Applications of computational fluid mechanics at Sandia National Laboratories

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Abstract

In the spirit of representing the industrial perspective (at least the high-end-application user) on computational fluid mechanics at this 3rd MIT Conference, we present the results of recent calculations in three areas of fluid mechanics of interest at Sandia National Laboratories. The ability to simulate these phenomena at extremely-high fidelity on massively-parallel, distributed, computer platforms has only recently been achieved using Sandia's SIERRA and NEVADA software architecture. These simulations represent the broad range of compressible fluid mechanics now being applied to problems of national security at Sandia National Laboratories.

Keywords: Fluid mechanics; Fire; Incompressible; Compressible; Low Mach number; Magnetohydrodynamics

1. Some simulation capabilities

Brief descriptions of three fluid mechanics modeling and simulation capabilities are given below.

1.1. Low Mach number reactive fluid mechanics – FUEGO/SYRINX

FUEGO and SYRINX, fire environment simulation software, are focused on predicting the thermal environment of large-scale pool fires and building enclosure fires (Fig. 1). FUEGO embodies the turbulent, buoyantly-driven incompressible flow, heat transfer, mass transfer, combustion, soot, and absorption coefficient model portion of the fire physics. SYRINX embodies the participating-media thermal radiation mechanics. FUEGO and SYRINX utilize the SIERRA framework for massively parallel computing, solution adaptivity, mechanics coupling on unstructured grids, parallel services, linear and nonlinear solvers, finite-element and I/O services, and configuration management.

1.2. Compressible fluid mechanics – PREMO

PREMO, aerothermodynamics simulation software, determines aerodynamic characteristics of bodies in compressible flight: subsonic compressible, transonic, and supersonic flow. Built using an edge-based, finite-volume scheme, PREMO utilizes explicit and implicit (Newton–Krylov) solvers to generate transient and steady-state solutions to inviscid, laminar and turbulent flows (Fig. 2). PREMO's infrastructure allows for the quick and easy introduction of new physics (i.e. new turbulence model, and chemistry) and of new solver methods and techniques (i.e. segregated physics, and operator splitting). PREMO also utilizes many of the application-developer services provided within the SIERRA framework.

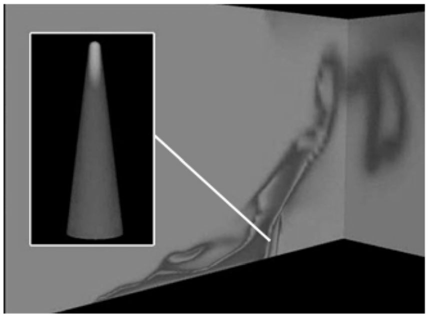

Fig. 1. Example of the three-dimensional, thermal response of an object coupled within a fully turbulent fire with crosswind.

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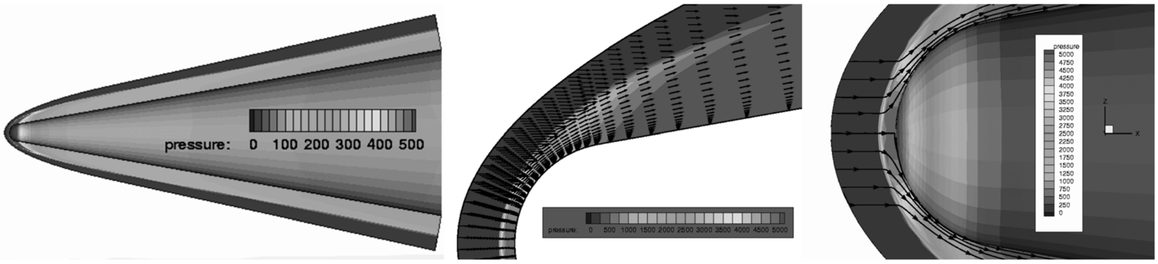

Fig. 2. Example of three-dimensional hypersonic flow over a blunt cone.

1.3. Magnetohydrodynamics – ALEGRA

The Arbitrary Lagrangian Eulerian Grid for Research Applications (ALEGRA) software is built on the NEVADA architecture and allows simultaneous computational treatment, within one code, of a wide range of strain-rates varying from hydrodynamic to structural conditions. This range encompasses strain rates characteristic of shock-wave propagation (10^7/s) to those characteristics of structural response (10^2/s). A three-dimensional resistive magnetohydrodynamics (MHD) option has been implemented in ALEGRA and is being used to simulate z-pinch wire array implosions. The three-dimensional MHD modeling capability in ALEGRA is crucial for understanding the instabilities that occur in z-pinch wire array implosions, which in turn are critical phenomena in determining the resulting radiation pulse generated in the Sandia National Laboratories intense X-ray source 'Z machine' (Fig. 3).

