymbol{\beta}$), such as the system's time-constant and steady-state gain. The essence of the various parts of the dynamic behavior of the theory-based models can similarly be encapsulated in identical terms. Thus, instead of supposing that theory will be entirely successfully confronted with data in the space of $\boldsymbol{y}$, by way of evaluating the validity of that theory, features of the macro-parameters of the *theory*-based model can be juxtaposed with those of the *data*-based model, and conclusions drawn from this juxtaposition in the space of $\boldsymbol{\beta}$ (about how theory diverges from observation). Along this continuum of transformations of "information"

$$\text{Theory} \leftrightarrows \text{Theory-based model} \leftrightarrows \text{Macro-parameters } (\boldsymbol{\beta}) \leftrightarrows \text{Data-based model} \leftrightarrows \text{Data}$$

the goal is to deduce useful insights about the relationship between theory and data, as reflected in their shared macro-parameters space (Lin and Beck, 2007b).

This continuum of transformations will readily and convincingly appear distanced from the immediacy of the (very) public debate over climate change and hurricane intensity (Mooney, 2007). Yet Mooney structures his book around those characters (scientists) promoting empiricism over theory, who plead for "the data to speak for themselves", and those who promote theory over empiricism. Thus he sculpts (with seemingly little literary license) the essential difficulty: of reconciling empiricism with theory, and the attaching computational complexity of VHOMs, about which such controversy has boiled. Theorists standing at the point of "Theory-based model" in the above continuum; empiricists mustered at their "Data" station; and no apparent meeting of minds anywhere in between. In less literary terms, that essential difficulty has to do with the vastly different orders of magnitude of the data bases to which we have had access — the orders and samples of [$\boldsymbol{u}$,$\boldsymbol{y}$] being customarily small — and these VHOMs with high-dimensional state ($\boldsymbol{x}$) and parameter vectors [$\boldsymbol{x}$,$\boldsymbol{\alpha}$]. It is akin to looking at the world and trying to comprehend it through a pair of binoculars, with one eye-piece a microscope, the other a telescope.

Focusing more constructively, then, on the right-hand end of this continuum of transcriptions, Figure 6(a) (essentially the "Data"), tells us something about the topographic control on climate-induced inter-annual vegetation variability over the US (White *et al*, 2005). Figure 6(b), "mined" from the "Data" using analysis of a suite (or tree) of regression relationships, typifying thus a "Data-based model", tells us *something else*. This we only but imagined earlier as "the archetypal Statistician interpreting the data, using the artful visualizations of the self-organizing maps of data-mining", when we were speculating on the novelty to arise from introducing the environmental cyber-infrastructure in the context of ***Challenge # 2*** (in Chapter 2.2). Now this manifestation of that "something else" should provoke novel insights of a kind not prompted by Figure 6(a), in the mind of the archetypal Terrestrial Ecologist (here), "who can proffer the hypothetical conjectures on why the correlation or curious anomaly is occurring". Indeed, running our eye along the foregoing continuum from right to left, White *et al* (2005) themselves conclude that:

> These findings suggest that the representation of vegetation dynamics in existing climate models, which do not incorporate [variability induced by topography], may be inadequate.

Insights of a similar nature from exploiting the continuum of transcriptions, in effect, are apparent in the work of Young and Parkinson (2002) on the global carbon cycle, as too in the work of Machu and Garçon (2001), who use wavelet analysis to enquire into the nature of phytoplankton distributions in the Agulhas Current off the south-western coast of Africa. Besides reconciling the extracted and distilled properties of models from rather different disciplinary traditions, such as those embodied in the "Macro-parameters ($\boldsymbol{\beta}$)", the key is that each transcription along the continuum should prompt questions that would otherwise *not* have been asked.

In a similar vein — in order to realize the "radical change of perspective" of their earlier work (Gupta *et al*, 1998) — Gupta *et al* (2008) propose that Lewis's "acts" might more fruitfully take place in the richer domain of what they call signatures (pattern extracts) and indices (pattern properties), i.e., at one or two levels of encryption removed from the conventional space of $\boldsymbol{y}$. In other words, model-referenced patterns are to be reconciled with data-referenced patterns, as a supplement to the more familiar "acts" of system identification in the space of $\boldsymbol{y}$ alone. The allusion, albeit inadvertent, to the "pattern-oriented" approach to IBMs of Grimm *et al* (2005) should not be allowed to pass without notice. And not least because Schröder and Seppelt (2006) are advocating bridging not just the one span of process-pattern (constituent micro-scale rule; collective macro-scale behavior), but also that of the heterogeneous traditions in modeling hydrology and modeling landscape ecology.

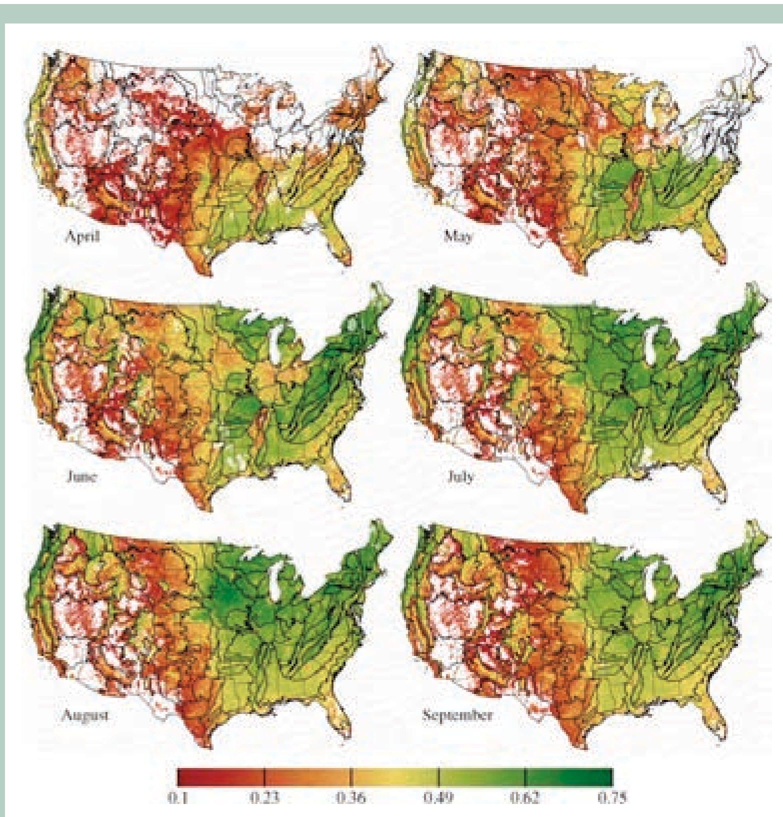
In the struggle to attain the broader perspective in responding to ***Challenge # 7*** lies thus the genesis of the kind of synthesis across previously disparate schools of thought and forms of model that ought to make the whole of the procedure more than the classical sum of its parts. System identification is a forensic science in which claiming the elusive "truth of the matter" is unlikely to yield to dogged, blinkered application of but the one approach alone.

Supportive Software Environment: Accommodating VHOMs and HVHQ Data

As much as in its unforgettable expression of the "tyranny of scales", so the NSF blue-ribbon committee on Simulation-based Engineering Science (SBES) identified "The Emergence of Big Data in Simulation and the Role of Visualization in SBES" as another of its six core issues (NSF, 2006). What drove the committee to this conclusion were issues primarily of handling uncertainty, as follows (NSF, 2006):

> For example, uncertainty quantification, a key component of SBES, will require data sets many orders of magnitude larger than those of traditional deterministic computing.
>
> Then there is the issue of interpreting the results of the simulation itself, a problem that can involve gigantic data sets.

(a)



(b)

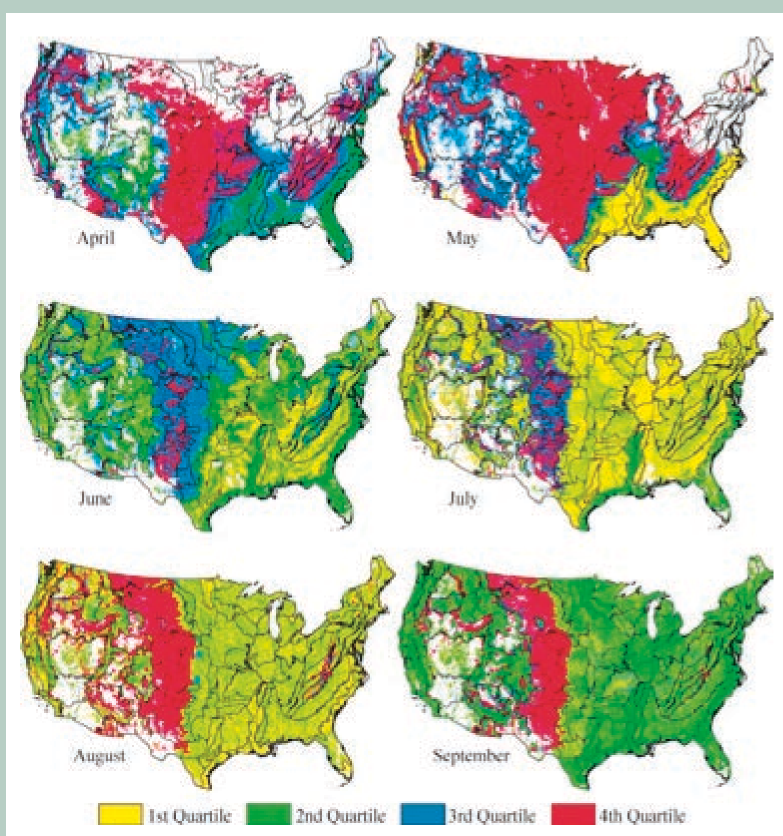


Figure 6
Moving back and forth along the continuum of transformations of information. Upper panel (a): "Data" on the topographic control of climate-induced inter-annual vegetation variability over the US. Lower panel (b): outputs from a "Data-based model" mined from the "Data" of (a). Reprinted with permission from White *et al* (2005).

> As we work to harness the accelerating information explosion, visualization will be amongst our most important tools.
>
> Visualization research must continually respond to and address the needs of the scientific community. For example, the ability to visualize measures of error and uncertainty will be fundamental to a better understanding of three-dimensional simulation data. This understanding will allow the validation of new theoretical models, improve the interpretation of data, and facilitate decision-making. With few exceptions, however, visualization research has ignored the need for visual representation of errors and uncertainty for three-dimensional visualizations. We need to create an SBES visualization framework for uncertainty and to investigate new visual representations for characterizing error and uncertainty.

These views are broadly shared with those of the committee investigating the role and needs of sensor technologies within the Environmental Observatory initiatives, who observed that "modeling and visualization tools are critical" (NSF, 2005).

"Big data"[18] occur prodigiously in applications of the algorithms of filtering theory and recursive estimation, with their various high-dimensional estimation error variance-covariance (and other) matrices propagating through the discretized time-space continuum — the kinds of uncertainties of which the SBES committee writes. The matrices must be propagated in addition to the like propagation of input, state, parameter, and output vectors. So why should visualization be highlighted in this manner in the context of ***Challenge # 7*** and in solving, in particular, the problems of model structure identification? Our response is this: because learning, discovery, and the forensic science of model structure identification, are all about the highly condensed visual apprehension of the myriad diagnostic facets of the comparisons and juxtapositions entailed therein, *especially in complex multivariable situations of HVHQ data and VHOMs*. How indeed should we reconcile a VHOM such as that of Figure 4 with any corresponding HVHQ data of the kind shown in Figure 2, or those of the GIS maps of Figure 6?

[18] The "big data" to which the SBES committee refers are clearly not identical to the "data" of Lewis's schema for the growth of knowledge, since they are dominated by numbers generated from a computer, without having any direct association with the observed behavior of the real system.

We need hardly be reminded of the startling expansion over the past few decades in our capacity to simulate the behavior of systems, in theory, in ever more detail and completeness on the computer. Likewise, the substantial impact of the EOs and environmental cyber-infrastructure in expanding our technical capacity for observation, i.e., the volume and quality of data streams, is obvious. By comparison, there has been no advance in the capacity of the human brain to juggle with a huge entanglement of computational estimates and observed facts — no advance in our capacities for lateral thinking, as we have already said — in order to reconcile bundles of obscurely and obliquely discerned anomalies, where data and theory seem to diverge, and not through the action of spurious chance occurrences. Imagine what is to be supported: reconstruction in a computational world of a complex assembly of experimental tests of multiple, constituent hypotheses; which hypotheses are of varying prior strengths, irreducible and impossible to isolate clinically from the whole for examination one by one as singlets; and whose observable causes and consequences all interact with each other.

What is called for, above all, is succinct visual representation of the structure of the model: probably not along the lines of the animation software of Figure 3; more along the lines of animating the branch-node network of Figure 4; and with the succinctness of the compression achieved through the enormous visual complexity of color, movement, and animation of the model's structure. Visualization is necessary just as much for the "acts" of system identification as it is (already) for the "data" and for the "set of concepts". It may take the form of that for the ELAM of Goodwin *et al* (2006) or the IBMs of Grimm *et al* (2005). It may be as familiar as the computer graphics of games, films, and the scientific reconstruction of history and the imagination of future threats (for the television programs of the *History* and *National Geographic* channels, for instance). In Box 3, however, an argument is developed for taking the conceptual visualization introduced in Box 2 and propelling it towards what we can already find in the software domain of molecular graphics.

The need has been long-standing: for the kind of software environment enabling rewiring of the constituents within the whole of the model, almost as quickly and easily as the serendipitous thought surfaces in the brain; for support of the "tinkering paradigm" of the on-line dialog between our archetypal Statistician and Marine Ecologist (of ***Challenge # 2*** above); and for

BOX 3

Structural Change

Animating Flexure and Collapse of Model Structure in Lewis's Acts of System Identification

In Box 2 the conceptual branch-node network diagram of Figure B2.5 conveys an "artist's impression" of a model's structure, representing there a prior candidate model structure (M_{prior}) with its apparent failings, as a step en route to that of an improved posterior structure ($M_{posterior}$), all in the overall process of model structure identification. In discussing (in Chapter 2.6) the ever-alert environmental cyber-infrastructure, poised to enact adaptive sampling and faced with acknowledging the associated need of an "adaptive model" (in response to ***Challenge # 6***), we introduced the idea of a model whose structure would change and evolve with time, from $M(t^{-})$ to $M'(t^{+})$. The threads of these two arguments establish a sense of fluidity in the structure of a model, which we shall elide with the ideas of movement, motion, and therefore animation. Figure B3.1 realizes three snapshots in time (t) of such motion, or structural change in the model.

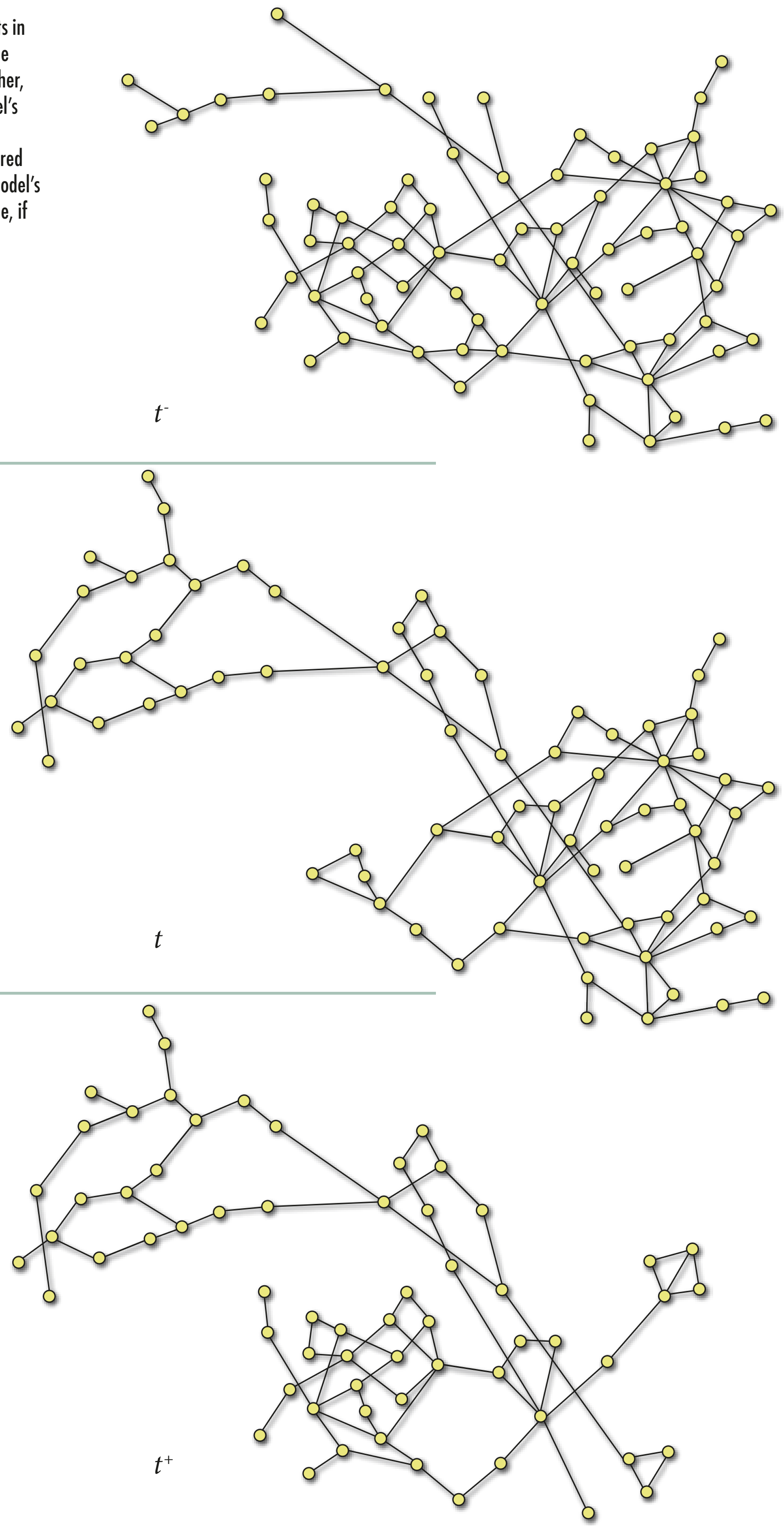
Alternatively, supposing our understanding of the behavior of the given environmental system could be resolved to some greater degree of refinement, the three snapshots of Figure B3.1 might be subsumed as merely a sequence of predominant facets of some more complete model, such as that of Figure B3.2 (just as, indeed, in the pictorial representations of the collapse of coastal ecosystems in Jackson *et al*, 2001). Coloring of the branches of Figure B3.2 follows the previous logic of that introduced in Box 2: with blue representing a secure, confidently supported constituent hypothesis, with relatively little uncertainty attaching to the associated model parameter estimates; and red signaling the opposite, i.e., a constituent hypothesis that has been stressed to the point of failure in the act of reconciling the candidate structure with the data. Animation would permit changes of color over time. And to color could be added the dimensions of flexure, deformation, and oscillation in these branches pinning together the nodes (state variables) of the structure.

The purpose of Figure B3.2 in the present argument is to establish some conceptual complements of Figure B3.1. Given the two, and the previous liberal use of these metaphors in Environmental Science (Beck, 2002), little further imagination is needed to proceed to Figure B3.3, as found in the Biomedical Sciences. If the two facets of animation and visualization in Figures B3.1 and B3.2 could be brought together in realizations such as those of Figure B3.3, then surely it could also be that the software platforms of molecular graphics have a role to play in model structure identification in responding to ***Challenge # 7***. For we already know that one of the algorithmic frameworks of Box 2, that of recursive estimation and the RPE algorithm, in particular, generates streams of digital information — on parameter estimates, variance-covariance matrices, and the like — sufficient to color and animate Figure B3.2 in a systematic manner, as its attaching "set of concepts" is reconciled with the "data", time-frame by time-frame.

Now imagine our colored and animated model structure as a three-dimensional object on the computer screens of our archetypal Statistician in city office and Marine Ecologist aboard ship at sea. And suppose the cyber-infrastructure enables them both simultaneously to freeze a frame in the film, arresting it at the point of detecting a red buckling to the rear of the model structure, rotating the object, and cutting out the buckled portion of the structure for closer inspection. Imagine, in fact, Figure B3.4. We ought indeed then to have the beginnings of the "tinkering paradigm" called for in our earlier response to ***Challenge # 2***.

BOX 3

Figure B3.1
Structural change: snapshots for three instants in time capturing evolution in the structure of the model. Over time, from one snapshot to another, it appears some constituent parts of the model's structure have fallen away, from significance into insignificance, while others, once considered insignificant (not worthy of inclusion in the model's structure), have arisen to assume considerable, if not dominant, significance.



BOX 3

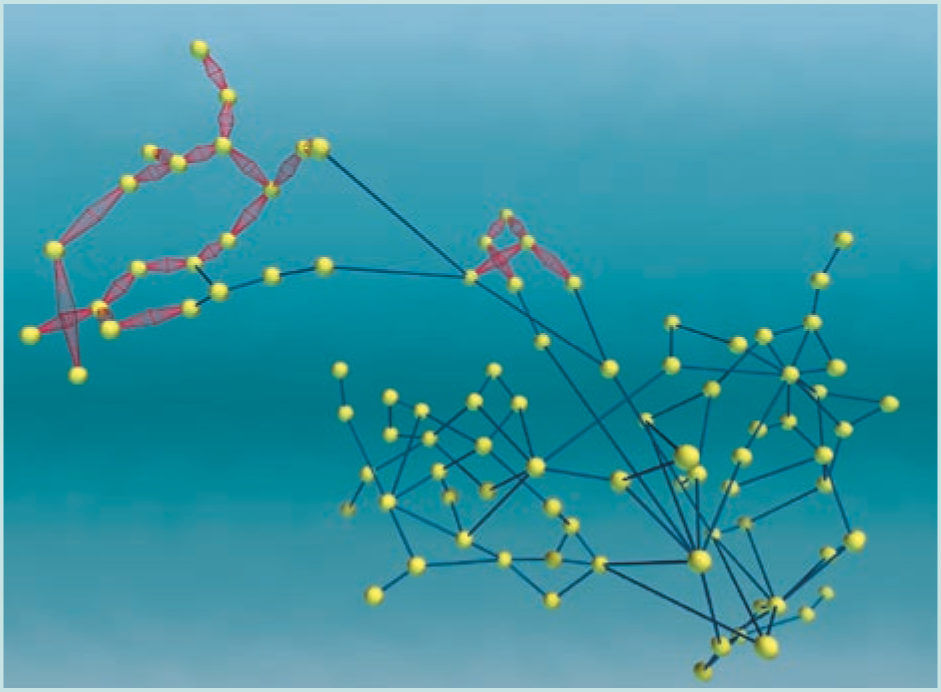


Figure B3.2
Towards model structure identification: three-dimensional representation of the model structure (previously depicted merely in two dimensions in Figure B2.5 of Box 2).

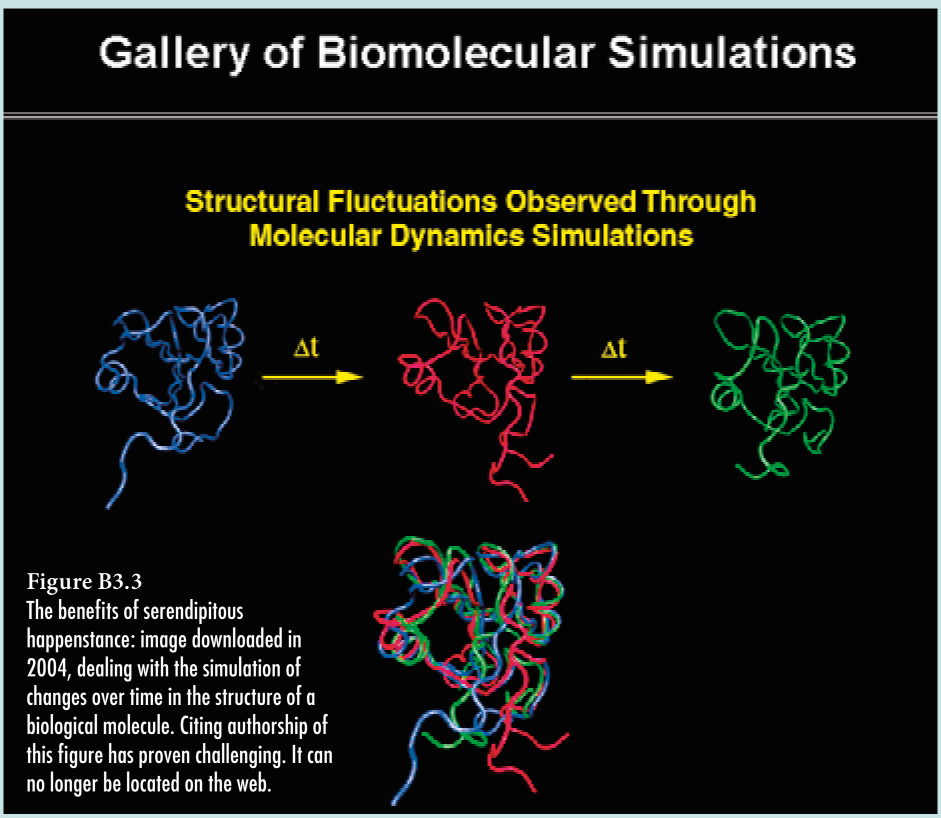
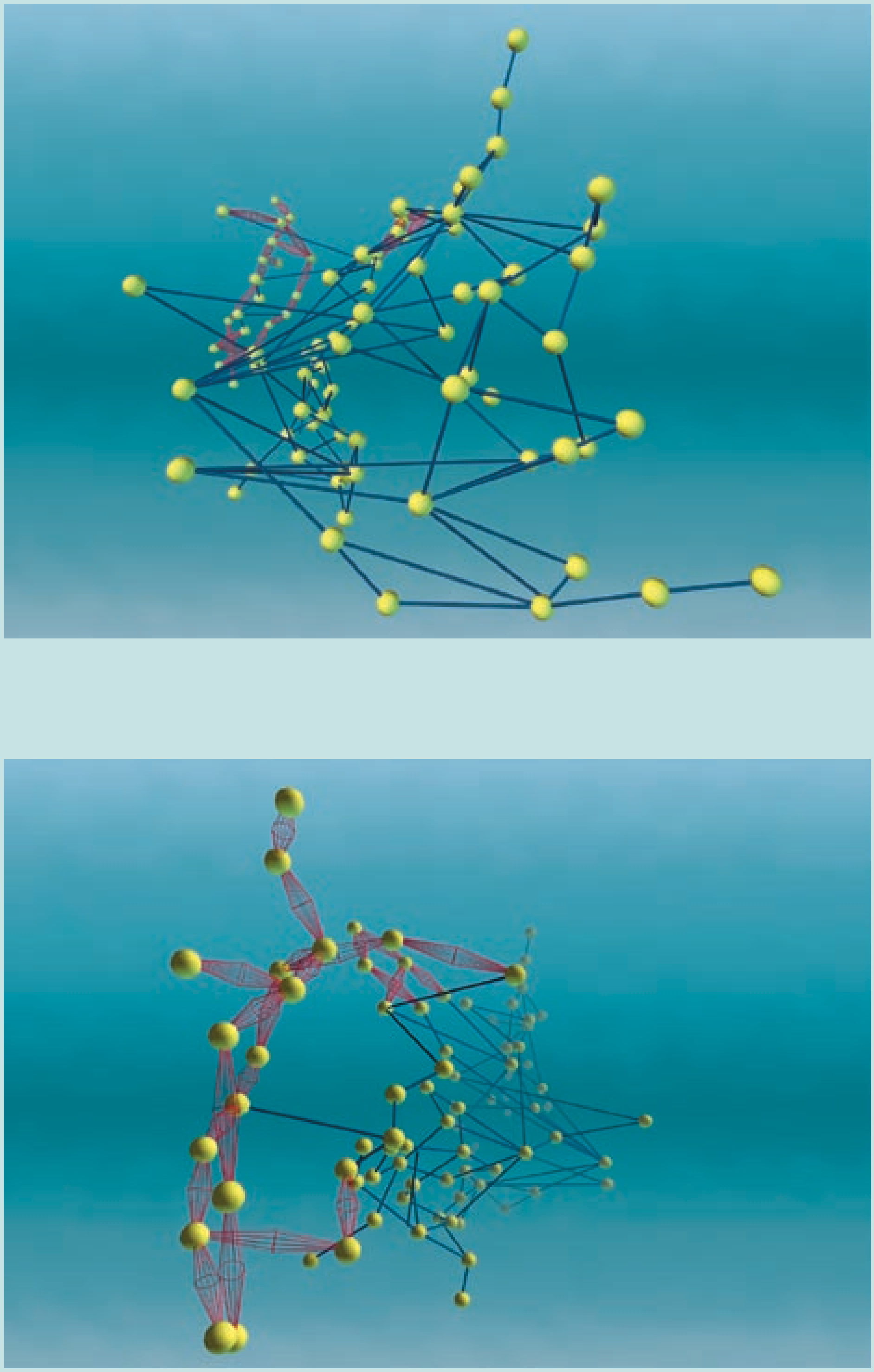


Figure B3.3
The benefits of serendipitous happenstance: image downloaded in 2004, dealing with the simulation of changes over time in the structure of a biological molecule. Citing authorship of this figure has proven challenging. It can no longer be located on the web.

BOX 3

(a)



(b)

Figure B3.4
Towards model structure identification through animation of flexure and collapse of model structure: (a) frozen frame of the animation as the analyst first detects a red web of faulty behavior to the rear of the three-dimensional model structure, as the model is in the process of being reconciled with a recorded span of field data; (b) same frozen frame as (a) but rotated in the three-dimensional space of the visualization of the model's structure in order to reveal more clearly the failing constituents (hypotheses) of the model's structure.

the kinds of scientific visualization that will enable the serendipitous thought to occur sooner rather than later. Much of what is called for in responding to ***Challenge # 7*** is likely to depend on an essential element of such serendipity, something which by definition defies full automation and systematization in any form of environmental cyber-infrastructure.

2.8 Predictive Science and Uncertainty

Everything, technically, is uncertain: $\boldsymbol{u}$, $\boldsymbol{M}$, $\boldsymbol{\alpha}$, and $\boldsymbol{y}$. And according to the SBES committee, uncertainty is clearly a significant matter, even in the more secure, "artificial", constructed world of engineering (the built environment). Given this, the important question is not so much that we should be concerned to take account of uncertainty, for once was the time when technically we were analytically and computationally largely unable so to do, but that we should be able to establish when such uncertainty, be it great or small, might be important. Looking back, it is important for the uncertainty and ambiguities in explaining past, observed behavior to be reduced to insignificance, expunged, and the explanation rendered as founded upon just *the* singular "set of concepts" alone. Peering ahead, it is important to be able to discern where forecasts of possible future patterns of behavior in the system can be relied upon, and where not.

As we introduce our next grand challenge, aligned with the second of our textbook problems, of "given $\boldsymbol{M}$ and $\boldsymbol{u}$ find $\boldsymbol{y}$", but not divorced from the prior problem of "given $\boldsymbol{u}$ and $\boldsymbol{y}$ find $\boldsymbol{M}$", our need is to pinpoint aspects of accounting for the various facets and types of uncertainty for which no solutions are yet readily apparent. For this — shortly to be expressed as ***Challenge # 8*** — our focus will be on uncertainty in knowledge and its consequences with respect to making statements about future behavior. ***Challenge # 10***, which is closely related, will subsequently be addressed to those consequences in the more pragmatic context of decision-making and decision support in environmental management. The former views the issue of prediction from the perspective of the scientist as stakeholder, the latter from the perspective of the policy-maker as stakeholder.

Moorcroft's Question

In his review paper, Moorcroft (2006) asks: "*How Close Are We to a Predictive Science of The Biosphere?*". The science plan for NEON released in September 2006 observes that "[m]oving ecology to a predictive science at the regional to global scale will require a coordinated program of theory development, testing, and refining" (NEON, 2006). Becoming a "predictive science" is thus a noble, widely shared goal; and its attainment, in respect of such massively complex, large-scale systems, must rest upon achieving what the community of peer scientists will judge to be secure, reliable models.

Moorcroft's response to his own question, which touches upon a number of the grand challenges in this *White Paper* — from the role of models in the process of core scientific discovery, i.e., from ***Challenge # 1***, onwards — entails the following:

> That there be no obvious, absurd discord between the "data" and the "set of concepts", echoing thus all of the preceding discussion under ***Challenge # 7***.

The "data" for Moorcroft will be an eclectic synthesis of cross-scale fragments, blocks, and patches of observed behavior spanning the time-space-biogeochemical continua (echoing thus the discussion of ecoinformatics in Jones *et al* (2006) under ***Challenge # 2***). His "set of concepts" are to cover subgrid-scale heterogeneity in the community of plants and their cross-scale dynamics. Omission hitherto of these features, he argues, has been responsible for (Moorcroft, 2006)[19]

> our current understanding of biosphere-atmosphere feedbacks [being] a collection of interesting, but largely untested, hypotheses for the future state of terrestrial ecosystems and climate.

But as we now know from the extensive discussion of the challenges of reconciling complex VHOMs with the anticipated yield of HVHQ data from the EOs, the archetype of the single curve of the model traveling demonstrably through the dots of the data can conceal a host of ambiguities and uncertainties, hence a plurality of interpretations. As Moorcroft (2006) expresses it:

> [A]lthough most models can replicate inferred patterns of potential vegetation and seasonal to interannual patterns of productivity, they diverge from each other significantly in their predictions of ecosystem composition, structure and functioning under novel climates.

And in this he epitomizes the challenge we are approaching.

If the uncertainties attaching to the various models as a result of replicating (uncertain) past observed behavior had been evaluated — for this is not disclosed in Moorcroft's discussion — and then accounted for in the predictions, the significance, or otherwise, of the divergence amongst the predictions (and of the models) could have been established. Furthermore, once qualified by such an account of the propagation of this uncertainty into the bundle of predictions, discerning where divergence is statistically significant or not should be revealing of the points of relative strength and weakness amongst the constituent hypotheses in the competing models. Accordingly, we can see how solving our two textbook problems, of identification and prediction, are in this way intertwined (Beck, 1987).

Looking to explanation of the past, how then should we judge whether the predictive science base is unblemished, without flaws? Looking to the future, how do we insure use of our forecasts against the propagated consequences of these blemishes and flaws, in order to be in any way confident in making statements about behavior in the future, especially behavior radically different from that observed in the past? For it is towards this objective — of being reliable in inferring such novel behavior — that becoming a predictive science is strongly inclined.

Sound Science

"Being reliable" is indeed the key — as may also be reiteration of our call (in Chapter 1.1) to professional philosophers of science to become involved in the particular challenges of developing models in Environmental Science.

On the one hand, adhering to what is understood as the paradigm of "sound science" (Fisher, 2007), uncertainty is, in principle, capable of being eliminated in due course, i.e., uncertainty in our knowledge bases is essentially a transient phenomenon. According to Funtowicz and Ravetz (1990), reliability in the status of the relevant science would evolve through the following stages:

> from "no opinion" with no peer acceptance;
>
> through an "embryonic field" attracting low acceptance by peers;
>
> "competing schools", with medium acceptance;

[19] At the scale of the spatial grids presently employed in models of the global atmosphere, biological cover on the earth appears as the uniform, monotone "canopy as big-leaf" (Moorcroft, 2006).

> a "theoretically-based model" accepted by "all but rebels";
>
> and on, in the end, to an "established theory" accepted by "all but cranks" (expressions quoted are those of Funtowicz and Ravetz).

In our domain of formal, computational modeling, this progression might be mirrored as:

> from perceived correlations within the data, derived from applications of techniques such as data mining, self-organizing maps, regression analysis, and the like;
>
> to the sets of rules of fuzzy logic and Bayesian nets;
>
> lumped-parameter ordinary differential equations, or several such model structures (with/without time-varying parameters);
>
> to culmination in sets of partial differential equations, with invariant parameters (without stooping to the expedient of estimation through model calibration).

In this climax a single and secure "set of concepts" should unquestionably have been achieved (in Lewis's terms).

