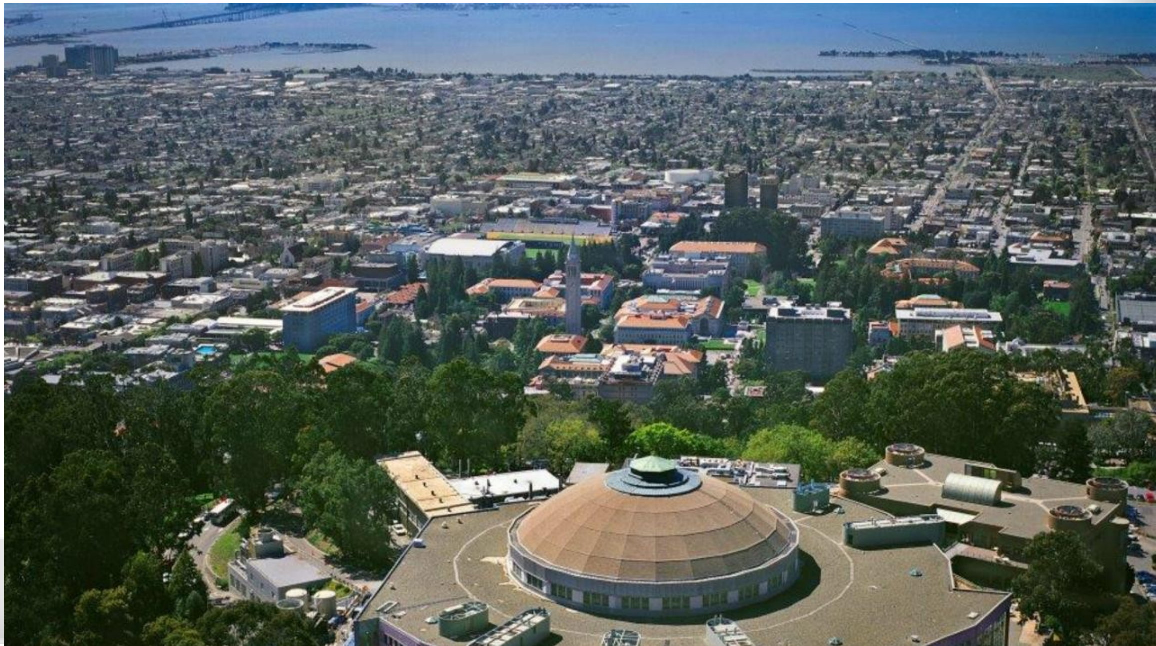
From Microscale Flow to Exploding Stars – Fluid Simulation at Lawrence Berkeley Lab

Andy Nonaka – Center for Computational Sciences and Engineering, LBL

UC Berkeley Fluids Seminar – 2/27/17

Lawrence Berkeley National Laboratory

- Department of Energy National Lab managed by University of California
- ~3,000 Staff in all areas of basic science (no weapons, no classified research)
- Physical, Energy, Earth, Environmental, Bio, and Computing Sciences



Computing Sciences

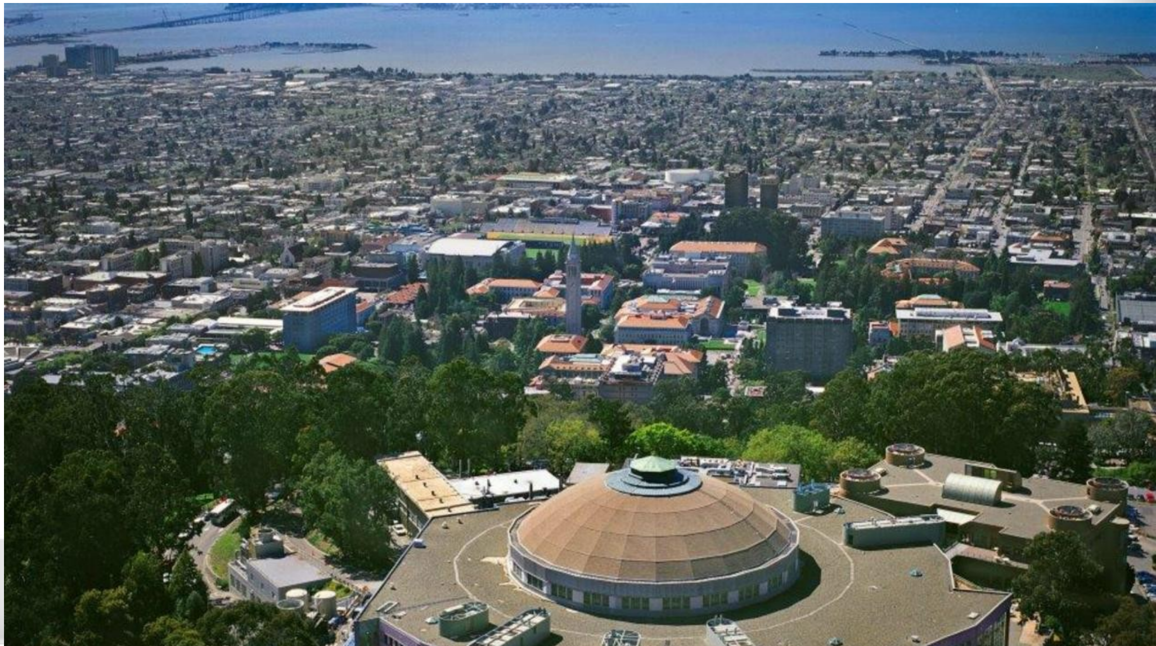
- Computing sciences accounts for ~10% of the lab staff.
  - NERSC: home to our supercomputing center

NERSC

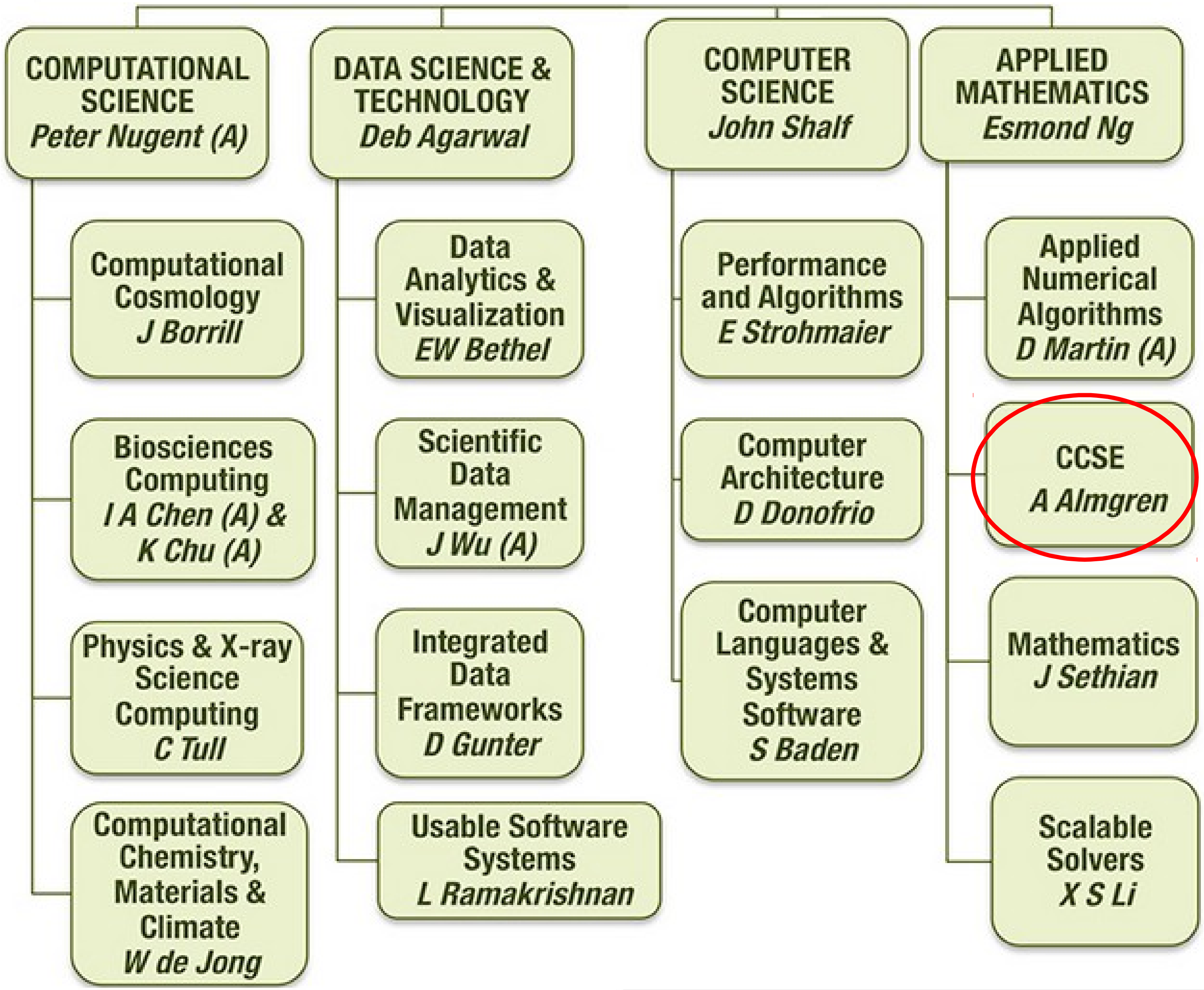
- **National Energy Research Scientific Computing Center:** “NERSC”
  - Home to “cori”, currently the 5th fastest supercomputer in the world.
  - ~600,000 CPUs, 28 petaflops
  - Electricity costs: ~$5 million per year
  - Recently moved on site to the new Computing Research and Theory building.

Computing Sciences

- Computing sciences accounts for ~10% of the lab staff.
  - NERSC: home to our supercomputing center
  - Computational Research Division: broad range of computing activities.

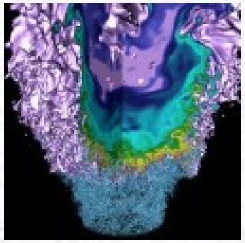


Computational Research Division

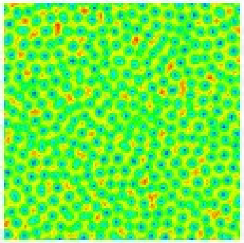


Center for Computational Sciences and Engineering

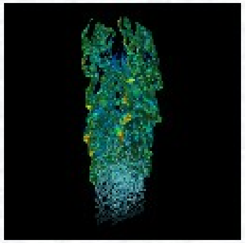
- CCSE focuses on simulations of “multiscale, multiphysics, partial differential equations”.
  - FLUIDS!!!



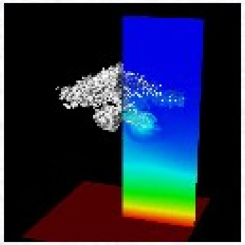
Laboratory-Scale Flames



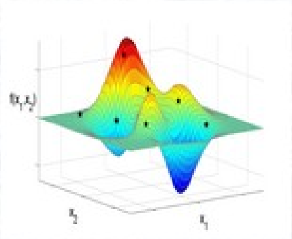
Fluctuating Hydrodynamics



ExaCT Co-Design Center

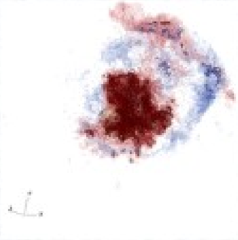


Low Mach Number Atmospheric Modeling



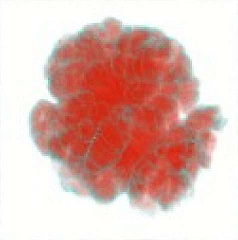
Optimization

Porous Media



Low Mach Number Astrophysics

Computational Cosmology

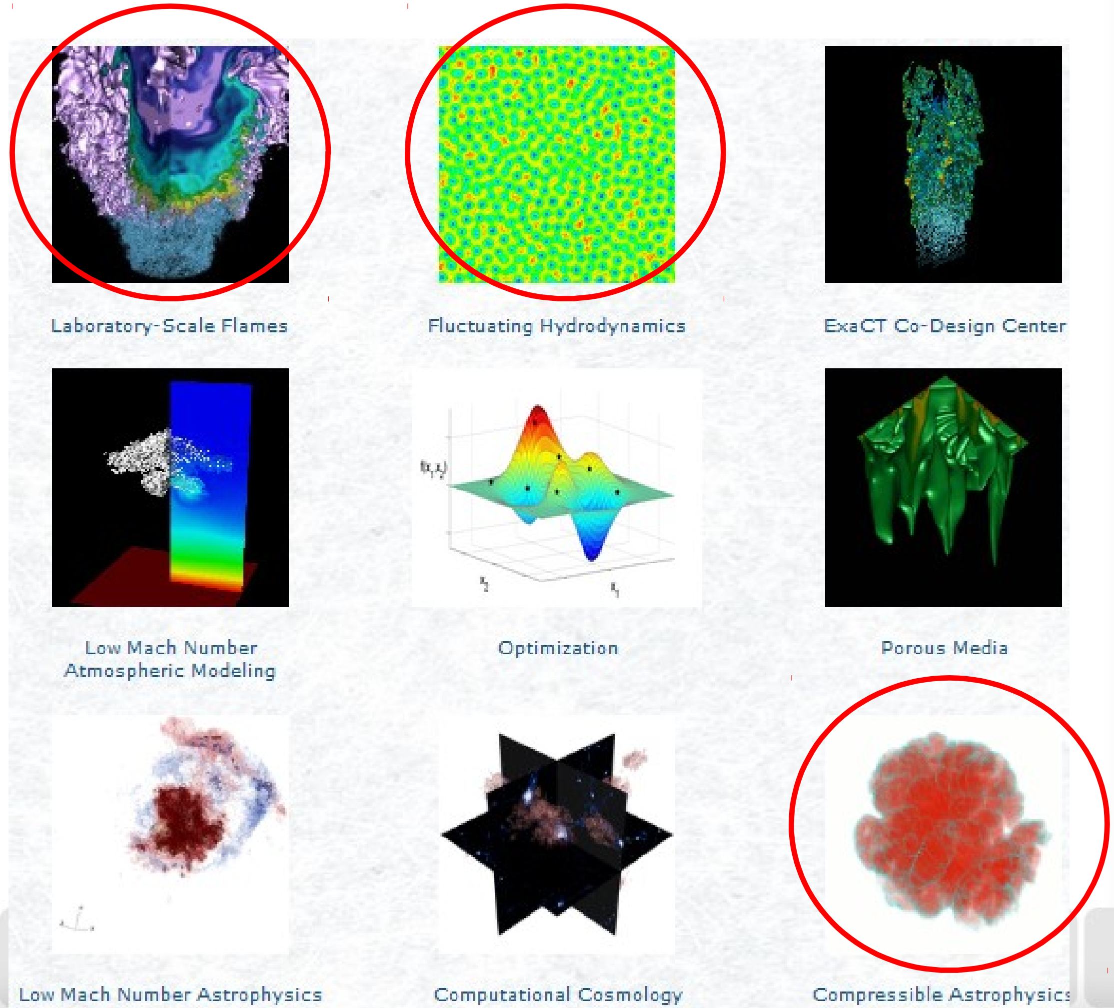


Compressible Astrophysics

ccse.lbl.gov

Center for Computational Sciences and Engineering

- Combustion, supernovae, mesoscopic flow – what do these have in common?



