Synopsis of a Workshop on Quantification of Uncertainties in Physics Simulations

Prepared by
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Executive Summary

The Workshop on Quantification of Uncertainties in Physics Simulations (QUIPS), held at the Los Alamos National Laboratory on September 9 and 10, 2002, brought together nearly 150 LANL scientists. The presentations and discussions covered a wide variety of applications, ranging from simulations of simple hydrodynamics and material dynamics to simulations of nuclear weapons. The workshop successfully met its primary goal of promoting discussions among LANL scientists about the problems associated with quantifying uncertainties in physics-based simulation calculations. The workshop made an important step toward developing a sense of common purpose among those engaged in different applications. This common interest should be fostered through local seminars, such as the Uncertainty Quantification Working Group seminar series. It would be valuable to hold further seminars and workshops, involving not only the LANL community, but also other DOE laboratories, to improve our understanding of the problems associated with uncertainty quantification of simulation codes, and how to solve them.[1]

1. Introduction

The Workshop on Quantification of Uncertainties in Physics Simulations (QUIPS) was held at the Los Alamos National Laboratory on September 9 and 10, 2002. The purpose of the workshop was to promote a Laboratory-wide discussion of the quantification of uncertainties in results obtained from physics-based simulation codes. The issues that were discussed included identification of perceived needs for uncertainty quantification, examples of approaches that have been used to assess simulation uncertainties, and new approaches to solving uncertainty quantification problems. We sought to involve those who play a role in the uncertainty quantification process, including experimentalists, physics modelers, code developers and users, computer scientists, engineers, statisticians, and analysts.

QUIPS came about at the suggestion of Stephen Lee (Deputy Division Leader, CCS Division), who sensed a growing concern at the Lab about uncertainty quantification of simulation codes, and that it was an appropriate time to organize a workshop on the subject. As the planning progressed, it became apparent that there was indeed a great deal of enthusiasm for such a meeting.

[1] This document is available on the web at http://public.lanl.gov/kmh/quips/.

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The QUIPS organizing committee represented a cross section of technical divisions that deal with uncertainty quantification (UQ) issues:

Kenneth Hanson (CCS-2), Chair

Robert Benjamin (DX-3)	Jane Booker (ESA-WR)
Shuh-Rong Chen (MST-8)	François Hemez (ESA-WR)
Valen Johnson (D-1)	James Kamm (CCS-2)
James Kao (X-4)	Jack Shlachter (P-22)
David Sharp (T-13)	Merri Wood-Schultz (X-2)

Administrative help was provided by Stephanie Ladwig and Mary Ann Lynch (CCS-2). The refreshments were sponsored by the ASC Verification and Validation Board, Alexandra Heath (X-5), Chair.

We wish to express our appreciation to Charles W. Nakhleh (X-2), George T. (Rusty) Gray III (MST-8), Len Margolin (X-DO), and François Hemez (ESA-WR) for serving as session chairs and presiding over the discussions. They also helped prepare this workshop summary.

The workshop consisted of four half-day-long sessions. Two classified sessions were held Monday, September 9, in the auditorium of the new Metropolis Center for Modeling and Simulation. The two unclassified sessions were held Tuesday, September 10, in the Oppenheimer Study Center. The committee structured the program to provide ample time for presentation and discussion. We scheduled 30 minutes at the end of each session for open discussion. Indeed, the discussion sessions were quite lively and productive.

Partly because of our desire to enhance open exchange of ideas, and partly to develop a sense of community among LANL researchers interested in UQ issues, the committee decided to restrict the workshop to LANL scientists and their colleagues. Nearly 150 people registered for QUIPS.

The QUIPS program is included at the end of this document in Appendix A. There were 18 talks and 6 posters presentations. In regard to uncertainty quantification, there were many questions about how to do it, as well as some solutions. Certainly, not all of the questions were answered.

Abstracts for the workshop presentations are listed in Appendix B.

2. Technical Presentations and Discussion

The presentations and discussions are briefly summarized in this section. The aim here is to provide a concise overview of the workshop.

Keynote Speaker – Ray Juzaitis (Associate Director – Weapons Physics)

Ray Juzaitis kicked off the workshop by talking about his vision of the importance of uncertainty quantification (UQ) in achieving the goal of robust and predictive simulation capability in weapons physics. He tied the need for UQ to certification methodology and performance gates. In the broader context of simulation science, for which the Laboratory is renowned, UQ must play a major role, for example, to provide decision makers with the appropriate information to critically assess a given situation. Juzaitis acknowledged that embracing UQ may be a tough cultural adjustment, but a necessary one. He stated that his directorate is strongly committed to understanding the uncertainties in weapon simulation codes, and will target funding to specifically support UQ work.

2.1 Session 1: Weapons Physics

(a) Presentations

Matt Kirkland (X-4) gave an overview of primary operation as well as a description of X-4's view of uncertainty quantification (UQ). He maintained that there is currently no consensus, either within LANL or between the Los Alamos and Livermore Labs, regarding essential details of UQ. He noted that existing impediments currently make it impossible to address certain critical issues. Finally, he described the common baselining methodology that X-4 is currently developing.

Merri Wood-Schultz (X-2) gave two presentations. She first discussed in general terms the important elements in simulations of secondary performance and described existing needs that, if met, could improve those simulations. She emphasized that existing simulations suffer from several defects and have not yet achieved a predictive capability. In her second presentation, Merri contrasted two distinct ways to calibrate computational physics simulations: those that match the data from a single experiment and those that match an ensemble of experiments. She described the relationship between these two approaches and their strengths and weaknesses.

Two classified posters were presented. Les Thode (X-1) gave a fascinating account of the development of a plasma physics model and described potential implications for high-energy-density simulation codes. Mike McKay (D-1) reported on a sensitivity analysis used to identify the dominant sources of uncertainty in a code output. Two unclassified posters were also presented; they will be described in Sect. 2.3.

(b) Discussion

The discussion period at the end of the session focused on ways in which the Laboratory might systematically attempt to reduce simulation uncertainties, including the undertaking of experiments aimed at reducing database uncertainties. Also needed are consistent mathematical approaches for combining individual uncertainties into an overall assessment.