In the latter stages, what drives matters is the quest for successively eliminating model parameters as temporary "parking places", as it were, for accounts of behavior regarded for the time being as too uncertain, too variable, too immature, or lying outside the "scale window" of what can be included in the model (Lermusiaux *et al*, 2006b). This is just as Moorcroft (2006) anticipates:

> The plant functional types represented within coupled DGVMs [Dynamic Global Vegetation Models] have *fixed* traits, such as their maximum photosynthetic rate and their patterns of carbon allocation between leaves, stem and root tissues. By contrast, empirical studies of terrestrial ecosystem responses to climate change have documented widespread evidence of plant *acclimation* to elevated levels of CO_2. [emphasis added]

The trait (parameter), currently treated for expedience as invariant, might better be regarded as temporally, if not spatially, varying, unless and until that parameter can be replaced by a more mature model, with a higher resolving power, wherein the expedient trait is acknowledged as crudely approximating interactions amongst several state *variables* at the more refined level of understanding.[20] This quest, as Popper puts it, is "unending" (Popper, 1976) — notwithstanding the ambition of enterprises such as the Human Physiome Project (Hunter and Borg, 2003), in descending to the ever smaller, or Earth System Analysis, tending towards the opposite end of the scale.

Current DGVMs, we could say, are subject to structural error/uncertainty, or epistemic uncertainty, i.e., uncertainty in the science and sets of concepts underpinning the model. If they were to attain the status of the predictive science in Moorcroft's question, the blue-ribbon committee on Simulation-Based Engineering Science (SBES; NSF, 2006) would nevertheless lead us rightly to expect them still to be subject to aleatory uncertainty — uncertainty, that is, attaching primarily to the parameterization of an otherwise agreed structure for the model, beyond dispute.[21] Until such a status is attained, what computational account (rhetorically) is to be given of the structural error/uncertainty?

At bottom, adoption of the sound-science paradigm expects progression in but one direction, with no substantial setbacks, except when the relevant science undergoes a Kuhnian shift of paradigm (Kuhn, 1962).

Deliberative Problem Solving

On the other hand, there is the paradigm of "deliberative problem solving", in which epistemic uncertainty is considered ineluctable (Fisher, 2007). This can be portrayed as having much of a Bayesian spirit about it. Beginning at some point in an iterative cycle, we:

[20] The "mixing-layer depth factor"in ocean science models seems likewise a candidate expedient, subject to temporal variability, and capable in principle of more satisfactory representation (Lermusiaux *et al*, 2006b), just as was the ratio of chlorophyll-*a* to carbon in phytoplankton biomass in the previously quoted work of Spitz *et al* (2001).

[21] To be clear about the use of terms here, the word epistemic is understood as "of, relating to, or involving knowledge or the act of knowing", whereas aleatory denotes "dependent upon chance, luck, or an uncertain outcome".

(i) identify some key sources of uncertainty;

(ii) explore the nature of experiments designed to reduce these — at a mature stage, after several cycles, some such designs of experiments will be using models for this purpose (just as we have seen in Chapter 2.6; ***Challenge # 6***);

(iii) quantify and record the uncertainty attaching to the model (***M***), both parametric and structural, as it is reconciled with the resulting data;

(iv) account for the propagation forward of this posterior model uncertainty in the making of predictions (and come to a current view on the problem being solved); and

(v) rank the sources of uncertainty compromising the reliability of those predictions — hence, to embark on the next cycle.

The cycle is that of identification-prediction-identification-prediction, and so on. Through it runs the continuous thread of accounting for uncertainty.

It is possible, in principle, for confounding data to cause the posterior model uncertainty, after identification, to be greater than that with which any given iteration began. System identification, as we have discussed it in response to ***Challenge # 7***, assumes now not merely the goal of explaining past behavior without ambiguity, but also the purpose of mapping the loci and extent of that which is more or less uncorroborated in the model. The resulting map is a faithful "fingerprint" of any and all the distortions wrought in the model as it is reconciled with the data. And this fingerprint of uncertainty determines, in part, the reliability of the predictions generated from the model (Beck, 1987).

It is not that this second paradigm does not seek utter clarity in explanation and prediction. Rather it seeks quality in this quest, presuming uncertainty cannot be made negligible, hence eliminated from consideration, not even when having attained the partial differential equations that are the target end-points of the sound-science paradigm. In fact, since this is precisely the argument Funtowicz and Ravetz (1990) wish to make, care must be taken not to make their thinking captive of just the sound science paradigm. Furthermore, all of us would want to see our science progress from no opinion to a fully fledged theory. If our nascent models are expressed in the rules of fuzzy reasoning and Bayesian nets, for example, uncertainty is axiomatic. But somewhere along the line of the sound science paradigm — for it is unclear whether there are the procedural and algorithmic means for graduating these forms of nascent models systematically into the forms of ordinary differential equations — models emerge without any formal account of uncertainty.

Being open about such uncertainty should be celebrated: in illuminating where our explanations and predictions can be trusted and in proceeding, then, in the cycle of things, to amending their flaws and blemishes. And so we come to expressing our next grand challenge.

Challenge # 8:

Recognizing the inevitably flawed and uncertain conceptual foundations of many environmental models — while acknowledging the possibility of natural features of biological acclimation, even evolution, over a longer-term horizon, especially in response to the introduction of invasive species, and the high likelihood of continual adaptation in the behavior of many types of environmental system — how are structural error/uncertainty and structural change in these models to be identified, quantified, rectified, and accounted for (in the propagation of prediction errors and the making of decisions)? What new schemes of generating environmental foresight will be needed to cope with these challenges?

What, in fact, must go into making environmental science a predictive science (a strong form of "environmental foresight")? What might be the role of the Environmental Observatories, and the data they are to generate, in facilitating this?

Computational Analyses of Uncertainty and Sensitivity

In 2003, scientists and engineers from a unusually large number of US federal government agencies came together for a Workshop on "Uncertainty, Sensitivity, and Parameter Estimation for Multimedia Environmental Modeling" (Nicholson *et al*, 2004). Uncertainty, whose analysis had historically been tied to the making of predictions, was thereby coupled to parameter estimation, i.e., to the prior process of identifying the model in the first place. This, then, was an embodiment of the Bayesian spirit of the identification-prediction cycle — recognition too of the role of past observations (and their uncertainties) in influencing the propagation of uncertainty in predictions of behavior in the future.

The titles of some of the programs prominent under the inter-agency collaboration hosting the Workshop convey much the same spirit: specifically, that on Joint Universal Parameter IdenTification and Evaluation of Reliability (JUPITER) and its manifestations in the peer-reviewed literature (Doherty and Johnston, 2003; Poeter and Anderson, 2005; Gallagher and Doherty, 2007). Given widespread acceptance of this Bayesian outlook today — indeed, its prominence in some fields, notably Hydrology (source of the procedure of Generalized Likelihood Uncertainty Estimation (GLUE; Beven and Freer, 2001)) — the intellectual effort originally invested in making such a connection between prior identification, uncertainty, and subsequent prediction (Beck, 1987) seems now superfluous.

Across the disciplinary domains germane to the EOs, the most expansive penetration of applications of the relevant computational methods of Uncertainty Analysis and Sensitivity Analysis (UASA) to higher-order, computationally expensive models is clearly apparent in Hydrology and the Ocean Sciences (Lermusiaux *et al*, 2006b). It is especially prominent in matters affecting systems of groundwater: in respect of bioremediation of contaminant plumes (for example; Mugunthan and Shoemaker, 2006); and in accounting for the exceptionally long-term, future behavior of such segments of the environment in the vicinity of storage facilities for high-level radioactive wastes, for example, over the scales of 10^3 and 10^6 years (Helton *et al*, 2006; Ye *et al*, 2007; see also the reference textbook of Saltelli *et al*, 2000).

From a slightly different conceptual and algorithmic heritage, but nevertheless heading towards the handling of uncertainty in very high order models, are some contemporary extensions of the seminal work of Hornberger and Spear (1981) on Regionalized Sensitivity Analysis (RSA)[22]. That sub-population of candidate parameterizations of the model, screened out under gross uncertainty, as generating acceptable matches of qualitative, subjective experience of past observed behavior (the signature feature of RSA), constitute the sample of candidate parameterizations of the model with which to generate forecasts of behavior in the future (every bit as much a characteristic feature of the Bayesian outlook). The extensions of RSA, currently tailored to an ecological foodweb model of modest order (Osidele and Beck, 2003, 2004), are to be incorporated into the FRAMES software system for human and ecological risk assessment constructed around a multi-media model (3MRA; Babendreier and Castleton, 2005), unquestionably a model meriting the assignation of being a VHOM.

To summarize, the ambition of attaining here computational facility in addressing and visualizing uncertainty in the very highest orders of models, is clearly shared with the recommendations from the NSF's blue-ribbon committee on Simulation-Based Engineering Sciences (NSF, 2006). Likewise broadly shared, of course, is the interest in having computational efficiency accompany computational facility, especially in the now dominant sampling-based schemes of accounting for uncertainty[23], as reported upon in Helton *et al* (2006), appropriately enough in a journal on reliability engineering. There is also a self-declared aim (Gallagher and Doherty, 2007) that developments in the enabling software of computational UASA become generic, i.e., applicable whatever the source of the model and, we would commend, compatible with protocols such as OpenMI (of which mention was made in Chapter 2.2).

Given a model $\boldsymbol{M}$, even a very high order model, we may conclude it is possible to compute the

[22] To which GLUE, as well as the set-membership approach of Keesman and van Straten (1990), owe much of their inspiration.

[23] Two decades ago the field of uncertainty and sensitivity analysis was greatly concerned to compare the performances of first- and second-order analyses of error propagation with those of sampling-based schemes (Beck, 1987). Today those approximate methods appear prominent primarily in but the prior analyses of model identifiability (and experimental design) discussed above in Chapter 2.6 (for example, Brun *et al*, 2001; Omlin *et al*, 2001), with the notable exception of Gallagher and Doherty (2007), who report on a comparative study in the analysis of uncertainty using both a first-order error analysis and a Markov Chain Monte Carlo (MCMC) sampling procedure.

uncertainties attaching to that model's parameters (**α**), as a result of reconciling the model with the data, and compute the consequences thereof in terms of the uncertainties attaching to the model's predictions (**y**). Hence, in principle, the specific loci of the strengths and weaknesses in that complex web of explanatory hypotheses, as well as in the bundle of predictive statements, can be illuminated, not left concealed, with therefore latent consequences. Should this help in addressing the problem of the (historical) impotence of the field data in discriminating amongst those models and their constituent hypotheses that are to be relied upon in making predictive statements about possibly radically different types of behavior, and those that are not? It ought.

Put less technically, more philosophically, and in the words of Funtowicz and Ravetz (1990): is exploration of the future to be dogged (or enhanced) by a plurality of plausible, candidate models under a regime of competing schools of scientific thought? In fact, could those candidate models be supported and promoted even as sharply contradictory certainties? Whatever the answers to such questions, the computational capacity of accounting for the propagation and modulation of uncertainty through the identification-prediction cycle is ready to be put to work.

Foresight: Coping with Structural Error/Uncertainty and Structural Change

Until environmental models attain membership of the set of predictive sciences, for they are yet falling short of this goal, what computational account is to be given of the structural error/uncertainty in them, in exploring possible patterns of behavior in the future? How are we to cope with such uncertainty in our conceptual knowledge base? When making predictions, what should be done about the recognized inadequacies of the fixed, macroscopic traits currently assigned to the behavior of vegetation in Dynamic Global Vegetation Models (Moorcroft, 2006)? Before delineating the beginnings of answers to these already substantial enough questions, let us ponder something of their still grander implications and origins.

In a contribution to an early text on evolutionary economics, Peter M Allen, a theoretical physicist who had worked with Nobel-laureate Prigogine on matters of complexity and self-organization in the 1970s and 1980s, took stock of his perspective on models and prediction in environmental science, following that experience. In the gap between the computationally tractable known (the model) and the truth (reality) lies the difference, as he would argue, between the behavior of mechanical and evolutionary systems (Allen, 1990):

> [I]f the world is viewed as some kind of 'machine' made up of component parts which influence each other through causal connections, then instead of simply asking how it 'works', evolutionary theory is concerned with how it got to be as it is.
>
> The Newtonian paradigm was not about this. It was about mechanical systems either just running, or just running down.
>
> The key issue is centred on the passage between detailed microscopic complexity of the real world, which clearly can evolve, and any aggregate macroscopic 'model' of this.
>
> The central question which arises is that in order even to think about reality, to invent words and concepts with which to discuss it, we are forced to reduce its complexity. We cannot think of the trillions of molecules, living cells, organisms, individuals and events that surround us, each in its own place and with its own history. We must first make a taxonomic classification, and we must also make a spatial aggregation.
>
> [I]f, in addition to our basic taxonomic and spatial aggregations, we assume that only average elements make up each category, and that only the most probable events actually occur, then our model reduces to a 'machine' which represents the system in terms of a set of differential equations governing its variables.
>
> But such a 'machine' is only capable of 'functioning', not of evolving. It cannot restructure itself or insert new cogs and wheels, while reality can!

What Allen imagines is the possibility of the structure of the web of interactions, of which we conceive in our models, dissolving, as it were, and then re-crystallizing into some other structure, with a different number of states and parameters and different inter-connections between the states.

The following are physical manifestations of Allen's conceptual imagination: the acclimation of vegetation to future changes in climate (Moorcroft, 2006); historic structural change charted in the foodwebs of estuarine and coastal ecosystems (Jackson *et al*, 2001) — just as already imagined in visualizing a model's changing structure in Box 3 (Chapter 2.7); and the structural adjustments to the same in river and lake ecosystems as a result of the introduction of exotic species (Strayer *et al*, 1999; Matthews *et al*, 2002). They are not matters of evolution in its literal sense, for what Allen went on to ask was: can we discover the rules by which the system will re-structure itself? But they are significant problems encountered in the practice of environmental science, and they are germane indeed to the expression of our present ***Challenge # 8***.

Conceptual error, or structural error/uncertainty in the model, may be thought of as a measure of the extent to which the expression of what is "known" diverges from the "truth". To reiterate from Box 2 of Chapter 2.7, it may be considered to have two important, significantly different dimensions: of error in the {presumed known} and of uncertainty about the {acknowledged unknown}. Addressing it as a matter of significance has been gaining ground in recent years, and yet again, notably in Hydrology, in the works of Neuman (2003), Poeter and Anderson (2005), Beven (2005), and Refsgaard *et al* (2006) (as well as Borsuk *et al*, 2004). Broadly, these all assume a plurality, if not a multitude, of candidate models, $\boldsymbol{M}_i$, $i = 1, 2, ..., m$, to each of which can be assigned a probability — in the present — of that model encapsulating the truth of the matter. This probability will vary with time in the Bayesian spirit of the identification-prediction cycle. At any point in the cycle, models $\boldsymbol{M}_i$, $i = 1, 2, ..., m$, with the accompanying distribution of likelihoods of encapsulating the truth, can be employed computationally in generating a sample of multiple bundles of predictions of possible behavior in the future. Our *Paper* has already touched upon this in respect of matters of adaptive modeling, adaptive sampling, and Environmental Observatory operations in the domain of the Ocean Sciences (under ***Challenge # 6*** in Chapter 2.6; Lermusiaux *et al*, 2006a).

There is a bigger picture here, however. Most of the foregoing has recently been brought together under the heading of a Bayesian Hierarchical Modeling framework, wherein the notion of hierarchy manifests itself as follows. Given the data from the EO, a posterior model structure ($\boldsymbol{M}_{posterior}$) can be obtained given $\boldsymbol{M}_{prior}$; whereupon, given $\boldsymbol{M}_{posterior}$, posterior estimates of the model's parameters are computable; so that then (ultimately) armed with $\boldsymbol{M}_{posterior}$ and these posterior parameter estimates, predictions of future behavior (as outputs $\boldsymbol{y}$) are calculable (Liu and Gupta, 2007). All this, these authors from the domain of Hydrology label "data assimilation", subsuming therein much of what has gone before under ***Challenge # 7***, the discussion of this present ***Challenge # 8***, and a good deal of what is to come in the next section in respect of ***Challenge # 9***. We shall choose there, however, to interpret the assimilation of data rather differently.

Looking back, with a grasp now of what it means to have a predictive science, we may conclude that what we practise as environmental modelers has yet to attain that noble goal. Looking back too, with an appreciation of the perhaps paradoxical illumination brought with analyses of uncertainty, the intent of these indicative lines of response to ***Challenge # 8*** is this: to make the utmost, under uncertainty, of the diversity of candidate models thriving under the competing schools of thought, presuming that within the span of the distribution of these models lies somewhere the truth. Attempts at detecting, gauging, quantifying, circumventing, or reducing the gap between the model and the (unknowable) truth come primarily under the preceding ***Challenge # 7***. Faithfully accounting for the consequences (for model-generated predictions) of this gap in our knowledge, with all its flaws and blemishes, is a matter of the current ***Challenge***.

Absent is the notion of supposing the gap will eventually be eliminated, notwithstanding its power of motivation. Not for nothing did Popper entitle his intellectual auto-biography an unending quest. There will always be a need for generating foresight — a less strong form of "prediction" — under the presumption of structural error/uncertainty, within which may reside structural change of a kind approximating that imagined by Allen (1990). The manifesto of Beck (2002) (in shorter form, in Beck (2005b)) is one perspective on the possible forms of response to the facet of foresight within ***Challenge # 8***. That manifesto was inspired in no small measure by Allen's description of his problem; and it embraces approaches — part computational, part conceptual — exploiting the idea of parameters ($\boldsymbol{\alpha}$) as stochastic processes, i.e., varying through time-space.

Chapter 3: Science and Engineering In "Real Time"

In 2010 half a century will have passed since Kalman published his seminal paper on a new approach to signal filtering and prediction (Kalman, 1960). Time enough, one might suppose, for real-time information processing and forecasting to have become a commonplace in the environmental sciences. It has not; and it is especially important to understand why this has been so. For the potential and scope of the EOs and accompanying environmental cyber-infrastructure are substantial, in precisely the domain of exercising "functions in real-time".

3.1 Assimilating Data and Processing Information in Real-time

Environmental Science did not want for early adopters of these algorithms of Kalman (and of recursive estimation more generally), themselves born of the then urgent needs of aerospace engineering. Real-time forecasting and control in hydrological and water resources systems, for both surface and ground waters, as well as the municipal water and wastewater treatment facilities of environmental engineering, had already been the object of considerable study throughout the 1970s (Wood, 1980). Bennett's original work on data assimilation in physical oceanography began in the 1980s (Bennett and Budgell, 1987).

All novel techniques emerging from applied mathematics and mathematical engineering tend to move through other disciplines as matters of fashion, some gaining more purchase in the new subjects than others. Why then has the field of environmental science been largely unreceptive to the processing of information in real-time? For this is more than a matter of technological barriers in sensor and communication technologies and the physical infrastructure for enacting controls in real-time.

Sir Alan Harris, an eminent engineer who regretted the intellectual and professional separation of mechanical engineering from civil engineering, put it this way: if an object is meant to move, that is mechanical engineering; if it is meant to stay put, that is civil engineering. Control engineering, taught in the disciplines of mechanical engineering, electrical engineering, aerospace engineering, and chemical engineering, is about engineering the dynamics of change and variability in the behavior of an entity — "movement" in an object — *after* its conception, design and construction. Civil engineering, which embraces engineering hydrology and environmental engineering, has generally had little pressing need to pay attention to the operational stage in the life cycle of its products, even over the past three to four decades.

When operating a built system, monitoring how the state of a system changes with time in response to disturbance, understanding how input disturbance and state are related, and intervening deliberately — in real time — to manipulate other system inputs in order to maintain the behavior of the system within some desired pattern or bounds (or avoid some feared threat), are all key. In particular, when the changes with time are relatively rapid, some form of real-time data-processing and decision-making scheme becomes crucially important. We have already seen something of this in the Dynamic Data Driven Applications Systems (DDDAS) of ***Challenge # 6*** (Chapter 2.6). With progressively increasing speeds of change, if not increasing complexity in the way the behavior of the system must be understood in order to exercise decision-making effectively, the associated schemes will need to become automated. Hence we have the typical context of real-time forecasting and control.

When the important elements of the system's dynamical behavior are perceived as being relatively slowly changing, processing data in real-time and making split-second, unerring decisions seem irrelevant, for all practical purposes. And in that we can find much of the reason why real-time forecasting and control have achieved such modest practical success in the environmental sciences. The attaching frustration, as well as a contemporary diagnosis of why this has been so, is chronicled in Beck (2005a).

Kalman, it is to be noted, published his seminal paper in the Transactions of the American Society of *Mechanical* Engineers. His triumph seems to have been so great as to have stifled significant algorithmic developments for quite some time thereafter — with perhaps the notable exception of Ljung, (1979), who in fact developed a filtering-like algorithm, designed for parameter (not state) estimation, starting from a premise rather different from Kalman's. In the past decade or so, however, all manner of variations on the basic theme of filtering theory have been unleashed: ensemble filter, particle filter, unscented filter, singular evolutive extended filter, singular evolutive partially local extended filter, all of which have been enjoying applications across the environmental sciences, from the ocean sciences (Hoteit *et al*, 2005; Lermusiaux *et al*, 2006a; Torres *et al*, 2006), through hydrology (Moradkhani *et al*, 2005a,b; Drécourt *et al*, 2006a,b; Andreadis and Lettenmaier, 2006; Liu and Gupta, 2007), and on to wildfire propagation (Douglas *et al*, 2006), terrestrial ecology (Williams *et al*, 2005), and population dynamics (Wang, 2007).

Environmental Science and Control Theory

It is *not* the case that applications of the algorithms of filtering theory and the like have not been useful for purposes other than just pragmatic real-time forecasting and control. Boxes 2 and 3 of Chapter 2.7 bear witness to this; to the legacy of the heady days of "youthful exuberance" characterizing early adoption of these algorithms in Environmental Science in the 1960s and 1970s. Present-day interest in data assimilation is significant, moreover, and the associated algorithms thereof have a strong cultural basis in filtering theory, hence control theory. Further details of both — control theory and data assimilation — will be placed in Box 4 below, along with the concepts of adaptive control and adaptive management (to become important in subsequent ***Challenges***). Neither has it been the case that, given sensors and instruments for observing some of the more difficult attributes of environmental systems in real time, no interesting or significant features of behavior have thereby been revealed, to challenge the knowledge bases encoded in contemporary models (developed essentially in the absence of such data).[24]

A large part of the problem has in fact been this: what exactly are the economic, policy, and socially relevant reasons — what are the practical incentives — for actually needing a forecast of environmental quality in the short-term? Responding constructively to this question will be a very important part of then fashioning a program of research for exploiting to the full the distinctive and unique opportunities for real-time computations with models, to be afforded by the advent of the EOs and the environmental cyber-infrastructure.

All three of our textbook problems (from Chapter 1.2) — given $\boldsymbol{u}$ and $\boldsymbol{y}$, find $\boldsymbol{M}$; given $\boldsymbol{M}$ and $\boldsymbol{u}$, find $\boldsymbol{y}$; and given $\boldsymbol{M}$ and desired, feared, and/or threatened $\boldsymbol{y}$, find $\boldsymbol{u}$ — may be considered under the next grand ***Challenge*** we are about to express. Its distinctive feature, as opposed to the foregoing ***Challenges # 8*** and ***# 7***, are identification, prediction, and management as a function of time in the near vicinity of the present (t, let us say).[25] In the sense that everything may be attempted in "real time", the approaching ***Challenge # 9*** cuts across much of what has gone before, perhaps courting duplication thereby, in particular in respect of ***Challenge # 6***.

To appreciate the full extent of our next grand challenge, however, and the central role of $\boldsymbol{M}$ within it, we shall need now to appreciate more of the detail of Kalman's filtering algorithm in the specific context of control theory, hence to appreciate too how the promise of data assimilation may be undermined by the security or otherwise of the model itself (Box 4). Under certain circumstances, our textbook problems may simply be demanding "something for nothing" or, to be precise, the reconstruction of too many unknowns from too few knowns.

As Box 4 shows, the essential role of a model $\boldsymbol{M}$ in assimilating observations is its capacity to unify interpretation of those observations across heterogenous scales of the time-space-biogeochemical continuua. This too is salient in differentiating some of the foregoing ***Challenge # 6*** from the present ***Challenge # 9***. Whereas ***Challenge # 6*** asked how might models be used to inform the deployment and re-deployment of observing capacity in a built, operational EO, our concern here is different. An important part of the challenge is one of reconstructing coherent, homogeneous fields of variables internal to the model ($[\boldsymbol{\alpha},\boldsymbol{x}_n,\boldsymbol{x}_m]$), in particular, from all manner of heterogeneous observing platforms and devices (subscripts m and n here distinguish between states

[24] For over a decade (1997-2008) the Environmental Process Control Laboratory of the University of Georgia generated such blocks of high volume high quality (HVHQ) data (in real time) for the C, N, P, and oxygen behavior of rivers, ponds, and biological wastewater treatment plants (Figure 2), albeit only touched upon in passing in the open literature (for example, Lin and Beck (2007a,b)).

[25] Although we can usefully relax this constraint of being "near real-time" for the purposes of considering issues of data assimilation.

BOX 4

Control Theory:
The Detailed Anatomy of Model State-Parameter Estimation

The model $\boldsymbol{M}$ relates inputs $\boldsymbol{u}$ to a variety of other entities: to state variables $\boldsymbol{x}_{\boldsymbol{m}}$ that are measurable (in effect $\boldsymbol{x}_m \approx \boldsymbol{y}$, the outputs); to states $\boldsymbol{x}_n$ that are to all intents and purposes not measurable, i.e., not accessible at a sufficiently fast sampling frequency (given current sensor technologies) or lacking the requisite intensity of spatial sampling; and to parameters $\boldsymbol{\alpha}$. Given the data $[\boldsymbol{u},\boldsymbol{y}]$ and given the current model $\boldsymbol{M}(t)$, the original motivation of filtering theory was to reconstruct current estimates of the unknowns within $\boldsymbol{M}$, now distinguished in more refined terms as $[\boldsymbol{\alpha},\boldsymbol{x}_n,\boldsymbol{x}_m]$. The quintessential feature of Kalman's filter is the manner in which forecasts of the fields $[\boldsymbol{\alpha},\boldsymbol{x}_n,\boldsymbol{x}_m]$ are updated (or adapted) on receipt of the current observations, as an elegant function of the balance between the uncertainties of these forecasts and those of the observations.

Technically speaking, adapting estimates in the near past (t^-) given $[\boldsymbol{u},\boldsymbol{y}]$ up to the present (t) is referred to as smoothing, while adapting them now (t) is the act of filtering; and not surprisingly, generating estimates into the short-term future (t^+) is the matter of forecasting. In these abstract terms, there is very little that distinguishes the notion of parameters $\boldsymbol{\alpha}$ from that of states $(\boldsymbol{x}_n,\boldsymbol{x}_m)$, merely their respective, presumed rates of change with time (and space). For $\boldsymbol{\alpha}$ these ought either to be zero, or tending towards zero, i.e., $\boldsymbol{\alpha}$ is truly constant or, at most, changing slowly.

Feedback Control:
When the Quality of the Model is Not Paramount

For the purposes of reconstructing estimates of $[\boldsymbol{\alpha},\boldsymbol{x}_n,\boldsymbol{x}_m]$ in the vicinity of the present, the quality, security, and reliability of the model structure ($\boldsymbol{M}(t)$) through which these quantities are inter-related, do not have to be paramount. They might be highly desirable properties of the model, but not necessary for the purposes of exercising (real-time) control: first, because the model needs only to be a reasonable approximation of the system's behavior over a very short span of time; second, because the deleterious consequences of acting on an erroneous basis will be quickly rectified, when actual behavior ($\boldsymbol{y}(t^+)$) is next checked against desired behavior, $\boldsymbol{y}_d(t^+)$ — at least where there is feedback control, as opposed to feedforward control. Indeed, it is the goal of feedback control to maintain adequate steering of the system's behavior in a desired manner in the face of an uncertain $\boldsymbol{M}$, as well as uncertain future incoming disturbances (elements of $\boldsymbol{u}$).[1]

Adaptive Control:
Seeking Deliberately to Improve the Quality of the Model

In adaptive control schemes it may be highly desirable to allow the parameters of the model ($\boldsymbol{\alpha}$) to change with time, such that model $\boldsymbol{M}(t)$ is always a reasonable approximation of what we might

[1] Feedforward (open loop) control presumes a secure model of how the system works, generates on that basis controlling actions intended to compensate for the anticipated consequences of the incoming disturbances that will impinge upon the system — but never acts upon any checks of whether actual and desired responses in the system's behavior are matching each other. Critical to the success of feedforward control is that the knowledge embodied in the model, and foreknowledge of what will be the future disturbances, are both subject to very low uncertainty.

call the actual, local, behavior of the system in the vicinity of the present. For in real-time control the priority is control of the behavior of $\boldsymbol{y}$, not acquisition of the best, most scientifically sound $\boldsymbol{M}$. However, given the uncertainty in $\boldsymbol{M}(t)$, and therefore in $\boldsymbol{\alpha}(t)$, it might be prudent for the manipulative, controlling, input actions applied to the system (in effect, elements in the vector $\boldsymbol{u}$) to be chosen so as to probe the behavior of the system in a manner deliberately designed to yield better estimates of $\boldsymbol{\alpha}(t)$, i.e., to reduce the uncertainty in our understanding of the system's behavior (encapsulated in $\boldsymbol{M}(t)$). Where such adaptive control entails choosing elements of the current controlling actions (say $\boldsymbol{u}(t)$) as a function of evaluating what it might take to have future $\boldsymbol{y}(t^{+})$ matching $\boldsymbol{y}_d(t^{+})$, i.e., predictive control (Woldt and Dahab, 2006), so the algorithmic scheme is solving all three of our textbook problems at one and the same time.

Hence — broadly speaking — we have the algorithmic basis of adaptive environmental assessment and management first so eloquently expressed in the book of Holling (1978). One essential difference between the apparent contemporary lack of pragmatic interest in real-time control and today's complete embrace of adaptive management of environmental systems, may reside in the difference in the scales of time to which each primarily refers: very short (days, hours, minutes, seconds) in the former; but over the medium term in the latter, where policy choices are to be made and implemented over the span of months and years.

The algorithmic and conceptual foundations of filtering theory and real-time control are thus applicable over scales of time and space far from what constitutes but the very local in space-time — literally, in the here and now. Relaxing our constraint of $[t^{-}, t, t^{+}]$ all being close to one another allows us now to enfold types of problems other than real-time forecasting and control into the same conceptual problem-solving framework.

When Quality of the Model is Crucial

There is one facet of real-time control, however, where we should want a model of the system $\boldsymbol{M}(t)$ to be very reliable. A defining feature of biological systems of water and wastewater treatment is the fact that one wishes to exercise control not so much on the basis of that which can be readily observed, i.e., $\boldsymbol{y}(t)$ and therefore $x_m(t)$, but on those states $\boldsymbol{x}_n(t)$ recalcitrant to easy observation in real-time, typically the biomasses of a microbial ecosystem (Beck, 1981; Chen and Beck, 1993). In the absence of a reliable model, it is in the nature of filtering algorithms to manipulate estimates of $\boldsymbol{x}_n(t)$, not to mention $\boldsymbol{\alpha}(t)$, such that the estimate of $\boldsymbol{x}_m(t)$ closely tracks $\boldsymbol{y}(t)$, at least to the extent that (logically) $\boldsymbol{x}_m \approx \boldsymbol{y}$. Choosing an action conditioned upon a highly uncertain, reconstructed estimate of $\boldsymbol{x}_n(t)$ would not be a good policy. Assessing the quality of the model $\boldsymbol{M}$ is therefore far from unimportant, even in real-time applications. It is just as important in the context of data assimilation, but in a different manner, as we shall see.

BOX 4

Data Assimilation:
Wresting Homogeneity of Estimated Fields
from Heterogeneity of Data Fragments

The generic character of data assimilation has already been expressed. It is, to reiterate: given the data [$\boldsymbol{u}$,$\boldsymbol{y}$] and given the model $\boldsymbol{M}$, find [$\boldsymbol{\alpha}$,$\boldsymbol{x}_n$,$\boldsymbol{x}_m$]. Of particular interest is the matter of solving this problem when the nature of the data is an eclectic mix of fragments of the (ideal) whole, as it is in the dynamic global vegetation models of Moorcroft (2006) (see, more specifically, for example, the complex of tower flux, flask, and satellite data discussed in Running *et al*, 1999). Let us suppose the mix of fragments, blocks, and patches of data across the various scales of space-time are denoted [$\boldsymbol{u}$,$\boldsymbol{y}$;Δt,$\boldsymbol{\Delta s}$], where Δt and $\boldsymbol{\Delta s}$ are a variety of (integer) multiples of the base numerical discretization of the time-space grid of the model $\boldsymbol{M}$, i.e., intervals δt and $\boldsymbol{\delta s}$. The heterogeneity of the data can be assimilated through the model — and an accompanying procedure of estimation — to generate the time-space fields of [$\boldsymbol{\alpha}$,$\boldsymbol{x}_n$,$\boldsymbol{x}_m$], wherein the orders of the vectors in the latter will typically be very much higher than the order of the vector $\boldsymbol{y}$ of observations, especially in respect of coverage in space. Insofar as $\boldsymbol{x}_n$ interpolates amongst and extrapolates beyond the "sampling points" of $\boldsymbol{x}_m$ characterizing the behavior of the system along the biogeochemical continuum, this complements assimilation (state reconstruction) along the dimensions of time and space.

The power of the assimilation, when working with the various *heterogeneous* fragments of data, lies in the manner in which the model inter-relates the components of behavior underlying all of these fragments, as a reflection of the behavior of the system as a *homogeneous* whole. This is exactly what we should expect of the environmental cyber-infrastructure to emerge in response to ***Challenge # 2*** (in Chapter 2.2). There are bounds on the possibilities, however. Again they have to do with the quality of $\boldsymbol{M}$, expressed now as a variation on the foregoing theme.

State-parameter Estimation or Model Evaluation
But Not *Both Simultaneously*

In order for the reconstructed time-space fields (of just [$\boldsymbol{x}_n$,$\boldsymbol{x}_m$] in fact) to be trustworthy in respect of provoking new scientific insights and hypotheses, model $\boldsymbol{M}$ should be maximally reliable in its encoded knowledge base. Ideally, the investigator should be in a position to assert that the model's parameters $\boldsymbol{\alpha}$ are known with certainty. If this is not the case, for example when the structure of $\boldsymbol{M}$ is considered known and correct, but some or all of $\boldsymbol{\alpha}$ must be treated as unknown constants, any significant mismatch between the structures of behavior underlying the model and the observations is likely to be channeled into untrustworthy and distorted reconstructions of [$\boldsymbol{x}_n$,$\boldsymbol{x}_m$], which distortions are likely to be magnified the higher the order of $\mathbf{x}_n$, in particular. Conversely, the capacity to evaluate the appropriateness of $\boldsymbol{M}$ when data are to be assimilated will be diminished, if not rendered entirely impotent. Comparing the total order of the three vectors in [$\boldsymbol{\alpha}$,$\boldsymbol{x}_n$,$\boldsymbol{x}_m$] with that of the lone vector $\boldsymbol{y}$, our metaphorical mathematical textbooks will tell us there is something of a challenge here: of "seeking too much from too little"; of attempting to reconstruct many more unknowns than there are knowns, which is not significantly vitiated by the potential to observe $\boldsymbol{y}$ repeatedly (in time).

that are readily observable (m) and those that are not (n); see Box 4).

Assimilating the observations alone, in reconstructing the fields of $[\boldsymbol{\alpha}, \boldsymbol{x}_n, \boldsymbol{x}_m]$, will result in massive sets of (computational) data (for example, Lermusiaux *et al*, 2006a). When coupled with the need to compute the uncertainties attaching to all the elements of these fields (Lermusiaux *et al*, 2006b), finding and developing innovative means of visualizing such "gigantic data sets", in the words of the NSF's blue-ribbon committee on Simulation-Based Engineering Science (NSF, 2006), become indispensable to scientific progress. Ecology, in particular, in its need to estimate net ecosystem exchange (NEE) of C between the land surface and the atmosphere, has but recently assumed an interest in data assimilation (for example, Williams *et al*, 2005), with evident energy, although not solely through the device of some algorithmic variation on the theme of filtering theory[26]. Hydrology, wherein such forms of data processing have now a mature history of at least three decades, has its own grand challenge: of reconstructing precipitation fields, soil-moisture patterns (McLaughlin, 2002), and mapping the recharge of sub-surface water systems "from space" (Entekhabi and Moghaddam, 2007).

