DRACO development for 3D Simulations

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Summary

Abstract

The Draco (r-z) lagrangian radiation-hydrodynamics laser fusion simulation code is being extended to model 3D hydrodynamics in (x-y-z) coordinates with hexahedral cells on a structured grid. The equation of motion is solved with a Lagrangian update with optional rezoning. The fluid equations are solved using an explicit scheme based on (Schulz, 1964) while the SALE-3D algorithm (Amsden, 1981) is used as a template for computing cell volumes and other quantities. A second order rezoner has been added which uses linear interpolation of the underlying continuous functions to preserve accuracy (Van Leer, 1976). Artificial restoring force terms and smoothing algorithms are used to avoid grid distortion in high aspect ratio cells. These include alternate node couplers along with a rotational restoring force based on the Tensor Code (Maenchen, 1964). Electron and ion thermal conduction is modeled using an extension of Kershaw's method (Kershaw, 1981) to 3D geometry. Test problem simulations will be presented to demonstrate the applicability of this new version of DRACO to the study of fluid instabilities in three dimensions.

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Summary of Results

Hydrodynamics

- A second order rezoner has been implemented in DRACO to provide more accurate rezoning
- Artificial smoothing forces have been added to damp out 2dx instabilities in high aspect ratio zones
- An example calculation is presented which demonstrates DRACO's ability to model fluid instabilities

Thermal Transport

- Kershaw's method has been extended to 3D
- Provides first order accurate thermal transport on non-orthogonal grids
- Several calculations are presented comparing DRACO's thermal transport to analytic results

Future Work

Validate new models in realistic simulations

Add 3D Radiation Transport

- 3D Implicit Monte Carlo Radiation Transport
  Radiation diffusion using Kershaw's Method

Add 3D Particle Transport

- Monte Carlo Alpha Particle Transport
- Alpha Particle Diffusion

Parallelize 3D Code

- Domain Decomposition

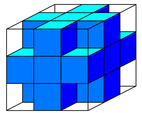
Kershaw 3D Thermal Diffusion

Extension of Kershaw's Method to 3D

- DRACO implements an implicit method for solving the thermal diffusion equation shown below

$$\rho C_v \frac{\partial T}{\partial t} = \nabla \cdot D \nabla T$$

- To achieve first order accuracy on a non-orthogonal grid, a 19-point finite difference scheme is required



- A set of finite difference equations based on Kershaw's method has been derived and added to DRACO

Defining the Matrices

- The matrix B is defined as shown below:

$$\begin{aligned}(Bf)_{K,L,M} = &\Sigma_{K,L,M}\left(f_{K+1,L,M} - f_{K,L,M}\right)\vec{R}_K^{\prime} \\ &+ \Lambda_{K,L,M}\left(f_{K,L+1,M} - f_{K,L,M}\right)\vec{R}_L^{\prime} \\ &+ \Gamma_{K,L,M}\left(f_{K,L,M+1} - f_{K,L,M}\right)\vec{R}_M^{\prime}\end{aligned}$$

- The variables Σ, Γ, and Λ are representations of the term $\sqrt{\frac{D}{j}}$ averaged over different faces of a zone.
- There are eight equally valid representations of the matrix B. These are averaged together to determine A

$$\sum_{K,L,M} f_{K,L,M}\left(Af\right)_{K,L,M} V_{K,L,M} = -\frac{1}{8}\sum_{i=1}^{8}\sum_{K,L,M}\left(B^i f\right)_{K,L,M}$$

Finite Difference Equations

$$\begin{aligned}V_{K,L,M}A_{(K,L,M)(K-1,L+1,M)} = &-\frac{1}{2}\left\{\Sigma_{K-1,L+1,M}\lambda_{K,L,M}(R_K)_{K,L+1,M}(R_L)_{K,L+1,M}\right. \\ &\left.+\Lambda_{K-1,L,M}\Sigma_{K-1,L,M}(R_K)_{K-1,L,M}(R_L)_{K-1,L,M}\right\}\end{aligned}$$