Numerous physics-modeling issues were mentioned, including ensemble modeling, sub-modeling, hierarchical modeling, and 2D and 3D modeling. The UQ tools and methodologies would have to incorporate the knowledge and experience of Laboratory experts. Peer review is an important part of the scientific method and should be part of UQ methodology. Uncertainties exist in the data, the models, and the solution methods, but it is the unknown aspects of the models and simulations that are the most difficult and troublesome to get a handle on. There is often a tendency to focus on the sources of uncertainty that are easiest to cope with, as opposed to those that are most important. Understanding and modeling the uncertainties in material models are as difficult as for physics models.

2.2 Session 2: Experimental Uncertainties

(a) Presentations

The speakers in this session discussed the status of experimental data in the areas of equation of state (JD Johnson, T-1; Dave Schiferl, C-PCS), alpha-curve measurement (Barry Warthen, P-22), radiochemistry (Anna Hayes, T-16), and radiographs of importance to weapon certification (Greg Cunningham, DX-3). They described the implications for uncertainties in current modeling and simulation implementations. They discussed the assumptions governing the data sought, the approximations, accuracies, and systematic errors in the experimental techniques used to quantify the data measured, material issues related to sample preparation, and the uncertainties in the data and their analysis. While each speaker presented specifics related to the uncertainties in their own experimental focus area, a number of common themes emerged. Several speakers voiced the critical importance of continuing dialog with the weapon designers and production engineers concerning setting priorities and providing guidance for needed experimental data to support baseline weapons materials assessment and the development of predictive materials physics models. There was consensus about the importance of developing a coupled experimental–modeling approach to address weapon certification issues.

(b) Discussion

The discussions of the modeling issues included the role of experimentation, especially integrated experiments. Because it may not be possible to develop predictive models from first principles, the utility of such large, expensive experiments comes into question. Large experimental facilities and programs are subject to political winds and funding and may not provide the fundamental data needed to validate models. The difficulties with topics like back propagation of uncertainty in models and images were discussed. Some specific topics regarding lack of knowledge (often called epistemic uncertainty) were identified, including those related to weapon-stockpile certification. As long as the changes made are small enough, the current experimental A-B comparisons may be sufficient for certification; however, the data may be so uncertain as to preclude detecting small cumulative changes in the stockpile.

One poignant question was asked, “Can someone focus on a specific performance gate (requirement), and drill down through the layers of the problem to define what issues and requirements are important, then work through the details, and present the results?” This suggestion brought into focus much of the concern expressed during the discussion, and seemed to have broad support from audience. This task may perhaps be too demanding to be fully carried out in detail in the near future. It does, however, indicate the sense of frustration expressed by many that something relevant needs to be undertaken in regard to UQ. Perhaps this kind of task could be taken as a focal point for further work and discussion, both on the experimental and the modeling sides.

2.3 Session 3: Uncertainties in Simulations

(a) Presentations

Several aspects of dealing with the uncertainties in physics simulations were presented in this session. Dave Sharp (T-13) talked in general terms about the need for UQ, and discussed the sources of uncertainties in simulation outputs, especially those caused by solution errors. John Grove (CCS-2) described a careful study of solution errors generated when shock waves interact. Ken Hanson (CCS-2) presented a Bayesian framework for modeling uncertainties in simulation predictions based on updating one's knowledge about model parameters as one analyzes a hierarchy of experiments of increasing complexity. Jim Kao (X-4) showed how data assimilation may be used to improve predictions of a 1D time-dependent shock process on the basis of observations made a several times during the evolution of the process.

Four unclassified posters were presented at the workshop. Jane Booker and François Hemez (ESA-WR) presented a poster on how to combine non-probabilistic measures of uncertainty with probabilistic ones. Cliff Josyln (CCS-3) described a way to express certain types of imprecise knowledge in terms of random intervals. Parick Talou (T-16) presented a Bayesian inference scheme that can provide the "best" estimate for physical quantities, such as nuclear cross sections. Tony Warnock (CCS-3) described quasi-Monte Carlo techniques and presented a useful way to estimate errors in their results.

(b) Discussion

Models are not the pathway to estimating truth, but are a means of addressing some answerable questions. Sometimes simulation errors can be controlled, and investigating space-time behavior of partial differential equations (PDE) can indicate model behavior and localized phenomena. There are different types of errors: equation errors from truncation and solution errors.

(c) Session chair's comments - Len Margolin

Two points were common to all of the talks in this session. First, the most difficult part of quantifying uncertainty in numerical simulations is defining the "truth". Second, an important and often neglected source of error is the solution procedure.

These are my own thoughts on these two points. First of all, in the case of computer simulation, I don't believe there is a unique 'truth.' In particular on a discrete grid, one can only specify the resolved scales. There are many choices of the unresolved scales, each consistent with the initial conditions. In many cases, however, it is possible to specify a most probable 'truth,' which will be some statistical characterization of the unresolved scales. If the unresolved scales matter, then the variability that would result from different realizations is itself an important source of uncertainty.

Second, there are many issues to consider within the general category of solution procedure. Much attention has been paid to improving individual algorithms/models. However, little attention has been paid to the coupling of different models. Indeed, most multiphysics codes, at Los Alamos and everywhere else as well, employ operator splitting. In stiff problems, where there is a broad range of scales of time or length, operator splitting has been shown to lead to significant errors.

2.4 Session 4: Engineering

(a) Presentations

Scott Doebling (ESA-WR) presented a broad overview of the model-validation research being done in ESA Division in the area of structural dynamics. James Coons (ESA-WMM) demonstrated a Monte Carlo approach to quantifying the uncertainties in the assessment of surveillance data from cushions and pads in the nuclear stockpile. Peter Moller (T-16) presented a detailed quantitative analysis of uncertainties in estimating mass and reaction Q values for unknown nuclei. Mark Marr-Lyon and Chris Tomkins (DX-3) showed results from an analysis of shock-tube experiments in which gas velocities are measured and compared to predictions made by a hydrodynamic code. The session ended with Bill Rider's (CCS-2) description of the use of multiscale image-analysis techniques to compare experimental data with simulation predictions of a complex nonlinear phenomenon.

(b) Discussion

The discussion started with the recognition that experimental data are critical to assessing the predictive accuracy of computer simulations and validate numerical models. The observation that validation can not be performed without experiments may seem trivial, but it is still occasionally debated whether indirect inferences or subjective opinions can replace physical measurements to provide a reference to reality. Beyond the need for test data, attendees stressed that the type of measurements available and their quality must be carefully defined because these two factors often limit what can be achieved in terms of uncertainty quantification and model validation.

