Workshop on Verification and Validation in Computational Science

Sunday, 16 October 2011

5:00 PM-7:00 PM, Welcome Reception and Registration; Donors' Room, Morris Inn

Monday, 17 October 2011

7:30-8:10, Registration/Coffee, Notre Dame Conference Center

8:10-8:15, Workshop Opening Remarks, *Joseph M. Powers* (University of Notre Dame) slides

8:15-8:25, Welcoming Remarks, *Christine Maziar* (Vice President and Senior Associate Provost for Budget and Planning, University of Notre Dame)

8:30-9:20, Keynote, Verification and validation in simulations of complex engineered systems, *Robert Moser* (University of Texas at Austin) slides

9:20-9:35, Break

9:35-9:55, Validation and verification in global atmospheric chemistry models, *Mauricio Santillana* (Harvard University) slides

9:55-10:15, Computing and verifying compressible fluid dynamics: the good, the bad and the ugly, *Tariq D. Aslam* (Los Alamos National Laboratory) slides

10:15-10:35, Enabling sensitivity analysis, uncertainty quantification, and data assimilation via a hybrid reduced order modeling framework, *Hany Abdel-Khalik* (North Carolina State University) slides

10:35-10:55, Verification, validation and uncertainty quantification theory meets aerospace practice: NASA experience with formal requirements for VV & UQ, *Thomas A. Zang* (NASA Langley), Timothy S. Barth (NASA Engineering and Safety Center), William J. Bertch (Jet Propulsion Laboratory), Wei A. Lin (NASA Ames), Gary E. Mosier (NASA Goddard), Martin J. Steele (Kennedy Space Center) slides

10:55-11:30, Discussion led by *William Oberkampf* (Consultant), Topic: Differing goals of validation, calibration, and predictive uncertainty slides

11:30-1:00, Lunch

1:00-1:50, Keynote, Perspectives on verification and validation in complex adaptive systems, *Werner Dahm* (Arizona State University) slides

1:50-2:05, Break

2:05-2:25, Compressible flow code verification problems: oldies but goodies, *James R. Kamm*, William J. Rider, Gregory Weirs, Edward Love (Sandia National Laboratories–Albuquerque), Scott D. Ramsey (Los Alamos National Laboratory), Frank X. Timmes (Arizona State University) slides

2:25-2:45, A predictive capability planning, tracking, and evaluation system, *Patrick Knupp*, Angel Urbina (Sandia National Laboratories–Albuquerque) slides

2:45-3:05, Verification techniques for incompressible viscous flows on deforming domains, *D. Pelletier*, A. Hay, S. Etienne, A. Garon (École Polytechnique de Montréal)

3:05-3:20, Break

3:20-3:40, Manufactured solutions for (U)RANS solvers, *Luis Eça* (Universidade Técnica Lisboa), Martin Hoekstra (Maritime Research Institute Netherlands) slides

3:40-4:00, Verification of computational constitutive models using the method of manufactured solutions, *Krishna Kamojjala*, Rebecca M. Brannon (University of Utah)

4:00-4:30, Discussion led by *Samuel Paolucci* (University of Notre Dame), Topic: What is Direct Numerical Simulation (DNS)?

4:30-6:00, Reception, Atrium, Notre Dame Conference Center

Tuesday, 18 October 2011

8:00-8:30, Registration/Coffee, Notre Dame Conference Cetner

8:30-9:20, Keynote, What makes a computational simulation good? or bad?, *William J. Rider* (Sandia National Laboratories-Albuquerque) slides

9:20-9:35, Break

9:35-9:55, Automated solution verification using the wavelet adaptive multiresolution representation, *Zachary Zikoski*, Samuel Paolucci, and Joseph M. Powers (University of Notre Dame) slides

9:55-10:15, Verification and validation at the micro- and nanoscale, Harvey Zambrano, *A. T. Conlisk,* (The Ohio State University) slides

10:15-10:35, Classification of ignition regimes in thermally stratified n-heptane-air mixtures using computational singular perturbation, Saurabh Gupta, *Hong G. Im* (University of Michigan), Mauro Valorani (University of Rome) slides

10:35-10:55, V&V for turbulent mixing and combustion, *James Glimm* (State University of New York at Stony Brook) slides

10:55-11:30, Discussion led by *Gretar Tryggvason* (University of Notre Dame), Topic: Innovative and/or Accurate—Finding the Right Balance?

11:30-1:00, Lunch

1:00-1:50, Keynote, Laminar-to-turbulent stability and transition, *Helen Reed* (Texas A&M University) slides

1:50-2:05, Break

2:05-2:25, Predicting and correcting for grid-induced errors in steady and time-accurate CFD solutions, *Tom I-P. Shih* (Purdue University) slides

2:25-2:45, New technical requirements for software tools in computational solid mechanics, *Barna Szabó* (Engineering Software Research and Development) slides

2:45-3:05, Framework for residual-based error estimation in computational fluid dynamics, *Christopher J. Roy* (Virginia Tech) slides

3:05-3:20, Break

3:20-3:40, Avoiding operator splitting of stiff source terms: a verification via two-fluid magnetohydrodynamics and a validation via astrophysical turbulence, *Dinshaw Balsara* (University of Notre Dame) slides

3:40-4:00, Multiscale modeling of particulate composited with co-designed experiments using micro-computer tomography, *Karel Matous* (University of Notre Dame) slides

4:00-4:30, Discussion led by *Christopher J. Roy* (Virginia Tech), Topic: Practical solution verification approaches for complex scientific computing applications

4:30-5:30, Free time

5:30-9:00 Studebaker National Museum tour and banquet at Tippecanoe Place

Wednesday 19 October 2011

8:00-8:30, Registration/Coffee, Notre Dame Conference Center

8:30-9:20, Keynote, V&V in image-based cardiovascular fluid dynamics: from mathematical models to patients, *Charles A. Taylor* (HeartFlow, Inc.; Stanford University)

9:20-9:35, Break

9:35-9:55, An overview of inverse material identification within the frameworks of deterministic and stochastic parameter estimation, *Miguel A. Aguiló*, Laura Swiler, and Angel Urbina (Sandia National Laboratories–Albuquerque)

9:55-10:15, Comparison of a pragmatic and versatile "real space" model validation framework against several other validation frameworks, *Vincente Romero* (Sandia National Laboratories-Albuquerque) slides

10:15-10:35, From validation set points to a continuum domain of validation, *Patrick J. Roache* (Consultant) slides

