

Overview of Eulerian Methods and Block Adaptive Mesh Refinement Techniques at Sandia

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Multi-material shock-physics Eulerian codes have undergone several generations of refinement in as many decades at Sandia. The widely used code, CTH, can trace its lineage to the one- and two-dimensional codes CHARTD and CSQ. An adaptive mesh refinement (AMR) strategy has been implemented in CTH, providing improved performance and memory utilization and evidence of improved scaling for large problems. The ALE (Arbitrary Lagrangian Eulerian) code ALEGRA combines the multi-material shock physics capabilities found in CTH with a finite element numerical technique. It functions as an Eulerian code by imposing a trivial remesh strategy. The open architecture of ALEGRA has made it a popular foundation for multi-physics applications.

Introduction

Multi-material shock-physics Eulerian codes have undergone several generations of refinement in as many decades at Sandia. The widely used code, CTH (McGlaun, 1987), can trace its lineage to the one- and two-dimensional codes CHARTD (Thompson, 1972) and CSQ (Thompson, 1975). It is supported on a wide variety of serial and parallel computers at Sandia and at more than 300 external license holders throughout the U.S., U.K. and Canada. CTH solves conservation of mass, momentum and energy by integrating finite difference approximations using an explicit two-step Lagrangian/remap formulation. A CTH calculation can contain up to 20 materials, each described with analytic or tabular equations-of-state, modern deviatoric strength models and modern fracture models that can be based on damage criteria.

The ALE (Arbitrary Lagrangian Eulerian) code ALEGRA combines the multi-material shock physics capabilities found in CTH with a finite element numerical technique. It functions as an Eulerian code by imposing a trivial remesh strategy. The open architecture of ALEGRA has made it a popular foundation for multi-physics applications. Although it originally operated only on unstructured meshes, a multi-block curvilinear mesh type has recently been added. This mesh type provides many of the efficiencies available to a structured mesh while allowing arbitrary connectivity between structured blocks.

Eulerian codes have the advantage of being able to handle large distortions with relative ease yet they suffer from dispersion. An adaptive mesh refinement (AMR) strategy to reduce dispersion through increased resolution was implemented in CTH by Crawford, et al. (2002), providing at least a factor of three improvement in performance and memory utilization at equivalent resolution and evidence of improved scaling for large problems.

With their complementary and overlapping capabilities, CTH and ALEGRA are being used for a wide variety of applications and research and development at Sandia. They both take advantage of common material models: equations-of-state and deviatoric (strength and failure) models and common material insertion (initial condition definition) and interface reconstruction techniques. This paper will discuss each code's Eulerian hydrodynamic capabilities with sample applications.

