Modeling Omega HED and ICF Experiments with MARBL

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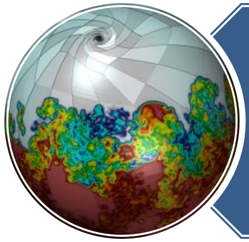
Mentor: Luc Peterson

September 9th, 2020

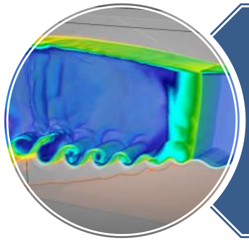
LLNL-PRES-814502

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under contract DE-AC52-07NA27344. Lawrence Livermore National Security, LLC

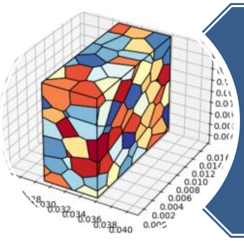
Outline for Today



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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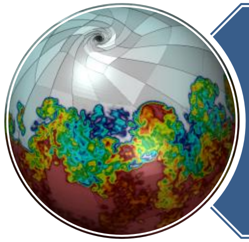

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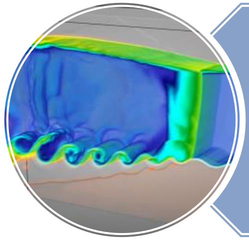

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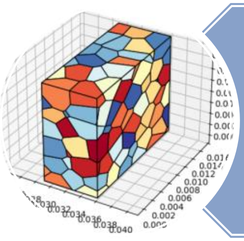
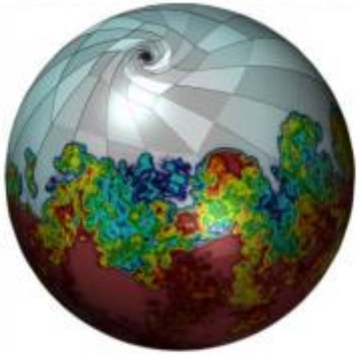


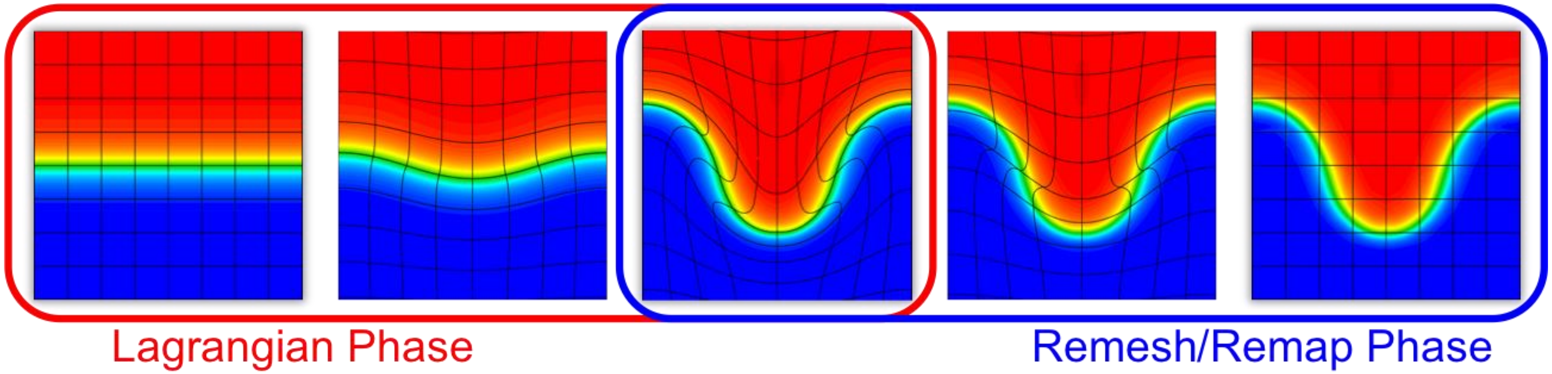
Part II: Modeling the microstructure of HDC ablators in rad-hydro simulations

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

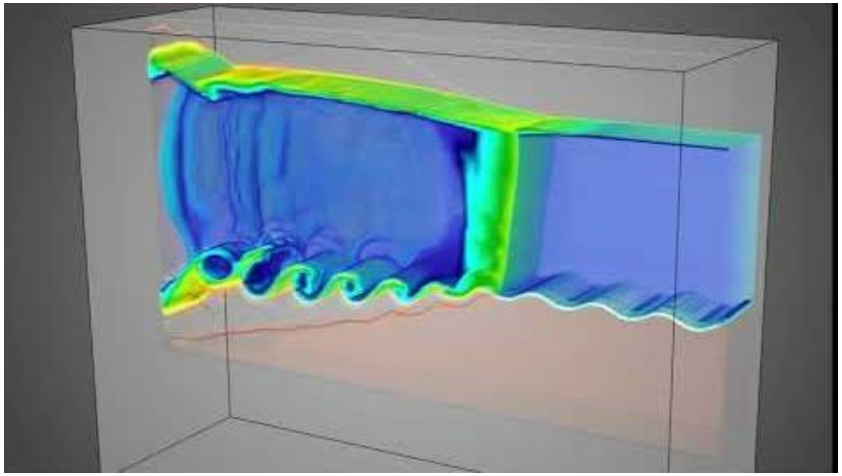




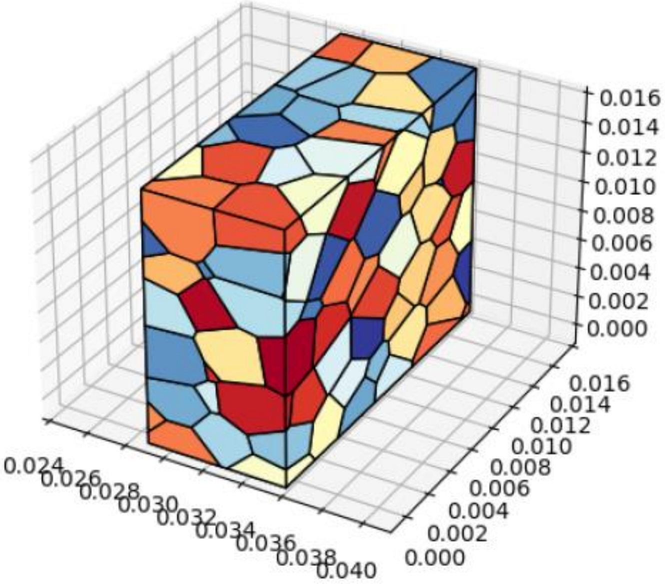
Bottom: https://computing.llnl.gov/projects/blast

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

Left: MARBL RKH simulation: https://www.youtube.com/watch?v=J-ANLAnc6WI

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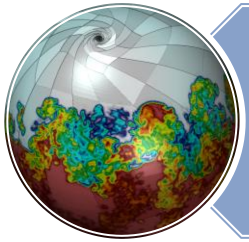

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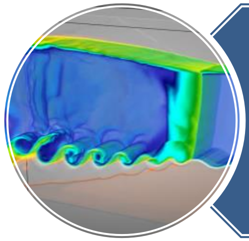

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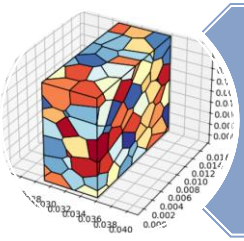


Part II: Modeling the microstructure of HDC ablators in rad-hydro simulations

Magnetic fields can potentially suppress the growth of fluid instabilities

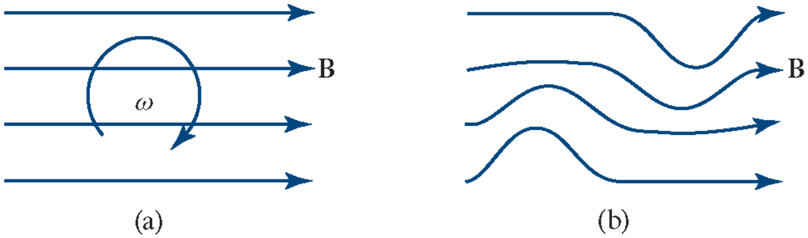
- The induction equation describes the evolution of a magnetic field in a conducting fluid with conductivity σ:

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

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

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

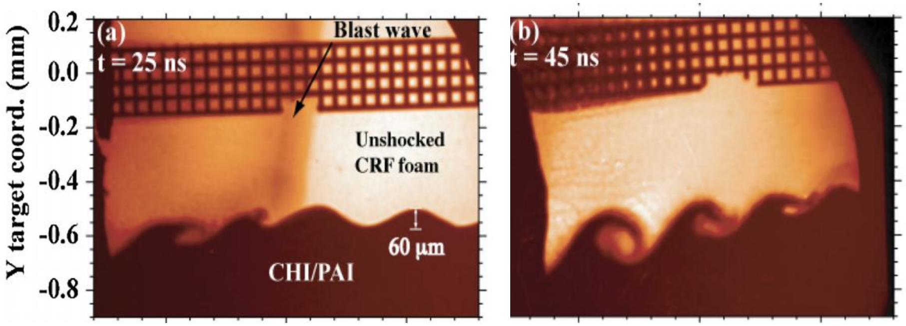
- In "ideal" MHD ($R_m \rightarrow \infty$), magnetic field lines are "frozen" into the flow, effectively serving as rebar for the fluid



