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University of Utah ASC Site Review, August 24-25, 2006

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Abstract

This report is a review of progress made by the Center for the Simulation of Accidental Fires and Explosions (C-SAFE) at the University of Utah, during the ninth year (Fiscal 2006) of its existence as an activity funded by the Department of Energy's Advanced Simulation and Computing Program (ASC).

The ten-member Review Team composed of the TST and AST spent two days (August 24-25, 2006) at the University, reviewing formal presentations and demonstrations by the C-SAFE researchers and conferring privately. The Review Team found that the C-SAFE project administrators and staff had prepared well for the review. C-SAFE management and staff openly shared extensive answers to unexpected questions and the advance materials were well prepared and very informative. We believe that the time devoted to the review was used effectively and hope that the recommendations included in this 2006 report will provide helpful guidance to C-SAFE personnel and ASC managers. The review team consisted of Dick Watson (LLNL), Tony Chen (SNL), Nels Hoffman (LANL), Bob Voigt (NNSA HQ), Thuc Hoang (NNSA HQ), Rod Schmidt (SNL), Tommy Sewell (LANL), Laura Monroe (LANL), Charlie Westbrook (LLNL), and Gene Hertel (SNL-TST Lead).

ACKNOWLEDGMENTS

This report was written by a dedicated group of DOE lab staff. The Tri-lab Support Team (TST) was responsible for the Year-9 Site Review in contract to the independent site review teams that have been a part of the ASC University Alliance Program for the previous 8 years. The current TST team members include Charlie Westbrook and John Gyllenhall of LLNL, Tommy Sewell and Laura Monroe of LANL, and Gene Hertel and Rod Schmidt of SNL. Charlie, Tommy, Laura, Rod, and myself contributed directly to this report. The authors would also like to thank the long-term contributions of Bob Voigt and Tina Macaluso who have supported the alliance program since its inception. Finally, the TST would like to acknowledge both the hospitality and technical exchanges with the University of Utah faculty, staff, students, and administration. Without their contributions, the program would have been an empty shell.

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NOMENCLATURE

1. EXECUTIVE SUMMARY

The 2006 Review Team commends the C-SAFE team for their first end-to-end full system simulation, which coupled three separate phases of the computation, fire dynamics, container heat-up, and violent reactions. The incorporation of the disparate time scales in a single executable was accomplished in a straightforward but effective manner.

The review team was impressed with the effectiveness of the Uintah Computational Framework (UCF) that enabled the blending of the three phases of the computation. In particular, the transition between MPM and ICE and the ease at which the radiation model was incorporated is an indication of the success of UCF. It was noted that the UCF has also been successful in attracting external funding to the program.

The review team was impressed with the extent to which the teams representing the different disciplines were integrated in the effort to produce the end-to-end simulation.

The external impacts of the C-SAFE project include an increased number of spin-offs this year. The review team suggests that the broader computational science community be targeted for additional spin-offs

The review team recommends that the Center should use the simulation pipeline and identify an end-goal problem that includes as much physics as possible and complete the simulation with sufficient time left in the project to evaluate the simulation and publish the results.

The review team also acknowledges that Utah has been very proactive in integrating Verification and Validation concepts into their program. They have been active in external workshops discussing these concepts, in particular, the Utah-Sandia Workshop on Fire Models and Validation.

2. ACCOMPLISHMENTS

Several noteworthy accomplishments can be attributed to the University of Utah's effort under ASC. The C-SAFE fire model is currently one of the two high fidelity fire models in the world for the simulation of large hydrocarbon fuel fires primarily due to the following features; the model:

- Is LES-based;
- contains detailed soot sub models;
- uses parameterization as the methodology for including first principle chemistry in the simulation;
- employs a surrogate fuel formulation developed by C-SAFE to accurately represent the chemical and physical characteristics of complex jet-fuel;
- calculates radiation using a discrete ordinates method so the directional-dependence of radiation can be included;
- utilizes robust nonlinear and linear solvers for large-scale, nonlinear sets of PDEs;
- has been rigorously verified and validated against extensive experimental measurements, and
- captures a wide range of length and time scales in the flow. The code is structured and highly parallelized, the algorithm includes an implicit pressure projection step, and the simulations can be run on terascale computing facilities.

C-SAFE large-scale simulations run on the ASC computers have created new requirements for visualizing large, time-varying data sets. Working in collaboration with the SCI Institute, C-SAFE scientists have produced major, new visualization techniques, including:

- new, high-speed, real-time ray tracing,
- new volume rendering algorithms,
- new AMR visualization techniques, and
- new methods for realistic rendering of luminous flames.

