Computational Modeling of Dynamic Interfaces in Explosive Systems

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Awards/Honors/Recognitions

- Lana Šteković - NSF Fellowship award 2015 (Lana is completing her first year of PhD studies and was an ONR intern at NAVAIR China Lake)
- D. Scott Stewart, Shao Lee Soo Professorship, University of Illinois, 2013 to date
- D. Scott Stewart, Fellow of the American Society of Mechanical Engineering (ASME) 2015
- Sushil Koundinya, DOD "Smart Scholar" awarded 2013, working at AFRL/RW Eglin AFB, FL

PhD Students Supported on AFOSR Computational Mathematics

- **Brandon Lieberthal**, PhD Student, Detonation Shock Dynamics and Geometrical Shock Dynamics
- **Alberto Hernández**, PhD Student, numerical methods for multi-material simulations related to energetic materials
AFOSR Supported Journal Papers


2. Embedded particle size distribution and its effect on detonation in composite explosives, B. Lieberthal, D. S. Stewart, submitted to Combustion Theory and Modelling

3. Geometrical shock dynamics applied to condensed phase materials in heterogeneous explosives, B. Lieberthal, A. Hernández, D. S. Stewart, to be submitted


5. An explicit algorithm for imbedding internal boundaries in Cartesian grids, A. Hernández, J. B. Bdzil and D. S. Stewart, to be submitted
Metal Loaded High Explosives

• Condensed high explosives consist of a high energy explosive fluid embedded with binder, combustible additives, and inert (metal or plastic) particles.
• By embedding inert material in the fluid, we can control the pressure and sustainability of detonation waves.
• Allows for carefully tailored explosive devices

Microstructure of PBX 9501 pressed piece embedded with HMX [Skidmore, et al. 1998]
Detonation Wave Propagation

- Fluid flow governed by Euler conservation laws and Rankine-Hugoniot relations
- Inert particles are embedded in high explosive material
- Detonation wave front propagates normal to surface
- DSD Theory: Velocity of propagation dependant on curvature
  \[ D_n = D_{CJ}(1 - \alpha \kappa) \]  
  [Stewart, et al. 1988]
- Interested in wave front propagation pattern over long time scales (hundreds of particles)
Cylindrical Approximation of Unit Cell

- Particles arranged unto cubic unit cells
- Use cylinder of radius 0.5 as approximation for cube
- Assumption of axisymmetry allows 1D computation of level set
- **Computation time of order** $O \left( \frac{1}{dx} \right)$ rather than $O \left( \frac{1}{dx^3} \right)$
- Simulation over hundreds of unit cells in hours, not days
- Memory requirements negligible on modern computers

Animation of the simple cubic array model [Stewart, et al. 2009]
DSD Passover Cell

- Horizontal outflow boundaries on top and bottom of cell
- Symmetric conditions along the lateral boundaries to simulate horizontal stacking
- Input wave of current cell is output wave of previous cell
- Linear $D_n - \kappa$ relation implies a level set evolution equation:
  \[ D_n = -\frac{\psi_t}{|\nabla \psi|}, \kappa = \nabla \cdot \left( \frac{\nabla \psi}{|\nabla \psi|} \right) \]
  \[ D_n = D_{CJ} (1 - \alpha \kappa) \Rightarrow \]
  \[ -\psi_t = D_{CJ} |\nabla \psi| \left[ 1 - \alpha \nabla \cdot \left( \frac{\nabla \psi}{|\nabla \psi|} \right) \right] \]
- Project goal: accurately model shock propagation inside of inert sphere
Expanding Shock Wave in Inert Material

- Expanding wave governed by Euler conservation equations:
  - **Mass:** \( \frac{d\rho}{dt} + \rho \left( \frac{\partial u}{\partial r} + 2 \frac{u}{r} \right) = 0 \)
  - **Momentum:** \( \frac{du}{dt} + \frac{1}{\rho} \frac{\partial p}{\partial r} = 0 \)
  - **Energy:** \( \frac{d}{dt} (\rho e) + (\rho e + p) \frac{\partial u}{\partial r} = 0 \)

- Constitutive relation: \( e(p, \rho) \)

- **Objective:** describe expanding shock wave with \( \dot{D}_n - D_n - \kappa \) relation
Expanding Shock Wave in Inert Material