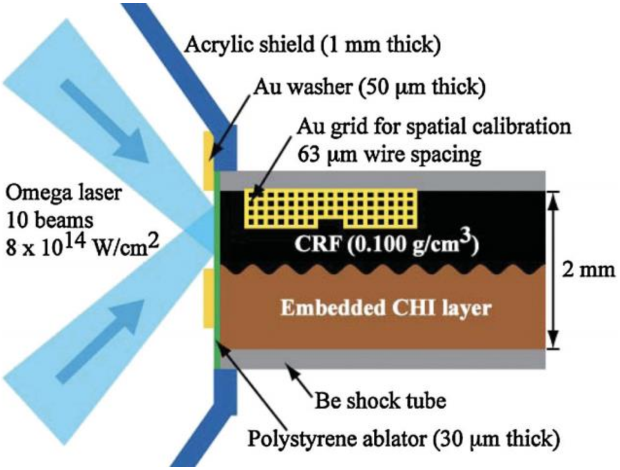
(a) (b)

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:



Experimental schematic

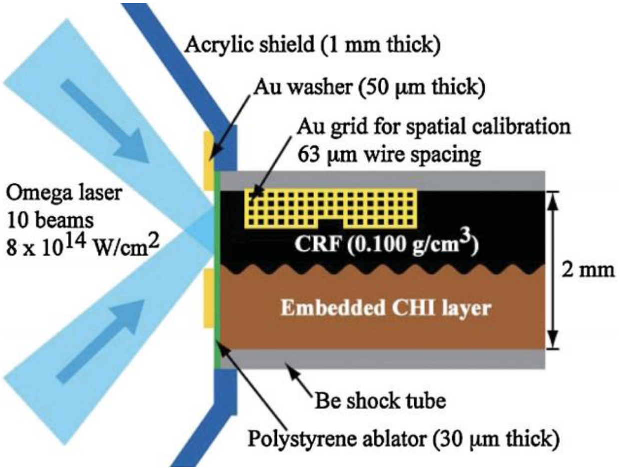


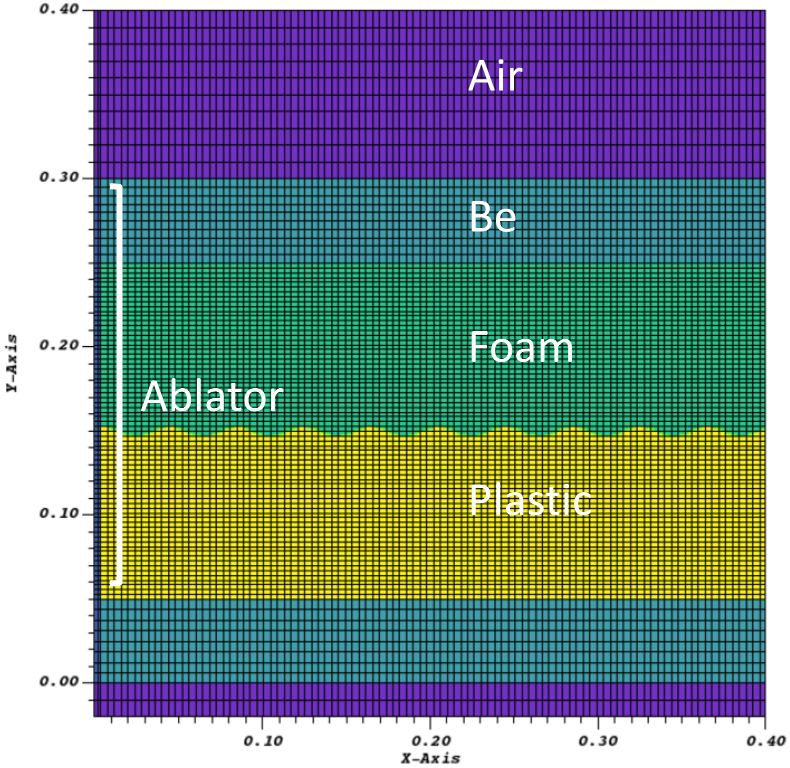
- Idea is to repeat w/ uniform B-field oriented in the shock direction

- Our goal is to try and model this new experiment using MARBL

Harding, E. C. et al. Phys. Rev. Lett. 103, 1–4 (2009).

The numerical setup is designed to closely mimic the experimental configuration





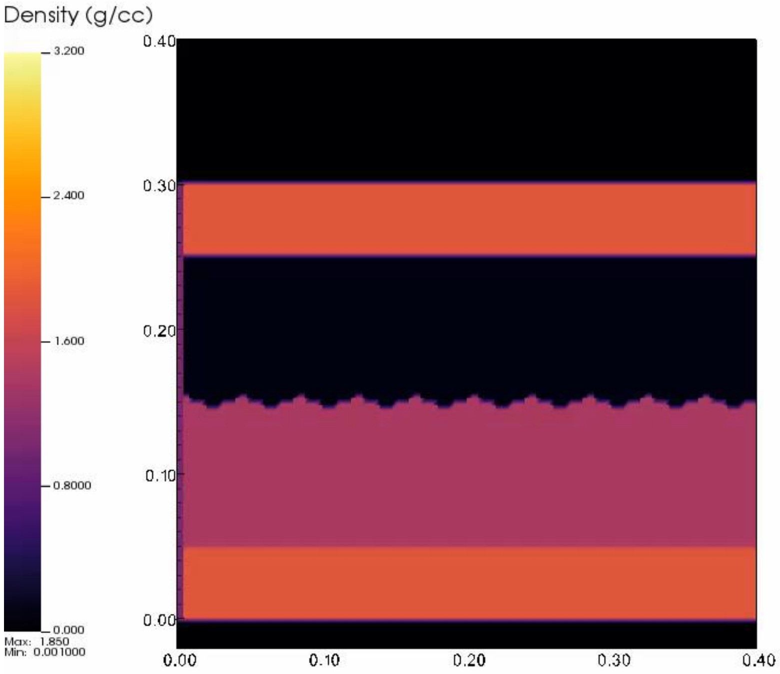
Numerical considerations

- 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.

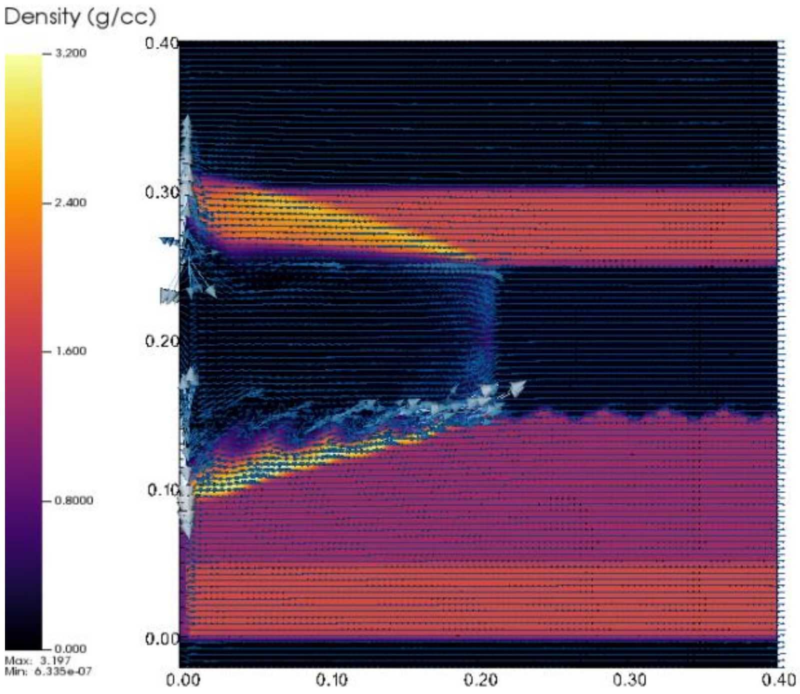
Top left: Harding, E. C. et al. Phys. Rev. Lett. 103, 1–4 (2009).
3D RKH simulations w/o MHD: Raman, K. S., et al. *Physics of Plasmas* 19.9 (2012): 092112.

