





Impact of Community Codes on Astrophysics

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Argonne Training Program in Extreme Scale Computing St. Charles, IL - 10 August 2015

Can NOT be overestimated!

Benefits of Community

- Open source is a good thing in science!
- Reproducibility
- No need to reinvent the wheel
- More science per funder dollar!
- Greater impact of methods development!
- Better documentation (?)

"Community" Astro Codes

FLASH
MESA
Enzo
yt
Gadget
CASTRO
MAESTRO

Athena
Ramses
Zeus
Einstein Toolkit
Pluto
many, many more....

see Astrophysics Source Code Library, <u>ascl.net</u> >800 codes listed!

Comm. Codes Have Greater Impact

| Code | Approx. Publications | | |
|--------|----------------------|--|--|
| Gadget | 3000 | | |
| Zeus | 1000 | | |
| FLASH | 800 | | |
| Enzo | 400 | | |
| MESA | 300 | | |

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Why Astro Comm. Codes?

- Monetization unlikely...
- Problems are complex and difficult for the lone coder
- Communal coding leads to greater return on investment

Why Astro Comm. Codes?

- More eyes on the code means more bugs found...
- Testing more rigorous

Multiphysics Complexity

Astrophysics Has It!

- Compressible hydrodynamics
- Magnetic fields
- Radiation transport/hydro
- Self-gravity

- Chemistry
- Nuclear burning
- Multifluids
- Detailed EOS
- Relativity

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Multiphysics Complexity

Mathematically...

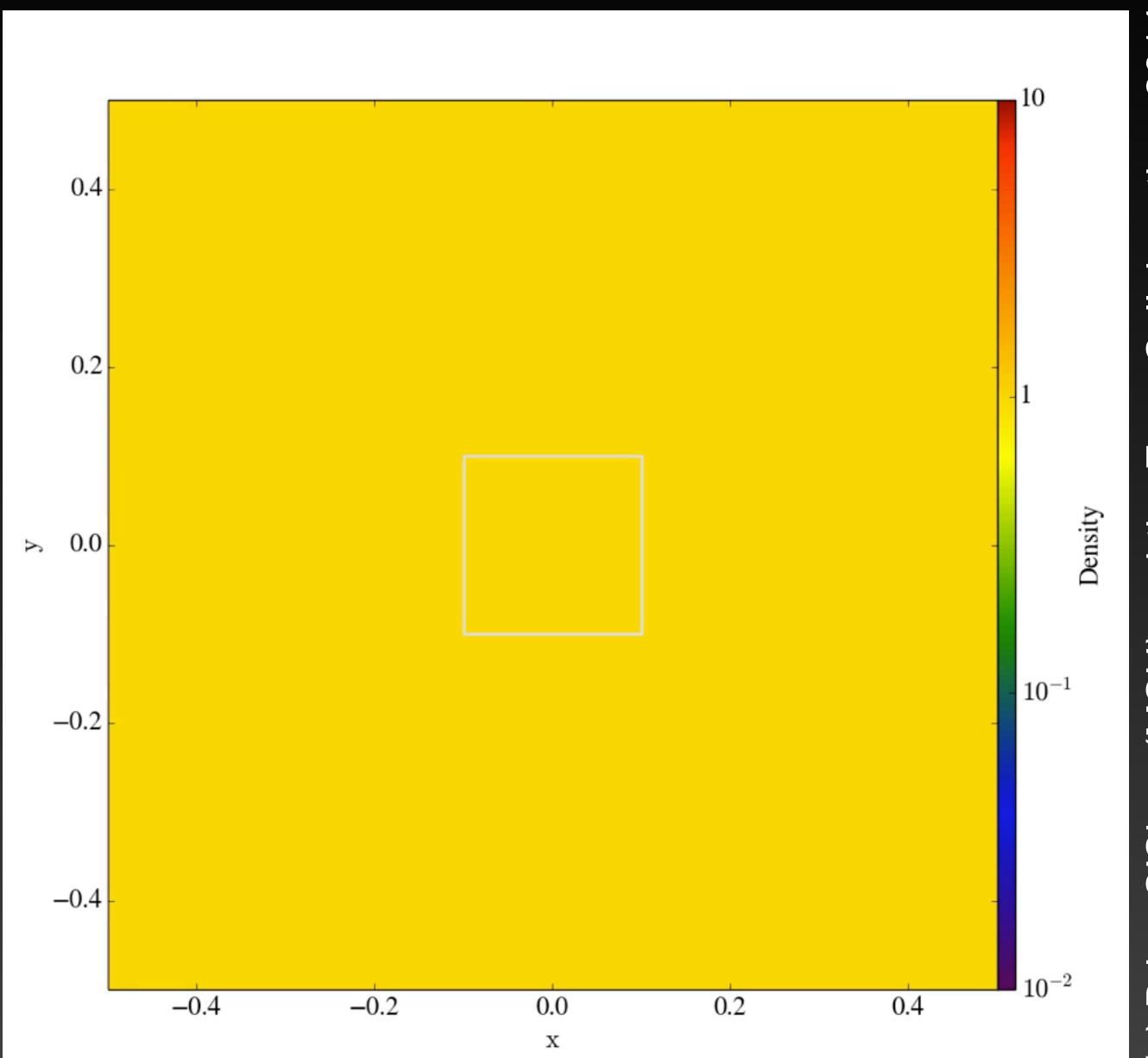
- Mix of:
- Hyperbolic PDEs
- Elliptical PDEs
- Parabolic PDEs
- Stiff equations
- etc., etc.