- Ideal gas: $e = \frac{p/p}{\gamma - 1}$
- Self similar properties allow for asymptotic solutions
- Taylor Blast Wave (high $\kappa$, $D_n$)
  \[ \dot{D}_n = -0.75 D_n^2 \kappa \]
- Geometrical Shock Dynamics (low $\kappa$, $D_n$)
  \[ \dot{D}_n = -c_0^2 \left( \frac{D_n}{c_0} \right)^2 \frac{1}{\lambda(D_n)} \kappa \]
Mie-Gruneisen Equation of State

• Constitutive relation:
  \[ e(p, \rho) = \frac{1}{\Gamma_0 \rho_0} \left[ p - \frac{\rho_0 c_0^2 \chi}{(1 - s \chi)^2} \left( 1 - \frac{\Gamma_0}{2} \chi \right) \right] \]
  \[ \chi = 1 - \frac{\rho_0}{\rho} \]

• Physical constants:
  \( \rho_0 \): inert density
  \( c_0 \): bulk speed of sound
  \( \Gamma_0 \): Gruneisen parameter
  \( s \): linear Hugoniot slope coefficient
Rankine-Hugoniot Equations

- Equations governing flow through shock front

  Mass Flux: \( u_1 = D_n \left( 1 - \frac{\rho_0}{\rho_1} \right) \)

  Momentum Flux: \( p_1 = \rho_0 u_1 D_n \)

  Energy Flux: \( e(p_1, \rho_1) = \frac{1}{2} p_1 \left( \frac{1}{\rho_0} - \frac{1}{\rho_1} \right) \)

- Solution for MG EOS:

  \( \rho_1 = \frac{D_n s \rho_0}{c_0 + D_n (s - 1)} \), \( u_1 = \frac{D_n - c_0}{s} \), \( p_1 = \frac{D_n (D_n - c_0) \rho_0}{s} \)

- Energy equation: \( e_1 = \frac{(D_n - c_0)^2}{2 s^2} \)
Strong Shock Limit

• In asymptotic limit of $D_n \gg c_0$:

$$e_1 \sim \frac{D_n^2}{2s^2} = \frac{p_1}{2(s-1)\rho_1}$$

• Euler equations become self-similar with characteristics $C = \frac{R}{t^{2/5}}$

• Taylor Blast Wave theory applies, so $\dot{D}_n - D_n - \kappa$ relation is

$$\dot{D}_n = -0.75D_n^2\kappa$$

• Note that shock wave must be extremely fast before this limit becomes relevant
Acoustic Limit

• In low curvature limit, Euler equations have a radial characteristic that governs flow behind the shock

\[ \frac{dp}{dr} + \rho c \frac{du}{dr} + \frac{\rho c^2 u}{u+c} \kappa = 0 \]

• Evaluated on the shock front in terms of \( D_n \), this equation becomes

\[ \left[ \frac{dp_1}{dD_n} + \rho_1 c_1 \frac{du_1}{dD_n} \right] \frac{1}{u_1+c_1} \frac{dD_n}{dt} + \frac{\rho_1 c_1^2 u_1}{u_1+c_1} \kappa = 0 \]

• Substituting the Rankine-Hugoniot solutions and solving for \( \dot{D}_n \), we find

\[ \dot{D}_n = -\frac{D_n(D_n-c_0)c_1^2 s}{2D_n^2(s-1)+D_n c_1 s+D_n c_0(3-s)-c_0^2} \kappa \]
Numerical Simulation Results for Aluminum

Simulation performed by NEWCODE of spherical expanding shock wave in aluminum

Transition from TBW to GSD state in dimensionless variables
DSD/GSD Hybrid Unit Cell

• **Objective**: complete simulation of aluminum sphere in PBX-N9 unit cell

• PBXN-9 properties:
  \[ D_{CJ} = 0.8559 \, \text{cm/\mu s} \]
  \[ \alpha = 0.07948 \, \text{cm} \]

• Aluminum sound speed
  \[ c_0 = 0.5328 \, \text{cm/\mu s} \]

• Interface boundary angles are computed by comparing to direct numerical simulation
• Simulation of detonation wave passing over five unit cells embedded with an aluminum sphere
• It takes about 6.2 μs for the wave to travel through the model
• Average effective propagation velocity is 0.81 cm/μs
• After initial unit cell, wave propagation pattern is almost perfectly periodic
HE: \[ P = \frac{\rho_0}{\gamma + 1} D_n^2 \]

Metal: \[ P = \frac{\rho_0 c_0}{s} D_n \left( \frac{D_n}{c_0} - 1 \right) \]

- Pressure is highest at regions of wave attachment and detachment
- Pressure inside sphere is initially high but decays to 0
- Profile consistent with experiments involving particle deformation
Comparison to Direct Numerical Simulation