Often the techniques employed to analyze simulation results differ from those used to analyze physical measurements. Such practices tend to introduce biases of different types, which can adversely affect their comparison and the assessment of the model's predictive accuracy. It was mentioned that there is a need to align the data-reduction methods for predicted data with those used for experimental data.

Even though subjective opinions cannot replace actual experimental data, it was suggested that in some situations, it is important to make use of the knowledge held by experts. The formal process of elicitation is a valuable means to capture experts' knowledge in as quantitative a manner as possible. Uncertainty in subjective opinion is not always best represented in terms of probability. When a probabilistic framework cannot be used because of a lack of specific information, other approaches to representing uncertainty may have to be applied. Examples are the Dempster-Shafer theory of plausibility and belief, interval arithmetic, fuzzy logic and the theory of information-gap.

ASC-size simulations generate huge amounts of results. More work needs to be put into analyzing large numerical simulations. For example, use the same techniques as those employed to analyze large experimental data sets.

In some applications, such as reliability assessment, one may need to characterize rare (catastrophic) events, which is different from characterizing the mean (average) behavior of the system. This process is more difficult because rare events occur in the tails of the statistical distributions.

3. Conclusions

The QUIPS workshop was enthusiastically received by LANL scientists. Nearly 150 people registered for the workshop, and attendance was good for all sessions. Interactions between people from different Laboratory organizations at the breaks and poster sessions confirmed that the goal of promoting open discussion was achieved. Feedback from attendees was very positive. The topics of the presentations and discussions covered a wide variety of issues and raised the level of awareness of uncertainty quantification issues. While Monday's presentations and discussions dealt primarily with problems that need uncertainty quantification, especially in the weapons program, Tuesday's presentations provided some promise of UQ tools and solutions.

The strong local interest demonstrated at the QUIPS workshop suggests that there is a growing awareness at the Lab of the importance of UQ in simulation physics. While there are many promising ideas and projects underway, there also seems to be a certain amount of confusion about how to go about addressing some basic UQ issues. It would be valuable to engage in further discussions and hold seminars at the Laboratory to improve our understanding of the problems associated with uncertainty quantification of simulation codes. It also seems appropriate to plan further forums to continue raising awareness of UQ issues, exchanging ideas, and presenting potential tools and methods for solutions. Such meetings might well include participants from other DOE Laboratories, and possibly from other scientific institutions, such as universities and industrial labs.

Specifically, here are some things we could do, as a Laboratory:

- Encourage participation in the existing Uncertainty Quantification Working Group, which is an dynamic forum for interchange and discussion of UQ problems and solutions. Information about UQWG: http://public.lanl.gov/kmh/uqwg/.
- Hold seminars and short courses on various aspects of UQ, for example, assessing uncertainties in experimental results, coping with UQ in data analysis and modeling, etc.
- Organize further workshops on UQ issues, with participation from other DOE Laboratories.
- Follow the suggestion that arose at the end of Session 2, namely, have a qualified team of designers, modelers, experimentalists, and statisticians take on the challenge of identifying what would be necessary to estimate the uncertainties in one particular gate in the certification methodology.

Appendix A. QUIPS Program

Workshop on Quantification of Uncertainties in Physics Simulations
September 9 and 10, 2002, Los Alamos National Laboratory
Los Alamos, New Mexico

Monday, September 9th – Metropolis Center for Modeling and Simulation

Classified Sessions (Q clearance and Sigmas 1-10 required)

7:45 Poster Session with Breakfast Burrito

8:30 Welcome - Goals and Vision for Workshop, Ken Hanson (CCS-2)

8:40 **Keynote Talk, Ray Juzaitis, Associate Director – Weapons Physics**

Session 1. Weapons Physics – Chair: Charles W. Nakhleh (X-2)

9:10 Primary modeling, QMU, and UQ, Matt Kirkland (X-4)

9:40 Uncertainties in secondary modeling, Merri Wood-Schultz (X-2)

10:10 Poster Session with Refreshments

10:50 Data and uncertainties in experimentally constrained physics simulations, Merri Wood-Schultz (X-2)

11:20 Discussion

11:50 **Lunch**

1:00 Poster Session with Dessert

Session 2. Experimental Uncertainties – Chair: George T. (Rusty) Gray III (MST-8)

1:20 Uncertainties in EOS's and what regions of pressure-temperature space are important: assigning uncertainties to ignorance and mistakes, J.D. Johnson (T-1)

1:50 Reliability of static equation of state determinations, David Schiferl (C-PCS)

2:20 Uncertainties in alpha curves, Barry Warthen (P-22)

2:50 Poster Session with Refreshments

3:10 Quantification of uncertainties in simulations of weapons radiochemistry, Anna C. Hayes and Gerard Jungman (T-16)

3:40 Uncertainty quantification for edge-location estimators on static radiographs taken at the DARHT facility, Greg Cunningham (DX-3)

4:10 Discussion

4:40 End of session

Classified Posters (Q clearance and Sigmas 1-10 required)

Functional Sensitivity Analysis (FSA): approaches to sensitivity and importance analysis based on functional output, Katherine Campbell and Michael McKay (D-1)

Temperature equilibrium rate in strongly coupled plasma, L.E. Thode, C.H. Chang, C.M. Snell, W.S. Daughton, and G. Csanak (X-1)

Unclassified Posters

Combined probabilistic and non-probabilistic uncertainty quantification applied to performance reliability, Jane M. Booker and François M. Hemez (ESA-WR)

Effective error estimates for quasi-Monte-Carlo computations, Tony Warnock (CCS-3)

Tuesday, September 10th – Oppenheimer Study Center

Unclassified Sessions (open to all LANL badge holders)

7:45 Poster Session with Breakfast Burrito

8:30 Welcome – Goals and Vision for Workshop, Ken Hanson (CCS-2)

Session 3. Uncertainties in Simulations – Chair: Len Margolin (X-DO)

8:40 Uncertainty estimates for predictive simulations, David H. Sharp (T-13)

9:10 Error distribution models for strong shock interactions, John W. Grove and Yunghee Kang (CCS-2)