Conspicuous by its absence here is environmental engineering, wherein applications of data assimilation might most have been expected. For there one has the fact of practical access to HVHQ data and the need to exercise control on the basis of reconstructed fields of unobserved microbial populations ($\boldsymbol{x}_n$) — colored and animated through computational visualization (to cultivate the right populations at the right times and right places in a biological wastewater treatment system, for example). But this is, significantly and distinctively, a matter of processing information in *real time*.[27]

And it is on this that our next grand challenge focuses.

Challenge # 9:

> ***In a world of increasing inter-connectedness and instantaneous communication, environmental vulnerability, and infrastructure systems fragility — subject in all probability to higher-amplitude extreme events, natural disasters, terrorist threats, and the like — how best can the expected innovations in cyber-infrastructure and sensors under the Environmental Observatories programs be used in developing models and real-time data-processing and forecasting algorithms: for the on-line detection of faults, failures, anomalies, and the weak signals portending imminent dislocations in system behavior; and for orchestrating/guiding rapid counter-measures for enhancing and resuscitating/reviving damaged system functioning, system survivability, and resilience?***

Time is of the essence. But so is the imploding intensity of society's interactions with the environment, *ergo* the more rapid propagation of consequences arising from natural events, faults, and failures. A conceptual argument can be mounted — for in general we lack sufficient data sampled with a sufficiently high frequency over sufficiently long (historical) periods to provide the basis of any empirical support — to suggest a growing preponderance of significant environmental perturbations of a higher-frequency character (at frequencies of days and hours, as opposed to months and years; Beck, 2005a)[28].

The hurricane epitomizes the extreme natural event, for which there is a cyber-infrastructure for forecasting its trajectory and evolution in real time (for example, Gopalakrishnan *et al*, 2002). Such archetypal storms in turn call for real-time forecasting of stream stages and discharges, as discussed in the context of data assimilation and adaptive forecasting by Romanowicz *et al* (2006). And likewise they call

[26] Phrasing, or terminology, continues to have the potential to confuse. Sacks *et al* (2007) write of a "model-data fusion analysis": in essence, calibration of a model $\boldsymbol{M}$ against data $[\boldsymbol{u}, \boldsymbol{y}]$, with then reconstruction of constituent fluxes internal to the model as a function of its estimated parameters and (deterministically computed) unobserved states, i.e., $[\boldsymbol{\alpha}, \boldsymbol{x}_n]$. Wylie *et al* (2007) report on a method of "adaptive data-driven models" — let us say, a family of identified regression relations, $\boldsymbol{M}(t_i, \boldsymbol{s}_j)$ for several discrete periods of time (i) and discrete areas (j) — for achieving much the same.

[27] Until 2007 (at least) the WATERS Network was entertaining the goal of detecting and forecasting the nation's water conditions in real time. By the time of issuing its eventual "*Draft* Science, Education, and Design Strategy" document (WATERS, 2008) emphasis appeared to have been withdrawn from the "forecasting" element, leaving "detecting" thus much more prominent. This *may* be evidence, then, of the magnitude of ***Challenge # 9***, notwithstanding any thrill at conquering some last technical frontier.

[28] The term "frequency" is used here to connote the speed of propagation of a disturbance, *not* the frequency of occurrence of such an event over a given span of time.

for schemes of real-time control over flows in urban sewer networks (Pleau *et al*, 2005), not least for the network to fulfil the function of "shock absorber" to the downstream wastewater treatment plant. The sudden spill of contaminant, deliberate or otherwise (from infrastructure failure), is another archetypal fast transient event. There, the purpose of an environmental observatory and its cyber-infrastructure, is to "pounce" immediately, as it were, onto the data streams in order to recognize "an event", and to diagnose what, when, where, and how to countervail, in order to protect the well-being of the public, the flora and fauna, and the continued functioning of the (protective) built infrastructure itself (an issue also of concern in ***Challenge # 6***).

There is a qualitative difference between an event whose propagation and consequences are broadly *known*, even in advance of its occurrence, from one of broadly unknown consequences and directions of propagation, even substantial uncertainty about whether an event has occurred. For the former, it could be that the grander of the challenges for the future reside not in the technical domain, but at the interfaces between science, policy, and society. Some of the Environmental Observatories will have the ambition of operating at these interfaces.

In 2005, the US National Water Research Institute (NWRI) facilitated a Workshop addressing this question: "What are the priority needs for social science research with respect to the hurricane forecasting and warning system?" (National Center for Atmospheric Research & the UCAR Office of Programs; www.sip.ucar.edu; accessed 11 March, 2007). As an issue, "Precision Versus Accuracy: Are Risks Adequately Expressed by Current Deterministic Forecasts?" was ranked seventh amongst 22 in the Workshop Report. As a counterpoint to the evident enthusiasm in the NSF's blue-ribbon committee on Simulation-Based Engineering Science, this hurricane Workshop Report challenges itself — and our community — on the matter of social accountability: "It Is in Color, and It Animates, So It Must Be Right". Outside our cloistered circles of research and scientific enquiry, it should not surprise us that the trustworthiness of a model may be gauged, by the stakeholder taking flight in the face of a forecast threat, in ways very different from either the model-builder or the model-user.

Point of Departure in Responding to Challenge # 9

At the technical level, the cyber-infrastructure for the Littoral Ocean Observing System (LOOPS/Poseidon) shown in Figure 7 and its attaching agenda of research (Lermusiaux *et al*, 2006a), stand ready and waiting to respond to ***Challenge # 9***. In Box 5, therefore, each component of that agenda is translated into the conceptual framework of Box 4, in order to make it more generally relevant across the domains of all the EOs. Not surprisingly, Figure 7 shares much in common with the environmental cyber-infrastructure of Mahinthakumar *et al* (2006) for addressing issues of threat-response in public, potable water supply systems, and depicted in Figure 5. Elements of ***Challenge # 6*** on adaptive sampling and Observatory operations are inevitably common to some of those in ***Challenge # 9***.

The schemes of detection, diagnosis, and counter-action for the broadly *unknown* event are where the technical and algorithmic emphases of future programs of research on environmental models might best be placed (in response to ***Challenge # 9***). The urban water distribution system is a microcosm of the "imploding intensity of society's interactions with the environment", as we have expressed it. And the cyber-infrastructure of Figure 5 was in turn described as "evert-alert ... continually primed and poised to detect" an unknown event. In the words, once more, of Mahinthakumar *et al* (2006):

> [A] typical network is highly interconnected and experiences significant frequent fluctuations in flows and transport paths. These design features unintentionally enable contamination at a single point in the system to spread rapidly via different pathways through the network, unbeknown to consumers and operators due to uncertainty in the state of the system. This uncertainty is largely a function of spatially and temporally varying water usage. When a contamination event is detected via the first line of defense, e.g., data from a water quality surveillance sensor network and reports from consumers, the municipal authorities are faced with several critical questions as the contamination event unfolds: Where is the source of the contamination? When and for how long…
>
> Real-time answers to such complex questions will present significant computational challenges.

The kinds of "answers" discussed above in Chapter 2.6 had to do with "how best to re-deploy finite observing capacity away from the previous regime $[\boldsymbol{u},\boldsymbol{y};t^-]^S$ towards $[\boldsymbol{u}',\boldsymbol{y}';t^+]^S$, where t^- marks time before t and t^+ marks time after t, the moment of the event." In that sense, the answers amounted to nothing more than passive observation alone of an unfolding contingency, albeit witnessed then in much greater detail.

Challenge # 9, in contrast, obliges us to contemplate the nature of actions intended deliberately to counter (enhance) the deleterious (desirable) consequences of the event — in real time. [29] At the very swiftest, subliminal level, there is no time for such actions to wait upon cogitation on the part of the human "User" in the cyber-infrastructure of either Figure 7 or Figure 5. This is why we have automated control systems.

[29] Of course, if the effect ($\boldsymbol{y}$) and the model $\boldsymbol{M}$ are known, and the unknown cause (event) is considered an element of the *observed* inputs ($\boldsymbol{u}$), then ***Challenge # 6*** has too the task, in this sense, of finding $\boldsymbol{u}$ given $\boldsymbol{M}$ and $\boldsymbol{y}$.

The Engineering of Control: Throughout the Life Cycle

Speaking of the urban water distribution system, Mahinthakumar *et al* (2006) note that it is the *design features* of such systems that *unintentionally* give rise to the sudden, transient, unpredictably propagating events their environmental cyber-infrastructure is intended to detect and counter. A substantial part of the historic, constrained capacity to implement controlling actions — in general, in real time — in the built environments of metropolitan water infrastructures, has been insufficiently detailed "thinking ahead", from within

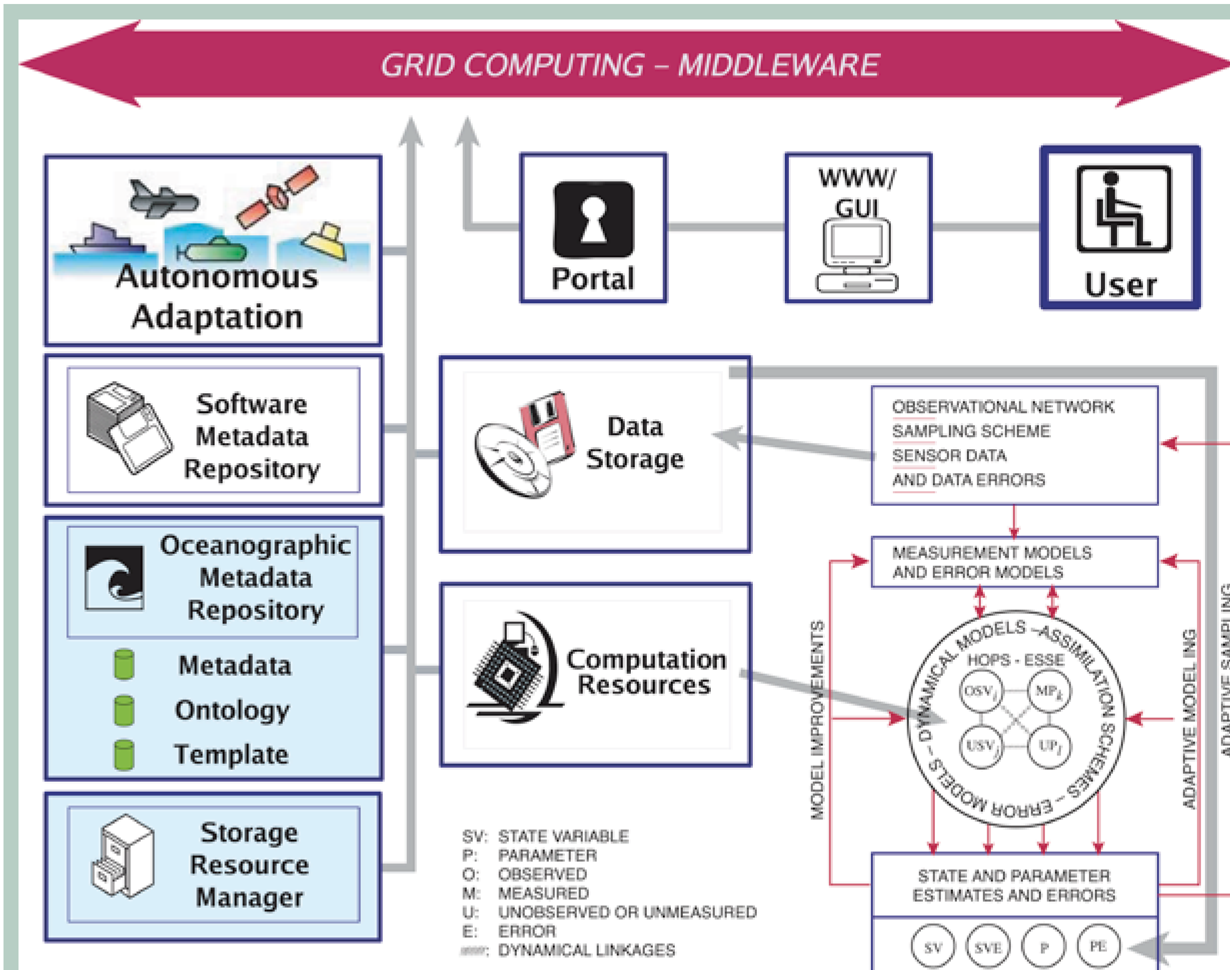


Figure 7
Schematic of the architecture of the Littoral Ocean Observing and Prediction System (LOOPS/Poseidon) from the work of N M Patrikalakis, J J McCarthy, A R Robinson, H Schmidt, W Cho, C Evangelinos, P J Haley, S Lalis, P F J Lermusiaux, R Tian, W G Leslie, and W Cho. Reprinted with permission from Lermusiaux *et al* (2006a).

BOX 5

An Ocean Sciences Research Program and Its Pursuit in Other Branches of Environmental Science

A research agenda for the Littoral Ocean Observing System (LOOPS/Poseidon) has been expressed in Lermusiaux *et al* (2006a). Set originally in the *specific* domain of the Ocean Sciences it can be re-cast in the *generic* conceptual framework elaborated in the preamble to ***Challenge # 9***, facilitating access thereto from the constituent disciplines of all the EOs.

The first component of the ocean sciences research agenda is (Lermusiaux *et al*, 2006a):

> (1) to integrate the various data with dynamical models to obtain optimal descriptions of the ocean and allow accurate process studies

which herein we would express as (1) reconstruct the temporal evolution of the fields of $[\boldsymbol{x}_n,\boldsymbol{x}_m]$, together with their respective uncertainties (see also Lermusiaux *et al*, 2006b) — the most customary format of data assimilation — with a view to (2) provoking novel insights and hypotheses, uniquely enabled by such visualization and animation, i.e., as originally expressed (Lermusiaux *et al*, 2006a):

> (2) to provide a foundation for hypothesis testing and model improvement, including estimating model and data errors (uncertainty modeling)

Under its respective EO, terrestrial ecology will increasingly have the novel opportunity of employing just the single, *homogeneous* model $\boldsymbol{M}$ with which to assimilate *heterogenous* fragments of data, across tower flux, flask, and satellite devices (Running *et al*, 1999). The ocean sciences have a diversity of ship, aircraft, satellite, buoy and submersible as observing platforms (Figure 7), from whose partial, differently angled "glimpses" into the behavior of marine systems — when brought together uniquely and distinctively within the whole of $\boldsymbol{M}$ — might spring the basis of discovery. We can see how "adaptive modeling" lies at the heart of Figure 7 and how within it state variables *and* parameters are conceptually separated into those that are measurable and those that are not, i.e., $[\boldsymbol{x}_m,\boldsymbol{x}_n]$ and $[\boldsymbol{\alpha}_m,\boldsymbol{\alpha}_n]$ respectively. Some, however, might question whether any model parameter is itself *directly* observable, as opposed to only calculable *indirectly* from the relationship, i.e., model, between the observable quantities in which it appears.

The ocean sciences agenda continues with a third component (Lermusiaux *et al*, 2006a):

> (3) to initialize ocean models, or the ocean component of coupled models, and assimilate subsequent observations for optimal forecasting

Since the order of the state vector $[\boldsymbol{x}_m,\boldsymbol{x}_n]$ of the model $\boldsymbol{M}$ to be employed in making forecasts into the future (t^+) is much larger than that of the states directly observable ($\boldsymbol{x}_m$), our expression of this challenge would be: (3) assimilate data from the past (t^-) up to the start t_0 of the forecasting horizon in order to provide the initializing estimates of $[\boldsymbol{x}_m,\boldsymbol{x}_n;\, t_0]$ (within $\boldsymbol{M}$).

Whereas our transcribed goals (1) and (2) deploy the unifying power (and presumed reliability) of $\boldsymbol{M}$ for the purpose of state reconstruction, a fourth goal seeks to channel processing of the collection of

BOX 5

data fragments into probing of that very reliability of the model, expressed originally as (Lermusiaux *et al*, 2006a):

> (4) to estimate model parameters and parameterizations, including forcing and lateral boundary conditions

We transcribe this goal as: (4) to reconstruct [$\boldsymbol{\alpha}$,$\boldsymbol{u}$], i.e., assimilate the data into the prior model $\boldsymbol{M}_{prior}$, in order to investigate any propensity for temporal-spatial variability in $\boldsymbol{\alpha}$, hence to arrive at an improved model from which any significant tendency for such parametric variability has been removed by restructuring of the model into an improved $\boldsymbol{M}_{posterior}$ (more or less as demonstrated in Spitz *et al*, 2001). The challenge in this, of course, is to constrain somehow the enormous computational freedom in reconstructing from the data the vast, unknown fields of states [$\boldsymbol{x}_n$,$\boldsymbol{x}_m$] at the expense of impotence in exposing unambiguously any structural error/uncertainty in $\boldsymbol{M}_{prior}$ — our ***Challenge # 7,*** in fact.

A fifth and final goal of the ocean sciences research agenda echoes our foregoing ***Challenge # 6*** (Lermusiaux *et al*, 2006a):

> (5) to provide the means to assess observing systems, measure the utility of new data and collect the most useful observations through adaptive sampling

Indeed, experience from the ocean sciences has been defining for that earlier grand ***Challenge*** (for models across all the environmental sciences), i.e.: (5) to assess the effectiveness of choices over what is to be observed [$\boldsymbol{u}$,$\boldsymbol{y}$] in respect of minimizing the uncertainties attaching to the reconstructed fields [$\boldsymbol{\alpha}$,$\boldsymbol{x}_m$,$\boldsymbol{x}_n$] and — in a quasi-real-time sense — to use these fields up to the present, let us say [$\boldsymbol{\alpha}$,$\boldsymbol{x}_m$,$\boldsymbol{x}_n$;t^-,t] in order change the current observing strategy [$\boldsymbol{u}$,$\boldsymbol{y}$;t^-,t] to another, [$\boldsymbol{u}'$,$\boldsymbol{y}'$;t^+].

the earliest stages of the life cycles of such systems (planning, design, and construction), to the needs and nature of their subsequent operation (Beck, 2005a). Such would be to the regret of Sir Alan Harris. Hence also, in no small part, have contributions to the topic of data assimilation from environmental engineering been conspicuous by their absence. The challenge now is obvious: using models $\boldsymbol{M}$ of the entire built infrastructure, to design for its survivability, resilience, and adaptability over the long span of the operational stage in its life cycle.

Some would argue (Holling, 1996) that the fragility, or "brittleness", arguably manifest in the behavior of current city water infrastructures, is a consequence, over the decades and centuries, of building into them but a kind of "engineering resilience". This is a form of resilience wherein control — perhaps quintessentially the control engineering of automated, real-time control — is utterly dedicated in concept to pursuit of operation at a narrowly defined target of desired system performance, caricatured as some singular point $\boldsymbol{y}_d$ invariant over time. For as long as the disturbances ($\boldsymbol{u}(t)$) impinging upon the system are of but modest amplitude, behavior can be confined to a very small domain about $\boldsymbol{y}_d$. Come the unexpectedly large disturbance, the achievement of engineering resilience is lost. Worse still, perhaps not even any kind of base-line protective function of the infrastructure is preserved over the future period of system recovery. For that, Holling argues, the system must possess a kind of "ecological resilience" (Holling, 1996; and ***Challenge # 5***), possibly something akin to the auto-immune response of the body. And that is truly the nature of the challenge just expressed, as well as a central reason for seeking a "biologizing" of control theory (Casti, 2002) in response to ***Challenge # 5***.

It does not have to be large disturbances towards which an observing and supervisory system must remain alert. Watts (2002) asks, for instance:

> How is it that small initial shocks can cascade to affect or disrupt large systems that have proven stable with respect to similar disturbances in the past?

And then he proceeds to answer his own question using a model network of agents, in other words, an agent-based model (or IBM). Studies of urban wastewater infrastructures using integrated sets of differential-equation models are already sufficiently mature for research to commence into identifying potentially risk-prone "hot spots" (Vanrolleghem *et al*, 2005).

Chapter 4: Science and Engineering for Policy and Society

Looking back over the preceding Sections and ***Challenges*** of this *White Paper*, a number of changes of emphasis are apparent, albeit with considerations of models (***M***) always central, against a constant background of, first, the motivation of the Environmental Observatories initiatives and, second, the seeming inevitability of the oncoming environmental cyber-infrastructure.

Expression of our ***Challenges***, their grounding in contemporary research, and the beginnings of indicative ways of responding to them, has shifted strategically: from a focus on science (the ***Challenges*** of Chapters 1 and 2) to an outlook embracing both science and engineering (***Challenge # 9*** in Chapter 3). This trend will be continued in the present Chapter, as the context in which the last three ***Challenges*** are elaborated turns towards addressing issues at the interfaces, *not* amongst the disciplines of the EOs as previously, but amongst Science, Policy, and Society. With this progression comes an expanding purview on the matter of who holds a stake in the outcomes of the ***Challenges*** being expressed: from primarily the scientist and model-builder as stakeholder hitherto, to gathering in of the policy-maker as stakeholder, and so to an all-inclusive awareness of the needs of the scientifically and technically lay members of the general public.

Our goal remains unchanging, however: to reflect on the challenges for *research* in the future on *environmental models*.

Problem-solving in the sense of the third of our triplet of textbook puzzles, i.e., find ***u***, given ***M*** and desired, feared, and/or threatened ***y***, is defining for both ***Challenges # 10*** and ***# 11*** to come. Having narrowed the span of attention to near real-time for the purposes of Chapter 3 (and ***Challenge # 9***), we shall immediately relax it in the following (for ***Challenge # 10***). "Real time" will be substituted by "slow time"; and short-term future horizons will become the "long view" across the generations (in ***Challenge # 11***; Chapter 4.2). The iconic "User" in the cyber-infrastructures of Figures 7 and 5 will be considered to have time enough for cogitation in the "feedback loop"; and the nature of the stakes held by that User will broaden, as we have said.

Two themes, then, will become central to the next pair of ***Challenges***. Both can be thought of as discussions along a continuum: along the extent to which the "human dimension" is projected into the formalities of the model (***M***); and a progressive uncovering and refinement of — an extension of — what is understood as Uncertainty. We begin with the latter (in Chapter 4.1), acknowledging its continuing prominence, and noting from our present vantage point how it emerged as far back as ***Challenge # 6***. Whereas uncertainty was key to assessment by the model-builder of the power of a model to explain past observed behavior unambiguously, under ***Challenges # 7*** and ***# 8***, its consideration will now be key to the policy-maker as well, whose concern is to know where the model can be relied upon and where not.

4.1 Management and Decision-support

In 1992, an article with an arresting title was published in the journal *Advances in Water Resources*: "Groundwater models cannot be validated", it proclaimed (Konikow and Bredehoeft, 1992). The title had three purposes: first, to shock the community of groundwater modelers — to jolt them out of the view of models being, or becoming, the "truth of the matter"; second, to affirm the kind of Popperian view on the growth of knowledge set out in introducing this *White Paper* (in Chapter 1.1); and third, to acknowledge the need not to mislead those scientifically lay members of the public, who hold a stake in the decisions to be made, into believing models encapsulate the (incontrovertible) "truth of the matter".

At the Interface With Society and the Community of Scientists

Some seven years later, in 1999, pandemonium broke out in the normally quiet world of environmental foresight in the Netherlands. Its National Institute for Public Health and the Environment (RIVM), officially charged with preparing the country's State of the Environment Reports, was publicly accused of lies, deceit, and shoddy workmanship with its computer models — by one of its own statisticians. The affair became front-page news, received prime-time coverage on television, and provoked questions and debate in the Dutch parliament (van der Sluijs, 2002; Petersen, 2006).

Throughout the 1990s the "headline" forecast of a change in global atmospheric temperature remained remarkably stable, anchored in the conclusion from the 1992 report from the Inter-governmental Panel on Climate Change (IPCC), which observed (Houghton *et al*, 1992):

> [T]he evidence from modelling studies, from observations and sensitivity analyses indicates that the sensitivity of global mean surface temperature to doubling CO_2 is unlikely to lie outside the range 1.5 to 4.5°C.

That the forecast should have remained so stationary over the years, in spite of all the research invested in reducing the scientific unknowns approximated in the models, was a curiosity to some of those studying the behavior of the scientific community involved (van der Sluijs *et al*, 1998). They argued that the constancy of the forecast may have fulfilled, primarily in fact, a sociological role: of maintaining coherence in the fragile process of building a global policy community, while not doing justice to the variegated, evolving understanding of the earth system (van der Sluijs *et al*, 1998).[30] Hardly surprising, then, was the way in which publication of Lomborg's *Skeptical Environmentalist* (Lomborg, 1998) was to rattle the (arguably) hard-won composure of the scientific establishment, in particular, some members of the global change and earth systems science communities.

Mathematical models, and the interpretations and forecasts derived from them, have become matters of both very public debate and popular concern. To his 2004 novel *State of Fear*, best-selling author Michael Crichton appends an illuminating "Author's Message", in which he offers his perspective on the state of play in modeling and forecasting the impact of climate change on sea levels: "all sides overstate the extent of existing knowledge and its degree of certainty" (Crichton, 2004; page 625); and subsequently, on page 628, he urges, "We need more people working in the field, in the actual environment, and fewer people behind computer screens".

Even if the level of effort devoted to both sides (observation and computation) were balanced, the divide may not be bridged. Indeed, what transpires at this seemingly esoteric divide can remain both very public and highly contentious. ***Challenge # 7*** is cast exactly there. So also is Mooney's (2007) popular account of *Storm World*, with characters to mirror the divide: Emanuel and colleagues set in the computational camp with their models (***M***); Gray and associates cast as empiricists. It makes for good reading to pit the two camps against each other, in this case without apparent inaccuracy in reporting. For there appears to have been no meeting of minds, i.e., no productive, inter-penetration of theory-based and data-based models, of the kind commended in response to ***Challenge # 7*** (in Chapter 2.7). Still others, not encamped on either side of the divide, can yet get caught in the cross-fire, and come to regret not having had the benefit of an education in debating science in public (Curry *et al*, 2006).
As if to echo the earlier Dutch (RIVM) "foresight scandal", and citing Konikow and Bredehoeft (1992), Lomborg (1998), and Crichton (2004), one side of the debate over the trustworthiness of environmental models and their forecasts has culminated in this contemporary title: *Useless Arithmetic: Why Environmental Scientists Can't Predict the Future*,

[30] Just as Schaffer (1993) has said: "the most apparently technical estimates of cometary [earth systems] science are very sensitive to public needs and attitudes".

written deliberately for a non-technical audience (Pilkey and Pilkey-Jarvis, 2007).

Such uncloaking and public exposure of the weaknesses of models is neither new nor about to cease. Models, it has been said (Rayner, 2008), allow the craft skills and expertise of the model-builder to be legitimated — made objective (as opposed to subjective) — such that that expertise may be presented in an impersonal manner. Some would say disparagingly "passed off as detached and impersonal". Model-building is thus merely the latest in a long tradition of creating oracles to be consulted. Deliberate shrouding of the soothsayer's device in a mystique is ages-old, Schaffer (1993) would remind us, doubtless to the delight of Pilkey and Pilkey-Jarvis (2007).

Modelers, as a professional sub-group, are by no means universally held in high social esteem amongst the broader community of scientists.[31]

At the Interface With Policy, Regulation, and Law

The US National Research Council's (2007) report, *Models in Environmental Regulatory Decision Making*, records the recent history of environmental models being put to use in the formulation of policy and promulgation of regulations (NRC, 2007). The executive branch of the US Federal Government, through its Office of Management and Budget (OMB), issued guidelines in 2001 calling for each regulatory agency to develop, in turn, their own guidance on ensuring the quality, objectivity, utility, and integrity of information employed in support of policy (OMB, 2001). The US EPA's Council for Regulatory Environmental Modeling (CREM) — itself established in 2000 in response to the same gathering political momentum, for assuring quality in the numbers put into and generated by models — issued subsequently its draft guidance document (Pascual *et al*, 2003). Krupnick *et al* (2006) — writing more recently on the communication and treatment of uncertainty in models employed in Regulatory Impact Assessments (RIAs), like the NRC committee — directly acknowledge two policy-related documents as the motivation for their work: an earlier NRC report on proposed regulations for air pollution (NRC, 2002); and an OMB circular giving specific and detailed guidance to EPA on analyses of uncertainty (OMB, 2003).

Where there is regulation, there is the law, from which may follow litigation, including over the validity of a model: just as Bair (1994) was to observe in the wake of the milestone of Konikow and Bredehoeft's (1992) contribution; and professional lawyers were to document a decade later (McGarity and Wagner, 2003). We see policy formation at a strategic level, therefore, with yet an interest in uncertainty penetrating to quite some technical depth. Conversely, uncertainty in the science encoded in the model must be articulated and addressed within the legal discourse, in largely non-technical terms understandable, in principle, to all (Pascual, 2005; Fisher, 2007).

Where assessment panels are dealing with such uncertainty at the Science-Policy interface — and, above all, its communication to a scientifically lay audience, as in the Intergovernmental Panel on Climate Change (IPCC) — Patt (2007) argues there is a need *not* to confuse uncertainty associated formally with the model (***M***) with uncertainty arising from conflict amongst scientific experts. Audiences (the public) may respond differently to the two sources of uncertainty (Patt, 2007).

Thrown into the spotlight of public policy and public scrutiny, models, their uncertainties, and their trustworthiness pose thus challenges of a different character, albeit — perhaps — at one stage removed from the principal scientific thrusts of the EOs and environmental cyber-infrastructure.

Trustworthiness of Models in Supporting Policy Tasks

On 29 August, 2003, the OMB issued a "Proposed Bulletin on Peer Review and Information Quality". The purpose of the Bulletin was to ensure "meaningful peer review" of science pertaining to regulation, as part of the "ongoing effort to improve the quality, objectivity, utility, and integrity of information disseminated by the federal government", to which we have already alluded. Responding to the manner in which the Bulletin was proposing to meet this intent, Jasanoff (2003) argued that, in short, making progress may depend more on getting stakeholders — the public, the regulators, the scientists, and so on — to agree in advance on appropriate methodologies and investigative protocols, than on subsequent scientific peer review, at least in

[31] See, for example, the report on the 13 February, 2008, Seminar "A New Look at the Interaction of Scientific Models with PolicyMaking", held within the Policy Foresight Programme of the James Martin Institute at the University of Oxford, UK (www.martininstitute.ox.ac.uk). The comments of Rayner (2008) reside in this report.

regulatory science. Establishing, and demonstrating, the reliability and credibility of the peer review process itself are every bit as crucial as the conventional challenge of establishing the reliability and credibility of the information to be reviewed in the process, including that from models. In what would be Jasanoff's preferred form of "extended peer review", it is the process, not the product, that matters; and the scientifically lay public, as legitimate stakeholders, should be engaged therein from the very beginning.

Jasanoff, let us be clear, was speaking on matters of science, not models (***M***), at the interface with public policy. So too are Nowotny *et al* (2001) in their book *Re-Thinking Science: Knowledge and the Public in an Age of Uncertainty*, portrayed somewhat more provocatively under the title of "Science's New Social Contract with Society" (in an article published in *Nature* — portentously perhaps — on the eve of the new millennium; Gibbons, 1999). Their book reveals the challenges and responsibilities of environmental science as key to their thinking.

When Funtowicz and Ravetz (1990) wrote their book on *Uncertainty and Quality in Science for Policy* they may not have had environmental policy primarily in mind. But their work has since risen to prominence in this domain (van der Sluijs, 2007), as indeed acknowledged at the outset of the monograph on *Environmental Foresight and Models: A Manifesto* (Beck, 2002; page 3):

> Today's problems of environmental protection differ significantly from those of the past in several respects. Most obviously, the scale of the current problems is often global (not local) and their dynamics are evolving with relatively long (as opposed to short) time constants. Analysis of such problems will require extrapolation of perhaps staggering proportions: of making statements about the entire mosaic having inspected just the nature of a single tile. Perhaps less obviously, but more directly indicative of the distinctive character of this Monograph, we must find solutions that are based on *inconclusive model evidence*, not conclusive field evidence. Our research must be conducted in a setting of *policy proximity and data poverty*, as opposed to policy remoteness and data richness (Funtowicz and Ravetz, 1990). And we shall be less concerned with optimising recovery under low costs of failure, rather with *avoiding disasters with high costs of failure*.

For all of these reasons, including the foregoing observations on the esteem in which modelers are held, there is cause for us to question how society and policy-makers might view environmental models. This is especially so in the light of the thought-provoking title of Gibbons' paper (Gibbons, 1999), questioning the manner in which major scientific expenditures are justified, such as self-evidently — and tellingly here — for the EOs and environmental cyber-infrastructure themselves.

In short, once the issue was of model (in)validation. It was cast in formal, technical terms, of matching scientifically observed history with satisfactory quantitative statistics (for example, Konikow and Bredehoeft (1992)). It was of concern primarily to those who had developed the model, or been professionally trained to use it; and it was of significant philosophical concern, treated with equally substantial authority in Oreskes *et al* (1994) (and Oreskes, 1998). Now this has become a matter of whether models are to be trusted by legal and policy persons, without the customary technical training; and by those members of the scientifically lay public affected by the outcomes of decisions informed by the forecasts generated by our models. It is also an issue of whether models are trusted by the vast majority of members of the professional scientific community who do not consider themselves modelers.

It is not unreasonable to expect that models, developed in the predominantly science- and research-oriented context of the EOs, will be deployed for the purposes of formulating policy, be subject increasingly to penetrating public scrutiny, and be vigorously disputed in both policy and public domains.

Challenge # 10:

> ***Under the prospect of lengthy and costly social negotiation and legal discourse over policy formation, wherein the placing of trust by various stakeholders in the models underpinning that policy is crucial, and where it has come to be recognized that the needs of model evaluation and peer review for conventional research science are different from those of regulatory science, what new methods of evaluating the alternative models designed to fulfil the predictive tasks of policy formation, decision-support, and management for environmental stewardship are urgently needed? How is the uncertainty associated with both the model and the***

decision-making context to be handled computationally and what new algorithmic and procedural developments will this warrant?

There is a paradox. The greater the degree of extrapolation from past conditions, so the greater must be the reliance on a model as the instrument of prediction; hence, the greater is the desirability of being able to quantify and evaluate the trustworthiness of the model, yet the greater is the degree of difficulty in doing just this.

Should the use of models be put aside in these situations? Pilkey and Pilkey-Jarvis (2007) argue they should, at least for all but what they call "qualitative models" (suggestive of Bayesian Belief Networks), in favor of the definitive field experiment. Their position is close to the oft-heard plea to "let the data speak for themselves", untainted by mediation through any model (***M***). Those raw untranslated data, nevertheless, may yet be used to tell a story quite different from that to which, in respect of global warming, we have become accustomed (Robinson *et al*, 2007).

There is, of course, a counter to the argument of putting models aside. It is founded upon a simple complement to the more familiar concept of a model as a "truth-generating machine", liberated by an insight first expressed long ago by Caswell (1976) in respect of ecosystem models, and now endorsed by the NRC report on *Models in Environmental Regulatory Decision Making* (NRC, 2007). It runs thus.

Conceive of the model as a *tool* designed to fulfil specified tasks, like a screwdriver or a computer program. Recall, from the discussion of algorithms for model calibration (in respect of ***Challenge # 7***), the algorithmic framework of Regionalized Sensitivity Analysis (RSA) of Hornberger and Spear (1981), with its capacity to function effectively under gross uncertainty, employing but "qualitative, subjective, experience of the system's apparent behavior" for the observed past. Recognize that behavior to be regulated in the future can be expressed formally for the RSA in just this same manner, as a (future) "behavior definition". This might be in the form of a bracket of high-end exposure of a population to a novel, xenobiotic substance never before released into the environment, or a behavior imagined in the future, such as essentially similar circulation of waters in the North Atlantic, or radically different patterns thereof. And then think of the model as a tool — as an instrument of prediction — the quality of whose design is to be evaluated against such a task specification (such an expression of desired, imagined, or feared future behavior). We would be *calibrating* the model against a (qualitative) definition of *future* behavior.

Is the model ***M*** fit for purpose, we should ask? Is it fit indeed for a predictive purpose calling for substantial extrapolation into the unknown? In principle, previously unutilized numerical, diagnostic material from the RSA test can be evaluated statistically and made available to inform one's judgement in coming to a view on this question (as sketched out in Beck and Chen, 2000).

Who is it, however, in a policy- and public-proximate setting, given Jasanoff's notion of "extended peer review" (Funtowicz and Ravetz, 1990) and Gibbon's call for "socially robust science" (Gibbons, 1999), who must come to such a judgement on the model?