- ALE3D: Numerical hydrodynamic solver from Lawrence Livermore National Laboratory
- Detonation triggered by CL-20 with programmed burn model
- PBXN-9 simulated with JWL reactive flow model
- Aluminum simulated with MG equation of state
- Visual comparison of unit cell test
Comparison of ALE3D and GSD Methods

My research
Hybrid shock dynamics
Computation time: 5 minutes

ALE3D software
Direct numerical simulation
Computation time: 8 hours
Future Work

• Rapid shock propagation simulations over arbitrary particle geometries

• Requires computation of level set function $\psi$ and velocity function $D_n$

• Intend to run DSD/GSD simulations on 2D slices of foam over arbitrary long time scales and observe variation in wave behavior

2D cross-section of aluminum foam cylinder

DSD simulation of an imported image of an airfoil [Hernández, et al. 2013]
Introduction to NEWCODE

- **NEWCODE**: 3D, TVD, compressible flow solver, fully parallel

- **Objective** – compressible mixing of high pressure and temperature jet fuel into ambient air

- A detonation driven mechanism compresses the jet fuel increasing pressure and temperature

- Reaction of the jet fuel follows an expansion of fuel into ambient air

- Comparable experiment by Professor Nick Glumac and his group at University of Illinois (UIUC)

- High speed video recording capturing the reaction

![Expansion phase of jet fuel]
### Test Case Numerical Simulation

<table>
<thead>
<tr>
<th>Time</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>t = 0</td>
<td>High pressure and high density gas (center) replicating the compressed jet fuel. Ideal gas EOS was applied.</td>
</tr>
<tr>
<td>t = 44.3 μs</td>
<td>High pressure gas expands outwards, forming a circular region with highest densities at outer edge</td>
</tr>
<tr>
<td>t = 710.8 μs</td>
<td>Jet fuel and air mix with the ideal gas reflecting off the walls causing vorticity</td>
</tr>
</tbody>
</table>
Intro to Numerical Approach

• Solving the 3D Reactive Euler equations

\[
\frac{\partial \mathbf{u}}{\partial t} + \frac{\partial \mathbf{f}(\mathbf{u})}{\partial x} + \frac{\partial \mathbf{g}(\mathbf{u})}{\partial y} + \frac{\partial \mathbf{h}(\mathbf{u})}{\partial z} + \mathbf{S} = 0
\]

with,

\[
\mathbf{u} = \begin{bmatrix} \rho \\ \rho u \\ \rho v \\ \rho w \\ \rho E \\ \rho \lambda \end{bmatrix}, \quad \mathbf{f} = \begin{bmatrix} \rho u \\ \rho u^2 + p \\ \rho uv \\ \rho uw \\ u (\rho E + p) \\ \rho u \lambda \end{bmatrix}, \quad \mathbf{g} = \begin{bmatrix} \rho v \\ \rho v^2 + p \\ \rho vw \\ \rho wv \\ v (\rho E + p) \\ \rho v \lambda \end{bmatrix}, \quad \mathbf{h} = \begin{bmatrix} \rho w \\ \rho wu \\ \rho wv \\ \rho w^2 + p \\ w (\rho E + p) \\ \rho w \lambda \end{bmatrix}
\]

and \( \mathbf{S} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \rho r \lambda \end{bmatrix} \)

\[
E = \rho e + \frac{1}{2} \rho (u^2 + v^2 + w^2)
\]

• Developing a multi-material model of expanding fuel into air, meanwhile defining each material with a different EOS
NEWCODE: Multi-material Reactive Euler Solver

• **Solid boundaries** – Developed a novel point-wise scheme to enforce reflective boundaries of arbitrary shapes. A stationary level set, $\Psi$, is used to describe the boundary (applied to DSD problems [Hernández et. al, 2013]).

• **Multi-material** – Adopted the Ghost-Fluid Method with density extension [Stewart et. al, 2007][Fedkiw et. al, 1999], and used a narrow banded level set, $\phi$, to represent the interface between the air and jet fuel.

![Level set convention applied to a horse internal boundary](image1)

![Narrow band](image2)

![Fuel/air domain for the multi-material simulation](image3)
Numerical Methods: Point-wise Reflective Boundaries

Why are the IB nodes coupled?