Early results (ideal MHD) were difficult to resolve and suggested the need for resistivity

Density vs. time



Magnetic field at $t \approx 4.0$ ns

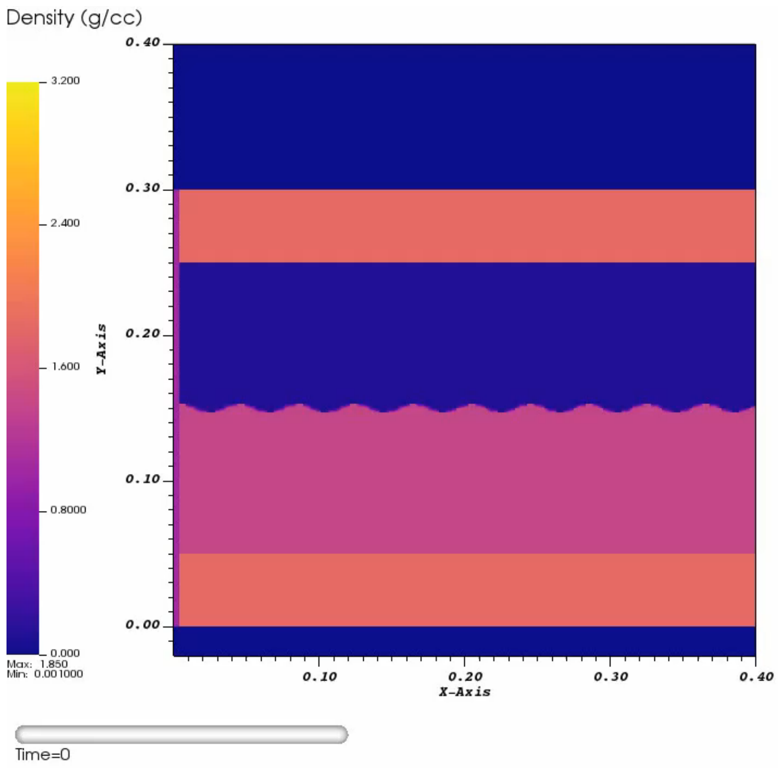


Jet of material along left-hand side boundary causes simulation to terminate prematurely around $t \approx 4.2$ ns upon impacting upper boundary of domain

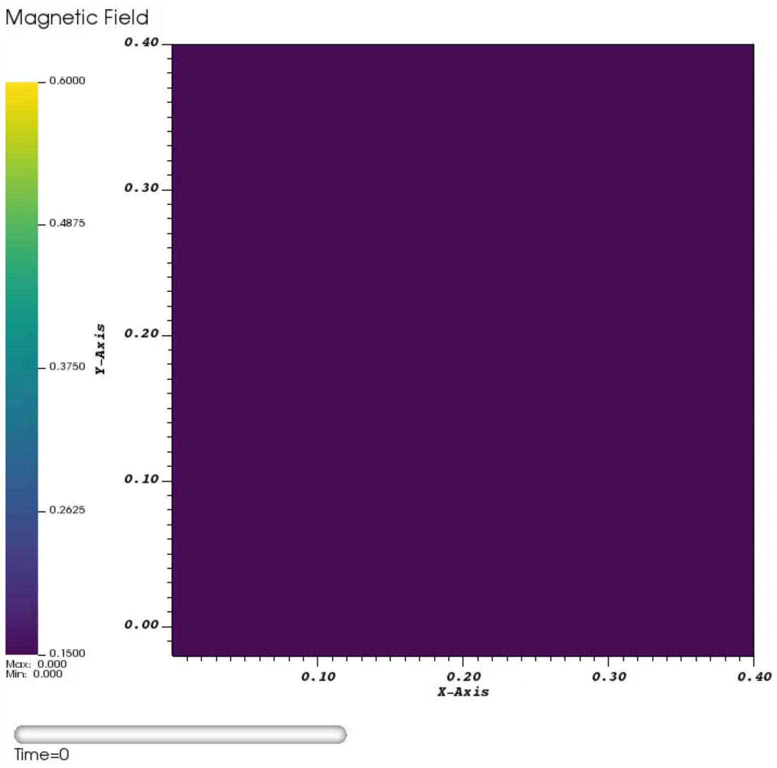
$\mathbf{B} = [B_0, 0, 0]$ where $B_0 = 40$ Tesla

Latest results with resistivity progress further but still suffer from numerical challenges

Density vs. time with B-field (arrows)



Magnetic field strength vs. time

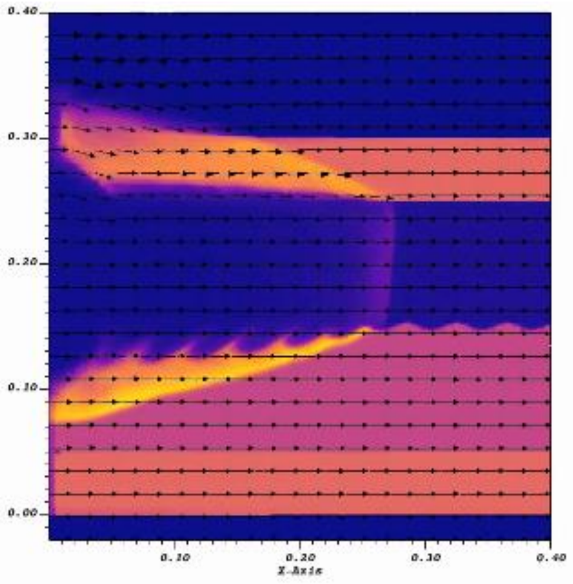


$\mathbf{B} = [B_0, 0, 0]$ where $B_0 = 40$ Tesla

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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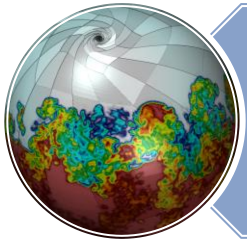

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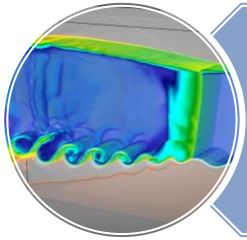
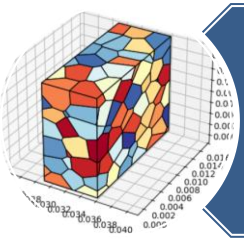


Part I: Radiation Kelvin-Helmholtz Instability in a Magnetic Field

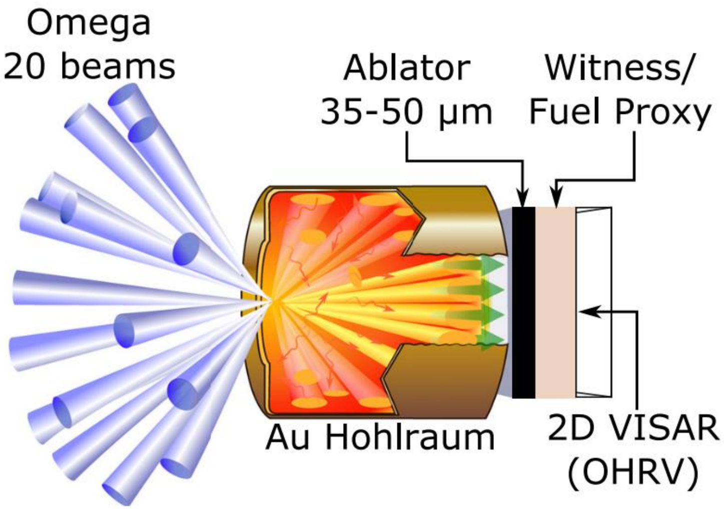


Part II: Modeling the microstructure of HDC ablators in rad-hydro simulations

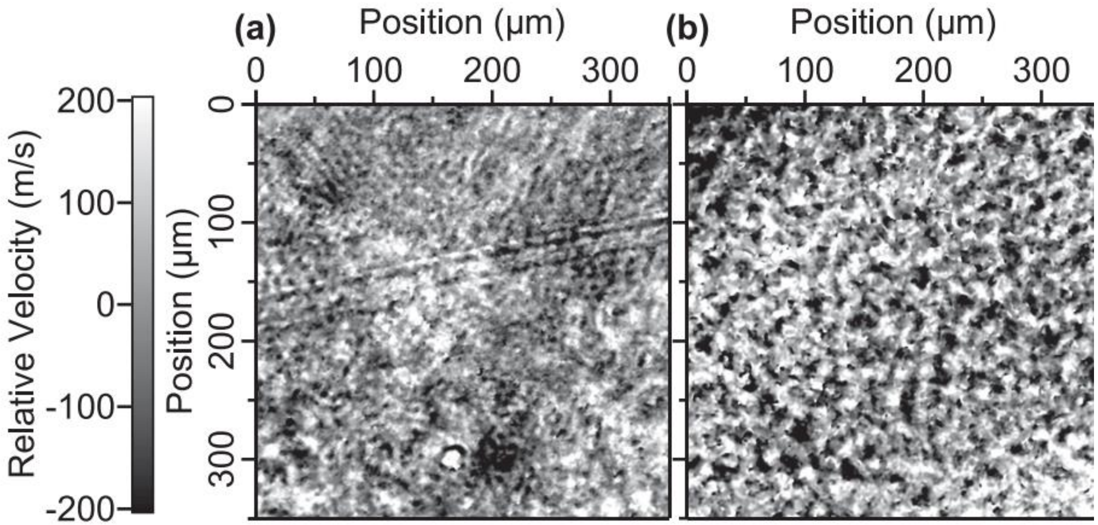
Experiments at Omega suggest that HDC microstructure may induce fluid instabilities

