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CTH: A Software Family for Multi-Dimensional Shock Physics Analysis

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Abstract. CTH is a family of codes developed at Sandia National Laboratories for modelling complex multi-dimensional, multi-material problems that are characterized by large deformations and/or strong shocks. A two-step, second-order accurate Eulerian solution algorithm is used to solve the mass, momentum, and energy conservation equations. CTH includes models for material strength, fracture, porous materials, and high explosive detonation and initiation.

Viscoplastic or rate-dependent models of material strength have been added recently. The formulations of Johnson-Cook, Zerilli-Armstrong, and Steinberg-Guinan-Lund are standard options within CTH. These models rely on the use of an internal state variable (typically the equivalent plastic strain) to account for the history dependence of material response. The implementation of internal state variable models will be discussed and several sample calculations will be presented. Comparison with experimental data will be made among the various material strength models. The advancements made in modelling material response have significantly improved the ability of CTH to model complex large-deformation, plastic-flow dominated phenomena.

The detonation of energetic material under shock loading conditions has been an area of great interest. A recently developed model of reactive burn for high explosives (HE) has been added to CTH. This model along with newly developed tabular equations-of-state for the HE reaction by-products has been compared to one- and two-dimensional explosive detonation experiments. These comparisons indicate excellent agreement of CTH predictions with experimental results. The new reactive burn model coupled with the advances in equation-of-state modeling make it possible to predict multi-dimensional burn phenomena without modifying the model parameters for different dimensionality. Most current burn models do not accurately predict both one-dimensional plate acceleration experiments and two-dimensional cylinder expansion experiments simultaneously. Our implementation is significant because it represents the first time a multi-dimensional model has been used to successfully predict multi-dimensional detonation effects without requiring a modification of the model parameters.

Examples of the features of CTH will be given. The emphasis in simulations shown will be in comparison with well characterized experiments covering key phenomena of shock physics.

Key Words: CFD, Shock Physics

1. Introduction

The CTH (McGlaun et al. 1990) software family is a complete package for the initialization, integration through time, and visualization of complex phenomena surrounding shock physics. The classes of problems that can be analyzed with CTH include penetration and perforation, compression, high explosive detonation and initiation phenomena, and hypervelocity impact. The software family currently consists of six major components along with several graphics post-processing tools. The major components are CTHGEN which sets up the initial configuration of the problem; CTHREZ which allows the user to rezone a problem and/or combine two or more problems into one; CTH which does the time integration on the conservation equations; CTHED which allows the user to query the problem data base for detailed cell-level information; CTHPLT which allows the user to produce black-and-white or color graphics at a given time of all computational and secondary variables; and HISPLT which allows the user to produce black-and-white or color graphics of all computational and secondary variables as a function of time.

A detailed description of CTH will be given in the next sections followed by a description of two simulations. The first CTH simulation is of a typical two-dimensional impact that demonstrates the effect of strain-rate dependent constitutive behavior. The second CTH simulation is one that is more typical of gas dynamics and demonstrates the use of exact solutions in the validation of large scale "hydrocodes".

CTH uses an Eulerian mesh to solve the conservation equations. Six geometry options are available in CTH: one-dimensional rectangular, cylindrical, and spherical; two-dimensional rectangular, and cylindrical; and three-dimensional rectangular. Up to ten materials and void can occupy a computational cell, although the maximum number of materials can be changed by modifying a single Fortran parameter statement. In general, all internal dimensions are controlled by Fortran parameter statements and can be easily modified by rebuilding the appropriate program or programs.

The conservation equations of mass, energy, and momentum are replaced by finite volume approximations. For those cases where exact conservation of mass, momentum, and energy is not possible, the user is allowed to control how the differences are rectified.

The mesh is generated from three sets of user specified spatial coordinates *x(i)*, *y(j)*, and *z(k)* which are logically connected. All quantities are cell centered except the velocities which are face centered. All cell-centered quantities are assumed to be constant across the cell. CTH uses a staggered mesh for the solution of the momentum conservation equation. However, this technique has been recently modified by including a method developed by Benson (1991) that advects face-centered quantities with a cell-centered algorithm. It has been found that the cell-centered solution technique for the momentum equation has simplified the numerical algorithms and improved the predictions of CTH.