Models conceived of as tools entail design spaces, in which searches and compromises are effected in achieving the triple goals of "fidelity" (to the science base), "transparency" (to the stakeholders), and "relevance" (to the task at hand). Judgements on the quality of design, however, may reside primarily in the eye of the beholder. The plurality of stakeholder solidarities amongst the public will view the trustworthiness of the model, and the policy it informs, in a variety of ways, and subject to negotiation. The government agency employing ***M*** must anticipate this plurality of perspectives in forming its provisional policy; in the political economy of the tussles over the trustworthiness of the model, a minimization of transaction costs might be sought, but not necessarily a consensus; and due process in a court of law may be needed to impose a singularity of outcome on the plurality of solidarity perspectives on the trustworthiness of ***M***. For but one course of action on environmental stewardship can be adopted over the next decision-period.

To be of practical policy significance, any such computational advances in the analysis of uncertainty and sensitivity for the purpose of evaluating a model in the context of regulatory science will have to be articulated within the coherent administrative framework likely to emerge from the rich and extensive procedural detail set down in the NRC report on *Models in Environmental Regulatory Decision Making* (NRC, 2007). Should a suitable procedure materialize therefrom, some amongst the stakeholders might take all of this detail into account in coming to a summary judgement on the trustworthiness of the model and its forecasts.

In the end, however, many others may not. Availing themselves only of the sparse heuristics these "many" are said to use in exercising judgement and making decisions (Kahneman *et al*, 1982), they might pragmatically place their trust in a model as a matter of mere faith, not the comprehension of voluminous procedural detail, much as the ancients would previously have ventured to consult an oracle (Ayton, 2007).

Uncertainty, Ignorance, Contradictory Certainties — and Making Decisions

There is a pragmatist, decision-focused position on uncertainty in the model ***M***. It will serve as our point of departure. This position has a distinctly different perspective from that of coping with uncertainty and the lack of model identifiability in solving the first of our textbook problems (of finding ***M*** given ***u*** and ***y***). Its goal is not to explain the past. It is different yet again from attempts at eliminating uncertainty in the pursuit of a predictive science of the biosphere (***Challenge # 8***). It is instead this:

> No matter the uncertainty in ***M***, and the uncertainty in the resulting forecasts of the future of the environment (***y***), or in the (predicted) effectiveness of the policy alternatives and assumed future disturbances (***u***), as long as one policy, say u^*, stands above the obfuscation of all the uncertainties, as that to be preferred — given the information currently to hand, and given too the various perspectives of all those holding a stake in the outcome of u^*.

The formal, classical analysis of decisions, for identifying u^*, can be simply portrayed in the tree-like graphical representation of Figure 8, with its sequences of nodes and branches: square nodes for the current and future decision points in time, with branches for each alternative course of action; circular nodes for events occurring over time into the future, with branches for the alternative, possible outcomes of these events, for future "states of nature", that is (denoted "outcome *j*", "outcome *j* + 1" in Figure 8). In other words, the event is considered a random event.

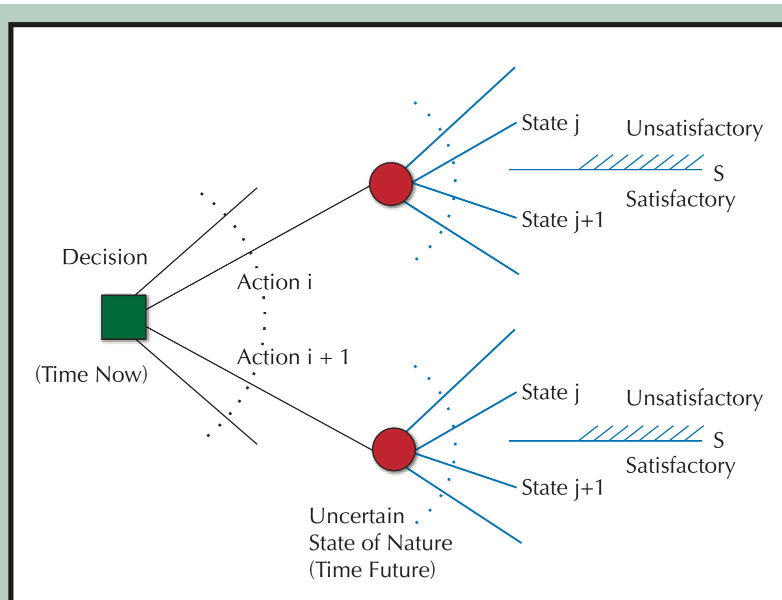
To appreciate now the approaching methodological challenges in using models to guide the making of decisions on environmental policy and management, some classifications of the extent, depth, and qualitatively different "manifestations" of Uncertainty must be introduced. That is the purpose of Figure 8. Within its idealized framework, therefore, uncertainty surrounding the analysis of a decision can be classified into three significantly different categories (for example, Krayer von Krauss and Janssen, 2005):

(i) The exhaustive set of (discrete) possible outcomes of the event (the future states of nature) is known, as too are the probabilities of occurrence of each outcome; this has been referred to as Statistical Uncertainty.

(ii) The exhaustive set of outcomes is known, but not all of the outcome probabilities, i.e., Scenario Uncertainty.

Figure 8

Archetypal tree graph of formal, mathematical, decision analysis: green square node for the decision now to be made; black branches emanating from this green node denote the alternative courses of action; red circular node for the future (unknown) state of nature, which event each action from the decision node will encounter; blue branches emanating from this red node represent the alternative outcomes of the future random event defining the future state of nature; and standard or regulation (*S*), above which the given combination of decision and event outcome will be deemed unsatisfactory (cross-hatched side of bar *S*) as opposed to satisfactory for those combinations ending up below bar *S*.



(iii) Not all of the outcomes are known, *ergo* nor can the set of probabilities be known, i.e, Ignorance.

Statistical Uncertainty

The analysis of decisions under Statistical Uncertainty is taught to undergraduate civil and environmental engineers. They have practical needs for solving the ubiquitous problem of "decision-making under uncertainty", such as assessing ground conditions (the uncertain future state of nature) prior to embarking on a construction project (the decision). In contemporary and vastly more complex schemes this classical form of decision analysis appears in what today are called environmental Decision Support Systems (DSS; see, for example, Matthies *et al*, 2007), well exemplified by the work of Reichert *et al* (2007) on river rehabilitation, and elaborated upon in Box 6.

Likewise taught to undergraduate civil and environmental engineers — and likewise dealt with in more detail in Box 6 — is the use of mathematical programming and optimization: to decide where to construct wastewater treatment facilities in a watershed with degraded water quality and how large to build each facility, including under uncertainty, as illustrated in Harrison's proposal of what he calls Bayesian Programming (Harrison, 2007). The current popularity of "triple bottom line" accounting in discriminating the less from the more unsustainable courses of action (Elkington, 1998) can indeed encourage the view of "becoming less unsustainable" as just such a matter of mathematical programming, where now the constraints (or goals) to be formally satisfied (or optimized) are those very bottom lines: of {environmental benignity}, {economic feasibility}, and {social legitimacy} (as we shall see in our subsequent ***Challenge # 11***).

In the traditions of both decision analysis and mathematical programming, the urge is to encapsulate in mathematical form (within $\boldsymbol{M}$) the attitudes of stakeholders towards Statistical Uncertainty. In particular, attitudes towards welcoming or shunning risk are encoded mathematically as utility functions. Exactly how far this common impulse should propel models, simulation, and computation into mimicking the human dimension is a matter for careful judgement, as addressed further in Box 6, again under ***Challenge # 11***, and beyond (for it raises important ethical issues, amongst others).

Scenario Uncertainty

The task of finding textbook-style the best course of action, u^*, given value-imbued preferences encoded in $\boldsymbol{M}$ and the desired outcomes of $\boldsymbol{y}_d$, is not indispensable to a DSS, however. Finding future outcomes $\boldsymbol{y}$, given a value-free $\boldsymbol{M}$ and an accompanying more or less sophisticated set of scenarios for $\boldsymbol{u}$, i.e., solving for textbook forecasting, can just as well serve the needs of a DSS (as again Box 6 shows). This was the basis of some of the work of the Millennium Ecosystem Assessment (Carpenter and Folke, 2006), and that of Schröter *et al* (2006) on the vulnerability of supplies of ecosystem services across Europe in the face of future climate change scenarios (Chapter 2.1).

Looking back to the formal archetype of Figure 8, at the branches of outcomes for the uncertain future state of nature — scenarios, in effect — Liu *et al* (2009) have this to say:

> There are no "true" likelihoods associated with scenarios in the sense that scenarios are not forecasts/predictions but descriptions of plausible alternative futures. However, for the purpose of risk assessment, scenarios can be categorized on whether they are possible, realizable, or merely desirable. Possible scenarios encompass all that are feasible; realizable scenarios are feasible scenarios operating under a set of defined and specified constraints; and desirable scenarios are possible scenarios that may not necessarily be feasible or realizable (Godet and Roubelat, 1996). In risk management, pair wise comparison of these relative "likelihoods" of the scenarios can be used to determine the priority of scenarios, for risks generally increase with scenario likelihoods and the undesirability (or severity) of consequences of scenarios.

In short, we can have uncertainty as type (ii) above, namely Scenario Uncertainty, typically here in the form of not knowing the probability that a forecast of future climate and meteorological patterns from a Global Circulation Model (GCM) will, in the event, turn out to be the case, as discussed in Box 6.

Whether either the discussion of Liu *et al* (2009) or the brief accounts of the two associated case studies in Box 6 imply Scenario Uncertainty strictly in the sense of Krayer von Krauss and Janssen (2005), is open to debate. What is clear is that nearly all works on decision-making under uncertainty have been studies

BOX 6

Decision Support Systems (DSS), Models, and the Human Dimension: Points of Departure for Responding to *Challenge # 10*

We begin with a question that will come to pre-occupy the discussion of this *Paper* regarding "Science and Engineering for Policy and Society". To what extent can, and to what extent should, the human dimension be formally encoded in the model (***M***)?

This Box has four segments, each serving the purpose of illustrating, through case studies, the role of models in supporting the making of decisions. Each segment also has the purpose of developing a response to the foregoing question. The first segment points to case studies incorporating human preferences formally into ***M***, and in a conventional manner. These mathematical accounts of preferences are then retracted from the model, successively in the two subsequent segments of this discussion. Finally, in the fourth segment, the human dimension is re-inserted into an ***M***, and in a rather unconventional manner.

Models Within Formal Decision Analyses

Within the formalism of Figure 8, the model ***M*** relating outcomes (***y***) to decisions (***u***) is typically, as it is in the case study of Reichert *et al* (2007), a graphical web of elementary cause-effect couples of the probability (or Bayesian) network models, such as developed in the water and aquatic ecology sectors by Reckhow (1999) and Borsuk *et al* (2004, 2006). Expression of the elementary cause-effect couples in such network models may be derived in a variety of ways, as already noted under ***Challenge # 1***, and with the following increasing levels of computational sophistication. First, they may simply be derived from expert judgement. Second, they may come from a regression relationship of this binary pair, i.e., an approximation identified from controlled experimentation with a full science-based model articulating the mechanisms by which single input stimulus *u* induces a response in single output *y*. The single *u*-*y* couple may be a part of a multivariable model accounting for multiple inputs and outputs (***u***,***y***), such as, for example, the floodplain vegetation model in Reichert *et al* (2007). Third, a differential-equation model may be available for simulating the cause-effect (*u*-*y*) relationship, without any of the preceding approximation and simplification.

Each cause-effect couple is an uncertain approximation of what may be the truth of the matter, hence it is assigned a probability of being correct. Outcomes from the probability network model, of concern to all holding a stake in the decision to be made, are likewise characterized by probability distributions. The attitudes of these stakeholders to Statistical Uncertainty, in particular, towards welcoming or shunning risk, are incorporated into the formal mathematical analysis of the DSS through the conventional means of elicited utility functions (in this matter, Reichert *et al* (2007) cite the procedures of von Winterfeld and Edwards (1986)).

BOX 6

Models Within Mathematical Programming

Generating optimal such decisions under Statistical Uncertainty has been treated in archetypal form in Burn and McBean (1985), for example. In the contemporary literature we can find the same problem treated as a matter of Bayesian Programming (Harrison, 2007), wherein all outcomes and their probabilities for all random events are assumed known, i.e., Statistical Uncertainty, founded on the classical form of the decision tree of Figure 8, with a multi-stage sequence of {... -decision-outcome-decision-outcome- ...} over time. Harrison employs the equally classical model ***M*** of Streeter and Phelps for longitudinal, spatial variations in river water quality — remarkably durable, given its original publication in 1925.

In the context of today's DSS, in particular, those supporting implementation of Integrated Water Resources Management (IWRM) and the search for less unsustainable arrangements of urban water infrastructure, methods of mathematical programming are currently being turned to the generic problem of multi-criteria analysis (Jakeman *et al*, 2006). The presently popular appeal to "triple bottom line" accounting in discriminating the less from the more unsustainable courses of action (Elkington, 1998) illustrates immediately the involved, tortuous nature of a multi-criteria analysis. Decisions should be seen by stakeholders to be {environmentally benign}, {economically feasible}, and {socially legitimate}. Driven by the European Union (EU) Water Framework Directive, with its emphasis on participatory approaches to watershed management, Giupponi (2007) argues the case for a new generation of DSSs:

> The proposed approach can be applied in decision processes in which a group of people (i.e., decision makers and stakeholders), share a common conceptual framework and procedure, to structure the problem, discuss the decision and communicate the proposed solution.

Following public release of the software, entitled *m*DSS, with "*m*" signaling "multi-criteria analysis", Giupponi (2007) records the fact that out of 1000 contacts through the project website, fewer than just 20 downloaded the software, all of whom were working in an academic environment. This experience, as he says, is typical of the field of environmental DSS as a whole, where adoption of these systems "by the targeted competent authorities ... is still substantially lacking" (Giupponi, 2007; p 256).

In the foregoing examples of how considerations of Statistical Uncertainty have been accommodated in situations of decision support, the scope and complexity of the model ***M*** have been subordinated to the (higher) task of finding *the* preferred strategy, u^*, including its property of being robust in the face of such uncertainty. Algorithmic interest was focused on achieving the attribute of "preferred", even "best", about u^*, whether in the mathematical domain of formal decision analysis, or optimization, or the combination of the two (as in Harrison (2007), for example).

In general, the purpose of any associated DSS is to render facile this computational burden, thus to focus the attention of stakeholders on matters of trading gains in achieving one goal against gains in attaining some other (incommensurate) goal, notwithstanding the fact that some of the value judgements of a stakeholder, for example, her/his attitude towards risk, may have been elicited from that individual and encoded in a computational algorithm.

BOX 6

On balance, projection of the human dimension into the formalities of ***M*** is here somewhat less than in the foregoing account of formal decision analyses. That projection will be foreshortened yet further in the following segment of this discussion.

Scenario Analysis

In their review of formally developing scenarios for environmental impact assessment, Liu *et al* (2008) are guided by the Intergovernmental Panel on Climate Change (IPCC) definition of a scenario, as:

> [A] coherent, internally consistent and plausible description of a possible future state of the world. It is not a forecast; rather, each scenario is one alternative image of how the future can unfold.

Standing back from the foregoing focus on the task of finding *u**, stakeholders can just as ably form their preferences on the basis of straightforward forecasts (***y***). The candidate alternative policies (***u***) can be assumed (as components of scenarios), threaded through a simulation model (***M***), and the outcomes (***y***) assessed by each stakeholder in respect of their proximity or otherwise to the hopes or fears of that stakeholder for the future.

In principle, the value judgements of stakeholders can remain external to the software, as they do in two similar integrated assessments of the impacts of future climate change on watershed behavior (Krysanova *et al*, 2007; Wilby *et al*, 2006). Both assessments concern themselves with the intersection between climate change and agricultural land use: the former (Krysanova *et al*, 2007) in respect of impacts of climate change on crop yields across the Elbe basin in central-north Europe; the latter in respect of potential consequences for in-stream water quality associated with the nitrogen cycle in a small, lowland watershed in the UK (Wilby *et al*, 2006).

The one acknowledges uncertainty through forecasts deriving from three GCMs, each themselves driven by the same pair of IPCC emission scenarios (Wilby *et al*, 2006). Since no probability is attached to any of these six future states of nature occurring, the assessment would be said to have been conducted under the condition of Scenario Uncertainty. The other case study accommodates uncertainty in the future pattern of climate change by taking a single forecast from a single Global Circulation Model (GCM) for a single IPCC scenario and then, through a downscaling procedure, constructs 100 (random) variations about this single theme (Krysanova *et al*, 2007). Interpreted within the archetypal decision-tree framework of Figure 8 we should have 100 branches emanating from the random (future) event nodes, each with a probability assignable according to the probability distribution assumed for the sampling of the 100 variations on the single theme — but *no* probability for that strategic theme proving true, in the event. Should you be a farmer from Lower Saxony viewing the changes of crop yield forecast by the model ***M***, standing on the threshold of your decision node in Figure 8, with an interest in the fate of your grandchildren in the decade of 2046-2055, you might well prepare to abandon cultivating winter wheat now, while taking up cultivation of silage maize — but you would essentially be banking on the single, strategic scenario becoming true (Krysanova *et al*, 2007).

BOX 6

Human Agency, Culture, and Values in the Model

In stark contrast to the absence of a human dimension from the models (***M***) of the Elbe study, Janssen and Carpenter (1999) populate their conventionally simulated watershed (for the migration of nutrients from the land surface to a water body) with farmers, as the agents in an agent-based model. Each of these agents — in the computer world — perceives the state of the simulated environment and receives signals from the market for agricultural produce; interprets this in terms of his/her individual (simulated) mental model of the Man-Environment relationship, according to the plurality of perspectives in Cultural Theory (for example, Thompson, 1997); is capable of learning from the actions of neighbors, and therefore engages in a rudimentary form of social transactions (if not negotiations); and acts accordingly, purchasing fertilizer and applying it to the land, affecting thus the future state of the (simulated) environment and economy. This is, of course, little different in algorithmic intent to Bennett and Tang's (2006) use of an IBM to simulate the migration of elk about a landscape, with the elk being treated as boundedly rational agents. It is also, however, a manifestation of what was intended in response to ***Challenge # 5*** (Chapter 2.5) as the benefit to be derived from fusing future developments in environmental modeling with those in the social (and biomedical) sciences.

Janssen and Carpenter's interest was in studying the resilience of coupled natural-human systems, not in the matters of making decisions under uncertainty and developing the software of DSS. Nevertheless, their work allows us to reveal something more of the continuum of the human dimension (for comparison and contrast with that of uncertainty, as it motivates the discussion of this Chapter 4.1). This continuum can now be seen to span from the pole of "human choice and subjective values" to that of "utterly dispassionate, objective algorithmic logic". The former can be embedded into the latter, almost as if to make subjectivity objective (as in the model of Janssen and Carpenter (1999)), whereas the choice of how to incorporate and parameterize objective, constituent, scientific hypotheses in ***M*** can be revealed as *subjective* and subject to differing cultural outlooks on the Man-Environment relationship (van Asselt and Rotmans, 1996; van Asselt and Rotmans, 2002).

Our models (***M***) are normally staunchly considered "value-free". It will be controversial to most of us, therefore, to read this from van Asselt and Rotmans (2002):

> An example of alternative quantities in perspective-based model route is the value for the CO_2-fertilisation factor β, which ranges from 0 (i.e., no effect) in the egalitarian model route, to 0.7 (i.e., substantial effect) in the individualistic model route.

where "egalitarian" and "individualistic" are two of the perspectives of the same Cultural Theory as that informing the computational studies of Janssen and Carpenter (1999).

In his summary of the 2004 Symposium on *Uncertainty and Precaution in Environmental Management*, van der Sluijs (2007) refers to this inter-penetration of the objective and the subjective as the "monster" of uncertainty at the Science-Policy interface:

BOX 6

> The categories that we thought to be mutually exclusive and that now tend to get increasingly mixed up to create monsters in the science-policy interface include: knowledge versus ignorance, objective versus subjective, facts versus values, prediction versus speculation, science versus policy.

Drawing upon certain philosophical and anthropological considerations, he suggests there are four styles in which such a monster, or abnormality, is treated in a community, such as that of scientists, engineers and those constructing computational models of environmental systems (van der Sluijs, 2007): one is to expel the problem, i.e., to presume the uncertainty is merely of a transient nature, redolent of the treatment of uncertainty in the sound-science paradigm discussed in Fisher (2007); another is to adapt the problem, by fitting it back into the (above) categories, notably through attempts at quantifying the uncertainties, just as in the present discussion of this Box and elsewhere in this *White Paper*.

Projection (retraction) of the human dimension into (from) the model (***M***) has something of the same "monster-like" character about it, as apparent in ***Challenge # 11*** on sustainability of the built environment (in Chapter 4.2).

in decision-making under Statistical Uncertainty, as defined above. Few systematic analyses in using models for environmental decision-making under Scenario Uncertainty have been reported; and Liu and her co-authors themselves conclude that much research on this is yet to be undertaken (Liu *et al*, 2009).

Ignorance

Extrapolation then to the third category of uncertainty, would suggest that fewer studies still can be expected to be found for the problem of decision-making under Ignorance. And this is in fact so.

When Lempert (2002) calls for "A New Decision Sciences for Complex Systems", he comes close to this. His "deep uncertainty" resonates with our foregoing definition of Ignorance (in the decision context), but it also has resonance with the (rather different) notion herein of epistemic uncertainty, or structural error/uncertainty, placed elsewhere therefore at the heart of ***Challenge # 8*** (in Chapter 2.8). That kind of uncertainty, in its deeper, vaguer manifestations — approximated technically by the {acknowledged unknown} in the model (***M***) — may prompt the question of how to design a model *expressly* for the purposes of discovery of our ignorance (Beck, 2002): for "probing the shores of ignorance" (Dennis *et al*, 2002); and decidedly in a policy-proximate setting (Dennis, 2002).

Contradictory Certainties

Even the category of Ignorance can be sub-divided according to van Asselt and Rotmans (2002), along the lines of increasing uncertainty, expressed colloquially as: "We don't know what we do not know"; "We will never know"; to "We cannot know". From some point along this continuum we can choose to single out a fourth in our categories of Uncertainty, as follows.

So great is the uncertainty in the decision framing that:

(iv) More than one version of Figure 8 is actively maintained and promoted, each alternative caricatured as having the certainty of but a single outcome branch emanating from the future uncertain state of nature, i.e., a plurality of Contradictory Certainties (Thompson, 1985).

Here (with some exaggeration) we are in a situation of arch disagreement: "What I know is the truth; what you know is utterly false". This is readily recognizable as a euphemism for disagreement not so much about the model and science from which it is drawn, but about what is desired as the outcome of the decision context, born of differing views on the Man-Environment relationship. Were a problem to lie within this seemingly paradoxical situation of Contradictory Certainties, we might find a plurality of such statements, each buttressed indeed by a quite different — but "certain" (in the eyes of its proponent) — model (***M***) (Thompson and Gyawali, 2007).

As we have progressed, then, from Statistical Uncertainty through Scenario Uncertainty and on into the more profound, more abundant uncertainty of Ignorance, our discussion has come to a point under Contradictory Certainties where the formal uncertainty of any particular model (***M***) is technically nil, while the decision context is replete with the uncertainty of disagreement amongst the various social groupings of stakeholders (some of whom might be the IPCC assessment "experts" said to be in disagreement in Patt (2007)). We have also reversed in this, backing away from the relative security of consensus on the decision framework (and chosen model of analysis), to the strident dissonance of competing schools of thought — on both the decision context and the model.[32]

However discomforting and unpalatable this might appear, two points are worth noting. First, it is already known that, as a consequence of a lack of model identifiability (***Challenge # 6***; Chapter 2.6), forecasts from a model of Lake Ontario's ecosystem, for instance, can give rise to what are statistically confident, but contradictory, statements about future behavior (from equally plausible candidate parameterizations of the same model structure; Beck, 1987).

Second, and strategically much more important in developing responses to ***Challenge # 10***, confronting uncertainty as Ignorance, or as Contradictory Certainties, as opposed to Scenario or Statistical Uncertainty, would seem to call for altogether different ways of developing environmental models

[32] Viewed from yet another perspective — to gauge the roles of models and the forms of uncertainty at the Science-Policy interface — Petersen (2006) has used a two-dimensional categorization of decision contexts according to the presence/absence of consensus, across (a) the (subjective) values shared in the heterogeneous groupings of stakeholders, and (b) the schools of scientific thinking.

and evaluating their trustworthiness in support of decision-making.

Observatories, Observations, Updating, and Adaptation

What the Environmental Observatories, the environmental cyber-infrastructure, and models (***M***) can collectively be to control and decision-making in real-time in Chapter 3 (and the preceding ***Challenge # 9***), so they might be to all of this policy material and decision-making in slow time, for the present ***Challenge # 10***.

At the core of the DSS prepared by Reichert *et al* (2007) for river rehabilitation is a probability (Bayes) network model (***M***), comprising a web of elementary cause-effect (*u*-*y*) couples with assigned probabilities of having given rise to observed behavior (if not probabilities of being accounts of the "truth of the matter"). As blocks of policy-driven data accumulate, as a consequence of the decisions being made, decade upon decade, say, learning in a Bayesian framework implies updating of those probabilities through reconciling the data with the model. Hence the distributions of probabilities for the policy outcomes (***y***) may be adapted over time and presented to stakeholders for their consideration and negotiation *via* the DSS. Though ***M*** therein is quite different in form from the partial differential equations of the VHOMs discussed by Neuman (2003), for the purposes of policy-forecasting in respect of the (very) long-term storage of high-level radioactive wastes, the principle of updating is identical.

The "blocks of policy-driven data" gathered over spans of years from the EOs are to decision-making in slow time what the observations at instant *t* are to DDDAS.

The sequential character of decision-making, of {... -decision-outcome-decision-outcome- ...}, is ubiquitous and indispensable to the notion of adaptive management, which embodies the principle of learning through the probing and experimental component of a policy (Holling, 1978). It is equally relevant, whether in real or slow time, as Box 4 in Chapter 3 is at pains to point out. Once the decision has been taken, everything entailed in its unfolding consequences — the science, the structure and trustworthiness of the model, the efficacy of the regulation and policy, the community's understanding of itself, its relationship with the environment, the model, and so on — will amount to an opportunity for learning and adaptation, ahead of the subsequent decision (Petersen *et al*, 2009). Adaptive policy design, to identify key uncertainties in ongoing ecosystem management, of both marine and terrestrial animal populations, and including through the use of simulation models, has both a substantial history and an active current research agenda (for example, Lessard *et al*, 2005).

Few, if any, DSS for environmental policy appear to deal with this inevitably sequential nature of making decisions, however. Policy analysis anticipates, in effect, a once-and-for-all decision, or one-stage decision tree, as Harrison (2007) observes in introducing his multi-stage Bayesian Programming procedure. Fewer still concern themselves with estimating the value of the information acquired through monitoring between one decision and the next.[33]

Looking out over a policy horizon of 45 years, for a river subject to pulp-mill effluent discharges, with a first decision at the beginning of year 1 and a second due at the beginning of year 15, Harrison estimates the worth of monitoring water quality between the two decision points to be equivalent to some 4-5% more pulp production for a given annual sum of transient violations of dissolved oxygen standards, or to a reduction of 10% in the latter for a given level of the former (Harrison, 2007). He goes on to argue, with an eye on the kinds of shifts in ecological regimes of interest to Lessard *et al* (2005) and their colleagues (for example, Carpenter and Folke, 2006), that the value of such information from monitoring — and of adaptive management itself — could be significantly greater, but that extension of his two-stage to a multi-stage analysis would quickly become computationally prohibitive for just a handful of decision stages (Harrison, 2007).

None of the DSS in Box 6 deal with the issue of scientific visualization for comprehending the implications of model uncertainty, which is so prominent in the recommendations of NSF's blue-ribbon committee on *Simulation-Based Engineering Science* (NSF, 2006; see also Lermusiaux *et al*, 2006b). None address the role of such visualization in communicating model and decision uncertainty to stakeholders, one of the two motivations for the work of Krupnick *et al* (2006). But even in the midst of

[33] Something to which Gabbert (2006) alludes in arguing the case for making more cost-effective reductions in parametric uncertainty in the RAINS integrated assessment model, under the Clean Air for Europe (CAFE) policy program.

decision-making in slow time — the 2004 Symposium on *Uncertainty and Precaution in Environmental Management* — one of the key insights of van der Sluijs (2007) is the essential need for "[s]ystematic long-term monitoring and learning".

The observing capacity of the EOs and their attaching cyber-infrastructures, of such obvious immediacy in respect of real-time control, is just as necessary in the slow time of policy formulation, assessment, adaptation, assessment, adaptation, and so on.

4.2 The Long View: Towards Sustainability of the Built Environment

Begun under ***Challenge # 10***, the changing emphasis in our discussion will continue, extending further away from the needs of Science alone, towards inclusion of those of Policy and Society, as we now compose ***Challenge # 11***. This will be the last of our "technical" challenges. For ***Challenge # 12*** (to follow in Chapter 4.3) relates to challenges to ourselves, as a community of professionals involved in building and applying models of environmental systems.

Triple Bottom Line: Just Another Mathematical Program?

Over the two decades since the Brundtland definition was famously given to the notion of "sustainability", scientific enquiries thereinto have come to acknowledge that what matters is neither just {environmental benignity} nor {economic feasibility}, but also {social legitimacy} of action, including those actions conditioned upon the outcomes of models. Given the foregoing discussion of decision support systems, and origination of these three {bottom lines} of sustainability (Elkington, 1998) in the quantitative methodology of accountancy, our instinct might well be to formulate problems of sustainability as ones of our textbook mathematical problems. The task would be to find preferred decisions ($\boldsymbol{u}$), given a model ($\boldsymbol{M}$) and desired outcomes ($\boldsymbol{y}$), by solving the following caricature of a mathematical program:

Find those $\boldsymbol{u}$ minimizing {unsustainability over the generations}

Subject to satisfying the constraints of

{environmental benignity}
{economic feasibility}
and, especially, {social legitimacy}

Were we to formulate the task in this way, it is clear that a good deal — arguably too much — of people's personal, subjective attitudes towards risk, uncertainty, the value of an environment, and so on, could have been quite inappropriately subordinated to mathematical approximations. Such insertion of "human agency, culture, and values in the model" was one of the topics singled out for consideration in Box 6 of Chapter 4.1. Inter-penetration of matters objective and matters subjective was discussed, in respect there of uncertainty at the Science-Policy interface (van der Sluijs, 2007).

At the heart of ***Challenge # 11*** lies a similar inter-penetration, of matters personal and matters computational, in models at the Science-Society interface. Driving in the one direction, computational technology and software have enabled the behavior of individuals and society to be incorporated into the model ***M*** (witness Janssen and Carpenter, 1999; Lempert, 2002). Moving in the counter direction, the general public and scientifically-lay individuals may increasingly be encouraged to assume the right, if not the obligation, to judge the quality and implications of those technical and scientific ***M***, all in the interest of attaining social legitimacy of policy actions.

If there has been discomfort in the scientific community over the handling of uncertainty (van der Sluijs, 2007; Box 6), so too should there be in the engineering community over accommodating the computational treatment of personal preferences — as in the above caricature of a mathematical program. In responding to the challenge about to be introduced, those who construct and use models of environmental systems may eventually be drawn by considerations of {social legitimacy} into the unfamiliar territory of unusual and novel questions of ethics. This human dimension to the use of models will come to dominate in the following. Uncertainty there will be too, in more than sufficient volume and depth; but we shall henceforth largely take for granted the need for analyzing it, coping with it, and going forward in spite of it.

More immediately, the builders and users of models may be projected into new ways of conceiving of, if not simulating, the behavior of environmental systems, because of significant changes in the conception of what constitutes {environmental benignity} in the triple bottom line of the foregoing mathematical program. Motivated by a metaphor, we conceive of a "grand conjecture" in the following — a salient into *terra incognita* — and then ask: how might observations be collected, and how might computations with what kinds of models, be employed to corroborate or refute such a conjecture. First people, and then technology, will need to be put more obviously into the frame of consideration as to what might constitute future challenges for environmental modeling.

We shall need to move with ease between ecological and engineering thinking, between animal and human agency in the rural and the urban landscapes, and between what differentiates a "natural" environment from a "built" environment (as in infrastructure). For some, such a blurring of distinctions between concepts and disciplines may be just as discomforting as the ethical matters that will arise at the very end of this discussion.

Re-engineering the Built Environment as a Force for Good in the Natural Environment

We begin by picking up again the biological metaphor, already familiar from ***Challenge # 5***, and seemingly everywhere appropriated.

That projects and products have life-cycles is a commonplace. We made use of it in developing the cases for ***Challenges # 9*** and ***# 10***. Having emerged in the late 1960s, life-cycle assessment (Frankl and Rubik, 2000) sees itself as addressing a form of cradle-to-grave analysis, which in turn can be extended to the concept of "cradle-to-cradle" analysis (Stahel, 1997; McDonough and Braungart, 2002). Much vaunted too is the notion of biomimicry, with its proposed access to the vast store of intellectual seed-corn for the technological innovations of the Second Industrial Revolution (Benyus, 1997). Industrial Ecology has been formally in place as an academic subject for two decades (Ayres and Ayres, 2002); the *Journal of Industrial Ecology* was first published in 1996. The city can be conceived of as having not only a calculable ecological footprint (Rees, 1992; Rees and Wackernagel, 1996) but also an appetite, a metabolism, a pulse, and so on (Wolman, 1965; Beck, 2005a; Barles, 2007; Bettencourt *et al*, 2007).

Thinking in terms of the attributes of an organism and of the manner in which that organism lives and prospers harmoniously within its environment is, we now appreciate, a powerful metaphor for engineering and industrial design. It augments the image of the clockwork mechanism as the earlier epitome of the same, manifest itself in the above caricature of a mathematical program. The image of the "sentient organism in the ecosystem" introduced in Chapter 2.5 (***Challenge # 5***) can be transcribed productively into that of the "{city and its infrastructure} in the {watershed}" (Beck *et al*, 2009). This alternative conceptual framework, for thinking about re-engineering the built environment, is neither an entirely new metaphor nor yet exhausted in its potential to reveal novel avenues of further research. It provides much of the impetus for the expression below of ***Challenge # 11***.

Beyond exploiting the biological metaphor, we need thoroughgoing inter-disciplinarity in our thinking. ***Challenge # 5*** also called for the pursuit of insights into the generic, dynamical properties of systems' behavior. Its discussion culminated in advocacy of further synthesis in classical systems thinking, amongst the construction and use of models across the Environmental, Biomedical, and Social Sciences (Chapter 2.5). We drew upon the work of Hawes and Reed (2006) and their vision of a cyber-infrastructure associated with agency in terrestrial and agricultural systems, to suggest it was but a short step from there to the metaphor of the city as a "large animal grazing in its pasture". This, Rees and Wackernagel (1996) had proffered earlier, as a means of engaging us in conceiving of the rather successful innovation of the urban ecological footprint — massive, of course, for cities such as Paris, New York, and the like. Needed too, then, is the kind of thinking already exposed in the culmination and synthesis of ***Challenge # 5***: the capacity for moving effortlessly amongst disciplines, metaphors, and images.

About 50% of the world's population is now (2009) classified as urban. Much of the built environment can be equated with infrastructure for sustaining the city's metabolism. And while Kaye *et al* (2006) may write of how "footprints depict negative impacts of cities without accounting for the probable efficiency of dense urban living", cities and the built environment are most likely viewed (in the popular mind-set) as inherent environmental "bads", with no extenuating circumstances.

Yet things do not have to be this way, no matter how hard it may today be to conceive of cities as forces for good in the environment. Far from the burden of infrastructures having to compensate for the ills of cities, the two should "act" deliberately to contribute positively to enhancement of the natural environment about them. Let us take therefore the metaphor of Rees and Wackernagel (1996), with its obvious basis in ecology, and see just how far it can be pushed to serve the purposes of an engineering turn of mind.

Viewed as an organism, the city takes in its "daily bread" and "daily water", together with life-sustaining "breath". And we have engineered the return of the residuals of this metabolism to the air, water, and land environments surrounding the city. In the Global North, a good deal of the city's daily water is used to convey the residuals of its daily bread — as wastewater — away from the confines of the urban space, so that citizens can lead healthy and productive lives. Much technological effort has been invested in treating that wastewater, not always to the good of the air, missing an opportunity to benefit the land, while not being a wholly unmitigated good for the water environment.

