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TECHNICAL REPORT

Is there Still More to Science than Simulation?

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Abstract:

The relationship between simulation and experimentation is a complex one. In this paper we examine this relationship in the context of a number of research programs. Some conclusions are drawn regarding the difficulty of undertaking computational science without linked experiments. A revised copy of this report is to appear in Computing in Science and Engineering 2007.

THE UNIVERSITY OF UTAH

Is There Still More to Science than Simulation?

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Abstract
The state of the art in computational science and the relationships between theory computation and experiment are explored in the context of large scale simulations being undertaken in the C-SAFE project at the University of Utah.

The State of the Art in computational simulations was described by the recent NSF Blue Ribbon panel report, [1], as follows. *Computer simulation represents an extension of theoretical science; it can and generally is based on mathematical models characterizing scientific theory, but it can be much more, because simulation can be used to explore the consequences of situations in which well-established theory breaks down.* The report also states that simulation *transcends the traditional pillars of science*. Similar statements are made by the PITAC report [2], with many good examples and convincing justifications. Given the increasing importance of simulation it is worthwhile to attempt to evaluate the role of simulation in 21st century science. In this article I will make a purely personal attempt to do this based on my broad experiences of software and computation and by using my recent experiences as part of the CSAFE (Center for the Simulation of Accidental Fires and Explosions), [3], project at the University of Utah to illustrate some of the points. Part of the rationale for this is that the state of the art in computation is perhaps exemplified by main target problem being considered by the large multi-disciplinary team in the C-SAFE center. This target problem is to simulate the rapid heating of a container with conventional explosives in a pool fire as shown in Figure 1(a).

Figure 1(a) CSAFE Model Problem

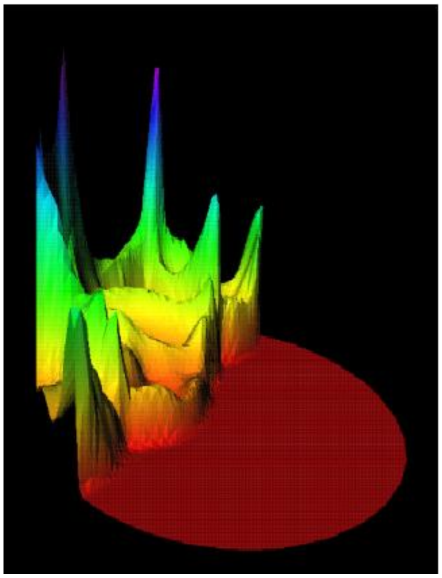

Figure 1(b) Pressure spikes in Knock Model

The simulations were each run on 200 processors on alc.llnl.gov. The simulation domain consisted of 550,000 cells containing 400,000 Lagrangian particles representing steel and energetic material. Total simulated time for each explosion was about 6 milliseconds, and required about 30 hours to complete. The results of the simulation are shown in Figure (2). In each case, ignition occurred at the interface between the hot steel and the material. Combustion gases then pressurized the interior, resulting in rupture of the container. In the case of the solid material simulation, the container ruptured in a single location, resulting in rapid depressurization and a relatively mild explosion. In contrast, in the case of the hollow material simulation, the combustion caused the material to collapse into the bore region, resulting in a large volume of burning material. When the container ruptured, fragmentation was extensive, and the violence of explosion was significantly increased. It is natural to ask how realistic these results are. The target simulation includes the combustion of the pool fire, heat transfer to the container, mechanical stress and rupture of the container, and the chemistry and physics of energetic material inside the vessel. The problem is naturally multiscale ranging from tens of meters for the fire to micrometers for the energetic material, [4]. The challenge for the CSAFE software, Uintah, [4], of computing an accurate (or indeed any) solution to this problem is considerable, but attainable. Recently, [5], two simulations of an exploding container were performed by CSAFE staff in order to demonstrate the effect of including a hollow bore region in the center of the energetic material inside the steel container.