Infrastructure Complexity

- Extremely high dynamic range in space and time!
- Adaptive mesh techniques common
- BIG problems => extreme scale computing
- Infrastructure (IO, grid, build, analysis)
- Many different classes of operators

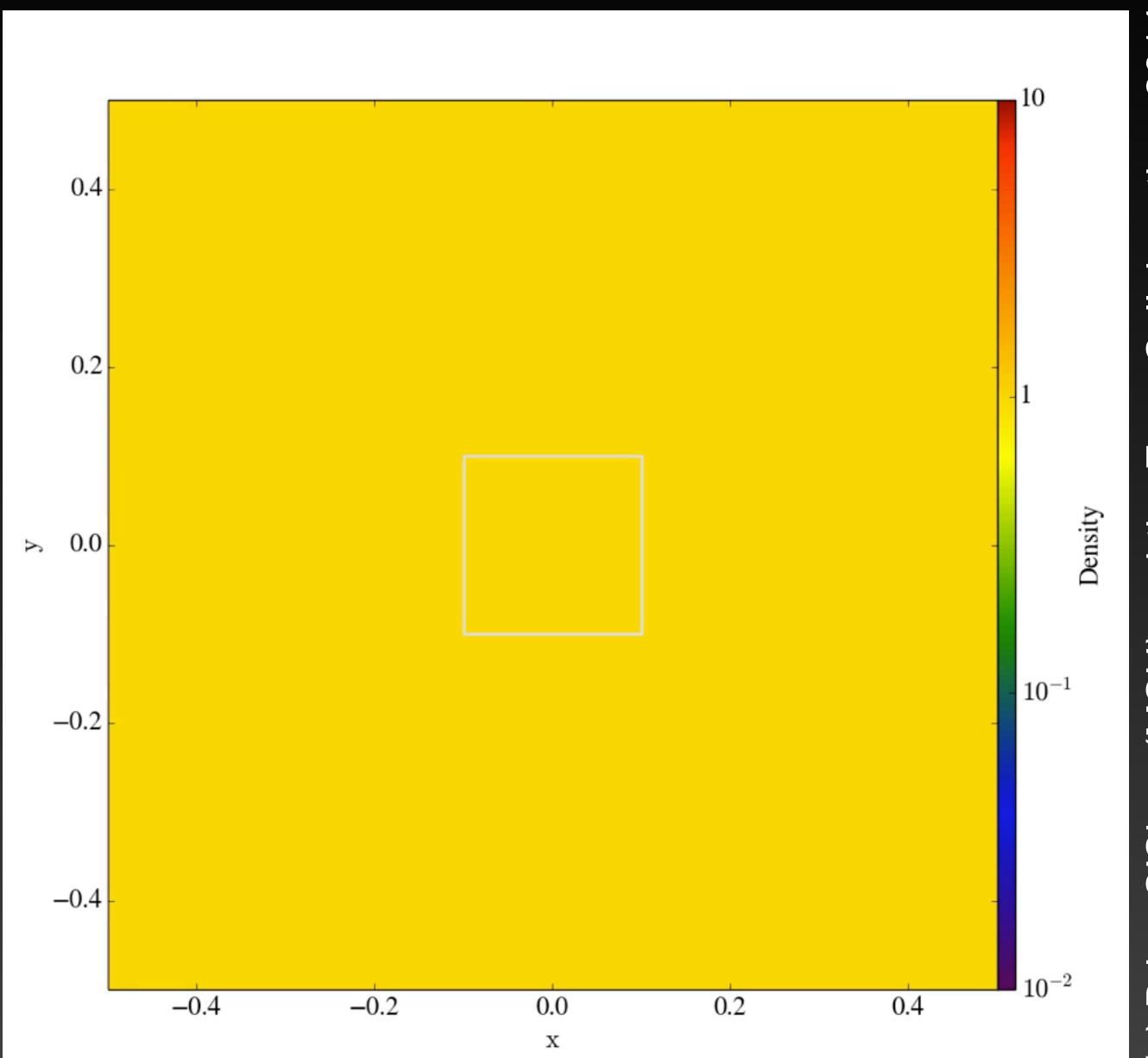
AMR

- Prolongation/restriction
- Guard (ghost) cell filling
- Fine/coarse flux correction
- Parallel load balancing



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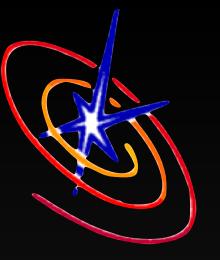