10:35-10:55, Development of a standard for verification and validation of software used to calculate nuclear system thermal fluids behavior,*Richard Schultz*, Edwin Harvego (Idaho National Laboratory), Ryan Crane (ASME) slides

10:55-11:30, Discussion/Wrap-up led by *Joseph M. Powers* (University of Notre Dame)

Monday, 17 October 2011

8:30-9:20, Keynote, Verification and validation in simulations of complex engineered systems, *Robert Moser* (University of Texas at Austin)

Computational simulation is a ubiquitous tool in engineering. Further, the explosion of computational capabilities over the last several decades has resulted in the use of computational models of unprecedented complexity to make critical design and operation decisions. One potential benefit should be to improve reliability of the engineered system while reducing margins, due to the more accurate predictions such models could produce. However, realizing this benefit requires that the models employed be carefully validated, and the simulations rigorously verified. The Center for Predictive Engineering and COmputation Sciences (PECOS) at the University of Texas at Austin is developing tools and methodologies for verification and validation in the presence of uncertainty for such simulations. Among the developments being pursued are techniques for code and solution verification, calibration and validation of physics-based models using uncertain data, characterizing the uncertainties in such data, representing uncertainty due to model inadequacy and validating predictions of unobserved quantities. Central to model validation is accounting for uncertainty, and at PECOS, it is represented using Bayesian probabilities, with calibration and validation processes formulated in terms of Bayesian inference.

In this talk, the PECOS approach to verification and validation in complex systems will be discussed with example applications to the prediction of reentry vehicles with ablative heat shields.

9:35-9:55, Validation and verification in global atmospheric chemistry models, *Mauricio Santillana* (Harvard University)

Understanding the global-scale dynamics of the chemical composition of our atmosphere is essential for addressing a wide range of environmental issues from air quality to climate change. Numerical modeling of this phenomenon presents an enormous challenge. On one hand, we need to formulate an appropriate mathematical model capable of describing the time evolution of the interactions of hundreds of chemical species with time scales varying from milliseconds to years in multiple spatial scales. On the other hand, we need to discretize the mathematical model, often in the form of coupled partial differential equations (PDE), to obtain a "computational model" that can be numerically solved using state-of-the-art high performance computers. Validation of our mathematical models is crucial since we use them to evaluate and devise appropriate environmental policies, such as the Kyoto Protocol on global greenhouse gases emissions. In practice, the validation process is often performed by comparing the numerical solution of the computational problem, with sparse (in time and space) measurements coming from satellite observations and monitoring stations. This validation approach assumes implicitly that the verification step (making sure that the numerical solution is close to the true solution of the differential equations) is negligible. The argument being that the errors and uncertainties coming from the discretization of the differential equations are small. In my presentation, I will show that this assumption may be incorrect in diverse real life circumstances. I will emphasize the need to formulate and include sub-grid parametrizations in our current global models in order to ensure consistency across spatial scales. I will also present evidence of structural deficiencies in our models that limit our ability to extract meaningful information from them in specific inverse modeling problems

9:55-10:15, Computing and verifying compressible fluid dynamics: the good, the bad and the ugly, *Tariq D. Aslam* (Los Alamos National Laboratory)

Many practical engineering calculations utilize the inviscid compressible Euler equations of fluid mechanics. And although many methodologies for constructing consistent numerical methods for these equations have been successful, there remain many outstanding issues. Several examples of “The Good,” “The Bad,” and “The Ugly” will be presented and discussed. The focus here will be on solutions containing discontinuities, and the variety of schemes built to handle them. For a single numerical method, one may observe high order, low order and zero order convergence depending solely on the chosen initial conditions.

10:15-10:35, Enabling sensitivity analysis, uncertainty quantification, and data assimilation via a hybrid reduced order modeling framework, *Hany Abdel-Khalik* (North Carolina State University)

Sensitivity analysis, uncertainty quantification, and data assimilation are integral tools to the success of any verification and validation activities. For example, in a typical validation plan,one needs to compare the predictions and measurements for quantities of interest and devise a rigorous mathematical device to calibrate the model in order to improve the quality of its prediction. This process is referred to as data assimilation. To complete data assimilation, one must have sensitivity information which captures the variations of the various quantities of interest with respect to the model parameters that can be calibrated by data assimilation. An important outcome of any validation plan is to identify where the key sources of uncertainties originate, which can be achieved via a coupled sensitivity/uncertainty analysis.

Applying these analyses to complex systems on a routine basis is challenging given the complexity of most real-world models. Reduced order modeling has been recognized as the most prominent approach to reduce the computational complexity without sacrificing the accuracy of the original complex model. This presentation overviews our recent developments on a hybrid framework intended to enable the application of reduced order modeling to routine design calculations. Recent research has shown that it is possible to combine the benefits of existing techniques using a hybrid approach that can be applied in a generic manner to a general code system. We discuss these developments and demonstrate their applicability to typical reactor design calculations. Finally, we introduced a new reduced order approach for verification employing the method of manufactured solutions to ensure proper coverage of the solution space- this is considered one of the limitations of the method of manufactured solutions.

10:35-10:55, Verification, validation and uncertainty quantification theory meets aerospace practice: NASA experience with formal requirements for VV & UQ, *Thomas A. Zang* (NASA Langley), Timothy S. Barth (NASA Engineering and Safety Center), William J. Bertch (Jet Propulsion Laboratory), Wei A. Lin (NASA Ames), Gary E. Mosier (NASA Goddard), Martin J. Steele (Kennedy Space Center)

In July 2008, NASA issued its Standard for Models and Simulations (NASA-STD-7009). This was one of the many agency-wide responses that NASA made to the 2003 Columbia accident. The overall goal for this standard is to ensure that the credibility of the results from models and simulations is properly conveyed to those making critical decisions, i.e., those technical decisions related to design, development, manufacturing, ground, or flight operations that may impact human safety or mission success criteria. It is intended to cover all systems, all disciplines, and all types of models and simulations. This is the only requirements-based standard for models and simulations yet issued by a government agency. A generic Guidebook for assisting practitioners in implementing the standard is near completion. The standard contains 49 requirements, 17 of which pertain to some aspect of verification, validation or uncertainty quantification.