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Compressible Euler Equations

$$\frac{\partial \rho}{\partial t} = -\nabla \cdot (\rho u)$$

conservation of mass

$$\frac{\partial \rho u}{\partial t} = -\nabla \cdot (\rho u u) + \nabla p$$

conservation of momentum

$$\frac{\partial \rho E}{\partial t} = -\nabla \cdot ((\rho E + p) u)$$

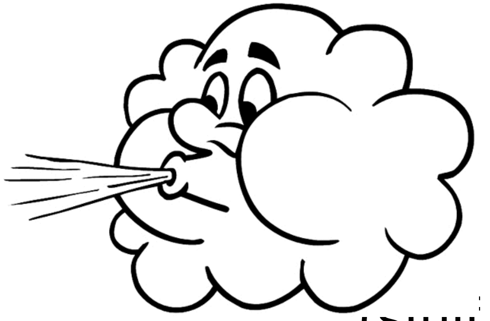
conservation of energy

ρ	mass density
u	velocity
E	total energy density
p	pressure

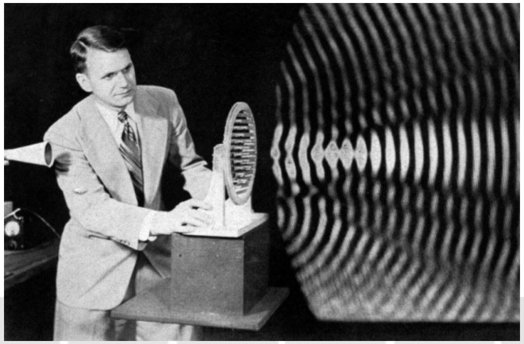
- Gas dynamics – suitable for e.g., air in this room.

Compressible Euler Equations

$$
\begin{aligned}
\frac{\partial \rho}{\partial t} &= -\nabla \cdot (\rho u) \\
\frac{\partial \rho u}{\partial t} &= -\nabla \cdot (\rho u u) + \nabla p \\
\frac{\partial \rho E}{\partial t} &= -\nabla \cdot ((\rho E + p) u)
\end{aligned}
$$



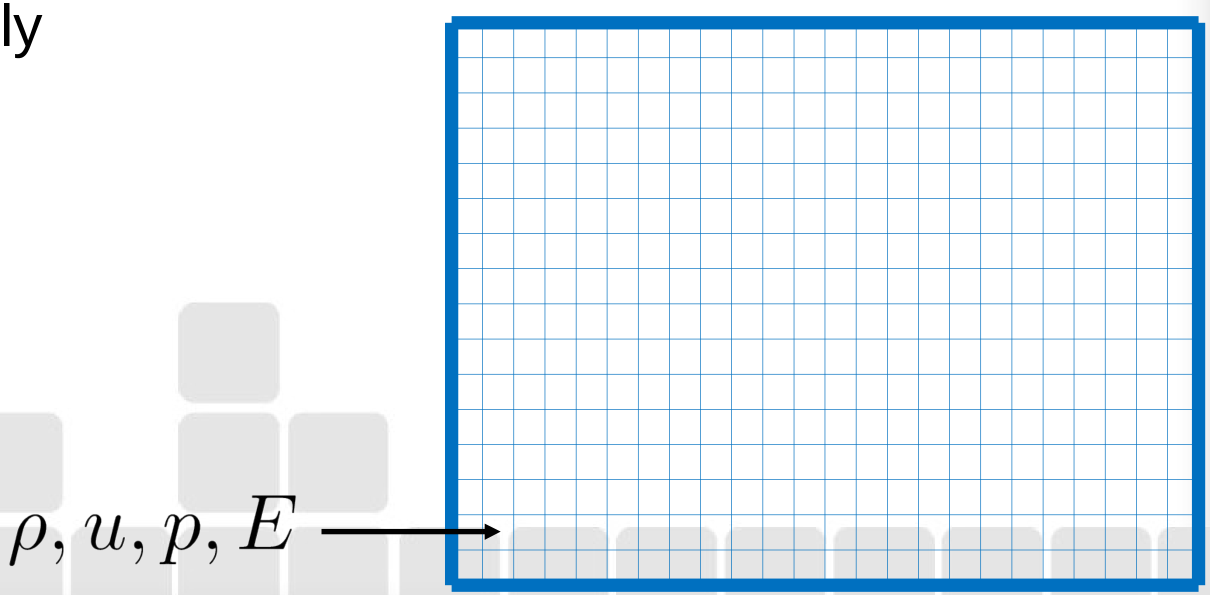
- What do these equations describe?
  - Convection/Advection (stuf blowing around)



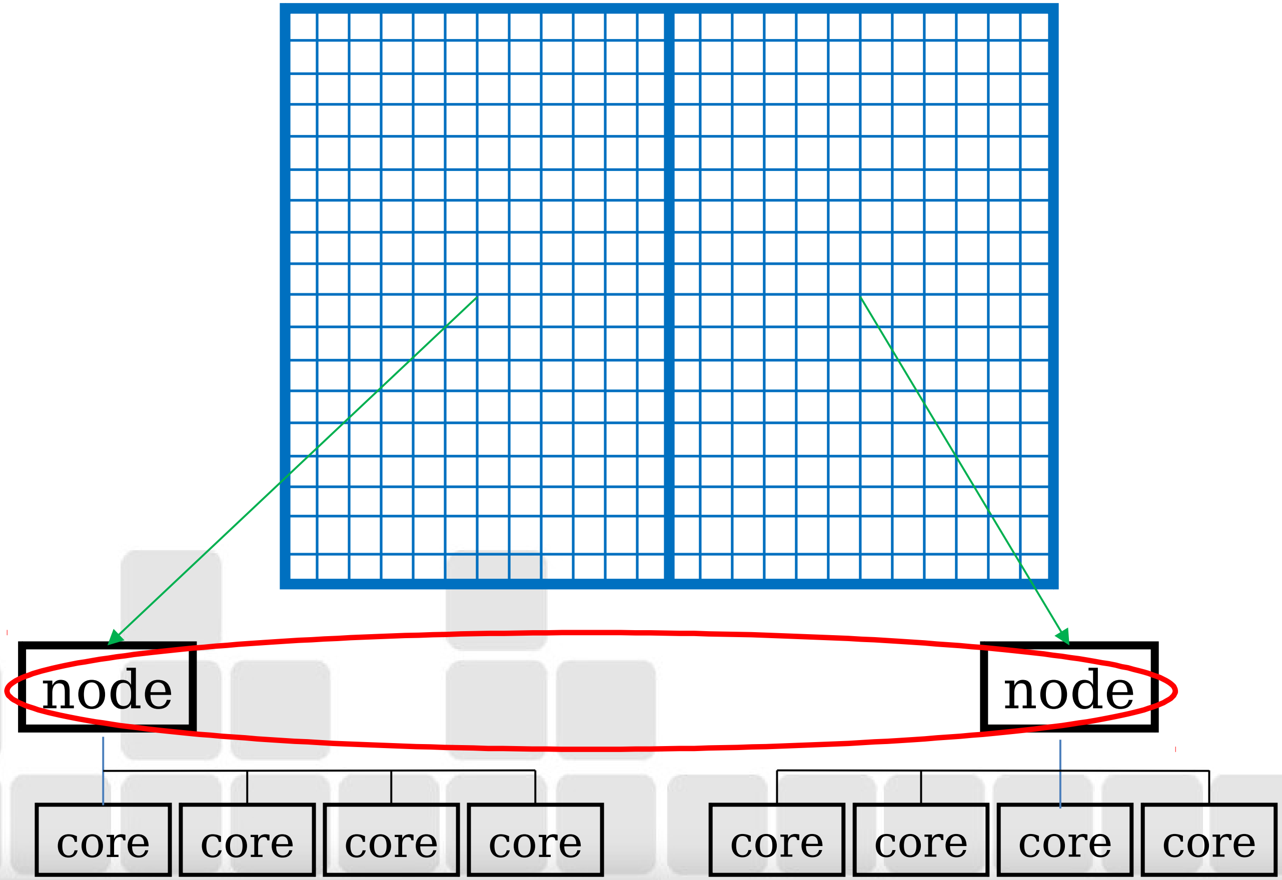
  - Sound waves

Numerical Simulation

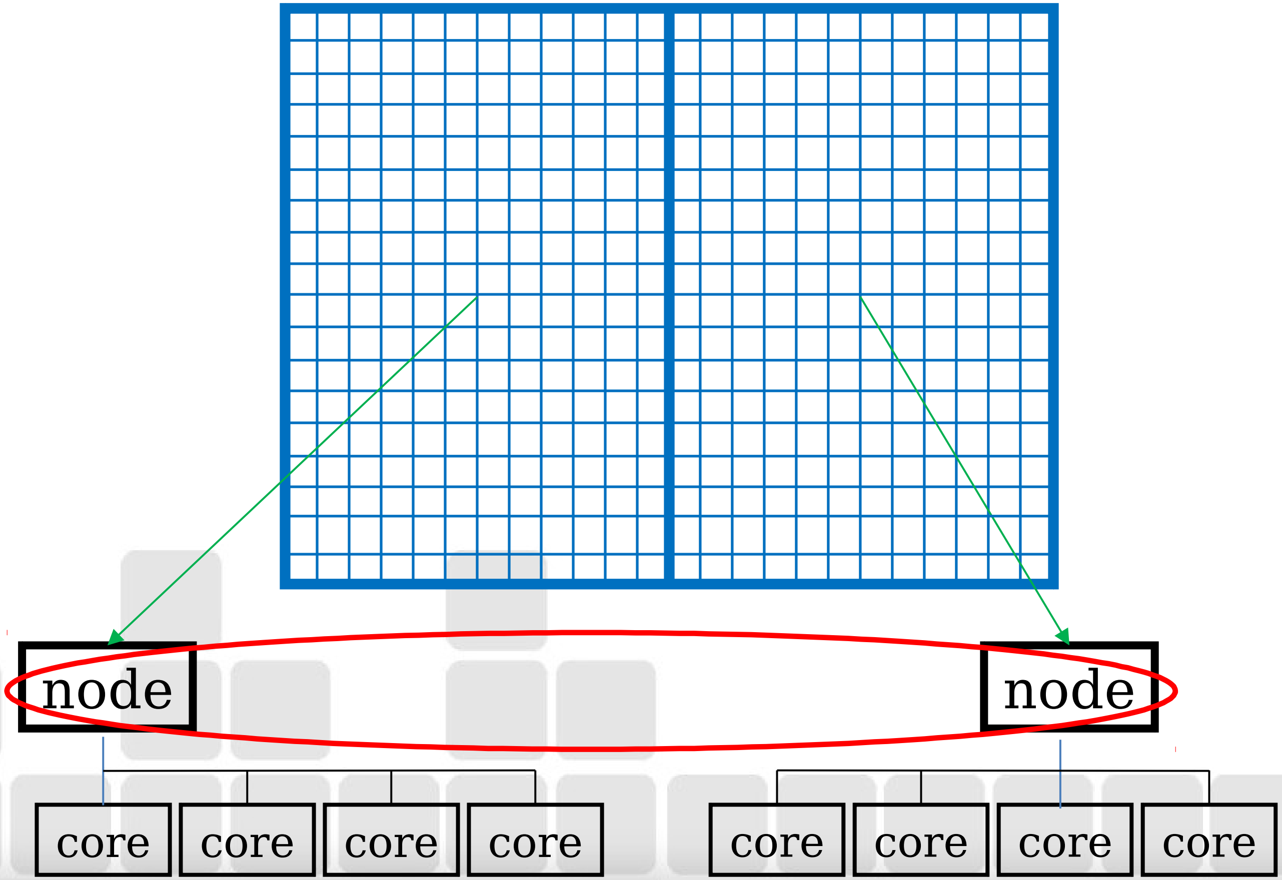
- These equations are well studied, both analytically and computationally.
- One approach is to use finite volume techniques.
  - Divide domain into cells
  - Use discrete representations of the spatial operators for divergence and gradient
  - Use numerical integration to advance solution over time incrementally



- Parallelization techniques are reasonably well established.
  - Divide domain into different grids.
  - Assign grids to nodes, which communicate with each other using MPI
  - Distribute work among cores using OpenMP



- “cori” has ~9,000 nodes, each capable of spawning 68 threads.
- Using this technique, many have been able to perform simulations on full supercomputers.



