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## **Prediction and Uncertainty in Computational Modeling of Complex Phenomena: A Whitepaper**

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# Prediction and Uncertainty in Computational Modeling of Complex Phenomena: A Whitepaper

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## Abstract\*

This report summarizes some challenges associated with the use of computational science to predict the behavior of complex phenomena. As such, the document is a compendium of ideas that have been generated by various staff at Sandia. The report emphasizes key components of the use of computational to predict complex phenomena, including computational complexity and correctness of implementations, the nature of the comparison with data, the importance of uncertainty quantification in comprehending what the prediction is telling us, and the role of risk in making and using computational predictions. Both broad and more narrowly focused technical recommendations for research are given. Several computational problems are summarized that help to illustrate the issues we have emphasized. The tone of the report is informal, with virtually no mathematics. However, we have attempted to provide a useful bibliography that would assist the interested reader in pursuing the content of this report in greater depth.

\*Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under Contract DE-AC04-94AL85000.



# Acknowledgment

This report summarizes input from many staff at Sandia, including John Aidun, Roy Baty, Rob Easterling, Eliot Fang, Richard Fye, Grant Heffelfinger, Sorin Istrail, Marlin Kipp, Dave Martinez, Bill Oberkampf, Tom Paez, Rich Pryor, John Red-Horse, Andrew Salinger, Mark Stevens, and David Womble. While it is being released under a single author's name, the potential reader should always keep in mind that the work represented here was a fully collaborative effort on the part of many people. The primary content was originally developed as a position paper on the subject of a new DOE Mathematics, Information, and Computer Science program in "Prediction of Complex Phenomena." Because of wider interest in the paper, we have elected to release it as a Sandia Report. We would like to thank Gene Hertel and Dan Carroll for reviewing this report.

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# Executive Summary

The purpose of this paper is to discuss some of the issues that we feel are important to prediction and uncertainty in the modeling of complex phenomena. Complex phenomena tend to have in common strongly nonlinear and tightly coupled physics, stochastic-like behavior, and the need for many spatial and temporal scales. Typical examples of what we mean by “complex phenomena” include: (1) climate modeling; (2) protein folding; (3) behavior of populations, as in agent-based economic modeling; and (4) materials aging problems associated with the Department of Energy (DOE) Science Based Stockpile Stewardship Program (SBSS). It is a paradigm that the main general method for producing quantitative predictions from models of such complex phenomena is through computation. This observation will underlie all of our subsequent discussion. With this in mind, we observe that these problems lie at the current frontier of computational difficulty. In fact, these and similar problems motivate the ongoing acceleration of computing hardware capability beyond the Tera-Op regime.

Because computation is such an important tool, we are naturally stimulated to study questions associated with computational complexity, efficient algorithm design, and correct implementation of these algorithms. However, focusing a discussion of prediction of complex phenomena only on the accuracy of fundamental models, numerical algorithms, and computational implementations misses certain additional important issues.

We suggest that the process of prediction is actually a complex interaction between the mechanics of computational simulation, the comparison with the real world, and the understanding that hopefully results from this effort. We must formally deal with several concepts to provide an appropriate framework to discuss prediction, including **Science**, **Uncertainty**, **Computation**, and **Data**, as well as **Prediction**. By “Science”, we mean the fundamental models that we use to describe the phenomenon. “Uncertainty” means the full range of uncertainty that enters into any prediction of the phenomenon, such as model, parametric, algorithmic, computational, as well as uncertainty in the basic data that are used to compare with the prediction. “Computation” includes both fundamental and practical algorithm issues, as well as implementation characteristics. “Prediction” includes constraints, such as associated consequences of the prediction, timeliness and accuracy requirements, as well as the formal predictive content of the model itself. “Data” enter in both the simulation of the phenomenon, as well as in assessments of the quality of the prediction, which is typically referred to as “Comparison with data.” The goal for performing a prediction is not isolated. Rather, we seek “Comprehension,” the achievement of better understanding of the phenomenon. The process is ultimately iterated, in a continual effort to improve our next prediction.

Capability for prediction is applied simultaneously to improve our fundamental comprehension of complex phenomena as well as to apply this comprehension to the solution of specific problems. One element in the struggle to be predictive is *predictive confidence*, in which we claim measurable confidence in the accuracy, hence utility, of our predictions. Another element is *predictive consequence*, in which we must deal with the possibilities that our predictions are insufficiently accurate for their planned application.

When high consequence is associated with the use of a prediction of a complex phenomenon, the element of risk increases drastically. Thus, in addition to the study of fundamental models, algorithms, and implementations, we must also quantitatively assess consequence in the application of a complex phenomenon model. Finally, we must define and quantify the full range of uncertainty associated with the complex phenomenon. High consequence applications are an important type of prediction that we are concerned with. In the main body of this paper, we introduce the notions of low-consequence and high-consequence prediction, to emphasize that consequence is an important factor in prediction.

As the consequence of an intended application increases, so does the importance of uncertainty quantification. For example, developing and implementing a clever two-phase flow algorithm, followed by publication in a journal such as the *Journal of Computational Physics*, is one end of the spectrum. Actually applying that algorithm in a formal nuclear reactor safety assessment is quite another. The consequences associated with publishing versus a reactor safety certification are worlds apart. It is our attempt to deal with this issue that leads us to fundamental questions about the nature of uncertainty in our simulations.

Uncertainty is in reciprocal relation to predictive content of complex phenomena models - as uncertainty increases, predictive content decreases. Uncertainty is currently studied technically using stochastic methods. Thus, if we include uncertainty in our discussion of prediction, we are also viewing the predictive content of our models in a stochastic manner. There is no reason to believe that the current technical emphasis on stochastic methods for analyzing uncertainty will change in the future. One of the best current applications for these stochastic approaches is found in the fields of nuclear reactor safety and waste repository assessment. This work has been evolving for more than thirty years. We believe that much of the existing work in these fields can be applied more generally to uncertainty quantification in many of the complex phenomena of interest to us.

The important technical problems to be solved in performing stochastic uncertainty quantification include application of statistical design of experiments to computational studies, propagation of uncertainty associated with model inputs to the model outputs, and improving our knowledge in a cyclical way via comparison with data. The latter task is a difficult inverse problem, and is commonly considered to be a natural application for Bayesian statistical inference. We say more about these problems in the main body of this report. Here we simply stress that while significant research problems underlie the solution of these problems for application to general complex phenomena, there are also a wide variety of existing methodologies that can be applied. A well-designed program needs to strike a balance between research and use of existing methodologies.

Serious efforts are underway at Sandia to introduce uncertainty-based technology in engineering and scientific simulations related to our DOE missions. We also generically refer to these efforts as “non-deterministic modeling.” Reduction of uncertainty is the most obvious goal of this effort. Our view is that uncertainty can be reduced only if we can

- Develop detailed identification of uncertainty in specific simulation tasks.

- Quantify uncertainty in such a way that statistical inference can be utilized.

Learn how to properly use this quantitative inferential framework in our simulation environment. We will refer to this as developing *uncertainty-based comprehension and engineering practice*.

In the body of this paper, we give three examples of recent complex phenomena studies at Sandia: an application in computational materials science, the prediction of tertiary structure in proteins, and a micro-agent-based macroeconomic model. These examples help illustrate critical interactions in attempting to "predict" complex phenomena, which we characterize with the following questions:

**C**omputation - How do we actually compute the complex phenomena?

**C**omparison - How do we compare our calculations with "reality"?

**C**omprehension - How do we know how predictive we really are?

These questions are canonical. Any programmatic attack on the problem of prediction of some specific complex phenomenon must to some degree attempt to answer all of these questions.

In the main body of this report, we recommend topics of a general nature that should be addressed as part of a broad research program in prediction of complex phenomena. A subset of these topics are given below, in no particular order by importance.

- We need scientific methodologies for accurate risk assessment associated with prediction of complex phenomena. Typical questions that should be answered are: Where does low consequence prediction end and high consequence prediction begin? How do we measure, let alone control, the risk attendant with high consequence applications in our simulations? We expect systems or operations research approaches to be particularly useful, as well as ideas in statistical quality control. A good starting point for applicable methodologies seems to be the nuclear reactor safety and waste repository assessment communities.
- We continue to be driven in practical problems by the need for algorithmic approaches that reduce fundamental computational "complexity", as in the protein folding problem. Is it possible to uncover powerful general principles that can guide algorithm development in the future for such combinatorially complex problems?
- What new ideas for comparing data with predictions from very complex simulations are likely to be effective? For example, how do we compare a multi-scale model which directly calculates from atomic scales to continuum scales with "data?" Are there more refined methods for assessing data quality and data importance applicable to the comparison of data with predictions of complex phenomena? What weight should specific data be given when comparing with a prediction to properly measure the predictive content of the simulation? In other words, which data count more heavily when we are trying to assess the predictive quality of simulations of complex phenomena?

- The entire framework for prediction of complex phenomena, boiled down to a core of “compute, compare, and comprehend”, probably requires new ideas to be executed in an optimal manner. We know that we are currently outstripping our ability to understand the largest problems that are running on our largest current massively parallel computers. This is because our interfaces to the data, such as graphical tools, lag the current rapid growth in computing power. What graphical tools are required to optimize the information we gain by performing comparisons with data. Another relevant issue, especially for high consequence simulations, is how do we deal with the possibility of human error in performing and analyzing such simulations. How can we minimize the potential impact of human error in performing simulations of complex phenomena for high consequence applications? Can we quantify the uncertainties that result from the potential for human error?

We also have given recommendations regarding particular technical issues that have arisen in our current computational work at Sandia. We list a few of these below to give a hint as to the nature of these recommendations. We suggest that any or all of these issues are specific technical topics which are relevant to the study of prediction of complex phenomena.