2. Solution Scheme

Eulerian codes like CTH use a mesh that is fixed in space, and material flows through the mesh in response to boundary and initial conditions. The conservation equations are solved in two steps, a Lagrangian step and a remap step. In the Lagrangian step, the Lagrangian forms of the governing equations are integrated across a timestep. The initial mesh distorts to follow the material motions and there is no mass flux across the cell boundaries. After the Lagrangian step, the remap step is performed. During the remap step, the distorted cells are remapped back to the initial fixed mesh. CTH also allows for a third step called the data base modification step. This step gives the user an opportunity to modify the data base in a few select cases.

The volume, mass, momentum, and energy must be conserved across the Lagrangian step. The mass is conserved trivially because the mesh moves with the material during the Lagrangian step and no mass crosses the cell boundaries. The remaining conservation equations are replaced with explicit finite volume representations of the original integral equations. Although the explicit equations are solvable, the time step must be controlled to prevent information from crossing more than one cell during a single timestep. The timestep is the minimum of a CFL condition derived by Hicks (1977) and a cell-volume change limiting step. The volume change limit prevents excessive compression or expansion of a cell.

An area of considerable interest is the modelling of material strength. As Eulerian shock physics codes are increasingly used for modelling relatively low speed impacts, the emphasis has switched from equation-of-state issues to details of material response. A linearly-elastic perfectly-plastic material strength model is available. This model has two yield surface options: a von Mises (constant) yield surface and a pressure dependent yield surface. Both surfaces limit the second invariant of the stress deviator. The pressure dependent surface has low strength at low pressure and increasing strength as the pressure increases. Both models have thermal softening and low density degradation corrections available to the user.

In addition to the simple elastic plastic model, three rate-dependent viscoplastic models are available in CTH: Johnson and Cook (1985), Zerilli and Armstrong (1987), and Steinberg et al. (1980). All of these models utilize complex functional forms of the yield surface which depends on both the local material state and some information about the history or rate-dependent state of the material. Complete descriptions of the functional forms are available in the noted references. The model of Johnson et al. (1990) describing the phenomena of brittle material failure is also available in CTH. This model replaces the normal CTH equation-of-state options with an internal description of the thermal response of the material.

Strength in compression is only one aspect of material response that is important for many of the current applications of CTH. Material fracture can also be critical in making accurate predictions. CTH has historically used a void insertion model to simulate failure. This model monitors the tensile state of a cell and relieves that tension by adding void. The model allows the user to select either pressure or principal stress as the criteria for tension relief. This technique is adequate to predict material failure due to hydrodynamic spall, but does not predict failure due to shear phenomena or large strains. An equivalent plastic strain based model of Johnson and Cook (1985) has been implemented in CTH. This model predicts failure due to shear deformation. The model is coupled with the void insertion model through the user specified cut-off tensile pressure or stress. If the user requests the Johnson-Cook fracture model, the user specified value for the maximum tension that can be supported is degraded by the fraction of failed material. As the failure due to shear deformation increases, the amount of tension that a cell can support decreases until the cell can support no tension. At this point the material has completely failed and will act like a fluid. Limited testing with this model indicates that it is stable and predicts reasonable results, but further testing is required.

A three term artificial viscosity is used to control the discontinuity associated with shocks and other instabilities. The form used to control shocks is a vector subset of the full viscosity tensor with linear and quadratic terms. The vector includes the diagonal elements *xx*, *yy*, and *zz*. The third viscosity term is linear and controls a singular point in the update of the stress deviators at the axis-of-symmetry for the two-dimensional cylindrical geometry option. Shear viscosity has been found to control non-physical oscillations sometimes seen in normal penetration simulations.

There are three high explosive detonation models in the production version of CTH. The oldest is the programmed burn model, which is appropriate for simple detonations where the initiation time and location

is well known. This model automatically calculates the appropriate amount of energy to be deposited in each cell of high explosive at the correct time. The two additional models are capable of modelling the shock initiation, as well as the detonation of high explosives. They are the Chapman-Jouguet and History Variable Reactive Burn models (Kerley 1992). Both of these models rely on the use of an internal state variable to monitor the reaction parameters of the high explosive initiation.

All of the models discussed above are applied during the Lagrangian step. After this step, the velocities, energies, stress deviators, and any internal state variables must be remapped back to the initial mesh. It is during the remap step where much of the cpu time is consumed and where numerical intricacies are important.

The remap step advects the appropriate mass, momentum, energy, and volume from the deformed mesh of the Lagrangian step to the original mesh. The volume flux between the old and new cells is calculated first. An interface tracking algorithm then decides which materials in the old cells are moved with the volume flux. Next, each material's mass and internal energy are moved from the old to the new cells. Finally, the momentum and kinetic energy are moved using the information from the interface tracker.