Imagine now the generic animal of Rees and Wackernagel as specifically a bull. The "bull" of intense social and economic activity in the city might be shod in the future with the "padded athletic trainers" of re-engineered infrastructures and imbued with a technological deftness and intelligence sufficient for restoring the business of running the environmental "china shop" in which it charges about. Pushing the metaphor yet further, the city might even profitably expand the shop's operations, by becoming a net contributor to some of the watershed's ecosystem services. Projections show that, by the compliance date (2015) of the EU Water Framework Directive, Paris might well look like the bull in the restored but vulnerable china-shop of the Seine watershed (Billen *et al*, 2007a,b; Even *et al*, 2007a), yet not at all self-evidently shod with padded trainers, nor necessarily in possession of the intelligence and technological deftness required for expanding the shop's operations.

With the ground thus prepared, our next Challenge can be cast upon it.

Challenge # 11:

> ***Since the greatest debate of our times is the "sustainability debate", with its significant implications for the design and operation of the built infrastructure at the interface between Man and Environment (most conspicuously so at the urban centers of socio-economic activity), how best should the Environmental Observatories be deployed and, more specifically, what kinds of models should be developed in order to promote a better strategic alignment of the study of urban metabolism with that of ecosystem services, all within the web of global biogeochemical cycles? How too, in the widest of possible terms, can innovations in information and communication technologies (ICT) — as realized in the environmental cyber-infrastructure — lead to tangible gains in reducing the unsustainability of current patterns of socio-economic behavior?***

How indeed could the built infrastructure be re-engineered to restore the natural capital and ecosystem services of the nature that occupied the land before the city? How could it be re-engineered to enable the city to act as a force for good, deliberately to compensate positively for the ills of the rest of Man's interventions in Nature?

How in particular, to echo ***Challenges # 4*** and ***# 5***, can the inter-disciplinary insights of applied systems analysis at the conjunction of ecology, computational science, and biomedical science — of damage limitation, self-repair and self-replication, and their relationships with the notion of ecological resilience — be developed and then exploited to answer such questions? In the face of all manner of threats, how can the technological parts of the infrastructure (organs and cells) within the city-infrastructure couple (body of the organism) be designed to function as does an auto-immune system (or as might a "self-healing energy infrastructure"; Amin, 2001)?

How can cities of the Global South avoid adopting the same historical technological trajectory, and sell back to the Global North what they have learned from taking another path? How, more profoundly, can the engineering of city infrastructure be deployed expressly so that those at the bottom of the pyramid of dignified human development (Maslow, 1943) may be brought to a level where they care to engage in such a debate, over such a grand challenge for the next century — of cities as forces for good — beyond their desperate needs of survival for just today and tomorrow?

One scenario — one candidate future path for cities of the Global North; one grand conjecture in response to this host of questions — runs as follows.

If the water- and nutrient-return infrastructures of those cities could be uncoupled and kept strictly separated (from the household or office block onwards), eventual recovery of a "perfect fertilizer" product from a re-arranged wastewater treatment plant can be imagined (Beck *et al*, 2009). This would be tantamount to realizing "Uncoupling [of] the Nutrient and Water Metabolisms of Cities" as called for in Box 1 of Chapter 2.1 and, once uncoupled, of then seeking to lower their respective rates of metabolism.

While this perfect fertilizer scenario is but *one* candidate path away from unsustainability, a number of conjectured benefits might flow therefrom, including, for instance:

(i) The product of a perfect fertilizer would generally be destined for direct return from the wastewater treatment plant to the agricultural sector, just as the city of Paris achieved through other means 150 years ago (Barles, 2007). From this should derive the benefit of rectifying some of the distortions wrought by the city in the pre-city global cycling of materials (nutrients, N and P, in particular) and exacerbated (arguably) by the advent of the water-based paradigm of the nutrient-return infrastructure of the 20th Century (see Box 7).

(ii) Given intelligence and (metaphorical) deftness of movement, i.e., the enhanced authority of real-time operational control arising from such re-engineering of the built environment (and ***Challenge # 9***), cities could from time to time re-allocate the recovered fertilizer product as nutrient supplements discharged to the river. The goal would thus be to contribute positively to the ecosystem services provided by the watershed's aquatic environment.

Our metaphor of "sentient beings within their environments" may now have been pushed to breaking-point.

Nevertheless, in conjecturing upon these beneficial consequences, what kinds of Environmental Observatories, and what kinds of models, would best assist in evaluating their conception and their promise? How should we design and operate an EO to gauge progress in compensating for the kinks induced by man and the built environment in the global cycling of materials, or to corrobate/refute the hypothesis that nutrient supplements delivered from the city are of benefit for the watershed's ecosystem, and therefore its service providers?

Observing The Big Picture

Gauging sustainability of the built environment, with its rich heterogeneity of disciplines and scales of enquiry, does not fall neatly across the three axes of the "data cube" of Figure 1. A sense of this can be obtained by examining each axis in turn, using the perfect fertilizer scenario as an anchoring device.

BOX 7

Sustainability, the Nitrogen Cycle, and Models

Consider the global N cycle (Galloway *et al*, 2003; Boyer *et al*, 2006) and place conceptually within it the metabolism of the city, connected to its surrounding watershed. To deal, on the one hand, with the deleterious consequences for the aquatic environment of employing water-based conveyance in removing from the city the metabolic residuals of its "daily bread", great effort and cost are invested in accelerated biological nitrification and denitrification of sewage during wastewater treatment. On the downside of the city, therefore, N is deliberately shunted into the atmosphere — in order to avoid historic problems of water pollution — whence it must then, also with great effort and cost, be fixed through the Haber-Bosch process for incorporation back into the production of artificial fertilizer, for application to the land, on the upside of the city. Roughly two-thirds of the N "removed" in this manner from urban wastewater during treatment, across the whole of Finland, is vented as gaseous emissions to the atmosphere (Sokka *et al*, 2004). This does not seem a sympathetic way of organizing the metabolism of the city and its compensatory wastewater infrastructure; of enabling the city to sit more comfortably within its surrounding environment and the web of global material cycles in which its metabolism participates (Beck, 2005a).

Challenge # 11 asks how, in the great sustainability debate, can studies of the metabolism of urban, built environments be better aligned with those of global biogeochemical material cycles and ecosystem restoration — and the restoration of natural capital and the ecosystem services derived therefrom. Taking the N cycle as exemplary, we review here three case studies at the watershed scale in how models might have been used to respond to this question, had it been asked of them. Our goal is to reveal the anatomy of each study according to: the features of the watershed; the nature of the models employed; and the policy actions related to matters of infrastructure, in particular. In conclusion, we shall revisit the metaphor of "sentient beings in their environments".

River Kennet, Thames, UK

The Kennet is a sub-watershed of the Thames, upstream of London, in the UK (and the subject of earlier discussion of scenario analysis in Box 6; Wilby *et al*, 2006). Annual and seasonal temperature and precipitation scenarios for 1960-2100, downscaled from three GCMs, each themselves driven by the same pair of IPCC emission scenarios (as noted in Box 6), are provided as inputs to a watershed hydrological model coupled to a water quality model, in order to generate six trajectories of in-stream concentrations of ammonium-N and nitrate-N over this 140-year span of time.

In essence, the sub-watershed is treated as an agricultural ecosystem. Although occupied in places by urban communities, no options for changes of infrastructure are considered (for this was not the purpose of the assessment). The metabolisms of the conurbations are not even traceable through the customary, time-invariant point-source discharges from their associated wastewater treatment plants.

BOX 7

Mississippi, USA

The Mississippi watershed needs no further geographical referencing (Mitsch *et al*, 2001). Observations of the areal extent of hypoxia (low levels of dissolved oxygen) in the Gulf of Mexico show an upward trend across the decade of the 1990s, a trend mirrored variously in: (i) the in-stream concentration of nitrate-N near the outlet of the watershed, from 1945 through the late 1990s; (ii) the estimated annual mass of N fertilizer applied to the watershed from 1955 to 1995; and (iii) the areal extent of (engineered) land drainage in the watershed from 1900 onwards. No model (***M***) is mentioned, for none was a part of the assessment.

As for the Kennet, the watershed can be viewed predominantly as an agricultural ecosystem. The single most important goal of watershed management is to promote denitrification wherever possible, i.e., the venting of gaseous N species to the atmosphere. This is to be realized through the preferred options of riparian buffer strips and, more so, wetlands, for changing both the rural (primarily) and urban (much less so) wastewater infrastructures. Whereas we have sought in this *White Paper* to push ecology into the image of the highly engineered city (the metaphor of the "large animal grazing in its pasture"), so here installing wetlands and buffer strips to compensate for the ills of agricultural activities (in the Mississippi) is tantamount to the reverse concept: of pushing the engineering of infrastructures out from the city into the companion vision of the highly managed rural landscape (similar exchanges of perspective are evident in Box 8).

Seine, France

The city of Paris dominates the Seine watershed, whose estuary discharges into the English Channel, off the northern coast of France (Billen *et al*, 2007a). An integrated set of four models is central to the assessment (Even *et al*, 2007a). It comprises (i) the watershed upstream of Paris, (ii) the watershed downstream of Paris, (iii) the Seine estuary, and (iv) the Seine Bight, a coastal portion of the English Channel (Figure B7.1). It is gathered around a consistent, core representation of the biogeochemistry of N, P, and Si (Even *et al*, 2007a) and inspired by the nutrient spiraling concept of Newbold *et al* (1981) and Elwood *et al* (1983). It is also the most complete account of the non-atmospheric portions of fluxes within the given global biogeochemical material cycles. Three annual hydrological sequences (wet, mean, dry) form the basis of a reconstruction of this biogeochemistry, for retrospective analyses of the entire watershed from a pristine era (pre-1000) through the 1500s and from 1850 through the present, and on to prospective behavior up to 2015, when the European Union Water Framework Directive will require waters in watersheds to have achieved a "good ecological status" (Billen *et al*, 2007b). Through an exercise in model structure identification typical of our ***Challenge # 7***, water quality downstream of Paris cannot be made to match observations without accounting for the effects of combined sewer overflows from Paris in the lower watershed model (Even *et al*, 2007b).

An especially illuminating historical analysis of the N-metabolism of Paris over the period 1801-1914, and the best account to hand of the dynamics of gross urban metabolism, reveals the following: that of this daily bread, as we have called it, one quarter was required for powering transport (by horse); that the residuals of the metabolism were returned to the land as (solid or liquid) fertilizer to support the production of food for the city; and that the introduction of "British-style" water-based, flushing toilets brought about the downfall of the previous fertilizer-focused infrastructure, which included “urine separating toilets”, presumably of a non-flushed, dry variety (Barles, 2007). In the suite of four models, metabolism of the entire current population of greater Paris (10,000,000 people) and the water/wastewater infrastructure to which it is connected, is approximated as the resultant, time-invariant concentrations of the pollutants (nutrients, even resources) in the effluent fluxes discharged from a handful of wastewater treatment plants.

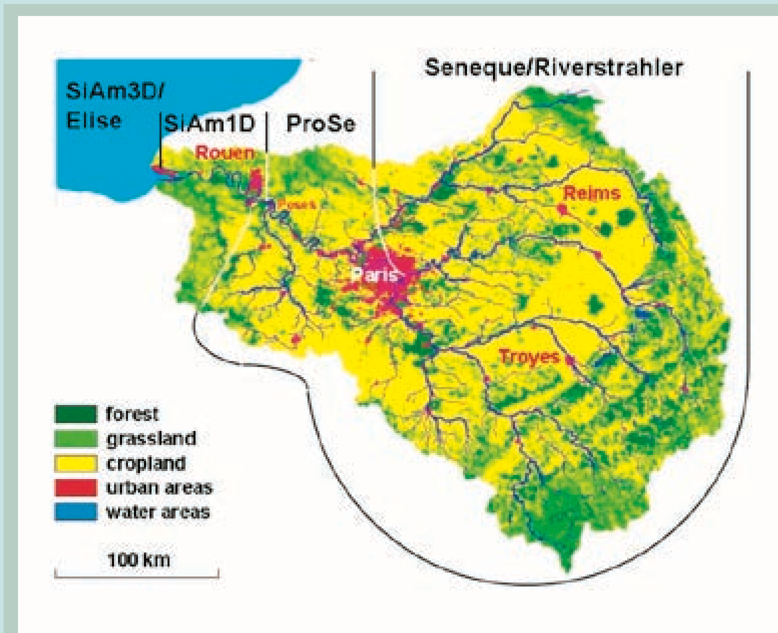


Figure B7.1
Geographical delineation of the suite of four models used in the case study of the Seine watershed in France and its accompanying coastal zone. Reprinted with permission from Even *et al* (2007a).

Viewing the watershed as an ecosystem, today’s spatial distribution of terrestrial autotrophic production and heterotrophic consumption shows the watershed as a surface with predominantly higher photosynthesis (P) than respiration (R), except for Paris, conspicuous through its P/R ratio descending to below 0.1 (Billen *et al*, 2007a). Future implementation of infrastructure options for metropolitan Paris, including *inter alia* wastewater treatment through biological nitrification-denitrification, is expected both to curb the occurrence of harmful algal blooms (HABs) and to return coastal marine primary production in the Seine Bight to a state of being P-controlled by 2015, as previously during the watershed’s earlier biogeochemical history of the traditional cottage economy of the 1200s through the 1700s (Billen *et al*, 2007b).

Synthesis: State-of-the-art Models

Our first conclusion is this. All three case studies are striking in their attainment of the “big picture”, conspicuously in respect of the time dimension, which is so distinctive of the idea of sustainability and its long view.

Second, and without exception, as far as we can tell, models of the watershed reduce description of the behavior of the entire city-water infrastructure couple to but a single vector of constants characterizing the point-source discharge to the river (as in Billen *et al*, 2007a). No feature of the city-infrastructure couple merits an account as a variable with a differential equation of state. On the other hand, the scope of current models of the urban wastewater infrastructure (sewer network and wastewater treatment plant) barely penetrates into the watershed, extending but a short distance down the receiving stream from the point-source discharge (Schütze *et al*, 2002; Vanrolleghem *et al*, 2005). The two, models of watersheds and models of wastewater infrastructure, are thus the unintended, perfect complements of each other. The latter also tend never to be coupled either to the potable water treatment and distribution network on the upside of cities or to the groundwater systems below them.

Technologies and Future Scenarios

While now not quite as novel as one might have thought, the single, simple technological device of the urine-separating toilet could short-circuit the onerous atmospheric diversion of N — in the big picture — as it cycles around the city's metabolism, at least in principle. For it would have to be socially legitimate, literally at an intensely personal, local scale in the individual household. And in the longer-term, extrapolating over the generations towards a vision of a drier, if not dry, metropolitan sanitation infrastructure, some deft technological capabilities (of real-time process control; Achleitner *et al*, 2007) might well be needed to navigate through a risk-prone phase of newly re-plumbed households and offices coupled to the current city-wide sewer network (Beck, 2005a; Larsen and Gujer, 1996; Borsuk *et al*, 2008).

The challenge in prospect is this. Once households are fitted with storage tanks for the separated urine, that material must be removed in a timely manner and transported to a place of treatment, for the eventual production of fertilizer. If the place of treatment is that of the customary end-of-pipe, centralized, municipal wastewater treatment plant; and if the "pipe" to be used for conveyance is a sewer network subject to precipitation-related flow variations with associated emergency overflows to the receiving water body; then the entire infrastructure — during this intermediate phase (say 5-20 years into the future) — will become highly vulnerable to fast, transient events of inadvertent releases of ammonium-rich liquors to the surrounding aquatic environment (Beck, 2005a; Larsen and Gujer, 1996; Lienert and Larsen, 2006).

Several stages for this scenario into the future can be imagined, all using the "business-as-usual" paradigm of cities of the Global North as both a point of departure and as a reference trajectory. These stages comprise: (i) installation of urine-separating toilets and storage cisterns in households and places of work, together with their associated re-plumbing and automation; (ii) operation of (i) for the purposes of producing a "designer sewage" flux leaving the existing combined sewer network and entering the centralized wastewater treatment plant, for improved performance there, albeit with N species regarded as pollutants of which to be rid (as in Achleitner *et al*, 2007); (iii) a possible re-orientation of stage (ii) wherein the N species are recovered as resources through re-arrangements of side-stream processes at the plant; (iv) installation at the plant of a dedicated nutrient recovery sub-system, with optimization of operating arrangements for (i) so as to maximize conveyance of urine-concentrated sewage to the plant — the risk-prone, "adolescent" phase colloquially referred to as real-time control of the "yellow wave" (Larsen and Gujer, 1996); and (v) installation of a second pipe network within today's combined sewer system for dedicated transfer of the urine concentrate from households to the dedicated nutrient recovery sub-system at the treatment plant.

To close, let us recall the metaphor of sentient beings in their environments, introduced in Chapter 4.2 by way of motivating ***Challenge # 11***. Suppose there were to be a city, such as Paris might become in the long view, deemed a sustainable "bull" in the sense of "shod with padded athletic trainers" and

BOX 7

“in possession of the technological deftness” required to intervene as a force for good in respect of the Seine’s ecosystem services, i.e., fit for “expanding the china shop’s operations” (Beck *et al*, 2009; also Box 8). Could or should such a city be developed deliberately in the watersheds of either the Kennet or the Mississippi, to compensate there for the loss of ecosystem services and the distortions of global material cycles as a consequence of their being (perceived as) essentially intensively managed, agricultural ecosystems (Hobbs *et al*, 2006) or rural-crops ecosystems (Kaye *et al*, 2006)? And to what extent is the platform of the suite of models (***M***) for the Seine-Paris system (Figure B7.1) appropriately oriented as a point of departure in responding to such a question?

Space

If we are to understand something about distortions in the cycling of nutrients, it will be necessary to track the movement of foodstuffs into the city (as opposed to water influxes) and to track the fate of the nutrients thereafter. If dry sanitation is to be the core principle in designing the urban nutrient-return infrastructure, the customary measurement of chemical species in water fluxes will doubly not suffice. Observing the city's nutrient metabolism cannot readily be cast into the mold of conventional measurement strategies for the aquatic environment.

Any EO turned thus to observing the big picture, of sustainability of the built environment, is self-evidently going to have to cover a dramatic span of scales along this dimension of space, without dropping the many significant scales at which the issue manifests itself, hence to focus solely on observing at either the global or the local scale. Box 1 reveals that span and the need to sample at many points along it: from the global trading of virtual water in the composition of the city's incoming foodstuffs (Allan, 2003; SIWI-IWMI, 2004); and the accompanying global movement of nutrients from soils in producer-export countries to coastal environments downstream of cities in consumer-import countries (Grote *et al*, 2005); across the prospect of urban growth in coastal zones fueled by membrane and desalination technology, with then the potentially distorting consequences of yet further enhanced eutrophication for marine ecosystems (Jackson *et al*, 2001); through the built infrastructure of water storage and diversion schemes, and their undermining of our capacity for managing watersheds as ecosystems (Poff *et al*, 2003; Arthington *et al*, 2006); and down to exercising control in real-time over the flushing of a myriad household toilets — at the local (and very personal) scale — in order to "re-design" the urban crude sewage flux for improved performance in a centralized wastewater treatment system (Achleitner *et al*, 2007).

Time

The Brundtland definition of sustainability, paraphrased as the following exhortation, is nothing if it is not about the long view:

> "Doing well now by the biosphere and the stock of natural capital and flow of services therefrom implies doing at least as well generations hence."

Adopting such a long view, however, is not to turn a blind eye to higher-frequency variations over hours, if not minutes and less. Measuring the "fast" cannot necessarily be sacrificed in favor of the "slow", any more than local observations might be sacrificed in favor of global observations (or *vice versa*) along the spatial dimension.

Introduction of the technological device of a urine-separating toilet — as part of a path towards fertilizer recovery — anticipates a years-long, if not decades-long, risk-prone phase in its imagined life-cycle (in Box 7). Having to control risky short-term behavior, over minutes and hours, may be a necessary precursor to achieving the eventual maturity of an infrastructure imagined currently as less unsustainable than today's arrangements. In not yielding to the common temptation to sacrifice the high-frequency detail in favor of an exclusive low-frequency focus, there will be sufficient heterogeneity of significant temporal variability to qualify the problem as fully subject to a tyranny of scales (NSF, 2006), every bit as much as in the spatial domain.

Indeed, we should be reminded of a well known saying: "for want of a nail a kingdom was lost" — as was the former symbiosis lost between nineteenth-century Paris and the Seine watershed with the introduction of the familiar WC (Barles, 2007; Box 7). Conversely, installing today the urine-separating toilet may become "the nail, given which a kingdom might be gained", with all of the cross-scale ramifications thus implied.

Biogeochemistry

Expression of the data cube of Figure 1 obliged us to think there (in Chapter 2.1) of sampling, sensors, and instrumentation ranging from very small biogeochemical targets to the very large, and to conceive of the intensity of consistent sampling in space-time of the species/individuals within that (bounded) biogeochemical range. Presently, and arguably (in the context of the sustainability of the built environment), observation of the minutiae of chemical species may suffice, together with — after some gap in sampling along the biogeochemical continuum — just the behavior of the human species moving about the built environment.

At the heart of the issue of re-engineering the city's nutrient-return infrastructure reside (at least) two personal and intimate matters of human agency: dietary needs and preferences; and the willingness to adopt one technology over another (as in re-plumbing the household for a urine-separating device, for example). A tyranny of scales may not reign here over sampling and observation in the biogeochemical dimension. But some other form of distorting power might (as we shall now argue).

People in the Picture; Agents in the Model

The Seine-Paris case study of Box 7 is indeed impressively complete in so many respects. Yet it is flawed by one omission of profound importance to using models (***M***) in exploring ways of moving towards greater sustainability of the built environment.

The vast and intense social and economic activities of 10,000,000 agents — people, that is, behaving as consumers, citizens, enfranchised stakeholders, adopters of technologies (urine-separating toilets, notably), holding a plurality of cultural perspectives on sustainability, having a growing interest in man's relationship with the environment, perhaps even contemplating Gibbons' (1999) suggestion of Science being in need of a new contract with Society — are compressed into but a single, inanimate vector of time-invariant boundary conditions of the watershed model. All this is compressed down to a point, as in a point-source discharge of treated wastewater.

The following words may only have been spoken in jest, but they make their point too: "Wastewater treatment plants would work well enough, if only people would eat salads in winter and goulash in summer" (Watts, 1993). Therein lies the unmistakable element of human agency in the urban landscape: choice over diet. That goes well beyond the concept of creating a "designer sewage" explored in Achleitner *et al* (2007), who take agency largely out of the hands of citizens, vesting it instead in an automated system of household storage-tank releases.

Why have we remained blind, almost wilfully so, to individual and collective human agency in the urban, built environment?

For we recognize — and must always (self-evidently) have known — that the river network is defined by the geographical and topographical features of the watershed, hence the movement of water above and below the land surface; that there are people, animals, plants, and vegetation on this surface; and that all the metabolism on, and attributes of, the surface cause materials (many considered, for a time, as pollutants) to be deposited on it and moved across it by precipitation-induced fluxes of water. Similarly, we can recognize that through the society and economy in which they participate, *people* cause degradation of water quality, *not* the inanimate "population equivalent" of engineering analysis, or the somehow "people-divorced" wastewater treatment plant of the local, municipal government, which entity itself may often be accused of "dumping" sewage into the environment.

This sense of detachment of the person from the problem, which is marked in the urban environment, cannot obtain so readily in the rural environment. There, individual farmers are unmistakably responsible for the distribution and manipulation of the behavior of plant and animal communities over the land surface (and thus the degradation, or improvement, of water quality).

People too participate much more than previously — in living memory — in *their* aquatic environment, partly because of the growing awareness of man's impact on the environment and the successful restoration of improved surface water quality (devoid, on average, in some places, of significant contamination from the social and economic metabolism of the city, as in prospect for the Seine by 2015). It is they, the people, and their domestic pets, who contract illnesses from contact with the water. It is they who are disadvantaged if the sport fishery, restored through a more complete wastewater infrastructure and thus healthier ecosystem in the lake or river, is threatened in the short-term by a treatment plant failure or in the long-term by climate change, or whatever (Beck, 2005a).

Accounting formally in a model ***M*** for human agency in the built, urban environment is just as important as in the rural/agricultural environment, if not much more so. Huge quantities of water and nutrients may be pushed through the rural systems of agriculture and livestock production. Increasingly, however, personal preferences and market signals as to what should be produced in those systems, if not how this daily bread is produced, will emanate from urban communities (SIWI-IWMI, 2004). In that sense, the social and economic activities of cities are primary drivers of the movement of materials around the globe.

A kind of hegemony — if not tyranny — of intellectual effort devoted to the theoretical (and computational) frameworks of rural landscapes/actors seems to have been exercised over that given to their urban counterparts.

In Box 6 (Chapter 4.1) we saw how Janssen and Carpenter (1999) had populated their simulated *rural/agricultural* landscape and its simulated drainage to a simulated eutrophy-prone lake, with computational agents (as simulated farmers). The same landscape was likewise the focus of the individual-based models and cyber-infrastructure of Hawes and Reed (2006). Shifting away from the pole of these "rural forest/crops" ecosystems and along the continuum of ecosystems types of Kaye *et al* (2006),[34] agent-based models are finding ever wider application in the contemporary discussion of sustainable management of water resources (Hare *et al*, 2006; Giupponi *et al*, 2006; see also Hare and Deadman, 2004). These address principally matters of utilizing infrastructure for conveying water around the various landscapes to furnish the agents — be they trees, crops, livestock, or humans, even urban citizens (Tillman *et al*, 2001) — with their daily water intake. Castelletti and Soncini-Sessa (2006, 2007) seem almost to celebrate the push towards greater participation of scientifically lay stakeholders, as if paradoxically to revitalize the application of formal, mathematical optimization in water resource systems analysis.

Further along the continuum, at the instance of a suburban "residential" ecosystem, a different kind of socially sensitive modeling, "participatory modeling", has attracted attention. Built within the STELLA™ software framework (Brown Gaddis *et al*, 2007), its purpose is to assist stakeholders at the urban-rural interface in managing nitrogen migration through the Solomons Harbor watershed, Chesapeake Bay, Maryland. Excessive amounts of reactive N-species arise there from the diffuse, nonpoint sources of household septic tanks and from residential agents applying artificial fertilizer to yards and gardens — in effect, bringing us back to the same problem context surrounding the farming agents of Janssen and Carpenter (1999).

[34] In enquiring whether there is "*A Distinct Urban Biogeochemistry?*", Kaye *et al* (2006) propose a continuum of ecosystem types: "urban core" and "rural-forest" bound its extremes, with "urban residential" and "rural-crops" as internal sampling points. Hobbs *et al* (2006) posit an alternative spectrum, or continuum. Theirs ranges from the "wild" (or natural/semi-natural) across to the "intensively managed" (agricultural), with "novel ecosystems" arising somewhere between these two poles — as a result of invasion, degradation, or abandonment. The reader, however, is left to presume that the "urban core" and "residential" ecosystems must lie off their scale, beyond the "intensively managed".

Moving on from the "residential", hence to end up at the urban/built ("urban core") pole of their continuum of ecosystems, Kaye *et al* (2006) have composed a diagram redolent of the icon-based interface of the STELLA™ software platform (Isee Systems Inc, Lebanon, New Hampshire), with controls on cause-effect relationships denoted by stick-figure humans. They make no further progress, however, beyond this conceptual recognition of human agency, towards formal model computations. Instead, they proceed to recommend three areas for future urban biogeochemical research, two of which concern:

> [H]ybrid engineering-ecology models ... linked to the energy and material demands generated by human demographic trends and household actions ...
>
> [M]odels that link demographics, diets and waste.

while the third (consideration of household-scale actions) concludes (Kaye *et al*, 2006):

> [W]e are unlikely to generate accurate predictive models of urban biogeochemistry without incorporating the actions that people take in managing their landscapes and households, and we are unlikely to be able to predict those actions without understanding their variation as a result of culture, attitudes, and socioeconomic setting.

They give us thus a foretaste of how — under the Environmental Observatories — we might respond to the challenges in pursuing the long view of sustainability of the built environment, whence ***Challenge # 11*** derives.

Technological Diversity and Ecological Resilience

To summarize, we have models for all manner of human agency in respect of harvesting from the landscape the intakes of daily bread and daily water fueling the city's metabolism, but yet not in respect of what is required to assimilate the residuals of this metabolism back into the city's environment. And it is human agency in this latter, as in choices over the adoption of one household technology over another, that will be key in moving towards greater sustainability of the built environment.

Does this lacuna arise because there is something rightly too intimate and personal about the choices we make over "diets and waste", as Kaye *et al* (2006) call them?

Perhaps not, for contrary to the widespread sense of our coming to a kind of historical closure in environmental engineering, typical of which is this from Brown Gaddis *et al* (2007),

> Remaining point sources of pollution are related to monetary and regulatory problems rather than technology shortfalls.

we stand instead on the threshold of potentially radically different ways of conceiving of the technologies of metropolitan water infrastructure, spurred on precisely by the sustainability debate. The customary "water-centric" view of the built environment of the city, wherein pollutants are to be removed from water in the wastewater infrastructure, has a complement: a nutrient-focused perspective, under which water is instead to be removed from the resources of nutrients (and other energy-carriers). Some of the principles for such re-thinking of the city's built environment are adumbrated in McDonough and Braungart (2002).

To conceive then of things in the round — to be confronted with computational assessment of a single, constituent, technical innovation (a novel membrane technology for chemical-species separation, for example) in respect of its long-term, inter-generational sustainability, within an entire infrastructure of a city, whose metabolism should be gauged for its impact on the web of literally global material cycles in which it is suspended — is an engineering challenge in its own right. It is one entirely consistent with the recommendations from the NSF's (2006) blue-ribbon committee on Simulation-Based Engineering Science (SBES). When such an enormous intellectual gap must be spanned — between the urgent pragmatism of today's municipal engineering (of the unattractive but essential services we would rather take for granted) and the radically different, imagined alternatives several generations hence in the future — grounding the debate in the quantitative analyses of environmental models ($\boldsymbol{M}$), including the computational virtual realities of SBES, will be indispensable.

For how else might we puzzle out the system-wide implications of constituent, technological innovation T_i within the host of other technological components of which entire infrastructures are comprised, i.e., $i = 1, 2, ..., m$, where m is large? How critical is the presence of some other technology (T_j) in the infrastructure for T_i to be a success? How else should we make even vaguely convincing the distant visions of the target "end-points" (E_k) of infrastructure re-engineering, with $k = 1, 2, ..., n$, and allowing these as necessary to be several, not singular, in line with the plurality of a community's aspirations for the future? Which immediate candidate innovations (T_i) might be key — under gross uncertainty — in enabling paths of transition away from today's *status quo* towards any, if not all, of the socially legitimate, inter-generational aspirations E_k? Through what framework of adaptive community (social) learning might quantitative assessment ($\boldsymbol{M}$) of the choices over T_i bestow {social legitimacy} on the paths of transition? Or how should we gauge progress away from unsustainability without the simulated means to approximate the behavior of the pre-existing natural capital, ecosystem services, and biogeochemical fluxes of the watershed prior to arrival of the city (in geological time)?[35]

When ***Challenge # 4*** was composed, on universal science issues of a biological nature, our discussion traversed an arc scaling up from the smallest of cellular details to an earth systems perspective and then back down to behavior within the cell (in Chapter 2.4). Facets of the same great expanse of heterogeneous scales of consideration have already re-surfaced in our brief examination of how the EOs might be turned towards observing the big picture, with people emphatically included therein. Now, in furthering responses to ***Challenge # 11***, with its call for a "better strategic alignment of urban metabolism with that of ecosystem services", the questions just posed — in respect of developing models for imagining and assessing the technological composition of the built environment — likewise fall unavoidably and untidily across a variety of scales of analysis, as related in Box 8.

The beginnings of possible answers to some of these questions raise other questions, not surprisingly, about the lines of responses to other facets of ***Challenge # 11***. In Box 8 we enquire in passing whether there might not be a "material-minimal" sequence of technological innovations, for example, implying that this would be more environmentally benign. ***Challenge # 11*** itself deliberately begged the rhetorical question: should it not be the case that Information and Communications Technologies (ICT), the essence of an environmental cyber-infrastructure, *are* more environmentally benign than other forms of technological innovations?

Motivated by ***Challenge # 9*** (of science and engineering in "real time") at least two schools of thought on the options are possible. Consider a scale of infrastructure

[35] All questions motivating the computational analyses in Beck *et al* (2009).

BOX 8

Scale-dependent Technology Assessment, Models, and Sustainability

Challenge # 11 asks "what kinds of models should be developed in order to promote a better strategic alignment of the study of urban metabolism with that of ecosystem services, all within the web of global biogeochemical cycles"?

Technically lay citizens make decisions about what technological apparatus deserves space in their households; municipalities and utilities must assess which technological innovations offer benefits on a system-wide basis, shunning the temptation to optimize the part, while pessimizing the whole; watershed authorities might eventually wish to evaluate innovation T_i as a net contributor to enhancing ecosystem services; while some other actor in a future institutional pattern of global governance could require assessment of T_i for its restitution of the pre-industrial global cycling of nitrogen.

In this Box, we examine what kinds of models and computational analyses could support responses to ***Challenge # 11*** along these lines. They must clearly recognize the predominant feature of scale, as well as the significance of cross-scale interactions. No amount of household re-plumbing could deliver benefits at the watershed scale without commensurate actions by municipalities, as we shall see.

Household

Within the long view of sustainability, there are those who argue that the General Agreement on Trade and Services (GATS) can only but add to the increasing role of private-sector actors in the provision of water infrastructure (Mondello, 2006). Others assert that good governance must flow from the involvement and essential leadership of public-sector actors (Hooper, 2006), while yet others note the significance of civil-society (non-governmental) actors, especially in respect of rural irrigation infrastructure (Mostert, 2006).[1] The three sets of actors have differing attitudes towards risk, fundamentally different outlooks on the Man-Environment relationship, and just as different a set of views on the economies (and dis-economies) of various scales of industrial production — hence different preferences on the nature of technological innovations each would adopt (Schwarz and Thompson, 1990; Thompson, 2004). Different public debates amongst the three typologies (Kwame, 2007), determining different outcomes of infrastructure development, will be engaged at the level of the household, the neighborhood, city district, the city, the watershed, and across and amongst these various levels. Society's aspirations E_j are scale-dependent, we should therefore suppose (IWA, 2007).

What Janssen and Carpenter (1999) achieved in applying agent-based models for studying the evolution of ecological resilience over the (very) long-term in coupled farmer-rural landscapes would be one point of departure into the present domain of examining, say, socially robust paths, patterns, and possibilities of metropolitan water infrastructure. There might even be elements of fashion (a "herd instinct") in the adoption of household technologies and appliances; and the model might be charged with exploring when mass change should/should not be induced or promoted, how exactly, and whether this is ethical.

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[1] There is historical evidence, nonetheless, of such cultures and traditions of rural water governance being introduced into the urban setting through the rural-to-urban migration of people and communities (Barraqué *et al*, 2006).

BOX 8

Local (city)

Assuming such sweeping, collective choices were to occur at the level of many households, enabling thus strategic, macroscopic innovation (T_i), of "separation at source" of the residual fluxes of the city's metabolism, we know that the conventional unit-process models of infrastructure simulation (Vanrolleghem *et al*, 2005) can be used to assess the system-wide implications of that innovation. So too can the caricature of the mathematical program in the introduction to this last technical ***Challenge*** (for instance, Tsai *et al*, 2004). Assessment could be referenced to the pejorative "end-of-the-pipe", or to locations within the watershed, but would require new criteria of assessment, even for the relatively straightforward bottom line of {environmental benignity}, as foreshadowed in Beck (2005a). Measuring progress towards the pristine spectrum of temporal disturbances of the watershed, which gave rise to the ecological assemblies, their dynamic resilience, and their portfolio of ecosystem services as found prior to the arrival of the city, would be subject to the now famous tyranny of scales recalled, yet again, above. Less immediately obvious is how any model might be constructed and applied in order to chart future paths of transition intended to serve the current paradigm of treating nutrients in wastewater as pollutants of which simply to be rid, if it turns out to be a conceptual *cul-de-sac*. How today should we plan to adapt contemporary engineering and technological upgrades, if they can already be discerned as potential "retrogrades" under an alternative, complementary paradigm where these nutrient fluxes are regarded as resources to be recovered? Is there a cost- and material-minimal sequence of initial adaptations that maximizes flexibility in subsequent adaptations driven by such a possible sea-change in outlook?

