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Parallel Adaptive Algorithms for Multi-Scale Problems

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Summary

New fast algorithms are being developed for simulating multi-scale phenomena. Target applications include the modeling of detonations in high-energy explosives, the modeling of multiphase mixtures and the modeling of shock waves in lithotripter devices. The adaptive numerical algorithms allow computational resources to be dynamically targeted at critical regions to increase the accuracy of the simulation. The algorithms are being developed to run efficiently on large scale parallel computers. The approach will enable accurate, high-resolution modeling of physical phenomena in complex three-dimensional regions.

As part of the Applied Math Research program, researchers at LLNL are developing fast new parallel algorithms for solving multi-scale problems. Target applications include the modeling of detonations in heterogeneous high-energy explosives, the modeling of shock waves in lithotripters (a medical device used to break up kidney stones) and the modeling of multi-phase mixtures of fluids and solids. Previous two-dimensional computations on serial computers have shown the efficacy of the approach [1][2]. The new three-dimensional parallel algorithms will enable the rapid simulation of problems with billions of degrees of freedom. This effort is part of a larger project, whose goal is the design, analysis and development of advanced new algorithms for the accurate and efficient solution of partial differential equations in complex moving geometry and the application of these algorithms to projects of critical interest to the DOE.

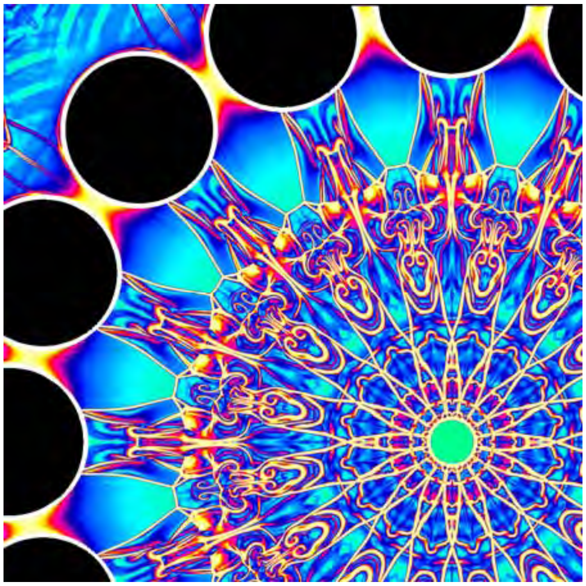

Figure 1: The intricate flow pattern from a cylindrically converging shock wave that diffracts around sixteen circular obstacles. Researchers are interested in the structure of the solution near the focus (green region). This high-resolution numerical solution was computed with the adaptive algorithms described herein.

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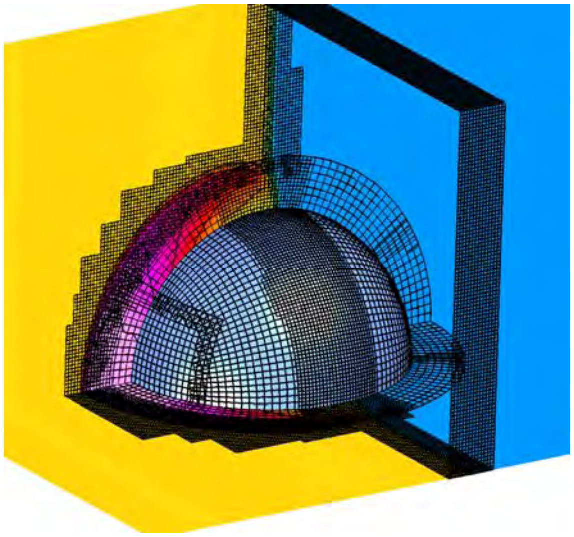

Figure 2: Parallel computation of the diffraction of a shock wave by a sphere using overlapping grids. The dark grid-lines indicate regions where the resolution and accuracy have been dynamically increased

The parallel adaptive algorithms are based on a domain decomposition approach using “overlapping grids”, as shown in Fig. 2. Efficient Cartesian grids are used throughout most of the domain (a “grid” defines the points where physical quantities such as density and velocity are represented). Curved boundary fitted grids are used locally near bodies. Dynamic, locally refined grids are added where needed, in order to increase the accuracy of the solution and thus avoiding the cost of using a fine grid everywhere. This is especially important for modeling multi-scale phenomena that can contain very small scale features that must be represented accurately. A detonation wave, for example, may be a fraction of a millimeter wide but travel at speeds of 1500 meters/s. The new multi-scale adaptive algorithms are being developed to perform well on large-scale distributed-memory parallel computers. The algorithms and data-structures are quite complex and their efficient implementation thus requires the creation of sophisticated software components. An important benefit of this algorithm and software development effort is that, through improved efficiencies in CPU time and memory, much larger problems can be simulated for a given size of computer.

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[1] W.D. Henshaw and D.W. Schwendeman, "Moving Overlapping Grids With Adaptive Mesh Refinement for High-Speed Reactive and Non-Reactive Flow”, J. Comput. Phys., 2006.

[2] J.W. Banks, D.W. Schwendeman, A.K. Kapila, W.D. Henshaw,”A High-Resolution Godunov Method for Compressible Multi-Material Flow on Overlapping Grids”, J. Comput. Phys., 2007.

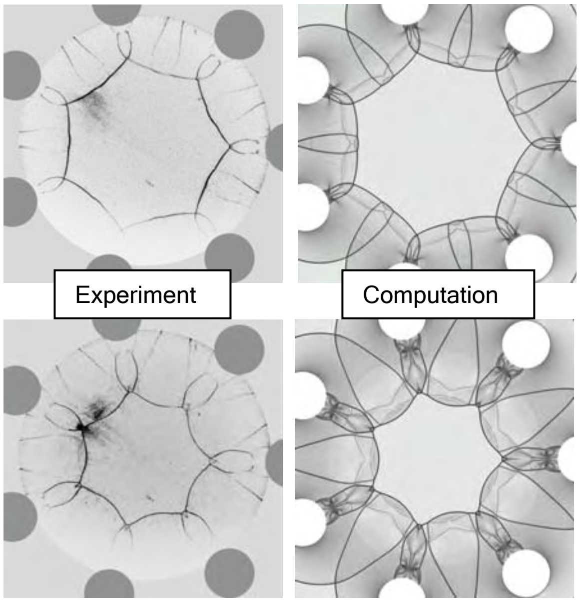

Figure 3: Left: experimental images of the diffraction pattern from a cylindrically converging shock that hits seven obstacles. Right: images from an adaptive numerical simulation, showing excellent agreement with the experiment.

For further information on this subject contact:

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