The NASA Standard for Models and Simulations is still in its initial period of trial use. This presentation will briefly summarize the VV&UQ requirements in the standard and then will focus on some of its applications (both notional and real) to NASA space flight projects. Examples will be drawn from such NASA operational and development projects as the Space Shuttle, crew capsules (Orion), government launch vehicles (Ares), commercial launch vehicles (Commercial Crew Transportation Program), planetary landers (Mars Science Laboratory), Earth satellites (Aquarius), and space telescopes (James Webb). Some of the concerns that have arisen in these applications are the upfront cost of the additional rigor, conflicts with specialized terminology and practices, perceived questioning of the integrity of the practitioners, the need for training and tools for uncertainty quantification, and, above all, resistance to the use of a "scale" to assess the rigor used to produce the results from models and simulations.

1:00-1:50, Keynote, Perspectives on verification and validation in complex adaptive systems, *Werner Dahm* (Arizona State University)

Verification and validation has taken on special interest within the Department of Defense, since it is the single greatest factor that limits our ability to establish "certifiable trust" in the software needed to enable highly adaptable autonomous systems and processes. Such systems hold enormous potential not just for developing far more advanced unmanned aircraft and other autonomous platforms, but for addressing the single greatest problem facing all DoD Services, namely reducing their ballooning manpower costs while at the same time increasing their capabilities. Both these objectives require developing the next generation of more highly adaptable autonomous systems and processes. As noted in the recent public-releasable Vol. 1 of U.S. Air Force "Technology Horizons," V&V of the complex adaptive software that enables such autonomous systems and processes will be a key focus area for Air Force science and technology over the next two decades.

These are near-infinite state systems that use a potentially huge number of inputs to make a potentially huge number of interdependent decisions and thereby take on a potentially huge number of system adaptations. Already today, the operational flight program (OFP) in a modern fighter like the F-35 is a near-infinite state autonomous system. Literally over half the cost of developing the F-35 has resulted from the need to V&V its amazingly capable but enormously complex OFP software. The fact that we cannot today adequately V&V such complex software systems is the reason we continue to discover serious problems in the OFP even very late in development, which then require astonishing amounts of money to fix because countless other parts of the OFP software must then also be V&Ved again.

Our current inability to V&V the complex adaptive software for such systems to achieve the "certifiable trust" needed to field them, let alone to field the far more highly adaptable autonomous systems and processes that we need for our generation-after-next capabilities, is one of the central problems facing DoD. Our potential adversaries also recognize the enormous capabilities they will gain from such highly-adaptable autonomous systems and processes, and may be entirely willing to field them without the enormous V&V burden that we place on ourselves. This could provide a major asymmetric advantage for our adversaries, and further highlights the critical importance of finding new ways to architect software to make it more "V&V-able," new ways to think about how software V&V might be done, and new thresholds for declaring near-infinite state software to be certifiable.

2:05-2:25, Compressible flow code verification problems: oldies but goodies, *James R. Kamm*, William J. Rider, Gregory Weirs, Edward Love (Sandia National Laboratories–Albuquerque), Scott D. Ramsey (Los Alamos National Laboratory), Frank X. Timmes (Arizona State University)

Code verification remains the definitive practice by which to quantitatively demonstrate the legitimacy of a software instantiation for a numerical algorithm. Specifically, code verification analyses form a technically essential computational foundation upon which to build further code confidence with solution verification and uncertainty quantification. Additionally, code verification can guide algorithm developers to improve the accuracy of their numerical methods, and associated error measurements can be used to compare the overall accuracy of different numerical schemes. The field of gas dynamics is particularly amenable to this practice, as the nonlinear PDEs possess a host of exact solutions containing nontrivial flow features. In this overview presentation, we review the systematic Lie group approach used to obtain similarity solutions of the one-dimensional Euler equations of gas dynamics for a polytropic gas with planar, cylindrical, and spherical symmetry. We spotlight a number of well-known exact solutions for compressible flow code verification, including the spherical flow triumvirate comprised of the Noh, Sedov, and Guderley problems; we discuss lesser known variants and aspects of these and other exact solutions. Despite the attention that these problems have received over many decades, there remain controversial code verification aspects regarding their computational setup and little-known details required for accurate evaluation of their exact solution. It is well established that the numerical methods for the nonlinear hyperbolic system of gas dynamics exhibit at best first-order convergence on such problems. We provide computational results with both Eulerian?frame and Lagrangian-frame codes, and examine some reasons why they do not always attain the theoretical result and the implications for verification acceptance tests.

2:25-2:45, A predictive capability planning, tracking, and evaluation system, *Patrick Knupp*, Angel Urbina (Sandia National Laboratories–Albuquerque)

There is currently sparse literature on how to implement systematic and comprehensive processes for modern V&V/UQ (VU) within large computational simulation projects. Important design requirements have been identified in order to construct a viable "system" of processes. Significant processes that are needed include discovery, accumulation, and assessment. A preliminary design is presented for a VU Discovery process that accounts for an important subset of the requirements. The design uses a hierarchical approach to set context and a series of place-holders that identify the evidence and artifacts that need to be created in order to tell the VU story and to perform assessments. The hierarchy incorporates VU elements from a Predictive Capability Maturity Model and uses questionnaires to define critical issues in VU. The place-holders organize VU data within a central repository that serves as the official VU record of the project. A review process ensures that those who will contribute to the record have agreed to provide the evidence identified by the Discovery process. VU expertise is an essential part of this process and ensures that the roadmap provided by the Discovery process is adequate. Both the requirements and the design were developed to support the Nuclear Energy Advanced Modeling and Simulation Waste project, which is developing a set of advanced codes for simulating the performance of nuclear waste storage sites. The Waste project served as an example to keep the design of the VU Discovery process grounded in practicalities. However, the system is represented abstractly so that it can be applied to other M&S projects

2:45-3:05, Verification techniques for incompressible viscous flows on deforming domains, *D. Pelletier*, A. Hay, S. Etienne, A. Garon (École Polytechnique de Montréal)

The paper will discuss issues arising in both code and simulation verification of incompressible viscous flows on deforming domains with applications to flows around moving bodies, free surface flows, flow induced vibrations, and fluid structure interaction. These flows have in common a rather broad spectrum of computational challenges:

- Incompressibility complicates the spatial discretization and imposes severe restrictions on time integrators when high order temporal accuracy is necessary;
- Fluid-structure interaction and flow induced vibrations result in additional restrictions and challenges if one wishes to use the same time-integrator for the fluid and structural domains in 2-D and 3-D problems;
- Methods that are effective for verification of first or second order time integrators, become impractical or infeasible when applied to high order time-integrators (3rd and 5th order) because of their excessive requirements in terms of computational resources;
- satisfaction of the GCL for high-order time-stepping schemes becomes a non-trivial task.