Regional (watershed)

Conservation and restoration ecologists, in concert with ecological economists, have elevated our thinking on sustainability to the heights of the grand economic and ecological notions of natural capital and ecosystem services (Aronson *et al*, 2006; Farley and Daly, 2006; Kremen, 2005). What form of model, under what EO operating protocol, could be tasked with computing how much natural capital and ecosystem services could be restored in the watershed (and beyond) by incorporating constituent technology T_i into the city's water infrastructure?

More specifically, how exactly might the classical technology of the activated sludge process of wastewater treatment be re-engineered (innovation T_i) so as to serve better this much broader objective? The question ranks as but the "smallness" of a footnote to Kremen's (2005) tabulation of the "largeness" of global ecosystem services classified according to the Millennium Ecosystem Assessment (Carpenter and Folke, 2006). And in that sense "thinking globally, acting locally" is epitomized — and the sweeping traversal across scales from ***Challenge # 4*** echoed, in its call for research on universal science issues of a biological nature (Chapter 2.4). Few ecosystems can be readily experimented with in the interests of advancing the *science* of Ecology. The microbial ecosystem of the activated sludge process is a salient exception, precisely because of its *engineered* form. Cited for this purpose by Kremen (2005), Graham and Smith (2004) promote the idea of "designed ecosystem services". Moreover, they look to the development and application of models (***M***) as the means to articulate and realize this idea (Saikaly and Oerther, 2004), rekindling the youthful exuberance, as it were, of systems ecology in the 1960s and 1970s, which had briefly penetrated environmental engineering (Curds, 1973a,b).

BOX 8

Just as the trading of permits between urban and rural actors is facilitated at the watershed scale, in the interests of reducing pollution of the aquatic environment through the discharge of nutrient fluxes as wastes, so too can the intermingling of technological innovations in the water, agricultural, and energy sectors be facilitated — at the watershed scale. Diffuse, nutrient-rich runoff from the spreading on pasture land of litter from intensive poultry production can be substituted by the recovery of a biofuel and a fertilizer. What kind of model and EO functions would be needed to further this kind of possibility and to assess its implications for the restoration of ecosystem services?

Global

Without courting the intellectual paralysis of the systems analyst,[2] we know that developments in all economic sectors are inter-related, in particular, in the water, energy, and agriculture sectors. We know too that in the late 20th Century industrial, anthropogenic N fixation from the atmosphere overtook natural terrestrial N fixation (Galloway and Cowling, 2002; Galloway *et al*, 2004); that Man's predominant appropriation of nutrients and water is in producing foodstuffs (and fiber) in the rural-agricultural domain; and that only 14% and 4% of the N applied to the land as fertilizer reaches our mouths in our daily bread, as a function of whether or not, respectively, we are vegetarian; but that soon the majority of the world's population will be urban dwellers; that it is in the cities where dietary choices may have the greatest scope for change; that the making of these choices will send increasingly clear signals to farmers in the rural surrounds and hinterlands of cities, as to what kinds of food the market desires to be produced (SIWI-IWMI, 2004); and that — beyond human choice over diet — historic changes in the technologies of urban water infrastructure, in particular, in respect of handling the biological residuals of the city's metabolism of its daily bread, can have an important impact on the paths by which nutrients and other materials cycle around the globe (Barles, 2007; Sokka *et al*, 2004; see also Box 7).

Skirting around the issue of whether personal diets can and should be adapted in the interests of lessening the unsustainability of the built environment, we put this question: what kind of model could be constructed for assessing which technological innovations (T_i), and which paths towards alternative future metropolitan water infrastructures, might lower the global nutrient (and water) metabolism, i.e., uncouple human and economic development from industrial N fixation, and all under the prospect of global climate change? Such questions are studied formally with models in the energy sector, in respect of strategies for mitigating climate change (Lempert, 2002). Why should this not be the case in the sectors central to this *White Paper*? Why also, to mirror the interchange of rural (ecological) and urban (engineering, infrastructure) perspectives noted in Box 7, should not agricultural-, chemical-, and energy-sector businesses begin to look more favorably and aggressively on resource recovery from the urban wastewater infrastructure (and its hitherto predominantly water-centric commerce)?

[2] Who recognizes that all things are related to each other, but analysis of their interactions is intractable, since every thing seems equally essential to everything else, leaving thus undecided what should be left out in composing the model (***M***).

reconstruction varying between 0% and 100%. To exaggerate, let it now be bounded at the two extremes by: (i) a 0% strategy, in which not one brick of the urban water infrastructure is therefore removed, except for inserting the small boxes housing instrumentation and real-time control devices — the essence of "intelligence" and "deftness of movement" enabling the city to act as a force for good in the environment; and (ii) a 100% strategy, in which everything is demolished — including the vast hull of the sunk historical investment in plumbing, pipe networks, channels, tanks, and so forth — as the prelude to building completely anew.

Elaborated thus, there might well be a *prima facie* case for asserting that the "hard path" of a 100% reconstruction strategy (changing the structure) should suffer from a large ecological/carbon footprint arising from the movement, if not the recycling, of so much material. In contrast, the "soft path" of the 0% strategy — the ICT path, of changing the function of the infrastructure — ought not to be so disadvantaged.[36] It might not, in other words, constitute a strategy of dematerialization, but it might avoid the prospect of serious further "materialization".

It could even be argued that in its "pure" form the "0% school of thought" should seek — in the spirit of ***Challenges # 4*** and ***# 5*** — to suffuse the entire system of infrastructure with ecological resilience by applying control "externally", without indeed moving barely a brick. This, however, could arguably make the system increasingly prone to cascading failures arising from a growing reliance on precisely the kind of ICT required for effecting communication and operations from "without" (Zimmerman, 2001; Rinaldi *et al*, 2001; Little, 2002). Such vulnerability would be heightened in the face of high-frequency (fast-acting), high-amplitude threats. The soft path of the pure strategy could thus yet run the risk of coming to epitomize (again) the brittleness of Holling's engineering resilience (Holling, 1996).

There could, then, be significant merit in the alternative: of something approaching the caricature of the 100% school of thought, whereby ecological resilience is progressively designed into the structure of the system, as opposed to somehow being enacted through real-time operations from "without". We take one last glance, therefore, at our biological metaphor of the city as a sentient organism, therefore, in order to add one further extension to the construction of ***Challenge # 9***, built upon the inter-disciplinary thinking of ***Challenge # 5***, under which Holling's notion of ecological resilience was first introduced.

We know from the preamble to those earlier ***Challenges*** that ecological resilience in behavior over time is a function of the inter-play amongst relatively slowly changing (low-frequency) and relatively swiftly changing (high-frequency) components of behavior, i.e., cross-spectrum interactions (Carpenter and Folke, 2006). We are aware from the present ***Challenge # 11*** (including Box 7) that an EO turned towards observing the big picture of sustainability should not abandon observation of the fast for observation of the slow alone, or *vice versa*. We are likewise aware from Box 8 of the multiple spatial scales over which candidate technological innovations within the built environment (T_i) are active and influential. We know too from the introduction of ***Challenge # 5*** that ecological resilience has companion interpretations in respect of cross-scale interactions. To recapitulate (Peterson *et al*, 1998):

> [E]cological resilience is generated by diverse, but overlapping, function within a scale and by apparently redundant species that operate at different scales, thereby reinforcing function across scales.
>
> The combination of a diversity of ecological function at specific scales and the replication of function across a diversity of scales produces resilient ecological function.

What principles for re-designing the dynamic performance of a city's water infrastructure could we derive from these, through merely substituting the word "species" by "unit process technology" T_i (and eliding thus, one last time, the disciplinary and conceptual distinctions amongst Engineering, Ecology, and Cellular Biology)?

In the absence of some study or assessment with a model (***M***), all this will readily be recognized for what in fact it is: yet more provocative, speculative questioning. Engaging in constructive disputation amongst the differing, archetypal schools of thought on infrastructure re-engineering will not progress far or fruitfully without, for instance, charging both with the

[36] Such a "soft path" towards distant community aspirations might not only be very different from that envisaged by Gleick (2003) in his original coining of this phrase. It might also even retain the hull of the city's sunk investment of past decades and centuries in its unreconstructed (and currently much denigrated; Niemcynowicz, 1993) centralized forms of sewerage and wastewater treatment.

task of coming up with strictly comparable accounts of the sustainability or otherwise of their respective paths — of soft (→0% reconstruction) *versus* hard (→100% reconstruction). Those alternative paths must proceed from the initial conditions of today's hull of conventional centralized wastewater infrastructure and arrive at, say, the target end-point of the perfect fertilizer aspiration (E_k), generations hence. The purpose of ***Challenge # 11*** is to invite considerations of what kinds of ***M***, novel or otherwise, will be needed to buttress — to corroborate or refute — such grand conjectures.

Empirical studies of ICT innovations, in general, beyond the water sector of the built environment, indicate rather a "rebounding" effect of re-materialization (Berkhout and Hertin, 2004; but see also Kander, 2005). Even in our narrower context of the EOs, in respect of the impact of ICT, ***Challenge # 11*** remains just that: an open question as to what exactly should be the role of models (***M***) in exploring the role of the future environmental cyber-infrastructure in the de-materialization of Society.

Separating Formal Model Computations from Public Debate and Democracy

Looking back to the 19th Century, medics, clerics, lawyers, and like members of the scientifically lay public offered their opinions on what should be done about urban sewage and sewerage; and they were heeded by the engineers of the day. By the second half of the 20th Century, in the then modern age of the technocracy, it became progressively easier to presume that scientific and engineering professionals would "know best" about the interaction between the built and the natural environment and, therefore, how to manage its growing technical sophistication. Less and less attention was paid to the perceptions and insights of lay members of the public.

With the arrival of the internet, all this has changed. Technocracy and a hegemony of expert knowledge in the affairs of environmental management are yielding to a form of participatory democracy (Darier *et al*, 1999). The lay public increasingly has an independent "voice", and the wherewithal to give expression to that voice with a rising volume to an ever larger audience, through websites and blogs, for instance. Scientists and engineers are no longer perceived as utterly in command of "value-neutrality", clinically distanced somehow from the problem to be dissected on the surgeon's operating table, but instead a part of the problem (witness Hare *et al*, 2006). Some have argued that the engineering professional's struggle to maintain value-neutrality is even an impediment to progress when it comes to shifting away from unsustainability of the built environment (Davis, 2008).

On the threshold of the millennium, Gibbons (1999) used the platform of a special supplement to *Nature* to argue that Science was in need of a new contract with Society; that for two centuries Science had spoken unto Society; but that now Society was increasingly likely to speak back to Science, as it were. In keeping with this contemporary mood, the 2006/7 Grand Challenges Committee of the US National Academy of Engineering insisted on its essays being understandable, in principle, by all. Whatever were to emerge as the grand challenges for engineering in the present century, they should have been fully debated by the public at large — through a dedicated Academy website (www.engineeringchallenges.org).

In introducing our last technical ***Challenge***, we began by drawing a caricature of a mathematical program, of how to determine "optimal" courses of action enabling Society to move along a path towards greater sustainability of the built environment. The expectation was of discomfort amongst our community over the computational treatment of personal preferences when reflected in our models (***M***).

There will indeed be those kinds of environmental problems that are amenable to being addressed and resolved using quantitative methods from the traditional engineering toolkit, in which case the fine line separating this form of technical analysis from public debate and democracy might well be able to penetrate deep into the property of {social legitimacy}. In others, it will be decidedly inappropriate, with that line barely able to penetrate the property of {environmental benignity}. This tension, in where to draw the "fine line", is encapsulated in Fenner (2008), who juxtaposes the sharply opposed and succinct *desiderata* of two pre-eminent Physicists (Lord Kelvin and Einstein) on the matters of measurement and quantification. There may even be no common ground for formal agreement amongst the various groupings of stakeholders on the science underpinning projections of what constitutes "doing well" by the biosphere, let alone on the form of democracy, debate, and governance through which the "doing well" can be witnessed by most, if not "all", as about to be done.

Models and their forecasts *are* of interest to the public: through works of fiction (Crichton, 2004); through programs on future threats to our environment aired on the *National Geographic* and like television channels; and through well informed accounts of

Science prepared for a general, scientifically lay readership (Mooney, 2007). In this instance (Mooney, 2007), as we have already observed, such accounts turn out to be shaped by questions we too have identified as core issues for this *White Paper* — ***Challenges # 9*** (on philosophy) and ***# 7*** (on system identification) — yet seemingly so subtle as to be generally regarded as at the edge of the mainstream, even for scientists and engineers.

Models — expressly — matter now at the Science-Society interface. The wheel, in this sense, never quite turns full circle. The means of supporting a two-way dialog between Science and Society are vastly different today than a century or so ago. The means to envision longer-term futures, and the possible paths towards them, including through the invention, diffusion, and adoption of novel technologies, would 100 years ago have seemed inconceivable. The technologies of scientific visualization and virtual reality (amongst the destinies of environmental modeling) must themselves have seemed unimaginable. Whereas once it was the artist's sketch that was used to convey an impression of our futures — and still must be used for succinctness on the printed page (as in Carpenter and Folke, 2006) — it will increasingly be the computer-animated film, the virtual simulator chamber (Hall and O'Connell, 2007), or encounters within the context of Second Life (WATERS, 2008). Achieving {social legitimacy} has risen to the status of *primus inter pares* amongst the three bottom lines in the global search for technical solutions contributing to progress away from unsustainability.

We are already sufficiently equipped to simulate the interaction over the decades between (simulated) man and (simulated) environment. In that virtual reality, "man" can be an agent primed with the rules of one perspective on the Man-Environment relationship, from amongst a plurality of such culturally conditioned outlooks, and be primed too with the capacity to learn and adapt "his" behavior as "he" moves through time in an environment populated by other agents (Janssen and Carpenter, 1999). Movement of the simulated agent through the simulated environment over a span of time, and the insults and injuries "he" suffers from exposure to harmful substances in that environment, can also be tracked in a complex suite of software for risk assessment (TRIM.Fate; www.epa.gov./ttn/fera/trim_fate; see also Efroymson and Murphy, 2001). There is talk of building "electronic crash test dummies" (Clarke, 2004). It is not hard to imagine the "span of time" eliding into the entire life of the simulated agent, with simulated preferences over modes of transport and other matters of life-style, presumably too "his" diet therefore, with all such preferences being conditioned and negotiated within the community of other simulated agents, through the computational game theory we already know (Dieckmann and Metz, 2005; Levin, 2006; or Ohtsuki and Iwasa, 2006).

As a real stakeholder observing *your* simulated, virtual self as participant in a proposed strategy for moving away from some unsustainable pattern of behavior — for example, in restoring a suburban watershed degraded by excessive use of garden fertilizer — what would you conclude and learn from such an exercise? Would the simulation add to, or detract from, the social legitimacy accorded to the strategy? And taking the long view, as your personal (private) simulated self becomes ever more life-like, what are the ethics of exploring options for collective, public policy in this manner? How comfortable should any of us feel about this?

4.3 Community Structure

Any self-respecting exercise in assembling grand challenges from any given community of scientists, engineers, and scholars, will face the final challenge regarding that community's self-determination and self-education in responding to the scientific and technical challenges it has expressed. Our *White Paper* will be no exception. Indeed, in many ways what is being recommended in the following (in Chapter 5) reiterates what has already been recommended in the National Research Council's earlier set of "*Grand Challenges in Environmental Sciences*" (NRC, 2001). We make no apologies for being repetitious in this respect. For some of the challenges we face — in changing ourselves — are recalcitrant, universal, and the very grandest of all.

Looking thus inwards, towards our own community, we offer this cartoon of the (May, 2006) Tucson workshop:

> Speaker A, from discipline X, presents his view of future challenges in his native discipline, and with some enthusiasm and conviction. Participant B, from discipline Y, quips that he has just heard a very nice presentation, but then he wonders — aloud — where speaker A has been for the past 30 years.

This exchange happened, specifically in respect of data assimilation (herein ***Challenge # 9*** now). Its expression in the form of a cartoon preserves anonymity, not least because the very same wonderment (at one's scientific whereabouts these past three decades), could have been leveled at Participant B himself, by Participant C from Discipline Z.

Challenge # 12:

> ***What steps can the community of model-builders in the Environmental Sciences take to pre-empt and reduce to a minimum the still readily apparent scope for re-inventing the "wheels" of modeling in contemporary research across the various disciplines of the EOs? How can our community best be organized so as to benefit as much as possible from novel developments in modeling in general, as they arise in, for example, the quite disparate disciplines of the biomedical sciences, social sciences, cognitive sciences, artificial intelligence, and artificial life? More broadly, how should the community of modelers best work with the community of primary field scientists to promote the development of models for basic scientific discovery at the interfaces amongst multiple disciplines? In the light of universal and ever-more urgent calls for profound changes in the manner in which the next generation of scientists and engineers is educated, trained, and formed — all of which calls focus on "inter-disciplinarity" — what special role can models serve in meeting these needs?***

Looking across the grand Challenges expressed above, none calls as much for investments in equipment, computing, specialized field campaigns, and so on, as it does for investments in changing habits of mind. These are mind sets, in particular, of a kind of "tunnel vision", with its part unconscious, part seemingly wilful "blind spots", fully capable of giving birth to the foregoing cartoon from the Tucson Workshop. Inasmuch as not all of us have the talents for becoming an astronaut or brain surgeon, not everyone is suited to engaging fully and effectively in inter-disciplinary work, including when the object of enquiry is the development and application of models.

Turning now to peer outwards from the enclaves of modeling, those of us who consider we are modelers first and foremost should readily admit to our ignorance: we should hesitate to venture opinions on how others ought to conduct their affairs in enquiring into the nature of the biogeochemistry of aluminum speciation in forest soils or the existence and role of the microbial loop in the foodweb of an impoundment. Just about everyone, however, whether modeler or not, appears to have an opinion on how modelers should conduct their affairs, and quite strong ones at that: witness the recent book of Pilkey and Pilkey-Jarvis (2007) and the earlier observations on how modelers, as a professional solidarity, are not always held in high social esteem amongst the broader community of scientists. While we believe that computational model-building should be viewed as a free-standing discipline in its own right, our purpose herein is not perversely to promote ignorance in others, by being deliberately obscure, opaque, or obfuscating in communications across from the domain of "modeling expertise" outwards to all others (just as Schaffer (1993) has recorded of the soothsayers of old). It is to nurture humility.

PART III:

RECOMMENDATIONS & CONCLUSIONS

Chapter 5: Ways Forward

After the NRC Committee (NRC, 2001) had expressed its *Grand Challenges for Environmental Sciences* it went on to make recommendations for immediate investments in research and then to discuss issues of implementation, including "building capacity for interdisciplinary, problem-oriented research", itself the subject of another, more recent NRC report on *Facilitating Interdisciplinary Research* (NRC, 2004). We too shall be much concerned with this issue, as we now go about indicating some ways forward in response to our own grand challenges, with special reference to models as the *lingua franca* for communication across many — but not all — of the disciplinary domains upon which those challenges touch.

5.1 Models, the *Lingua Franca*, and Becoming Inter-disciplinary

Consider again, as in the introduction to this *White Paper*, the image of a model as the vessel into the holds of which the contributions from all of the relevant disciplines must be poured in a consistent and compatible manner. The systematic character of model-building, together with the discipline imposed by the formal algorithmic and mathematical logic of the models themselves, can at the least assist in eliminating daft ideas — constituent hypotheses from different disciplines that do not mesh logically together — sooner rather than later. From the demands of such consistency derives the metaphor of models affording us a *lingua franca*. And in this, it is the process (of model building) that may be as important as the product (the model), if not more so.

Assembling our *White Paper* has itself been an exercise in becoming inter-disciplinary, even a reflexive self-study. It began by introducing the simple, abstract triplet {$\boldsymbol{u}$, $\boldsymbol{M}$, $\boldsymbol{y}$}, of the observed inputs ($\boldsymbol{u}$), model ($\boldsymbol{M}$), and observed outputs ($\boldsymbol{y}$), and then setting out the attaching tasks of modeling as those of the archetypal mathematical textbook: given two out of these three unknowns, find the third. Essentially everything from there onwards can be tied back to the reference framework of this piece of elementary abstraction.

Horizontal Integration: Across and Beyond the Disciplines of the Environmental Observatories

Armed with the common language of modeling, we are better equipped to achieve "internal", horizontal integration across the disciplines of the Environmental Observatories. Thus, for example, in setting up ***Challenge # 8***, we were able to shed light on how Environmental Engineering has been largely conspicuous by its absence from the study of data assimilation, as commonly found in Hydrology and the Ocean Sciences, albeit less so in Ecology. Something of the reverse then followed. Given the triplet of {$\boldsymbol{u}$, $\boldsymbol{M}$, $\boldsymbol{y}$}, and the notational conventions flowing from it, a research agenda in response to ***Challenge # 8*** could be transcribed (in Box 5) from the specific domain of the just the Ocean Sciences — the Littoral Ocean Observing System (LOOPS/Poseidon; Lermusiaux *et al*, 2006a) — into a more generic framework, embracing all four disciplines (Environmental Engineering, Hydrology, and Ecology, in addition to the Ocean Sciences).

We suggest our *lingua franca* should likewise enable extrapolation to the achievement of a significant measure of "external", horizontal integration, not to mention significant innovation, outside the span of all four of these disciplines: *via* the development of models, into the biomedical sciences, on the one hand, and the social sciences, on the other. Ideally, we should be able to move with ease through and across the different disciplines. This was the culmination of our preliminary response to ***Challenge # 5***.

We evoked there (under ***Challenge # 5***) the image of simulating the sentient individual organism within its ecosystem, i.e., its environment containing individuals from its own and other species, as the means to mark out where some of the frontiers of research now stand in respect of generating novel insights into the generic, dynamical properties in the behavior of *all* systems. We then lifted up this image, transfigured it into an association with the urban ecological footprint, itself another metaphor, and set the result down as defining of a way of thinking about the kinds of model that might be needed for exploring sustainable development of the built environment (in ***Challenge # 11***). One should just as effortlessly be able to switch amongst different images and metaphors for problem-solving.

Issues of scale, brought together in ***Challenge # 3*** as a core scientific challenge in their own right, returned to prominence as matters inextricable from designing Observatories and developing models, when (again in ***Challenge # 11***) the long view was taken over pragmatic, policy-oriented tasks of re-engineering the built environment.

And in Box 7 under that ***Challenge # 11***, and in the spirit of classical systems thinking (we may note in passing), some *generic* (and complementary) limitations in models (***M***) are extracted from three superficially quite different *specific* case studies of the N cycle in whole watersheds.

Vertical Integration: Outreach to Non-Modeling Communities

What works well about a jargon in this horizontal sense can become an impediment, as so obvious in the strident reactions of Pilkey and Pilkey-Jarvis (2007), when we are confronted with the need to achieve "vertical integration": from the computational science of the environmental cyber-infrastructure, up through our own modeling community, to the primary field scientists, and on ultimately to scientifically lay members of the public.[37] A high degree of transparency about the essence of the model is crucial to the equally vital building of trust amongst these other communities (Pascual, 2009).

This capacity for seeing through the inescapable complexity, especially of very high order models, is reflected in the advocacy of scientific visualization devoted *expressly* to the structure of the model, so that the office-bound Statistician may work with the ship-board Marine Ecologist, in responding to ***Challenge # 7***. It is just as vital when the stakeholder is not the model builder, but the policy person seeking support and guidance in the making of decisions (***Challenge # 10***), or the ordinary member of the public witnessing the treatment of personal preferences along the bottom line of attempting to achieve {social legitimacy} in those policy decisions (***Challenge # 11***).

[37] As already noted (Chapter 4.1) in respect of the report on the Seminar "A New Look at the Interaction of Scientific Models with PolicyMaking" (www.martininstitute.ox.ac.uk).

We all belong to a community, perhaps several of them. Each community has its prejudices. And models are not always viewed in a favorable light, as now abundantly clear. We observed this in introducing those policy-directed ***Challenges # 10*** and ***# 11***. Models, it has been said, allow the craft skills and expertise of the model-builder to be legitimated — made objective, as opposed to subjective — such that that expertise may be presented in an impersonal manner (Rayner, 2008). Since some would be much less detached in expressing their resentment of models and modelers, it is clear that our community suffers from a problem of "image". We should be obliged to attempt to overcome it.

Lingua Franca*: Acquiring the Skill*

If the *lingua franca* of modeling holds out the promise of such advantages, when is the skill of "speaking it" generally acquired, and is that the best of times for acquiring such a skill?

No-one takes a Bachelor's degree majoring in computational environmental modeling. For this is an advanced subject, arguably a secondary science (as we have said), certainly a second scientific language, learned later in one's professional life (if at all), customarily in the years of a PhD or shortly thereafter. Becoming inter-disciplinary in one's thinking needs to happen immediately after the first, primary specialization of tertiary study and training. The timing may be critical and the window of opportunity but briefly ajar. A balance must be struck between pre-empting onset of the mono-disciplinary tunnel vision at the earliest possible juncture, while not breaking the nascent self-confidence of those starting to engage in the process of being inter-disciplinary. Each of us needs to be reassured of having acquired some of the intellectual clothing of being an expert — in something, some single discipline, or some specialization — before disrobing to stand ignorant and humble before the expertise and disciplines of others. For as long as we have the pressures of gaining tenure in an academic system (NRC, 2004), the window of opportunity for acquiring the life-long skill of communicating across disciplines, using the language of modeling (in our case), will not remain open for long around the pre- and post-doctoral years.

To summarize, developing responses to many of the grand challenges of this *Paper* implies investments in the structure of our community (***Challenge #***

12), including in the education and training of the next generation of environmental modelers. In line with the ubiquitous calls for realizing greater inter-disciplinarity in the conduct of Environmental Science (and elsewhere, further afield; NRC, 2004), we argue that model-building has a special role to play. Yet despite this as the focus of the project's (May, 2006) Tucson Workshop, even the mechanism of communicating amongst ourselves — as modelers from just the constituent disciplines of the Environmental Observatories — is not in perfect working order.

5.2 Recommendations

Within Community Orchestration: Substance Not Form

All that said, our first recommendation has to be this:

Recommendation # 1:

> ***Having brought a significant proportion of the community together, through a Workshop, and now — by virtue of the literature reviewed herein — this* White Paper*, it would be a missed opportunity not to provide the wherewithal for the continuing* active *maintenance, development, and scientific prosperity of the modeling community under the EO initiatives.***

But what might be the *substance* of such active management? For we can readily reach for various *forms* of organized activity: network, workshop, center, summer school, task force, specialist technical group, and so on; with each assuming either a real or virtual form, as enabled through the cyber-infrastructure. No matter their intensity and extent, however, the formalities of organization may not be the key to successful implementation of this recommendation.

We have the *lingua franca* of modeling; how should we now best put it to work within these various forms of activity?

The archetypal procedure of Applied Systems Analysis is supposed to function ideally as follows. A problem *specific* to "foreign" discipline F lacks a solution. That problem, nevertheless, has certain prominent, *generic* features, crudely recognizable to the applied systems analyst working predominantly on problems specific to his/her "native" discipline N. This analyst has a solution to the generic problem, albeit a solution attuned to the specific needs of discipline N. Working with a partner in discipline F, initially to re-shape F's unsolved problem, to fit it better within the mold of N's (solved) problem, the *generic* problem-solution couple can be transcribed from N to F, thus to liberate a solution to the previously unsolved problem *specific* to F. But this is not an end to the process. Given an ever improving understanding of the problem set — if not solution set — of the foreign discipline (F), our archetypal analyst has growing access to translations of a set of problems rarely, if ever, uncovered in his/her native discipline N.

Things could begin just as well from the opposite perspective, of course: of a frustrated analyst in discipline F looking outwards from his/her own discipline, scanning other disciplines for a matching of their problem-solution couples with his/her unsolved problem. But s/he would have to be provoked into "looking outwards" in the first place. And what training would incline anyone so to do?

Levin (2006) gives tangible and succinct form to such clinical abstraction of systems thinking, in his case on the matter of extracting generic insights into the nature of adaptive dynamics in systems (and in our case, under our ***Challenge # 5***):

> Moving from the ecological to the social or economic situation simply completes the loop — these are ideas that had their origins in economics, were adapted and modified for biology, and now find new application in their original setting.

Success in implementing our first recommendation, then, is unlikely to be entirely a matter of form or format, or of the intensity, or superficially visible structure, of the organization behind any given activity. Alas, it is more likely to be dependent upon the correct mix of people, their personalities, and their outlooks on what constitutes a scientific problem worthy of their sustained attention.

Time is manifestly a vital factor in inter-disciplinary work, and in various ways:

(i) time to be given up for a brief period, such as at a workshop, to step out of the specifics of one's personal research interests — groundwater contaminant transport; settling and compaction of biological flocs in wastewater treatment — to recognize the shared challenge, in modeling and forecasting the generic features of transient pollution events;[38]

(ii) time for the younger researcher on a fixed-term contract to ensure the first flush of naïve curiosity, in collaborating widely across disciplines, is rewarded sufficiently quickly, before the next career position has to be secured; and

(iii) time in the sense of age being on the side of the applied systems analyst, who must accumulate the experience of sufficient case studies in solving specific problems to be able to discern with increasing clarity those recurring problem-solution couples of a more generic character.[39]

In 1986 Holling expressed his synthesis of the "Myths of Nature" and their mapping onto the cyclical, longer-term dynamics of ecological systems (Holling, 1986). Over the subsequent decade, anthropologist Thompson was able to map the social transactions amongst the fundamental typologies of Cultural Theory onto Holling's cyclical behavior in ecosystems, with powerful implications for Applied Systems Analysis in general (Thompson *et al*, 1990; Price and Thompson, 1997; and Thompson, 1997). That is one important exemplar of the very best of inter-disciplinary research; and surely an indicator of the time such can take.

Personality too will be important:

(i) in the sense of suppressing any tendency to scoff in disbelief at the utter simplicity of the problem specifications — gross distortions of the real-world problem — essential to initiating a novel procedure of solution;

(ii) in the dogged persistence of the solution-provider, to work with the problem-owner in removing each gross assumption, one by one, as the solution procedure matures, instead of forsaking the ardor of the path back to the messy problems of the real world for the relative ease and appeal of the next pristine, elegant, but abstract, alternative, wherever it may present itself (elsewhere); and

[38] Experience has shown, rather consistently, that such does not tend to happen.

[39] And that aging analyst would do well to retain a degree of naïvety, tolerant of the seemingly impossible and outlandish (at first sight).

(iii) in simply holding on to humility — an absence of pontificating on how others should mobilize their uniquely acquired expertise.

And there will probably be a need for a *dirigiste* style of orchestration, drawn along by the vision of a well targeted, tangible, and substantial end-point:

(i) the book on *Panarchy* by Gunderson and Holling (2002) was the product of a deliberately orchestrated network activity (the Resilience Alliance) sustained over several years;

(ii) that on *Evolutionary Economics* by Dosi et al (1990) resulted from a sequence of meetings and workshops dedicated expressly to achieving the sole outcome of the monograph; and

(iii) production of the monograph on *Environmental Foresight and Models: A Manifesto* (Beck, 2002) was fashioned after the process employed by Dosi and colleagues (and all told, took a decade to complete).

We recommend no specific form of community orchestration, therefore, merely sustaining an active awareness of the foregoing considerations of group sociology, as the basic ingredients of eventual success, when it comes to developing any given activity.

Having offered these general principles of community orchestration aimed expressly at achieving inter-disciplinary work, our next recommendation is likewise *not* prescriptive. Rather, it is indicative of the kinds of actions that could be taken following publication and dissemination of this, our full *White Paper.*

Cross-Community Communication: Attaining the Bigger Picture

Whereas ***Recommendation # 1*** looked primarily inwards, to our own professional community, this second recommendation is oriented towards what we have labeled as “outreach”, thus:

Recommendation # 2:

> ***Given that modeling cannot proceed in a vacuum, detached from reality, case studies and case histories should be prepared and packaged in forms designed to serve the ever-present need of the modeling community to build and maintain fruitful relationships with a variety of other communities — of philosophers, scientists, engineers, scholars, policy-makers, and the public — in developing the beginnings of responses to the Grand Challenges.***

It is important to achieve a strategic sense of perspective, a sense of history. The long view is as important as looking outwards from our own professional community.

Our over-arching ***Challenge # 0***, for example, calls for a perhaps unusual collaboration to be initiated between modelers and philosophers of science. Constructive engagement of the two, however, is unlikely to be established in the absence of the empirical evidence of case histories in how models *and* the sciences of, say, Ecology or Hydrology have evolved *in tandem* over the past four decades. Only now, with the benefit of such a significant span of history, might we be able to discern innovations of a strategically important philosophical nature.

Challenge # 7 has its sights set on a cyber-infrastructure capable of supporting the lateral thinking necessary for reconciling large, very high order models (VHOMs) with extensive sets of data. Making progress on that front will require computational scientists and software engineers[40] to be led through our more substantial case histories in the systematic identification of environmental models, to the points where they can diagnose why current software frameworks frustrate realization of the needed “tinkering” paradigm. Enabled now to take the long view over four to five decades of environmental modeling, significant shifts in schools of thought, which may have seemed imperceptible at the time, can be more sharply illuminated, even to dramatize

[40] Typically, those who generate the toolboxes of the MATLAB-SIMULINK® platform or who, like The DHI Group, are promoting the production of software that is “OpenMI™ Compliant”; atypically, perhaps, also those who have worked on the graphics design of the visualizations in Boxes 2 and 3 of ***Challenge # 7***.

why access to such a tinkering paradigm should be so important (Schertzer and Lam, 2002; Dennis, 2002).

The Seine-Paris case study (Billen *et al*, 2007a) is of strategic importance for a variety of reasons, not merely for its long view (which spans a thousand years or so), nor its relevance to opening out responses to the essentially scientific (***Challenge # 1***) and the urgently pragmatic alike (***Challenge # 11***). Indeed, we should be enquiring into what, therefore, in the nature of the funding mechanisms and community structures underpinning this Seine-Paris program, has made it something of an exemplary, inter-disciplinary case study — at least according to the public accounts of its outcomes.

Models for Design/operation of the EOs

To this general rule of mere indicative responses to our various ***Challenges***, there is one notable exception, expressed as follows:

Recommendation # 3:

> ***Given the maturity of Observing System Simulation Experiments (OSSEs), and their obvious potential role in the design of* all *the Environmental Observatories, investment in the work needed to respond to this facet of* Challenge # 6 *is recommended. In seeking progress on a variety of fronts, however, such investment should be directed beyond the pragmatic needs of EO design, for example: to furthering the social and professional aspects of bridging any divides between the field-science and model-building communities; and to propelling OSSEs as much as possible beyond the current state of their art.***

The WATERS Network proposes to do precisely that (WATERS, 2008). Its second phase of planning will focus on designing its EO to answer scientific questions informed by the somewhat heterogeneous means of fixed *and* mobile observing platforms. If formulated as an OSSE, embedding therein some of the principles of data assimilation (from ***Challenge # 9*** and the LOOPS/Poseidon initiative recounted in Box 5), new research ground should be broken in the process.

Given the initial momentum of this *White Paper*, in bringing together disciplines and schools of thought that might otherwise have remained apart, quite other lines of research are discernible. Mobile observing platforms, after all, are (intelligent) agents moving about the field. Those carrying forward the new frontiers in Individual Based Modeling (IBMs) in Ecology (Grimm *et al*, 2005) might therefore be encouraged to bring unexpected and novel challenges to this rather mature domain of OSSEs, data assimilation, and adaptive sampling, with its basis in models alternatively as (traditional) sets of differential equations.

What, however, does Society want of the EOs? Just as cultivation of the Grand Challenges for the 21st Century by the US National Academy of Engineering was enacted (2006/7) through public debate and the priorities set (2007/8) by a public voting system — and just as Gibbons (1999) has argued for a new contract between Science and Society — some of the goals of the EOs might similarly be so determined. How should models (***M***), scientific visualization, and all the facilities of the environmental cyber-infrastructure be turned then to such a purpose?