More Elaborate Models

- Our models for combustion, supernovae, and mesoscopic flow are based on the compressible Euler equations, but with more physics
  - Diffusion of mass, momentum, and energy
  - Reactions
  - Thermal fluctuations in the form of stochastic (random) noise fields

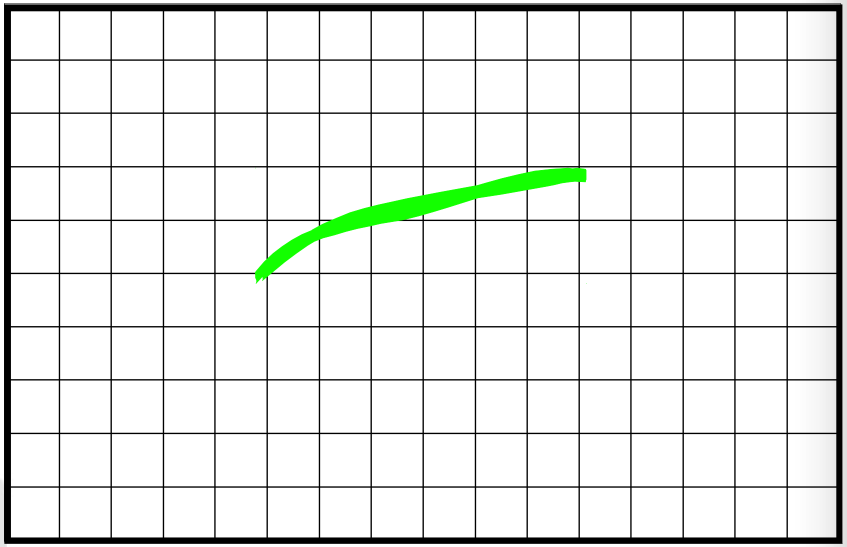
Computational Challenges

- Even with supercomputers, high resolution simulations can be very <u>expensive</u>.
  - Combustion models can have hundreds of reactions, and species, requiring ~hundreds of billions of degrees of freedom to resolve features appropriately
  - Stars are very large, dividing them up into billions of cells is still very poor resolution (1km zones).
  - Mesoscopic simulations need to run for very long times in order to generate proper statistical results for how thermal fluctuations affect the flow field.

- Solutions:
  - More efficient algorithms
  - More efficient models (can be numerically solved faster).

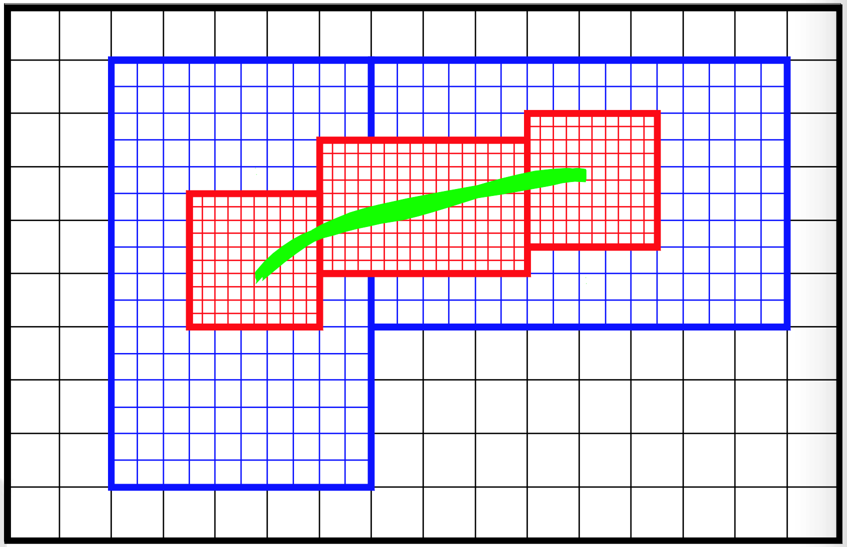
Adaptive Mesh Refinement

- Say we are running a simulation, and there is some interesting feature we would like to take a closer look at.

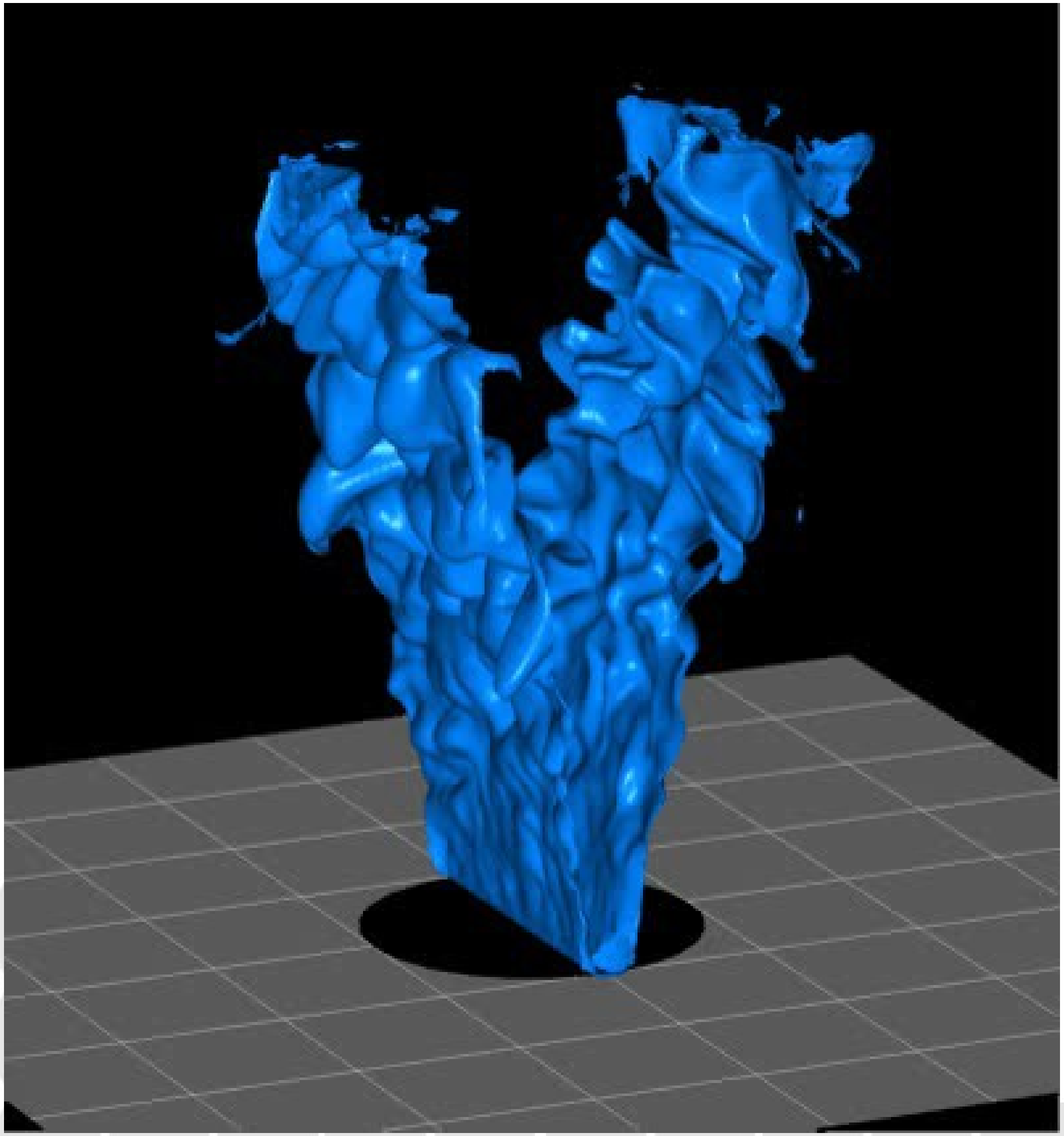


Adaptive Mesh Refinement

- We can use Adaptive Mesh Refinement (AMR) techniques to enhance spatial resolution in regions of interest.
- Furthermore, we can focus the use of smaller time steps (for increased accuracy) in regions of interest.

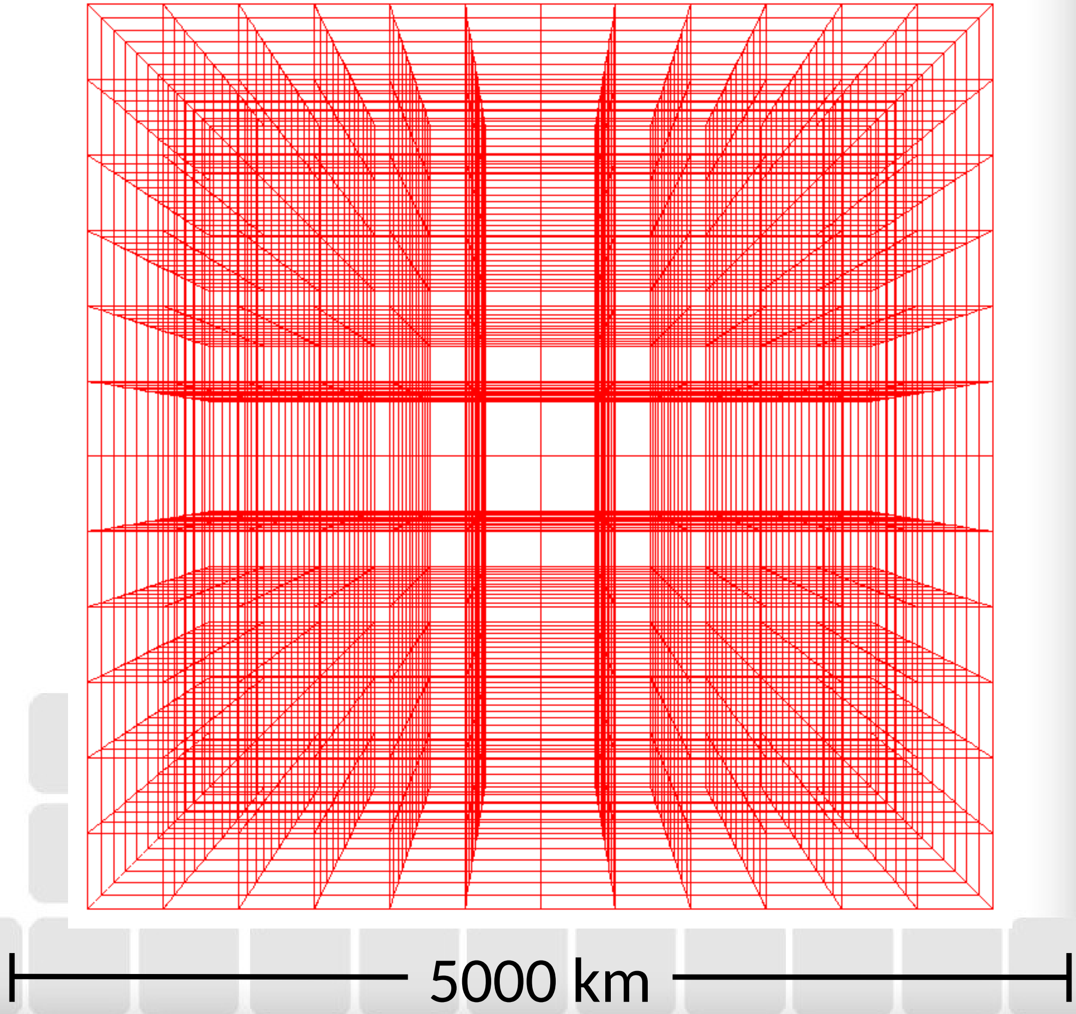


AMR in Combustion



- Depending on the application, you can gain 1-3 orders of magnitude of efficiency using AMR.
- Another example: full star simulations of convection preceding the explosion phase of supernovae