- 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

Experimental setup

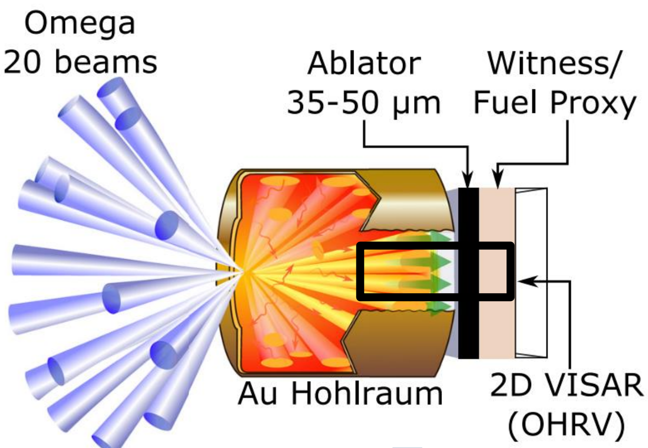


2D VISAR of HDC at (a) 10 Mbar (b) 7 Mbar



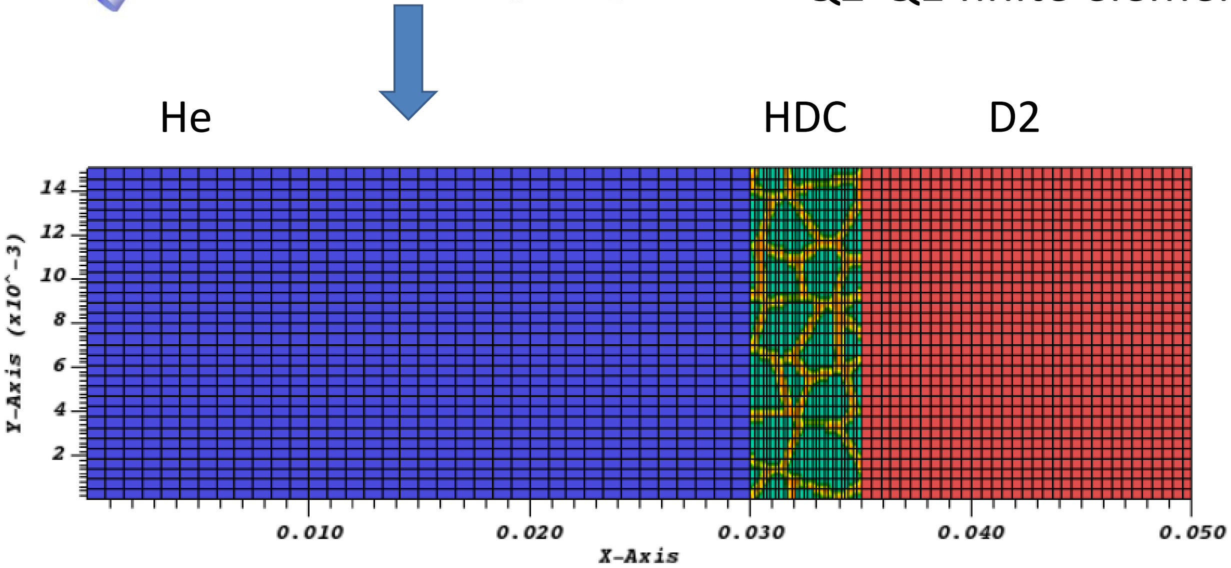
Bottom: Ali, S. J. et al. Probing the seeding of hydrodynamic instabilities from nonuniformities in ablator materials using 2D velocimetry. Phys. Plasmas 25, (2018).

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



$\Delta x_{He} = 8.3\ \mu\text{m}$

$\Delta x_{HDC} = 1.9\ \mu\text{m}$

$\Delta x_{D2} = 4.5\ \mu\text{m}$

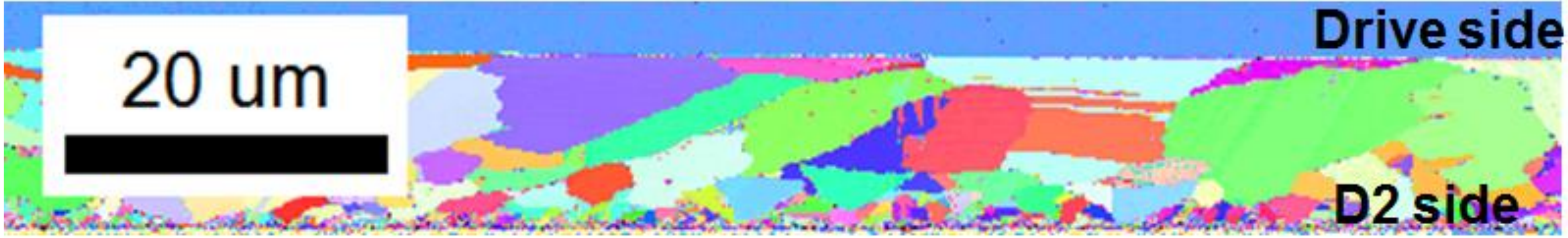
$\Delta y = \Delta z = 4.7\ \mu\text{m}$

Top left: Ali, S. J. et al. Probing the seeding of hydrodynamic instabilities from nonuniformities in ablator materials using 2D velocimetry. Phys. Plasmas 25, (2018).

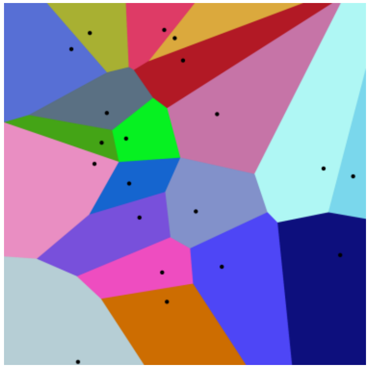
We can simulate a realistic HDC microstructure via a Voronoi tessellation

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

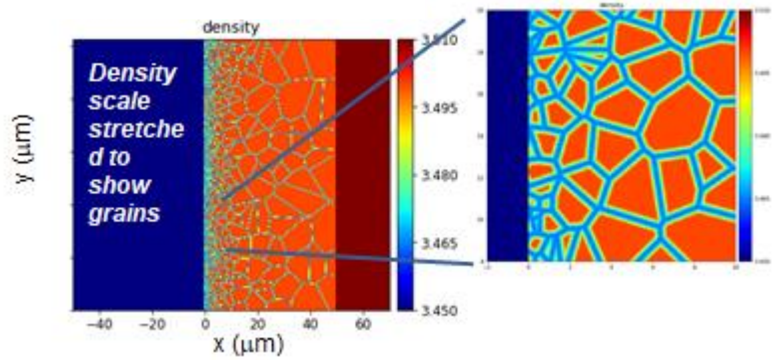
Cross section



Voronoi tessellation



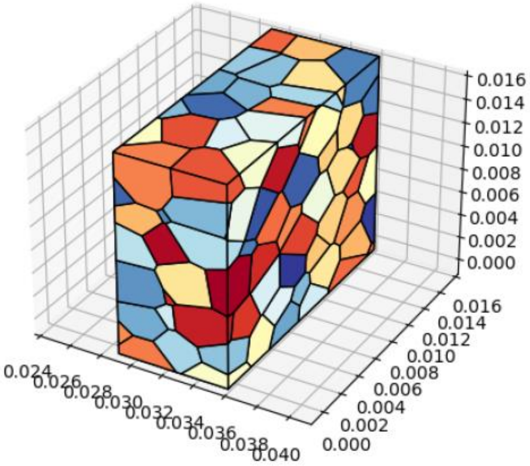
Previous 2D microstructure modeling by Chris Weber using HYDRA



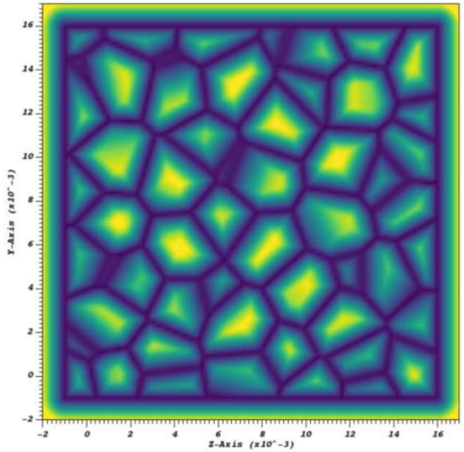
Top: Data collected and processed by D. Rosas, D. Bober, and E. Sedillo
Bottom right: Weber C. APS. 2019;2019:GI3-001.

Axom allows us to create a full workflow for generating 3D Voronoi microstructures

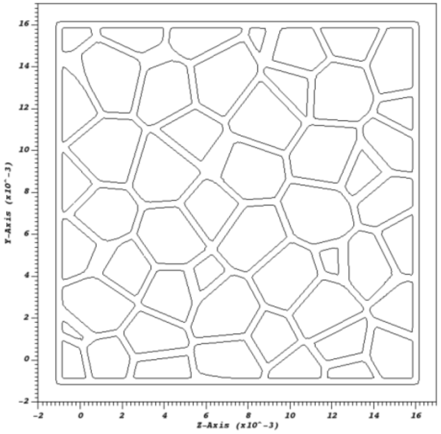
Creation of polygon mesh using MicroStructPy