Manufactured solutions will be presented for code verification of the finite element solver that we have developed for this class of flow problems including interaction of a viscous incompressible flow with a solid undergoing large displacements, flow over solid bodies in relative motion with respect to each other, free surface flows, and flow induced vibrations.

When high order time-integrators are used, the usual time-step and mesh size refinement technique becomes impractical. Halving the time-step size reduces the temporal error by factor of 32. Ensuring an equivalent reduction of the spatial error for a second order discretization of space results in a reduction of the mesh size by a factor of $4\sqrt{2}$ or 5.6. This amounts to increasing the number of grid points by a factor of 32 in 2-D and 187 in 3-D for each halving of the time step. We will discuss an alternative approach for time-integrator verification. Results of simulation verification will also presented for the same class of flow problems.

3:20-3:40, Manufactured solutions for (U)RANS solvers, *Luis Eça* (Universidade Técnica Lisboa), Martin Hoekstra (Maritime Research Institute Netherlands)

In this presentation, the focus is on uncertainty quantification for the Reynolds-Averaged Navier-Stokes ((U)RANS) equations for both time-averaging (statistically steady) and ensemble averaging (statistically unsteady) approaches. The (U)RANS equations are still the most common model for the solution of engineering flow problems characterised by high Reynolds numbers (above 10^6). The demand on quality assessment of solutions obtained with this model is increasing. Because the RANS equations do not form a closed system due to the presence of the Reynolds stresses (produced by the statistical handling of the Navier-Stokes equations), a turbulence model is an essential part of the system of equations, which complicates quality assessment.

Quality assessment is based on error evaluation (Code Verification) and error estimation (Solution Verification). In the first case, the Method of Manufactured Solutions [1] is essential due to the inexistence of analytical solutions of the (U)RANS equations. For the latter problem, the difficulties are mostly linked to the difficulties to attain the "asymptotic range" in turbulent flows at high Reynolds numbers, as discussed in the three Lisbon Workshops of 2004 [2], 2006 [3], and 2008 [4]. This makes the evaluation of procedures for Solution Verification troublesome, because most of the methods available in the literature assume that the data are in the "asymptotic range." A straightforward way to assess the ability to perform uncertainty estimates with data outside the "asymptotic range" is to use a manufactured solution. This was exactly one of the strategies followed in the 2006 and 2008 Lisbon Workshops.

A first example of a manufactured solution for Code Verification of RANS solvers (and hopefully for checking procedures for uncertainty estimation) supplemented by eddy viscosity models has been presented in [5]. The manufactured flow field resembled a nearwall flow with a divergence free velocity field and a velocity component parallel to the "wall" defined by the error (erf) function. Analytical expressions were also proposed for the dependent variables of several one and two-equation eddy-viscosity models. Although the usefulness of this MS has been widely demonstrated [3, 4], there are several features that can be improved:

- The horizontal mean velocity profiles have a shape factor which is much closer to a laminar flow than to a turbulent flow.
- The "shear-stress" at the wall (normal derivative of the tangential velocity component) is much smaller than what is obtained for a near-wall turbulent flow.
- Simple products of polynomial and exponential functions were used to define the turbulence quantities, leading in some cases to unphysical [6] or unreasonably complex behaviour of the damping functions [7] for some turbulence models.

The main consequence of the choices made in [5] is that the mean flow field is too simple, i.e. it is fairly easy to attain the asymptotic range (even for equally-spaced grids) and in some cases the turbulence quantities are too complicated.

In order to avoid the shortcomings mentioned above, this presentation introduces a new set of manufactured solutions for incompressible flows governed by the (U)RANS equations supplemented by eddy-viscosity models. The set includes two-dimensional and three-dimensional solutions for statistically steady and periodic flows. The main ideas behind the newly proposed manufactured solutions are the following:

- The flow field is divergence free, i.e. the manufactured velocity field satisfies mass conservation.
- The near-wall flow mimics a zero pressure gradient turbulent boundary-layer flow, with a skin friction coefficient matching a simple empirical correlation and with the near-wall velocity profiles including a viscous sub-layer.
- The flow field is defined as a function of the Reynolds number, allowing the choice of values in the range of 10^6 to 10^9.

- The near-wall behaviour of the turbulence quantities is determined by expressions available from "automatic wall functions" [8] combined with an exponential decay in the outer region of the flow.

For each of the cases mentioned above, the manufactured solutions define the mean velocity and pressure fields, an undamped eddy-viscosity ($\tilde{\nu}$), the turbulence kinetic energy (k), the turbulence frequency ($omega$) and the eddy-viscosity (ν_t) of several one- and two-equation eddy-viscosity models. The balancing source terms of the momentum equations and of the turbulence quantities transport equations are also determined for the same eddy-viscosity models. The presentation will also discuss the consequences of the inclusion of max/min functions (as for example in the SST $k-\omega$ model) in the turbulence models for Code and Solution Verification procedures.

The present manufactured solutions are defined in simple rectangles or rectangular prisms. However, we will also exemplify how a simple coordinate transformation may generalize the present manufactured solutions to domains with curved boundaries.

References

[1] Roache P.J. - Code Verification by the Method of the Manufactured Solutions - ASME Journal of Fluids Engineering, Vol. 114, March 2002, pp. 4-10.

[2] Proceedings of 2nd Workshop on CFD Uncertainty Analysis - Instituto Superior Técnico, Lisbon, October 2006.

[3] Proceedings of 2nd Workshop on CFD Uncertainty Analysis - Instituto Superior Técnico, Lisbon, October 2006.

[4] Proceedings of 3rd Workshop on CFD Uncertainty Analysis - Instituto Superior Técnico, Lisbon, October 2008.

[5] Eça L., Hoekstra M., Hay A., Pelletier D. - A Manufactured Solution for a Two-Dimensional Steady Wall-Bounded Incompressible Turbulent Flow - International Journal CFD, Vol. 21, No 3-4; March-May 2007, pp. 175-188.

[6] Rumsey C.L., Thomas J.L. - Application of FUN3D and CFL3D to the Third Workshop on CFD Uncertainty Analysis - 3rd Workshop on CFD Uncertainty Analysis - Instituto Superior Técnico, Lisbon, October 2008.