$$\begin{aligned}V_{K,L,M}A_{(K,L,M)(K-1,L,M+1)} = &-\frac{1}{2}\left\{\Sigma_{K-1,L,M+1}\Gamma_{K,L,M}(R_K)_{K,L,M+1}(R_M)_{K,L,M+1}\right. \\ &\left.+\Sigma_{K-1,L,M}\Gamma_{K-1,L,M}(R_K)_{K-1,L,M}(R_M)_{K-1,L,M}\right\}\end{aligned}$$

$$\begin{aligned}V_{K,L,M}A_{(K,L,M)(K,L,M)} = &-\Sigma_{K,L,M}^2(R_K)_{K+1,L,M}^2 - \Lambda_{K,L,M}^2(R_L)_{K,L+1,M}^2 - \Gamma_{K,L,M}^2(R_M)_{K,L,M+1}^2 \\ &-\Gamma_{K,L,M-1}^2(R_M)_{K,L,M-1}^2 - \Lambda_{K,L-1,M}^2(R_L)_{K,L-1,M}^2 - \Sigma_{K-1,L,M}^2(R_K)_{K-1,L,M}^2 \\ &-\left(\Gamma_{K,L,M}^2 + \Gamma_{K,L,M-1}^2\right)(R_M)_{K,L,M}^2 \\ &-\left(\Lambda_{K,L,M}^2 + \Lambda_{K,L-1,M}^2\right)(R_L)_{K,L,M}^2 \\ &-\left(\Sigma_{K,L,M}^2 + \Sigma_{K-1,L,M}^2\right)(R_K)_{K,L,M}^2 \\ &+\left(\Gamma_{K,L,M-1} - \Gamma_{K,L,M}\right)\left(\Lambda_{K,L,M} - \Lambda_{K,L-1,M}\right)(R_L)_{K,L,M}(R_M)_{K,L,M} \\ &+\left(\Gamma_{K,L,M-1} - \Gamma_{K,L,M}\right)\left(\Sigma_{K,L,M} - \Sigma_{K-1,L,M}\right)(R_K)_{K,L,M}(R_M)_{K,L,M} \\ &+\left(\Lambda_{K,L-1,M} - \Lambda_{K,L,M}\right)\left(\Sigma_{K,L,M} - \Sigma_{K-1,L,M}\right)(R_K)_{K,L,M}(R_L)_{K,L,M}\end{aligned}$$

Diffusion Operator

The diffusion operator is first re-written in terms of the continuous variables K, L, and M, as shown below, where subscripts denote derivatives:

$$\begin{aligned}\nabla \cdot D\nabla f = \frac{1}{j}\Bigg\{&\left(\frac{D}{j}\vec{R}_K{}^2 f_K\right)_K + \left(\frac{D}{j}\vec{R}_L{}^2 f_L\right)_L + \left(\frac{D}{j}\vec{R}_M{}^2 f_M\right)_M + \\ &\left(\frac{D}{j}\vec{R}_K \cdot \vec{R}_L f_K\right)_L + \left(\frac{D}{j}\vec{R}_L \cdot \vec{R}_K f_L\right)_K + \left(\frac{D}{j}\vec{R}_K \cdot \vec{R}_M f_K\right)_M + \\ &\left(\frac{D}{j}\vec{R}_M \cdot \vec{R}_K f_M\right)_K + \left(\frac{D}{j}\vec{R}_L \cdot \vec{R}_M f_L\right)_M + \left(\frac{D}{j}\vec{R}_M \cdot \vec{R}_L f_M\right)_L\Bigg\}\end{aligned}$$

where,

$$\vec{R}_K^{\prime} = \begin{pmatrix} y_L z_M - y_M z_L \\ z_L x_M - z_M x_L \\ x_L y_M - x_M y_L \end{pmatrix},\ \vec{R}_L^{\prime} = \begin{pmatrix} y_M z_K - y_K z_M \\ z_M x_K - z_K x_M \\ x_M y_K - x_K y_M \end{pmatrix},\ \vec{R}_M^{\prime} = \begin{pmatrix} y_K z_L - y_L z_K \\ z_K x_L - z_L x_K \\ x_K y_L - x_L y_K \end{pmatrix}$$

and,

$$j = \det\begin{pmatrix} x_K & y_K & z_K \\ x_L & y_L & z_L \\ x_M & y_M & z_M \end{pmatrix}$$