- 576^3 (8.7 km)
  - 1728 · 48^3 grids
  - 191 Million Cells

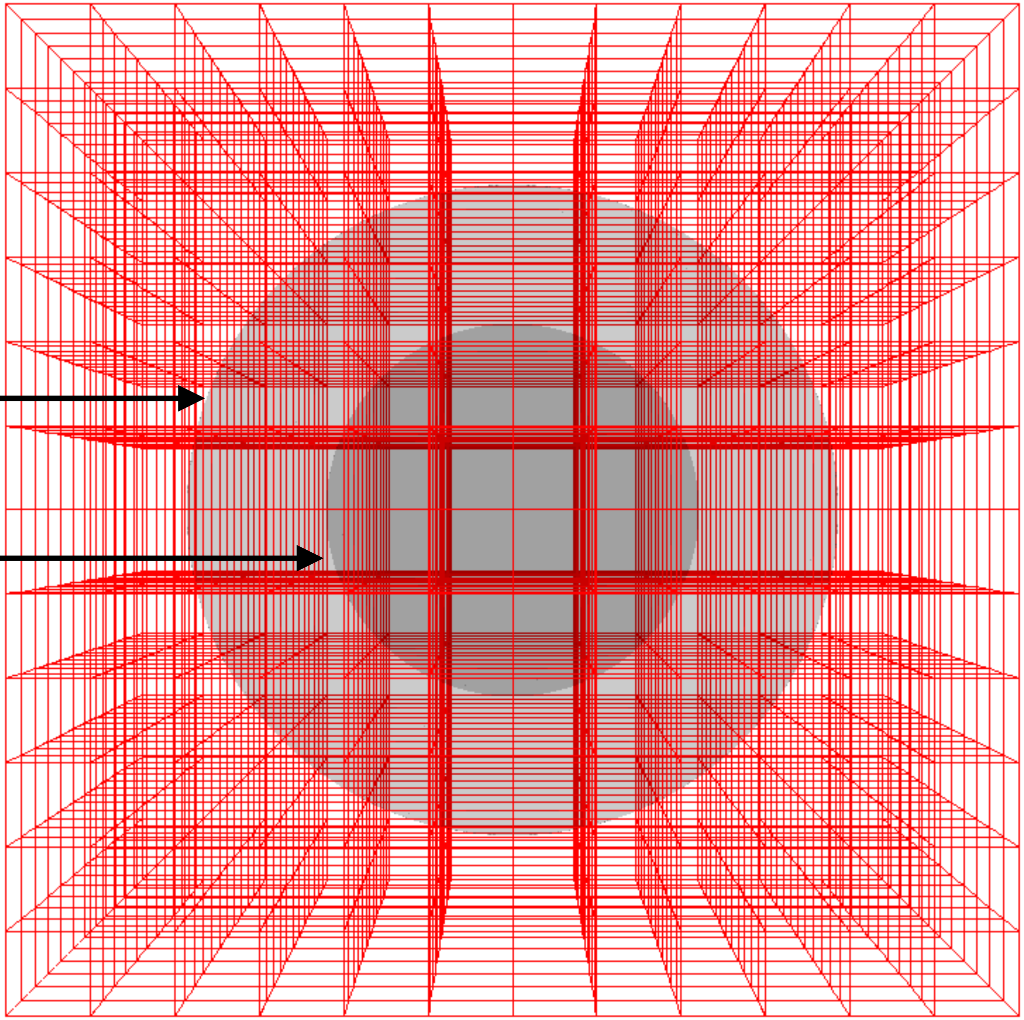


Adaptive Mesh Refinement

- 576^3 (8.7 km)
  - 1728 · 48^3 grids
  - 191 Million Cells

Edge of Star

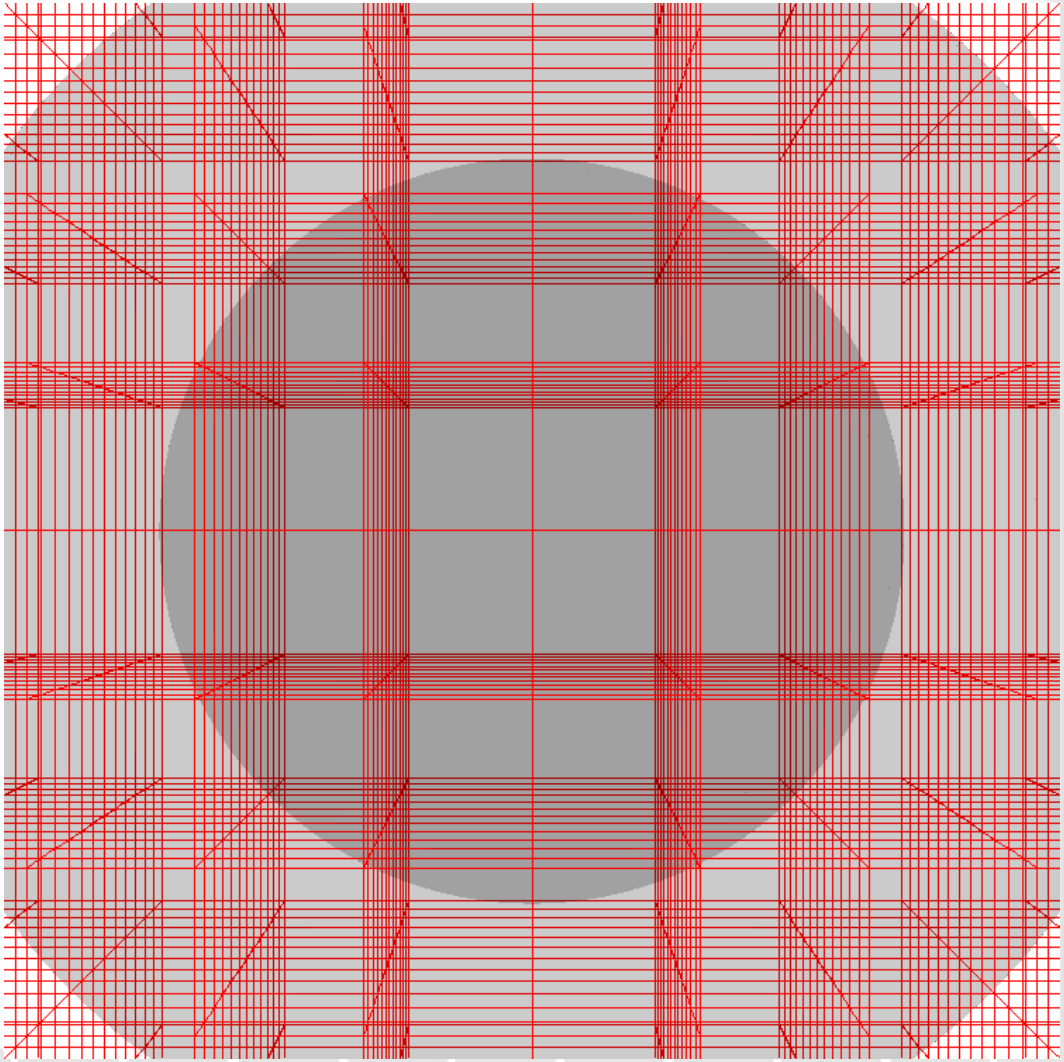
Boundary encapsulating most energetic reactions



5000 km

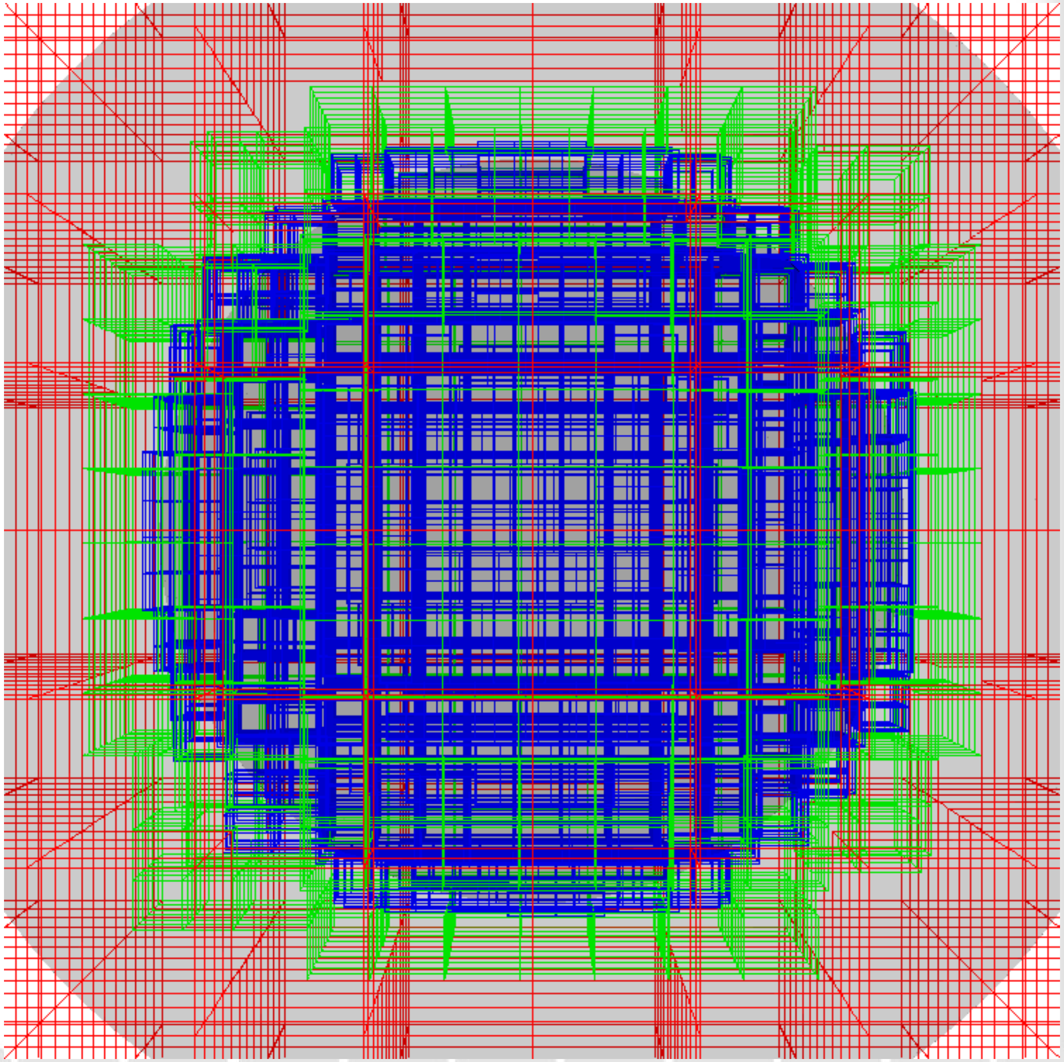
Adaptive Mesh Refinement

- 576^3 (8.7 km)
  - 1728 · 48^3 grids
  - 191 Million Cells



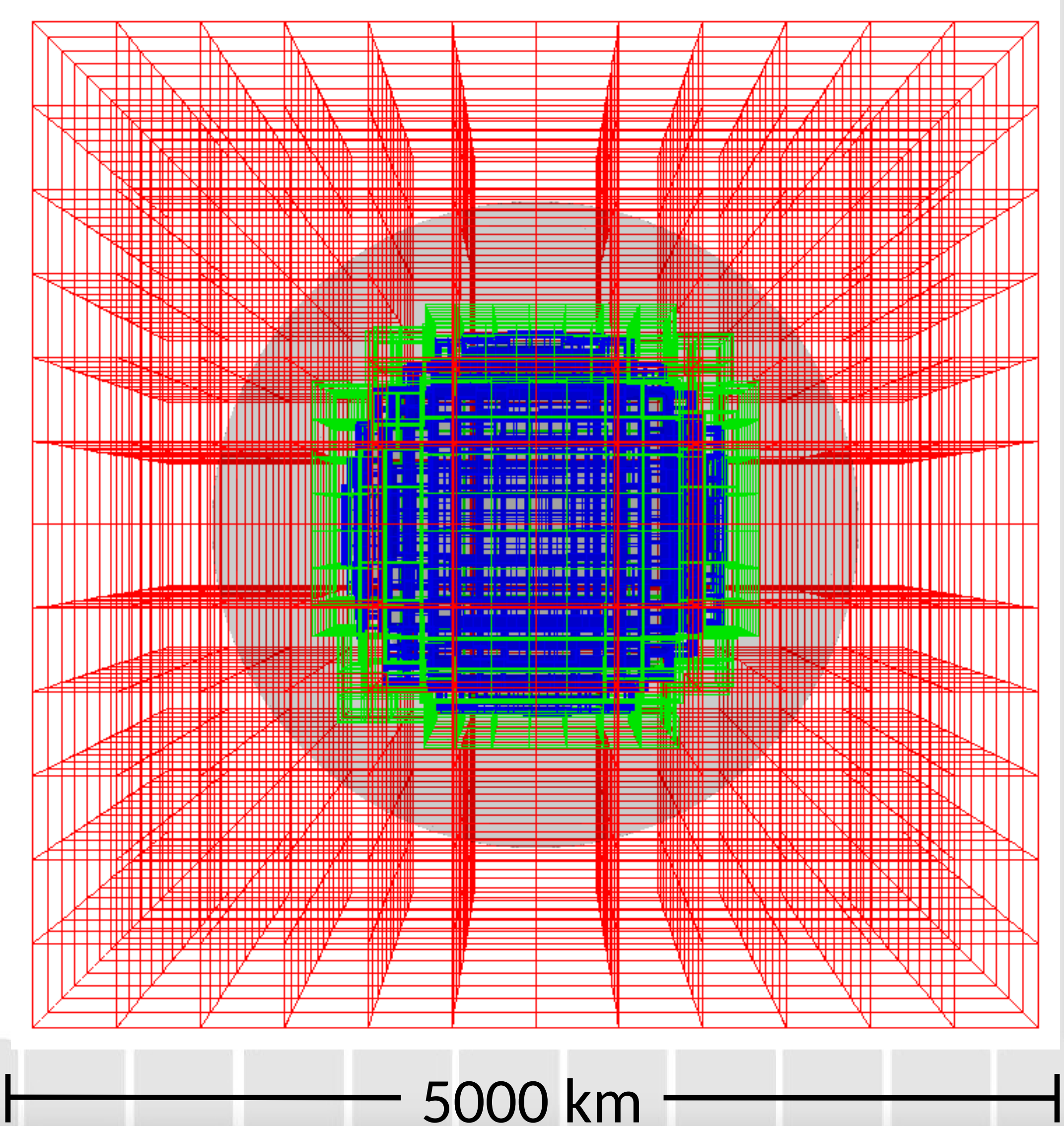
Adaptive Mesh Refinement

- 576^3 (8.7 km)
  - $1728 \cdot 48^3$ grids
  - 191 million cells
- 1152^3 (4.3 km)
  - 1684 grids
  - 148 million cells
  - 9.7% of domain
- 2304^3 (2.2 km)
  - 3604 grids
  - 664 million cells
  - 5.4% of domain



Adaptive Mesh Refinement

- A 2304^3 simulation with no AMR would contain 12.2 billion cells.
- Our simulation contains a total of 1.0 billion cells, requiring a factor of 12 less work.

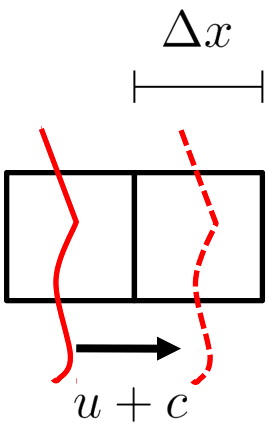


Low Mach Number Flow

- Another common feature to the applications I will discuss is that they have low speed flows.
  - Fluid velocity is much smaller than the sound speed.
  - Sound waves carry little energy, do not significantly affect the solution.
  - These are so-call “low Mach number flows”, since the Mach number is defined as Ma = U / c
    - Characteristic fluid velocity divided by characteristic sound speed.
  - In our applications, the Mach number (Ma) is ~O(0.01)

Compressible Time Step Limit

- Sound waves are very expensive to compute. Why? The sound speed, “c”, is often much larger than the fluid velocity, “u”.



Front propagating at “u+c”.