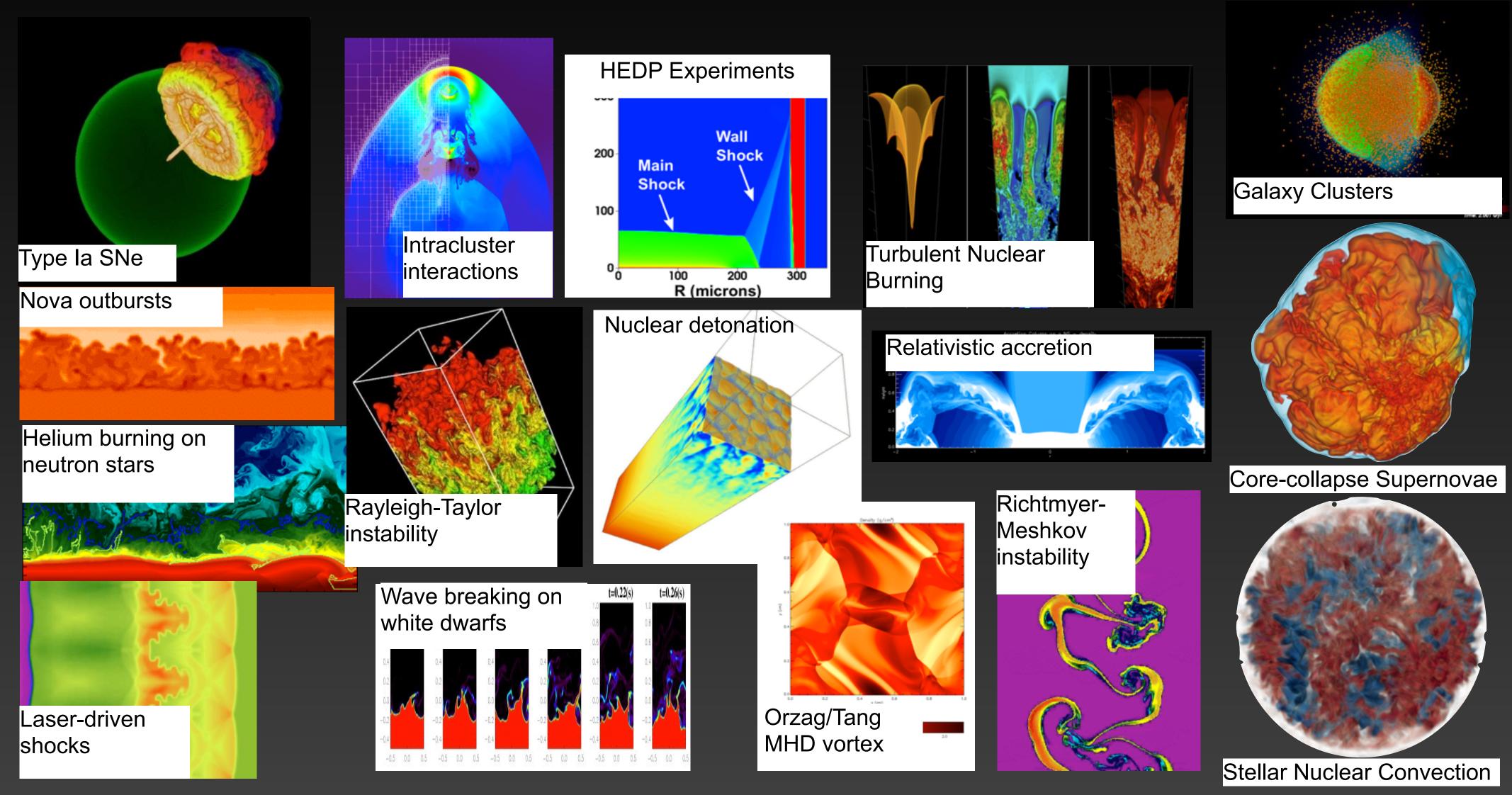
- Writing to disk from >100k cores is beyond me.
- 100's of TB's of output for a project
- 100's of GB's per write
- Big savings from machine-specific tuning

Particles

- Lagrangian tracers
- Active (i.e., gravitating, SPH)
- Laser ray tracing
- Fluid-structure interactions