Training the Next Generation

Our fourth and final recommendation follows directly from ***Challenge # 12*** (community structure):

Recommendation # 4:

> ***Having argued a case in favor of the special role of models, as the* lingua franca *of inter-disciplinary research, we recommend investigating the merits of complementary alternatives to vehicles such as NSF's Integrated Graduate Education Research and Training (IGERT) schemes for the purpose of training the next generation of environmental modelers.***

The Education Committee of the WATERS Network has recently recommended a Workshop for all of the Environmental Observatories on the topic of Education and Outreach (WATERS Network, 2007b), just as our own project has been supported in hosting the Tucson Workshop of May, 2006. There is every reason, therefore, for us not to recommend duplication of such effort.

Instead, noting that in 2007 the International Institute for Applied Systems Analysis (IIASA) celebrated its 35th Anniversary and, more importantly, the 30th anniversary of its Young Scientists Summer Program (YSSP; www.iiasa.ac.at/YSSP), we suggest there may be much to be gained from reviewing the merits of that kind of Program in meeting our present needs.

A candidate description of what constitutes "inter-disciplinarity" (for the environmental systems analyst) has been embedded in the foregoing discussion of ***Challenge # 12*** and ***Recommendation # 1*** regarding the structure of our community (see also Chapter 5.1). Given this as a point of departure to be disputed and improved upon, alongside the NRC's more wide-ranging report (NRC, 2004) what — we should ask — has the YSSP correctly encapsulated, and what has escaped its purview, in sowing the seeds of successful inter-disciplinary thinking in young minds? How might we benefit, if at all, from the longevity and consistency of the YSSP, in identifying whether and how its alumni have actually become leaders in the science and practice of inter-disciplinary thinking?

Chapter 6: Conclusions

NSF's Environmental Observatory initiatives promise access to unprecedented streams of observations on the behavior of environmental systems *in situ*. Excellence in developing models of that behavior is not achievable without both such volume *and* quality in those expected data streams.

Talk of things being "transformative" and "unprecedented", however, can become a commonplace when large sums of money are in prospect for supporting ambitious programs of research. We are using these words advisedly, therefore.

There is a subtle, but significant point of dislocation — a threshold — beyond which the scope for progress and achievement in model-building becomes qualitatively different from that to which we have become accustomed. Hitherto, it has been typical for any divergence — between a model (of growing complexity, in general) and the relatively sparse and inadequate data (with which conditions, incidentally, we shall always have to deal) — to be dismissed as a consequence of those inadequate data. High volumes of high quality (HVHQ) data should deny such all-too-easy dismissal in future. Hard thought will have to be invested in diagnosing why the model is failing, not as a *whole*, but in which particular *parts*. And even harder thought will be called for in extracting the failed parts from the complex whole; coming up with novel hypotheses; expressing them in mathematical form; and re-configuring the structure of the model so as to accommodate the new and revised constituent hypotheses. This is especially true today in understanding the behavior of chemical and biological species in our environment, beyond the more customary measures of pH, conductivity, and dissolved oxygen concentration, for example.

For some members of this Committee, with access to monitoring platforms capable of generating HVHQ data, the beginnings of the transformation to such a qualitatively different domain of opportunities for research in environmental modeling have already been experienced.[41] In so many of our ***Challenges*** this same kind of question recurs: what exactly is it that causes model and reality not to match; and how should we observe, diagnose, probe, and explore such a mismatch in order to understand and resolve it as swiftly as possible?

Whether we also stand on the threshold of qualitative change in other ways is less clear. For there has always been monotonic progression in our models of environmental systems, towards an ever greater scope (such as an Earth Systems perspective) and the inclusion of ever more detail (down to the biochemical metabolism of the individual cell and below). This progression seems now, however, on the verge of being cross-fertilized in rather novel ways by simulation of the behavior and functioning of the individual organism (in the biomedical sciences) and simulation of that individual as it negotiates a natural environment populated by like and other individuals (in the social sciences).

This same irrepressible advance in environmental models — and their increasing embrace of the personal and the private in human affairs — will eventually cause our professional community to step over another threshold, there to confront some uncommon ethical challenges.

[41] And Kirchner *et al* (2004) talk enthusiastically and convincingly of "catching this new wave" in the Hydrologic Sciences.

REFERENCES

Achleitner, S, Möderl, M, and Rauch, W (2007), "Urine Separation as Part of a Real-time Control Strategy", *Urban Water*, **4**(4), pp 233-240.

Allan, J (2003), "Virtual Water — The Water, Food and Trade Nexus: Useful Concept or Misleading Metaphor", *Water International*, **28**, pp 4-11.

Allen, P M (1990), "Evolution, Innovation, and Economics", in *Technical Change and Economic Theory* (G Dosi, C Freeman, R Nelson, G Silverberg and L Soete, eds), Pinter, London, pp 95-119.

Alvarez-Vasquez, F, Sims, K L, Cowart, L A, Okamoto, Y, Voit, E O, and Hannun, Y A (2005), "Simulation and Validation of Modelled Sphingolipid Metabolism in *Saccharomyces Cerevisiae*", *Nature*, **433**, pp 425-430 (27 January).

Amin, M (2001), "Toward Self-Healing Energy Infrastructure Systems", *IEEE Computer Applications in Power*, (January), pp 20-28.

Andersen, M E, Dennison, J E, Thomas, R S, and Conolly, R B (2005), "New directions in Incidence-dose Modeling", *TRENDS in Biotechnology*, **23**(3), pp 122-127.

Anderson, M C, Kustas, W P, and Norman, J M (2003), "Upscaling and Downscaling — A Regional View of the Soil-Plant-Atmosphere Continuum", *Agronomy J*, **95**, pp 1408-1423.

Andreadis, K M, and Lettenmaier, D P (2006), "Assimilating Remotely Sensed Snow Observations Into a Macroscale Hydrology Model", *Advances in Water Resources*, **29**, pp 872-886.

Arnold, C P, and Dey, C H (1986), "Observing-systems Simulation Experiments: Past, Present and Future", *Bulletin American Meteorological Society*, **67**(6), pp 687-695.

Aronson, J, Blignaut, J, Milton, S, and Clewell, A (2006), "Natural Capital: The Limiting Factor", *Ecological Engineering*, **28**, pp 1-5.

Arthington, A H, Bunn, S E, Poff, N L, and Naiman, R J (2006), "The Challenge of Providing Environmental Flow Rules to Sustain River Ecosystems", *Ecological Applications*, **16**(4), pp 1311-1318.

Ayres, R U, and Ayres, L W (eds) (2002), "*Handbook of Industrial Ecology*", Edward Elgar, Northampton, Massachusetts, 680pp.

Ayton, P (2007), Personal Communication (30 July).

Babendreier, J E, and Castleton, K J (2005), "Investigating Uncertainty and Sensitivity in Integrated, Multimedia Environmental Models: Tools for FRAMES-3MRA", *Environmental Modelling and Software*, **20**, pp 1043-1055.

Bair, E S (1994), "Model (*In*)validation — A View from the Courtroom", Ground Water, **32**, pp 530-531.

Baretta, J W, Ebenhöh, W, and Ruardij, P (1995), "The European Regional Seas Ecosystem Model, a Complex Marine Ecosystem Model", *Netherlands J Sea Research*, **33**, pp 233-246.

Barles, S (2007), "Feeding the City: Food Consumption and Flow of Nitrogen, Paris, 1801-1914", *Science of the Total Environment*, **375**, pp 48-58.

Barraqué, B, Juuti, P S, and Katko, T S (2006), "Urban Water Conflicts in Recent European History: Changing Interactions Between Technology, Environment and Society", in *Urban Water Conflicts*, UNESCO Working Series **SC-2006/WS/19**, International Hydrological Programme (IHP), UNESCO, Paris, pp 7-24.

Beck, M B (1981), "Operational Estimation of Nitrification Dynamics in the Activated Sludge Process", *Water Research*, **15**, pp 1313-1330.

Beck, M B (1987), "Water Quality Modeling: A Review of the Analysis of Uncertainty", *Water Resources Research*, **23**(8), pp 1393-1442.

Beck, M B (ed) (2002), "*Environmental Foresight and Models: A Manifesto*", Elsevier, Oxford, 473pp.

Beck, M B (2005a), "Vulnerability of Water Quality in Intensively Developing Watersheds", *Environmental Modelling and Software*, **20**(4), pp 381-400.

Beck, M B (2005b), "Environmental Foresight and Structural Change", *Environmental Modelling and Software*, **20**(6), pp 651-670.

Beck, M B, and Young, P C (1976), “Systematic Identification of DO-BOD Model Structure”, *Proceedings American Society of Civil Engineers*, *J Environmental Engineering Division*, **102**(EE5), pp 909-927.

Beck, M B and Chen, J (2000), “Assuring the Quality of Models Designed for Predictive Tasks”, in *Sensitivity Analysis* (A Saltelli, K Chan, and E M Scott, eds), Wiley, Chichester, pp 402-420.

Beck, M B, Kleissen, F M, and Wheater, H S (1990), “Identifying Flow Paths in Models of Surface Water Acidification”, *Reviews of Geophysics*, **28**(2), pp 207-230.

Beck, M B, Jiang, F, Shi F, and Villarroel Walker, R (2009), “Technology, Sustainability, and Business: Cities as Forces for Good in the Environment”, in *Integrated Urban Water Management in Temperate Climates* (C Maksimovic, ed), UNESCO/Taylor & Francis, London, (in press).

Bennett, A F, and Budgell, W P (1987), “Ocean Data Assimilation and the Kalman Filter: Spatial Regularity”, *J Physical Oceanography*, **17**, pp 1583-1601.

Bennett, D A, and Tang, W (2006), “Modelling Adaptive, Spatially Aware, and Mobile Agents: Elk Migration in Yellowstone”, *International Journal of Geographical Information Science*, **20**(9), pp 1039-1066.

Benyus, J M (1997), “*Biomimicry: Innovations Inspired by Nature*”, William Morrow, New York.

Berkhout, F, and Hertin, J (2004), “De-materializing and Re-materializing: Digital Technologies and the Environment”, *Futures*, **36**, pp 903-920.

Bettencourt, L M A, Lobo, J, Helbing, D, Kühnert, C, and West, G B (2007), “Growth, Innovation, Scaling, and the Pace of Life in Cities”, *Proceedings National Academy of Sciences*, **104**(17), pp 7301-7306.

Beven, K J, (2002), “Towards a Coherent Philosophy for Environmental Modelling”, *Proceedings Royal Society of London*, **A460**, 458, pp 2465–2484.

Beven, K J (2005), “On the Concept of Model Structure Error”, *Water Science and Technology*, **52**(6), pp 167-175.

Beven, K J, and Freer, J (2001), “Equifinality, Data Assimilation, and Uncertainty Estimation in Mechanistic Modelling of Complex Environmental Systems”, *J Hydrology*, **249**, pp 11-29.

Billen, G, Garnier, J, Mouchel, J-M, and Silvestre, M (2007a), “The Seine System: Introduction to a Multidisciplinary Approach of the Functioning of a Regional River System”, *Science of the Total Environment*, **375**, pp 1-12.

Billen, G, Garnier, J, Némery, J, Sebilo, M, Sferratore, A, Barles, S, Benoit, P, and Benoît, M (2007b), “A Long-term View of Nutrient Transfers though the Seine River Continuum”, *Science of the Total Environment*, **375**, pp 80-97.

Bitbol, M, and Luisi, P L (2004), “Autopoiesis With or Without Cognition: Defining Life at the Edge”, *J Royal Society Interface*, **1**, pp 99-107.

Blöschl, G, and Sivapalan, M (1995), “Scale Issues in Hydrological Modelling: A Review”, *Hydrological Processes*, **9**(3-4), pp 251-290.

Borsuk, M E, Stow, C A, and Reckhow, K H (2004), “A Bayesian Network of Eutrophication Models for Synthesis, Prediction, and Uncertainty Analysis”, *Ecological Modelling*, **173**(2-3), pp 219-239.

Borsuk, M E, Reichert, P, Peter, A, Schager, E, Burkhardt-Holm, P (2006), “Assessing the Decline of Brown Trout (*Salmo trutta*) in Swiss Rivers Using a Bayesian Probability Network”, *Ecological Modelling*, **192**, pp 224-244.

Borsuk, M E, Maurer, M, Lienert, J, and Larsen, T A (2008), “Charting a Path for Innovative Toilet Technology Using Multicriteria Decision Analysis”, *Environmental Science and Technology*, **42**(6), pp 1855-1862.

Boyer, E W, Howarth, R W, Galloway, J N, Dentener, F J, Green, P A, and Vörösmarty, C J (2006), “Riverine Nitrogen Export From the Continents to the Coasts”, *Global Biogeochemical Cycles*, **20**, GB1S91, doi:10.1029/2005GB002537.

Brown Gaddis, E J, Vladich, H, and Voinov, A (2007), “Participatory Modeling and the Dilemma of Diffuse Nitrogen Management in a Residential Watershed”, *Environmental Modelling and Software*, **22**, pp 619-629.

Brun, R, Reichert, P, and Künsch, H R (2001), “Practical Identifiability Analysis of Large Environmental Simulation Models”, *Water Resources Research*, **37**(4), pp 1015-1030.

Brun, R, Kühni, M, Siegrist, H, Gujer, W, and Reichert, P (2002), “Practical Identifiability of ASM2d Parameters — Systematic Selection and Tuning of Parameter Subsets”, *Water Research*, **36**(16), pp 4113-4127.

Burn, D H, and McBean, E A (1985), “Optimization Modeling of Water Quality in an Uncertain Environment”, *Water Resources Research*, **21**(7), pp 934-940.

Carpenter, S R, and Folke, C (2006), "Ecology for Transformation", *TRENDS in Ecology and Evolution*, **21**(6), pp 309-315.

Castelletti, A, and Soncini-Sessa, R (2006), "A Procedural Approach to Strengthening Integration and Participation in Water Resources Planning", *Environmental Modelling and Software*, **21**(10), pp 1455-1470.

Castelletti, A, and Soncini-Sessa, R (2007), "Bayesian Networks and Participatory Modelling in Water Resources Management", *Environmental Modelling and Software*, **22**(8), pp 1075-1088.

Casti, J L (1979), "*Connectivity, Complexity, and Catastrophe in Large-scale Systems*", Wiley, Chichester.

Casti, J L (2002), "'Biologizing' Control Theory: How to Make a Control System Come Alive", *Complexity*, **7**(4), pp 10-12.

Caswell, H (1976), "The Validation Problem", in *Systems Analysis and Simulation in Ecology* (B C Patten, ed), Academic, New York, **Vol IV**, pp 313-325.

Chen, J and Beck, M B (1993), "Modelling, Control and On-line Estimation of Activated Sludge Bulking", *Water Science and Technology*, **28**(11-12), pp 249-256.

Chen, J, and Beck, M B (2002), "Detecting and Forecasting Growth in the Seeds of Change", in *Environmental Foresight and Models: A Manifesto* (M B Beck, ed), Elsevier, Oxford, pp 351-373.

Choi, H T, and Beven, K J (2007), "Multi-period and multi-criteria Model Conditioning to Reduce Prediction Uncertainty in an Application of TOPMODEL Within the GLUE Framework", *J Hydrology*, **332**, pp 316-336.

Chow, F K, Kollet, S J, Maxwell, R M, and Duan, Q (2006), "Effects of Soil Moisture Heterogeneity on Boundary Layer Flow With Coupled Groundwater, Land-surface, and Mescoscale Atmospheric Modeling", Paper 5.6, in *Preprints 17th Symposium on Boundary Layers and Turbulence*, American Meteorological Association.

Ciavatta, S, Pastres, R, Lin Z, Beck, M B, Badetti, C, and Ferrari, G (2004), "Fault Detection in a Real-time Monitoring Network for Water Quality in the Lagoon of Venice (Italy)", *Water Science and Technology*, **50**(11), pp 51-58.

Clark, J S, and Gelfand, A E (2006), "A Future for Models and Data in Environmental Science", *TRENDS in Ecology and Evolution*, **21**(7), pp 375-380.

Clarke, D (2004), "Models *à la Mode* — the Promise and Peril of Integrated Environmental Modeling", *White Paper*, Foresight and Governance Project, Woodrow Wilson International Center for Scholars (Washington, DC) (http://wwics.si.edu/foresight).

Crichton, M (2004), "*State of Fear*", Avon, New York.

Crutzen, P J, Beck, M B, and Thompson, M (2007), "Cities", Essay (posted at website www.engineeringchallenges.org), Blue Ribbon Panel on Grand Challenges for Engineering, US National Academy of Engineering (see also *Options* (Winter, 2007), International Institute for Applied Systems Analysis, Laxenburg, Austria, p 8).

CUAHSI (2006), "High Performance Computing for Hydrological Sciences", *Internal Report*, CUAHSI, November.

Curds, C R (1973a), "A Theoretical Study of Factors Influencing the Microbial Population Dynamics of the Activated Sludge Process — I: The Effects of Diurnal Variations of Sewage and Carnivorous Ciliated Protozoa", *Water Research*, **7**, pp 1269-1284.

Curds, C R (1973b), "A Theoretical Study of Factors Influencing the Microbial Population Dynamics of the Activated Sludge Process — II: A Computer-simulation Study to Compare Two Methods of Plant Operation", *Water Research*, **7**, pp 1439-1452.

Curry, J A, Webster, P J, and Holland, G J (2006), "Mixing Politics and Science in Testing the Hypothesis that Greenhouse Warming is Causing a Global Increase in Hurricane Intensity", *Bulletin American Meteorological Society*, August, pp 1025-1037 (DOI:10.1.1175/BAMS-87-8-1025).

Darema, F (2005), "Grid Computing and Beyond: The Context of Dynamic Data Driven Applications Systems", *Proceedings IEEE*, **93**(3), pp 692-697.

Darier, E, Gough, C, De Marchi, B, Funtowicz, S, Grove-White, R, Kitchener, D, Guimarães-Pereira, Â, Shackley, S and Wynne, B (1999), "Between Democracy and Expertise? Citizens' Participation and Environmental Integrated Assessment in Venice (Italy) and St Helens (UK)", *J Environmental Policy & Planning*, **1**, pp 103-120.

Davis, C K (2008), "Ethical Dilemmas in Water Recycling", Chapter 15, in *Water Reuse — An International Survey*, (B Jimenez and T Asano, eds), IWA Publishing, London, pp 281-298.

Dennis, R L (2002), "The Ozone Problem", in *Environmental Foresight and Models: A Manifesto* (M B Beck, ed), Elsevier, Oxford, pp 147-165.

Dennis, R L, Arnold, J R, and Tonnesen, G S (2002), "Probing the Shores of Ignorance", in *Environmental Foresight and Models: A Manifesto* (M B Beck, ed), Elsevier, Oxford, pp 375-412.

Dieckmann, U, and Metz, J A J (eds) (2005), "*Elements of Adaptive Dynamics*", Cambridge University Press, Cambridge.

Dieckmann, U, and Metz, J A J (2006), "Surprising Evolutionary Predictions From Enhanced Ecological Realism", *Theoretical Population Biology*, **69**, pp 263-281.

Dippner, J W (2006), "Future Aspects in Marine Ecosystem Modelling", *J Marine Systems*, **61**, pp 246-267.

Dohan, K, and Whitfield, P H (1997), "Identification and Characterization of Water Quality Transients Using Wavelet Analysis. I Wavelet Analysis Methodology", *Water Science and Technology*, **36**(5), pp 325-335.

Doherty, J, and Johnston, J M (2003), "Methodologies for Calibration and Predictive Analysis of a Watershed Model", *J American Water Resources Association*, **39**(2), pp 251-265.

Dosi, G, Freeman, C, Nelson, R, Silverberg, G, and Soete, L (eds) (1990), "*Technical Change and Economic Theory*", Pinter, London, 646pp.

Douglas, C C, Beezley, J D, Coen, J, Li, D, Li, W, Mandel, A K, Mandel, J, Qin, G, and Vodacek, A (2006), "Demonstrating the Validity of a Wildfire DDDAS", in ICCS 2006, Part III, (V N Alexandrov and others, eds), Springer, Berlin, *Lecture Notes in Computer Science*, **3993**, pp 522-529.

Drécourt, J-P, Maden, H, and Rosbjerg, D (2006a), "Bias Aware Kalman Filters: Comparison and Improvements", *Advances in Water Resources*, **29**, pp 707-718.

Drécourt, J-P, Maden, H, and Rosbjerg, D (2006a), "Calibration Framework for a Kalman Filter Applied to a Groundwater Model", *Advances in Water Resources*, **29**, pp 719-734.

Duan, Q Y, Gupta, V K, and Sorooshian, S (1993), "Shuffled Complex Evolution Approach for Effective and Efficient Global Minimization", *J Optimization Theory and Applications*, **76**(3), pp 501-521.

Efroymson, R A, and Murphy, D L (2001), "Ecological Risk Assessment of Multimedia Hazardous Air Pollutants: Estimating Exposure and Effects", *Science of the Total Environment*, **274**, pp 219-230.

Elkington, J (1998), "*Cannibals With Forks: The Triple Bottom Line of 21st Century Business*", New Society, Stony Creek, Connecticut.

Elwood, J W, Newbold, J D, O'Neill, R V, and Van Winkel, W (1983), "Resources Spiraling: An Operational Paradigm for Analyzing Lotic Ecosystems", in *Dynamics of Lotic Ecosystems* (T D Fontaine and S M Bartell, eds), Ann Arbor Science, Ann Arbor, Michigan, pp 3-28.

Emanuel, K A (2005), "Increasing Destructiveness of Tropical Cyclones Over the Past 30 Years", *Nature*, **436**, pp 686-688.

Entekhabi, D, and Moghaddam, M (2007), "Mapping Recharge From Space: Roadmap to Meeting the Grand Challenge", *Hydrogeology J*, pp 105-116.

Even, S, Billen, G, Bacq, N, Théry, S, Ruelland, D, Garnier, J, Cugier, P, Poulin, M, Blanc, S, Lamy, F, and Paffoni, C (2007a), "New Tools for Modelling Water Quality in Hydrosystems: An Application in the Seine River Basin in the Frame of the Water Framework Directive", *Science of the Total Environment*, **375**, pp 274-291.

Even, S, Mouchel, J-M, Servais, P, Nicolas Flipo, Poulin, M, Blanc, S, Chabanel, M, and Paffoni, C (2007b), "Modelling the Impacts of Combined Sewer Overflows on the River Seine Water Quality", *Science of the Total Environment*, **375**, pp 140-151.

Farley, J, and Daly, H (2006), "Natural Capital: The Limiting Factor — A Reply to Aronson, Blignaut, Milton and Clewell", *Ecological Engineering*, **28**, pp 6-10.

Fenner, R A (2008), "Editorial: Can Sustainability Count?", *Engineering Sustainability, Proc Institution of Civil Engineers*, **161**(ES1), pp 1-2 (Special issue on "Assessment Frameworks, Indicators and Metrics: Part 2).

Fisher, E (2007), "*Risk Regulation and Administrative Constitutionalism*", Hart, Oxford.

Flikkema, P G, Agarwal, P K, Clark, J S, Ellis, C, Gelfand, A, Munagala, K, and Yang, J (2006), "Model-driven Dynamic Control of Embedded Wireless Sensor Networks", in *ICCS 2006*, (V N Alexandrov and others, eds), Lecture Notes in Computer Science, **3993**(III), pp 409-416.

Folke, C, Carpenter, S R, Walker, B H, Scheffer, M, Elmqvist, T, Gunderson, L H , and Holling, C S (2004), "Regime Shifts, Resilience, and Biodiversity in Ecosystem Management", *Annual Reviews of Ecological and Evolutionary Systems*, **35**, pp 557-581.

Frankl, P, and Rubik, F (2000), "*Life Cycle Assessment in Industry and Business*", Springer, New York, 280pp.

Funtowicz, S O, and Ravetz, J R (1990), "*Uncertainty and Quality in Science for Policy*", Kluwer, Dordrecht, The Netherlands, 229pp.

Gabbert, S (2006), "Improving Efficiency of Uncertainty Analysis in Complex Integrated Assessment Models: the Case of the RAINS Emission Module", *Environmental Monitoring and Assessment*, **119**, pp 507-526.

Galindo, H M, Olson, D B, and Palumbi, S R (2006), "Seascape Genetics: A Coupled Oceanographic-Genetic Model Predicts Population Structure of Caribbean Corals", *Current Biology*, **16**, pp 1622-1626.

Gallagher, M, and Doherty, J (2007), "Parameter Estimation and Uncertainty Analysis for a Watershed Model", *Environmental Modelling and Software*, **22**, pp 1000-1020.

Galloway, J N, and Cowling, E B (2002), "Reactive Nitrogen and the World: 200 Years of Change", *Ambio*, **31**(2), pp 64-71.

Galloway, J N, Aber, J D, Erisman, J W, Seitzinger, S P, Howarth, R W, Cowling, E B, and Cosby, B J (2003), "The Nitrogen Cascade", *BioScience*, **53**, pp 341-356.

Garrett, K A, Dendy, S P, Frank, E E, Rouse, M N, and Travers, S E (2006), "Climate Change Effects on Plant Disease: Genomes to Ecosystems", *Annual Review of Phytopathology*, **44**, pp 489-509.

Gibbons, M (1999), "Science's New Social Contract with Society", *Nature*, **402** (Supplement), pp C81-C84 (2 December).

Giupponi, C (2007), "Decision Support Systems for Implementing the European Water Framework Directive: the MULINO Approach", *Environmental Modelling and Software*, **22**, pp 248-258.

Giupponi, C, Jakeman, A J, Karssenberg, D, and Hare, M P (eds) (2006), "*Sustainable Management of Water Resources: An Integrated Approach*", Edward Elgar, Northampton, Massachusetts.

Gleick, P H (2003), "Global Freshwater Resources: Soft-path Solutions for the 21st Century", *Science*, **302**, pp 1524-1528.

Godet, M, and Roubelat, F (1996), "Creating the Future: The Use and Misuse of Scenarios", *Long Range Planning*, **29**, pp 164-171.

Goodwin, R A, Nestler, J M, Anderson, J J, Weber, L J, and Loucks D P (2006), "Forecasting 3-D Fish Movement Behavior Using a Eulerian-Lagrangian-agent Method (ELAM)", *Ecological Modelling*, **192**, pp 197-223.

Gopalakrishnan, S G, Bacon, D P, Ahmad, N N, Boybeyi, Z, Dunn, T J, Hall, M S, Jin, Y, Lee, P C S, Mays, D E, Madala, R V, Sarma, A, Turner, M D, and Wait, T T (2002), "An Operational Multiscale Hurricane Forecasting System", *Monthly Weather Review*, **130**(7), pp 1830-1847.

Graham, D W, and Smith, V H (2004), "Designed Ecosystem Services: Application of Ecological Principles in Wastewater Treatment Engineering", *Frontiers in Ecology and Environment*, **2**(4), pp 199-206.

Green, K C, and Armstrong, J S (2007), "Global Warming: Forecasts by Scientists Versus Scientific Forecasts", *Energy and Environment*, **18**(7,8), pp 997-1021.

Grimm, V, Revilla, E, Berger, U, Jeltsch, F, Mooij, W M, Railsback, S F, Thulke, H-H, Weiner, J, Wiegand, T, and DeAngelis, D L (2005), "Pattern-oriented Modeling of Agent-based Complex Systems: Lessons from Ecology", *Science*, **310**, pp 987-991 (11 November).

Grote, U, Craswell, E, and Vlek, P L G (2005), "Nutrient Flows in International Trade: Ecology and Policy Issues", *Environmental Science and Policy*, **8**(5), pp 439-451.

Gunderson, L H, and Holling, C S (eds), "*Panarchy: Understanding Transformations in Human and Natural Systems*", Island, Washington DC.

Gupta, H V, Wagener, T, and Liu, Y (2008), "Reconciling Theory With Observations: Elements of a Diagnostic Approach to Model Evaluation", *Hydrologic Processes*, DOI:10.1002/hyp.6989.

Gupta, H V, Sorooshian, S, and Yapo, P O (1998), "Toward Improved Calibration of Hydrologic Models: Multiple and Noncommensurable Measures of Information", *Water Resources Research*, **34**(4), pp 751-763.

Hall, J, and O'Connell, P E (2007), "Earth Systems Engineering: Turning Vision into Action", *Civil Engineering, Proc Institution of Civil Engineers*, **160** (CE3), pp 114–122.

Harrison, K W (2007), "Test Application of Bayesian Programming: Adaptive Water Quality Management Under Uncertainty", *Advances in Water Resources*, **30**, pp 606–622.

Hare, M P, and Deadman, P (2004), "Further Progress Towards a Taxonomy of Agent-based Simulation Models in Environmental Management", *Mathematics and Computers in Simulation*, **64**, pp 25–40.

Hare, M P, Barreteau, O, Beck, M B, Letcher, R A, Mostert, E, Tàbara, J D, Ridder, D, Cogan, V, and Pahl-Wostl, C (2006), in *Sustainable Management of Water Resources: An Integrated Approach* (C Giupponi, A J Jakeman, D Karssenberg, and M P Hare, eds), Edward Elgar, Northampton, Massachusetts, pp 177-231.

Hawes, C, and Reed, C (2006), "Theoretical Steps Towards Modelling Resilience in Complex Systems", in *ICCSA 2006*, (M Gavrilova and others, eds), Lecture Notes in Computer Science **3980**, Springer, Berlin, pp 644–653.

Henze, M, Gujer, W, Mino, T, Matsuo, T, Wentzel, M C, Marais, GvR, van Loosdrecht, M C M (1999), "Activated Sludge Model No 2d (ASM2d)", *Water Science and Technology*, **39** (1), pp 165–182.

Helton, J C, Johnson, J D, Sallaberry, C J, and Storlie, C B (2006), "Survey of Sampling-based Methods for Uncertainty and Sensitivity Analysis", *Reliability Engineering and Systems Safety*, **91**, pp 1175-1209.

Hobbs, R J, Arico, S, Aronson, J, Baron, J S, Bridgewater, P, Cramer, V A, Epstein, P R, Ewel, J J, Klink, C A, Lugo, A E, Norton, D, Ojima, D, Richardson, D M, Sanderson, E W, Valladares, F, Vilà, M, Zamora, R, and Zobel, M (2006), "Novel Ecosystems: Theoretical and Management Aspects of the New Ecological World Order", *Global Ecology and Biogeography*, **15**, pp 1–7.

Holling, C S (1973), "Resilience and Stability of Ecological Systems", *Annual Reviews of Ecological Systems*, **4**, pp 1–23.

Holling, C S (ed) (1978), "*Adaptive Environmental Assessment and Management*", Wiley, Chichester.

Holling, C S (1986), "The Resilience of Terrestrial Ecosystems: Local Surprise and Global Change", in *Sustainable Development of the Biosphere*, (W C Clark and R E Munn, eds), Cambridge University Press, Cambridge, pp 292–317.

Holling, C S (1996), "Engineering Resilience Versus Ecological Resilience", in *Engineering Within Ecological Constraints*, (P Schulze, ed), National Academy Press, Washington DC, pp 31–44.

Hooper, B (2006), "Integrated Water Resources Management: Governance, Best Practice, and Research Challenges", *J Contemporary Water Research and Education*, **135**, pp 1–7.

Hornberger, G M, and Spear, R C (1981), "An Approach to the Preliminary Analysis of Environmental Systems", *J Environmental Management*, **12**, pp 7–18.

Hornberger, G M, Beven, K J, Cosby, B J, and Sappington, D E (1985), "Shenandoah Watershed Study: Calibration of a Topography-based, Variable Contributing Area Hydrological Model to a Small Forested Catchment", *Water Resources Research*, **21** (12), pp 1841–1850.

Horsburgh, J S, Tarboton, D G, Piasecki, M, Maidment, D R, Zaslavsky, I, Valentine, D, and Whitenack, T (2009), "An Integrated System for Publishing Environmental Observations Data", *Environmental Modelling and Software*, (in press).

Hoteit, I, Triantafyllou, G, and Petihakis, G (2005), "Efficient Data Assimilation Into a Complex, 3-D Physical-biogeochemical Model Using Partially Local Kalman Filters", *Annales Geophysicae*, **23**, pp 3171–3185.

Houghton, J T, Callander, B A and Varney, S K (eds) (1992), "*Climate Change 1992, The Supplementary Report to the IPCC Scientific Assessment*", Cambridge University Press, Cambridge.

Howard, K W F, and Gelo, K K (2003), "Intensive Groundwater Use in Urban Areas: The Case of Megacities", in *Intensive Use of Groundwater: Challenges and Opportunities* (R Llamas, and E Custodio, eds), Balkema, Lisse, pp 35–58.

Hunter P J, and Borg, T K (2003), "Integration from Proteins to Organs; The Physiome Project", *Nature Reviews Molecular Cell Biology*, **4**, pp 237–243.

Ijspeert, A J (2001), "A Connectionist Central Pattern Generator for the Aquatic and Terrestrial Gaits of a Simulated Salamander", *Biological Cybernetics*, **84**, pp 331–348.

Ijspeert, A J, and Kodjabachian, J (1999), "Evolution and Development of a Central Pattern Generator for the Swimming of a Lamprey", *Artificial Life*, **5**, pp 247–269.

IWA (2007), "*Sanitation 21*", International Water Association, The Hague.

Jackson, J B C, Kirby, M X, Berger, W H, Bjorndal, K A, Botsford, L W, Bourque, B J, Bradbury, R H, Cooke, R, Erlandson, J, Estes, J A, Hughes, T P, Kidwell, S, Lange, C B, Lenihan, H S, Pandolfi, J M, Peterson, C H, Steneck, R S, Tegner, M J, and Warner, R R (2001), "Historical Overfishing and the Recent Collapse of Coastal Ecosystems", *Science*, **293**, pp 629-638 (27 July).

Jakeman, A J, Norton, J P, Letcher, R A, and Maier, H R (2006), "Integrated Modelling, Construction, Selection, and Uncertainty", in *Sustainable Management of Water Resources: An Integrated Approach*, (C Giupponi, A J Jakeman, D Karssenberg, and M P Hare, eds), Edward Elgar, Northampton, Massachusetts, pp 263-286.

Janssen, M A, and Carpenter, S R (1999), "Managing the Resilience of Lakes: A Multi-agent Modeling Approach", *Conservation Ecology*, **3**(2), 15 [online].

Jasanoff, S (2003), Personal communication (an e-mail comment of 16 December).

Jones, M B, Schildhauer, M P, Reichman, O J, and Bowers, S (2006), "The New Bioinformatics: Integrating Ecological Data from the Gene to the Biosphere", *Annual Review of Ecology and Evolutionary Systems*, **37**, pp 519-544.

Kahneman, D, Slovic, P, and Tversky, A (eds) (1982), "*Judgment Under Uncertainty: Heuristics and Biases*", Cambridge University Press, Cambridge.

Kalman, R E (1960), "A New Approach to Linear Filtering and Prediction Problems", *American Society of Mechanical Engineers Transactions, J Basic Engineering*, **83D**, pp 95-108.

Kander, A (2005), "Baumol's Disease and Dematerialization of the Economy", *Ecological Economics*, **55**, pp 119-130.

Kaye, J P, Groffman, P M, Grimm, N B, Baker, L A, and Pouyat, R V (2006), "A Distinct Urban Biogeochemistry?", *TRENDS in Ecology and Evolution*, **21**(4), pp 192-199.

Keesman, K J, and van Straten, G (1990), "Set Membership Approach to Identification and Prediction of Lake Eutrophication", *Water Resources Research*, **26**(11), pp 2643-2652.

Kirchner, J W, Feng, X, Neal, C, and Robson, A J (2004), "The Fine Structure of Water-quality Dynamics: The (High-frequency) Wave of the Future", *Hydrological Processes*, **18**, pp 1353-1359.

Kohring, G A (2006), "Avoiding Chaos in Wonderland", *Physica A*, **368**, pp 214-224.

Konikow, L F, and Bredehoeft, J D (1992), "Ground-water Models Cannot Be Validated", *Advances in Water Resources*, **15**(1), pp 75-83.

Krajewski, W F, Anderson, M C, Eichinger, W E, Entekhabi, D, Hornbuckle, B K, Houser, P R, Katul, G G, Kustas, W P, Norman, J M, Peters-Lidard, C, and Wood, E F (2006), "A Remote Sensing Observatory for Hydrologic Sciences: A Genesis for Scaling to Continental Hydrology", *Water Resources Research*, **42**, W07301, doi:10.1029/2005WR004435.

Krayer von Krauss, M P, and Janssen, P H M (2005), "Using the W&H Integrated Uncertainty Analysis Framework with Non-initiated Experts", *Water Science and Technology*, **52**(6), pp 145-152.