- We need continued research and development of advanced molecular dynamics and advanced Monte Carlo methods. These techniques are increasingly important for small scales in multi-scale problems (e. g. cracking prediction, microstructural evolution, etc.). Advanced Monte Carlo techniques might also be leveraged for uncertainty propagation sampling strategies. Better understanding of extreme statistics from Monte Carlo calculations is additionally of physical interest, as well as useful for quantitative uncertainty assessment.
- General approaches for multi-time scale and multi-length scale problems are needed, Multi-scale methods appropriate for long-time problems seem to be particularly needed. How careful (rigorous) do we have to be in blending different length/time scale approaches in unified simulation frameworks?
- What are the key issues that are driven by computational complexity when we study predictability of complex phenomena? For example, how important and canonical is the strategy of replacing a complex phenomenon by one which is approximate but solvable with polynomial time algorithms?
- How do we progress beyond operator splitting - the approximate weak coupling or full decoupling of physics - in simulation of strongly coupled, physically complex systems?
- We recommend continued study of the connections between recent computer science developments, for example, and statistical mechanics.
- Well-validated computational libraries for complex phenomena studies should be developed. This involves sharing and standardization, as well as procedures for determining candidate algorithms.

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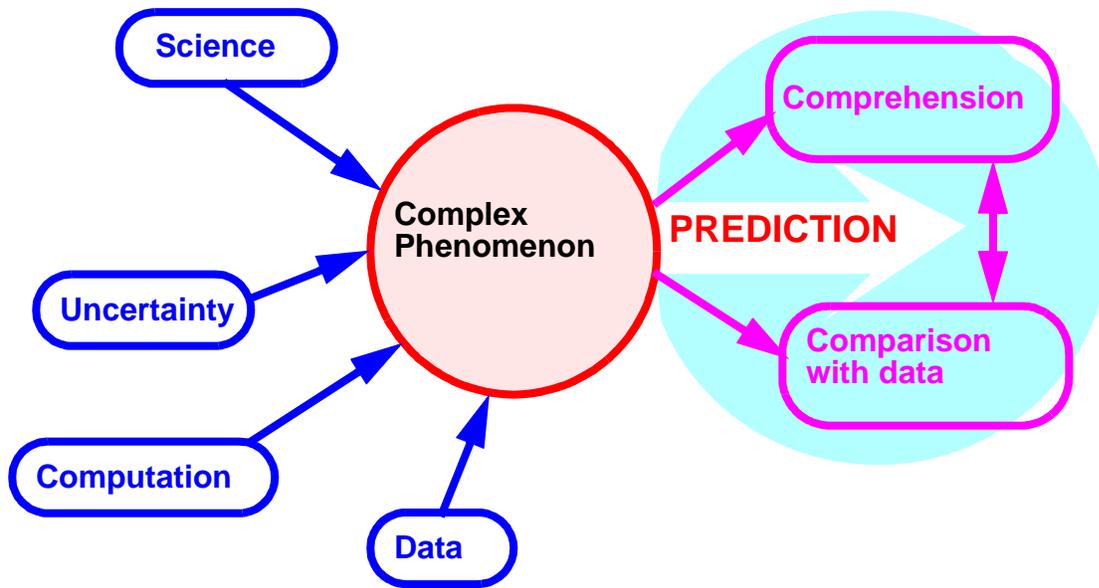
## 1. Introduction

The purpose of this paper is to discuss some of the issues that we feel are important to the modeling of complex phenomena, focusing on prediction and uncertainty in the modeling of such phenomena. As will be clear in the following, we view the latter concepts as reciprocal to one another. In other words, the quality of being predictable is in inverse relationship to the quality of being uncertain. In a purely operational sense, therefore, predictive confidence will and should logically increase when our determined uncertainty is reduced. Thus, we should attempt to reduce uncertainty in studies of complex phenomena if we hope to produce reasonable predictions. Much of what we are attempting when we predict complex phenomena is also nuanced by the overall need to be performing non-deterministic prediction. This view will be clarified below, but we emphasize that what is involved is larger than the fact that the physical phenomena themselves might be non-deterministic.

The study of complex phenomena is a battleground. Elements of fundamental science, large-scale computation, complicated experimental data, and uncertainties associated with these components fiercely mix in our efforts to develop meaningful predictions. We schematically depict the overall complex phenomenon prediction process in Figure 1.

We have suggested in Figure 1 that the process of prediction is actually a complex interaction between the mechanics of computational simulation, the comparison with the real world, and the understanding that hopefully results from this effort. By “Science”, we mean the fundamental models that we use to describe the phenomenon. “Uncertainty” means the full range of uncertainty that enters into any prediction of the phenomenon, such as model, parametric, algorithmic, computational, as well as uncertainty in the basic data that are used to compare with the prediction. “Computation” includes both fundamental and practical algorithm issues, as well as implementation characteristics. “Prediction” includes constraints, such as associated consequences of the prediction, timeliness and accuracy requirements, as well as the formal predictive content of the modeling itself. “Data” enter in both the simulation of the phenomenon, as well as in assessments of the quality of the prediction, “Comparison with data.” Finally, “Comprehension” implies that the goal for performing a prediction to begin with is not isolated. Rather, we seek to use prediction to achieve better understanding of the phenomenon, and then iterate to improve our next prediction.

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**Figure 1.** Components for prediction of complex phenomena.

The factors of computational predictability or uncertainty that are commonly discussed and analyzed are (1) algorithmic errors and inaccuracy; (2) software implementation errors; and (3) fundamental model inaccuracies. However, in our view there are two additional challenges associated with attempts to increase the predictive content of simulations of complex phenomena. These additional challenges are the association of *application consequence* with the computational model and the *full range of uncertainty* which must be captured in quantifying the uncertainty of a prediction.

Prediction is applied simultaneously to improve our fundamental comprehension of complex phenomena as well as to apply this comprehension to the solution of specific problems. One element in the effort to be predictive is *predictive confidence*, in which we claim measurable confidence in the accuracy, hence utility, of our predictions. Another element is *predictive consequence*, in which we must deal with the possibility that our predictions are insufficiently accurate for their planned application. When high consequence is associated with the use of a prediction of a complex phenomenon, the element of risk associated with an incorrect or insufficiently accurate prediction increases drastically. We might normally ask whether our prediction was right or wrong according to some chosen measure. Paying attention to consequence of the application of the prediction, on the other hand, the question we now must ask is whether our prediction is *good enough* for the intended application.

We believe that important issues are ignored if we focus only on the accuracy of fundamental models, algorithms, and their implementations. In fact, this concern is more properly the subject of *verification* - demonstrating the correctness of the implementation and accuracy of the algorithms - and *validation* - demonstrating the correctness of the fundamental models. Achieving verification and validation is often summarized by the simple statements “solving the equations correctly” and “solving the correct equations,”

respectively. (See Knepell and Arangno [25] or the Defense Modeling and Simulation Organization (DMSO) document [37] for relevant discussions of verification and validation. In general, this topic is beyond the scope of this paper.)

That something important is missing is simply illustrated by one example. Suppose that we are given a verified and validated numerical model (assuming this is even possible to begin with), so that we are solving the correct equations correctly. Apply this code to a high-consequence application, such as climate or a nuclear weapon. A human being must do this. How do we deal with the possibility that our human user may make a variety of errors in the use of the code, such as a bad specification of the problem to be solved? Scientists and code developers might argue that such a question is beyond the scope of their charter, and so not appropriate for discussing problems of prediction of complex phenomena. However, this issue is a clear and large component in the overall quantification of uncertainty associated with that high-consequence modeling activity and so part of our subject. It is also interesting that such a question becomes more important as the consequence of the application increases. Thus, the range of uncertainty that should be understood is related to the consequence of the application.

Our view is that uncertainty is a fundamentally stochastic concept. Probabilistic indeterminacy has been fundamental in modeling of complex phenomena for as long as we have had formal definitions of probability. Whether we are discussing stochastic variation in manufactured parts, or whether we are applying a Monte Carlo algorithm to compute a prediction of a complex phenomenon, direct treatment of stochastic behavior has been one of our tools for prediction for the past century. However, we now also include the probability of having incorrectly parameterized fundamental models, of having incorrect values for the parameters, of making mistakes in either execution of a simulation or in the analysis of its results. Worrying about these possibilities under a logical umbrella of probability is more akin to work that has been done for the past thirty years in nuclear reactor safety studies and waste management than in classical non-deterministic physics and engineering.

If “predictive” is indeed the reciprocal of “uncertain”, then the result is that necessary concepts of prediction themselves are stochastic. This statement demands that “confidence assessments” associated with high-consequence computational simulation go well beyond the classic concerns of numerical analysis. We believe that this is true, and that simple principles can be defined which clarify the need for stochastic inference in discussions of prediction for complex phenomena.

Having set the stage, we will now summarize the content of the remainder of this paper. Section 2 will expand our above discussion. The main point of that section is that an important variable for consideration in the discussion of prediction of high consequence phenomena is the product of consequence and complexity, not simply isolated measures of the two. Our argument, of course, is mere persuasion. Theorems are lacking in this area. We will discuss the broad scope of modeling uncertainty in Section 3, as well as its influence on prediction. We will also discuss particular issues related to the propagation of uncertainty in simulations and the need to optimize the inferential content of simulations in

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the presence of uncertainty. The only equations that appear in this paper are presented in this section. Particular, and particularly difficult, complex phenomena modeling activities at Sandia are sampled in Section 4. A major reason for doing this is to make more concrete our philosophical framework, as well as to guide the reader's thinking as they move into Section 5. There, we give our recommendations regarding important needs and future directions for any program which seeks to address uncertainty and prediction of complex phenomena. Finally, we conclude this paper in Section 6 by taking the preacher's advice and saying it all again, in a far less wordy manner of course!

Where our discussion is technically specific, we will tend to mainly focus on applications at Sandia, as well as Sandia bibliographic references. This not because we are parochial, but simply because we understand our own context considerably better than other efforts. This understanding is important for the purposes of this Whitepaper.