FLASH: A Multiphysics Simulation Framework



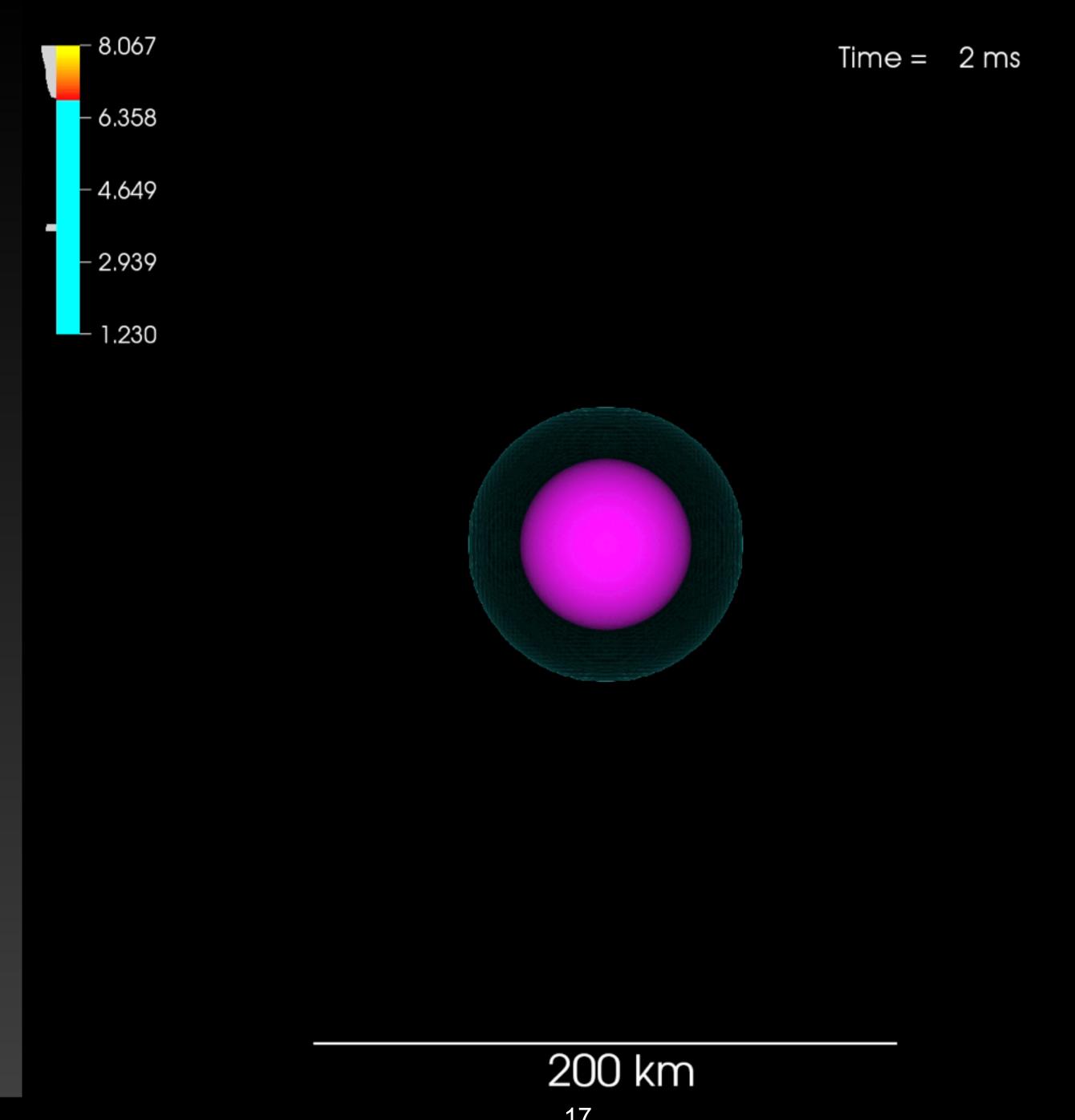


Adaptability: FLASH

- Originally: thermonuclear burning in degenerate stars
- Then many other problems in Astro!
- Not for the core-collapse supernova mechanism