- Many computational approaches have limits on the time step, dictated by the fact that information cannot move more than one cell per time step (or the method becomes unstable)

$$\Delta t_{\text{compressible}} < \frac{\Delta x}{|u| + c}$$

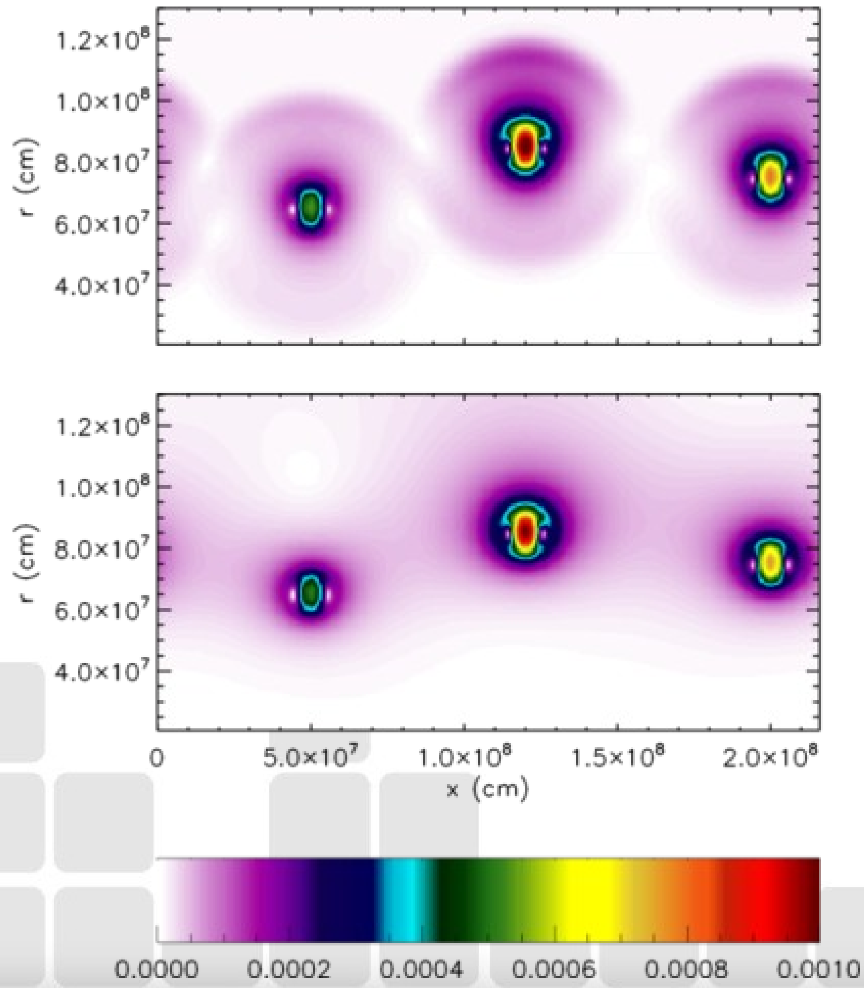
Low Mach Number Time Step Limit

- We research asymptotic models that contain most of the important physics (convection, diffusion, reaction, stochastic noise), while eliminating sound waves.
- Net result – fast sound waves are not part of our model, and we can take time steps that are orders of magnitude larger!

$$\Delta t_{\mathrm{lowMach}} < \frac{\Delta x}{|u|} \qquad \rightarrow \qquad \Delta t_{\mathrm{lowMach}} \gg \Delta t_{\mathrm{compressible}}$$

- To be more precise, the time step is a factor of ~1/Ma larger.

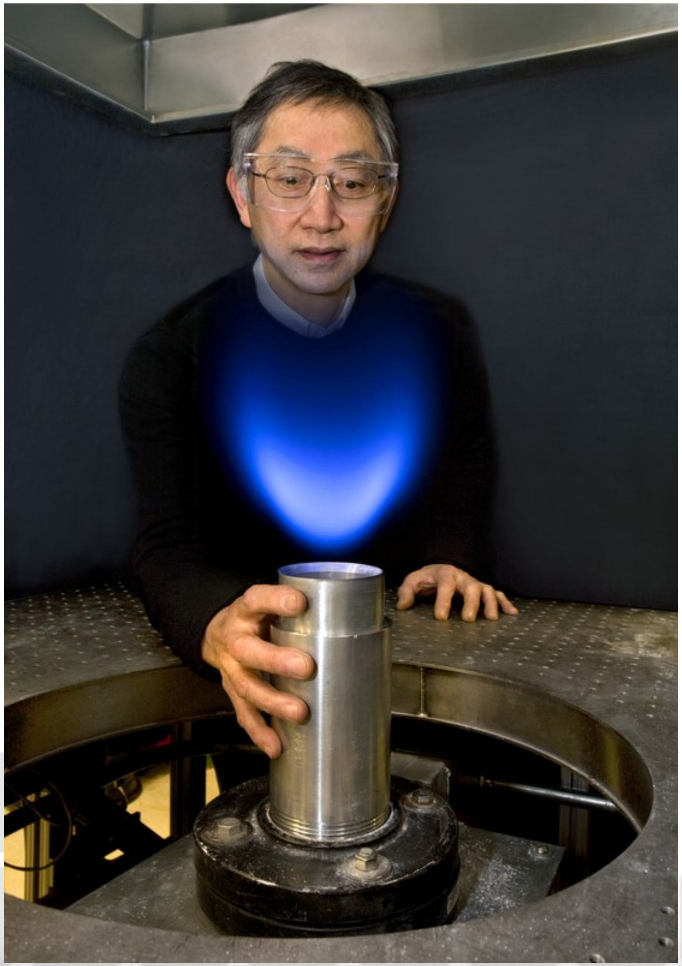
- White dwarf stellar environment with rising hot bubbles. Top is a compressible code, bottom is a low Mach code.
  - Low Mach code captures the same dynamical movement without sound/pressure waves



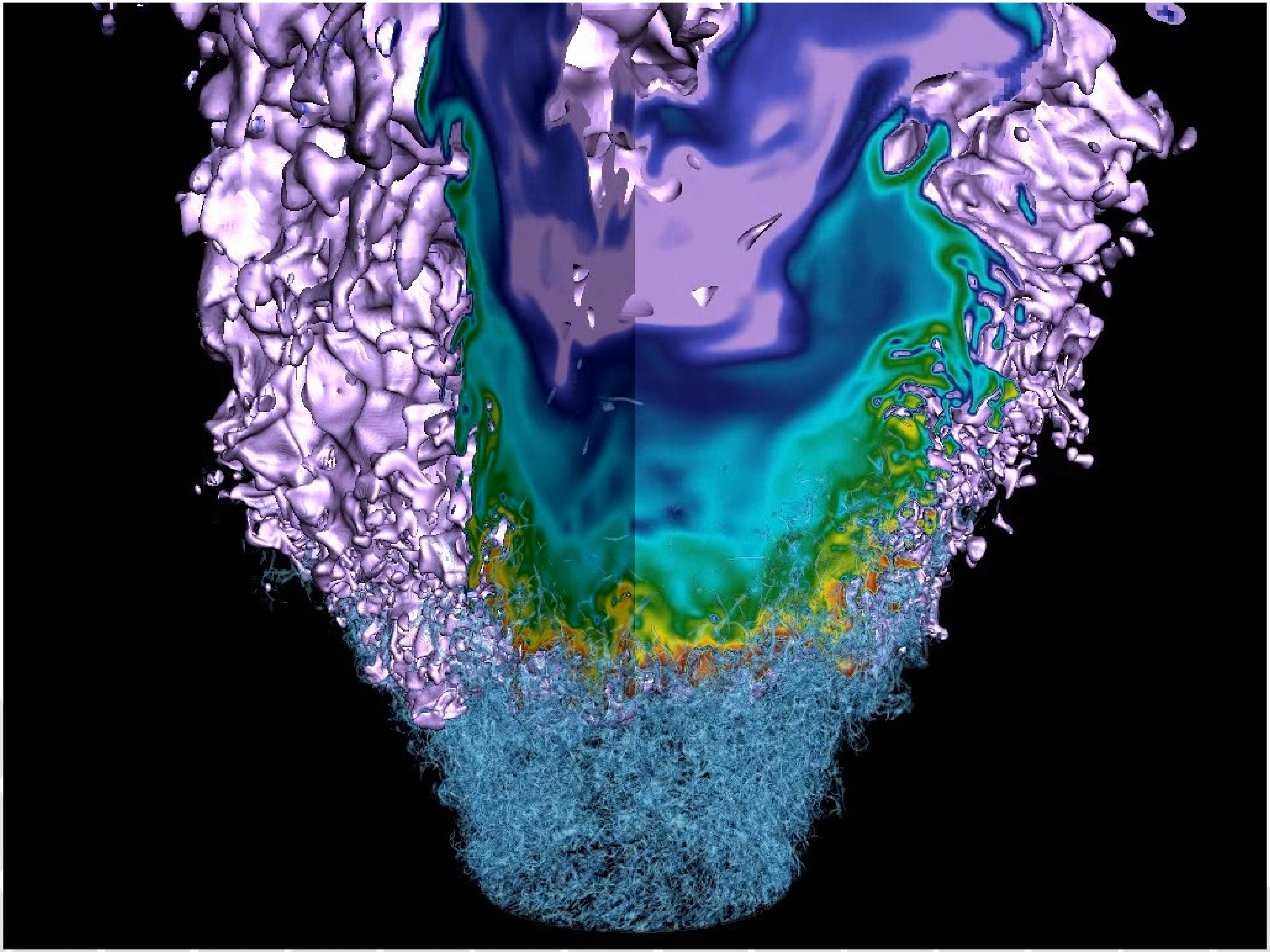
- Altogether, combining AMR with low Mach number modeling, we can perform computations 10,000x (or greater) more efficiently than standard single-grid, compressible approaches.
- Combine this with the factor of 100,000x increase in computational power over the last 20 years…

Combustion

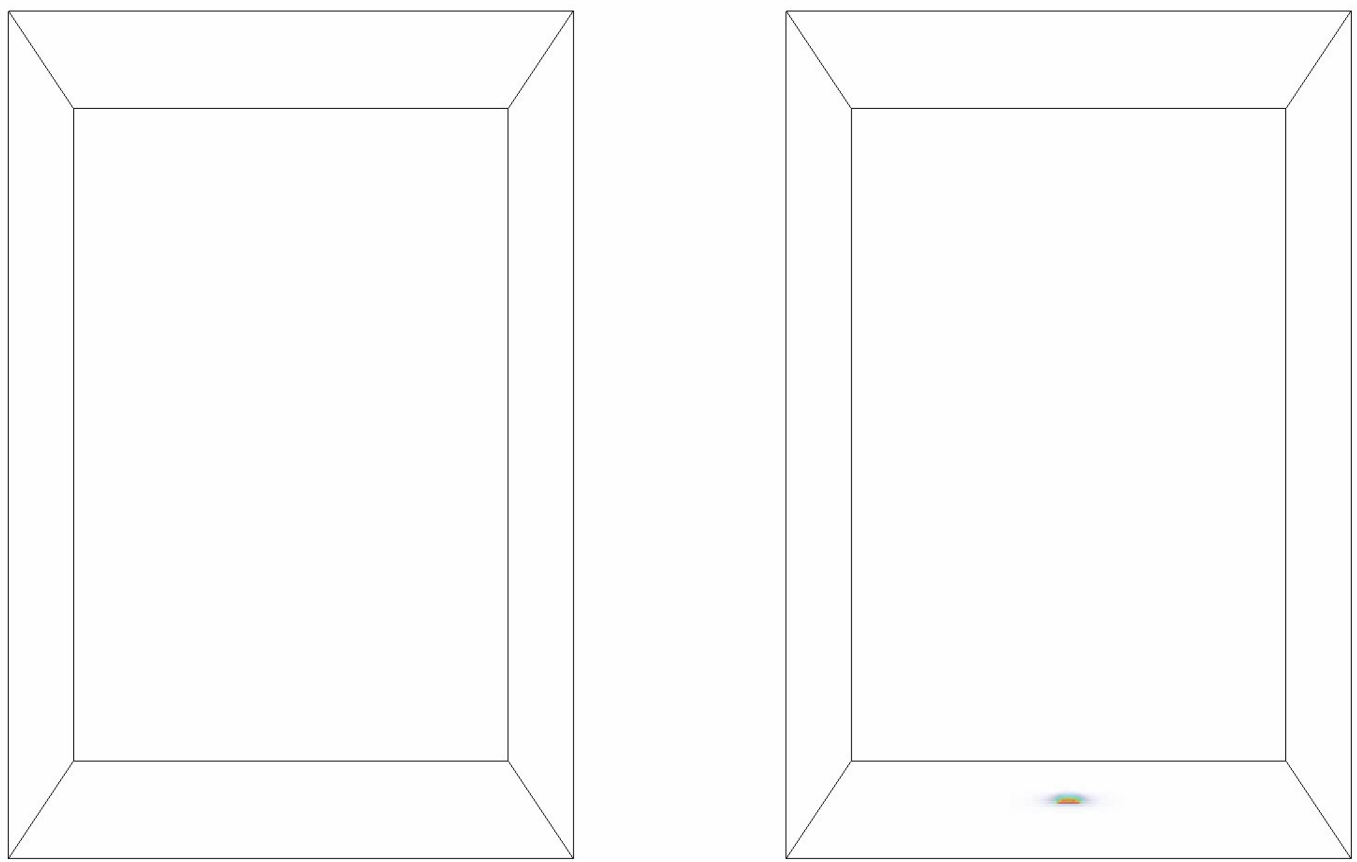
- We work with combustion scientists to perform comparison and characterization of laboratory-scale flames.