Typically in the past, an iterative approach has been used to set the IB nodes (i.e: point Jacobi, Gauss-Siedel, SOR) [Xu et. al, 1997][Stewart et. al 2007]
Numerical Methods: Point-wise Reflective Boundaries

Simplifying the algorithm resulting in a **local and fully explicit** scheme by breaking the IB node interdependence

Resulting in the following advantages

- No need for an iterative solve, instead we use simple function evaluations to set IB node
- No convergence and tolerance criteria
- Local scheme
- Improved parallel performance using MPI (reduced parallel overhead)

Priority 0 (**circles**): no other IB nodes in their interpolation stencils

Priority 1 (**squares**): one or more Priority 0 IB nodes in the interpolation stencil

Priority 2 (**triangles**): one or more Priority 0 or 1 IB nodes in the interpolation stencil
Numerical Methods: Point-wise Reflective Boundaries

Case (a): just use bilinear interpolation on each state variable

Case (b): Here the interpolation stencil includes the IB node which is being set.

For momentum we end up with a system of 4 equations

\[
\phi_{IB}^u = P_u - 2\psi_u \frac{\vec{\psi} \cdot \vec{P}}{||\vec{\psi}||^2}
\]

\[
\phi_{IB}^v = P_v - 2\psi_v \frac{\vec{\psi} \cdot \vec{P}}{||\vec{\psi}||^2}
\]

\[
\alpha P_u = \phi_{IB}^u N_{IB} + \sum_{i=1, i \neq IB}^{4} N_i \phi_i^u
\]

\[
\alpha P_v = \phi_{IB}^v N_{IB} + \sum_{i=1, i \neq IB}^{4} N_i \phi_i^v
\]

\[
N_1 = (x_2 - x_p)(y_2 - y_p)
\]

\[
N_2 = (x_p - x_1)(y_p - y_1)
\]

\[
N_3 = (x_2 - x_p)(y_p - y_1)
\]

\[
N_4 = (x_p - x_1)(y_p - y_1)
\]

\[
\alpha = (x_2 - x_1)(y_2 - y_1)
\]
Experimental Comparison

Top: Numerical density Schlieren plots

Bottom: Experimental density shadowgraph plots [Sivier et. al, 1993]
Experimental Comparison

- **a** - horizontal distance from the nose of the wedge to the reflected shock
- **r** - vertical distance from the midline of the wedge to the highest point of the reflected shock
- **vcx** - distance from the back of the wedge to the geometric center of the vortex
- **vcy** - distance from the midline of the wedge to the geometric center of the vortex

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**Primary Shock Structure Comparison**

![Graph showing primary shock structure comparison](image)

**Vortex Comparison**

![Graph showing vortex comparison](image)

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Frame: 2 4 6 8 10 12
Distance [cm]: 0.2 0.4 0.6 0.8 1.0 1.2 1.4 1.6 1.8
Distance [cm]: 1.5 2.0 2.5 3.0 3.5 4.0 4.5 5.0 5.5 6.0

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Iterative Scheme Comparison

How does this compare to the iterative scheme?

[Xu et. al, 1997] iterative solver comparison (SOR with \( w = 0.9 \) and \( \epsilon = 10^{-4} dx \))

<table>
<thead>
<tr>
<th>Iterative Method</th>
<th>Our Method</th>
</tr>
</thead>
<tbody>
<tr>
<td>25 iterations (or no convergence)</td>
<td>6 priority groups</td>
</tr>
<tr>
<td>25 calls to MPI communication</td>
<td>6 calls to MPI communication</td>
</tr>
<tr>
<td>High parallel overhead</td>
<td>Considerably lower parallel overhead</td>
</tr>
</tbody>
</table>

Approximately 4X more calls to MPI communication routines!

- Per iteration (going from \( t=t_n \) to \( t=t_{n+1} \)) we have 25x3 = 75 calls to MPI Com. Routines just for the IB update
NEWCODE (In-House Code) Summary

**Underlying Solver**
- Semi-discrete approach to solve the system of PDEs
- Lax-Friedrich flux splitting and 5th order WENO [4]
- 3rd Order TVD RK scheme for advancing in time
- Fully Parallel (MPI)

**Simulation Capabilities**
- Ideal and Jones-Wilkins-Lee (JWL) EOS
- Multi-components/species
- Nonlinear PT-Equilibration (well mixed, common P, T, u)
- Solid boundaries and multi-material

*Single vortex field test case*  
[Salih et. al, 2009]
Future Work

• Compare the experimental test data with the numerical results
• Adaptive Mesh Refinement (AMR) in NEWCODE

Impact on Other Projects

• Multi-material thermites/intermetallics: Copper Oxide and Aluminum
• Thermite / Titanium-Boron high energy mixing
• Heterogeneous explosives: high explosive/metal hybrids
• Microstructure of solid oxides
• Premixed combustion
• Turbulent combustion