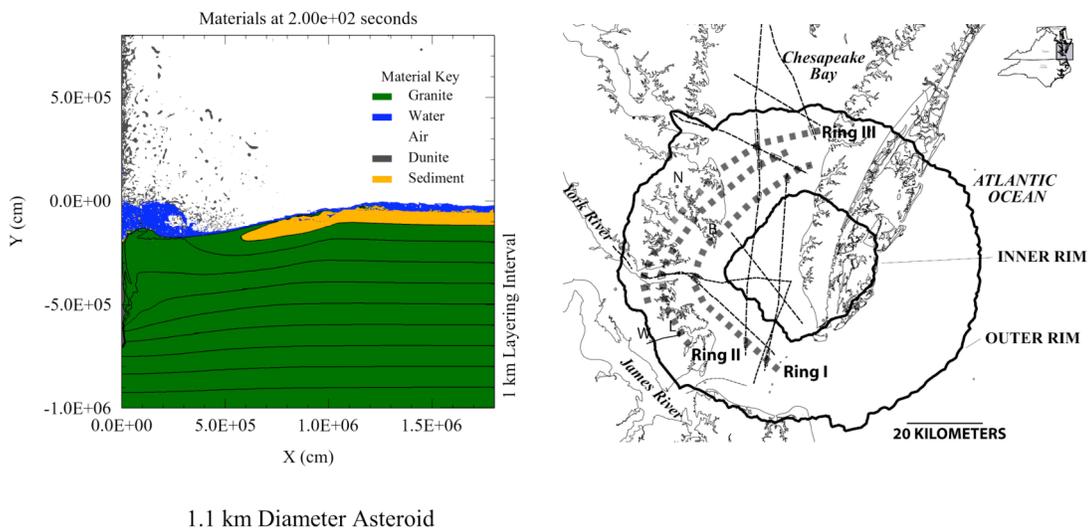
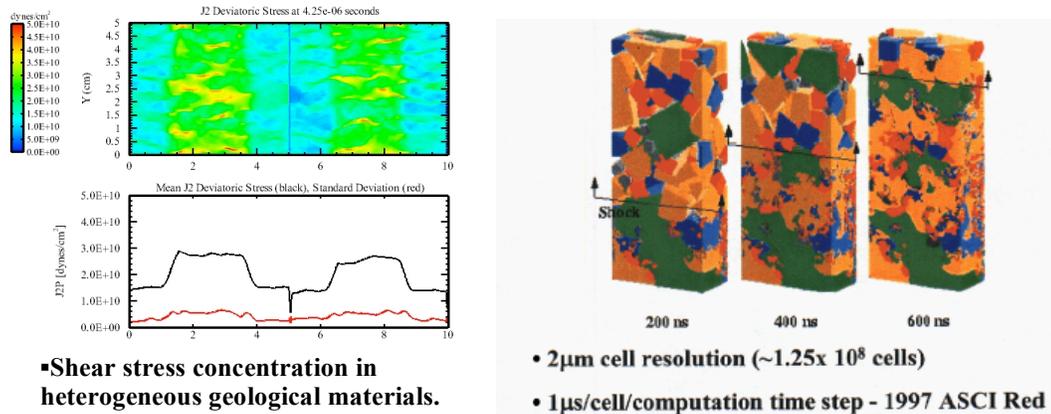


Figure 1. A CTH calculation at large scale: modeling the impact of an asteroid that formed the 35 million year old Chesapeake Bay Impact structure (Crawford and Barnouin-Jha, 2004). The map at right (from Powers et al., 2003) is the present day extent of the buried impact structure near the entrance of Chesapeake Bay, Delaware/Maryland/Virginia, USA.

CTH

CTH is an Eulerian shock physics code solving conservation equations of mass, momentum and energy for up to twenty materials. It contains analytic and tabular equation-of-state representations for gases, fluids, solids and reactive materials and advanced strength and fracture models. With an adaptive mesh refinement capability, CTH is being widely used throughout the U.S. for solving problems across many spatial scales with increasing complexity (Figures 1 and 2). CTH is designed to be easy to use with straightforward and flexible mesh description, material geometry insertion, built-in parameters for common materials and easy to use post-processing tools that are all self-contained as part of the code package. A single text file input can be used to control all

aspects of CTH code behavior from problem setup through integration and post-processing. Written primarily in Fortran and C, CTH is fast and robust, enabling rapid problem solving for the analyst. It has been extensively verified and validated by an estimated 1,000 users throughout the United States.



•Shear stress concentration in heterogeneous geological materials.

Figure 2. CTH calculations at small scale: modeling mesoscale response to shock loading of geological materials (Crawford and Barnouin-Jha, 2004) (left) and explosives (Baer, 2003) (right).

CTH has six geometry mesh options: one dimensional rectilinear, cylindrical and spherical, two dimensional rectilinear and cylindrical and three dimensional rectilinear. It integrates the mass, momentum and energy conservation equations through time in a two-step process: a Lagrangian step followed by an immediate remap step. In the remap step, second order Van Leer is used along with interface tracking to minimize distortion of material interfaces. We are presently investigating potential improvements to the Lagrangian step (Schmitt, this proceedings).