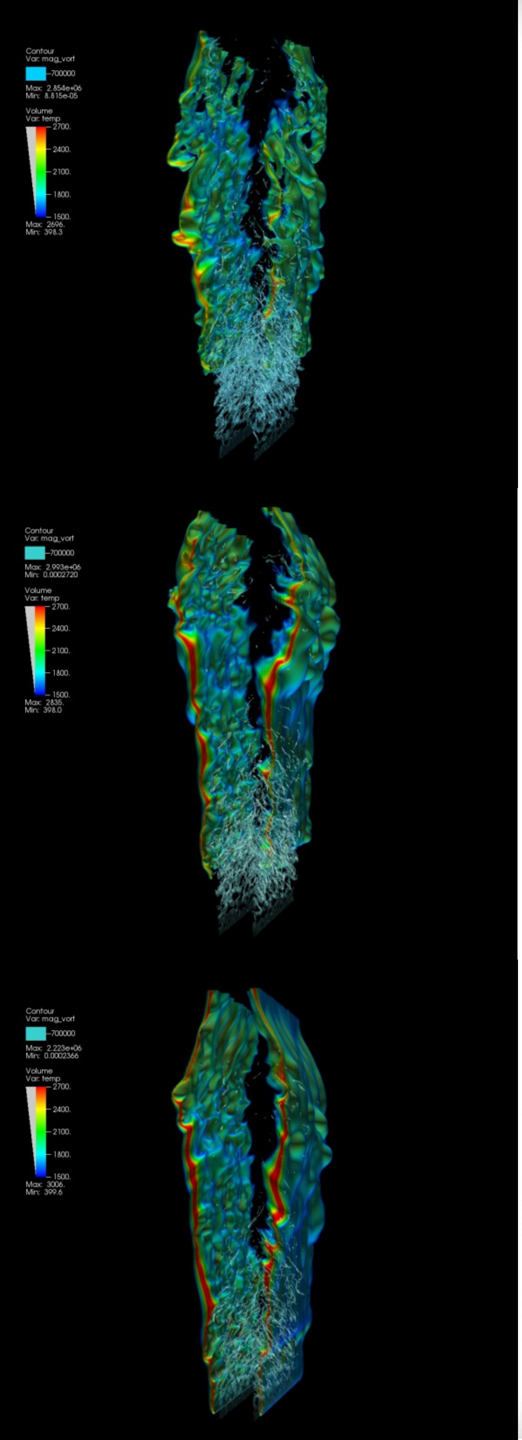


- A hydrogen flame run using NERSC resources (a few thousand CPUs). Color is the mass fraction of OH^- "Clouds" are contours of vorticity.

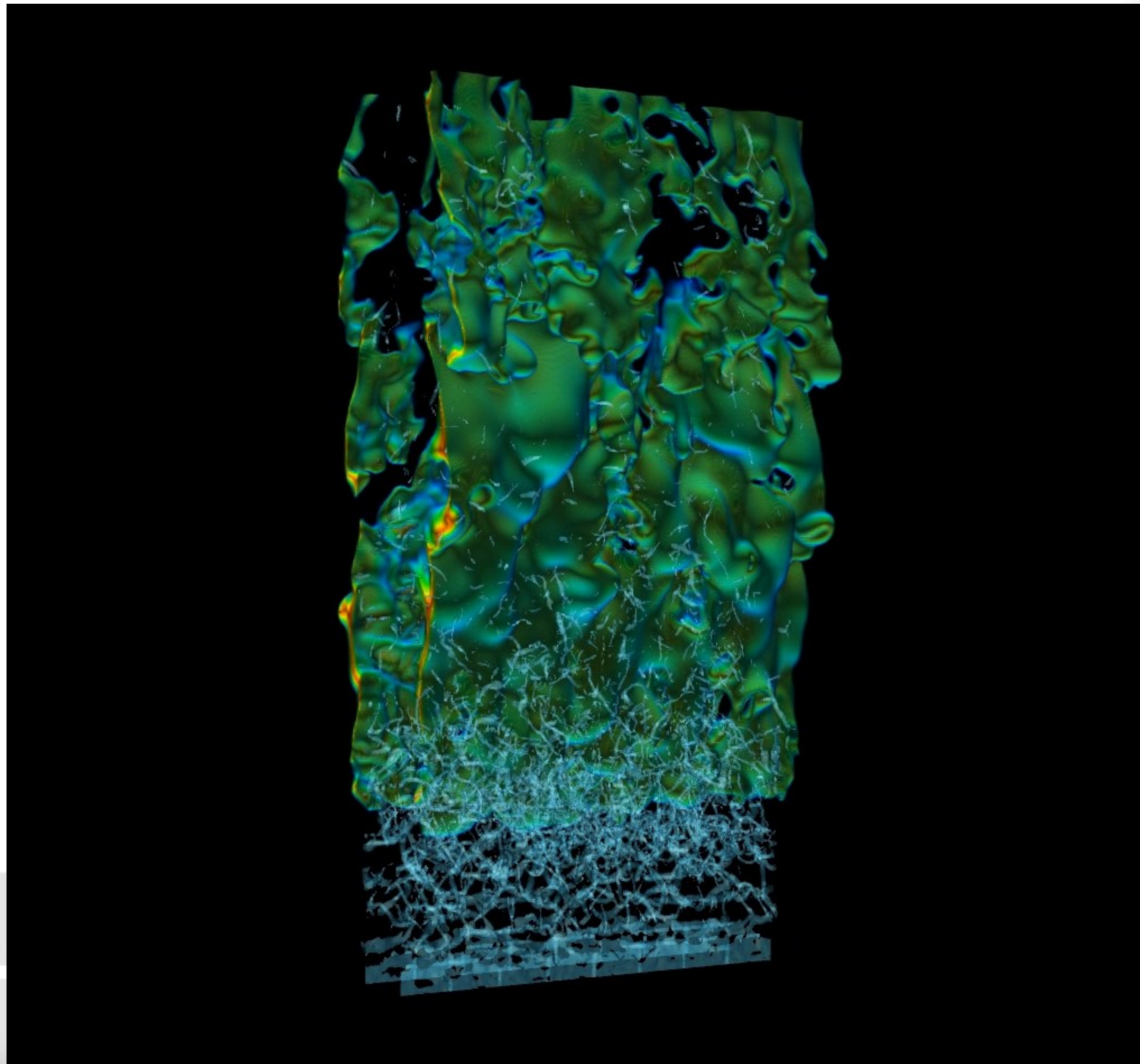


- A “small” calculation (done on my desktop) of a Dodecane jet flame. (temperature on left, vorticity on right)





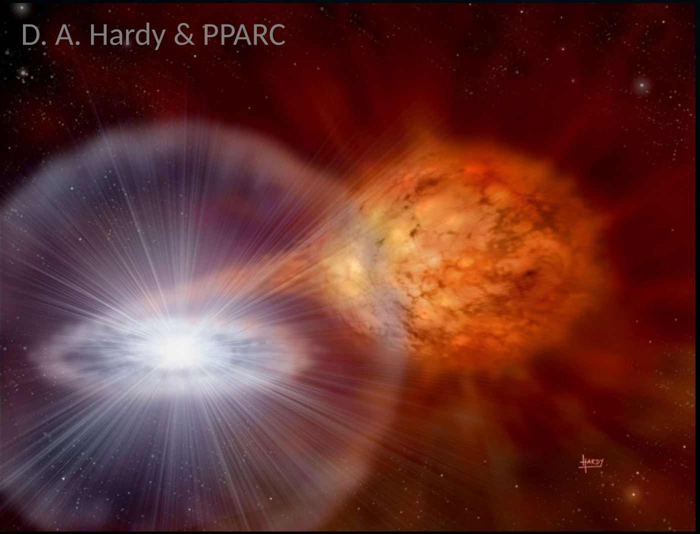
- A dimethyl ether flame run on NERSC resources (a few thousand CPUs). Color is temperature.



Astrophysics

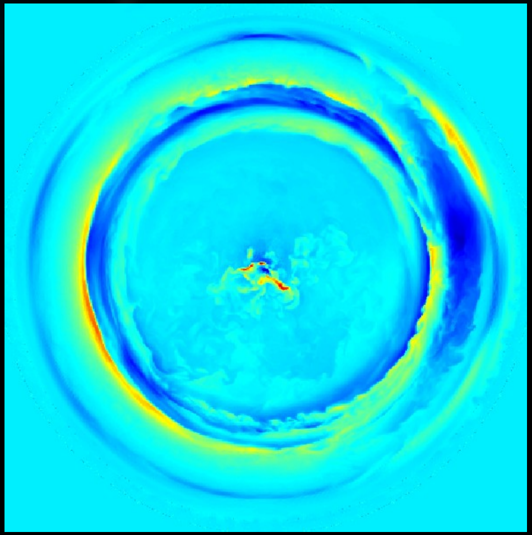
- We work with astrophysicicists to come up with models for supernovae.

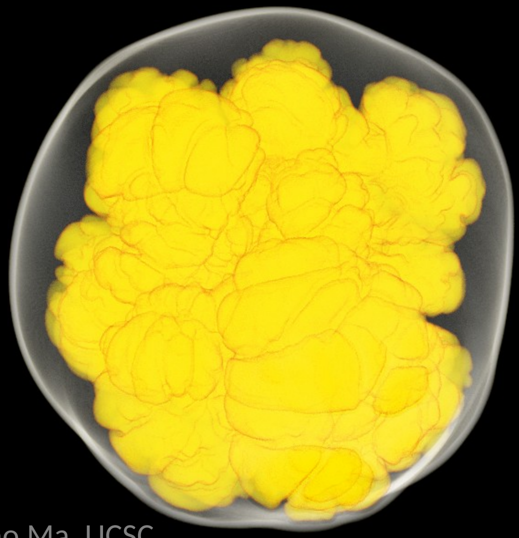
THE PHASES OF TYPE IA SUPERNOVAE: SINGLE DEGENERATE MODEL



A white dwarf accretes matter from a binary companion over millions of years.

Smoldering phase characterized by subsonic convection and gradual temperature rise lasts hundreds of years.





Flame (possibly) transitions to a detonation, causing the star to explode within two seconds.

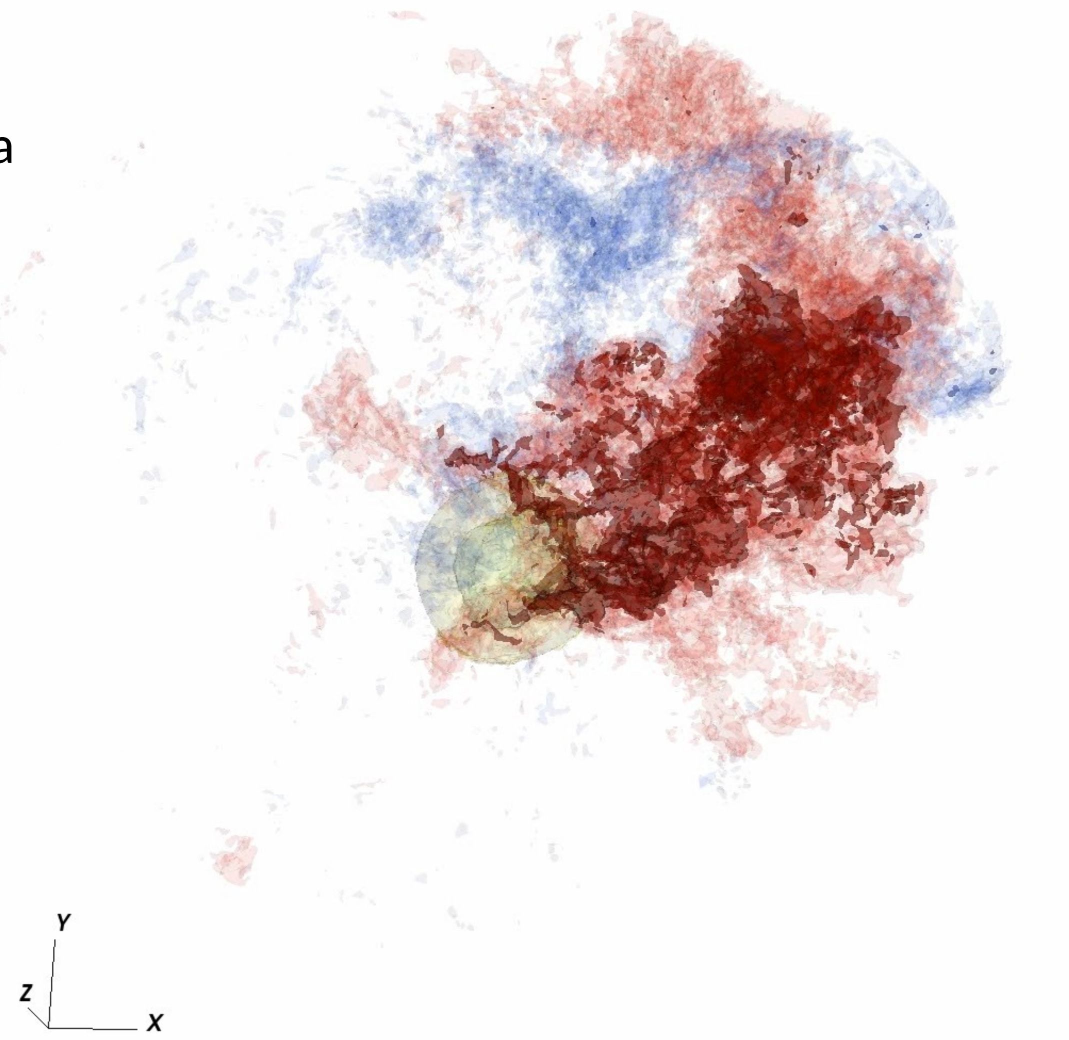
The resulting event is visible from Earth for weeks to months.