## 2. Complex Phenomena and Complex Calculations

### Complex Phenomena - Physical Complexity is Important

The complexity we are concerned with must be described more precisely than to simply say that we are interested in problems which are harder than solving single ordinary differential equations, and easier than predicting the local weather over the United States one year from now. Attempting to specify the "complexity" in complex phenomena, someone with a sense of humor might observe that, while we can't exactly define this complexity, we sure know it when we see it. Recent general references that seek to capture at least some of the broad scope of what "complex" really means are the books of Badii and Politi [2] and Bar-Yam [3].

A more formal attempt at definition could involve comparison with a precise metric of complexity. A complex phenomenon would then be one that satisfies the metric. For example, Feldman and Crutchfield [13] argue in favor of a statistical metric, in which limits of fully ordered and fully disordered systems are considered to be simple, and intermediate systems are (roughly speaking) complex. Such metrics might be algorithmic as well. If computer models which simulate complex phenomena enter the picture we might as well center metrics on the complexity of the code itself.

Anderson [1] has suggested a taxonomy of attributes of complex systems, including algorithmic complexity, complex adaptivity, randomness, and emergence. He also suggests that a truly complex system possibly contains all of the taxonomic features he catalogs. The important point we are stating here is that the way we approach and think about complexity may be more a matter of intellectual *texture* than technical *content*, in the sense that the word "texture" captures a little better the more integrated viewpoint that is required when we examine very complex phenomena. This is certainly a reasonable way to view our difficulties in discussing predictability of these same complex phenomena.

“Emergence” is worth isolating in the context of our focus on simulations. It is generally believed that complexity manifests itself in the emergence of complicated behavior from a collective of simple behaviors. For example, the information that can emerge from simple computational cellular automata can be enormously complex. It is also believed that the emergence of simplicity from seemingly extraordinarily complicated dynamics hints at complexity. An example of this phenomenon is the appearance of coherent structures in turbulent flows.

A simulation framework can also support emergence, even in a formal sense. The ability of simulations to produce emergent behavior is studied abstractly, for example, by Rasmussen and Barrett [31]. Anybody who has spent a fair amount of time performing complex modeling tasks does not need an abstract treatment to know that complicated computer models are likely more than the sum of their parts, possibly producing emergent (and unwanted) behavior in many situations. We might reasonably claim that attempting to make a rational, consequential prediction from an enormous calculation like that performed in climate modeling, or what ASCI hopes to accomplish, is an act of emergent simplicity. Along these lines, a general question is whether or not complex phenomena fundamentally require complex simulations. Conversely, are complex simulations truly representative of the complex phenomena they purport to simulate?

The paper of Brown, *et al* [8] captures important notions of physical complexity in modeling that are present in the examples we present in Section 4. The common drivers for complex phenomena and their correspondingly complex simulations suggested in [8] are nonlinearity, stochasticity, and the presence of multiple time and length scales. In addition, a wide range of physics is usually important. Hence, for example, to perform predictive materials modeling a suitable simulation might utilize micro-scales and quantum mechanics, meso-scales and statistical mechanics, and macro-scales and continuum mechanics, with a dense fabric of nonlinearity and stochasticity coupling these scales tossed in. Such a problem seems to be so physically formidable that we automatically tend to weakly couple or actually decouple the physics when we approach such problems currently. Macro-scales are modeled mainly independently of the micro-scales, for example, with ad hoc prescriptions serving as the only means for providing even weak coupling. This approach has seemed to work in the past mainly because the engineering applications of natural materials have, for the most part, been amenable to macro-scale treatments. Metastable engineered materials, of increasing importance to human technology, are far less amenable to this approach. One of the deep conceptual issues mentioned in [8] is to develop better rational understanding of reductions in the complexity of physics coupling for simulation of complex phenomena.

A similar point could be made about each of the complex phenomena - SBSS, climate, financial (and political) modeling, and so on - which happen to be mentioned in Reference [8]. The general methodological issues that arise in complex phenomena include complexity of “real” data, multi-scale treatments, fundamental versus perceived stochasticity, fundamental measures and treatment of uncertainty in models, and complexity of simulation implementations. These methodological issues are a fundamental

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current running through all of our attempts to predictively simulate complex phenomena and capture a good part of the pulse of the associated complexity.

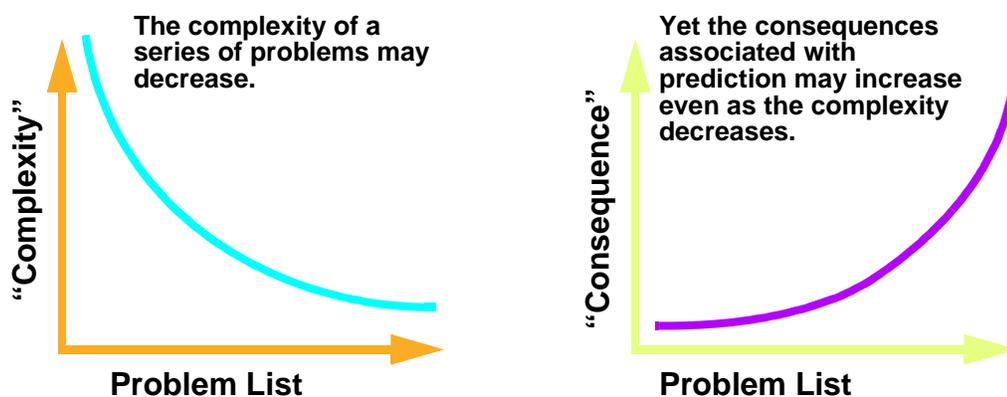
There is at least one other issue which is equally important. This is the impact of formal algorithmic complexity, and its transmutation into formal computational complexity in real simulation implementations. Some discussion of this is found in the books mentioned above [2, 3], as well as in Svozil's book [36]. We will illustrate this current specifically in the examples we present in Section 4.

### Complex Phenomena - Consequence is Important

In high-consequence applications of predictions of complex phenomena, the results of modeling error become dramatic. This could be as straightforward as the result that people may die if an aircraft control system software implementation is faulty. As a more subtle example, which is more closely related to the scientific modeling that we are most interested in, there is also now increasing consequence associated with climate modeling. This is because there is more national and world policy dependence upon the predictions of climate modeling. The long term impact of determining uncertainty in such a policy consequential scientific simulation is not clear, but is potentially large. Although climate modeling is such a complex scientific problem that it is on anybody's list of grand challenge simulation problems, we should not let complexity alone dwarf the other issues. The coupling of significant risk to climate simulations places a much greater burden on those who must extract predictions from this modeling. Such a situation certainly lends itself to further discussion. An alternative example that we could have used here is increasing dependence upon accurate earthquake prediction.

Consider another example. This is the challenge of high consequence simulation resulting from the movement of the maintenance and evolution of the U. S. nuclear weapons stockpile from an underground test centered program to a program with an intended real, predictive, consequential simulation component. This so-called **Science Based Stockpile Stewardship** program will dramatically increase the quantitative consequences of simulations focused on stockpile applications, and will almost certainly increase the qualitative consequences as well. The Accelerated Strategic Computing Initiative (ASCI) [27, 38] is designed to be the major technology enabler for this transformation of the computing component of the stockpile program. Many of the software and hardware issues that are at the core of ASCI combine overwhelming technological complexity with almost overwhelming application consequence.

Figure 2 presents a notional view of a key observation. There, we have depicted a generic list of problems (it could start with climate modeling and end with predicting the dynamics of a gyroscope - the reader is invited to provide their own favorite starting and ending problems). This list is arranged so that the apparent and formal complexity of the modeling task is decreasing as we move from left to right through the list of problems. At the same time, we suggest that there is some consequence or risk associated with each problem that grows (again, we do not claim that this consequence is particularly easy to measure objectively) as we move through the list.



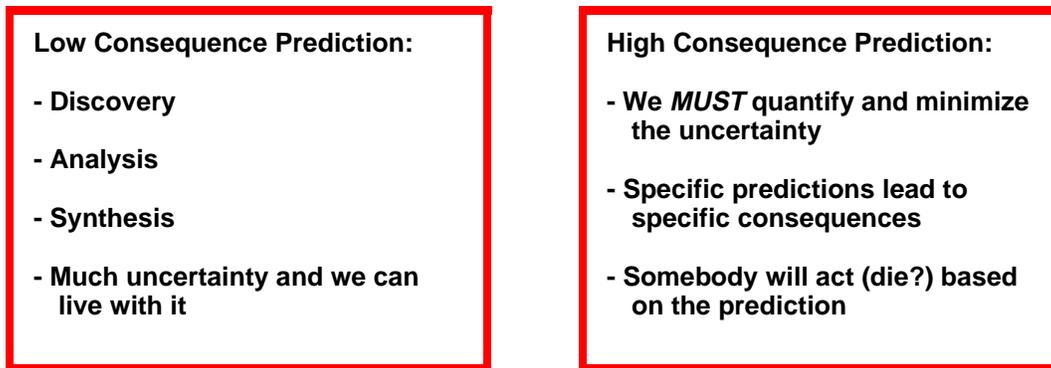
**Figure 2.** The formal modeling complexity of a problem may decrease, yet the predictive challenge might become more difficult.

It may be harder to “predict” with suitable accuracy the physically simpler, but higher consequence, problems. Our confidence in the prediction of more consequential problems may decrease simply due to increased consequence, even if the purely technical challenge may be dramatically simplified.

