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

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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.
Center for Computational Sciences and Engineering

• CCSE focuses on simulations of “multiscale, multiphysics, partial differential equations”.

  – FLUIDS!!!
Center for Computational Sciences and Engineering

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

\[ \frac{\partial \rho}{\partial t} = -\nabla \cdot (\rho u) \]  
conservation of mass

\[ \frac{\partial \rho u}{\partial t} = -\nabla \cdot (\rho uu) + \nabla p \]  
conservation of momentum

\[ \frac{\partial \rho E}{\partial t} = -\nabla \cdot ((\rho E + p)u) \]  
conservation of energy

\( \rho \) mass density
\( u \) velocity
\( E \) total energy density
\( p \) pressure

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

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

- What do these equations describe?
  - Convection/Advection (stuff 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 expensive.
  – 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)
  – $1728 \cdot 48^3$ grids
  – 191 Million Cells
Adaptive Mesh Refinement

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Edge of Star
Boundary encapsulating most energetic reactions

5000 km
Adaptive Mesh Refinement

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Adaptive Mesh Refinement

- $576^3$ (8.7 km)
  - 1728 · $48^3$ 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.

5000 km
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 $Ma = \frac{U}{c}$
    - Characteristic fluid velocity divided by characteristic sound speed.
  - In our applications, the Mach number (Ma) is $\sim O(0.01)$
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”.

- 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!

\[ \Delta t_{\text{lowMach}} < \frac{\Delta x}{|u|} \quad \rightarrow \quad \Delta t_{\text{lowMach}} \gg \Delta t_{\text{compressible}} \]

• To be more precise, the time step is a factor of \( \sim 1/\text{Ma} \) 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 astrophysicists 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.
White Dwarf Convection Preceding Ignition

- Convective flow pattern a few minutes preceding ignition
  - Inner 1000 km³ of star
  - Effective 2304³ resolution (2.2km) with 3 total levels of refinement
  - Red / Blue = outward / inward radial velocity
  - Yellow / Green = contours of increasing burning rate

![Image of convective flow pattern]
Post Ignition Simulations

Slice through MAESTRO results of magnitude of velocity

Convective region

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