In memoriam: Michael Welcome 1957 - 2014 RIP





Low Mach Number Models in Computational Astrophysics

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Introduction

We often associate astrophysics with explosive phenomena:

- novae
- supernovae
- gamma-ray bursts
- X-ray bursts



Type la Supernovae

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- Largest thermonuclear explosions in the universe
- Brightness rivals that of host galaxy, L 10⁴³ erg / s
- Definition: no H line in the spectrum, Si II line at 6150A.

But explosions are often preceded by long periods of non-explosive fluid dynamics, characterized by low Mach number convective flows.

We need to be able to understand, and simulate, both types of phenomena. Take SNe la as an example.

Why are SNe Ia so important?

1915: Einstein assumed the universe is static – theory of general relativity then needs a "cosmological constant"

1929: Hubble observed all galaxies are moving away from us

 \Rightarrow universe is expanding

1930s - 1970s: rotational speed of galaxies, orbital velocity of galaxies in clusters, gravitational lensing all provide evidence

 \Rightarrow dark matter

Does all this mass mean we are headed for the Big Crunch?



1998 Science Breakthrough of the Year and 2011 Nobel Prize

(Supernova Cosmology Project and High-z Supernova Search Team)



- By observing the duration of distant SNe Ia one could determine their absolute magnitude (standard candles).
- absolute vs. apparent brightness \rightarrow distance
- distance vs. redshift → Hubble diagram.

This led to the discovery that the rate at which the Universe is expanding is increasing.

 \Rightarrow dark energy

A popular (but not the only) model for SNe Ia is the thermonuclear explosion of a carbon/oxygen white dwarf.



A carbon-oxygen white dwarf accretes mass from a binary companion (≈ 10 million years to reach Chandrasekhar limit)

- Over a period of centuries, carbon burning near the core drives convection and temperature slowly increases.
- Over the last few hours, convection becomes more vigorous as the heat release intensifies and convection can no longer carry away the heat.
- Eventually, the star ignites, and finally explodes within seconds.

SNe Ia: Modeling

Traditional modeling approaches focus on the last few seconds.



Initial conditions:

- Radial profile from 1d stellar evolution code
- Assumptions about when & where of ignition "hot spots"

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Initial conditions:

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- But... the simulated explosions are very sensitive to the initial conditions.
- \Rightarrow We need to know more about how SNe Ia ignite.



Modeling of Type Ia Supernovae

Typically, numerical simulations of SNe Ia have used the compressible Navier-Stokes equations with reactions:

$$\frac{\partial(\rho X_k)}{\partial t} + \nabla \cdot \rho U X_k = \rho \dot{\omega}_k$$
$$\frac{\partial(\rho U)}{\partial t} + \nabla \cdot (\rho U U + \rho) = -\rho g \mathbf{e}_r$$
$$\frac{\partial(\rho E)}{\partial t} + \nabla \cdot (\rho U E + U \rho) = -\rho g (U \cdot \mathbf{e}_r) + \rho \sum_k \rho q_k \dot{\omega}_k$$

ρ	density	
U	flow velocity	
p	pressure	
$E = e + U^2/2$	total energy	

е	internal energy
X _k	mass fractions
$\dot{\omega}_k$	X_k production rate
ġ	gravity

with Timmes equation of state:

$$p(
ho, T, X_k) = p_{ele} + p_{rad} + p_{ion}$$

where

$$p_{ele} = \text{fermi}, \ p_{rad} = aT^4/3, \ p_{ion} = \frac{\rho kT}{m_\rho} \sum_m X_k/A_m$$

We can write the compressible equations as a set of hyperbolic conservation laws with source terms:

 $\mathbf{U}_t + \nabla \cdot \mathbf{F} = \mathbf{S}$

Standard approach: use a time-explicit method to solve the compressible equation set.

Advantages:

- easy to program
- easy to parallelize great weak scaling to 200K cores
- straightforward with AMR (synchronization is explicit as well)

Compressible models work well for modeling the explosion of the star but to capture ignition we need to simulate 2 hours, not 2 seconds.

Convection leading up to ignition is basically infeasible with standard explicit compressible codes (and hasn't been done).

But We Have Supercomputers!

Why not just use a compressible method with AMR and lots of processors?



Even with a code that scales perfectly, explicit methods are **not** parallel in time.

Time-explicit compressible codes use a time step

$$\Delta t < \min\left(\frac{\Delta x}{u+c}\right)$$

We want to eliminate acoustic waves (so they don't limit the time step) but make as few additional limiting assumptions as possible. Specifically we don't want to assume that the density and temperature are always close to the background state or the star will never ignite!

New model needs to incorporate

- Buoyancy
- Background stratification
- Nonideal equation of state
- Reactions and heat release
- Overall expansion of the star

and needs to allow a larger Δt and have lower time-to-solution.