The Finite Difference Equations

- Once the B matrices are determined, the finite difference equations can be found using the following relation

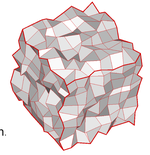
$$VA = -\frac{1}{8}\sum_{i=1}^{8}\left(B^i\right)^T \cdot \left(B^i\right)$$

- Due to the size and number of terms involved in performing this operation, a symbolic equation manipulator was used.
- Only 10 of the 19 non-zero matrix elements are presented. The other elements can be determined by the symmetry of A

$$\begin{aligned}V_{K,L,M}A_{(K,L,M)(K+1,L,M)} = &-\frac{1}{2}\Sigma_{K,L,M}\left\{-2\Sigma_{K,L,M}\left((R_K)_{K+1,L,M}^2 + (R_K)_{K,L,M}^2\right)\right. \\ &+\left(\Gamma_{K+1,L,M} - \Gamma_{K+1,L,M-1}\right)(R_K)_{K+1,L,M}(R_M)_{K+1,L,M} \\ &+\left(\Gamma_{K,L,M-1} - \Gamma_{K,L,M}\right)(R_K)_{K,L,M}(R_M)_{K,L,M} \\ &+\left(\Lambda_{K+1,L,M} - \Lambda_{K+1,L-1,M}\right)(R_K)_{K+1,L,M}(R_L)_{K+1,L,M} \\ &\left.+\left(\Lambda_{K,L-1,M} - \Lambda_{K,L,M}\right)(R_K)_{K,L,M}(R_L)_{K,L,M}\right\}\end{aligned}$$

Non-Orthogonal Grid Calculations

- The following two calculations were run to compare DRACO to analytic results with constant conductivities
  1. Steady state solution to conduction between fixed temperature boundaries
  2. A delta function source in time and space
- The grid was generated by randomly perturbing points on an orthogonal mesh.



The Variational Method

- Using the above equation, an expression for the gradient operator can be obtained in terms of K, L, and M

$$\begin{aligned}\int f\nabla \cdot D\nabla f dxdydz &= -\int D(\nabla f)^2 dxdydz \\ &= \int\left[\sqrt{\frac{D}{j}}\left(\vec{R}_K^{\prime} f_K + \vec{R}_L^{\prime} f_L + \vec{R}_M^{\prime} f_M\right)\right]^2 dKdLdM\end{aligned}$$

- The matrix form is shown below, where A and B are the matrix representations of the diffusion and gradient operators, respectively.

$$\sum_{K,L,M} f_{K,L,M}\left(Af\right)_{K,L,M} V_{K,L,M} = -\sum_{K,L,M}\left(Bf\right)_{K,L,M}$$

Finite Difference Equations

$$\begin{aligned}V_{K,L,M}A_{(K,L,M)(K,L,M+1)} = &\frac{1}{2}\Gamma_{K,L,M}\left\{2\Gamma_{K,L,M}\left((R_M)_{K,L,M+1}^2 + (R_M)_{K,L,M}^2\right)\right. \\ &+\left(\Lambda_{K,L-1,M+1} - \Lambda_{K,L,M+1}\right)(R_L)_{K,L,M+1}(R_M)_{K,L,M+1} \\ &+\left(\Lambda_{K,L,M} - \Lambda_{K,L-1,M}\right)(R_L)_{K,L,M}(R_M)_{K,L,M} \\ &+\left(\Sigma_{K-1,L,M+1} - \Sigma_{K,L,M+1}\right)(R_M)_{K,L,M+1}(R_K)_{K,L,M+1} \\ &\left.+\left(\Sigma_{K,L,M} - \Sigma_{K-1,L,M}\right)(R_M)_{K,L,M}(R_K)_{K,L,M}\right\}\end{aligned}$$