CTH has many primary equation-of-state models ranging from simple ideal gas, polynomial shock-particle-velocity relationships and Jones-Wilkins-Lee explosive reaction products to tabular models that can express the full range of equilibrium thermodynamic behavior. A model for material porosity is incorporated into several equations-of-state. CTH has composite equations-of-state to describe explosive detonation and phase transitions. In conjunction with the conservation laws, the equation-of-state models form a closed set of equations for solution of shock hydrodynamic problems. Most of these models are also used by ALEGRA.

When material strength is important, CTH has a number of constitutive models for computing the deviatoric components of the stress tensor. These range from simple elastic-perfectly-plastic to sophisticated visco-plastic and visco-elastic models that incorporate damage and failure. They typically incorporate strain and strain-rate dependence, thermal, density and pressure effects. Models are available for ductile, brittle, composite, porous (fluid/gas filled) and reactive materials. Most of these models are also used by ALEGRA.

Adaptive mesh refinement in CTH

Adaptive mesh refinement (AMR) has been used for improving computational

resolution when resources are limited and has been used for hyperbolic problems on an experimental basis for years (Berger and Olinger, 1984; Berger and Colella, 1989; Tang and Scannapieco, 1995; Jones, 1997). For a mature Eulerian multi-material shock-physics code family like CTH and its predecessors, adaptivity is considered a natural next step in code development.

In order to achieve adaptivity yet retain the man-years of effort that have been expended on the development of physics routines, the refinement is block-based, where each block consists of a small patch of cells (typically 10x10x10). An example of this approach, showing the outline of each AMR block, is shown in Fig. 3. In order to facilitate its implementation on massively parallel platforms, each block communicates with its neighbors using a generalization of the message-passing paradigm developed for multiprocessor CTH. A maximum 2:1 resolution difference across block boundaries is strictly enforced. Block refinement and un-refinement is isotropic. In multiprocessor AMR-CTH calculations, blocks are distributed across processors and CPU loading is optimized.

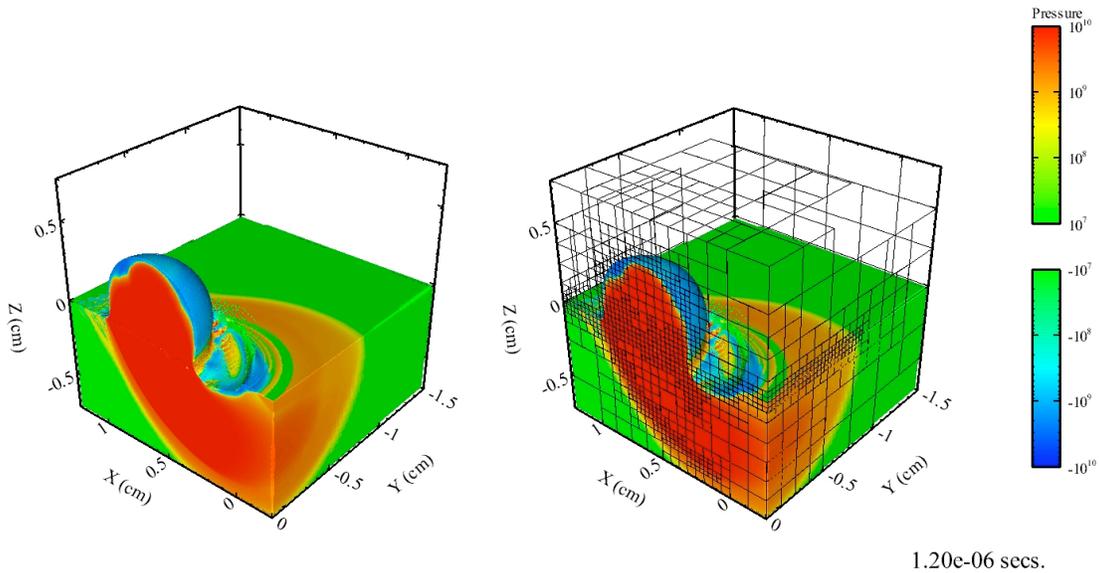


Figure 3. Highly oblique impact of 1/4" spherical aluminum projectile onto aluminum half-space target. Level 7 adaptive mesh (equivalent to 160 cells across the projectile diameter) is shown. Block outlines are shown in the figure on the right.