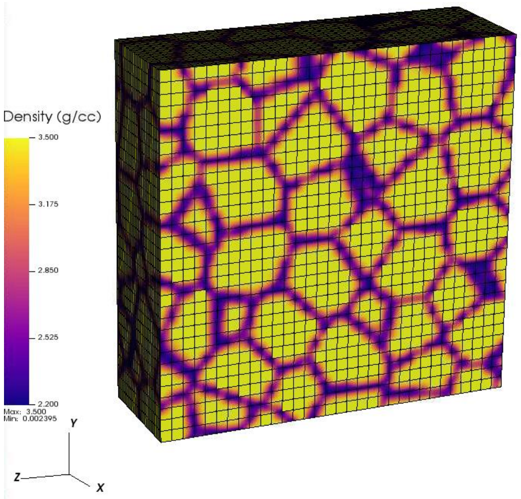
Generate distance field using Axom



Use an isosurface to define grain boundaries



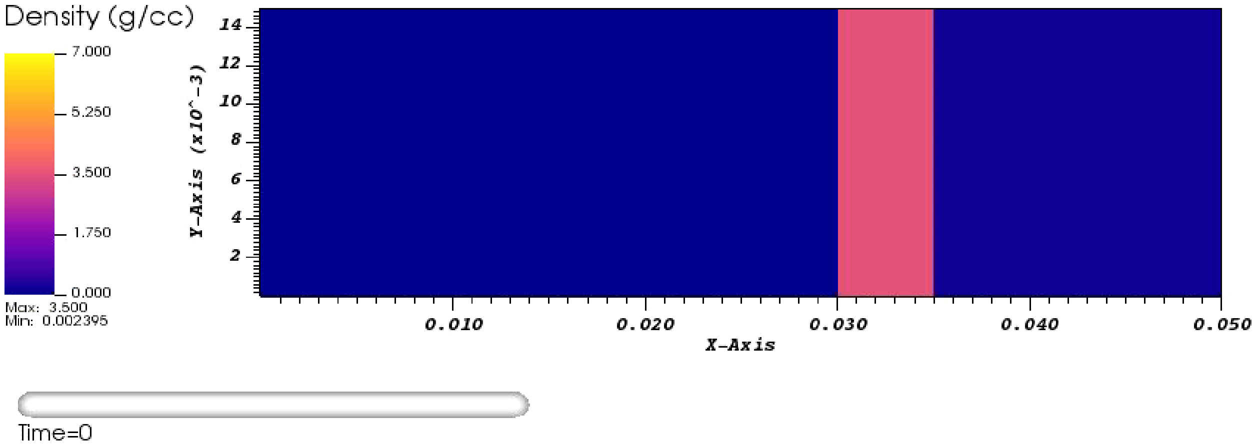
Generate initial density for MARBL using Axom



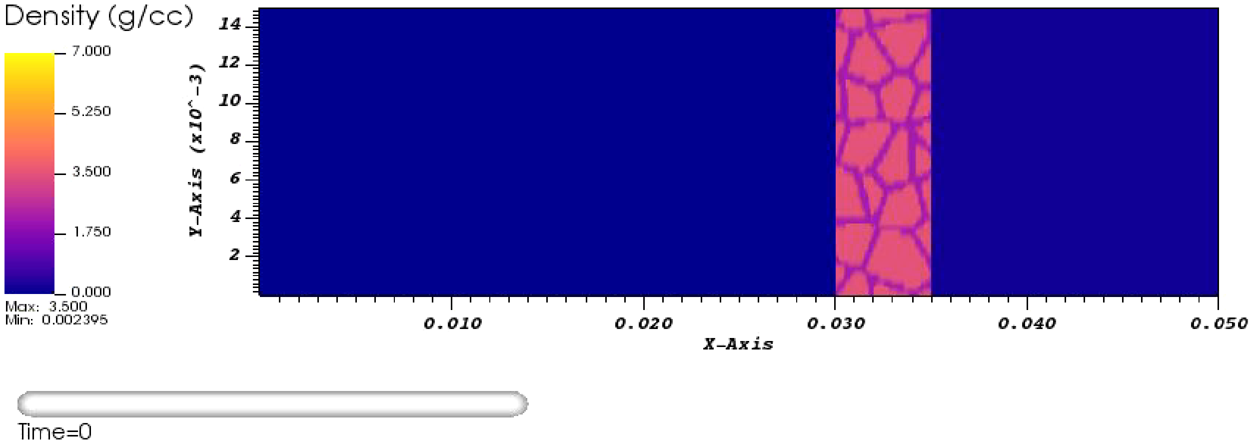
MicroStructPy: K. A. Hart and J. J. Rimoli, *Computer Methods in Applied Mechanics and Engineering*, 370 (2020), pp. 113242.

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

Nominal

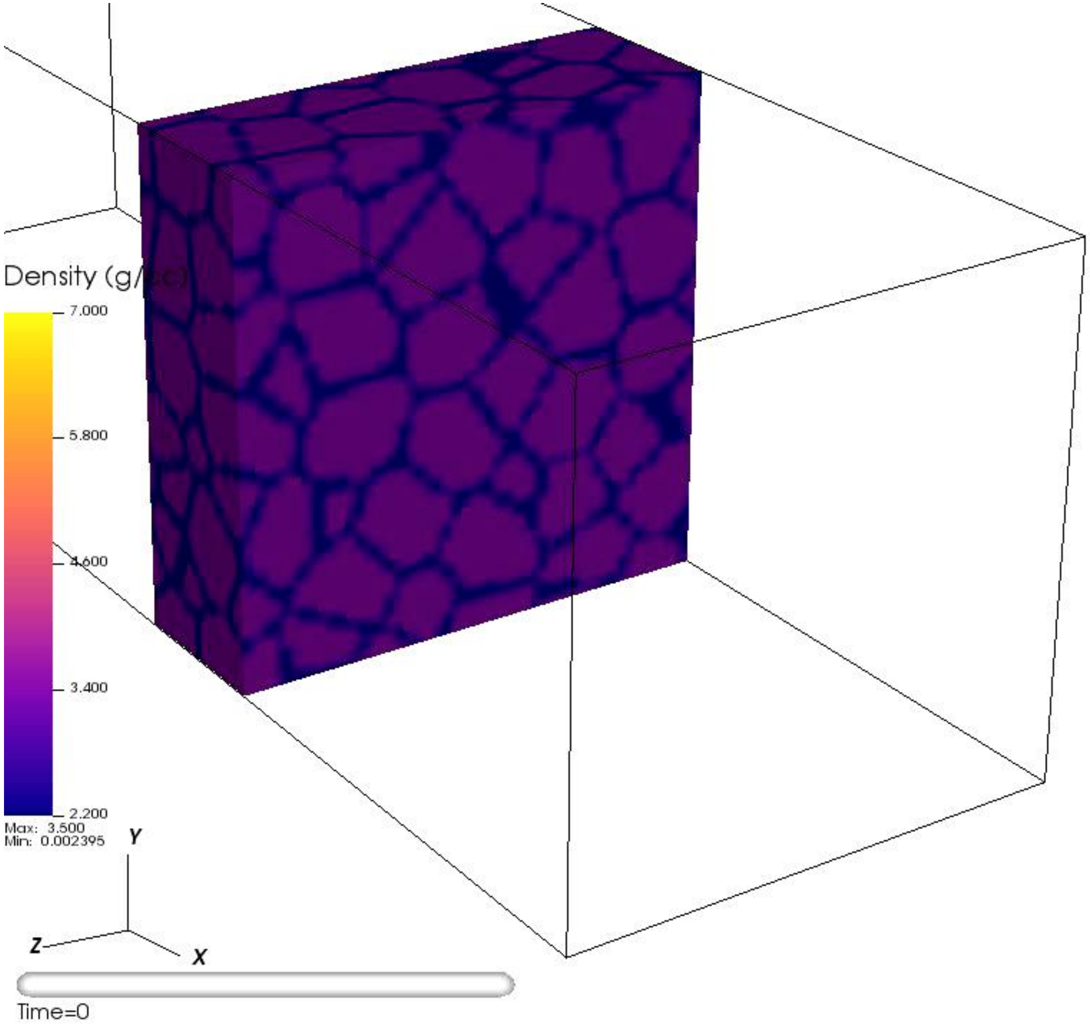


Microstructure



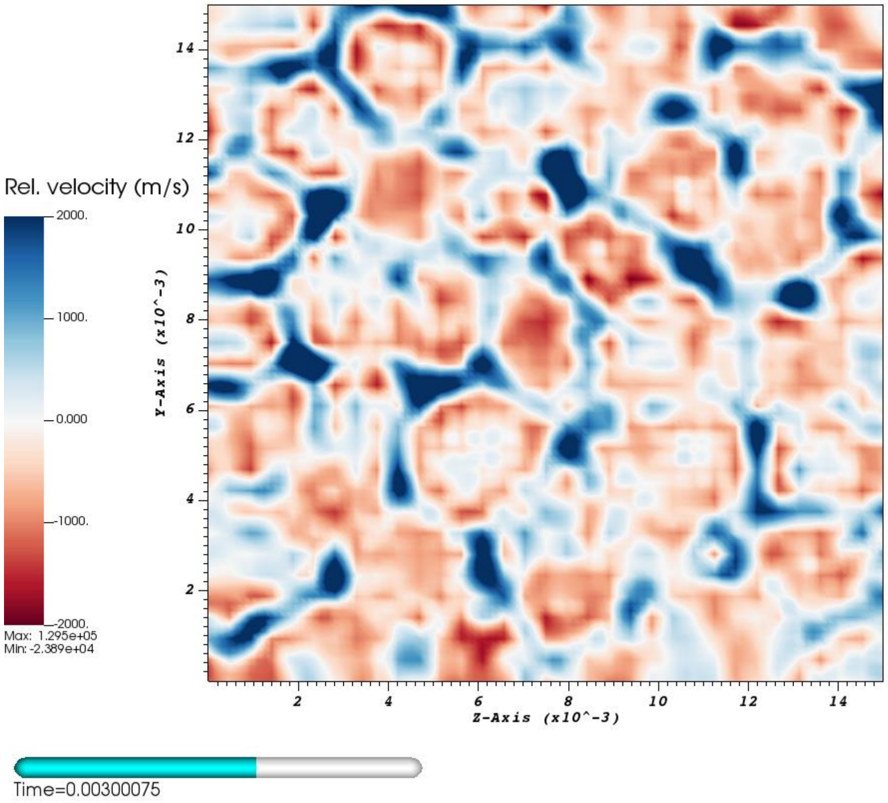
* These are both 3D MARBL simulations viewed from the side