9:40 Uncertainty quantification of simulation codes using experimental data: Taylor impact tests, Ken Hanson (CCS-2), François Hemez (ESA-WR), and Shuh-Rong Chen (MST-8)

10:10 Poster Session with Refreshments

10:50 Data assimilation with extended Kalman filter, Jim Kao and Sarah Frey (X-4)

11:20 Discussion

11:50 **Lunch**

1:00 Poster Session with Dessert

Session 4. Engineering – Chair: François Hemez (ESA-WR)

1:20 Computational model verification, validation, and uncertainty quantification from an engineering analysis perspective, Scott Doebling (ESA-WR)

1:50 Incorporation of model uncertainties and experimental errors in the assessment of surveillance data from cushions and pads in the nuclear stockpile, James E. Coons (ESA-WMM) and Michael D. McKay (D-1)

2:20 Quantification of mass-model uncertainties and the reliability of mass and reaction Q-value calculations for unknown nuclei, Peter Moller (T-16)

2:50 Poster Session with Refreshments

3:10 Code validation experiments with 2D velocimetry, Mark Marr-Lyon, Chris Tomkins, Kathy Prestridge, Paul Rightley, Robert Benjamin (DX-3), Cindy Zoldi (X-2), Jim Kamm, Bill Rider (CCS-2), and Peter Vorobieff (UNM)

3:40 Multiscale techniques for the analysis of high-resolution experimental data and simulation result, William J. Rider and James R. Kamm (CCS-2)

4:10 Discussion

4:40 End of workshop

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Posters (Unclassified)

Combined probabilistic and non-probabilistic uncertainty quantification applied to performance reliability, Jane M. Booker and François M. Hemez (ESA-WR)

Uncertainty quantification of simulation codes using probability intervals, Cliff Joslyn (CCS-3) and Bill Oberkampf (SNLA)

Uncertainties assessment in nuclear data evaluations, Patrick Talou (T-16)

Effective error estimates for quasi-Monte-Carlo computations, Tony Warnock (CCS-3)

Refreshments sponsored by ASC V&V

QUIPS web site http://protected.lanl.gov/kmh/quips/ (LANL internal only)
QUIPS external web site http://public.lanl.gov/kmh/quips/

Appendix B. QUIPS Abstracts

The abstracts are listed in the order in which they were presented at the workshop. Abstracts for the poster presentations appear at the end. Where the author did not supply an abstract, the editors created one.

Session 1. Weapons Physics

Primary modeling, QMU, and UQ

Matt Kirkland (X-4)

In this talk, I discuss the current state of development of the primary certification methodology. The concept of a framework for the Quantifications of Margins and Uncertainties (QMU) is introduced, and the role of uncertainty quantification (UQ) in this framework is presented. Within the context of the detailed operation of a nuclear weapon, the specific areas contributing to uncertainties in primary modeling are described. I discuss the current status of our work to quantify these uncertainties, highlight the difficulties, and suggest paths forward.

Uncertainties in secondary modeling

Merri Wood-Schultz (X-2)

There are many potential sources of uncertainty in simulations of the performance of secondaries, including uncertainties in physics models, numerical methods, data bases, and input data. When simulations are tuned to match any particular experiment, the concern is that there may be compensating errors, that together account for the experimental data, but individually are incorrect. I discuss various ways to model physical phenomena and describe how to merge them to obtain the best overall model. [Editors' abstract]

Data and uncertainties in experimentally constrained physics simulations

Merri Wood-Schultz (X-2)

Calibrations of computational physics simulations to match sets of experimental data can be viewed as falling into two classes: those designed to reproduce as precisely as possible the specific detail and data from a single experiment, sometimes called point models, and those optimized to capture the physical dependencies observed in variations among a set of experiments, the ensemble model. An ensemble model developed for a set of experiments will in general not reproduce the results of each experiment with the fidelity possible with a point model. The ensemble model is, however, more appropriate for extrapolating or interpolating results to new experimental conditions, precisely because it is developed to capture the physical dependencies of one or more (preferably all) important parameters in the experiments. To understand the reliance that can be placed on such predictions, it is important to understand the ways in which the experimental data that support the models influence the results of both point and ensemble models. [Editors' abstract]

Session 2. Experimental Uncertainties

Uncertainties in EOS's and what regions of pressure-temperature space are important: assigning uncertainties to ignorance and mistakes

J. D. Johnson (T-1)

Models for equations of state are at the heart of any hydrodynamic simulation. Unfortunately, most experimental data provided either in the literature or books do not provide estimates of the uncertainties in the tabulated data. There are also typically large gaps in the data that have to be filled in using models and the intuition of the modeler. Hence, the reliabilities of EOSs often need to be judged by the modeler. I will give examples of situations where there are distinct differences in the data from several laboratories for the EOS of the same material. The true answer is difficult or impossible to sort out. I will close by stating a number of concerns that I have about assigning uncertainties to tabulated EOS data, including coping with data that lack quantified uncertainties, and dealing with systematic uncertainties and uncertainties in judgment calls. On a positive note, I do feel that it is practical to perform sensitivity studies, determining what is important and what is not and thus focusing us on where to devote our efforts and improve all our work. I will discuss what I know of the regions of pressure-temperature space that are important.

Reliability of static equation of state determinations

David Schiferl (C-PCS)

Over the last several decades, the static equations of state determined in numerous laboratories often disagree with each other and with the results of dynamic experiments. In this talk, the procedures to determine equations of state with static high-pressure apparatus will be reviewed. The possible reasons for the problems encountered will be discussed in detail. The current experimental situation will be critically reviewed. Finally, suggestions will be made for future static equation-of-state experiments using new tools that have recently been developed.

Uncertainties in alpha curves

Barry Warthen (P-22)

Since the end of testing at the Nevada Test Site (NTS), the P-22 Analysis and Archiving Team has been reanalyzing the reaction history data collected at the NTS. The main focus of the reanalysis has been to more or less reproduce the original analysis to generate electronic data files for the flux and alpha curves similar to those in the original reaction history analysis reports. We are in the process of improving our analysis procedure and developing uncertainty analysis methods for the reaction history measurements

The reaction history measurement recorded the currents generated by detectors responding to a gamma-ray flux from an exponentially increasing source. The signals from the detectors were generally recorded on film from Rossi oscilloscopes using several scopes per detector to cover the linear range of the detector. At most, one scope per detector was common timed. Each detector viewed the gamma-ray source through a collimated line of sight. The flux a detector received was determined by the geometric effect and attenuating materials of the line of sight. The uncertainties of the reaction history curves due to the analysis and compositing of the Rossi data and the experimental effects are not addressed in our existing analysis method.