[7] Eça L., Hoekstra M., Hay A., Pelletier D. - On the Construction of Manufactured Solutions for One and Two-Equation Eddy-Viscosity Models -International Journal of Numerical Methods in Fluids, Wiley, Vol. 54, 2007, pp. 119-154.

[8] Menter, F., Esch, T. - Elements of Industrial Heat Transfer Predictions- 16th Brasilian Congress of Mechanical Engineering, November 2001.

3:40-4:00, Verification of computational constitutive models using the method of manufactured solutions, *Krishna Kamojjala*, Rebecca M. Brannon (University of Utah)

Verification and validation of solid mechanics codes with complicated numerical constitutive models is crucial to establish confidence in the appropriateness of the governing equations and the accuracy of their solution. Verification is evidence that the computational model solves the governing equations correctly, whereas validation is evidence that the equations themselves are realistic [1]. Recognizing that verification must precede validation, two large-deformation verification problems are constructed based on the method of manufactured solutions (MMS) [2]. In the MMS, the computational model is verified by running the simulation with an external body force that has been analytically determined to achieve a pre-determined material motion. The error in the simulation is quantified by the error between the predicted material motion and the exact pre-determined motion. Even though the MMS can be applied to any arbitrary constitutive model to test accuracy and robustness, it has been relatively rare in the solid mechanics community. To date, MMS has been limited to simple constitutive models because of the mathematical complexity involved in deriving the analytical body force. To alleviate this problem, a series of increasingly complicated verification problems is presented that can be applied to any arbitrary constitutive model provided that the response of the model to standard loading (such as simple shear, uniaxial strain, etc.) is known. The first problem involves traction-free boundary conditions with all points in the domain subjected to simple shear with superimposed rotation. The other problem is similar except that the shared deformation is uniaxial strain, and there is traction on the boundary. These problems not only confirm basis and frame indifference, but also verify the implementation of traction boundary conditions in the computational model, which is quite complicated in particle and Eulerian methods. Convergence properties are assessed as a function of deformation intensity.

References

[1] L. E. Schwer, et al., Guide for Verification and Validation in Computational Solid Mechanics, ASME V&V, (2006).

[2] P. Knupp and K. Salari, Verification of Computer Codes in Computational Science and Engineering, Chapman and Hall/CRC, (2003).

Tuesday, 18 October 2011

8:30-9:20, Keynote, What makes a computational simulation good? or bad?, *William J. Rider* (Sandia National Laboratories-Albuquerque)

Each passing year computational simulation plays a ever greater role in science and engineering. Increasingly, research and high consequence decision-making relies upon computed results. Why should someone believe the results? What distinguishes a good calculation from a bad calculation? For example, if a calculation is part of a publication in an esteemed journal, is it good? Some journals have moved in the direction of instituting policies to enforce quality computational simulation. Increasingly this question is being addressed in a systematic manner by well-funded research such as the DOEs ASC program or nuclear energy research. This umbrella of activities is known a verification, validation and uncertainty quantification (VVUQ), and software quality assurance (SQA). We will explore the universe of computational quality and the means to providing defensible bounds on the credibility of simulated results. In the end, these efforts seek to provide a firmer foundation for simulation to play its advertised role in the scientific-engineering enterprise.

There is a maxim in computational science exists stating that "everyone believes the experiment, but the experimenter and no one believes the calculation, except the one who did it." A more optimistic expression of the state of affairs comes from Yuan T. Lee, Nobel Laureate in Chemistry, "Because of recent improvements in the accuracy of theoretical predictions based on large scale *ab initio* quantum mechanical calculations, meaningful comparisons between theoretical and experimental findings have become possible." Finally, Bertrand Russell adds to our closing stream of consciousness, "Although this may seem a paradox, all exact science is dominated by the idea of approximation." Just how approximate is still a question that must be answered in more quantified fashion

9:35-9:55, Automated solution verification using the wavelet adaptive multiresolution representation, *Zachary Zikoski*, Samuel Paolucci, and Joseph M. Powers (University of Notre Dame)

Solution verification is necessary to demonstrate a particular numerical result reflects, to a desired accuracy, the underlying physical model. This is often accomplished through *a posteriori* error estimation through application of extrapolation or grid convergence studies, as examples.

As an alternative, the Wavelet Adaptive Multiresolution Representation (WAMR) provides a robust method for generating verified numerical simulations on a spatially adaptive grid. A wavelet transform used in the WAMR method yields a direct measure of local error at each collocation point in an adaptive grid. By thresholding on the wavelet amplitudes, the WAMR algorithm automatically constructs sparse grids which represent a solution to within a prescribed error tolerance. Subsequently, appropriate grid resolution is maintained based on the demands of the evolving solution, while also supplying substantial reductions in computational time and effort.

9:55-10:15, Verification and validation at the micro- and nanoscale, Harvey Zambrano, *A. T. Conlisk* (The Ohio State University)

For the purposes of this paper we use the AIAA guide definition of Verification as "the process of determining that a model implementation accurately represents the developers conceptual description of the model and the solution to the model." In the simplest interpretation verification means that the given equations have been numerically solved correctly. Verification procedures are unchanged when continuum calculations are performed at the micro and nanoscale. Validation is the term given to the process of determining whether the the simulation accurately represents the physical problem of interest. Validation answers the question: Is the computational model an accurate physical representation of the actual real-world problem? Most often validation is performed by comparing with experimental data. However experiments that yield velocity and other profiles are extremely difficult at the microscale and virtually impossible at nanoscale. This paper discusses the use of dimensional analysis to validate nanoscale computations using microscale experiments for liquid flows of an electrolyte mixture. In addition, the system response quantities (SRQ) appropriate to nanofluidics are also discussed [1]. The use of an alternative plausible model to validate electroosmotic flow in nanochannels is also described.

Reference

[1] Oberkampf, W. L. and Roy, C. J., *Verification and Validation in Scientific Computing*, Cambridge University Press, Cambridge, UK, 2010.