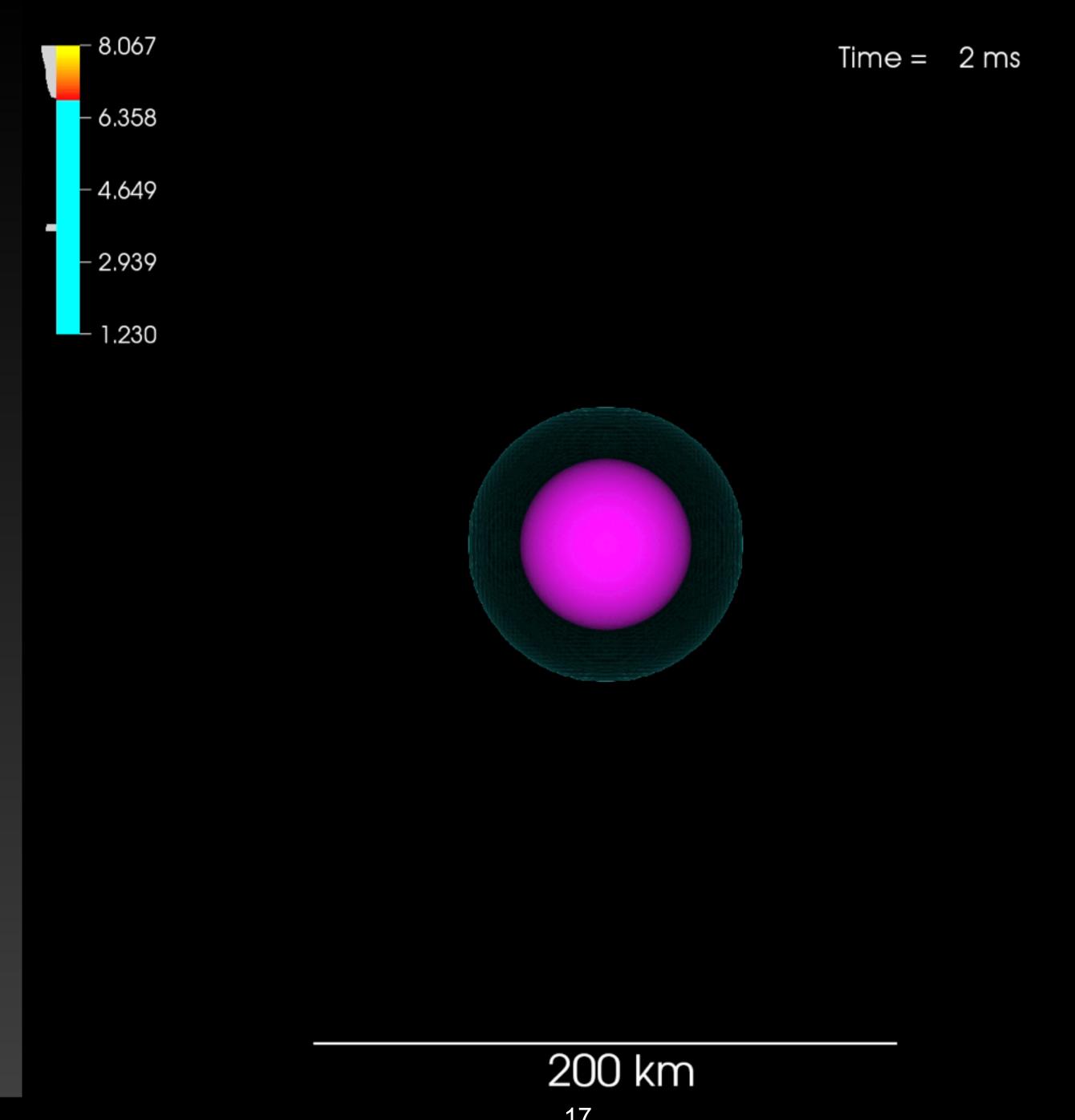
Adaptability: FLASH

- FLASH had: Hydro, gravity, AMR, I/O, data analysis/viz tools
- I could focus on just new stuff: nuclear equation of state, neutrino physics



SMC & Ott 2013, ApJL, 778, L7

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SMC & Ott 2013, ApJL, 778, L7

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Petascale Simulation of Magnetorotational CCSNe

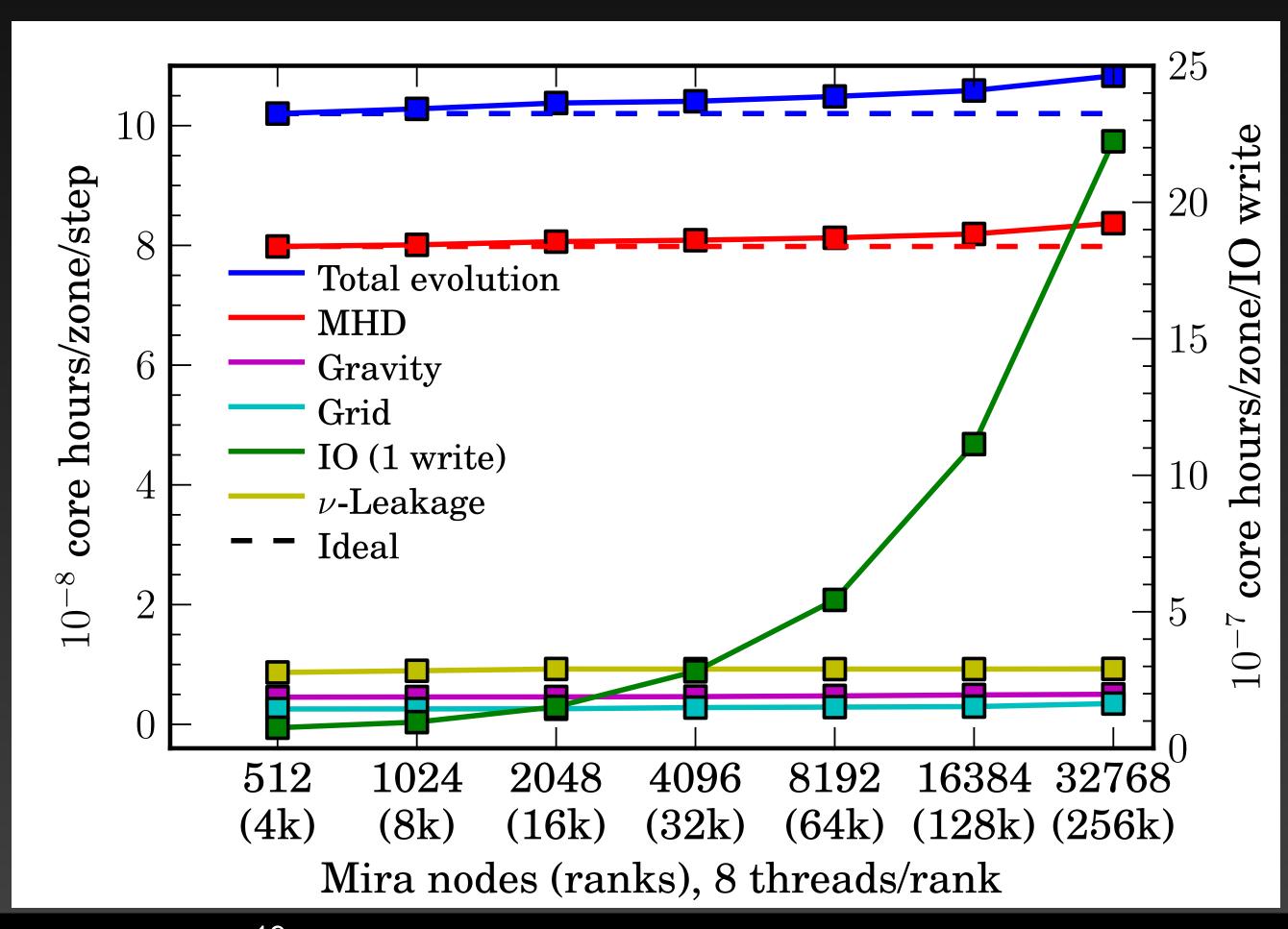
- Argonne Leadership
 Computing Facility: Mira
- 30 million DD hours per year in 2013 & 2014.
- Awarded DOE INCITE
 allocation of 50 million core hours per year for
 2015-2017.



