Modeling Omega HED and ICF Experiments with MARBL

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Outline for Today

Introduction to MARBL, a next-gen multiphysics code

Part I: Radiation Kelvin-Helmholtz Instability in a Magnetic Field

Part II: Modeling the microstructure of HDC ablators in rad-hydro simulations
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Introduction to MARBL, a next-gen multiphysics code

Part I: Radiation Kelvin-Helmholtz Instability in a Magnetic Field

Part II: Modeling the microstructure of HDC ablators in rad-hydro simulations
The next-gen code MARBL has recently added physics necessary to model complex HED systems

Some of the strengths of MARBL include

- High order finite elements
- Flexible Lua interface
- Axom: Modular CS infrastructure
- Ascent in-situ visualization
- BLAST: Arbitrary Lagrangian-Eulerian (ALE) package for simulating magneto-radiation-hydrodynamics phenomena

Bottom: https://computing.llnl.gov/projects/blast
The two projects I worked on demonstrate MARBL’s strengths and unique capabilities.

Radiation Kelvin-Helmholtz Instability with a Magnetic Field

Modeling HDC* microstructure in a rad-hydro simulation

*HDC – high density carbon
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**Part I:** Radiation Kelvin-Helmholtz Instability in a Magnetic Field

**Part II:** Modeling the microstructure of HDC ablators in rad-hydro simulations
Magnetic fields can potentially suppress the growth of fluid instabilities

- The induction equation describes the evolution of a magnetic field in a conducting fluid with conductivity $\sigma$:

$$\frac{\partial \mathbf{B}}{\partial t} = \nabla \times (\mathbf{u} \times \mathbf{B}) + \left( \frac{1}{\mu_0 \sigma} \right) \nabla^2 \mathbf{B}$$

- The relative importance of the two terms on the right is governed by the magnetic Reynolds number, $R_m$:

$$R_m = \frac{(U/L)B}{B/(\mu_0 \sigma L^2)} = \frac{\mu_0 \sigma UL}{D_m} \approx \frac{\text{induction/advection}}{\text{diffusion}}$$

- In "ideal" MHD ($R_m \to \infty$), magnetic field lines are "frozen" into the flow, effectively serving as rebar for the fluid.
An experiment at Omega plans to explore this in the context of the radiation Kelvin-Helmholtz instability

- The Rad-KH instability has been previously demonstrated in a HED environment using the setup shown to the right:

- Idea is to repeat w/ uniform B-field oriented in the shock direction

- Our goal is to try and model this new experiment using MARBL
The numerical setup is designed to closely mimic the experimental configuration

- Q2Q1 finite elements
- \( \mathbf{B} = [B_0, 0, 0] \) where \( B_0 = 40 \) Tesla
- Shock driven by 90 kJ of radiation energy deposited in the upper region of the ablator (next to the foam) for 1 ns. Simulation runs for 120 ns.
Early results (ideal MHD) were difficult to resolve and suggested the need for resistivity

Jet of material along left-hand side boundary causes simulation to terminate prematurely around $t \approx 4.2$ ns upon impacting upper boundary of domain

$B = [B_0, 0, 0]$ where $B_0 = 40$ Tesla
Latest results with resistivity progress further but still suffer from numerical challenges

Density vs. time with B-field (arrows)

Magnetic field strength vs. time

\[ B = [B_0, 0, 0] \] where \( B_0 = 40 \) Tesla
Key takeaways and future work for Part I

- **Key takeaways**
  - First application of MARBL utilizing both MHD and radiation transport
  - Early results are promising but the simulations require further tuning in order to be able to run to late times

- **Future work**
  - Continue to iterate on numerical challenges
  - Consider using more realistic conductivities for fully ionized plasmas
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**Part I: Radiation Kelvin-Helmholtz Instability in a Magnetic Field**

**Part II: Modeling the microstructure of HDC ablators in rad-hydro simulations**
Experiments at Omega suggest that HDC microstructure may induce fluid instabilities

- Material heterogeneity can seed instabilities. Due to shock speed varying as it passes through grains of differing orientations.
- Can use 2D VISAR to measure the velocity nonuniformity at the shock front after it passes through the ablator
To resolve the physics in the experiment, we focus on a small section of the irradiated area.