Our new focus of reanalysis is to provide reaction history curves that include uncertainty estimates. These new curves should be useful both to ongoing certification efforts and for validation of new computer codes. The tasks we are working on are as follows: (a) produce high resolution digital images of the Rossi and linear traces from the event films and scan all logbooks and supporting documents; (b)develop a process that uses computer-aided determination of the trace location and uncertainty from the digital images and calculate the flux and alpha curves with uncertainties for each indicator; (c) develop a method for estimating the uncertainty introduced by the process of producing composite flux and alpha curves from the individual indicators; (d) develop a process for estimating experimental calibration uncertainties when the actual values are not available.

A detailed description of the reaction history measurement and our initial progress on improving our analysis technique will be presented in this talk.

Quantification of uncertainties in simulations of weapons radiochemistry

Anna C. Hayes and Gerard Jungman (T-16)

Weapons radiochemistry is the analysis of radioactive isotopes produced during a thermonuclear explosion. Radiochemistry is a key diagnostic that helps provide a detailed physics understanding of these highly complex systems. Comparisons between the observed and predicted abundances of isotopes produced in a nuclear explosion are used to constrain design calculations and to determine yields. Additionally, radiochemical analysis is used to monitor the different energy components of the neutron spectrum.

At present the largest uncertainties in radiochemical analyzes arise from theoretical uncertainties in the nuclear cross sections that determine the pathways for production/destruction of the radioactive isotopes of interest. In this talk we will discuss the present uncertainties in radiochemistry simulations and their implications for yields and for assessing device performance. We will propose methods to reduce these uncertainties and a scheme to allow radiochemistry to be used as a more powerful tool for Stockpile Certification.

Uncertainty quantification for edge-location estimators on static radiographs taken at the DARHT facility

Greg Cunningham (DX-3)

At the end of construction in June 1999, the first axis of DARHT was used to radiograph two static objects, labeled A and B. The static objects were created so that the x-ray transmission through the objects matched the x-ray transmission through two devices in our stockpile, at radiographic time. The static radiographs were analyzed, and the rms errors on the inferred "inner" and "outer" edges were reported as the highest-level performance metrics for the machine. The fact that DARHT met requirements on these tasks (<200 microns rms error on the inner and outer edge for object A, <500 microns rms error on the inner edge, and <200 microns rms error on the outer edge for object B) was essential in declaring DARHT a technical success despite the fact that the spot size and dose did not meet expectations (the high performance of the detector exceeded expectations and compensated somewhat for these issues). In preparing for a similar set of experiments at the end of construction for the second axis of DARHT, a set of eight objects was defined (4 pulses for each device). The Bayes Inference Engine (BIE) was used to simulate the performance of DARHT's second axis under various assumptions on machine performance (energy, dose, spot size). The probability that the second axis would successfully meet the edge-finding requirements under each performance scenario was tabulated using the BIE's uncertainty quantification capability. In this talk I will review the first-axis results, the definitions for the static objects for the second-axis commissioning, the simulations, the methodology used in the BIE for uncertainty quantification, and the final results (probability of success).

Session 3. Uncertainties in Simulations

Uncertainty estimates for predictive simulations

David H. Sharp (T-13)

As simulation based predictions are called on to play a larger role in supporting high impact decisions about complex problems, estimates of the accuracy and reliability of the simulation results will form an indispensable part of the answer. If large scale simulations are to be used with confidence as predictive tools, one will have to show that the codes are giving the correct answers, for the correct reasons.

The keys to establishing confidence in predictive simulations are high quality and relevant data, high quality and relevant physics models, and, of course, elimination of outright discrepancies between simulations and observations. Within this context, the role of uncertainty quantification is to assess the overall level of agreement between simulations and data, to make maximum use of all available sources of data to constrain and reduce model uncertainties, and to provide guidance on the design of further experiments and experimental facilities. To do this with the necessary rigor, uncertainty quantification must supply a systematic procedure for identifying and estimating uncertainties arising from poorly known input parameters, incomplete or insufficiently accurate physics models, limited accuracy solutions of the governing equations and, from experimental measurement errors.

In this talk I will illustrate some of the issues that arise in uncertainty quantification with examples drawn from shock wave physics and petroleum reservoir engineering.

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Error distribution models for strong shock interactions

John W. Grove and Yunghee Kang (CCS-2)

A key problem in developing methods to quantify uncertainty in a numerical simulation is to understand the dynamic propagation and generation of solution error in a complex flow. For a given numerical method, the solution error for a specific realization can be regarded as the solution to a model equation obtained by the addition of the appropriate higher order diffusion and dispersion terms to the original set of PDE's being solved numerically. Since this model equation depends on the specific numerical method as well as the basic physical flow equations the utility of this abstract approach is limited in real problems, especially for complex nonlinear systems and complex numerical methods.

In this talk we will discuss an alternative approach that attempts to build empirical models for error generation based on a stochastic analysis of wave interactions. For simplicity we will focus our attention on describing the probability distribution of error generated due to the interaction of two shock waves. The basic method is an extension to stochastic flows of the fundamental random choice numerical method. Briefly we seek to determine the probability distribution for solution error as a function of the probability distribution for the Riemann problem data. We model this error using a linear superposition of a deterministic component and a random component, where by deterministic we mean a probability density function (PDF) that is a deterministic function of the pdf of the data. The random component is then a function of the numerical method and is modeled as an independent Gaussian.

This talk will describe the basic approach for performing the stochastic analysis, the evaluation of specified fitting forms for the deterministic component of the solution error, and estimations of the variance of the random, numerical method dependent, component of the solution error.

Uncertainty quantification of simulation codes using experimental data: Taylor impact tests

Kenneth Hanson (CCS-2), François Hemez (ESA-WR), and Shuh-Rong Chen (MST-8)

With the increasing reliance on simulation codes, understanding their uncertainties is clearly becoming a critical issue to address. The uncertainty quantification process consists of developing an uncertainty model for the simulation code through comparison of the code's output to experimental measurements.