A single time step, determined by a Courant-Friedrichs-Lewy (C.F.L.) condition in the highest resolution mesh, is used to advance the problem through time. At first glance, advancing the solution of the lower resolution mesh with the same time step as the highest resolution mesh may seem wasteful. A closer look, however, suggests that most computational cells are often at the highest resolution (Fig. 3) and the potential for improving performance with sub-cycling the highest resolution mesh must be offset by the additional algorithmic complexity. Additional research will be conducted to determine if the advantages of sub-cycling certain calculations can outweigh the costs.

Figure 3 shows a 3D calculation of a ¼” aluminum projectile striking an aluminum target half-space at a highly oblique incidence (15° from horizontal) and an impact velocity of 5 km/s. Several AMR calculations were performed of this scenario for maximum effective resolutions of 10, 20, 40, 80 and 160 cells across the projectile diameter (maximum refinement levels of 3, 4, 5, 6 and 7). The calculations were performed on as many as 512 processors.

The CPU times for the five 3-D adaptive cases and two non-adaptive cases are plotted in Figure 4. While the lowest resolution test case exhibited no significant performance improvements, the higher resolution cases exhibited substantial improvement with the highest resolution case (level 7) showing an improvement by about a factor of fifteen over the projected non-adaptive case. Furthermore, the highest resolution adaptive cases exhibit improved scaling. A non-adaptive 3-D calculation will require 16 times the CPU time for every additional level of refinement but here the highest resolution adaptive cases required only 8 times the CPU per refinement level.

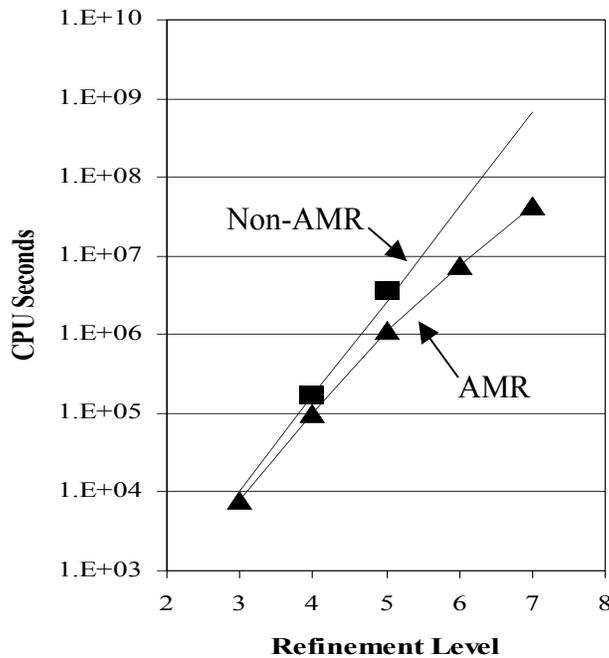


Figure 4. CPU time (equal to CPU-per-processor times number-of-processors) required to complete the 3-D CTH AMR test problem shown in Figure 1. At the highest level of refinement, the CTH AMR calculation ran fifteen times faster than the non-AMR equivalent.

Curvilinear Multi-Block Structured ALEGRA

The ALEGRA multi-material shock physics code uses an Arbitrary Lagrangian Eulerian (ALE) finite element formulation running on either an unstructured or curvilinear multi-block structured solution domain. An ALEGRA time step consists of a Lagrangian sub-step followed by a remesh and remap sub-step. ALEGRA functions as an Eulerian code when the remesh and remap sub-step returns nodes to their pre-step coordinates.