The resulting three-dimensional volume-rendered images of fires and of explosives have enhanced our understanding of the structure and physics in these systems where experimental data are difficult to obtain.

C-SAFE developed an advanced, Computational Framework (Uintah) that has allowed engineers to transform existing serial codes into high-speed parallel codes without being bogged down by parallel programming details, in particular, this fact can lead to a substantial reduction in the cost to develop new analysis codes. Uintah can balance computational loads across thousands of processors and

provide high-speed graphics interfaces. The university has developed techniques that allow integration of components developed by third parties including non-linear and linear solvers designed for solving complex-flow problems (PETSc and Hypre).

C-SAFE developed a true multi-material structures code (based on the material point method) that is capable of simulating complex, irregular geometries undergoing extremely large deformations (e.g. a truck of HMX exploding).

The molecular fundamentals effort at C-SAFE has resulted in a methodology that enables prediction of continuum-scale constitutive descriptions of polymer composites based on direct incorporation of molecular dynamics simulation results within a hierarchical homogenization scheme.

C-SAFE experiments have demonstrated that the most dangerous location for high-energy explosives in an accidental fire is adjacent to the fire (*not* in the middle of the fire). This was subsequently confirmed by computer simulation.

Utah has received a grant from NSF for multi-materials interaction dynamics that would not have happened without C-SAFE. Also an NIH grant on Angiogenesis and the extra cellular matrix were received that build on C-SAFE advancements. Other proposals have been submitted that are heavily leveraged with Uintah and other C-SAFE advancements. Integrated simulations using the C-SAFE code have moved simulation science from a dream to reality by helping real people solve real problems in terms of the following externally funded projects currently underway at Utah:

- rapid analysis of terrorism threats,
- design of large scale fire experiments,
- developing protocols for transportation classification of hazardous materials,
- protection of the environment through proper flare design, and
- investigation of an extremely violent transportation accident.

3. RESEARCH

Fire Science

Fire science involves a host of complex coupled non-linear phenomena occurring over a wide range of length and time scales, and involves seeking an understanding of many fundamental physical mechanisms as well as developing the ability to accurately simulate the overall process. From material presented to the reviewers it is clear that in the area of large pool fires, the ASC funded Utah C-SAFE work has made, and continues to make, major contributions.

An important strength of the C-SAFE work has been to fully recognize and actively embrace the need for a comprehensive verification and validation strategy. For JP-8 fire simulations they have developed a well thought-out verification and validation hierarchy that identifies specific cases, problems, and processes at different levels, and which has defined and organized their research and development efforts. As an example of work completed this year, results from a rigorous plume validation study (based on recent large-scale Helium plume data obtained from Sandia) were highlighted and a summary was presented of activities and results discussed at the Utah-Sandia Workshop on Fire Models and Validation (held July 2006). An important finding of this latest workshop was the importance of sufficient mesh resolution, a result that highlights the importance of their effort to fully implement AMR into the large-scale code. In short, the V&V effort is clearly first-rate, is a model for others to follow, and the review team commends the C-SAFE team for this aspect of their work.

A major contributor to high fidelity fire simulation is the radiation heat transfer model, and a key component of this is the ability to accurately model the formation, evolution, and transport of soot. Excellent progress has clearly been made in developing and demonstrating a scalable algorithm for the discrete ordinance radiation model that is independent of medium properties, and in performing the required V&V. Progress was also noted in migrating the radiation model that is currently in ARCHES into the ICE code that is used in the end-to-end simulations. Addressing the minor issues that remain in ICE concerning how radiation is absorbed by solid (particle-based) objects and the overall strategy for a correct thermodynamic treatment of energy should clearly be a priority. Another important question highlighted in this years review is how soot breaks through from the fuel side to the air side. Fundamental DNS simulations and the application of novel new models (e.g. One Dimensional Turbulence, ODT) are being pursued in an effort to understand and model this process - both activities which are supported by the review team. As will be discussed later, C-SAFE staff continue to be national leaders in the fundamental modeling of soot chemistry, formation, and evolution. However, it was noted in the review that the soot models used in the end-to-end simulation have not yet effectively incorporated results obtained from fundamental MD simulations, apparently due in part to the departure of two key personnel from C-SAFE (Violi and Voth). While lauding the fine progress in the fundamental science, the review team would encourage continued efforts to embed the results of this more fundamental work into the models used in the large-scale fire simulations.