SMC (PI, MSU)
Almudena Arcones (Darmstadt)
Manos Chatzopoulos (Chicago)
Carla Frohlich (NC State)
Dongwook Lee (UCSC)
Evan O'Connor (NC State)
Daan van Rossum (Chicago)
Petros Tzeferacos (Chicago)
J. Craig Wheeler (Texas)

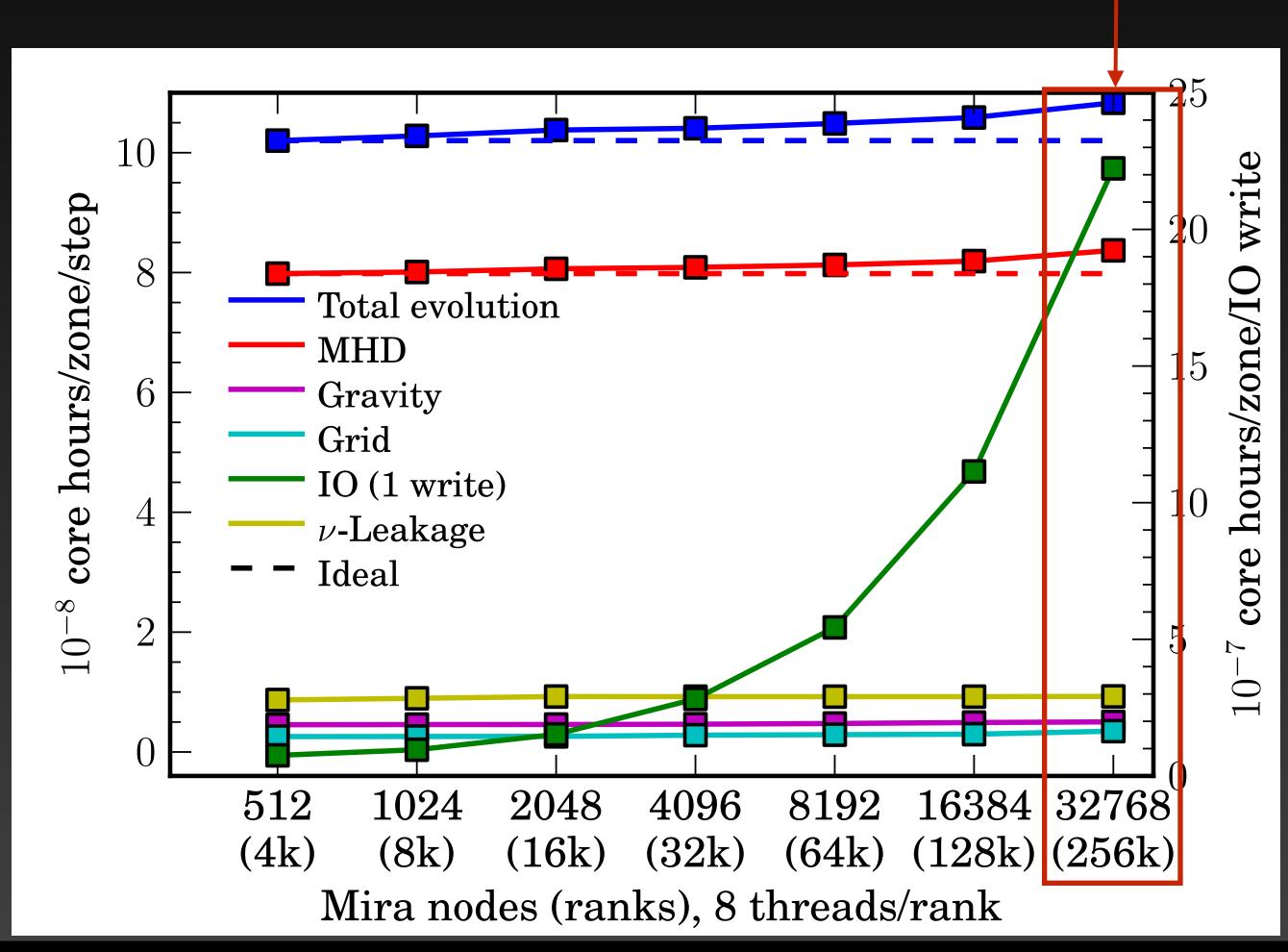


E.g. FLASH Scaling



E.g. FLASH Scaling

524k cores! >2 Million threads!



FLASH is Special

- Well-funded development for ~20 years
- Professional design/maintenance
- Core group of devs in central location
- Most astro codes done "on the cheap"

B.W. O'Shea

- Compressible MHD
- Cosmology
- Active (gravitating) particles
- Self-gravity
- Heating/cooling
- Radiation