A hierarchy of possible models

Possible "soundproof" models for convective motion:

All of these models allow $\Delta t < \min\left(\frac{\Delta x}{u}\right)$

	Heating-			
	induced		large	General
Model	Buoyancy?	Stratification?	ho', T'?	EOS?
Incompressible	No	No	No	No
Boussinesq	Yes	No	No	No
Anelastic	Yes	Yes	No	No
Pseudo-				
incompressible	Yes	Yes	Yes	No
Low M	Yes	Yes	Yes	Yes

In addition, the low Mach number model allows the background state of the star to expand with large-scale heating

Buoyant bubble rise



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Low Mach Number Approach

Asymptotic expansion in the Mach number, M = |U|/c, leads to a decomposition of the pressure into thermodynamic and dynamic components:

$$p(\mathbf{x},t) = p_0(r,t) + \pi(\mathbf{x},t)$$

where $\pi/p_0 = O(M^2)$.

- p_0 affects only the thermodynamics; π affects only the local dynamics,
- Physically: acoustic equilibration is instantaneous; sound waves are "filtered" out
- Mathematically: resulting equation set is no longer strictly hyperbolic; a constraint equation is added to the evolution equations
- Computationally: time step is dictated by fluid velocity, not sound speed.

Low Mach Number Model

$$\begin{aligned} \frac{\partial(\rho X_k)}{\partial t} &= -\nabla \cdot (U\rho X_k) + \rho \dot{\omega}_k ,\\ \frac{\partial(\rho h)}{\partial t} &= -\nabla \cdot (U\rho h) + \frac{Dp_0}{Dt} - \sum_k \rho q_k \dot{\omega}_k ,\\ \frac{\partial U}{\partial t} &= -U \cdot \nabla U - \frac{1}{\rho} \nabla \pi - \frac{(\rho - \rho_0)}{\rho} g \mathbf{e}_r ,\\ \nabla \cdot (\beta_0 U) &= \beta_0 \left(S - \frac{1}{\overline{\Gamma} \rho_0} \frac{\partial p_0}{\partial t} \right) \end{aligned}$$

where

$$\mathcal{S} = -\sigma \sum_{k} \xi_k \dot{\omega}_k + rac{1}{
ho \mathcal{P}_
ho} \sum_{k} \mathcal{P}_{X_k} \dot{\omega}_k$$

Use average heating to evolve base state.

$$\frac{\partial p_0}{\partial t} = -w_0 \frac{\partial p_0}{\partial r} \quad \text{where} \quad w_0(\mathbf{r}, \mathbf{t}) = \int_{\mathbf{r}_0}^{\mathbf{r}} \overline{\mathbf{S}}(\mathbf{r}', \mathbf{t}) \, \mathrm{d}\mathbf{r}'$$

MAESTRO: Low Mach number method

- Numerical approach based on generalized projection method
- 2nd-order accurate fractional step scheme
 - Advance velocity and thermodynamic variables
 - Project solution back onto constraint
- Strang splitting for reaction terms (same as CASTRO)
- Also need to advance background state
- Built in BoxLib, a reusable software framework for block-structured AMR application codes:
 - supports block-structured AMR
 - scales to 100000's of processors
 - linear solvers for solving elliptic and parabolic equations
 - hybrid MPI / OpenMP
 - modular EOS and reaction networks "plug 'n play"

- Physically:
 - Acoustic waves are no longer part of the solution;
 - Compressibility effects due to stratification, heat release and compositional changes are still included
- Mathematically:
 - No longer a purely hyperbolic system,
 - Divergence constraint on velocity ⇒ ellitpic equation for pressure to be solved at every time step
- Computationally:
 - Can run with Δ*t* based on advective, not acoustic, velocity
 - Solving variable coefficient elliptic equation fundamentally changes communication patterns
 - Multigrid is an efficient iterative solver
 - Computational cost dominated by communication rather than computation

In the end, we care about time-to-solution.

White dwarf convection





Convective flow pattern on inner 1000 km of star

- Red / blue is outward / inward radial velocity
- Yellow / green shows burning rate

Two dimensional slices of temperature a few minutes before ignition

Where does the star ignite?

We would like to know the the distribution of ignition sites (note there is not a single "answer")

Monitor peak temperature and radius during simulation

Filter data

Bin data to form histogram

Assume that hot spot locations are "almost" ignitions



What we know about the velocity field before ignition:





Using MAESTRO to initialize a CASTRO simulation

Courtesy of C. Malone et al.

From Convection to Breakout: porting results from MAESTRO to CASTRO Malone, Nonaka, Almgren, Bell, Dong, Ma, Woosley, Zingale

Simulations run at NCSA Blue Waters ESS and OLCF jaguarpf



Summary

MAESTRO

- Low Mach number model
- Adaptive mesh refinement
- Hybrid parallel implementation
- Enables previously infeasible simulations

Other MAESTRO applications

- Convection in some sub-Chandra SNIa scenarios
- Type 1 XRB
- Convection in main sequence stars
- Nuclear flame microphysics