In the experimental arena, plans were described to develop and apply a new tomographic spectroscopy-based flame diagnostic system to obtain high resolution flame data. This work is to be done in collaboration with Prof. Axel Schonbacher of the Univ. of Duisberg-Essen. This appears to compliment recent work performed at Sandia. The review team hopes that the results can be obtained in time to impact the model and code development effort.

The full potential of “simulation science,” as applied to fire science or any other area, can only be achieved when each of the contributing physical processes are brought together in a validated, robust, and sufficiently accurate overall model (or code) that enables one to reliably perform desired simulations in a reasonable amount of time and whose results can be meaningfully interrogated. Results presented in this years review suggest that this objective is in fact becoming a reality in the Utah C-SAFE effort. The dynamic visualization of results for a ~20 m diameter pool fire in a cross wind showing the two large counter-rotating columnar vortexes that formed behind a large cylindrical object in the fire is very impressive. Likewise the visualization of results illustrating the team’s progress on performing a full-physics end-to-end simulation coupling all of the different aspects of the problem (including fire) at high resolution was remarkable. To accurately perform the desired high fidelity end-to-end simulations, all key aspects of the ARCHES fire model are being migrated into the ICE code. Finishing all remaining aspects of this work in time to perform the desired high-fidelity end-to-end simulations should be an important goal of this final year.

Heat-up

Cookoff of energetic materials, including high explosives, solid rocket propellants, and gun propellants is an important problem. Cookoff concerns affect operations and handling of munitions and can have a major impact on life cycle costs. Although there are some qualitative differences between “fast” and “slow” cookoff, and separate qualification tests are typically prescribed, fundamentally the same types of physical processes occur in both types. During an accident event, energy transfer occurs between a source (typically a fire) and a target system (munition, rocket, or other device containing propellant and/or high explosive). That energy transfer manifests itself in a rise of temperature in the target through thermal conduction, convection, and radiation. The organic materials that make up the energetic materials chemically decompose, generating heat and gas (decomposition products) while undergoing a thermo-mechanical process that can give rise to internal damage. A major difference between fast and slow cookoff is the level of thermal penetration that occurs in the energetic material. In a slow cookoff event, most of the energetic material is affected by the temperature rise and can undergo a damage process. The result of the damage is an increase in internal porosity (surface area). In a fast cookoff event, the thermal penetration and damage is generally limited to a small fraction of the energetic material. As the heating continues, the exponential nature of temperature-dependent chemistry leads to a thermal runaway or ignition state.

Their approach has been to address different time scales by developing a bridge. They are conducting some basic verification of an explicit heat conduction code (a relatively new algorithm). Utah has been conducting numerical experiments of 1D transient heat conduction and doing comparisons with analytical solutions. They are looking at both single materials and composite materials. They compared these 1D heat conduction calculations with Finite Element calculations and found good agreement for arbitrary single material and composite material.

The Utah program is unique in that they are addressing all the key elements of energetic material cookoff in a fully coupled computational framework. Substantial work has been done over the last nine years on key aspects of this problem with much success.

Explosions

Our understanding of cook-off is as follows: an energy transfer occurs between a source (typically a fire) and the target material; that energy transfer manifests itself in a rise of temperature in the target through thermal conduction, convection, and radiation; the organic materials that make up energetics chemically decompose, generate heat and gas (decomposition products), and undergo thermo-mechanical processes that give rise to internal damage; the exponential nature of temperature-dependent chemistry leads to a thermal run-away; at this point the model system becomes a coupled race wherein chemical energy release competes with confinement (either inertial or from a container). Details of how a chemically reacting fluid interacts with the damaged energetic material dominate the final steps of a cook-off event; pressure enhanced combustion can lead to shock driven flows and possibly a detonation. The ultimate result of a cookoff insult (violence of reaction) is due to this competition between confinement dynamics and energy generation. Weak confinement typically results in little or no violence, due to early failure of the container. However, when the confinement is substantial, there can be adequate time for significant combustion acceleration and the system response can be a violent explosion or detonation. The dominant processes in cook-off lead to a natural division of the problem into two major, sequential temporal regimes: a long-heat up phase with a characteristic time of minutes or hours, and a much faster runaway phase (containment failure/explosion/detonation) that occurs on a time scale of microseconds.