Our approach to understanding simulation codes combines the principles of physics and Bayesian analysis. The focus is on understanding and quantifying the uncertainties in the simulation-code submodels and the numerical errors introduced in solving the dynamical equations. Bayesian analysis provides the underpinning for quantifying the uncertainties in models inferred from experimental results, which possess their own degree of uncertainty. The aim is to construct an uncertainty model that is based on inferences drawn from comparing the code's predictions to relevant experimental results. In the context of the proposed framework, it is possible to design new experiments that can best provide data for reducing prediction uncertainty.

The sources of uncertainty in a simulation-code prediction of the outcome to a hypothesized physical situation include a) uncertainties in the dynamical equations, b) uncertainties in submodels that describe material properties, c) numerical-solution errors, and d) uncertainties in the initial and boundary conditions of the physical situation being simulated.

We demonstrate our proposed approach by analyzing the results of a Taylor impact test, in which a metal cylinder is propelled into a rigid wall. The profile of the deformed cylinder is typically measured. We show how such profile data can be used to refine an uncertainty model for the simulation code, which can then be used to predict how well the code should be able to predict the results of the next Taylor test.

Data assimilation with extended Kalman filter

Jim Kao and Sarah Frey (X-4)

Data assimilation attempts to optimally determine the state of a physical system from a limited number of observations. While such a methodology has been used extensively in ocean and atmospheric modeling, the current study represents the very first attempt of applying data assimilation within the framework of shock wave physics. The extended Kalman filter (EKF) is characterized by solving the full nonlinear state evolution, and by using successive linearizations about the currently estimated state to advance the error-covariance matrix in time. It thus provides a consistent first-order approximation to the optimal estimate of the nonlinear state at the observation time. The EKF method combines the observations and modeled state variables to obtain the "assimilated" field variables through an optimal gain matrix coefficient. This coefficient, as a function of the forecast error-covariance, the observational error, and the observation procedure, are obtained through the minimization of the error-covariance matrix. The assimilated state variables and their associated errors (or uncertainties) can then be used as initial conditions for further model prediction until the next available data or for "extrapolation" purposes, if data are no longer available.

In this talk, I will present results of using EKF in the MESA code with real pressure data from a 1-D flyer plate experiment. The fidelity of EKF is further investigated with synthetic data, numerically generated from so-called "identical-twin experiments" in which the variations of numerous measurement techniques and strategies are feasible. Future applications of using EKF on production codes with radiography data in pit certifications will be introduced.

Session 4. Engineering

Overview of structural dynamics model validation activities at the Los Alamos National Laboratory

Scott W. Doebling (ESA-WR)

This presentation will provide a summary of the research and applications of structural dynamics model validation at Los Alamos National Laboratory. In this context model validation refers to the assessment of confidence in the usefulness of computational structural dynamics predictions for a particular application. A general process for approaching model validation, applicable to a wide range of engineering analysis problems, will be presented. Supporting technologies such as conceptual modeling, feature and metric definition, uncertainty quantification, global sensitivity analysis, metamodeling, model revision, and design of experiments will be discussed, along with their role in model validation. The model validation techniques will be demonstrated by application to the propagation of an explosive shock through a complex threaded joint that is a surrogate model of a system assembly.

Incorporation of model uncertainties and experimental errors in the assessment of surveillance data from cushions and pads in the nuclear stockpile

James E. Coons (ESA-WMM) and Michael D. McKay (D-1)

A Monte Carlo technique is applied to a foam aging model to predict changes in load-deflection properties that are directly comparable to surveillance test data taken on cushions and pads aged in the nuclear stockpile. The objective of the core surveillance program (CSP) is to assess changes that may impact the performance, reliability, and safety of the nuclear stockpile. Load-deflection tests have been performed under CSP on cushions and pads for decades, but considerable scatter in the data creates difficulties in assessing changes and trends. However, a foam aging model, developed under the Enhanced Surveillance Campaign, provides the ability to predict changes in load-deflection properties as the material ages in the stockpile. The material model has two components, a compression set model and a load-deflection model. The model parameters are based on an independent set of data taken from a nine-year aging study conducted in the 1970s and 80s. The compression set model predicts changes in the material thickness that result from being stored under compression. The load-deflection model predicts the load required to compress the material after it has been allowed time to recover its zero stress condition, a feature very similar to the recovery that occurs after foam parts are removed from weapons for surveillance tests. Limited test data salvaged from the historical aging study allow the optimum model parameters and codependencies to be determined. The aging model requires initial part thickness, storage thickness, storage temperature, and test thickness(es) as input, which vary between parts and systems. Therefore, the model input must be tailored to represent the aging conditions in each weapon system.

A Monte Carlo approach is used to quantify the variation in load-deflection properties that are expected to originate from a variety of sources. In addition to errors in the model parameters and variations in storage conditions and part dimensions, experimental errors are also thought to contribute to the scatter in surveillance data. Load-deflection tests are taken at the time each part is manufactured and again after the part is removed for surveillance. The absence of controls to mark the test positions results in the likelihood of multiple test sites being used for production and surveillance. Measurement errors originating from the load cell and linear variable differential transformers (LVDTs) are thought to be much smaller than the variability of material stiffness in any given part. Therefore, the largest contributor to the scatter of test data is thought to be due to the lack of common test sites on a given part. The Monte Carlo approach provides a means to incorporate variations in aging conditions, model parameter error, and experimental error in the model predictions as the components age. The result is a confidence band that represents the most likely region for surveillance data as the weapon ages. A direct comparison of the confidence region to surveillance data provides an independent and less subjective assessment of the integrity of aging cushions and pads in the nuclear stockpile.

Quantification of mass-model uncertainties and the reliability of mass and reaction Q-value calculations for unknown nuclei

Peter Moller (T-16)

In theoretical nuclear physics a basic nuclear property is the nuclear mass, which is a function of the proton number Z and neutron number N. Many nuclear mass models have been developed over the past 70 or so years, and a special series of conferences has been devoted to nuclear masses. In most or all nuclear mass models, there are a number of model constants that are determined by fitting the model to known nuclear masses, that is the model constants are adjusted so optimum agreement is obtained between calculated and measured masses for a set of nuclei. Normally this set of nuclei consists of all nuclei whose masses are known at the time the model constants are determined. About 2000 nuclear masses are known today.