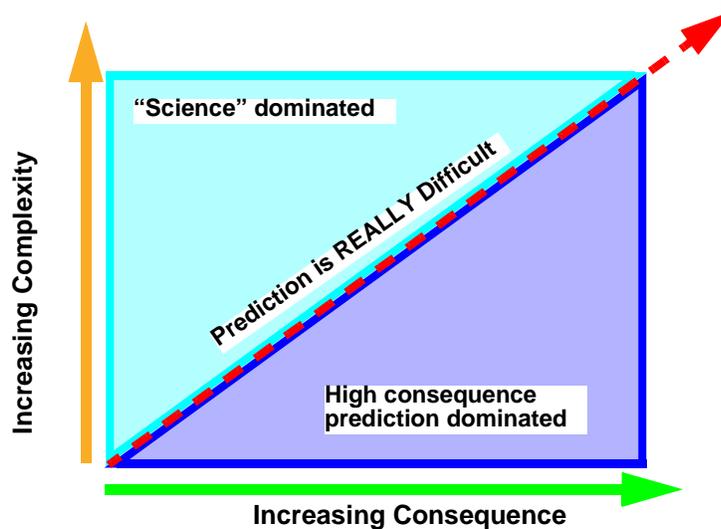
At the risk of an unfair simplification, we choose to distinguish *high consequence prediction* from *low consequence prediction*. We believe that much of the energy which we devote to studying prediction in complex phenomena should be aimed at the first kind of prediction, rather than the second. This is certainly where the thrust of applications in SBSS lies, for example. The ultimate purpose of the general complex phenomena discussed in [8] also points in this direction. We have summarized a few distinctions between low and high consequence prediction in Figure 3.

Our intention is to persuade the reader that consequence is an important variable in prediction for complex phenomena. It may become the dominant variable depending upon the necessity for high consequence prediction. This suggests that an appropriate scaling for effort (and funding) in prediction and uncertainty of complex phenomena relies on a product of complexity and consequence, rather than isolated contributions from each. We have captured this notion in Figure 4, although a three-dimensional plot, with “effort” as the third axis, would make this easier to appreciate.

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**Figure 3.** The transition from low consequence prediction to high consequence prediction is necessary for high consequence predictions of complex phenomena.



**Figure 4.** High complexity and high consequence really makes things tough.

### Complex Phenomena - Computation is Fundamental

We stress that very large scale computing is the common denominator which appears in all of the complex phenomena modeling with which we are concerned. The problems that are subsumed by the phrase “complex phenomena” are, for the most part, too complex for any predictive attack other than via computing. Computing is the heart and soul of all of our efforts to be predictive when we confront problems of complex phenomena.

If we focus on computation, and consider our general view presented in Figure 1, then there are three questions that we need to associate with predictive simulations of complex phenomena. These questions serve to provide general structure to our discussion of particular examples in Section 4. Any programmatic effort devoted to prediction of complex phenomena should attempt to answer all of these questions. These questions are:

**C**omputation - How do we actually compute the complex phenomena?

**C**omparison - How do we compare our simulations with “reality”?

**C**omprehension - How do we understand how predictive our simulations really are?

Computation is generally centered around issues of algorithmic complexity, serves as a driver for hardware development, and directly reflects issues of “fidelity” which are often heard when discussions of grand challenge computing problems arise.

Comparison is a rather more subtle problem. The primary need for care appears by asking what exactly we mean by “reality?” One of the apparent facts that we can’t quite seem to formally characterize for complex systems is that complex systems pose significant difficulties to revealing their secrets by experimental probing. For one thing, it may be hard to gather any data at all. For another, there are fundamental problems in distinguishing the important and relevant data from the trash. (Ransacking a garbage dump for a valuable antique comes to mind as an analogy.) Finally, even if we have a set of critical data that we actually believe, the act of comparing that data with a complex calculation may involve research in and of itself.

Comprehension brings consequence into our picture. If we *really* understand, we are more willing to risk the consequences associated with the application our predictions. Lack of comprehension is measured by increasing uncertainty in the effectiveness of the predictions.

## 3. Calculations

### What is Uncertainty and Why Do We Care?

As claimed above, correctly addressing the dimension of consequence in prediction of complex phenomena requires fully grasping the scope of uncertainty in our modeling endeavors. We have opined in Section 1 that the true range of uncertainty in high-consequence complex simulations goes beyond the traditional concerns of only algorithms, implementations, and fundamental models. One of the largest sources of uncertainty is the category often referred to as “the unknown unknowns.” In other words, what is it that will destroy our predictive effectiveness and about which we have no clue? Generally speaking, one way that science progresses is through chasing, capturing, and elucidating the unknown unknowns through the confrontation with data. This is very much the way that unknown unknowns in simulations must also be identified.

Gell-Mann [17] has addressed the influence of unknown unknowns in the consideration of the limits of predictability of a very fundamental model. There are two specific points in that lecture that are worth keeping in mind when we speculate about simulation predictability of complex phenomena. First, he emphasizes the role of our information gathering ability, which effectively operates to smooth or average uncertainty. In this

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regard, we find it helpful to consider a software system as an information gatherer about the complex phenomenon it is modeling. Second, Gell-Mann emphasizes that the details of the models can serve to amplify our uncertainty (or ignorance). He mentions the presence of chaos as a clear example of this, but this effect is also quite apparent in the operational aspects of performing simulations of complex phenomena.

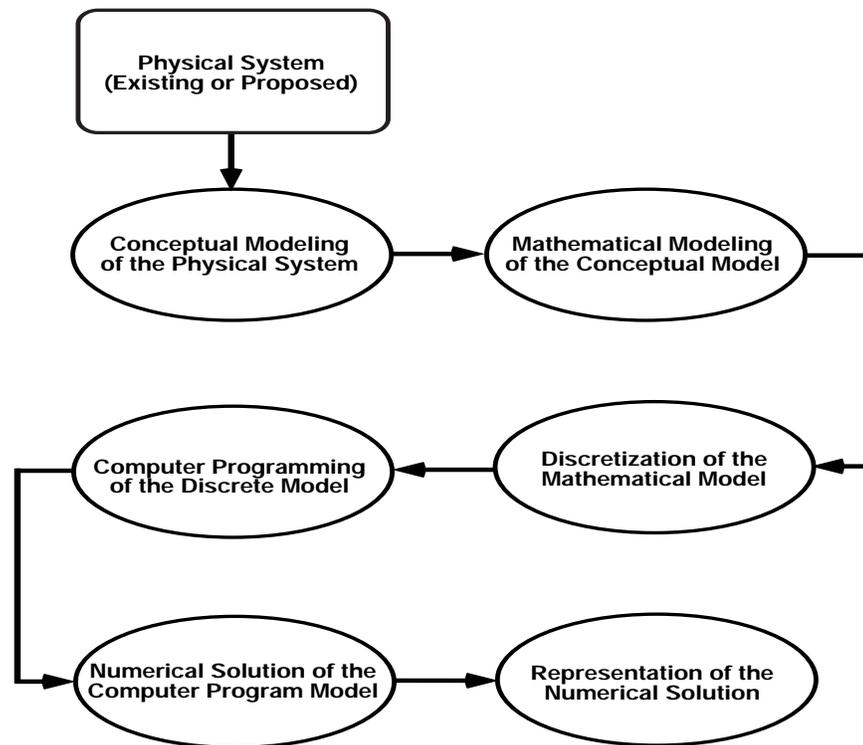
It is important to emphasize that the numerical accuracy of a simulation is only one factor in the overall assessment of uncertainty associated with that simulation and its application. Once again, as the consequence of the intended application increases, the scope of the uncertainty quantification effort also transcends the question of accuracy. For example, developing and implementing a clever two-phase flow algorithm, followed by publication in a journal such as the *Journal of Computational Physics*, is one issue. Actually applying that algorithm in a formal nuclear reactor safety assessment is quite another. The consequences associated with publishing versus a reactor safety certification are worlds apart. It is our attempt to deal with this that leads us to fundamental questions about the nature of uncertainty in our simulations.

Oberkampf and his colleagues [28] have recently taken a systems approach to assess the very wide range of uncertainty issues arising in simulation of complex phenomena. Here, we will simply summarize a few of the main points. The interested readers can study the article themselves.

Figure 5 depicts the phases needed to develop a computational prediction of a complex phenomenon as discussed in [28]. Oberkampf, *et al* propose to distinguish variability, uncertainty, and error in the development of the prediction. *Variability* means inherent variation in the physical system or environment that is under consideration. Thus, while we do not expect the laws of quantum chromodynamics to vary, if we are called on to model a complex manufactured component, such a thing is indeed subject to stochastic variations associated with production, handling history, usage, and other factors. *Uncertainty* is used in [28] to capture the notion of deficiency in any phase or activity of the simulation process that originates in lack of knowledge. *Error* is then defined to be a recognizable deficiency in any phase or activity of the simulation process that is not due to lack of knowledge.

A systematic characterization is offered of the simulation components addressed in Figure 5 in these terms. These results are simply summarized in Figure 6. We feel that such a systems approach to studying sources of limitations in simulations is extremely useful. We also emphasize how difficult the process of identifying variability, uncertainty, and error in particular complex phenomenon can be.

The authors of [28] call for the development of more comprehensive procedures for “representing, aggregating, and propagating individual sources [of variability, uncertainty, and error] through the entire modeling and simulation process.” Let us now turn our attention to some specifics associated with the quantifiability of uncertainty in simulations.