The Utah program approaches the technical needs of cook-off by separating the mechanical response of the confinement from the boundary conditions applied to the container by the fire. The Material Point Method (MPM) was chosen for container dynamics for several reasons. Utah is viewed as a leader in MPM as a result of their work under C-SAFE. In addition to the container dynamics, models that represent the behavior of the metals and energetic materials are necessary. In general, Utah has chosen existing models to represent these phenomena. At this time, they have all the pieces necessary to address problems of interest to many government agencies.

Molecular Fundamentals

The C-SAFE project has made impressive advances using computational science to study pool fires and the soot that they produce. These are complex phenomena that involve detailed reactive chemical kinetics, radiation transport, 3D fluid mechanics, turbulent flow, and multiphase phenomena. The University of Utah group has used massively parallel computing techniques to revolutionize the ability to describe fires and soot production in their computer simulations, placing them in a leading position in this subfield of combustion.

The chemistry of pool fires of hydrocarbon and related fuels is intricately connected to the chemistry of soot formation, soot oxidation and radiation transport. The pool fire is an inherently non-premixed flame, depending on evaporation of a fuel of relatively low volatility, followed by mixing of the vaporized fuel with air and then combustion. The presence of significant pockets of very fuel-rich gases make it difficult to burn all of the fuel. The chemical products of incomplete fuel combustion are the building blocks for soot in the flame, and this soot then plays a key role in controlling the emission and transport of radiation through and out of the pool flame. The C-SAFE researchers have treated each of these big problems, first examining each application in great detail as an isolated problem, but also recognizing their strong interconnections that lead to significant non-linear couplings between them.

The C-SAFE researchers have established the current state-of-the-art in both pool fire simulations and soot production kinetics. Important features that can now be explained in basic terms, based on C-SAFE computational studies, include the variation in fire properties with changes in pool size, such as the “puffing” frequency between the large scale features. Other features that can now be accurately predicted include effects of fuel properties such as volatility and chemical composition. Detailed chemical kinetic reaction mechanisms used in these pool fire simulations included such fuels as n-heptane and a surrogate set of components designed to represent the jet fuel JP-8. The n-heptane is an acceptable surrogate fuel to describe combustion of diesel fuel, so these fuels are appropriate to simulate fuel fires resulting from transportation accidents involving either trucks or aircraft. The C-SAFE program has led the field of development of surrogate hydrocarbon fuels for practical transportation fuels, which have hundreds or often thousands of components and cannot be simulated by exhaustive submodels for every component. Instead, mixtures of a few specific major components are used with the expectation that they can, collectively, reproduce the behavior of the real practical fuel and still be modeled successfully. The work of the C-SAFE group to build a surrogate for JP-8 produced the first meaningful surrogate chemistry papers in this emerging field.

Since the accident scenarios of concern to the C-SAFE program include cases in which the pool fires burn in open-air environments, the influence of atmospheric phenomena, especially windy conditions, are of considerable importance. Their modeling capabilities include the inclusion of crosswinds in the vicinity of the pool fire.

In addition to being expected in real-life accident scenarios, crosswinds introduce an enormous level of computational complexity and greatly increase the cost of these computations. In both of these flames, the production of soot and the details of the transport of energy via radiation have a strong influence on the way each fire heats the metal container and the explosive fuel within the container.

The C-SAFE researchers have made outstanding contributions to each of these areas. These models can predict the mechanisms by which atmospheric conditions can alter the rate of heat release from the pool fire and variations in the amounts of soot produced from changes in wind conditions.

The only significant modeling task for flames and soot chemistry that remains is a careful, general treatment of radiation transport. Considerable progress has been made [see recommendations 6-8 in the Container Heat-Up section of Appendix 1]. Both spectral and gray approximations have been employed for the optical properties in the flames, and both show some promise, coupled with a discrete ordinates model for the radiation transport. While this is often a satisfactory level of detail for these flames, some more complex behaviors cannot be simulated, often in situations where soot formed in one region of the fire affects features of a different fire region. Currently, the approach is to use a combination of experimental and computational analyses to produce heat transfer data in tabular form that can be inserted into the combined fire/canister simulation, and the intent is to improve the pool fire simulation to enable them to compute the heat transfer information directly; the use of this type of intermediate treatment is highly appropriate, and the technical direction of the approach is good. The nature of the research seems appropriate and the pace of progress is good, but the radiation simulation is as complex or even more challenging than the basic fuel chemistry, and this is an especially difficult task. The final year of the C-SAFE project may provide a good, serviceable submodel for this final, challenging part of the pool fire/sooting/radiation transport/heat transport/canister heating problem.