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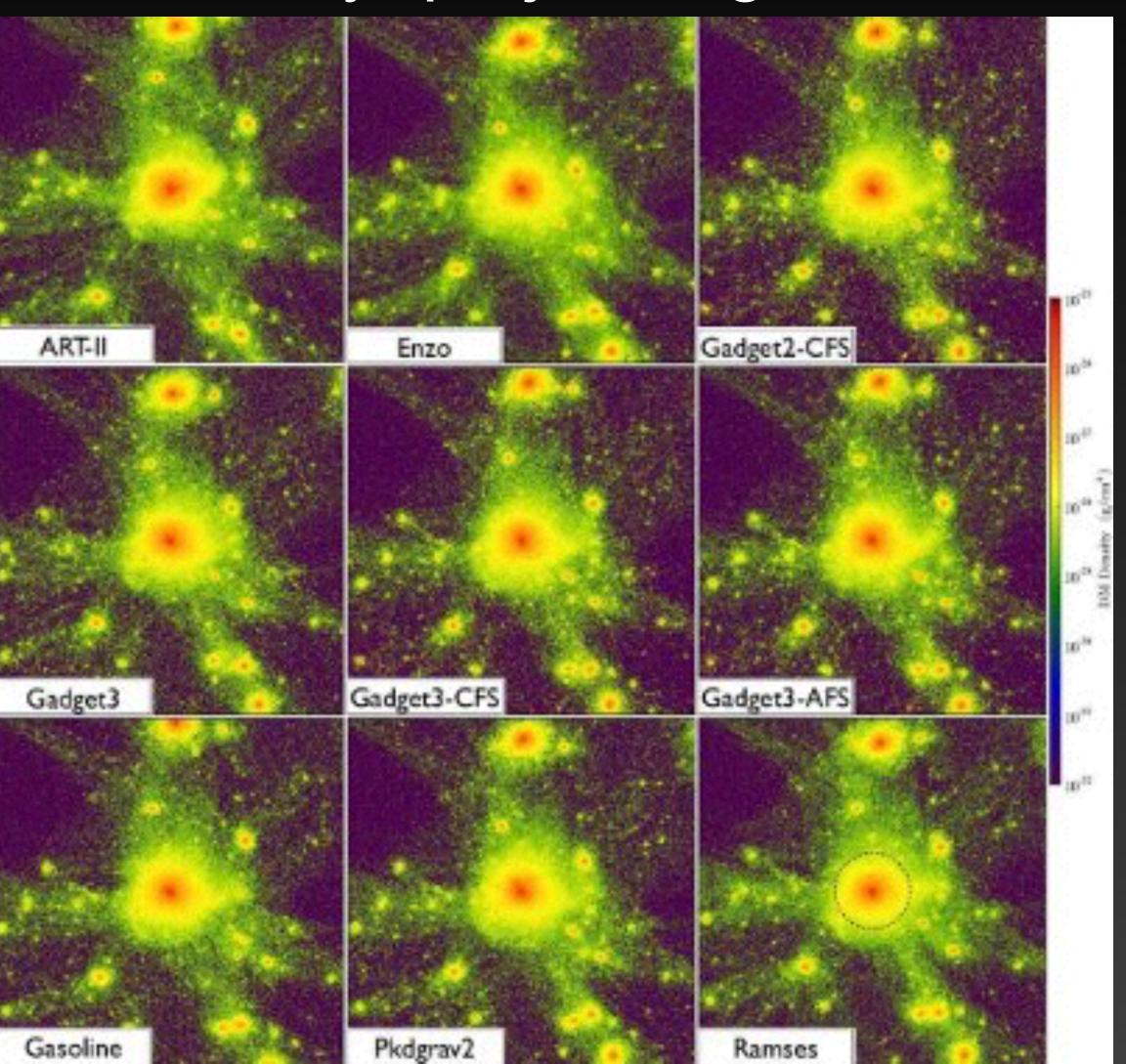
Enzo

- ~12 core developers in very different locales
- Heavy use of online collaboration tools
- distributed version control (!)

yt

- Started as part of Enzo collaboration
- Data analysis and visualization
- Glued together with Python
- Grew to many other codes
- Amazing dev community

yt-project.org



Not all areas of Astro

- Stellar evolution
- Radiation transport

Massive Stars

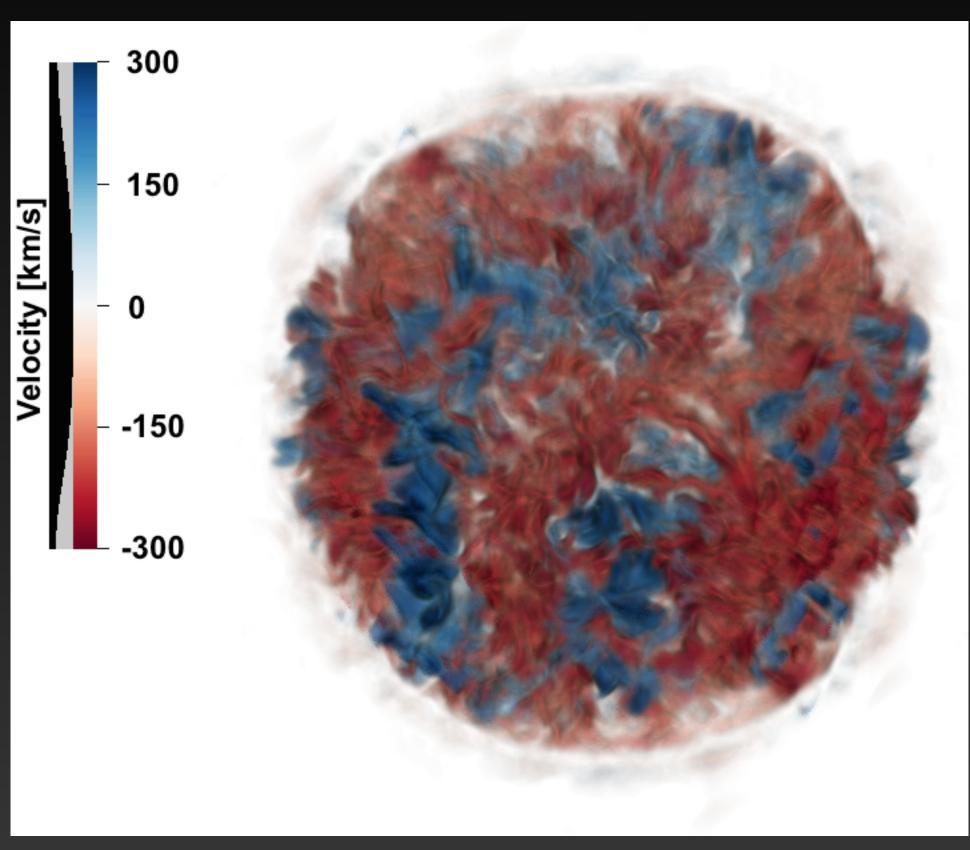
- Core-collapse supernova progenitors
- One code, one group for decades!
- New community code: MESA