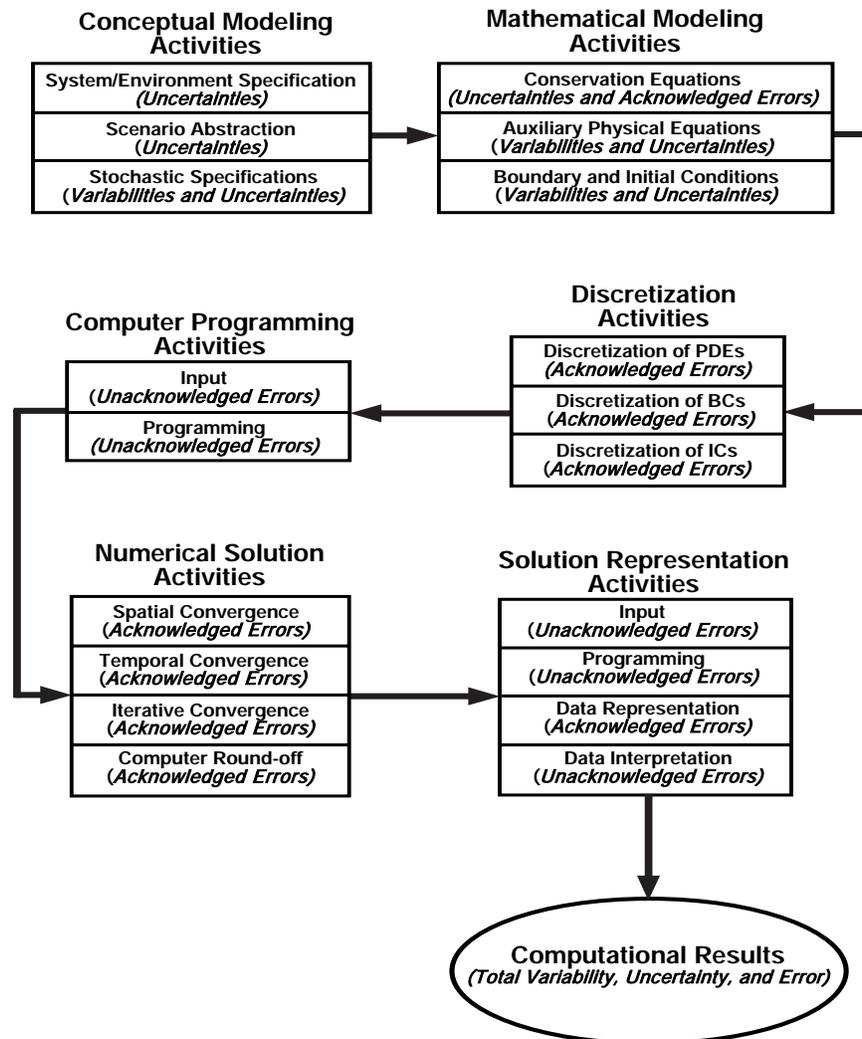
**Figure 5.** Phases for development of a simulation of complex phenomena.

## Uncertainty Quantification

The discussion in the above section was oriented at discussing needs and problems associated with identifying uncertainty. Quantifying and using uncertainty and its inferential methods is a problem that many people have studied and are continuing to study. A key part of our view of the problem of prediction of complex phenomena is simply to begin applying existing research and methodology to a wider class of scientific problems. Uncertainty quantification of the kind we seek to apply is perhaps best discovered in work over the past few decades associated with nuclear reactor safety and waste repository assessments. We will not attempt to even briefly summarize the methodologies in this work which hold promise for application to predictions for more general complex phenomena. Helton's article [22] is recommended for those readers interested in studying the nuclear reactor safety analog for these problems more deeply.

In almost all technical treatments of uncertainty quantification and its associated problems, the underlying framework is assumed to be stochastic. This immediately provides an inferential framework that is statistical, rather than deterministic. If understanding prediction requires understanding the simulation uncertainty, which we believe, then understanding prediction requires a similar inferential framework. A recent survey of various aspects of probabilistic methods for use in risk, reliability and uncertainty analysis is Robinson [34].

## Prediction and Uncertainty in Computational Modeling of Complex



**Figure 6.** Identifying primary variability, uncertainty, and error in simulation phases.

Serious efforts are underway at Sandia to introduce uncertainty quantification methodologies into engineering and scientific simulations related to our DOE missions. We also generically refer to these efforts as “non-deterministic modeling.” Systematic reduction of uncertainty is the most obvious goal of this effort. Generally, our view is that uncertainty can be reduced only if we can

Develop detailed identification of uncertainty in specific simulation tasks.

Quantify uncertainty in such a way that statistical inference can be utilized.

Learn how to properly use this quantitative inferential framework in our simulation environment. We will refer to this as developing uncertainty-based judgement and engineering practice.

To facilitate the following discussion, the only equations that appear in this paper will now be written. It is convenient to summarize the problem of simulating some particular complex phenomenon as

$$F(I) = O \tag{1}$$

Here,  $F$  is merely an input-output relationship which could be as simple as an algebraic equation or as complex as a 1 million line shock wave physics code. We will refer to it as an “operator” below.  $I$  is a set of inputs that drive the simulation. These could be geometries, boundary conditions, material properties, parameters appearing in fundamental models, or anything that someone could control when performing the simulation.  $O$  is the output of the operator  $F$ .

Stochasticity may arise in equation (1) in a variety of ways. In one case, a stochastic procedure might have been used to develop some of the data used by the operator  $F$ . More directly, the equation (1) might manifestly represent a fundamental stochastic process underlying its models. An example of what we have in mind by this is the Kardar-Parisi-Zhang equation [4]:

$$\frac{\partial}{\partial t}y(\vec{x}, t) = v\nabla^2y + \frac{\lambda}{2}(\nabla y)^2 + \eta(\vec{x}, t) \tag{2}$$

in which a stochastic term is explicitly present, the uncorrelated white noise term  $\eta(\vec{x}, t)$ . Equation (2) emerges in a particular sense as the macroscopic limit of a random, microscopic process, in this case random particle deposition on a surface with an interaction.

More directly related to the sense of our concerns for uncertainty quantification is the simple random linear wave equation governing longitudinal waves in a randomly varying one-dimensional medium:

$$\frac{\partial^2 P}{\partial t^2} = \hat{c}^2(x) \cdot \frac{\partial^2 P}{\partial x^2}. \tag{3}$$

In equation (3),  $\hat{c}(x)$  might be a one-dimensional random field that describes stochastic variation in the sound speed of the medium. However, we could also simply claim that we don't know what the sound speed of this particular medium is. We might believe that it lies between two logical limits, but that may be all that we know. We may know that we can assign a particular stochastic distribution to this variable. Or we may only be able to state that we simply don't know precisely what it is. We typically are concerned with how our characterization of this variable may influence the solution of the equation (3). In a recent paper [19], Glimm and Sharp address stochastic issues in partial differential equations. Complementary discussion can also be found in Glimm's review [18].

## Prediction and Uncertainty in Computational Modeling of Complex

There are two classes of problems associated with addressing uncertainty in the general equation (1). The first problem is *uncertainty propagation*. There are several tasks associated with uncertainty propagation. First and most generic is to answer the following question: given  $I$  as well as an associated probability distribution which measures its uncertainty, what is the resulting probability distribution for  $O$ ? A subsidiary question which is obviously of considerable interest is how well does the inferred probability distribution actually characterize the uncertainty in  $O$ ? This question can not be answered using uncertainty propagation alone. Another important question is to assess the sensitivity of the output  $O$  to the parameter family  $I$ . This is most simply measured in terms of partial derivatives of various orders of  $O$  with respect to the elements of  $I$ . A further question is exactly how the probability distribution that characterizes uncertainty in  $I$  is chosen in specific problems.

We will not attempt to summarize the literature that exists on uncertainty propagation and sensitivity analysis. Sensitivity analysis, for example, has a vast number of papers associated with deterministic methods such as adjoint differentiation, direct differentiation, automatic differentiation, finite difference differentiation approximation, and others. For example, in-line direct differentiation approaches coupled with perturbation theory (restricting attention to first order sensitivity coefficients) are being implemented at Sandia in the area of thermal conduction problems, with the intent to apply them to more general problems occurring in simulation of fire environments [6].

Sensitivity can also be determined as part of the uncertainty propagation treatment. Stochastic uncertainty propagation begins with attempts to characterize the output distribution by sampling it. Our greatest concerns arise when the cost of determining the output is very large. We are also typically interested in situations where  $I$  is a very large vector (perhaps hundreds or thousands of parameters). Sensitivity analysis might allow us to ultimately reduce the size of this vector. Sampling strategies then become very important. Monte Carlo based methods are discussed in [19], but clearly more sophisticated sampling strategies are required for very complex and expensive problems. This topic is of recognized importance and is discussed, for example, in [29, 26], as well as the vast literature associated with risk analysis for nuclear reactors and waste repositories.

An important problem in all uses of stochastic methods for propagating uncertainty, such as reliability techniques or response surface constructions, is the precise characterization of the probability distributions that must be associated with  $I$ . A deeper issue is whether quantitative characterization of our uncertainty in these parameters actually can be captured by probability theory, or is something more general required. For example, we could fundamentally question whether we have even captured most of the important characteristics of a complex phenomenon with a fixed choice of parameters. Is this question solvable using a stochastic inference framework? Such a question does not arise if the phenomena which are parameterized using  $I$  are “truly” stochastic (as in non-deterministic phenomena such as manufacturing variabilities). A great deal of work remains to be done simply applying existing stochastic methods to current complex phenomenon prediction

problems. We believe that it is best to pursue this direction until we have sharper understanding of where this approach may fail for specific phenomena.

The notion of synthesis of the output uncertainty leads naturally to the inverse problem of using uncertainty analysis to “improve” the operator  $F$  in (1) itself. In other words, how can knowledge of the output be used to learn more about  $F$  and  $I$ ? A Bayesian framework for doing this, in which a posterior distribution for  $I$  is inferred from its prior distribution and the  $O$  distribution, seems to be the first recourse, although there are other possibilities. Reference [19] discusses this problem specifically for applications associated with multiphase dynamic fluid mixing and porous flow in geologic media. A more general discussion is found in Draper [10], who casts the entire issue of fundamental modeling uncertainty associated with equation (1) in a Bayesian framework. Determining “improved” input parameters from outputs in this sense is also called a *system identification problem*. An excellent discussion of this can be found in Beck’s article [5], while a more recent reference to current research activities at Sandia is Red-Horse [32].

The practical problems of statistical design of experiments appropriate for computational simulations remain important. The experimental design has a strong influence on the inference of a posterior from a prior distribution on  $I$ . Once a design strategy has been defined and performed, one can also proceed to approximate the operator  $F$  by a surrogate or “approximate” operator  $\hat{F}$ . The major advantage of an operator such as  $\hat{F}$  is that it may have far less expense associated with evaluating it. The issues of sensitivity analysis, statistical parsimony (that is, the assumption that only a few of the parameters  $I$  are really statistically important), and parameter interactions may then be studied using  $\hat{F}$ . If, indeed, only a few parameters are then found to be important, one can proceed with a strategy of redoing the uncertainty analysis restricted to these parameters with the exact operator and a denser sampling scheme, such as Monte Carlo. See Romero and Bankston [35] for some recent work which studies this approach. Red-Horse and Paez [33] also discuss improving understanding of the probabilistic content of surrogates using statistical bootstrapping techniques.