Operator splitting techniques are used to preform the multi-dimensional remap operation. The resulting one-dimensional convection equations use a second-order accurate conservative scheme developed by van Leer (1977). The scheme used in CTH replaces a uniform distribution in the old cell with a linear distribution. To reduce the asymmetry resulting from the operator splitting, a permutation scheme in direction is applied.

The volume flux is calculated from the geometry of the cell-face motion. Once that is calculated, the volume of materials to be advected must be estimated. The interface reconstruction algorithms are used to estimate the amount of each material to be advected. Two interface reconstruction algorithms are available in CTH. The Simple Line Interface Calculation scheme developed by Noh and Woodward (1976) is available for all geometries. This technique is exact for one-dimensional geometries and effectively first-order for other geometries. A higher resolution (second order) interface reconstruction scheme developed by McGlaun et al. (1990) is also available for two-dimensional geometries.

In most formulations of the momentum advection equation, a staggered mesh is constructed in space and time. The staggered mesh is only used to advance the face-centered (velocity) variables for use by the next Lagrangian step. The staggered mesh requires additional storage and a second and different formulation of the difference equations for momentum advection. A technique developed by Benson (1991) has been recently implemented in CTH as a part of other upgrades. This technique maps the portions of the face-centered information to cell-centered locations and then performs the advection on the cell-centered data. The method requires advection of twice as much information but reduces the complexity of the advection scheme significantly. Figure 1 displays a schematic of the process. The first step is to map the respective

Figure 1. Cell Centered Momentum Advection Scheme

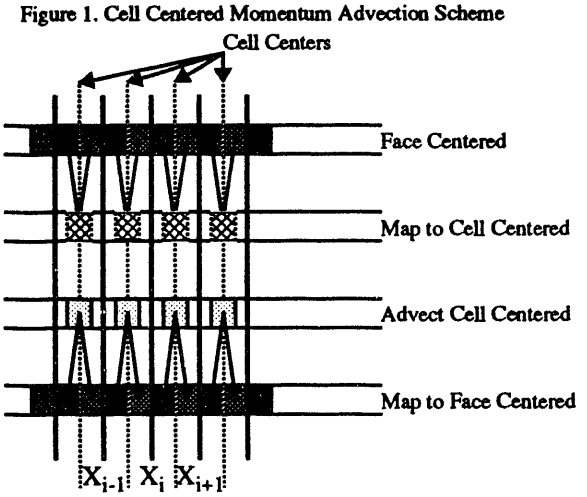
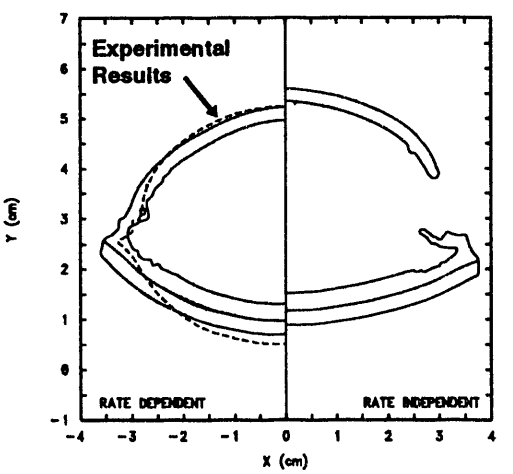


Figure 2. Strain Rate Dependent Material Deformation



halves of the momentum to the adjacent cell-centers. The step leaves two pieces of data at the cell-centers for advection. The second step advects the new cell-centered data using the normal advection algorithm for cell-centered data. After the advection step is complete, the separate halves of the cell-centered momentum is mapped back to the face locations and a face-centered velocity is calculated. This technique has been found to be very effective and guarantees that the accuracy of the advection scheme is maintained and has

the additional benefit of also being a monotone scheme.

The three basic variables of mass, momentum, and kinetic energy are calculated from two data base quantities: mass and velocity. As a result, the three basic variables cannot all be conserved across the remap step. The options available to the user to account for the non-conservation of both the momentum and kinetic energy are: 1) the momentum is conserved and any kinetic energy discrepancy is transformed into an internal energy source or sink; 2) the kinetic energy is conserved and the momentum is not; 3) the momentum is conserved and the kinetic energy is discarded in all cases except if the momentum fluxed into the new cell has the opposite sign as that cell. In this case, the energy is deposited into internal energy. The third option is conceptually similar to an inelastic collision and generally gives the best results.