Kremen, C (2005), "Managing Ecosystem Services: What Do We Need to Know about Their Ecology?", *Ecology Letters*, **8**, pp 468-479.

Krupnick, A, Morgenstern, R, Batz, M, Nelson, P, Burtraw, D, Shih, J-S, and McWilliams, M (2006), "*Not a Sure Thing: Making Regulatory Choices Under Uncertainty*", Resources for the Future, Washington, DC, 233pp.

Krysanova, V, Hatterman, F, and Wechsung, F (2007), "Implications of Complexity and Uncertainty for Integrated Modelling and Impact Assessment in River Basins", *Environmental Modelling and Software*, **22**, pp 701-709.

Kuhn, T S (1962), "*The Structure of Scientific Revolutions*", University Press, Chicago.

Kumar, P, and Foufoula-Georgiou, E (1997), "Wavelet Applications in Geophysics: A Review", *Reviews of Geophysics*, **35**, pp 385-412.

Kwame, D S (2007), "Domestication of Excreta: A Cultural Theory Analysis of Ecosan Dry Toilet Schemes in Peri-Urban Accra, Ghana", *MSc Dissertation*, Environment and Development Studies, Norwegian University of Life Sciences, Ås, Norway.

Larsen, T A, and Gujer, W (1996), "Separate Management of Anthropogenic Nutrient Solutions", *Water Science and Technology*, **34**(3-4), pp 87-94.

Lempert, R J (2002), "A New Decision Sciences for Complex Systems", *Proceedings National Academy of Sciences*, **99**(suppl 3), pp 7309-7313.

Lermusiaux, P F J, Malanotte-Rizzoli, P, Stammer, D, Carton, J, Cummings, J, and Moore, A M (2006a), "Progress and Prospects of U.S. Data Assimilation in Ocean Research", *Oceanography*, **19**(1), pp 172-183.

Lermusiaux, P F J, Chiu, C-S, Gawarkiwiecz, G G, Abbot, P, Robinson, A R, Miller, R N, Haley, P J, Leslie, W G, Majumdar, S J, Pang, A, and Lekien, F (2006b), "Quantifying Uncertainties in Ocean Predictions", *Oceanography*, **19**(1), pp 92-105.

Lessard, R B, Martell, S J D, Walters, C J, Essington, T E, and Kitchell, J F (2005), "Should Ecosystem Management Involve Active Control of Species Abundance", *Ecology and Society*, **10**(2), 1 [online].

Letcher, R A, Croke, B F W, and Jakeman, A J (2007), "Integrated Assessment Modelling for Water Resource Allocation and Management: A Generalised Conceptual Framework", *Environmental Modelling and Software*, **22**, pp 733-742.

Levin, S A (1998), "Ecosystems and the Biosphere as Complex Adaptive Systems", *Ecosystems*, **1**, pp 431-436.

Levin, S A (2000), "Multiple Scales and the Maintenance of Biodiversity", *Ecosystems*, **3**, pp 498-506.

Levin, S A (2005), "Self-organization and the Emergence of Complexity in Ecological Systems", *BioScience*, **55**(12), pp 1075-1079.

Levin, S A (2006), "Learning to Live in a Global Commons: Socioeconomic Challenges for a Sustainable Environment", *Ecological Research*, **21**, pp 328-333.

Lighthill, J (1986), "The Recently Recognized Failure of Predictability in Newtonian Mechanics", in *Predictability in Science and Society* (Mason, J, Mathias, P, and Westcott, J H, eds), the Royal Society of London and British Academy, London, pp 35-50.

Lin, Z, and Beck, M B (2007a), "On the Identification of Model Structure in Hydrological and Environmental Systems", *Water Resources Research*, **43**, W02402, doi:10.1029/2005WR004796.

Lin, Z, and Beck, M B (2007b), "Understanding Complex Environmental Systems: A Dual Thrust", *Environmetrics*, **18**(1), pp 11-26.

Lindner, P F O, and Hitzmann, B (2006), "Experimental Design for Optimal Parameter Estimation of an Enzyme Kinetic Process Based on the Analysis of the Fisher Information Matrix", *J Theoretical Biology*, **238**, pp 111-123.

Little, R G (2002), "Controlling Cascading Failure: Understanding the Vulnerabilities of Interconnected Infrastructures", *J Urban Technology*, **9**(1), pp 109-123.

Liu, Y, and Gupta, H V (2007), "Uncertainty in Hydrologic Modeling: Towards an Integrated Data Assimilation Framework", *Water Resources Research*, **43**, W07401, doi:10.1029/2006WR005756.

Liu, Y, Mahmoud, M, Hartmann, H, Stewart, S, Wagener, T, Semmens, D, Stewart, R, Gupta, H V, Dominguez, D, Hulse, D, Letcher, R, Rashleigh, B, Smith, C, Street, R, Ticehurst, J, Twery, M, van Delden, H, and White, D (2009), "Towards a Formal Scenario Development Approach for Environmental Impact Assessment Studies", in *Environmental Modelling and Software and Decision Support — Developments in Integrated Environmental Assessment (DIEA)*, **3**, (A J Jakeman, A Voinov, A E Rizzoli, and S Chen, eds), Elsevier, Oxford, (in press).

Ljung, L (1979), "Asymptotic Behaviour of the Extended Kalman Filter as a Parameter Estimator", *IEEE Transactions on Automatic Control*, **24**, pp 36-50.

Loehle, C (2006), "Control Theory and the Management of Ecosystems", *J Applied Ecology*, **43**, pp 957-966.

Lomborg, B (1998), "*The Skeptical Environmentalist: Measuring the Real State of the World*", Cambridge University Press, Cambridge.

Long, J D, Smalley, G W, Barsby, T, Anderson, J T, and Hay, M E (2007), "Chemical Cues Induce Consumer-specific Defenses in a Bloom-forming Marine Phytoplankton", *Proceedings National Academy of Sciences*, **104**(25), pp 10512-10517.

Luisi, P L (2003), "Autopoiesis: A Review and Reappraisal", *Naturwissenschaften*, **90**, pp 49-59.

MacFarlane, A G J (1990), "Interactive Computing: A Revolutionary Medium for Teaching and Design", *Computing and Control J*, **1**(4), pp 149-158.

Machu, E, and Garçon, V (2001), "Phytoplankton Seasonal Distribution from SeaWiFS Data in the Agulhas Current System", *J Marine Research*, **59**, pp 795-812.

Mahinthakumar, K, von Laszewski, G, Ranjithan, R, Brill, D, Uber, J, Harrison, K, Sreepathi, S, and Zechman, E (2006), "An Adaptive Cyberinfrastructure for Threat Management in Urban Water Distribution Systems", in *ICCS 2006*, (V N Alexandrov and others, eds), Lecture Notes in Computer Science, **3993**(III), pp 401–408.

Maslow, A H (1943), "A Theory of Human Motivation", *Psychological Review*, **50**, pp 370–396.

Matthews, D A, Effler, S W, Brooks Matthews, C M, Siegfried, C A and Spada, M E (2002), "Responses of Onondaga Lake, New York, to Early Stages of Rehabilitation: Unanticipated Ecosystem Feedbacks", *Water Environment Research*, **73**(6), pp 691–703.

Matthies, M, Giupponi, C, and Ostendorf, B (2007), "Environmental Decision Support Systems: Current Issues, Methods and Tools" (preface to special issue of journal), *Environmental Modelling and Software*, **22**(2), pp 123–127.

McDonough, W, and Braungart, M (2002), "*Cradle to Cradle: Remaking the Way We Make Things*", North Point Press, New York.

McGarity, T O, and Wagner, W E (2003), "Legal Aspects of the Regulatory Use of Environmental Modeling", *Environmental Law Reporter*, **33**(10), pp 10751–10774.

McLaughlin, D (2002), "An Integrated Approach to Hydrologic Data Assimilation: Interpolation, Smoothing, and Filtering", *Advances in Water Resources*, **25**, pp 1275–1286.

Mitsch, W J, Day, J W, Gilliam, J W, Groffman, P M, Hey, D L, Randall, G W, and Wang, N (2001), "Reducing Nitrogen Loading to the Gulf of Mexico from the Mississippi River Basin: Strategies to Counter a Persistent Ecological Problem", *BioScience*, **51**(5), pp 373–388.

Mondello, G (2006), "Policy Setting for Sustainable Water Management: GATS Rules and Water Management Systems", in *Sustainable Management of Water Resources: An Integrated Approach* (C Giupponi, A J Jakeman, D Karssenberg, and M P Hare, eds), Edward Elgar, Northampton, Massachusetts, pp 27–46.

Mooney, C (2007), "*Storm World — Hurricanes, Politics, and the Battle Over Global Warming*", Harcourt, Orlando, Florida.

Moorcroft, P R (2006), "How Close Are We to a Predictive Science of the Biosphere?", *TRENDS in Ecology and Evolution*, **21**(7), pp 400–407.

Moore, C, and Doherty, J (2006), "The Cost of Uniqueness in Groundwater Model Calibration", *Advances in Water Resources*, **29**, pp 605–623.

Moradkhani, H, Hsu, K-L, Gupta, H V, and Sorooshian, S (2005a), "Uncertainty Assessment of Hydrologic Model States and Parameters: Sequential Data Assimilation Using the Particle Filter", *Water Resources Research*, **41**, W05012, doi:10.1029/2004WR003604.

Moradkhani, H, Sorooshian, S, Gupta, H V, and Houser, P R (2005b), "Dual State-parameter Estimation of Hydrological Models Using Ensemble Kalman Filter", *Advances in Water Resources*, **28**, pp 135–147.

Morton, A (1993), "Mathematical Models: Questions of Trustworthiness", *British Journal of Philosophy of Science*, **44**, pp 659–674.

Mostert, E (2006), "Participation for Sustainable Water Management", in *Sustainable Management of Water Resources: An Integrated Approach* (C Giupponi, A J Jakeman, D Karssenberg, and M P Hare, eds), Edward Elgar, Northampton, Massachusetts, pp 153–176.

Mugunthan, P, and Shoemaker, C A (2006), "Assessing the Impacts of Parameter Uncertainty for Computationally Expensive Groundwater Models", *Water Resources Research*, **42**(10), W10428, doi:10.1029/2005WR004640.

Mugunthan, P, Shoemaker, C A, and Regis, R G (2005), "Comparison of Function Approximation, Heuristic, and Derivative-based Methods for Automatic Calibration of Computationally Expensive Groundwater Bioremediation Models", *Water Resources Research*, **41**(11), W11427, doi:10.1029/2005WR004134.

NEON (2006), "*Integrated Science and Education for the National Ecological Observatory Network*", Early Release Edition, NEON, 84pp (September).

Neuman, S P (2003), "Maximum Likelihood Bayesian Averaging of Uncertain Model Predictions", *Stochastic Environmental Research and Risk Assessment*, **17**, pp 291–305.

Newbold, J D, Elwood, J W, O'Neill, R V, and Van Winkel, W (1981), "Measuring Nutrient Spiraling in Streams", *Canadian J Fisheries and Aquatic Science*, **38**, pp 860–863.

Nicholson, T J, Babendreier, J E, Meyer, P D, Mohanty, S, Hicks, B B, and Leavesley, G H (2004), "Uncertainty, Sensitivity, and Parameter Estimation for Multimedia Environmental Modeling", Proceedings of International Workshop, *Report* **NUREG/CP-0187**, US Nuclear Regulatory Commission, Washington, DC.

Niemczynowicz, J (1993), "New Aspects of Sewerage and Water Technology", *Ambio*, **22**(7), pp 449-455.

Nowotny, H, Scott, P, and Gibbons, M (2001), "*Re-Thinking Science. Knowledge and the Public in an Age of Uncertainty*", Polity/Blackwell, Malden, Massachusetts.

NRC (2001), "*Grand Challenges in Environmental Sciences*", National Research Council, National Academy Press, Washington, DC, 96pp.

NRC (2002), "*Estimating the Public Health Benefits of Proposed Air Pollution Regulations*", National Research Council, National Academy Press, Washington, DC, 170pp.

NRC (2004), "*Facilitating Interdisciplinary Research*", National Research Council, National Academy Press, Washington, DC, 306pp.

NRC (2007), "*Models in Environmental Regulatory Decision Making*", National Research Council, National Academy Press, Washington, DC, 267pp.

NSF (2003), "Revolutionizing Science and Engineering Through Cyberinfrastructure", *Report of the NSF Blue-Ribbon Advisory Panel on Cyberinfrastructure, January 2003*, National Science Foundation, 84pp.

NSF (2005), "Sensors for Environmental Observatories", *Report of the NSF-sponsored Workshop, December 2004*, National Science Foundation, 64pp.

NSF (2006), "Simulation-Based Engineering Science: Revolutionizing Engineering Science Through Simulation", *Report of the National Science Foundation Blue Ribbon Panel*, National Science Foundation, 65pp.

NSF (2007), "Cyber-Enabled Discovery and Innovation (CDI)", *Program Solicitation* **NSF 07-603** (www.nsf.gov).

Ohtsuki, H, and Iwasa, Y (2006), "The Leading Eight: Social Norms That Can Maintain Cooperation by Indirect Reciprocity", *J Theoretical Biology*, **239**, pp 435-444.

OMB (2001), "Guidelines for Ensuring and Maximizing the Quality, Objectivity, Utility, and Integrity of Information Disseminated by Federal Agencies", Office of Management and Budget (OMB), Executive Office of the President, Washington, DC [Available at www.whitehouse.gov/omb]

OMB (2003), "*Circular A-4*", Office of Management and Budget (OMB), Executive Office of the President, Washington, DC [Available at www.whitehouse.gov/omb]

Omlin, M, Brun, R, and Reichert, P (2001), "Biogeochemical Model of Lake Zürich: Sensitivity, Identifiability and Uncertainty Analysis", *Ecological Modelling*, **141**(1-3), pp 105-123.

Oppenheimer, M, O'Neill, B C, Webster, M, and Agrawala S (2007), "The Limits of Consensus", *Science*, **317**, pp 1505-1506, (14 September).

Oreskes, N (1998), "Evaluation (Not Validation) of Quantitative Models", *Environmental Health Perspectives*, **106**(Supplement 6), pp 1453-1460.

Oreskes, N, Shrader-Frechette, K, and Belitz, K (1994), "Verification, Validation, and Confirmation of Numerical Models in the Earth Sciences", *Science*, **263**, pp 641-646.

ORION Executive Steering Committee (2005), "*Ocean Observatories Initiative Science Plan*", Ocean Research Interactive Observatory Networks (ORION), Washington DC, 102pp.

Osidele, O O, and Beck, M B (2003), "An Inverse Approach to the Analysis of Uncertainty in Models of Environmental Systems", *Integrated Assessment*, **4**(4), pp 265-283.

Osidele, O O, and Beck, M B (2004), "Food Web Modelling for Investigating Ecosystem Behaviour in Large Reservoirs of the South-eastern United States: Lessons from Lake Lanier, Georgia", *Ecological Modelling*, **173**, pp 129-158.

Otterpohl, R, Albold, A, and Oldenburg, M (1999), "Source Control in Urban Sanitation and Waste Management: Ten Systems with Reuse of Resources", *Water Science and Technology*, **39**(5), pp 153-160.

Pang, L, and Hunt, B (2001), "Solutions and Verification of a Scale-dependent Dispersion Model", *J Contaminant Hydrology*, **53**, pp 21-39.

Pascual, P (2005), "Wresting Environmental Decisions From an Uncertain World", *Environmental Law Review*, **35**, ELR, pp 10539-10549.

Pascual, P (2009), "Rational Regulations Through Model Evaluation", *Environmental Science and Technology*, (in press).

Pascual, P, Stiber, N, and Sunderland, E (2003), "*Draft Guidance on the Development, Evaluation, and Application of Regulatory Environmental Models*", Council for Regulatory Environmental Modeling, US Environmental Protection Agency, Washington, DC.

Patt, A (2007), "Assessing Model-based and Conflict-based Uncertainty", *Global Environmental Change*, **17**, pp 37-46.

Petersen, A C (2006), "*Simulating Nature: A Philosophical Study of Computer-Simulation Uncertainties and Their Role in Climate Science and Policy Advice*", Het Spinhuis, Apeldoorn, The Netherlands.

Petersen, A C, Martin, K C, and van der Sluijs, J P (2009), "Dealing with Uncertainty in Environmental Law Making: A Comparative History of Particulate Matter Regulation in the United States and the European Union", *Harvard Environmental Law Review*, (in preparation).

Petersen, B, Gernaey, K, and Vanrolleghem, P A (2001), "Practical Identifiability of Model Parameters by Combined Respirometric-Titrimetric Measurements", *Water Science and Technology*, **43**(7), pp 347-355.

Peterson, G, Allen, C R, and Holling, C S (1998), "Ecological Resilience, Biodiversity, and Scale", *Ecosystems*, **1**, pp 6-18.

Pickett, S T A, Cadenasso, M L, and Grove, J M (2004), "Resilient Cities: Meaning, Models, and Metaphor for Integrating the Ecological, Socio-economic, and Planning Realms", *Landscape and Urban Planning*, **69**, pp 369-384.

Pilkey, O H, and Pilkey-Jarvis, L (2007), "*Useless Arithmetic: Why Environmental Scientists Can't Predict the Future*", Columbia University Press, New York.

Pleau, M, Colas, H, Lavallée, P, Pelletier, G, and Bonin, R (2005), "Global Optimal Real-time Control of the Québec Urban Drainage System", *Environmental Modelling and Software*, **20**(4), pp 401-413.

Poeter, E, and Anderson, D (2005), "Multimodel Ranking and Inference in Ground Water Modeling", *Ground Water*, **43**(4), pp 597-605.

Poff, N L, Allan, J D, Palmer, M A, Hart, D D, Richter, B D, Arthington, A H, Rogers, K H, Meyer, J L, and Stanford, J A (2003), "River Flows and Water Wars: Emerging Science for Environmental Decision Making", *Frontiers in Ecology and Environment*, **1**(6), pp 298-306.

Popper, K R (1972), "*Objective Knowledge: An Evolutionary Approach*", Oxford University Press, Oxford.

Popper, K R (1976), "*The Unending Quest: An Intellectual Autobiography*", Fontana-Collins, Glasgow.

Price, M F, and Thompson, M (1997), "The Complex Life: Human Land Uses in Mountain Ecosystems", *Global Ecology and Biogeographical Letters*, **6**, pp 77-90.

Raicich, F (2006), "The Assessment of Temperature and Salinity Sampling Strategies in the Mediterranean Sea: Idealized and Real Cases", *Ocean Science*, **2**, pp 97-112.

Raick, C, Soetart, K, and Grégoire, M (2006), "Model Complexity and Performance: How Far Can We Simplify?", *Progress in Oceanography*, **70**, pp 27-57.

Railsback, S F (2001), "Concepts from Complex Adaptive Systems as a Framework for Individual-based Modelling", *Ecological Modelling*, **139**, pp 47-62.

Rayner, S (2008), As reported in the Record of a Workshop on "A New Look at the Interaction of Scientific Models and Policymaking", Policy Foresight Programme, The James Martin 21st Century School, University of Oxford, UK (available at http://www.martininstitute.ox.ac.uk/jmi/networks/Policy+Foresight+Programme.htm)

Reckhow, K H (1999), "Water Quality Predictions and Probability Network Models", *Canadian J Fisheries and Aquatic Sciences*, **56**, pp 1150-1158.

Rees, W E, "Ecological Footprints and Appropriated Carrying Capacity: What Urban Economics Leaves Out", *Environment and Urbanization*, **4**(2), pp 121-130.

Rees, W E, and Wackernagel, M (1996), "Urban Ecological Footprints: Why Cities Cannot Be Sustainable — and Why They Are Key to Sustainability", *Environmental Impact Assessment and Review*, **16**, pp 223-248.

Refsgaard, J-C, van der Sluijs, J P, Brown, J, and van der Keur, P (2006), "A Framework for Dealing with Uncertainty Due to Model Structure Error", *Advances in Water Resources*, **29**, pp 1586-1597.

Reichert, P, Borsuk, M E, Hostmann, M, Schweizer, S, Spörri, C, Tockner, K, and Truffer, B (2007), "Concepts of Decision Support for River Rehabilitation", *Environmental Modelling and Software*, **22**(2), pp 188-201.

Rinaldi, S M, Peerenboom, J P, Kelly, T K (2001), "Identifying, Understanding, and Analyzing Critical Infrastructure Dependencies", *IEEE Control Systems Magazine*, December, pp 11-25.

Risbey, J, Kandlikar, M, and Patwardhan, A (1996), "Assessing Integrated Assessments", *Climatic Change*, **34**, pp 369-395.

Rizzoli, A E, and Argent, R M (2006), "Software and Software Systems: Platforms and Issues for IWRM Problems", in *Sustainable Management of Water Resources: An Integrated Approach*, (C Giupponi, A J Jakeman, D Karssenberg, and M P Hare, eds), Edward Elgar, Northampton, Massachusetts, pp 324-346.

Robinson, A B, Robinson, N E, and Soon, W (2007), "Environmental Effects of Increased Atmospheric Carbon Dioxide", *J American Physicians and Surgeons*, **12**, pp 79-90.

Romanowicz, R J, Young, P C, and Beven, K J (2006), "Data Assimilation and Adaptive Forecasting of Water Levels in the River Severn Catchment, United Kingdom", *Water Resources Research*, **42**, W06407, doi:10.1029/2005WR004373.

Rosen, C, Rieger, L, Jeppsson, U, and Vanrolleghem, P A (2008), "Adding Realism to Simulated Sensors and Actuators", *Water Science & Technology*, **57.3**, pp 337-344.

Ruardij, P, Veldhuis, M J W, and Brussaard, C P D (2005), "Modeling the Bloom Dynamics of the Polymorphic Phytoplankter *Phaeocystis globosa*: Impact of Grazers and Viruses", *Harmful Algae*, **4**, pp 941-963.

Running, S W, Baldocchi, D D, Turner, D P, Gower, S T, Bakwin, P S, and Hibbard, K A (1999), "A Global Terrestrial Monitoring Network Integrating Tower Fluxes, Flask Sampling, Ecosystem Modeling and EOS Satellite Data", *Remote Sensing and Environment*, **70**, pp 108-127.

Sacks, W J, Schimel, D S, and Monson, R K (2007), "Coupling Between Carbon Cycling and Climate in a High-elevation, Subalpine Forest: A Model-data Fusion Analysis", *Oecologia*, **151**, pp 54-68.

Saikaly, P E, and Oerther, D B (2004), "Bacterial Competition in Activated Sludge: Theoretical Analysis of Varying Solids Retention Times on Diversity", *Microbial Ecology*, **48**, pp 274-278.

Saltelli, A, Chan, K, and Scott, E M (eds) (2000), "*Sensitivity Analysis*", Wiley, Chichester, 475pp.

Sanderson, W C (1994), "Simulation Models of Demographic, Economic, and Environmental Interactions", in *Population, Development, Environment: Understanding Their Interactions in Mauritius*, (W Lutz, ed), Springer, Berlin, pp 33-71.

Schaffer, S (1993), "Comets and the World's End", in *Predicting the Future* (L Howe and A Wain, eds), Cambridge University Press, Cambridge, pp 52-76.

Schellnhuber, H J (1999), "'Earth System' Analysis and the Second Copernican Revolution", *Nature*, **402**(Supp), pp C19-C23 (2 December).

Schellnhuber, H J, Crutzen, P J, Clark, W C, and Hunt, J (2005), "Earth System Analysis for Sustainability", *Environment*, **47**(8), pp 12-25.

Schertzer, W M, and Lam, D C L (2002), "Lake Erie and Evolving Issues of the Quality of its Water", in *Environmental Foresight and Models: A Manifesto* (M B Beck, ed), Elsevier, Oxford, pp 105-130.

Schröder, B (2006), "Pattern, Process, and Function in Landscape Ecology and Catchment Hydrology — How Can Quantitative Landscape Ecology Support Predictions in Ungauged Basins?", *Hydrology and Earth System Sciences*, **10**(6), pp 967-979.

Schröder, B, and Seppelt, R (2006), "Analysis of Pattern-process Interactions Based on Landscape Models — Overview, General Concepts, and Methodological Issues", *Ecological Modelling*, **199**, pp 505-516.

Schröter, D, Cramer, W, Leemans, R, Prentice, I C, Araújo, M B, Arnell, N W, Bondeau, A, Bugmann, H, Carter, T R, Gracia, C A, de la Vega-Leinert, A C, Erhard, M, Ewert, F, Glendining, M, House, J I, Kankaanpää, S, Klein, R J T, Lavorel, S, Lindner, M, Metzger, M J, Meyer, J, Mitchell, T D, Reginster, I, Rounsevell, M, Sabaté, S, Sitch, S, Smith, B, Smith, J, Smith, P, Sykes, M T, Thonicke, K, Thuiller, W, Tuck, G, Zaehle, S, and Zierl, B (2005), "Ecosystem Service Supply and Vulnerability to Global Change in Europe", *Science*, **310**, pp 1333-1337 (25 November).

Schütze, M R, Butler, D, and Beck, M B (2002), "*Modelling, Simulation, and Control of Urban Wastewater Systems*", Springer, Berlin.

Schwarz, M, and Thompson, M (1990), "*Divided We Stand: Redefining Politics, Technology, and Social Choice*", University of Pennsylvania Press, Philadelphia.

Schweitzer, F (2003), "*Brownian Agents and Active Particles: Collective Dynamics in the Natural and Social Sciences*", Springer, Berlin.

SIWI-IWMI (2004), "*Water — More Nutrition Per Drop. Towards Sustainable Food Production and Consumption Patterns in a Rapidly Changing World*", Policy Paper, Stockholm International Water Institute (SIWI) and International Water Management Institute (IWMI), Stockholm, Sweden, 35pp.

Sokka, L, Antikainen, R, and Kauppi, P (2004), "Flows of Nitrogen and Phosphorus in Municipal Waste: A Substance Flow Analysis in Finland", *Progress in Industrial Ecology*, **1**(1-3), pp 165-186.

Spitz, Y H, Moisan, J R, and Abbott, M R (2001), "Configuring an Ecosystem Model Using Data from the Bermuda Atlantic Time Series (BATS)", *Deep-Sea Research II*, **48**, pp 1733-1768.

Stahel, W R (1997), "The Service Economy: 'Wealth Without Resource Consumption'?", *Philosophical Transactions of the Royal Society of London*, A **355**, pp 1309-1319.

Stigter, J D, Vries, D, and Keesman, K J (2006), "On Adaptive Optimal Input Design: A Bioreactor Case Study", *AIChE J*, **52**(9), pp 3290-3296.

Strayer, D L, Caraco, N F, Cole, J J, Findlay, S and Pace, M L (1999), "Transformation of Freshwater Ecosystems by Bivalves: A Case Study of Zebra Mussels in the Hudson River", *BioScience*, **49**(1), pp 19-27.

Sumaila, U R, and Walters, C J (2005), "Intergenerational Discounting: A New Intuitive Approach", *Ecological Economics*, **52**, pp 135-142.

Tao, S, Cao, H, Liu, W, Li, B, Cao, J, Xu, F, Wang, X, Coveney, R M, Shen, W, Qin, B, and Sun, R (2003), "Fate Modeling of Phenanthrene with Regional Variation in Tianjin, China", *Environmental Science and Technology*, **37**, pp 2453-2459.

Thompson, M (1985), "Decision Making Under Contradictory Certainties: How to Save the Himalayas When You Can't Find Out What's Wrong With Them", *Applied Systems Analysis*, **12**, pp 3-34.

Thompson, M (1997), "Cultural Theory and Integrated Assessment", *Environmental Modeling and Assessment*, **2**, pp 139-150.

Thompson, M (2004), "Technology and Democracy: A Cultural Theory Approach", in *Power and Democracy: Critical Interventions*, (F Engelstad and Ø Østerud, eds), Ashgate, Aldershot, pp 185-208.

Thompson, M, and Gyawali, D (2007), "Uncertainty Revisited or the Triumph of Hype Over Experience", New Introduction, Republication of Thompson, M, Warburton, M, and Hatley, T, "*Uncertainty on a Himalayan Scale*", (Milton Ash Editions, Ethnographica, London, 1986), Himal Books, Lalitpur, Nepal.

Thompson, M, Ellis, R, and Wildavsky, A (1990), "*Cultural Theory*", West View, Boulder, Colorado.

Tillman, T, Larsen, T A, Pahl-Wostl, C and Gujer, W (2001), "Interaction Analysis of Stakeholders in Water Supply Systems", *Water Science and Technology*, **43**(5), pp 319-326.

Torres, R, Allen, J I, Figueiras, F G (2006), "Sequential Data Assimilation in an Upwelling Influenced Estuary", *J Marine Systems*, **60**, pp 317-329.

Tsai, J C C, Chen, V C P, Beck, M B, and Chen J (2004), "Stochastic Dynamic Programming Formulation for a Wastewater Treatment Decision-making Framework", *Annals of Operations Research*, **132**, pp 207-221.

Tushingham, A M, and Peltier, W R (1992), "Validation of the ICE-3G Model of Würm-Wisconsin Deglaciation Using a Global Data Base of Relative Sea Level Histories", *J Geophysical Research*, **97**(B3), pp 3285-3304.

Vaché, K B, and McDonnell, J J (2006), "A Process-based Rejectionist Framework for Evaluating Catchment Runoff Model Structure", *Water Resources Research*, **42**, W02409, doi:10.1029/2005WR004247.

van Asselt, M B A and Rotmans, J (1996), "Uncertainty in Perspective", *Global Environmental Change*, **6**(2), pp 121-157.

van Asselt, M B A and Rotmans, J (2002), "Uncertainty in Integrated Assessment Modelling: from Positivism to Pluralism", *Climatic Change*, **54**, pp 75-105.

van der Sluijs, J P (2002), "A Way Out of the Credibility Crisis for Models Used in Integrated Environmental Assessment", *Futures*, **34**, pp 133-146.

van der Sluijs, J P (2007), "Uncertainty and Precaution in Environmental Management: Insights From the UPEM Conference", *Environmental Modelling and Software*, **22**, pp 590-598.

van der Sluijs, J P, van Eijndhoven, J, Shackley, S, and Wynne, B (1998), "Anchoring Devices in Science for Policy: the Case of Consensus Around Climate Sensitivity", *Social Studies in Science*, **28**(2), pp 291-323.

Vanrolleghem, P A, Kong, Z, and Coen, F (1996), "Full-scale On-line Assessment of Toxic Wastewaters Causing Change in Biodegradation Model Structure and Parameters", *Water Science and Technology*, **33**(2), pp 163-175.

Vanrolleghem, P A, Benedetti, L, and Meirlaen, J (2005), "Modelling and Real-time Control of the Integrated Urban Wastewater System", *Environmental Modelling and Software*, **20**(4), pp 427-442.

Veldhuis, M J W, and Wassmann, P (2005), "Bloom Dynamics and Biological Control of a High Biomass HAB species in European Coastal Waters: A *Phaeocystis* Case Study", *Harmful Algae*, **4**, pp 805-809.

Voit, E O, Neves, A R, and Santos, H (2006), "The Intricate Side of Systems Biology", *Proceedings National Academy of Science*, **103** (25), pp 9452-9457 (20 June).

von Winterfeld, D, and Edwards, W (1986), "*Decision Analysis and Behavioural Research*", Cambridge University Press, Cambridge.

Wagener, T, McIntyre, N, Lees, M J, Wheater, H S, and Gupta, H V (2003), "Towards Reduced Uncertainty in Conceptual Rainfall-runoff Modelling: Dynamic Identifiability Analysis", *Hydrological Processes*, **17**, pp 455-476.

Wang, G (2007), "On the Latent State Estimation of Nonlinear Population Dynamics Using Bayesian and Non-Bayesian State-space Models", *Ecological Modelling*, **200**, pp 521-528.

WATERS (2007a), "An Engineering Research Plan for the WATERS Network", Report, Environmental Engineering and Science Committee (C Driscoll and D Reible, Co-Chairs), WATERS Network Project Office, Arlington, Virginia.

WATERS (2007b), "Education Plan for WATERS Net Incorporated", Report, Education Committee (E Eschenbach and J Johnson, Co-Chairs), WATERS Network Project Office, Arlington, Virginia.

WATERS (2008), "Draft Science, Education, and Design Strategy for the WATer and Environmental Research Systems Network", *Report*, WATERS Network Project Office, Arlington, Virginia, (February).

Watts, J B (1993), Personal communication (June).

Watts, D J (2002), "A Simple Model of Global Cascades on Random Networks", *Proceedings National Academy of Sciences*, **99**(9), pp 5766-5771.

Wheater, H S, Bishop, K H, and Beck, M B (1986), "The Identification of Conceptual Hydrological Models for Surface Water Acidification", *Hydrological Processes*, **1**, pp 89-109.

White, A B, Kumar, P, and Tcheng, D (2005), "A Data Mining Approach for Understanding Topographic Control on Climate-induced Inter-annual Vegetation Variability over the United States", *Remote Sensing of Environment*, **98**, pp 1-20.

Whitfield, P H, and Dohan, K (1997), "Identification and Characterization of Water Quality Transients Using Wavelet Analysis. II Application to Electronic Water Water Quality Data", *Water Science and Technology*, **36**(5), pp 337-348.

Wilby, R L, Whitehead, P G, Wade, A J, Butterfield, D, Davis, R J, and Watts, G (2006), "Integrated Modeling of Climate Change Impacts on Water Resources and Quality in a Lowland Catchment: River Kennet, UK", *J Hydrology*, **330**, pp 204-220.

Williams, M, Schwarz, P A, Law, B E, Irvine, J, and Kurpius, M R (2005), "An Improved Analysis of Forest Carbon Dynamics Using Data Assimilation", *Global Change Biology*, **11**, pp 89-105.

Woldt, W, and Dahab, M (2006), "Adaptive Management of Community Water and Wastewater Infrastructure: A Conceptual Approach", in Proceedings American Water Resources Association (AWRA) Conference on *Adaptive Management of Water Resources*, Missoula, Montana, (June).

Wolman, A (1965), "The Metabolism of Cities", *Scientific American*, **213**(3), pp 179-90.

Wood, E F (ed) (1980), "*Real-Time Forecasting/Control of Water Resource Systems*", Pergamon, Oxford.

Woods, J D (2005), "The Lagrangian Ensemble Metamodel for Simulating Plankton Ecosystems", *Progress in Oceanography*, **67**, pp 84-159.

Wu, J, Zheng, C, and Chien, C C (2005), "Cost-effective Sampling Network Design for Contaminant Plume Monitoring Under General Hydrogeological Conditions", *J Contaminant Hydrology*, **77**, pp 41-65.

Wylie, B K, Fosnight, E A, Gilmanov, T G, Frank, A B, Morgan, J A, Haferkamp, M R, and Meyers, T P (2007), "Adaptive Data-driven Models for Estimating Carbon Fluxes in the Northern Great Plains", *Remote Sensing of Environment*, **106**, pp 399-413.

Ye, M, Pan, F, Wu, Y-S, Hu, B X, Shirley, C, and Yu, Z (2007), "Assessment of Radionuclide Transport Uncertainty in the Unsaturated Zone of Yucca Mountain", *Advances in Water Resources*, **30**, pp 118-134.

Young, P C (1978), "General Theory of Modelling Badly Defined Systems", in *Modelling, Identification and Control in Environmental Systems*, (G C Vansteenkiste, ed), Elsevier, New York, pp 103-135.

Young, P C (1984), "*Recursive Estimation and Time Series Analysis: An Introduction*", Springer, New York.

Young, P C (1998), "Data-based Mechanistic Modelling of Environmental, Ecological, Economic and Engineering Systems", *Environmental Modelling and Software*, **12**, pp 105-122.

Young, P C, and Parkinson, S (2002), "Simplicity out of Complexity", in *Environmental Foresight and Models: A Manifesto* (M B Beck, ed), Elsevier, Oxford, pp 251-301.

Young, P C, and Ratto, M (2008), "A Unified Approach to Environmental Systems Modeling", *Stochastic Environmental Research and Risk Assessment*, DOI10.1007/s00477-008-0271-1.

Young, P C, Hornberger, G M, and Spear, R C (1978), "Modelling Badly Defined Systems — Some Further Thoughts", *Proceedings, SIMSIG Simulation Conference*, Australian National University, Canberra, pp 24-32.

Zimmerman, R (2001), "Social Implications of Infrastructure Network Interactions", *J Urban Technology*, **8**(3), pp 97-119.