10:15-10:35, Classification of ignition regimes in thermally stratified n-heptane-air mixtures using computational singular perturbation, Saurabh Gupta, *Hong G. Im* (University of Michigan), Mauro Valorani (University of Rome)

The computational singular perturbation (CSP) technique is applied as an automated diagnostic tool to classify ignition regimes encountered in thermally stratified n-heptane air mixtures, at pressure conditions relevant to homogeneous charge compression ignition (HCCI) combustion. Homogeneous, one- and two-dimensional high-fidelity simulations are conducted for n-heptane-air system, and the simulation data are analyzed by CSP to identify the physical characteristics of the auto-ignition event. The present study builds on our earlier work on the hydrogen-air system by considering more complex and realistic fuel chemistry. The CSP analysis applied to a complex n-heptane combustion system allows an automated identification of rate-limiting transport and chemical modes in the overall combustion behavior such as auto-ignition and combustion duration. The automated detection capability serves as a useful tool in verification and validation in the development of improved reaction mechanisms, such as those applicable to a wider range of operating conditions and different fuel blends, by isolating the essential subprocesses and assessing their impact on the key observables under consideration (e.g. ignition delay, pressure rise).

In the present study, the CSP analysis is systematically applied to detailed simulation data for homogeneous, one- and two-dimensional systems. For homogeneous systems, fundamental understanding is obtained on the characteristics and roles of various reactive modes during the two-stage ignition process for the n-heptane system. Subsequently, one- and two-dimensional simulations are investigated in order to investigate the role of mixing and transport in the auto-ignition of stratified mixtures. In particular, the important index for transport, defined as the sum of the absolute values of the importance indices of diffusion and convection of temperature to the slow dynamics of temperature, is used as a criterion to identify different ignition regimes. The systematic study showcases the potential benefit of the CSP analysis in the development and validation towards reliable predictive simulation of mixed-mode combustion encountered in modern internal combustion engines.

10:35-10:55, V&V for turbulent mixing and combustion, *James Glimm* (State University of New York at Stony Brook)

Practical simulations for turbulent mixing and combustion are generally limited to large eddy simulations (LES), with some but not all of the active turbulent length scales resolved. We present a novel notion of convergence, based on a stochastic interpretation of the simulation, to bin nearby points into a statistical ensemble. The ensemble is indexed by its space time localization, and thus defines a space time dependent probability, with space time resolution somewhat coarser than the original, but with an explicit representation of the statistical fluctuations that are an important aspect of turbulence. The simulation is thus interpreted as a probability distribution function (PDF), not a point valued solution, also called a Young measure. Convergence of the Young measure to a Young measure (PDF) limit is assessed by standard norms on probability measures, such as the L_1 norm on the associated probability distribution function (the indefinite integral of the PDF). The advantage of this point of view is that the fluctuations of the solution are captured, and that nonlinear functions of the solution, such as reactive chemistry source terms, converge through weak limits. As a further consequence, subgrid scale (SGS) models for chemistry are not needed if the chemical length scales are resolved. LES models for the turbulent SGS terms are still needed. Since models are the weakest link in most V&V studies, and since the turbulence models are better understood than those for processes built on top of turbulence, this point of view has the potential to benefit V&V studies for turbulent mixing and combustion. This point of view has been subject to verification and validation studies. These studies are ongoing and not complete. Their current status will be reviewed. Mathematical theorems to support this methodology will also be presented.

1:00-1:50, Keynote, Laminar-to-turbulent stability and transition, *Helen Reed* (Texas A&M University)

Laminar-to-turbulent transition location can be a significant source of uncertainty in the accurate prediction of aerodynamic forces (lift and drag) and heating requirements in applications ranging from high-altitude long-endurance unmanned aerial vehicles, to energy-efficient transports and hypersonic reentry systems. For example, in high-speed flows, transition causes heat transfer to rise by a factor of about five.

Transition is highly initial- and operating-condition dependent, and the availability of careful, archival experiments is the main validation issue. Following AIAA Transition Study Group guidelines (Reshotko, Saric), it is critical for an experimentalist to fully document the flowfield as a companion data set to transition measurements. This includes physical properties, background-disturbance details, initial amplitudes, and spatial variations. It is also good practice, whether one is involved in the experiments or in computations and regardless of the objectives of the study, to try to show that the linear problem is correct. That is, if one can show the comparison with linear theory for the particular flowfield, then the basic state is probably as thought.

Because of the extreme sensitivity of the stability and transition process to initial and operating conditions, advances have particularly come from those groups working hand-in-hand performing complementary computations and experiments on the same geometries. Not only are experiments important to validate computations, but also vice versa. For high-speed, flight-Reynolds-number, and complex-geometry flows, this kind of collaboration becomes even more critical, as detailed measurements are often more difficult and costly so that computations can guide the experiments as to what effects are important and what needs to be measured.

The community has demonstrated that if the environment and operating conditions can be modeled and input correctly, computations agree quantitatively with the experiments. A review of recent results, lessons learned, and future challenges for 3-D boundary layers, high-speed flows, and receptivity problems is presented.

2:05-2:25, Predicting and correcting for grid-induced errors in steady and time-accurate CFD solutions, *Tom I-P. Shih* (Purdue University)

For realistic engineering problems, the number of grid points or cells that can be used is restricted by either the available computer resource or a need to have a practical turnaround time in generating a solution. In addition, it is generally not feasible to do a grid-independent study so that there could be errors from poor quality cells and from inadequate spatial and/or temporal resolution. This talk describes a method based on the discrete-error-transport equation (DETE) to estimate grid-induced errors in CFD solution. The usefulness of DETE is demonstrated by applying it to three PDEs with known exact solutions: the linear advection equation, the linear wave equation, and the inviscid Burger equation with a discontinuity. This is followed by a discussion on methods for modelling the residual in the DETE. These methods include those that are based on a single grid and those that involve generating CFD solutions on two or more successively refined grids. The usefulness of these models are evaluated by applying them to estimate grid-induced errors in CFD solutions of the following problems: steady flow past a circular cylinder, steady transonic flow about an airfoil, unsteady flow of a translating vortex, and vortex shedding behind a circular cylinder.

2:25-2:45, New technical requirements for software tools in computational solid mechanics, *Barna Szabó* (Engineering Software Research and Development)

The importance of achieving substantial improvements in the reliability of predictions based on numerical simulation is now generally recognized. It is also recognized that such improvements are possible only through systematic application of the principles and procedures of verification and validation. This imposes certain technical requirements on software tools used in numerical simulation. Two key requirements are stated and methods for meeting those requirements will be described with reference to applications in structural and mechanical engineering practice.