The final stage of the remap step has to do with fragments smaller than a computational cell. These cannot be placed by the interface reconstruction algorithms since no portion of that object is known to intersect a boundary. CTH assigns a random location to the fragment's center of mass. Once the center of mass is known, its future location is simple to determine. Using this model, the fragments move through the mesh with the correct statistical velocity. If a fragment subsequently impacts another object, the correct impulse is imparted to that object. As with most options within CTH, the user can control the advection of fragments smaller than a computational cell. At this point, the simulation has advanced one timestep and can be continued.

The CTH software family allows the user two options to modify the simulation during execution. The user can discard unwanted material from the spatial domain. Current options include spatial, temporal, and data base variable (pressure, density, and temperature) filters. This option is particularly useful for removing the low pressure and density gas that results from high explosive detonation. This gas quickly fills the computational mesh and has little effect on the evolution of most simulations. The second option allows the user to apply a velocity transformation to the mesh (moving mesh option). Many simulations (explosively-formed-projectile and debris formation) require an object or objects to translate through the computational mesh. This typically requires the user to add mesh to allow for the translation. Appropriate use of the velocity transformation can significantly reduce the meshing requirements for many simulations.

3. Equations-of-State

Strong shock simulations require sophisticated and accurate models of the thermodynamic behavior of materials. Phase changes, nonlinear behavior, and fracture can be important for accurate predictions. CTH has two major equation-of-state packages available to the user: the Analytic Equation-of-State (ANEOS) package of Thompson and Lauson (1972) and the SNL-SESAME package of Kerley (1991).

The ANEOS package uses a Helmholtz potential to calculate the internal energy as a function of mass density and temperature. The use of a Helmholtz potential assures thermodynamic consistency. The ANEOS package allows for three-phase (liquid-vapor, liquid-solid, and solid-vapor) equations-of-state. In addition to the multi-phase analytic forms, there are three simple analytic expressions within the ANEOS package. Expressions for a linear U_s-u_p (Mie-Gruneisen), Jones-Wilkins-Lee, and ideal gas equations-of-state are subsets of the multi-phase analytic forms. The drawbacks of the ANEOS package are that it can be difficult for the novice to parameterize and is computationally inefficient.

The SNL-SESAME package is based on the SESAME tabular equation-of-state representation. The tabular form allows the equation-of-state to be as sophisticated as the information contained in the table. The tabular representations may contain multiple liquid-vapor, liquid-solid, and solid-solid transitions whereas, ANEOS is restricted to at most three. Table look-up schemes can be made very efficient on vector and parallel computers. Once the tables have been constructed, they are accessible to all users. In addition to the tabular representations, analytic forms for linear U_s-u_p (Mie-Gruneisen), Jones-Wilkins-Lee, and ideal gas equations-of-state are also available. The SNL-SESAME package contains two models that can be used to represent porous media. A "two-state" model can be used to model reversible compaction and the p-α model can be used for irreversible compaction.

4. Multi-Material Cell Thermodynamics

Each computational cell can contain up to ten materials and void. The thermodynamic state of the cell must be determined from the volume, energy, and mass of the constituent materials. If only one material occupies the cell, the determination of the thermodynamic state is straight forward. If many materials occupy the cell, the determination of the thermodynamic state is more complicated. Three models are currently available. The first model assumes that all materials in a cell are at the same temperature and pressure. Complex non-linear algebraic equations govern the energy partition for this model. These equations are solved by a multi-variable Newton's iteration. There are several drawbacks associated with this model.

It exhibits unrealistic energy flows from hot to cold materials. Also, solid material in a cell containing vapor will not fracture because no tension can be supported. In addition, the iterations can be extremely time consuming.

The second model allows all materials to have different temperatures but identical pressures. In general, this model is superior to the previous model described above but also has deficiencies. In some circumstances, cells containing solid and vapor can unrealistically partition energy between the solid and vapor leading to extreme temperatures in the vapor. This model also suppresses fracture in solid/vapor cells.

The third model allows all materials to have different temperatures and pressures. Cell quantities for this model are volume weighted averages of the constituent materials. The principal deficiency of this model is that there is no pressure relaxation feature for mixed material cells. In general, this model is the simplest computationally and gives the best results.