Haitao Ma, UCSC

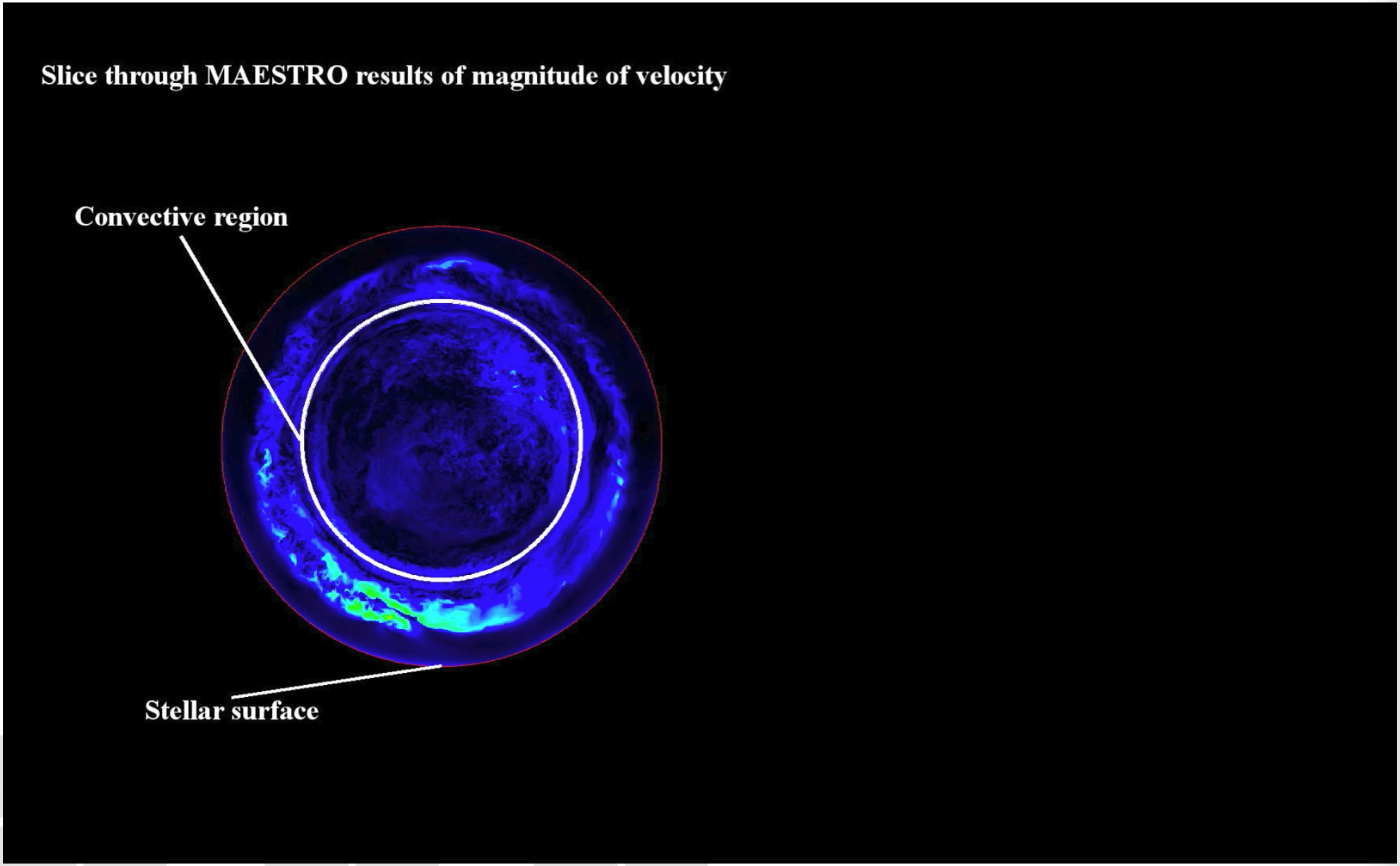
SN 1994D (High-Z SN Search team)

White Dwarf Convection Preceding Ignition

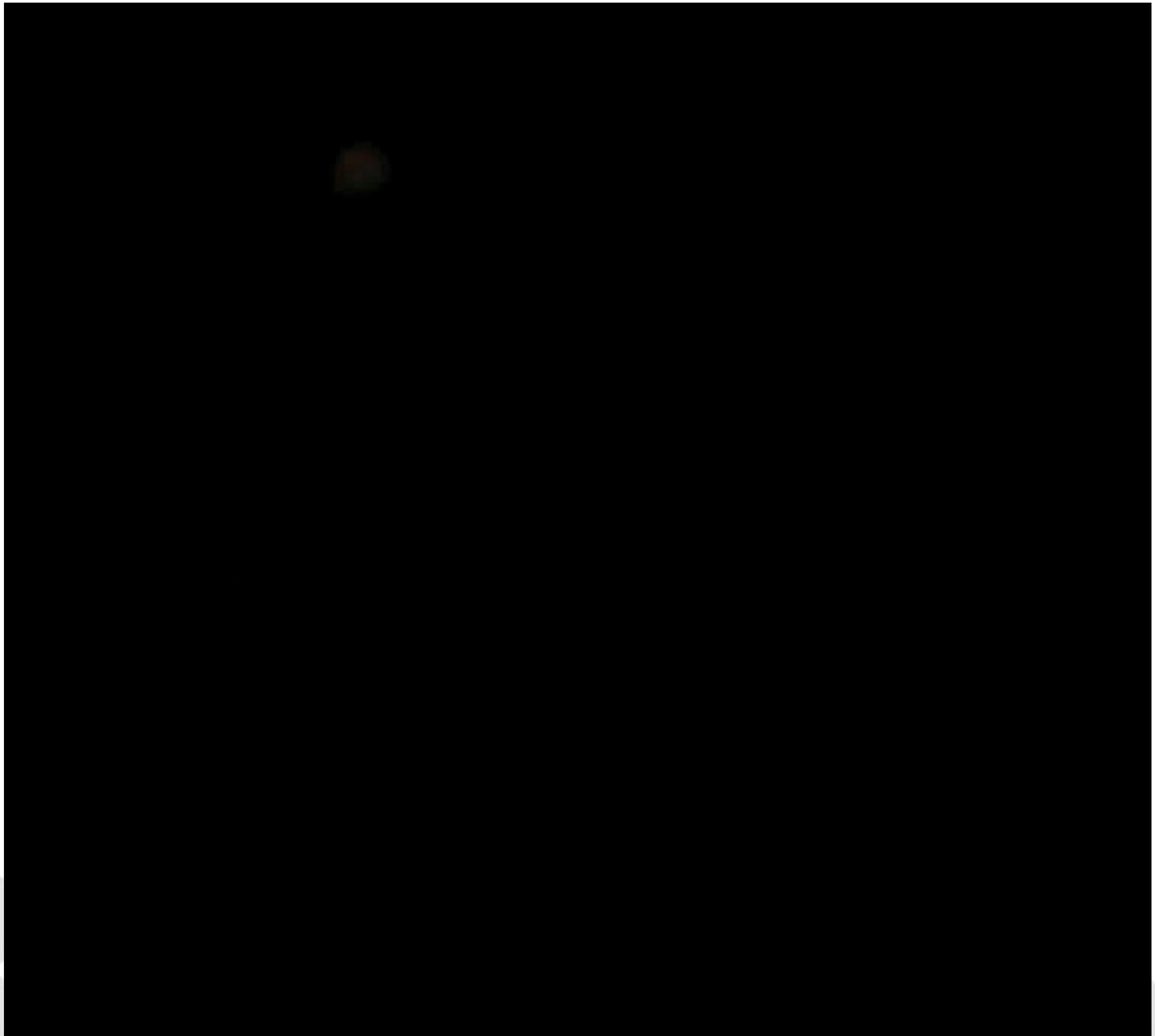
- Convective flow pattern a few minutes preceding ignition
  - Inner 1000 km^3 of star
  - Effective 2304^3 resolution (2.2km) with 3 total levels of refinement
  - Red / Blue = outward / inward radial velocity
  - Yellow / Green = contours of increasing burning rate



Post Ignition Simulations

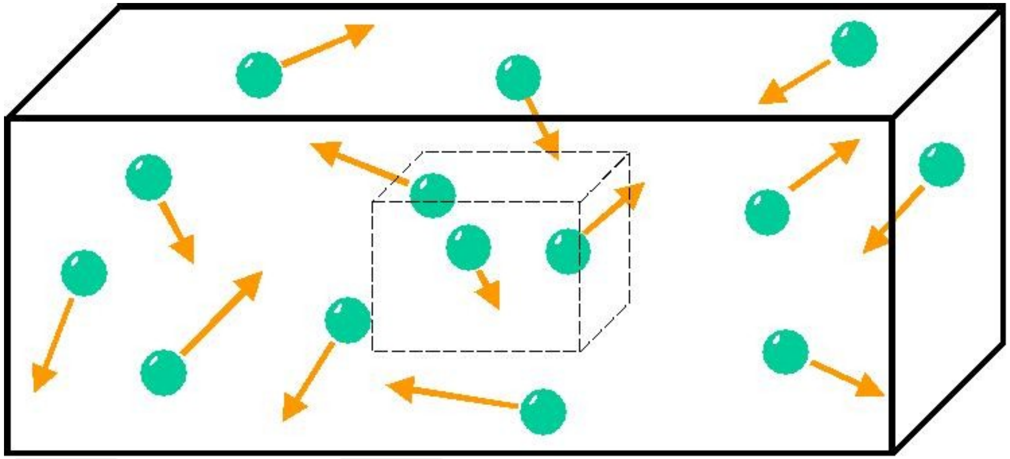


Post Ignition Simulations



Fluctuating Hydrodynamics

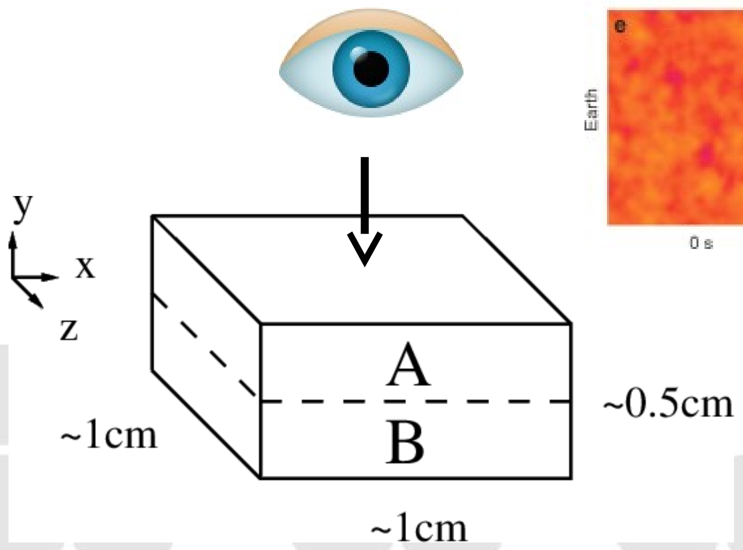
- We seek to understand the dynamics of fluid mixing at the microscale. Fluids are composed of molecules whose positions and velocities are random at thermodynamic scales. Long-range correlations between fluctuations causes macroscopic structures to form.

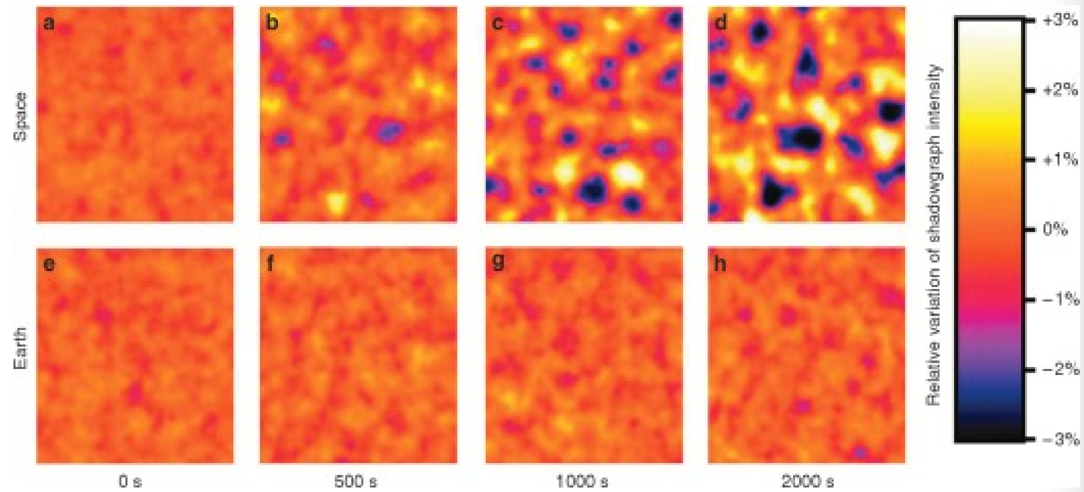


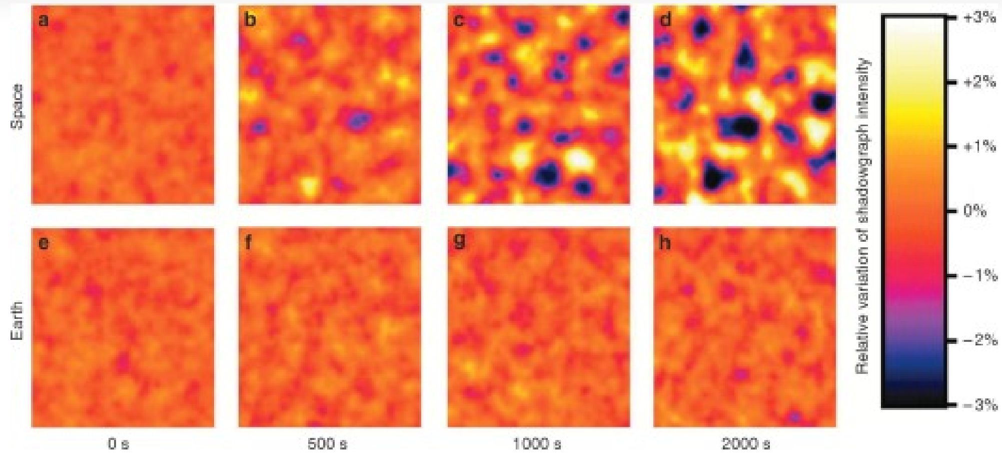
- We derive low Mach number models for stochastic PDEs with random forcing representing thermal fluctuations.