The first technical requirement is related to verification: Determine the approximate value of a set of system response quantities $\Phi_i(u_{FE})(i = 1, 2, ..., n)$ and show that

$$|\Phi_i(u_{EX}) - \Phi_i(u_{FE})| \leq \tau_i |\Phi_i(u_{EX})|$$

where u_{EX} (resp. u_{FE}) is the exact (resp. approximate) solution, τ_i are prescribed error tolerances. In other words, it is necessary to estimate the relative errors $\tau_i^{(R)}$ and show that $\tau_i^{(R)}$ satisfy $\tau_i^{(R)} \leq \tau_i$.

The second technical requirement is related to the process of conceptualization, the end product of which is a mathematical model: Show that the system response quantities $\Phi_i(u_{EX})$ are not significantly affected by any of the restrictive assumptions incorporated in the mathematical model conceived to represent the physical reality being modeled.

The first requirement can be met through extrapolation from finite element solutions corresponding to a hierarchic sequence of finite element spaces, the second requirement can be met through access to a hierarchic sequence of mathematical models.

The role of the stated technical requirements in the formulation of phenomenological models for prediction of the probability of fatigue failure of mechanical and structural components subjected to cyclic loading will be outlined.

2:45-3:05, Framework for residual-based error estimation in computational fluid dynamics, *Christopher J. Roy* (Virginia Tech)

In computational mechanics, the discretization error is often the largest and most difficult numerical approximation error to estimate. While the finite element community has a rich history in residual-based error estimation, these techniques are not easily extended to other discretization schemes. This talk will present a new framework for developing residual-based error estimation methods for finite difference and finite volume schemes, the two approaches most commonly used for computational fluid dynamics. This framework is based on the Generalized Truncation Error Expression which relates the discrete equations to the governing partial differential or integral equations in a very general manner. The residual-based error estimation methods to be discussed include error transport equations, defect correction, and adjoint methods, all three of which can be developed in either continuous or discrete form. Residual-based methods offer an alternative to methods such as Richardson extrapolation where solutions on two (or even three) systematically-refined grids are used to produce the discretization error estimate. For complex 3D applications, this refinement is usually limited to a factor of two in each coordinate direction, thus resulting in an order of magnitude increase in computing effort for each subsequent level of refinement. Residual-based methods produce error estimates by solving an additional problem on the same grid; furthermore, they have the potential to produce more reliable error estimates since they use additional information about the problem being solved (as compared to Richardson extrapolation which simply post-processes the solutions). Approaches for assessing the reliability of these error estimators will also be discussed.

3:20-3:40, Avoiding operator splitting of stiff source terms: a verification via two-fluid magnetohydrodynamics and a validation via astrophysical turbulence, *Dinshaw Balsara* (University of Notre Dame)

Several problems in fluid and magneto-fluid flow require the treatment of stiff source terms in addition to the base level flow solver. Since the base level flow solver, as well as the stiff source solution, represent algorithms that are difficult to implement, the usual simplification is to resort to operator splitting. As a result, the typical situation in this field consists of developing a very sophisticated flow solver while ignoring the source terms, obtaining the most detailed ODE solver for stiff source terms that one can obtain and then patching the two together. In this talk we examine the consequences of that approach. For a two-fluid MHD problem involving stiff source terms, we show that (in certain situations) the equations have an exact analytical solution in one-dimension and then we try and verify whether the operator splitting approach succeeds or fails. We find that it fails miserably in the strong coupling limit. This is a serious deficiency.

We then present ADER-WENO schemes as an alternative. Such schemes take a space-time approach to solving the PDE. As a result, they naturally couple the hyperbolic terms to the stiff source terms without resort to operator splitting. We then verify that the newly-designed schemes perform significantly better than their operator split cousins. The great utility of avoiding operator splitting wherever possible is, therefore, established. Consequently, we also demonstrate the value of analytical solutions in the verification process.

We then focus on astrophysical turbulence as a system where the simulations can be validated. A puzzling aspect of observing astrophysical turbulence in molecular clouds stems from the fact that the neutrals have larger line widths than the ions for certain isophotologues. We confirm this result using simulations.

3:40-4:00, Multiscale modeling of particulate composited with co-designed experiments using micro-computer tomography, *Karel Matous (University of Notre Dame)*

Wednesday 19 October 2011 *8:30-9:20, Keynote, V&V in image-based cardiovascular fluid dynamics: from mathematical models to patients,* Charles A. Taylor *(HeartFlow, Inc.; Stanford University)*

Heart disease is the number one killer worldwide. Each year in the U.S. more than 6 million patients go to the Emergency room and there are 9 million physicians office visits for patients with symptoms of heart disease. Restrictions in the coronary arteries resulting from atherosclerosis are the principal cause of heart disease. The severity of these restrictions and their effect on blood flow to the heart are difficult to measure, yet this information is critical for treating patients. Currently, only invasive diagnostic cardiac catheterization can provide critical flow information through coronary arteries, but this procedure is expensive and poses risk to the patient. A recent breakthrough in imaging technologies with CT scanners and image-based cardiovascular flow modeling software is enabling an inexpensive and potentially much safer diagnostic tool to emerge.

I will describe technology to analyze a patient's coronary CT scan images and, using high performance computing and computational fluid dynamics, to solve for coronary blood flow and pressure. This technology has been verified with comparison to analytical solutions including Womersleys solution for fully-developed pulsatile flow in elastic vessels. In addition, I will describe the validation of this technology for modeling pulsatile blood flow in physical models. Finally, I will present initial clinical data in 103 patients that has demonstrated significant improvements in diagnostic accuracy as compared to other noninvasive technologies. This latter clinical study involved comparison between CFD solutions and direct measurements of intra-arterial pressure during diagnostic cardiac catheterization.

9:35-9:55, An overview of inverse material identification within the frameworks of deterministic and stochastic parameter estimation, Miguel A. Aguiló*, Laura Swiler, and Angel Urbina (Sandia National Laboratories–Albuquerque)*

This work investigates the problem of stochastic parameter estimation in the context of a particular problem: determining the elastic properties for a beam given an observed displacement field. The approaches fall in two main classes: Bayesian calibration and Maximum a posteriori estimation (MAP). For the Bayesian calibration, we used Monte Carlo Markov Chain methods to calculate the posterior parameter estimates to calculate the posterior parameter estimates. We investigate several formulations for the likelihood function: standard likelihood function, a likelihood function that incorporates the error in the constitutive equation (ECE), and a likelihood function that incorporates the modified error in constitutive equation (MECE). Results for this case study show that computational savings are possible with the ECE and MECE likelihood functions. The other stochastic method we investigate is the MAP method. In the MAP approach, we do not generate a full posterior distribution via sampling, but we determine the mode or most likely value of the posterior parameter distribution using deterministic optimization methods. Results will be show for the standard, ECE, and MECE likelihoods functions.

