

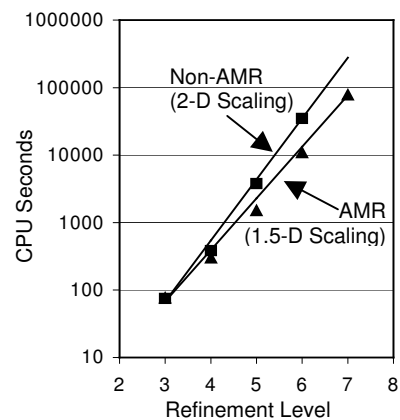
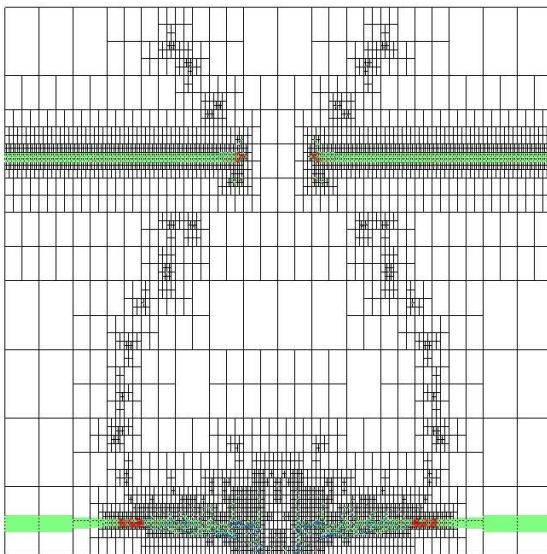
Adaptive Mesh Refinement and Multi-Phase Flow in the CTH

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Sandia has been developing a multi-material, multi-dimensional Eulerian shock physics analysis package known as CTH for almost 20 years. CTH was the natural progression from earlier one- and two-dimensional tools (CHARTD and CSQ). It started life as a serial-vector code best suited for use on Cray supercomputers. Shared memory parallelism (on a DO loop level) was added due to advances in computing capabilities in the early 1990s. When distributed data parallelism became practical in the mid 1990's, CTH was extensively modified to work in a data parallel environment. As computing hardware and software continue to improve our development emphasis has switched to improving the physics used in simulations. In this regard, we have implemented an adaptive mesh refinement scheme into and a multi-phase reactive flow model into CTH. The coupling of these two new capabilities allow use to address a new class of diffusion limited mixing problems where gas dynamics and shock physics play equal roles.

Adaptive mesh refinement (AMR) has been widely hailed for improving computational resolution when resources are limited and has been used for hyperbolic problems on an experimental basis for years. 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. It is a capability that allows full exploitation of today's limited computational resources and efficient use of tomorrow's substantial resources.

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. The refinement is isotropic with a maximum 2:1 resolution difference across block boundaries. Blocks are not allowed to overlap. In multiprocessor calculations, blocks are dynamically load-balanced among processors and CPU usage is optimized.



An example (see above) using the AMR feature in CTH shows a two-dimensional calculation of a copper ball striking a steel bumper shield. On the left, the outline of each block (6x12 cells per block) is shown. To perform this calculation without AMR would require 1.2 million cells. Including ghost cells, this seven level AMR calculation requires 277,312 cells. On the right, the CPU time required to perform this calculation with and without AMR at 5 different refinement levels is shown (each increment in refinement level equals a factor of two in linear resolution).

A multiphase continuum mixture theory has been developed that couples the mechanical response, damage evolution, and combustion of energetic materials. In addition to coupling the mechanical and reactive behavior of energetic materials, it can also treat a differential velocity due to phase separation. This coupled damage and reaction model is demonstrated to capture shock-to-detonation transition and deflagration-to-detonation transition. The modeling approach has also been demonstrated to simulate delayed detonation for rocket propellants and to investigate the violence of reaction in thermal explosion experiments. The multiphase mixture model couples the mechanical response and the dynamic damage evolution with combustion. The continuum mixture theory formulation allows for a thermodynamically consistent mathematical representation of the condensed-phase energetic material and the fluid-phase reaction products. A key aspect to applying this model is the specification of the phase interactions (i.e., mass, momentum, and energy source terms) in a manner consistent with the second law of thermodynamics. Discussions of this application of the multi-phase framework and AMR to advanced combustion model development will be discussed.

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