Fluctuating Hydrodynamics

- We simulate a diffusive layer convection instability, where a salt solution on top of a denser sugar solution in the absence of gravity leads to giant fluctuations



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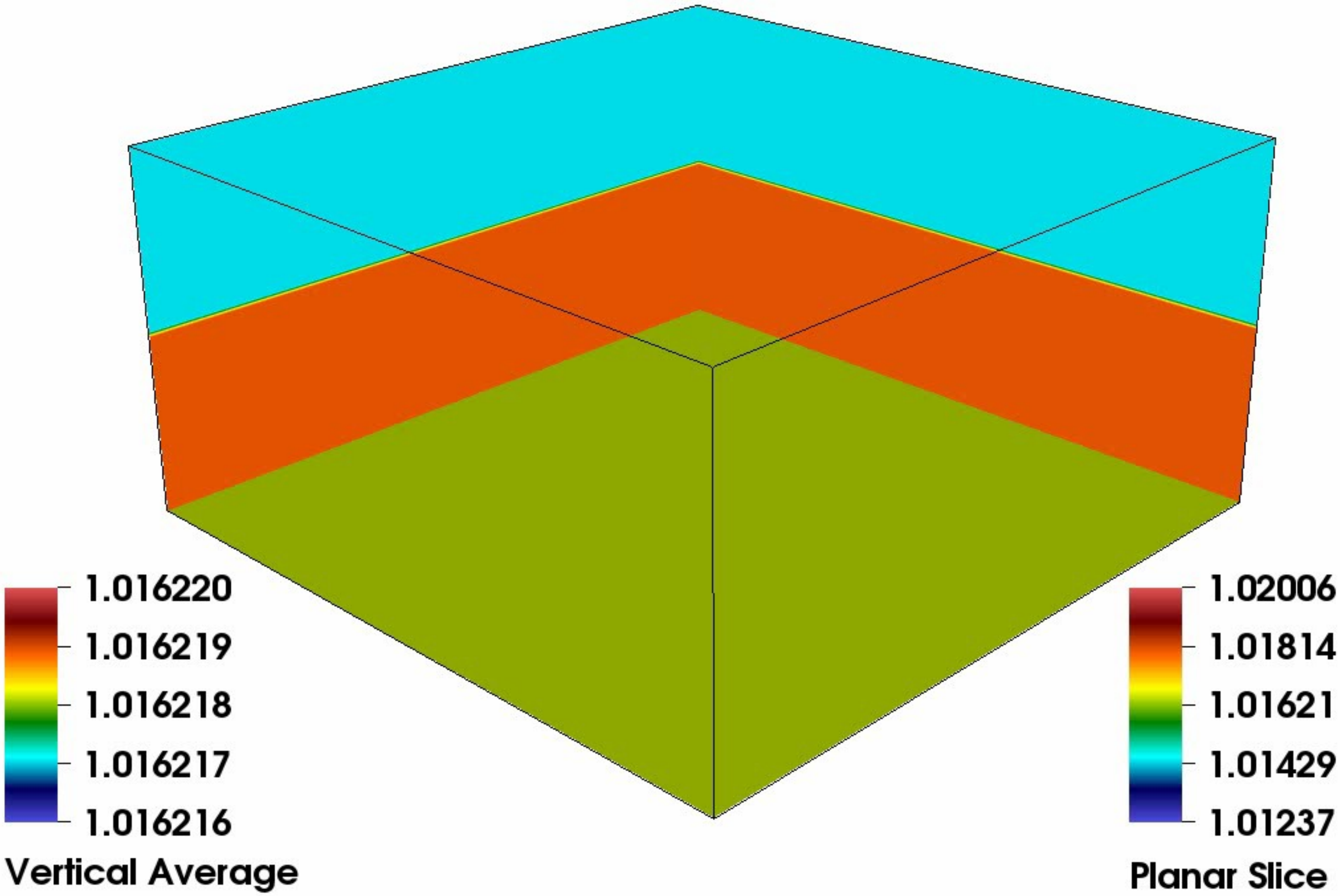
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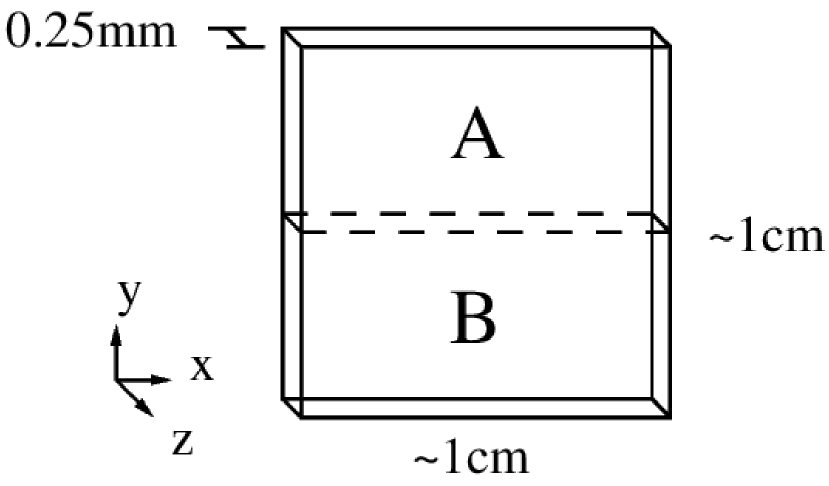
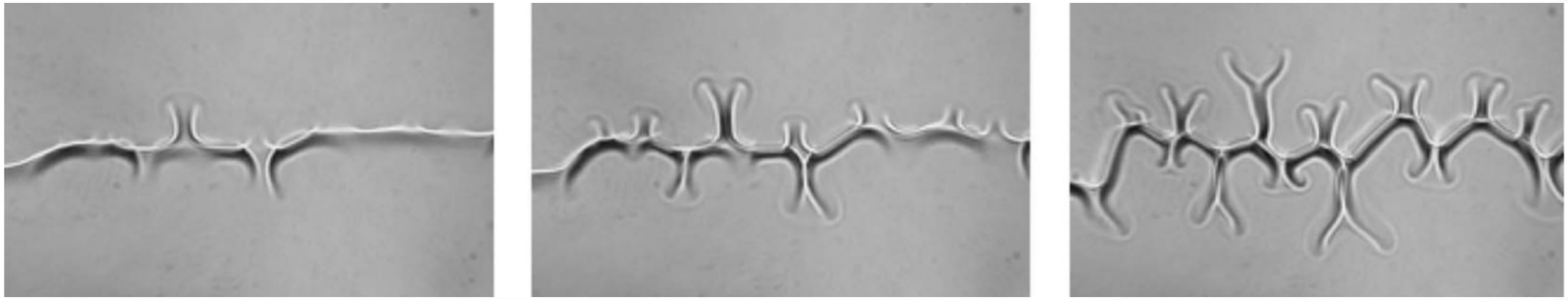
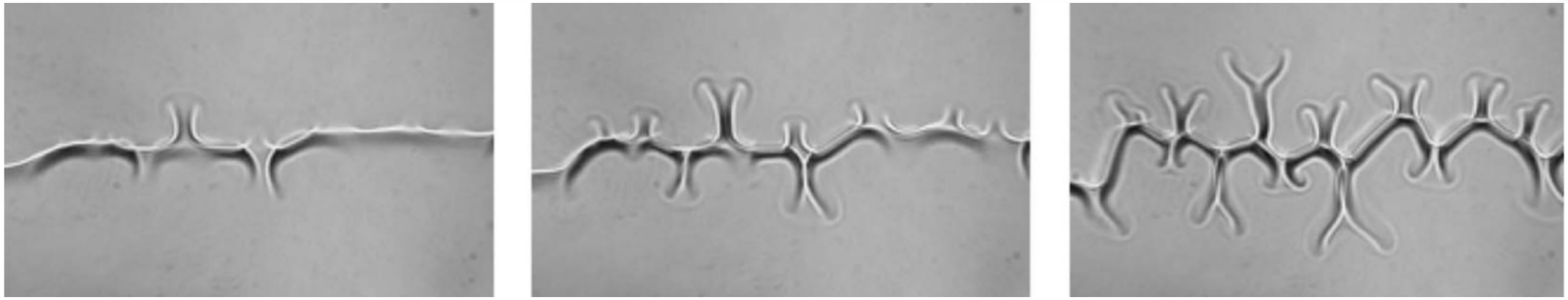
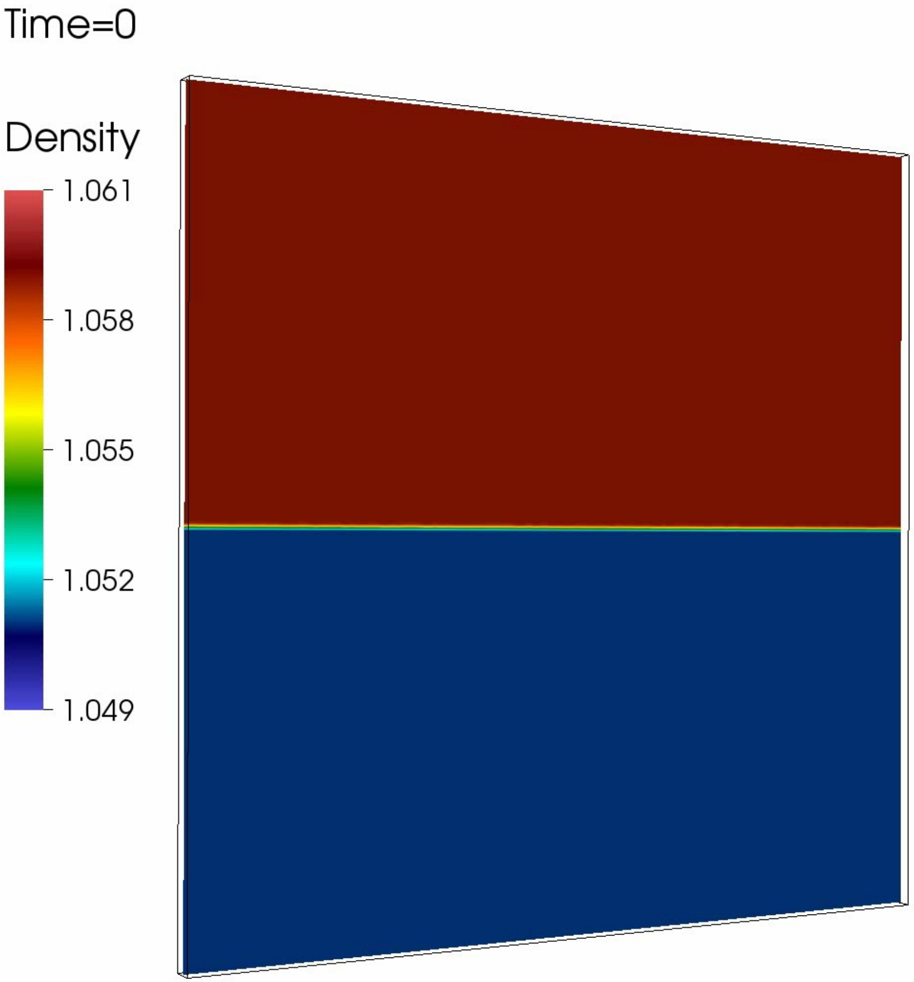
Planar Slice

- We simulate a mixed-mode instability, where a dense salt solution on top of a less-dense sugar solution develops Y-shaped fingers.





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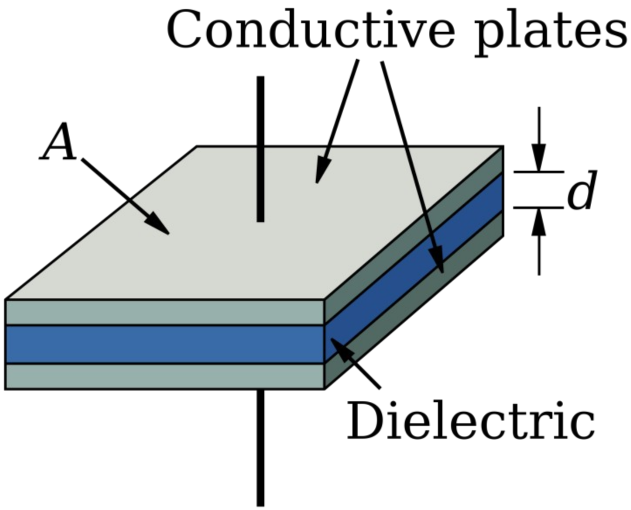
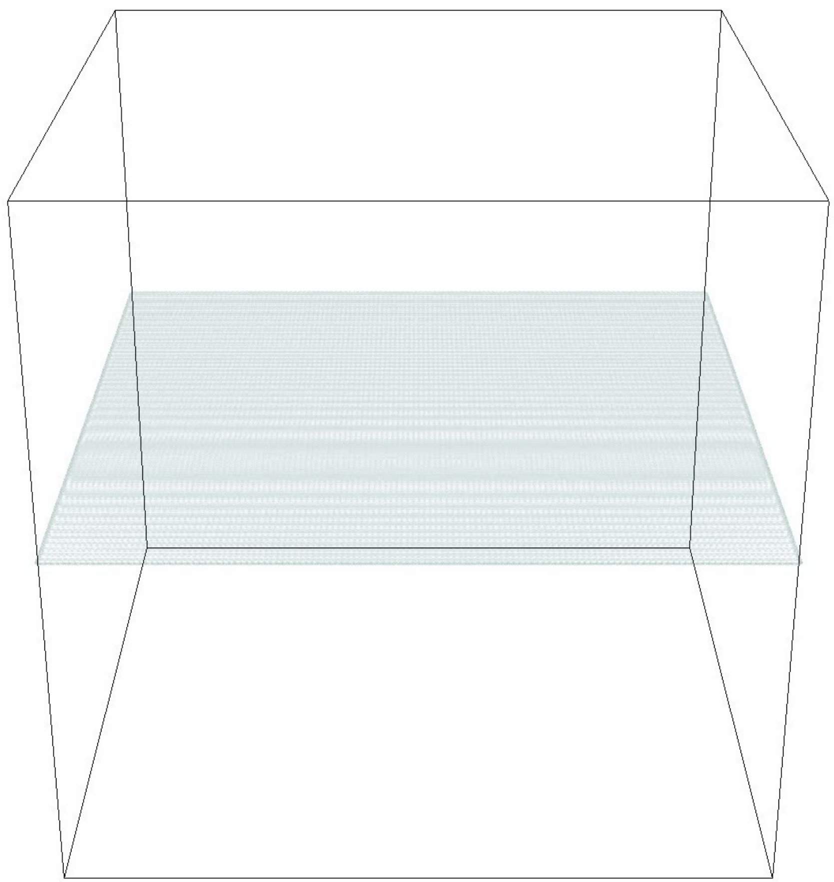
- We model instabilities in ionic solutions when exposed to an electric potential.
  - Salt water on top of fresh water





Summary

- Mathematical models derived from classic compressible fluid equations.
- Advanced numerical techniques such as AMR
- Supercomputing resources
- Collaboration with application scientists

- Cutting edge simulations in a variety of fluid mechanics applications.