9:55-10:15, Comparison of a pragmatic and versatile "real space" model validation framework against several other validation frameworks, Vincente Romero *(Sandia National Laboratories-Albuquerque)*

This presentation will outline a practical and versatile Real Space approach to model validation ([1] [4]) and then compare it against other selected approaches such as the ASME V&V20 framework [5] and the Oberkampf & Roy framework [6]. The comparison will be in terms of the how the issues of model accuracy and adequacy are framed and assessed, including the versatility and workability (complexity and cost) of the UQ techniques used to handle various sources of random and systematic uncertainties (correlated and uncorrelated, interval and probabilistic) in the experiments and models/simulations.

The Real-Space approach does not employ "Transform Space" discrepancy measures and acceptance criteria to assess model accuracy and adequacy. A large variety of mathematical transforms such as the subtraction transform in [5] and the area validation metric in [6] can be used to characterize discrepancy between experiment and simulation results. The transform measures in the literature can be relatively sophisticated and involved, with varying transparency and interpretability of the physical and decision-making significance of the numerical values yielded by the discrepancy measures. The transforms can also put constraints on what forms and types of uncertainty can be addressed. Furthermore, workable criteria to assess adequacy of model/experiment agreement in terms of transform measures are still elusive, whereas a simple criterion can be applied in Real Space that assesses the relative risk and adequacy of a model.

The Real-Space validation methodology reflects a pragmatism and versatility evolved from working a broad variety of industrial-scale problems involving complex physics and constitutive models, steady-state and time-varying nonlinear behavior and boundary conditions, and various categories of uncertainty in experiments and models in the areas of heat transfer, structural mechanics, irradiated electronics, and combustion in fluids and solids.

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10:15-10:35, From validation set points to a continuum domain of validation, Patrick J. Roache *(Consultant)*

It has been argued [H. Mair], and is a justifiable position, that "Validation" only at discrete experimental set points is nearly useless for practical applications, and that a model should not be declared "Validated" unless the set-point Validation results have been extended to some useful continuum Domain of Validation. The several recent V&V Guides [AIAA, V&V10, V&V20] all are limited to set-point Validation, deferring the necessary interpolation (or extrapolation or curve fitting) to analysts with expertise in the various application areas. However, there are features that are applicable generally. Oberkampf and Roy have presented a model validation framework that includes interpolation for model form uncertainty. They also consider procedures necessary for inclusion of interval-valued uncertainties. These procedures are rather complex, computationally expensive, and difficult to interpret; unfortunately, these may be necessary if significant interval uncertainties cannot be avoided.

The present work considers extension to a continuum Domain of Validation within the model Validation framework of V&V20. The ASME Committee V&V20 intends to publish a supplement that will include such an extension. The present paper is somewhat a work-in-progress, although some of these results have already been published (not to be understood as approved or authorized by the V&V20 Committee nor ASME). Essential elements are: model quality vs. validation quality; what quantities are to be interpolated; comparison of terms "Total Validation Uncertainty" vs. "model form uncertainty;" combination of aleatory and epistemic uncertainties; and reporting uncertainties for new simulations. Additionally, some consideration is given to the following issues: realism of interval-valued probabilities obtained from datasets or elicitation of expert opinion; Bayesian "beliefs;" and a suggested modification of the V&V20 Total Validation Uncertainty formulation to make the treatment of numerical uncertainty more easily justifiable and conservative for high-consequence applications

10:35-10:55, Development of a standard for verification and validation of software used to calculate nuclear system thermal fluids behavior, Richard Schultz, *Edwin Harvego (Idaho National Laboratory), Ryan Crane (ASME)*

To address the need for internationally recognized standards for verification and validation (V&V) of software used in the thermal-hydraulic analyses of advanced nuclear power plants, the V&V30 Committee was established to develop an ASME standard for verification and validation of computational fluid dynamics and system analysis software to be used in the design and analysis of advanced nuclear reactor systems, with an initial focus on High-Temperature Gas-Cooled Reactors. The title of the committee is "Verification and Validation in Computational Nuclear System Thermal Fluids Behavior." As defined in its charter, the committee "Provides the practices and procedures for verification and validation of software used to calculate nuclear system thermal fluids behavior. The software includes system analysis and computational fluid dynamics, including the coupling of this software."

The processes and procedures that will be addressed in the new standard will be used in the design and analysis of advanced reactor systems to be licensed in the U.S. As such, the standard should conform to Nuclear Regulatory Commission (NRC) practices, procedures and methods for the licensing of nuclear power plants as embodied in the Code of Federal Regulations and other pertinent documents including regulatory guidelines. In addition, the standard should be consistent with applicable sections of ASME Standard NQA-1 ("Quality Assurance Requirements for Nuclear Facility Applications (QA)").

Recently the V&V20 standard was released: Standard for Verification and Validation (V&V) in Computational Fluid Dynamics and Heat Transfer. As noted in the V&V20 Standard: "The scope of this Standard is the quantification of the degree of accuracy of simulation of specified validation variables at a specified validation point for cases in which the conditions of the actual experiment are simulated." In support of the V&V20 scope, the aim of the V&V30 Standard is to expand the domain of validation to encompass points beyond the range defined by the V&V 20 Standard. In other words, the V&V30 standard, to be defined by the committee, will complement the V&V20 Standard by defining a methodology for experimental validation of an expanded calculation envelope that encompasses the operational and accident domain of the nuclear system. Therefore V&V30 is expected to address: (a) applicable NRC requirements for defining the operational and accident domain of a nuclear system that must be considered if the system is to be licensed, (b) the corresponding calculation domain of the software that should encompass the nuclear operational and accident domain to be used to study the system behavior for licensing purposes, (c) the definition of the scaled experimental data set required to provide the basis for validating the software, (d) the ensemble of experimental data sets required to populate the validation matrix for the software in question, and (e) the practices and procedures to be used when applying a validation standard, such as the V&V20 Standard, to demonstrate that the validated software is capable of performing the needed licensing calculations. The presentation discusses the above topics together with the need for the V&V30 standard. Finally, a summary of possible approaches that may be taken to achieve the committee objectives will be summarized.