5. CTH Simulations

The first simulation discussed here is a problem that describes material deformation and failure that is inherently two-dimensional and requires a model that describes rate dependent constitutive behavior. The initial conditions for this simulation consist of a stationary 6 mm thick tantalum disk and a 3 mm thick tantalum disk that is traveling at 403 m/s. The CTH initial conditions are a simplification of an actual experimental configuration. Both target and projectile are 740 mm in diameter. The axis-symmetric geometry option with square zoning of 0.02 X 0.02 cm was chosen to represent the experimental conditions.

Since tantalum is known to possess significant rate dependent constitutive behavior, the Steinberg-Guinan-Lund model was chosen to represent the material. To assess the effect of rate dependent behavior, two simulations were completed, one with the full rate dependent treatment and one with the rate term set to zero. Figure 2 displays the results of the two simulations. The right hand half of Figure 2 displays the terminal state of the target disk 170 μs after impact when the rate dependent term was set to zero. The left hand side of Figure 2 displays the target disk at the same time when the full rate dependent model was used. A digitized cross section from the experiment is also shown (as a dashed line) on Figure 2. One can readily see the effect of the strain-rate hardening that the Steinberg model predicts. On the right hand side of Figure 2, the material does not possess adequate strength to resist the shear forces that are deforming the target. The disk thins and finally separates at the margin. When the full rate-dependent model is applied (see Figure 2, left side), the additional strength though strain hardening is sufficient to resist the shear forces at the margin of the disk. In the second case, the agreement with the experimental result is excellent. None of the experimental targets were sectioned, so comparisons of the internal structure are not possible.

The second simulation discussed here is the classic shock tube or Sod (1978) problem. This problem consists of a one-dimensional shock tube in which a higher density and pressure ideal gas is allowed to expand into a lower pressure and density ideal gas. For this simulation, the initial conditions are shown in Figure 3. This problem is a classical Riemann problem where an exact solution can be derived as long as

Figure 3. Sod Problem Initial Conditions

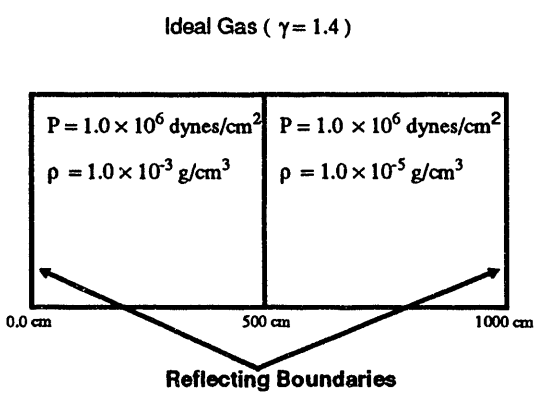
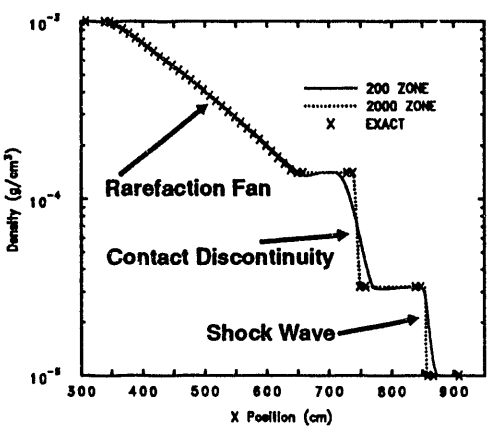


Figure 4. Sod Problem Solutions



the generated waves do not interact with the boundaries. In addition, it is a standard test problem for shock

physics models because three typical wave structures—a rarefaction fan, a contact discontinuity, and a shock wave occur in the simulation. Figure 4 displays the density field for 200 and 2000 zone CTH simulations as compared to the exact solution. Both CTH simulations are accurate representations of the exact solutions, although the 2000 zone simulation is obviously more accurate. The 200 zone simulation is of principal interest since that represents a typical domain size for two-dimensional simulations and is close to the upper limit for three-dimensional domains. The 200 zone CTH simulation has a small amount of post-contact discontinuity ringing as seen the particle velocity plot. Both the contact discontinuity and the shock are slightly smeared by the diffusion in the advection scheme and the artificial viscosity, respectively. Both of these effects are substantially reduced in the higher resolution simulation.

Both of the simulations shown here demonstrate the effectiveness of the numerical schemes and mechanical models embodied in CTH. It has been shown to possess state of the art numerical treatments and models to represent the mechanical and energetic behavior of materials and can be used to predict a wide variety of shock based phenomena.

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