Once an inferential approach involving both uncertainty propagation and the inverse problem has been established, regardless of how it is actually accomplished, one can think about trying to optimize predictions emerging from an equation like (1). This might involve directly optimizing some aspects of the operator  $F$ , or improving the apparent output accuracy by modifying the inputs and parameters systematically. An illustration of optimizing material parameters using such an approach is given in Fossum’s work [14-16], as well as in a recent study by Booker and colleagues [7]. Systematic procedures might be utilized to optimally select simulation parameters, such as nonlinear regression techniques suggested by Cox and his colleagues [9]. But, the computational requirements associated with such an approach for function evaluations that might take hours or days on a teraflop computer, and codes that may have 1000 input parameters, are overwhelming. Clearly, deep investigations of these methodologies will be required in the future to understand their limits of applicability to simulation problems associated with various complex phenomena.

## Prediction and Uncertainty in Computational Modeling of Complex

At Sandia, significant effort is being expended to make methodologies for this kind of uncertainty inference available as standard tools for simulation practitioners working on key engineering problems. One example is the implementation of experimental design procedures and uncertainty propagation techniques within the DAKOTA [11] optimization software framework. Problems of interest that seem to be likely candidates for melding stochastic uncertainty techniques with high complexity and high consequence simulations to better assess prediction quality include risk assessment, predictive engineering, predictive materials modeling, reverse engineering, certain grand challenge computing problems such as protein folding (leading to drug design methodologies), SBSS applications, and ASCI code verification and validation needs.

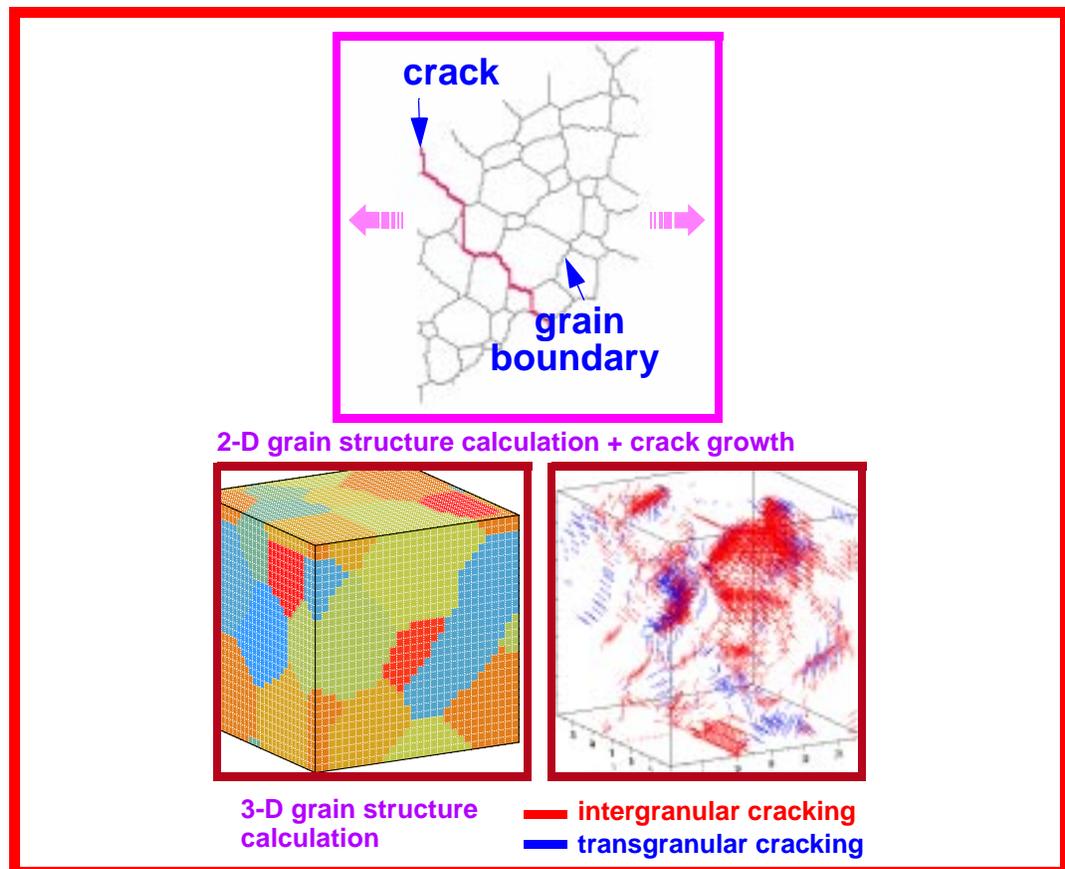
### 4. Some Examples

In this section, we will illustrate some of the issues discussed above by examining a series of problems of current topical interest at Sandia. While far from inclusive of all of the prediction problems that we are concerned with, each of these problems highlights the way that questions of computation, comparison, and comprehension are woven through the work in progress.

#### Multi-Scale Materials Modeling

Our first illustration is an example of a type of problem that will become increasingly important under the guise of predictive materials science. In Figure 7, we illustrate a simulation approach aimed at predictive modeling of anisotropic thermal strain induced 3-D cracking in polycrystalline materials. The straightforward goal of this effort is to make apriori (and accurate) predictions of the thermomechanical fatigue of solder joints under a potentially wide variety of environmental effects [12].

To perform such a task requires a wide range of length and time scales, as well as the coupling of complex nonlinear physics. In other words, the problem is characteristic of our general view of what makes up a complex phenomenon. The figure illustrates some of the elements necessary for possible success. First, an accurate material grain structure must be produced. Second, a microscopic and accurate model of crack nucleation, growth, and interaction must be implemented. There are at least two types of crack dynamics that must be explicated in the illustrated case: so-called inter-granular cracking, and so-called intra-granular cracking. There may also be grains of different material types, adding to the variety of possible cracking characteristics that must be modeled. Third, not depicted, the mechanisms at the microscopic scales illustrated in the figure must be related in an accurate and self-consistent way to phenomena at scales that are relevant for assessing the electrical behavior of actual macroscopic solder joints. Finally, the macroscopic behavior of the joints must then be calculated in a way that has substantive predictive content.



**Figure 7.** Illustration of a multi-scale materials modeling challenge - grain scale stress cracking [12].

The problem is fundamentally stochastic. Solution algorithms are used, such as Monte Carlo Potts modeling for developing the grain structure, which are fully stochastic. The “environmental” component of the problem - the thermal and mechanical history as well as current driving terms - are also characterized with random components. Finally, some randomness is introduced by the manufacturing variabilities in producing actual solder joints. Quantifying the environmental and manufacturing uncertainties associated with this problem is non-trivial. All of these factors directly contribute to uncertainty in predictions emerging from the model.

The computing challenge associated with this problem is significant, ultimately requiring multi-teraflops of computing power. Part of the algorithmic complexity emerges from the significant challenge of proper coupling of the non-linear processes across disparate time and length scales. Current computational issues are how to develop more efficient algorithms and best use massively parallel computing to increase the fidelity of these simulations

The complexity of the physics coupling and of bridging length scales does not lend itself to easy resolution through comparison with experimental data. Dynamic (time-resolved)

## Prediction and Uncertainty in Computational Modeling of Complex

meso-scale data are hard to come by. It is interesting that much of the significant macro-scale data associated with solder joints are electrical, not mechanical, in this particular problem. Yet the modeling we are discussing is purely mechanical at this time. Again, there are certain issues to be addressed associated with the predictive nature of this model when assessed via electrical data.

Because of the difficulty of determining exactly how tightly coupled the multiple processes are (and must be) in this problem, it is unlikely that computation by itself will allow full understanding of this phenomenon, especially in the absence of time-resolved meso-scale data.

The intended application of this modeling implies a high level of consequence associated with the modeling. Thus, the amount of risk associated with incorrect predictions from this simulation effort should be considered to be large.

## Protein Folding

The basic problem underlying this example is designing computational tools for predicting protein conformations using physical lattice models [20, 21]. Predictive solutions to problems of this general type have significant applications to a variety of pharmacological problems. The main intent for such applications is to increase the fidelity and speed with which drugs are designed and brought to the market. It is implicit that the use of such predictions in the pharmaceutical industry is accompanied by significant financial consequence.

These statistical mechanics lattice models provide a simplification of the biophysical process; they preserve some of the protein-like properties of the naturally occurring proteins. As the computational complexity of various models for protein folding has been found to be computationally intractable, i.e., NP-complete (see [23]), in order to provide tools for biophysicists to validate their models, one has to consider approximate predictions. In this context, the research needs to focus on approximations of the native conformations that can be constructed in polynomial time, and have mathematically guaranteed error bounds on the accuracy of prediction. This work [20, 21, 23] provided the first such near-optimal approximation algorithms for protein lattice models.

The structures of the naturally occurring proteins recorded in the Protein Data Bank provide the atomic coordinates of the atoms in the native structures. The statistical mechanics of lattice models cannot be compared directly with the off-lattice conformations of the real proteins. They provide avenues of "comprehension" of the principles of protein folding. Such avenues include initial - close to optimal - structures for molecular simulations, data for inferring empirical energy potentials, methods for simulations of the stability of predictions, and sequence-to-structure threading potentials.

The image in Figure 8 shows near to optimal conformation (better than 99% of the optimal energy) of a naturally occurring protein from PDB for a lattice model with explicit side chains. We used linear time algorithms based on the self-assembly of protein side-chains

(as self-assembly of materials), paired with threading algorithms to obtain the guaranteed error-bounds conformation.