$$\begin{aligned}V_{K,L,M}A_{(K,L,M)(K,L+1,M)} = &-\frac{1}{2}\Lambda_{K,L,M}\left\{-2\Lambda_{K,L,M}\left((R_L)_{K,L+1,M}^2 + (R_L)_{K,L,M}^2\right)\right. \\ &+\left(\Gamma_{K,L+1,M} - \Gamma_{K,L+1,M-1}\right)(R_L)_{K,L+1,M}(R_M)_{K,L+1,M} \\ &+\left(\Gamma_{K,L,M-1} - \Gamma_{K,L,M}\right)(R_L)_{K,L,M}(R_M)_{K,L,M} \\ &+\left(\Sigma_{K,L+1,M} - \Sigma_{K-1,L+1,M}\right)(R_L)_{K,L+1,M}(R_K)_{K,L+1,M} \\ &\left.+\left(\Sigma_{K-1,L,M} - \Sigma_{K,L,M}\right)(R_L)_{K,L,M}(R_K)_{K,L,M}\right\}\end{aligned}$$

$$\begin{aligned}V_{K,L,M}A_{(K,L,M)(K,L+1,M+1)} = &\frac{1}{2}\left\{\Lambda_{K,L,M}\Gamma_{K,L+1,M}(R_L)_{K,L+1,M}(R_M)_{K,L+1,M}\right. \\ &\left.+\Lambda_{K,L,M+1}\Gamma_{K,L,M}(R_L)_{K,L,M+1}(R_M)_{K,L,M+1}\right\}\end{aligned}$$

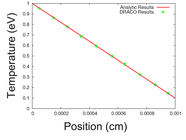
$$\begin{aligned}V_{K,L,M}A_{(K,L,M)(K-1,L,M+1)} = &-\frac{1}{2}\left\{\Lambda_{K,L-1,M+1}\Gamma_{K,L,M}(R_L)_{K,L,M+1}(R_M)_{K,L,M+1}\right. \\ &\left.+\Lambda_{K,L-1,M}\Gamma_{K,L-1,M}(R_L)_{K,L-1,M}(R_M)_{K,L-1,M}\right\}\end{aligned}$$

$$\begin{aligned}V_{K,L,M}A_{(K,L,M)(K+1,L+1,M)} = &\frac{1}{2}\left\{\Sigma_{K,L,M}\Lambda_{K+1,L,M}(R_K)_{K+1,L,M}(R_L)_{K+1,L,M}\right. \\ &\left.+\Lambda_{K,L,M}\Sigma_{K,L+1,M}(R_K)_{K,L+1,M}(R_L)_{K,L+1,M}\right\}\end{aligned}$$

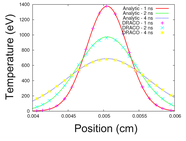
$$\begin{aligned}V_{K,L,M}A_{(K,L,M)(K+1,L,M+1)} = &\frac{1}{2}\left\{\Sigma_{K,L,M}\Gamma_{K+1,L,M}(R_K)_{K+1,L,M}(R_M)_{K+1,L,M}\right. \\ &\left.+\Sigma_{K,L,M+1}\Gamma_{K,L,M}(R_K)_{K,L,M+1}(R_M)_{K,L,M+1}\right\}\end{aligned}$$

Non Orthogonal Grid Calculations

Fixed Temperature Boundaries



Delta Function Source



Hydrodynamics

Lagrangian Fluid Dynamics

Higher Order Rezoner

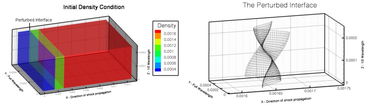
- The computational mesh can easily tangle during Lagrangian calculations
- To alleviate this problem, a second order rezoner has been added to DRACO in 3D
- The rezoner uses mesh point positions to linearly interpolate rezoned quantities within a cell
- This interpolation reduces the error associated with rezoning

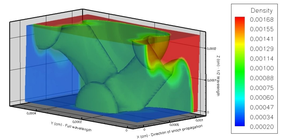
2dx Instabilities

- These numerical instabilities occur when low aspect ratio zones are encountered
- An alternate node coupler has been added to DRACO in 3D which smooths out instabilities by averaging velocities of nearby zones

Perturbation Calculation

- To demonstrate DRACO's fluid capabilities, an example problem has been run to simulate the Richtmyer-Meshkov instability
- Two regions containing a low and high density fluid are adjoined with a slightly perturbed interface
- A shock wave is then launched at the interface generating the instability



Perturbation Calculation

After the calculation has run for 150 ns, several bubbles can be seen forming at the interface between the two regions.