The C-SAFE program has made particularly noteworthy technical contributions in the area of modeling of soot production in liquid fuel pool fires and other related combustion systems. Led by Professors Adel Sarofim and Phil Smith, this group has built on a program of many years duration, involving soot chemistry experts from all over the country, to study the inception and growth of soot particles. This conceptual description of soot production, formulated by the University of Utah group, is being used throughout the combustion community.

While dozens of groups around the world are working in the area of soot formation, the work at Utah is unique in its particularly strong emphasis on simulations, although there is also strong coupling to an experimental program with Professors Ron Pugmire and Eric Eddings. Overall, the large-scale emphasis on chemistry of pool fires, fuel surrogates and soot production at the University of Utah has led to major accomplishments that lead their respective disciplines and are important products of the C-SAFE efforts.

Reliable knowledge of the thermo-mechanical properties of the energetic composite, its final reaction products, and physico-chemical states in between is vital to obtaining a true predictive capability for cook-off scenarios. Among the properties of most interest are the composite thermal conductivity, specific heat, elastic mechanical properties, plastic yield surface, melt phase properties, and reaction products equation of state. Some of these are sensitive functions of temperature and pressure, though in many cases lack of data has led to the use in continuum models of constant values that are empirically adjusted to match experiment for some property (for example the shock hughoniot) that involves two or more of them. Such approaches/approximations do not lend themselves well to robust predictive capability.

The C-SAFE molecular fundamentals group has made considerable progress toward obtaining several of the important fundamental equilibrium properties mentioned above for HMX, binder materials, and material interfaces through the development and careful application of molecular simulation; this work is available in numerous publications, and represents the state-of-the-art for potential energy function development and practical molecular simulation of materials properties and behaviors.

The molecular fundamentals group has recently developed and implemented a hierarchical multiscale homogenization scheme that allows prediction of continuum constitutive response of model composites directly from a set of calculated (or measured) fundamental properties; a particularly relevant application was the development of an atomic-based ViscoSCRAM description, including temperature dependence, for a model plastic-bonded explosive. The temperature effect is expected to be of key importance due to the significant variation of polymer viscoelastic properties over comparatively modest intervals of temperature; similar comments apply to pressure dependencies, as evidenced by calculations shown by the molecular fundamentals group during the review.

Development of ViscoSCRAM descriptions based on atomic-scale information about composite constituent materials and interfacial properties should enable a “closing of the loop” in the C-SAFE project. Specifically, engineering-scale continuum simulations for (homogenized) composites can now be performed using constitutive descriptions that were parameterized using information initially calculated on the nanometer spatial scale using atomistic molecular dynamics. This is significant and, while the studies done to date correspond to highly idealized models of composites, it is incumbent upon the engineering coterie to begin to use these results in their own studies, including temperature and pressure dependencies where feasible, to strengthen the ties between these two communities.

Computer Science

Computer science is basic to any ASC Alliance project. The efforts of C-SAFE have been most notable in the area of their Uintah framework, which this year has supported a multi-scale end-to-end run, and also in their visualization.

They have developed the Uintah framework over the 8-year time span of the C-SAFE project. Uintah is based on a CCA component architecture, and provides domain decomposition, inter-processor communication, parallel I/O, load balancing and other features. In theory, using a component-based approach enables flexibility and easier integration of new parts, and in practice, C-SAFE has been able to achieve such integration, completing an end-to-end simulation this year of a steel container filled with an explosive and engulfed in fire.

A notable success is the fact that C-SAFE is running large-scale simulations, showing the applicability of a component-based architecture to large problems. This scalability is achieved while retaining the flexibility of a component-based system.

Work continues on the integration of AMR into Uintah. Load balancing is a traditional issue in implementations of AMR. This year, C-SAFE has implemented a space-filling curve algorithm into Uintah to assist in this. The mesh is refined, and a path (the space-filling curve) is generated passing through each cell of the new mesh. The processor partition is then defined following the path. Regridding is done using a version of the Berger-Rigoutsous algorithm. On Thunder, C-SAFE reports performance increases of 23% for Berger-Ritsoutsous over hierarchical regridding using the space-filling curve.