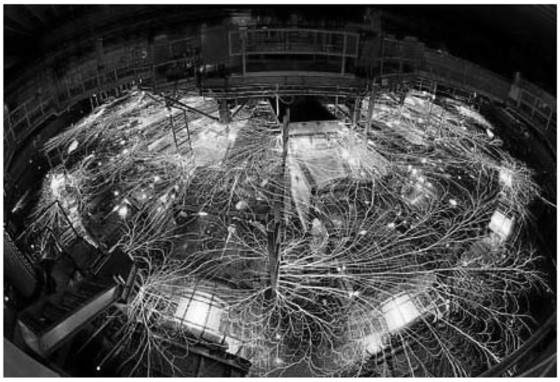

Fig. 3. Photograph during operation of the 'Z-machine' at Sandia National Laboratories.

2. The ASCI program

The ability to simulate the complex engineering sciences phenomena, as outlined above, is a direct result of the United States Department of Energy/National Nuclear Security Agency (NNSA) Accelerated Strategic Computing Initiative (ASCI) program. In 1994, NNSA established a ten-year ASCI vision for the use of computational models to achieve its national security mission goals. In ten years, there have been remarkable achievements within the ASCI program, including breaking the 10^{12} floating point operations/sec boundary with the goal of a petaflop, achieving a $>10^4$ increase in the fidelity of the computational models, realizing tremendous increases in our ability to manipulate and visualize data, introducing new computational software architectures, and utilizing new numerical approaches to nonlinear computational mechanics.

In addition to the development of these new tools, we require extensive verification and validation (V&V) processes to build trust in these simulations accurately portray the observed phenomena. Our ability to verify the mathematical basis of our software, to explore new validation technologies for the comparison of experiment and simulation, and to develop new methods to quantify the uncertainty not only of computational results but also of experimental results, limits us today. Recognizing this, the NNSA has focused on V&V as a critical element of the program to avoid the pitfall voiced by Ferziger [1]:

> *The greatest disaster one can encounter in computation is not instability or lack of convergence but results that are simultaneously good enough to be believable but bad enough to cause trouble.*

3. Conclusions

Sandia National Laboratories continue to develop and enhance a full suite of massively-parallel, engineering software that efficiently scales on thousands of processors on distributed-memory (and shared-memory) computation platforms. We are using this capability in our national security mission. The examples shown represent the fluid mechanics breadth of our capability.

A graphic of our full suite of our engineering software is shown in Fig. 4.

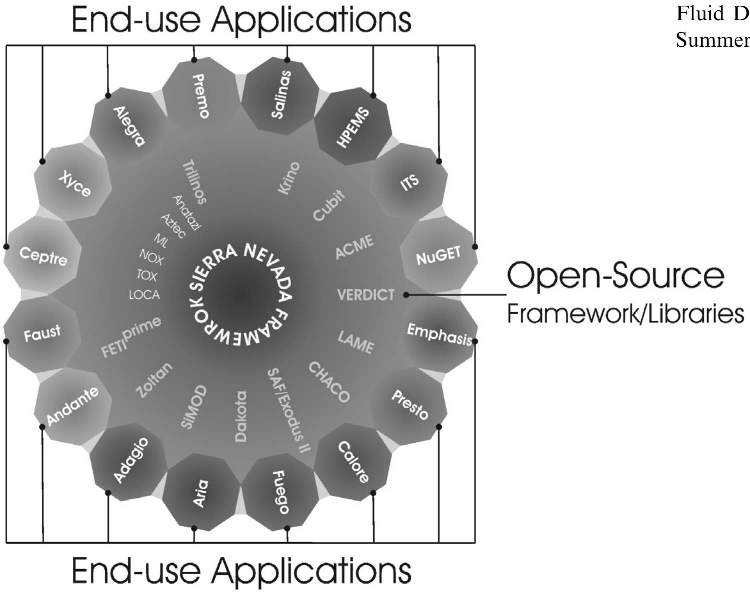

Fig. 4. Schematic of engineering end-use applications within Sandia National Laboratories' SIERRA and NEVADA frameworks.

Reference

[1] Ferzinger JH. Estimation and reduction of numerical error. In: Quantification of Uncertainty in Computational Fluid Dynamics, ASME FED Vol. 158, ASME Division Summer Meeting, Washington, DC, 20–24 June, 1993.