ALEGRA's Finite Element Formulation

ALEGRA supports quadrilateral elements in two dimensions (cartesian and cylindrical) and hexahedral elements in three dimensions. All element quantities are represented at the center of the element at a single integration point. Each element may contain an arbitrary number of materials. These materials may have dissimilar states and are not required to be in equilibrium. The state of each material in each element is determined by that material's equation of state, constitutive model, and the deformation rate of the element. The velocity field of the problem is carried on the nodes.

The Lagrangian step in ALEGRA begins by accumulating masses, internal forces (material stress state), and external forces (artificial viscosity, hourglass control, and boundary condition) to the nodes. The equation $F=ma$ is then integrated forward in time using a staggered time step: $v(n+1/2) = v(n-1/2) + a(n)*\text{delt_mid}$. Contributions to material internal energy are accumulated and individual material states are updated using the element deformation rate and internal energy incremental changes. The size of the next time step is calculated based on material sound speeds and advection velocities.

For an Eulerian simulation, the remap step of ALEGRA uses a directional splitting approach to remap materials, element quantities, and nodal quantities. The remap includes an interface reconstruction step and is based on the volume fluxes associated with moving nodal coordinates back to their location at the beginning of the time step. Multiple copies of nodal quantities (momenta) are shifted to the center of each element attached to the node. These quantities are then advected. The new nodal quantities (velocities) are then recovered from the residual values (of momenta) in the element centers.

Multi-Block Framework

The multi-block curvilinear framework of ALEGRA provides the storage and cycle time efficiencies of a structured mesh while allowing many of the advantages (such as conformal geometry, and element budget management) of an unstructured mesh. This flexibility is available because ALEGRA allows:

- Arbitrary sizes for blocks (number of elements in indicial directions)
- Arbitrary locations for nodes within blocks (reasonable element quality is required)
- An arbitrary number of blocks

- Arbitrary connectivity between blocks (provided nodes and element faces are contiguous)

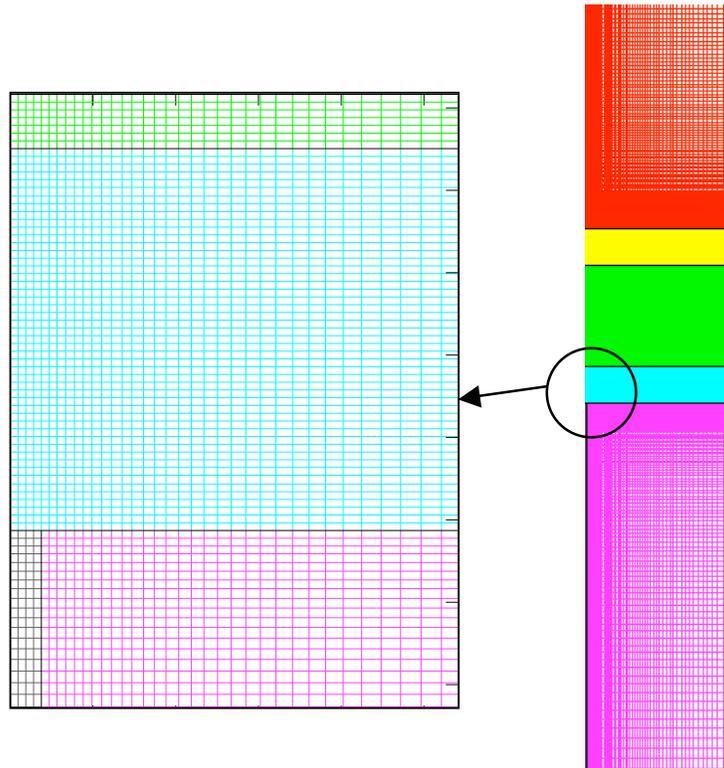


Figure 5. Two views of a two-dimensional cylindrical curvilinear multi-block mesh. The mesh is graded in the radial and axial directions to increase resolution in areas of interest. The mesh includes six blocks (each a different color) with varying numbers of elements in the i , j , and k indicial directions. The blocks are connected with each other such that the face of one block matches with a portion of an adjacent block.