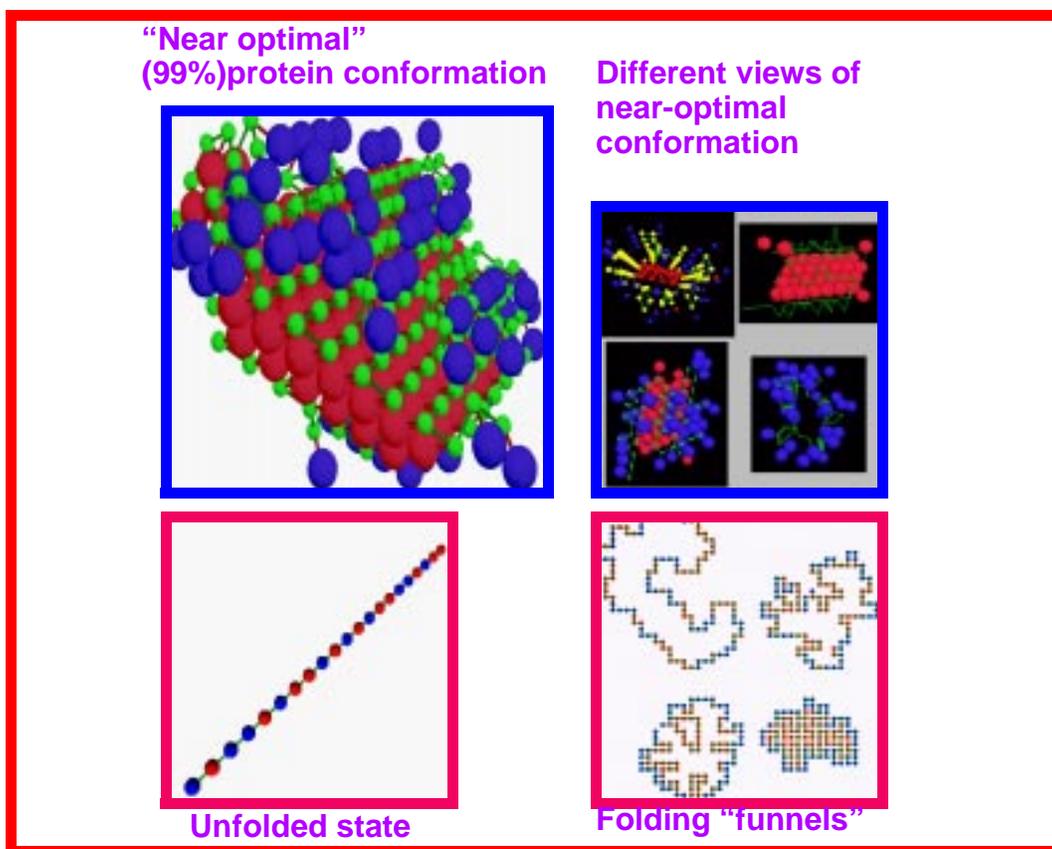
This problem illustrates how far removed we can be from real comprehension (of the type necessary for hard prediction, at any rate). Our ability to predict protein structure has undergone very limited progress, even after decades and enormous effort in the laboratory. What we mean by comprehension is not even clear at this point in time. Yet the consequences of reasonably confident modeling could be enormous.

### Agent-Based economic modeling

The problem we summarize here is developing agent-based microanalytic models which accurately predict features of the U. S. macroeconomy. A particular model, **ASPEN**, has been formulated and implemented [30]. The intent is to use this type of model, or its extensions, to perform quantitative economic forecasting. One particular result from **ASPEN** is shown in Figure 9, where the appearance of business cycles is predicted by the model. Cycles are rarely predicted by most financial forecasting models, and could be considered to be emergent behavior in the underlying dynamical system of the model. This application is effectively a complex adaptive system. Its implementation relies upon evolutionary learning strategies, as well as massively parallel computing techniques.

Requirements for massively parallel (MP) computing are driven by fidelity considerations and the need for ensemble averaging to produce prediction. Many simulations of given initial conditions or statistically varying initial conditions are performed to produce predictions which are appropriate averages. Unlike the protein problem, however, computation is not the central issue. Rather, it is understanding a complex adaptive system and its emergent behavior.

Suitable macroeconomic data exists, but in this case using it to tune the micro-scale agent behavior is a difficult inverse (backward prediction) problem. Using uncertainty methodologies to develop appropriate surrogates for optimizing agent behaviors would be an interesting research problem. The difficulty inherent in this inverse problem is typical also of one facet of complexity that we mentioned earlier - emergent *simplicity*. The predicted macroeconomic cycles represent simplification of the myriad, adaptive, complicated micro-interactions simulated by **ASPEN**. It is difficult to use simple, or simplified, information to tune the details of a more complex, collective behavior.



**Figure 8.** “Near-optimal” protein configuration computed using lattice techniques [21].

Simulations produce a very rich data set. Even attempting to extract cause and effect from the data produced is a difficult problem, and characteristic of many other kinds of complex adaptive systems. The model is one attempt at predicting the behavior of groups, one of the major complex phenomena areas of study called out in [8]. Comprehension problems produced by this model are thus characteristic of problems that will arise in general attacks on that area.

## 5. General Needs and Future Directions

In this section we will briefly discuss general needs in the prediction of complex phenomena that can be addressed by a research program. We also draw attention to some specific activities that are of interest within the Sandia research community. We feel that the following logic constrains elements of mathematical research in this program: *application needs*, or the predictive accuracy requirements implicit in investigating a complex phenomenon, drive *algorithmic requirements*, which create useful directions for *mathematical research*.

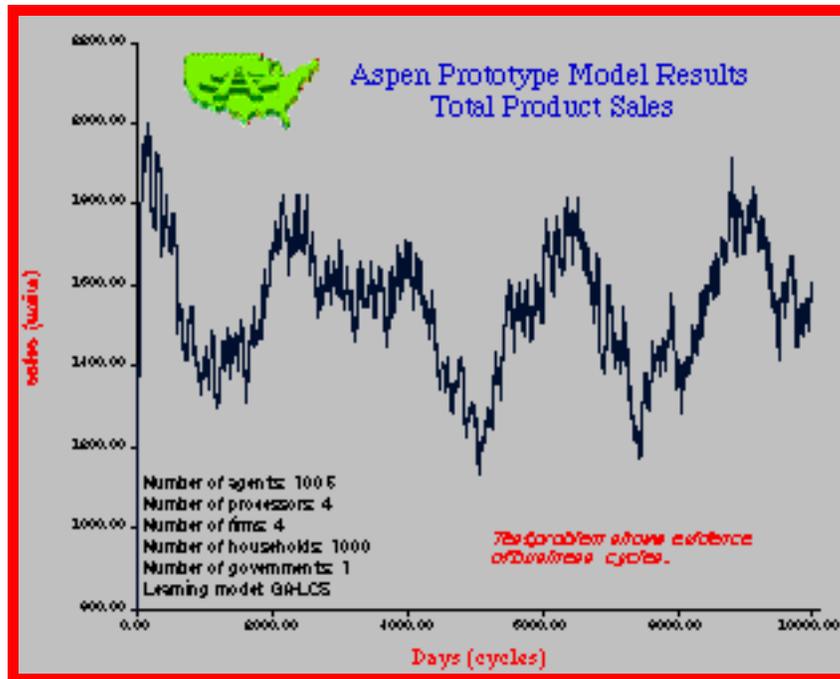


Figure 9. Macroeconomic oscillations from micro-scale agent based interaction [30].

## Recommended General Directions for Study of Prediction of Complex Phenomena

Below, we give recommendations regarding important technical directions that are required to support the extraction of reasonable predictions from simulations of complex phenomena for high consequence applications. These recommendations are listed below, in no particular order by importance.

- We need scientific methodologies for accurate risk assessment associated with prediction of complex phenomena. Typical questions that should be answered are: Where does low consequence prediction end and high consequence prediction begin? How do we measure, let alone control, the risk attendant with high consequence applications in our simulations? We expect systems or operations research approaches to be particularly useful, as well as ideas in statistical quality control. A good starting point for applicable methodologies seems to be the nuclear reactor safety and waste repository assessment communities.
- We need to fully understand the applicability of statistical (or more general) methodologies for dealing with uncertainty in large scale scientific computation. Our experience applying uncertainty quantification to high consequence scientific applications, such as climate or SBSS-related phenomena, is limited. Also, there is a fundamental challenge which concerns the general applicability of stochastic methods for quantifying the uncertainty in scientific calculations. Would fuzzy logic be more appropriate?

## Prediction and Uncertainty in Computational Modeling of Complex

- We continue to be driven in practical problems by the need for algorithmic approaches that reduce fundamental computational “complexity”, as in the protein folding problem. Is it possible to uncover powerful general principles that can guide algorithm development in the future for such combinatorially complex problems?
- Alternatively, are there alternate approaches to, e.g., NP-complete problems which allow one to obtain well-controlled answers to the scientifically relevant questions? One possibility is large-scale Monte Carlo simulations. Another more recent example is the density matrix renormalization group (DMRG) approach, which can be used to obtain high- or even machine-precision expectation values for certain statistical mechanics problems where explicitly computing the partition function is formally NP-complete (e.g., 2D Ising models with more than nearest-neighbor interactions).
- What new ideas for comparing data with predictions from very complex simulations are likely to be effective? For example, how do we compare a multi-scale model which directly calculates from atomic scales to continuum scales with “data?” Are there more refined methods for assessing data quality and data importance applicable to the comparison of data with predictions of complex phenomena? What weight should specific data be given when comparing with a prediction to properly measure the predictive content of the simulation? In other words, which data count more heavily when we are trying to assess the predictive quality of simulations of complex phenomena?
- How can we develop a simplified or “approximate” model of the complex phenomenon that can be used to predict and understand uncertainty in a more complete, more complex model? Our ability to develop such an “approximate” model is part of the process of comprehension.
- The entire framework depicted in Figure 1, boiled down to a core of “compute, compare, and comprehend”, probably requires new ideas to be executed in an optimal manner. We know that we are currently outstripping our ability to understand the largest problems that are running on our largest current massively parallel computers. This is because our interfaces to the data, such as graphical tools, lag the current rapid growth in computing power. What graphical tools are required to optimize the information we gain by performing comparisons with data. Another relevant issue, especially for high consequence simulations, is how do we deal with the possibility of human error in performing and analyzing such simulations. How can we minimize the potential impact of human error in performing simulations of complex phenomena for high consequence applications? Can we quantify the uncertainties that result from the potential for human error?