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

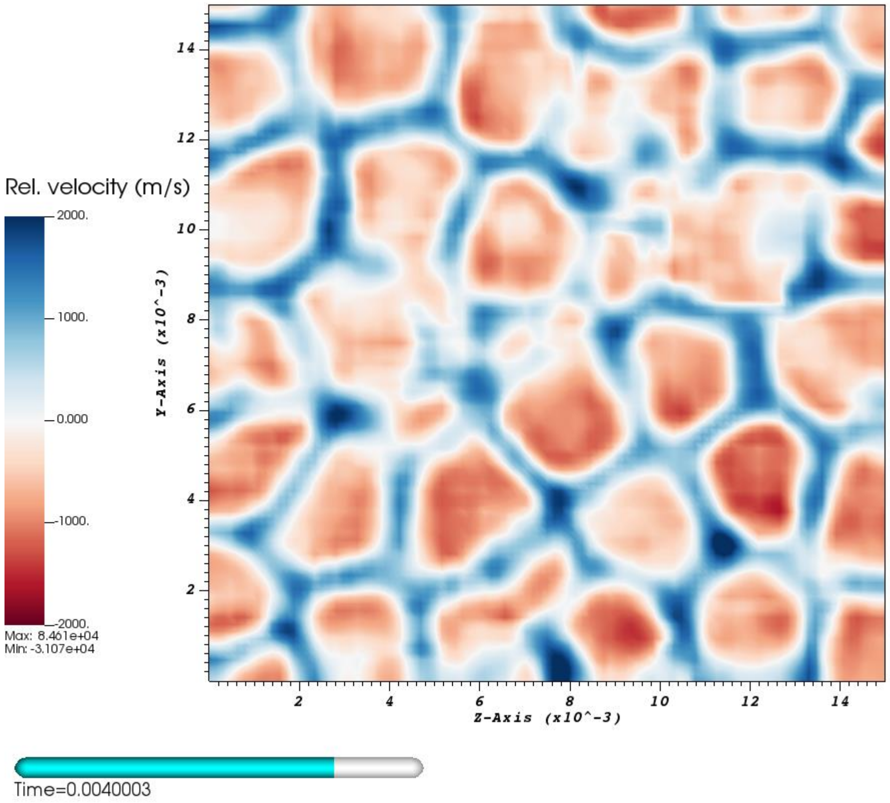


Visualizing the shock front gives insight into how the microstructure affects shock propagation

Relative velocity at the shock front 1 ns after breakout

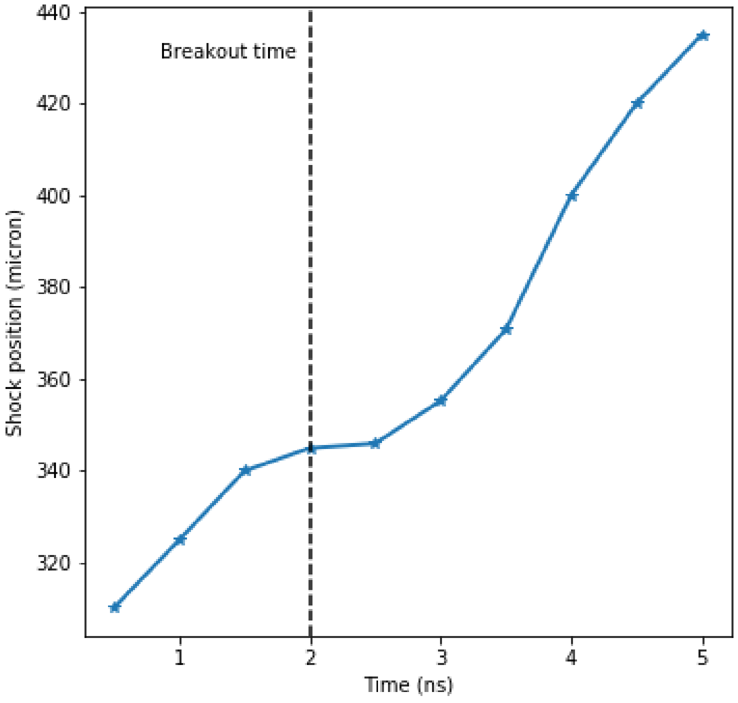


Relative velocity at the shock front 2 ns after breakout

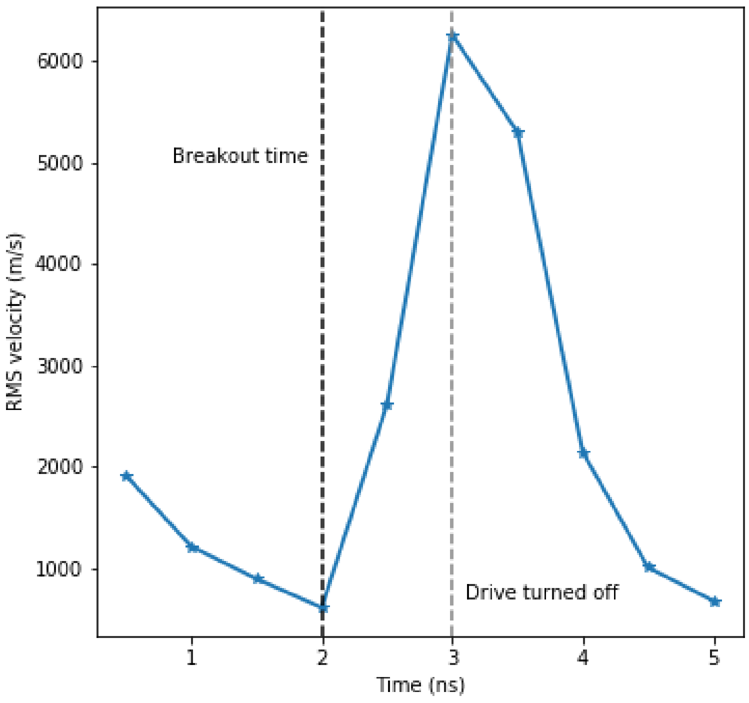


Ascent in-situ visualization provides us with quantitative information about the shock front

Shock position



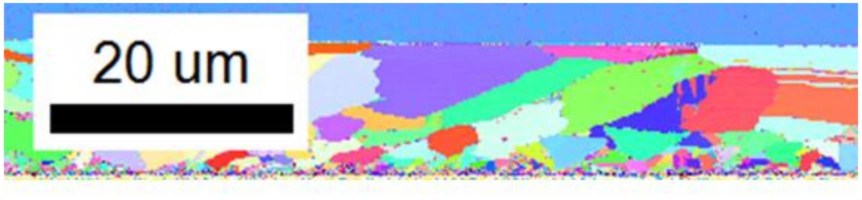
RMS velocity of the shock front



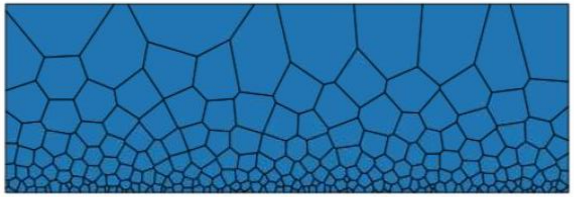
Key takeaways and future work for Part II

- 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

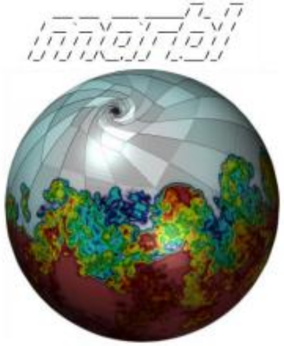
SEM Image



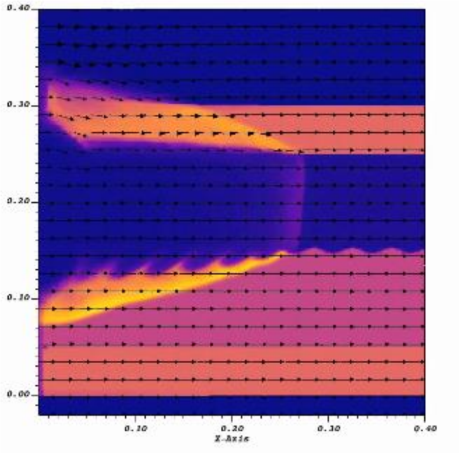
Early results for simulated microstructure

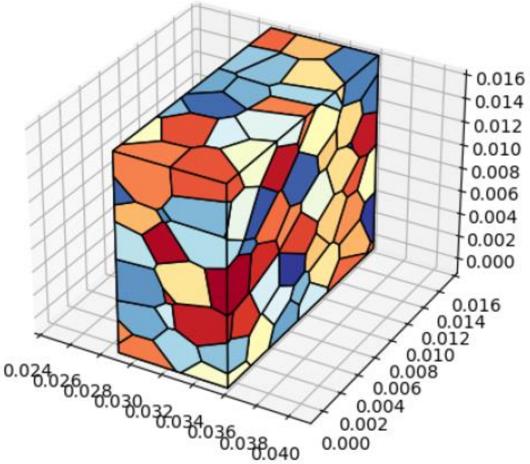


In conclusion



- 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





Acknowledgements

- Mentor
  - Luc Peterson
- LLNL Collaborators
  - Rob Rieben, Kenny Weiss, Matt Larsen, Dan White, Suzanne Ali
- HEDP Program
  - Lee Ellison, Perry Chodash, Kim Rivera

Questions?