The multi-block curvilinear mesh type relies on unstructured mesh specification files as its input format. Adopting an unstructured mesh format as input to the multi-block capability allows ALEGRA users familiar with unstructured analysis processes to adapt unstructured meshing techniques to structured analysis. Unstructured mesh files must satisfy a single requirement: the topology of each unstructured block must be able to be re-ordered into a structured block. Unstructured meshes meeting this requirement can be read into ALEGRA and translated at run time by a component library, or they may be translated by a free standing application into an augmented Plot-3D file which is later read into ALEGRA. The Plot 3D file is enhanced to include block to block communication and boundary condition domain information.

Support for arbitrary block to block connections has influenced block to block and inter-processor communications in ALEGRA. The fixed topology of structured blocks prevents the use of ghost elements for arbitrary connections between blocks. Instead of ghost elements, swap and add operations are used on the common nodes between blocks.

These operations must occur more frequently than ghost element updates would occur, but they involve significantly smaller messages.

ALEGRA Applications

The multi-block capability of ALEGRA was developed for modeling domains in which it is desired to resolve features of disparate length scales. The ability to manage the element budget through block transitions and mesh grading allows resolution of features in domains such as geologic structures. Eulerian structured domains provide the target domain for coupled Eulerian-Lagrangian methods being developed within ALEGRA.