When a model of this type is presented, its "accuracy" is normally given as the root-mean-square (rms) deviation between calculated and measured masses. When new measurements become available, the model accuracy for the new region of nuclei to which the model constants were not adjusted is again usually given as an rms deviation.

Several mass models agree with measured data up to about 0.7 MeV. Since mass measurements in regions of nuclei far from stability are often associated with errors in the range 0.2 - 2.0 MeV, it is clearly unsuitable to use the root-mean-square deviation as a measure of the model accuracy since the experimental mass uncertainties also contribute to the rms deviation.

Using a maximum-likelihood (ML) approach, we derive a measure for a model error that is insensitive to the error associated with the experimental measurements. We use actual case examples to compare the (unsuitable) rms deviation and our ML results as a characterization of the model error for several mass models and show that quite different conclusions are reached if the unsuitable rms deviation is used as the basis of this analysis, instead of the ML estimate.

We quantify the uncertainties of a very successful mass model developed here at Los Alamos over the past 20 years. The model constants were determined from adjustments to 1654 nuclei known in 1989. We compare it to more than 400 new nuclei discovered since then and show, using the ML approach to characterize the model error, that the model error does not increase in regions of newly discovered nuclei far from stability. This result is of great importance, for example, in calculating various Q-values for reactions on nuclei far from stability in weapons environments, for which experimental quantities are sometimes not available.

Code validation experiments with 2D velocimetry

Mark Marr-Lyon, Chris Tomkins, Kathy Prestridge, Paul Rightley, Robert Benjamin (DX-3); Cindy Zoldi (X-2); James Kamm, William Rider (CCS-2); and Peter Vorobieff (UNM)

Uncertainty quantification requires the meticulous comparison of computational simulations with experimental data. We have elevated such code validation to a higher standard by measuring the 2D velocity fields of complex flows induced by shock-wave acceleration, and by applying a variety of quantitative methods for comparing the simulations with experimental data. We describe the series of shock-tube experimental results, including gas curtain, one-cylinder and two-cylinder, that have not only been used for code validation, but also for model validation. We also describe extensions of PIV (Particle Image Velocimetry) techniques to explosively-driven flows with either radiographic or optical images that use either persistent flow features, marker particles, or ejecta particles to map the flow. These data are presenting new challenges to the capability of flow simulation to accurately create and transport vorticity.

In addition to the comparison of velocity fields and histograms, we present sample results of other analysis methods, including fractal dimension and structure function, which lend themselves to uncertainty quantification of incipient turbulent flows. We also show detailed studies of initial conditions in the shock-tube experiments to determine the effects of differential diffusion between the gases and the tracer particles.

In summary, these detailed experiments raise the standard of validating codes designed to simulate complex, shock-accelerated flows. These experiments yield data of high spatial and time resolution, and their reproducibility enables ensemble averaging so we can accurately assess the uncertainties.

Multiscale techniques for the analysis of high-resolution experimental data and simulation result

William J. Rider and James R. Kamm (CCS-2)

In both experimentally observed and computationally simulated phenomena, there are multiscale effects that are difficult to examine quantitatively. Such quantitative analysis is key to achieving a measure of simulation fidelity and ultimately assigning the relative uncertainty of the simulation. Hydrodynamic instabilities are a prototypical example of such a phenomenon. Often the only recourse is to rely upon statistical means of examination. Here we will discuss both methods for such examinations and their connection to various physical models or idealizations. These methods include fractals, wavelets, and a variety of statistical measures. We will discuss results obtained when applying these measures to both experimental data and simulations. We will compare and contrast among the measures discussed above and more rudimentary measures that are more commonly applied to such datasets.

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Posters

Combined probabilistic and non-probabilistic uncertainty quantification applied to performance reliability

Jane M. Booker and François M. Hemez (ESA-WR)

Probability theory may not always be sufficient for characterizing the different kinds of uncertainties existing in complex computer or physical system models. Two different examples of reliability problems are presented: one involving the test-analysis correlation of data with a computer model and the other involving estimating the reliability of a new concept system before prototyping or testing. Each involves ambiguous or imprecise information, with the lack of test data, and therefore, the need for mathematical theories for handling these kinds of uncertainty.

In the first case, an alternative to the theory of probability is applied to assess the reliability of model predictions to sources of uncertainty. The application involves the propagation of a shock through an assembly of structural components. The analysis technique is based on the theory of information-gap, which models the clustering of uncertain events in families of nested sets instead of assuming a probability structure. Conventional, probabilistic models of covariance are combined with information-gap models of uncertainty to study the adverse but also the beneficial effects of uncertainty on the correlation between measurements and predictions. Parametric calibration under uncertainty is also illustrated.

In the case of the reliability for a new concept system design, test data are lacking and expensive to obtain. Before prototypes of new parts/systems are built, the designers want to compare the potential performance of competing designs, using reliability as the metric for performance. Because the designers tend to think in terms of reliability as a probability, they wish to estimate performance in probabilistic space; however, not all of the available information for the new components and systems is in the form of probabilities. This example shows how more vague and ambiguous information about the new design is best captured using fuzzy sets. The analysis challenge then becomes one where probabilistic information must be combined with fuzzy information to estimate reliability, requiring a theoretical linkage between probability theory and fuzzy set theory. Such a linkage has been established and is illustrated in the example.

Functional Sensitivity Analysis (FSA): approaches to sensitivity and importance analysis based on functional output

Katherine Campbell and Michael McKay (D-1)

The outputs of physics-based computer models are often functions of time, space or other continuous variables. There are several options for dealing with outputs of this type for the purposes of model sensitivity and uncertainty analysis. First, of course, standard sensitivity analysis methods can be applied to the outputs at each point in space or time. This can lead, for example, to displays of indices of importance, such as R^2, as a function of the natural coordinate system. When this coordinate system is time, and the importance of the various inputs is naturally evolving over time, this approach can be quite successful.

When the natural coordinate system is related to space, however, we have frequently found that these analyses are not readily interpretable. Another option might be to extract scalar descriptors of the functional outputs (means or other moments, indicators of skewness or tail weight) to which standard analysis methods can be applied. The selection of such indicators, however, is highly problem specific and requires considerable insight into the physical problem.