Lawrence Livermore National Laboratory

Extra slides

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under contract DE-AC52-07NA27344. Lawrence Livermore National Security, LLC

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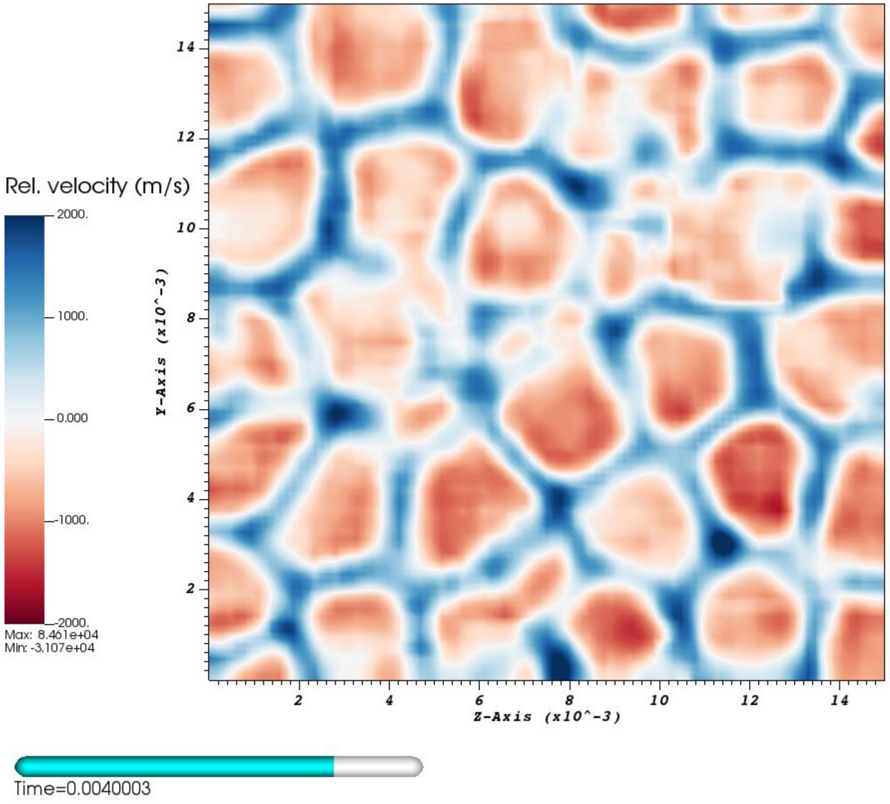
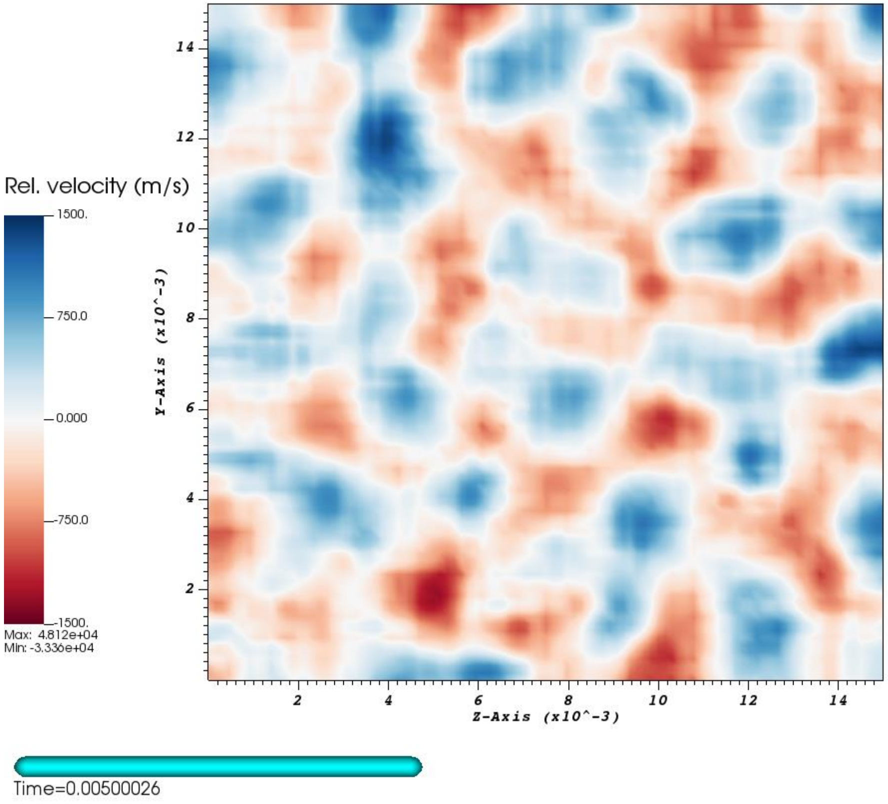
Visualizing the shock front gives insight into how the microstructure affects shock propagation



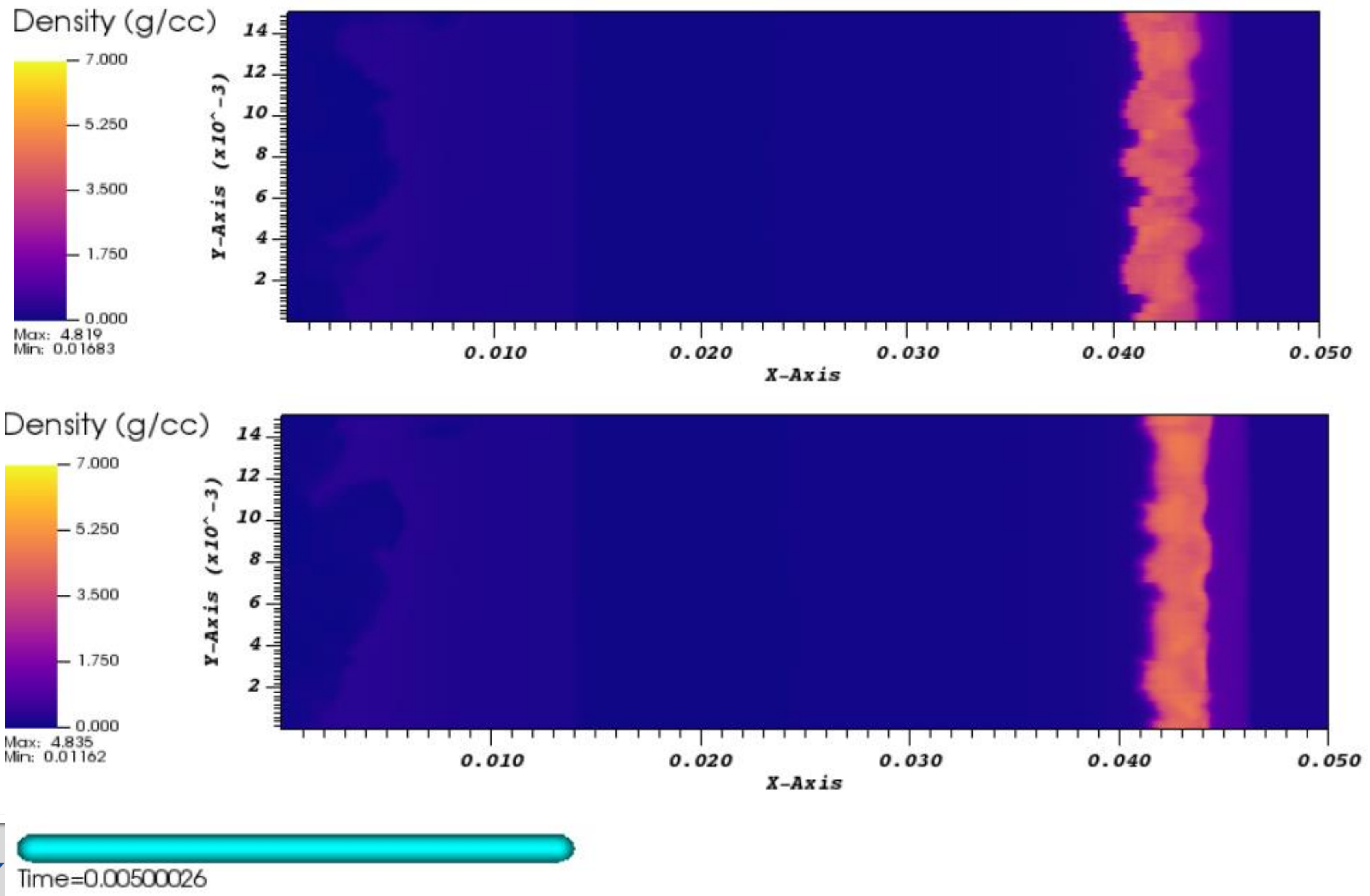
Relative velocity at the shock front 2 ns after breakout



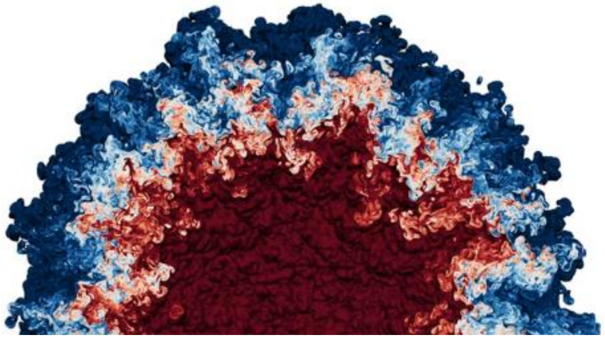
Relative velocity at the shock front 3 ns after breakout

Bottom: Ali, S. J. et al. Probing the seeding of hydrodynamic instabilities from nonuniformities in ablator materials using 2D velocimetry. Phys. Plasmas 25, (2018).