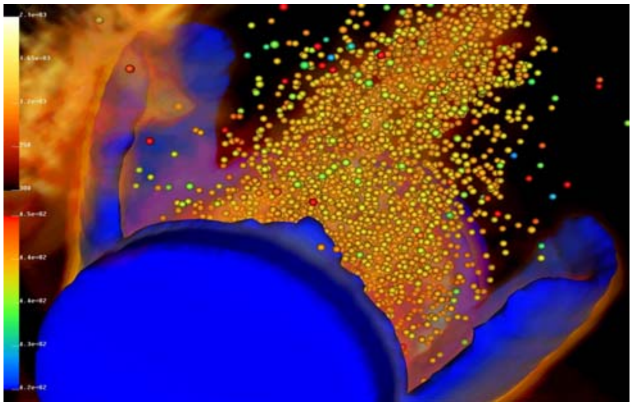

Figure 2(a) CSAFE Solid Case

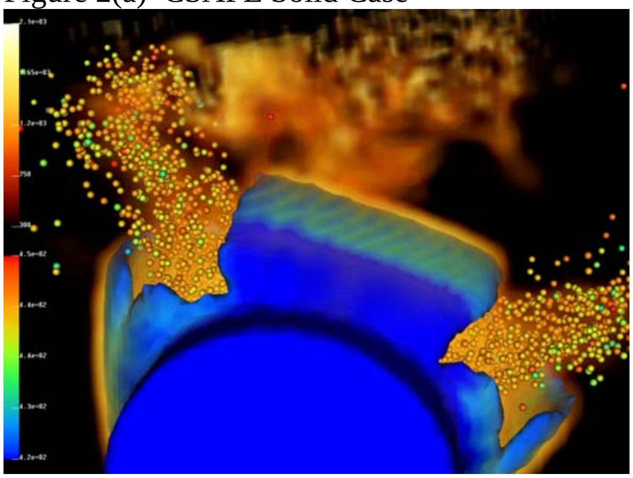

Figure 2(b)   CSAFE Hollow Case}

Theory, Experiments Verification and Validation In order to understand whether or not a computation is valid it is important to evaluate the theory behind both the mathematical models and the numerical methods used in the code. It is also important to match any available experimental results to those of the code. One of the most perplexing aspects of the availability of massive parallelism is that our ability to perform experiments outraces our corresponding efforts in the theory of both the mathematical models and the computational algorithms. This is despite outstanding advances in the theory of computational methods by researchers such as Babushka and Oden to name but two, [6]. Such theory is perhaps not yet comprehensive enough to apply to all aspects of complete multiphysics simulation codes such as those used in C-SAFE, however. Furthermore in order to solve the next generation of problems it is sometimes necessary to rapidly generate broadly plausible theories for the calculations that need to be done. The challenge of verifying and validating such codes and models is significant, outstanding and costly. A significant issue with all codes is the fact that they are far from bug-free, [7]. There are also inherent problems with systems built from large numbers of components. It is well understood that both the individual components and the system as a whole need to be tested individually, [8]. It is also well known that it is almost impossible to test all the potential paths in a code. Even if the codes are correct it is also understood, [1], that: *Ultimately, the most confounding aspect of V and V has to do with uncertainty in the data characterizing mathematical models of nature. In some cases,* *parameters defining models are determined through laboratory tests, field measurements, or observations, but are always variable in measured data from one sample to another or from one observation to the next.* These different levels of errors in our simulations can, clearly, be overcome in specific cases where enough time and resources are available. One additional complication arising from the development of a large complex code is that it may be difficult for others to replicate the results without knowing all the algorithmic intricacies of the original software. This knowledge is sometimes not documented or may have been lost.

In the case of CSAFE numerous validation experiments are undertaken in a continuous and thorough testing program. Furthermore the C-SAFE problem solution is being validated by rigorous comparison with experimental data for a variety of conditions. The experiments of Eddings Ciro and White, [9] show remarkable differences in the violence of the explosion in the hollow and solid cases and indeed motivated the computational experiments described above. These experiments show that in the hollow and solid cases the numerical solutions are in broad agreement with the experiments. Without the experimental results it might well not have been the case that this scenario was used as a test for the computational models.

Sometimes however even experiments do not provide enough information. For example in a simpler but still challenging combustion model of knock in an idealized car engine cylinder the onset of 'knock' is seen when large pressure pulses interact with the edges of the cylinder, [10], see Figure 1b. The important aspect of the numerical results is the size of any pressure spikes to reach the boundary. The maximum recorded values of the pressure on the boundary obtained by computation could not be verified as the pressure transducers in the corresponding experiment were not able to sample frequently enough. Thus even experimentation may not always be enough to convince us of correctness. The major change is that perhaps we are now entering an era in which simulation now drives theory and experiment. The observations and discussion above suggest that complex simulations of multiphysics phenomena will still need to be linked to as much theory and experimentation as is possible for a considerable time to come.
The most fundamental change that has occurred is that the ease and range of experimentation possible now make it possible to use simulation as a major tool in probing likely scenarios for experiments and for trying to investigate how possible theories may fit the results. Of course it is also true that, [1], *Simulation also provides a unique alternative to experimental science and observation, for it can be used to study events not observable or for which measurements are impractical or too expensive*. A major challenge for the next decade is to properly quantify the uncertainty in any such calculation. For example in the C-SAFE calculation the user should be able to know what level of reliance may be placed on the time of fragmentation of the container, of the energy of the process and of the final size and shape of the container fragments.

The future is bright in that the problem solving capability of codes such as those used in CSAFE will do much to encourage further theory and experimentation and to produce solutions to complex problems where none were possible before. In response to the question raised in the title the answer is yes, but simulation is clearly playing an increasingly dominant role for some classes of problems and even helping design future experiments.

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