The end-to-end simulation comprised three phases: the fire simulation, the heat-up and the explosion. The ICE CFD algorithm was used to model the fire and the products of the explosion, and MPM was used to model the container and solid explosive. C-SAFE also used Uintah to model the Spanish Fork accident that occurred in 2005 in the Wasatch mountains, and discovered that explosives with hollow bores explode much more violently than do solid explosives. Plans this year for further integrated simulations include exploration of the effects of winds and geometry on the violence of the explosion. Also planned is further work on AMR, in particular, combining radiation with AMR, and fixing a memory leak that becomes troublesome only on larger problems.

C-SAFE has achieved a component-based system with no single performance bottleneck. Analysis of the system was done with the TAU performance system, and C-SAFE worked with the TAU researchers so that they could see the performance of the task graphs the framework is built upon using TAU.

Uintah runs on a variety of platforms. C-SAFE is working on a general release of the Uintah framework. Uintah is already available at LLNL. A users' version soon will be available on CD for Linux, and this release will also include the SCIRun Problem Solving Environment. A developers' release is planned for mid-2007. These releases are specifically intended as outreach to the labs, and indeed, C-SAFE reports lab interest in this product, as well as outside interest. We encourage C-SAFE to complete this release, as one of the legacies of this Center.

Visualization is one of the strengths of the C-SAFE project, and the project has made major contributions to the visualization of large data, working in tandem with the world-class SCI Institute. Many of the SCI researchers are also on the C-SAFE project, which adds to the quality of C-SAFE visualization. Their integration with the labs is good, with ongoing collaborations, interns placed, and two graduates hired at the labs.

This year, they have concentrated on ray-tracing, improved fire visualization and use of the Graphical Processing Unit (GPU) in visualization. They have achieved impressive results in all of these, in particular in the real-time visualization of C-SAFE datasets. This allows quick and interactive exploration of the large C-SAFE datasets.

Improved methods of visualizing particle datasets from MPM simulations were presented. They have developed new algorithms for ray-tracing, and have been able to visualize datasets as large as 2.8 million particles at 22 frames per second on a single high-end desktop. C-SAFE and SCI Institute are leaders in this technique and organized a symposium this year on real-time ray-tracing. Also presented were techniques for rendering flames with realism, and these were used to render a methane pool fire. Finally, the C-SAFE researchers have incorporated the GPU-based AMR volume visualization technique shown last year into their Uintah visualization tools.

C-SAFE researchers also have been exploring the power of programmable GPUs in visualizing different types of data. They have used the GPU to visualize MPM particle data and particle-based flows mapped onto a texture for a volumetric visualization, and have implemented the UFLIC algorithm (which is a line integral convolution algorithm for flows) on the GPU and applied it to the visualization of pool fires. This is a promising area for future work, in that the speed of GPUs is increasing so fast and their programmability allows for GPU integration of graphics algorithms.

Convincing visual motivation for the value of enhanced shading effects was presented, including side-by-side visualizations of particle-based MPM datasets, with and without shadowing and with and without global illumination. They also ran a user study, which showed that such advanced shading methods do indeed enhance perception and help performance in shape-matching.

Overall, the computer science at C-SAFE is one of their strengths, and the Uintah framework and the many visualization techniques they have developed is a major contribution to the C-SAFE legacy.

4. IMPACTS AND LEGACY

The C-SAFE program catalyzed the development of the Computational Engineering and Science graduate program, which includes both an MS degree and a Certificate. This led to a new PhD degree in Computing with tracks in Scientific Computing, Graphics and Visualization, and Robotics.

The ASC funding has caused a fundamental culture shift over the past decade at the university. At the beginning of this program essentially no faculty members in Engineering or Science were carrying out parallel computations; now everyone doing scientific computing at the University wants access to 1000 processors. This is particularly true with current NFS funded projects that build on the C-SAFE legacy.

ASC funding has spurred the development of simulation tools that are truly multiphysics and multiscale. Information from the molecular scale is transferred to the resolved scale through sub grid scale models, parameterization of molecular scale data, and by hierarchical homogenization of nano-scale MD simulation results to yield continuum scale composite constitutive response. This allows researchers to resolve length and time scales that were previously ignored, leading to more accurate, physically-based solutions of complex problems.

Based on the C-SAFE developed simulation infrastructure, the C-SAFE fire model is currently one of the two high fidelity fire models in the world for the simulation of large hydrocarbon fuel fires.

Collaborative relationships with scientists and engineers at the DP labs have more than quadrupled since the program began. This has stimulated joint proposal efforts, research collaborations, and ongoing workshops that are of mutual interest to the DP labs and to the C-SAFE program.