Numerical considerations:

- Shock driven by radiation temperature set at left boundary: $T_r(x = 0) = 135$ eV
- Pulse duration of 3 ns; simulation time is 5 ns
- Reflected BC on other boundaries
- Q2-Q1 finite elements

\[ \Delta x_{He} = 8.3 \, \mu m \]
\[ \Delta x_{HDC} = 1.9 \, \mu m \]
\[ \Delta x_{D2} = 4.5 \, \mu m \]
\[ \Delta y = \Delta z = 4.7 \, \mu m \]
We can simulate a realistic HDC microstructure via a Voronoi tessellation

- HDC has a polycrystalline microstructure with grains ranging from 1 to 20 microns in size

Voronoi tessellation

Previous 2D microstructure modeling by Chris Weber using HYDRA
Axom allows us to create a full workflow for generating 3D Voronoi microstructures

Creation of polygon mesh using MicroStructPy

Generate distance field using Axom

Generate initial density for MARBL using Axom

Use an isosurface to define grain boundaries

The presence of the microstructure has a clear impact on the dynamics of the shock.

Nominal

Microstructure

* These are both 3D MARBL simulations viewed from the side
The presence of the microstructure has a clear impact on the dynamics of the shock.
Visualizing the shock front gives insight into how the microstructure affects shock propagation

Relative velocity at the shock front 1 ns after breakout

Relative velocity at the shock front 2 ns after breakout
Ascent in-situ visualization provides us with quantitative information about the shock front.

**Shock position**

**RMS velocity of the shock front**
Key takeaways and future work for Part II

- **Key takeaways**
  - We’ve created a general workflow for embedding a specified microstructure into MARBL 3D rad-hydro simulations
  - Simulations demonstrate the potential microstructure has for seeding fluid instabilities

- **Future work**
  - Better replicate experimental microstructures (i.e. smaller grain sizes and considering spatial gradients)
  - Minimize computational cost as the problem becomes increasingly multiscale due to the extremely fine grain structures
In conclusion

- The new multiphysics code MARBL is now at the stage where it can be used as a tool for scientific discovery
- We’ve successfully used MARBL to model two high energy density experiments at Omega:
  1. Radiation Kelvin-Helmholtz instability in a Magnetic Field
  2. HDC microstructure seeding fluid instabilities
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Questions?

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Extra slides
Visualizing the shock front gives insight into how the microstructure affects shock propagation.

Relative velocity at the shock front 2 ns after breakout

Relative velocity at the shock front 3 ns after breakout

Changing limit scale from 8 to 3 and using mesh adaptation
Fluid instabilities during ICF experiments lead to reduced capsule compression

- ICF experiments can experience:
  1. Rayleigh-Taylor instabilities
  2. Richtmyer-Meshkov instabilities
  3. Kelvin-Helmholtz (KH) instabilities

- In all cases, the net result is mixing of cold fuel / ablator material into the forming hotspot, thereby decreasing fusion yield

- My work has explored two interesting avenues of research:
  1. Can magnetic fields be used to suppress fluid instabilities, e.g. the Kelvin-Helmholtz instability?
  2. How does the microstructure of polycrystalline ablator material like high-density carbon (HDC) affect/trigger these instabilities?
Present simulations (currently with no HDC microstructure) run as expected (e.g. desired $P_{abl}$)

The following are 3D simulations viewed at the $z = 0$ plane

- **Ablation of the HDC region**
  - Volume fraction

- **Propagation of the shock wave**
  - Pressure (Mbar)

- **Goal 1:** want first shock pressure > 12 Mbar so HDC is fully melted
- **Goal 2:** want sufficient time after breakout to observe shock front

$T_r = 150$ eV applied on LHS boundary for 3 ns
Next steps include modeling the HDC microstructure in 3D using a Voronoi tessellation

- HDC has a polycrystalline microstructure with grains ranging from 1 to 20 microns in size

Cross section

Previous 2D microstructure modeling by Chris Weber

Laguerre-Voronoi tessellation