OPPORTUNITIES FOR THE
MATHEMATICAL SCIENCES
JUNE 26-27, 2000 WORKSHOP

Risk Assessment for the Solutions of Partial Differential Equations

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STATEMENT OF GOALS

Technology relies increasingly on simulations to support high impact decisions. Global climate change, environmental remediation, and computer assisted design for manufactured products are important examples. Sufficient and timely information to evaluate integrated system behavior will not be available from full system tests, as the necessary tests may be forbidden for political or environmental reasons, they may be too expensive or too time consuming, or they just may not be feasible.

Nonetheless, decisions will be made and predictive simulations will be requested to support decision making. This means that new levels of assurance will be expected to accompany simulations as increased reliance is placed upon them. Increasingly a simulation must be accompanied by estimates of accuracy, applicability, and an overall assessment of its degree of predictive confidence. In other words, decision makers need *certified* predictions. In many cases (for example involving optimized solutions or control) they need automated predictions.

Risk assessment is the quantification of the uncertainty resulting from accumulated errors in data, models, and solutions. Risk assessment is a necessary, but presently missing step, that will enable a significant increase in the role played by mathematical models [1], [2].

The work proposed here is based on rapid solution methodologies through upscaling for multiscale differential equations. Upscaling is used for climatology, turbulence, composite materials, and flow in porous media, among other problems. The development of novel methods in numerical and mathematical analysis will be needed for the analysis of errors in the solutions. Statistical inference will relate these errors and the observations, which have their own errors, to a probability model. The probability model thus yields confidence intervals and quantified measures of assurance of validity for prediction. The methods will be applied to risk assessment for many problems in computational physics, geology, biology, etc., including chaotic multiscale fluid flows, composite nanostructured materials, climatology, and protein folding. The methods will be broadly applicable to decision making based on mathematical models.

The assessment of uncertainty is more than an analysis of errors propagating and growing through the solution process. Information as well as error is introduced at numerous stages of a solution process. Information at any stage can be used to reduce uncertainty at that or other stages of the solution process. The solution process, with its ability to transfer information through solution stages, provides the ability to reduce uncertainty at multiple locations in the solution process. When the information is transferred to an earlier stage, such as the solution input, this is called the solution of an inverse problem. In practice, it is only through accumulated (but imperfect) observations that are we able control the growth of accumulated solution errors in a complex multi-stage problem and obtain reliable answers. Even the observations, which ultimately are often the reading on a dial, are related to the solution only through an additional modeling process.

We propose methodologies that will advance the leading edge of research in order to address each of these requirements. The methodologies define a new generation of mathematically based risk assessment concepts, algorithms and tools to predict scientific and engineering phenomena with quantification of uncertainty.

THE SCIENTIFIC APPROACH

We propose a program to develop risk assessment methodology based on three key ideas:

1. Rapid Solution Methodology. Multiscale equations have solutions with overwhelming detail, due to rapid solution oscillation, fine scale equation heterogeneities, and nonlinear solution instabilities. This structure cannot be ignored, but it must be simplified if it is to be understood. Very high levels of computational speed up have been achieved by upscaling (use of subgrid models, or coarse graining) in (a) turbulent mixing and transport, (b) flow in porous media, and (c) effective properties of microstructured materials, among other topics. Upscaling allows effective simulation sampling of an ensemble to assess uncertainties and risk. The research problem is to extend this capability and to understand its limitations.

2. Error Models. Errors result from the limits of validity of subgrid models, from approximations in the numerical integration of solutions, and from data acquisition. Analysis of errors is needed for risk management, when solutions are used for prediction. Probability models for solution and observational error are at the heart of a computationally assisted decision strategy. Error models applied to the comparison of simulation with observation test the simulation model and allow its systematic improvement. They furnish the probabilities which enter into the final confidence intervals of prediction. Solution error models exist only in a primitive form. The research problem is to develop them.

3. Statistical Inference and Variance Reduction. Inference furnishes the link connecting solution, observation and prediction error probabilities. Improved methods of statistical inference will be achieved through Monte Carlo sampling, latin hypercubes, response surface designs, moment expansions, sensitivity analysis, and parallel algorithm development.

REFERENCES

[1] J. Glimm and D. H. Sharp, Stochastic methods for the prediction of complex multiscale phenomena. Quarterly J. Appl. Math., 56: 741 - 765, 1998. Back to Text
[2] J. Glimm and D. H. Sharp, Prediction and the quantification of uncertainty. Physica D, 133: 152 - 170, 1999. Back to Text

Last Modified:
Oct 17, 2001

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Last Updated: 10/17/01
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