The C-SAFE program has already graduated 29 Ph.D. and 21 M.S. students trained in modern computational science techniques. In addition, another 34 graduate students and 22 research staff members currently supported under C-SAFE will ultimately push the total computationally trained graduate students and post docs to over 100.

A fundamental shift has occurred in the approach to achieving predictability in simulation science based on a foundation of Verification and Validation as proposed by Oberkampf and coworkers at SNL. Utah and SNL are working to push this issue to the forefront of simulation science.

Gene: Either pick up some scientific legacy items from the preceding text or at a comment here like “Additional scientific legacies may be found throughout the preceding text.”

Appendix 1: Status of 2005 Recommendations

End Goal

- 1) **Identify a well-defined end-to-end fire and explosion simulation as an end goal.**

C-SAFE has planned a parametric study of the effects of crosswinds up to 6 m/s on heating of a 4" diameter x 4" long cylindrical steel container of PBX9501 suspended 0.3 m above a 1 m diameter JP-8 pool fire. This study will be carried out in Year 10 and the results published in a joint paper with several C-SAFE authors.

Fire Science

- 1) **A molecular dynamics based soot constitutive model should be included in the final end-to-end simulation.**

The soot models in the end-to-end simulation have not incorporated the MD simulation results, in part due to the departure of 2 key personnel from C-SAFE (Violi and Voth). C-SAFE resources in the Fire Science area were instead focused on V&V activities.

- 2) **Completion of the radiation model into the ICE code.**

Implementation of radiation in ICE was completed this year. There are some minor issues that remain concerning how radiation is absorbed by solid (particle-based) objects and the overall strategy for correct thermodynamic treatment of energy.

- 3) **Further improvement of the ICE boundary conditions to allow for long time numerical integration.**

Progress on improving the boundary conditions was a major effort in previous years. The current efforts are focused on use of AMR to provide larger domains at lower resolution near the boundaries.

- 4) **Conduct rigorous plume validation studies using data from Sandia.**

Significant resources were invested this year on rigorous plume validation studies based on the Helium plume data from Sandia. One post-doc (Zhaosheng Gao) spent full time on performing these validation studies this last year. The work was presented at the Utah-Sandia Workshop on Fire Models and Validation held in Albuquerque on May 7-9, 2006 and at the 7th World Congress on Computational Mechanics in the session on "Accomplishments and Challenges in Verification and Validation" chaired by W.L. Oberkampf held in Los Angeles on July 16-22, 2006. The work is being prepared for publication by invitation of the session chair.

Container Heat-up

1) **Explore improvements for the implicit solver used for MPM.**

Performance improvements have been implemented, specifically in the setup phase of the implicit solve. The implicit heat conduction algorithm has been reworked to improve conduction within multi-material problems and additional capabilities have been added to the implicit heat conduction algorithm to eliminate the information loss that was occurring from particle to grid interpolations.

2) **Perform analytical or numerical investigation of spatial convergence properties of MPM in multi-dimension.**

An extensive study was performed to improve the error and convergence properties of MPM, and these improvements were implemented in the end-to-end code.

3) **Continue to work with mathematicians to analyze stability and dispersion properties of MPM.**

Stability and dispersion issues have been examined in detail and several improvements made by carrying additional state vectors on the Lagrangian particles and by modifying the method by which properties are interpolated to and from the Eulerian grid, especially with respect to AMR.

4) **Enhance AMR algorithms in MPM, especially the robustness of state and field variables during refinement in large deformation analysis.**

AMR is now fully implemented in MPM.

5) **Present MPM advancements at national and international conferences.**

C-SAFE sponsored a national workshop on the Material Point Method this year. They contributed to a mini-symposium on MPM at the World Congress on Computational Mechanics in July 2006, and gave presentations on fracture and plasticity of metals and wood at other national meetings.

6) **Include the propellant constitutive models in the end-to-end simulations.**

The ViscoSCRAM constitutive models were used in the end-to-end simulations last year. Temperature dependent viscoelastic properties of PBX9501 (ViscoSCRAM-T) have been implemented and committed this year.

- 7) Explore computational efficiency and sensitivity of results to the trigger strategies used to determine detonation.**

The trigger strategies for ignition of the PBX have been investigated and modified to be responsive to stimuli such as presence of hot gases or solids in the cell and the existence of sufficient surface area. These criteria are much more realistic than the artificial triggers used previously based only on the bulk temperature of the propellant.