## Recommended Specific Technical Directions Based On Work At Sandia

We also have recommendations regarding particular technical issues that have arisen in our current computational work at Sandia, similar to that illustrated in Section 4 of this paper

## General Needs and Future Directions

are listed below. We suggest that any or all of the following are specific technical topics which are relevant to the study of prediction of complex phenomena.

- We need continued research and development of advanced molecular dynamics and advanced Monte Carlo methods. These techniques are increasingly important for small scales in multi-scale problems (e. g. cracking prediction, microstructural evolution, etc.). Advanced Monte Carlo techniques might also be leveraged for uncertainty propagation sampling strategies. Better understanding of extreme statistics from Monte Carlo calculations is additionally of physical interest, as well as useful for quantitative uncertainty assessment.
- General approaches for multi-time scale and multi-length scale problems are needed, Multi-scale methods appropriate for long-time problems seem to be particularly needed. How careful (rigorous) do we have to be in blending different length/time scale approaches in unified simulation frameworks?
- We need to better understand how to balance brute force computational power and more sophisticated statistical inference procedures for uncertainty analysis.
- We need to understand the limitations of the “approximate” models defined above for use in both forward and backward prediction in physically complex phenomena. In addition, can we automate the process of constructing such “approximate” models from more elaborate simulation results?
- What are the key issues that are driven by computational complexity when we study predictability of complex phenomena? For example, how important and canonical is the strategy of replacing a complex phenomenon by one which is approximate but solvable with polynomial time algorithms?
- What are the important model descriptions that logically follow mean field theory and which are relevant to non-equilibrium statistically complex systems? As an example, what are appropriate algorithms and data structures for the general void percolation problem?
- How do we progress beyond operator splitting - the approximate weak coupling or full decoupling of physics - in simulation of strongly coupled, physically complex systems?
- What are the limits of application of agent-based modeling?
- How do we map empirical information about computational bottlenecks onto rigorous knowledge about algorithmic deficiencies?
- What are optimal strategies for calculating parameter sensitivity coefficients for complex and expensive code calculations?
- Can the stochastic finite element method be made into a general and useful tool for performing forward prediction in complex phenomena governed by systems of partial differential equations?
- We should continue to study the connections between recent computer science

## Prediction and Uncertainty in Computational Modeling of Complex

developments, for example, and statistical mechanics.

- Well-validated computational libraries for complex phenomena studies should be developed. This involves sharing and standardization, as well as procedures for determining candidate algorithms.
- How far can we push formal software verification techniques for application to codes for predicting complex phenomena?
- We are interested in quantitative studies that tell us how software may or may not introduce its own complexity into the simulations of complex phenomena.

## 6. Conclusions

We have stressed in this whitepaper that the predictability of complex phenomena has several strands that pass beyond fundamental model development, algorithm development and implementation, and calculation. We drew attention to the need to perform computation, compare with data, and develop improved comprehension of the phenomenon from this process as an integrated problem. We also emphasized that uncertainty, both in scope and in the risk it imposes, must be analyzed for high consequence predictions.

Our experience tells us that a computer program which implements models of complex phenomena on a massively parallel computer is itself a complex system. A host of problems must be addressed which are associated with model validity, and with algorithm and implementation correctness. Also, we note that the system which produces predictions - including code developers, the code itself, and its users - behaves somewhat like a complex adaptive system.

On top of this, we observed that the current exponential increase in computer power is already leading to grave difficulties in assessing the content of simulations of complex phenomena, as well as comparing them with high quality experimental data. Among other challenges, this situation leads to the erroneous possibility of thinking that because output is complex, we must be successfully modeling complex phenomena.

Because increasing consequence may dramatically weight the effectiveness of prediction we now suggest that formal calculation of consequence, or of the risk of inadequate prediction, should also be one of the main themes in the study of prediction of complex phenomena. We believe that the entire computational process for extracting predictions from models of complex phenomena needs to be enhanced to suitably quantify this latter factor. Programs that aim to study predictability of complex phenomena should aim to achieve this enhancement.

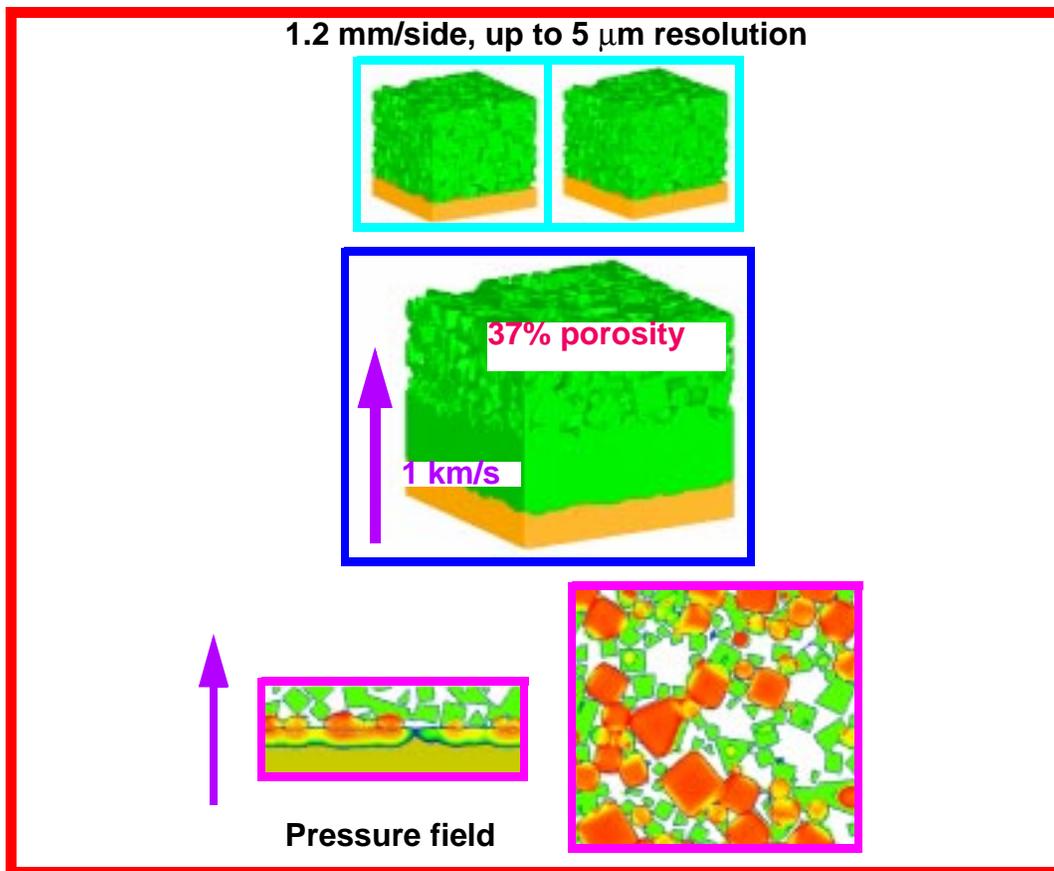
Let us conclude with one last example. We regard the computation shown in Figure 10 [24] as a paradigm for our concerns in this paper. There, an Eulerian shock wave calculation is shown. The shock wave is reactive, propagating through a bed of HMX crystals. The mesh

resolution is such that individual crystals can be resolved. The shock is induced by the impact of a copper plate at 1.0 km/s. Thus, this calculation models a relatively straightforward shock initiation experiment that can be performed at a variety of facilities worldwide. On any scale of complexity, this calculation is of only fair complexity. Solving the fundamental equations, and the code technology for doing this usefully (the Sandia code CTH), has been available for a long time. What is new is the resolution. To run 1.2 billion cells in such a calculation requires a currently unique piece of computing hardware, the DOE/Intel Teraflop computer located at Sandia in Albuquerque. This resolution bends our minds so to speak. Straightforward questions, such as does the reaction induced by the shock grow to detonation, rapidly become complex questions, such as: how sensitive is the computed reaction evolution to microscopic details of the crystal array (an ensemble question); are there collective effects that have an influence on the reaction evolution; how poor is the chemistry treatment; is there any data that can resolve reactive flow details down to the level of individual grains.

If such a simulation should be used to, say, assess the environmental degradation of a granular reactive material for larger purposes than scientific investigation, we are also led to ask: How reliable is the calculation? How accurate is the calculation? What are the largest uncertainties that influence the calculation? We don't even ask questions like: is the code implemented correctly? We already know the answer - NO. No person who uses any large computer code can claim that the code is bug free. Will lurking errors in our code be dramatically amplified in such calculations? Or, will their effect, heretofore undiscovered, remain in the background? How long will it be until we discover an important bug? Given this point of view, what do we mean by asking such calculations to be predictive, anyway? Such questions must be answered as the consequence of such a calculation rapidly increases.

The calculation in Figure 10 is also complex in that it is difficult to understand what it is telling us. The sheer volumes of data that are produced in a 1 billion cell calculation far exceeds our ability to comprehend at this time. We literally have difficulties even moving the data to something that could be used to produce the plots shown in this figure. The really novel information problems generated by the technology that ASCI is developing are well known at this time and of major concern to ASCI.

Thus, even such a "straightforward" calculation as that in Figure 10 gives us clear illustrations of the four challenges that we have emphasized in this paper: Computation, Comparison, Comprehension, and Calculated consequence. We state again: the product of complexity and consequence seems to be the most important variable that we must deal with in high-consequence simulations of complex phenomena.



**Figure 10.** “Typical” ASCI-scale physical modeling is mind-boggling. In this calculation, up to 1.2 billion cells are used in an Eulerian calculation. The calculation is performed on the DOE/Intel ASCI “Red” MP computer at Sandia. The calculation is of a copper plate striking an HMX crystal array with simplified chemical reactions at 1 km/s.

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