A third and natural alternative is to represent the function in another basis system. Possible transformations include both standard choices such as Fourier transformations, Legendre transformations, and spherical harmonics, or adaptive transformations, such as principal components and partial least squares. For sensitivity or importance analysis, as for these other types of analyses, the standard methods can be successfully applied to the coefficients of the expansion of the output functions in the new basis.

The advantages of using standard transformations are most evident when a series of problems is to be considered, and it is desired to compare the results. Variability across problems is then confined to the coefficients of the transformations, rather than affecting the basis functions themselves. Standard transformations are, however, seldom perfectly tailored to the problem in hand, and this leads to simple effects (sensitivities) being spread out across several terms in the expansion and also to the obscuring of more subtle effects. Data adaptive transformations achieve good compression of information, and their analysis can be both more interpretable and more revealing.

We will show examples of some of these options for a specific problem with a view towards learning when each is most likely to be successful.

Uncertainty quantification of simulation codes using probability intervals

Cliff Joslyn (CCS-3) and Bill Oberkampf (SNLA)

The Epistemic Uncertainty Project (http://www.sandia.gov/epistemic/) is evaluating new approaches to Uncertainty Quantification (UQ) and propagation for risk and reliability analysis of simulation codes. The project is collaboration between the Sandia and Los Alamos National Laboratories and Applied Biomathematics Corp. of Setauket, New York, through the ASCI V&V program element.

Codes of interest are typified by high run times, on the order of days; the necessity of accessing the codes as "black boxes"; and on the order of hundreds of inputs and outputs. The parametric uncertainties are complex: semantically, they may be determined either by eliciting expert opinion or making measurements; and they may be intended to represent distinct *kinds* of uncertainty: **aleatory** uncertainty, expressing inherent variability or stochasticity; or **epistemic** uncertainty, expressing ignorance or imprecision in its measurement or specification.

Where possible, we should quantify uncertainties mathematically as probability distributions. But when information is sparse, imprecise, or vague, for example a small distribution of points, an interval, or a statistical collection of intervals, a precise probability distribution may not be available.

We are developing mathematical methods for UQ which can accurately and properly represent these different forms of uncertainty. The goal is to be able to use all the information given, while not requiring the introduction of assumptions to accommodate the sparse information. Such methods require a tolerance for imprecision in the UQ, which under these circumstances is actually a very healthy exchange for both greater accuracy and for respecting the data as given.

We focus on cases where uncertainty is expressed as collections of intervals, arising from the elicitation of interval opinions from; observations made with relatively imprecise instruments; the collection of error bounds on measurements from multiple experiments; the extreme values of measured points; or from other sources. Rather, such statistical collections of intervals are best represented by a **random interval**, a probability distribution expressed at the level of intervals on the line.

Such data specify a *collection* of specific probability distributions, each of which is *consistent* with the data; and each region of the input space becomes equipped with an **interval probability** consisting of an **upper** and **lower** probability. In turn, when these structures are propagated through a simulation code, the resulting output random interval expresses the range of probability for an event of interest, for example the risk of a certain event.

Our ultimate target application is thermal response sensitivity and uncertainty quantification of weapon system safety in abnormal environments, modeled as a simplified component response. We discuss a Monte Carlo sampling approach to random interval propagation for estimating upper probabilities of risk events in this model.

Uncertainties assessment in nuclear data evaluations

Patrick Talou (T-16)

Crucial applications in the field of nuclear physics, e.g., weapons design, civil reactors, particle accelerators, astrophysics, nuclear medicine, to name but a few, rely heavily on accurate nuclear data, and in particular on accurate nuclear reaction cross sections. An important part of our work in T-16 is devoted to provide the overall nuclear physics community with very precise nuclear data evaluations. Such evaluations are usually the result of various physical models, continuously improved, along with experimental data sets, especially important when the available nuclear models are known to fail.

While experimental results are unavoidably subject to uncertainties, both statistical and systematic, a Bayesian inference scheme can help determine a "best" estimate for the physical quantities studied. We have recently used such a scheme to infer an evaluation of the neutron-induced fission cross section on Pu-239 below 20 MeV. Such a reaction is of prime importance in the quest of nuclear waste transmutation, as studied in the Advanced Fuel Cycle Initiative (AFCI) Program and in primary weapon design.

I will present both the method and results regarding our latest evaluation of the Pu-239 (n,f) cross section. I will introduce new techniques to be used in future evaluations (sensitivity analysis, robustness, etc.). I will also discuss how uncertainty/covariance tools are being developed in the nuclear data community to determine the impact of cross section uncertainties on physical simulations of neutron transport systems.

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Temperature equilibrium rate in strongly coupled plasma

L.E. Thode, C.H. Chang, C.M. Snell, W.S. Daughton, and G. Csanak (X-1)

A laser-driven experiment investigating electron-ion equilibrium in strongly coupled plasma was performed in 1995 [1]. At that time, standard estimates for the electron-ion equilibrium time were two to three orders of magnitude faster than observed experimentally. As a result, the electron-ion equilibrium time was taken as a fitting parameter to understand the experimental results.

Based on guidance from nonequilibruim molecular dynamics mixture calculations [2] and comparison with strongly coupled resistivity experiments [3], we have developed a consistent binary-collision theory to understand the electron-ion equilibrium results. The improved theory has been implemented in a newly developed multi-species, multi-temperature high-fidelity physics code, HiFi, which was subsequently used to successfully simulate the experiment. The main effect that brought about agreement with the data is the modified Coulomb logarithm.

Implications for high-energy-density codes will be discussed.

[1] Ng, Celliers, Xu, and Forsman, *Phys. Rev. E* **52**, 4299 (1995).
[2] Thode, Daughton, Murillo, and Sanbonmatsu, LANL Memo X-1-99-02 (U), October 14, 1999.
[3] Thode, Daughton, and Csank, LANL Memo X-1-00-39 (U), November 12, 2000.

Effective error estimates for quasi-Monte-Carlo computations

Tony Warnock (CCS-3)

Quasi-Monte-Carlo methods are based on sampling over a low-discrepancy point set rather than a randomly chosen point set as is used in traditional Monte-Carlo. Although Quasi-Monte-Carlo methods have a superior convergence rate compared to traditional Monte-Carlo methods, they have suffered from a lack of an effective error estimate. I describe an effective error estimate that is based on independent replications of Quasi-Monte-Carlo computations.