- 8) Continue to evaluate if soot deposition is important to heat transfer.**

This continues to be a strong focus of experimental activities in the center. Results of the studies on soot deposition and chemical analysis were published recently in the peer reviewed literature.

Computer Science

- 1) Undertake a study to determine the costs and benefits of preserving the UCF as a resource for the wider computational community.**

Uintah is currently designed as a plug-in to the larger open-source SCIRun code. Consideration is now being given to how Uintah and the UCF will be maintained in the future, as a separate code with its own development plan, or as a PowerApp in SCIRun to take fullest advantage of advances in visualization technologies.

- 2) Details of the UCF should be published in top venue journals and include performance metrics of the most challenging computations.**

Portions of the UCF have been described already in several publications. More detailed information and performance data will be provided in subsequent papers.

Applied Mathematics

- 1) Continue to implement AMR in Implicit ICE.**

This has been a major focus of activity in the Center this year. The AMR team discovered critical bugs in our code and in HYPRE. These are being resolved now.

- 2) Explore selection of a multigrid linear solver within HYPRE.**

C-SAFE selected HYPRE as its multigrid solver, completed a front end to take fullest advantage of the solver speed and accuracy, and implemented the code. The code works well with single-physics codes (ICE or MPM), and the HYPRE team has been working with C-SAFE to resolve remaining issues and bugs to achieve a full implementation in the multiphysics codes (MPMICE). The only issue with HYPRE is related to the AMR-ICE semi-implicit pressure solve. Otherwise the multigrid linear solver's performance is satisfactory: simply choosing a different solver reduced the solve time substantially.

3) Continue the analysis of the accuracy and stability of MPM.

Martin Berzins' group has been working with Jim Guilkey and his team to do this, and several major advances in MPM code stability and accuracy were reported.

4) Analyze the instability in the fire code with a first look at far-field boundary conditions.

Far-field boundary conditions have been a long standing issue in ICE and a significant amount of work has gone into implementing and debugging non-reflective boundary conditions. Initial simulations using these boundary conditions show promise; however, there are still unresolved bugs, particularly with reacting flows. The majority of effort of the ICE developers' time has gone into AMR.

Validation and Verification

1) The same level of code verification should be carried out for ICE as was done for Arches.

The Fire Science team conducted extensive side-by-side validation studies of Arches and ICE fires at the single resolution level. Continuation of the comparison studies will wait on the completion of the AMR implementation and HYPRE bug fixes for ICE fires.

2) Continue to validate the fire simulation model using ICE.

During the past year the fire validation work continued as defined in our Fire Validation Hierarchy. Work in each of the boxes of the hierarchy was conducted with ICE and with ARCHES. Some of the results of these studies were presented at the Utah-Sandia Workshop on Fire Models and Validation held in Albuquerque on May 7-9, 2006.

3) Repeat the thoroughness of the fire simulation V&V for all aspects of the final end-to-end calculation.

V&V efforts during the past year have been focused on supporting studies, where experimental data are more accessible. This year, there were extensive efforts to validate the MPM algorithm, as well as material models using Taylor Impact experiments, high velocity impact, and flyer plate. Work is underway to obtain experimental data for the end-to-end scenario, and validation comparisons will take place over this next year.

Education and Training

1) Students should participate in publishing in archival journals.

Students are being encouraged to participate as co-authors, and in some cases as primary authors.

- 2) **Interested staff should be encouraged to take the role of co-authors on papers of students they supervise.**

This is being done.

- 3) **There should be a regular seminar for students to present their research to one another across disciplines.**

C-SAFE did not implement a planned student seminar program this year, primarily because there are active student seminar programs in the individual departments. Information about these seminars is routinely disseminated through the C-SAFE lists to faculty students and staff. In addition, C-SAFE personnel are encouraged to participate in the new Computational Engineering and Science seminar program.

APPENDIX 2: SUMMARY LIST OF 2006 RECOMMENDATIONS

The review team makes the following recommendations:

1. You have one year left ... make sure you prioritize ...
2. We suggest that you finish incorporating AMR with radiation and exercise it in the simulation suite.
3. We suggest that you work with the CRT to define your requirements for the end-to-end simulations.
4. We suggest that you complete the Uintah release and focus on external users as resources permit.
5. We suggest that you incorporate homogenized MD simulation results into the end-to-end simulation.
6. Finally, we suggest that you pursue the ability to model soot break out physics.

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