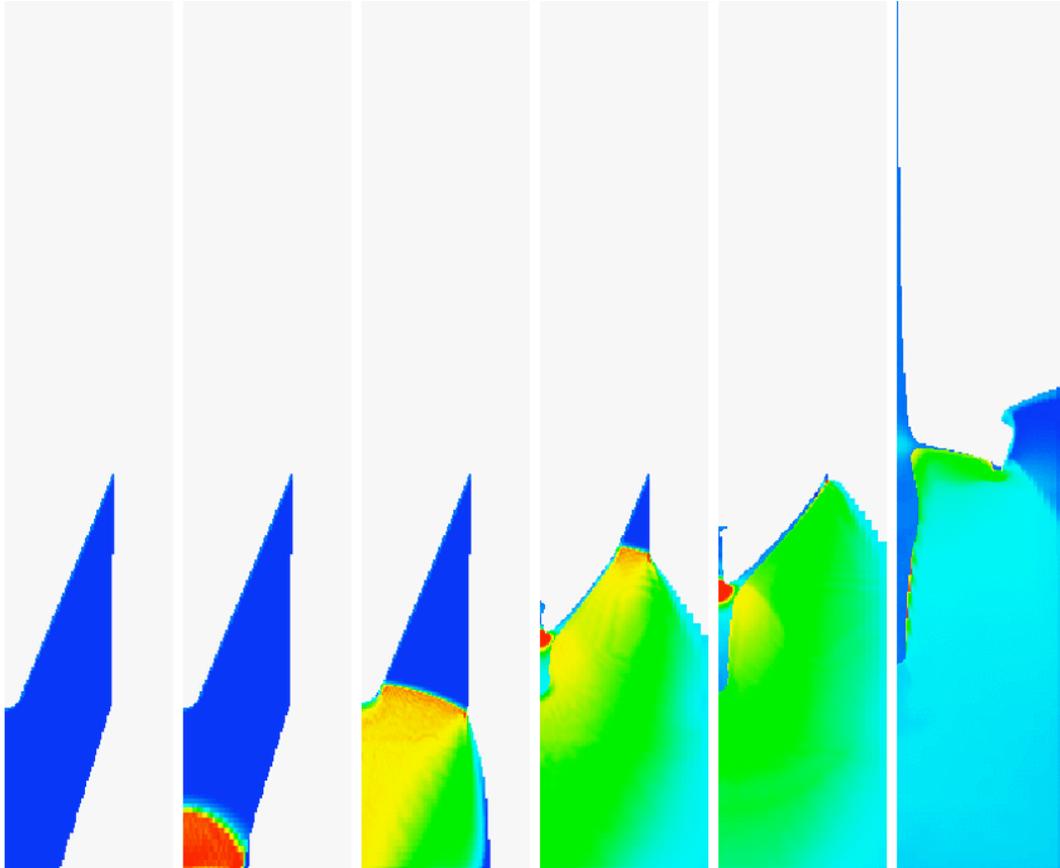


Figure 6. The images shown above are from a 2D shaped charge jet calculation run on curvilinear multi-block ALEGRA. In this Eulerian solid dynamics simulation, a soft copper liner was driven by an explosive material.

Conclusions

Because of its ease of use, performance and robustness, CTH will continue to be widely used for general purpose shock physics applications. ALEGRA fulfills a need as a platform to conduct research and development in modern numerical methods for shock physics and coupling techniques with other physics. As CTH and ALEGRA share many material models and solution techniques, so they share a common vision for shock physics solutions. Both are part of Sandia's long term strategy for the future.

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References

- Baer, Mel, "Theoretical and Experimental Studies of the Mesoscale Response of Shock-Loaded Explosive Materials", presented at the 3rd Joint Meeting of the U.S. Section of the Combustion Institute, (2003).
- Berger, M. J. and J. Olinger, "Adaptive Mesh Refinement for Hyperbolic Partial-Differential Equations", *J. Comp. Phys*, 54, 484-512 (1984).
- Berger, M. J. and P. Colella, "Local Adaptive Mesh Refinement for Shock Hydrodynamics", *J. Comp. Phys*, 82, 64-84 (1989).
- Crawford, D. A., et al., "Adaptive Mesh Refinement in the CTH Shock Physics Hydrocode" in *New Models and Hydrocodes for Shock Wave Processes in Cond. Matter*, Edinburgh, U.K., May 19-24, (2002).
- Crawford, D. A. and O. S. Barnouin-Jha, "Computational Investigations of the Chesapeake Bay Impact Structure", *Lunar and Planetary Science Conference*, Houston, Texas, (2004).
- Crawford, D. A. and O. S. Barnouin-Jha, "Mesoscale Computational Investigation of Shocked Heterogeneous Materials: Strength of Rocks Under Impact Loading", presented at the 67th Annual Meeting of the Meteoritical Society, (2004).
- Jones, B., "SHAMROCK – an adaptive, multi-material hydrocode", in *International Workshop on new Models and Numerical Codes for Shock Wave Processes in Condensed Media*, St. Catherines College, Oxford, UK, (1997).
- McGlaun, J. M., F. J. Zeigler and S. L. Thompson, "CTH: A Three-Dimensional, Large Deformation, Shock Wave Physics Code", *APS Topical Conference on Shock Waves in Condensed Matter*, Monterey, CA, July 20-23, (1987).
- Powars, et al., "ICDP-USGS Workshop: Deep Drilling in the Central Crater of the Chesapeake Bay Impact Structure", Reston, VA, 22-24 Sept. (2003).
- Tang, P.K and A. J. Scannapieco, "Modeling Cylinder Test, in Shock Compression of Condensed Matter", *Proceedings of the Conference of the American Physical Society Topical Group on Shock Compression of Condensed Matter held at Seattle, Washington, August 13-18, 1995*, 449-452 (1995).
- Thompson S. L., "Improvements in the CHARTD Radiation- Hydrodynamics Code II: A Revised Program", SC-RR-710713, Sandia National Laboratories (1972).
- Thompson S. L., "CSQ – A Two-Dimensional Hydrodynamic Program with Energy Flow and Material Strength", SAND74-0122, Sandia National Laboratories (1975).