Changing limit scale from 8 to 3 and using mesh adaptation



Fluid instabilities during ICF experiments lead to reduced capsule compression



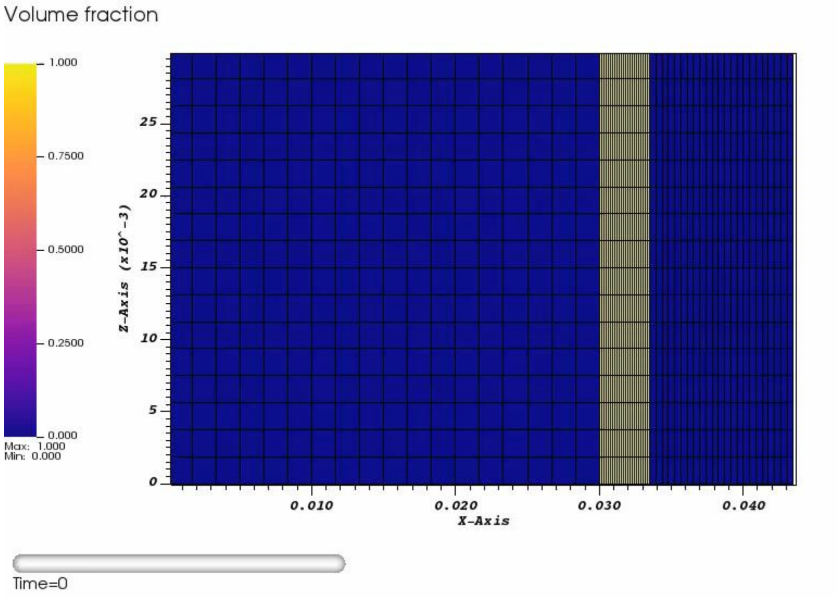
- ICF experiments can experience:
  1. Rayleigh-Taylor instabilities
  2. Richtmyer-Meshkov instabilities
  3. Kelvin-Helmholtz (KH) instabilities
- In all cases, the net result is mixing of cold fuel / ablator material into the forming hotspot, thereby decreasing fusion yield
- My work has explored 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?

Top right: https://doi.org/10.1103/APS.DFD.2019.GFM.V0002

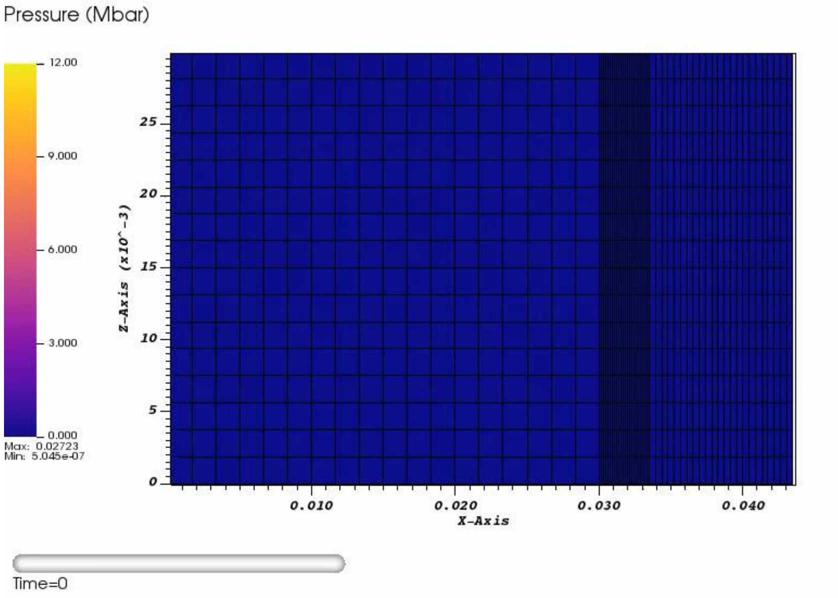
Present simulations (currently with no HDC microstructure) run as expected (e.g. desired P_{abl})

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

Ablation of the HDC region



Propagation of the shock wave

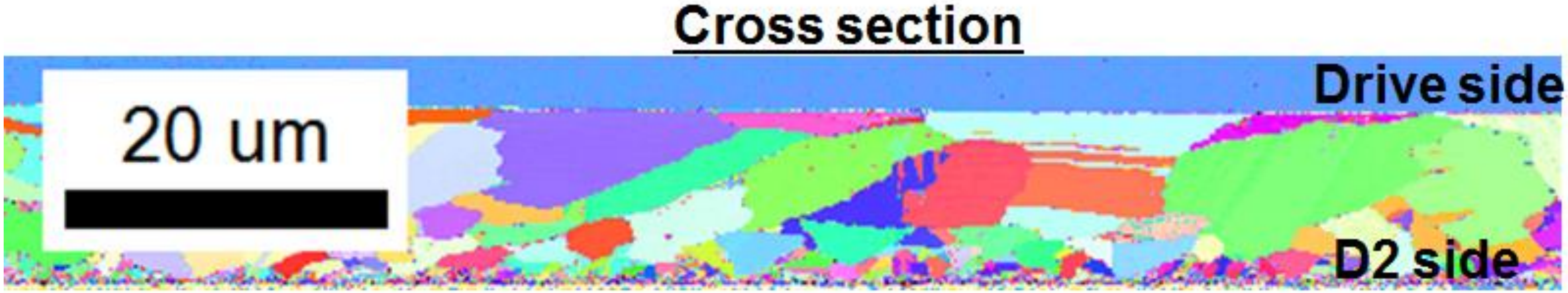


- Goal 1: want first shock pressure > 12 Mbar so HDC is fully melted
- Goal 2: want sufficient time after breakout to observe shock front

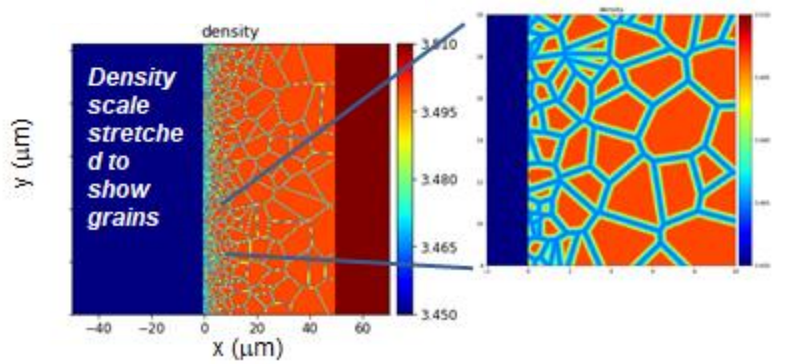
$T_r = 150$ eV applied on LHS boundary for 3 ns

Next steps include modeling the HDC microstructure in 3D using a Voronoi tesselation

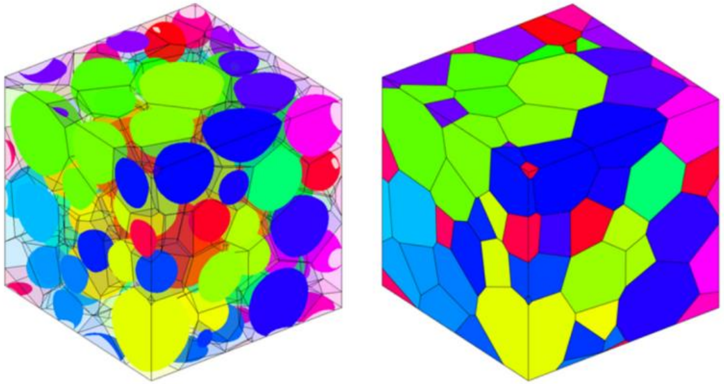
- HDC has a polycrystalline microstructure with grains ranging from 1 to 20 microns in size



Previous 2D microstructure modeling by Chris Weber



Laguerre-Voronoi tessellation



Top: Data collected and processed by D. Rosas, D. Bober, and E. Sedillo
Bottom right: Falco, S., Jiang, J., De Cola, F. & Petrinic, N. Comput. Mater. Sci. 136, 20–28 (2017).