MESA

Modules for Experiments in Stellar Astrophysics

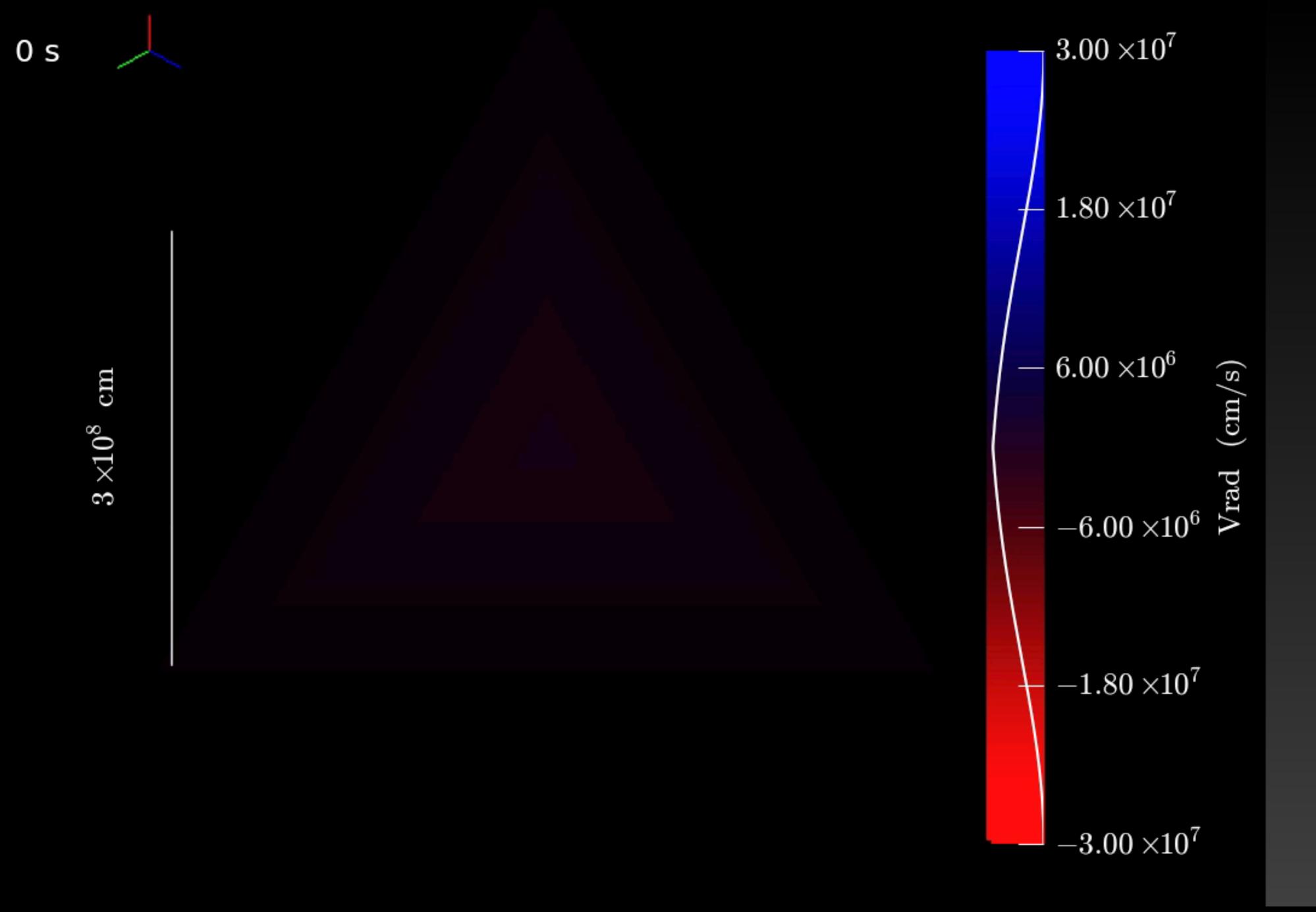
- mesa.sourceforge.net
- Started with one principal dev (Bill Paxton)
- Grown into large, active community
- Distributed development
- Contributions generally go through Bill

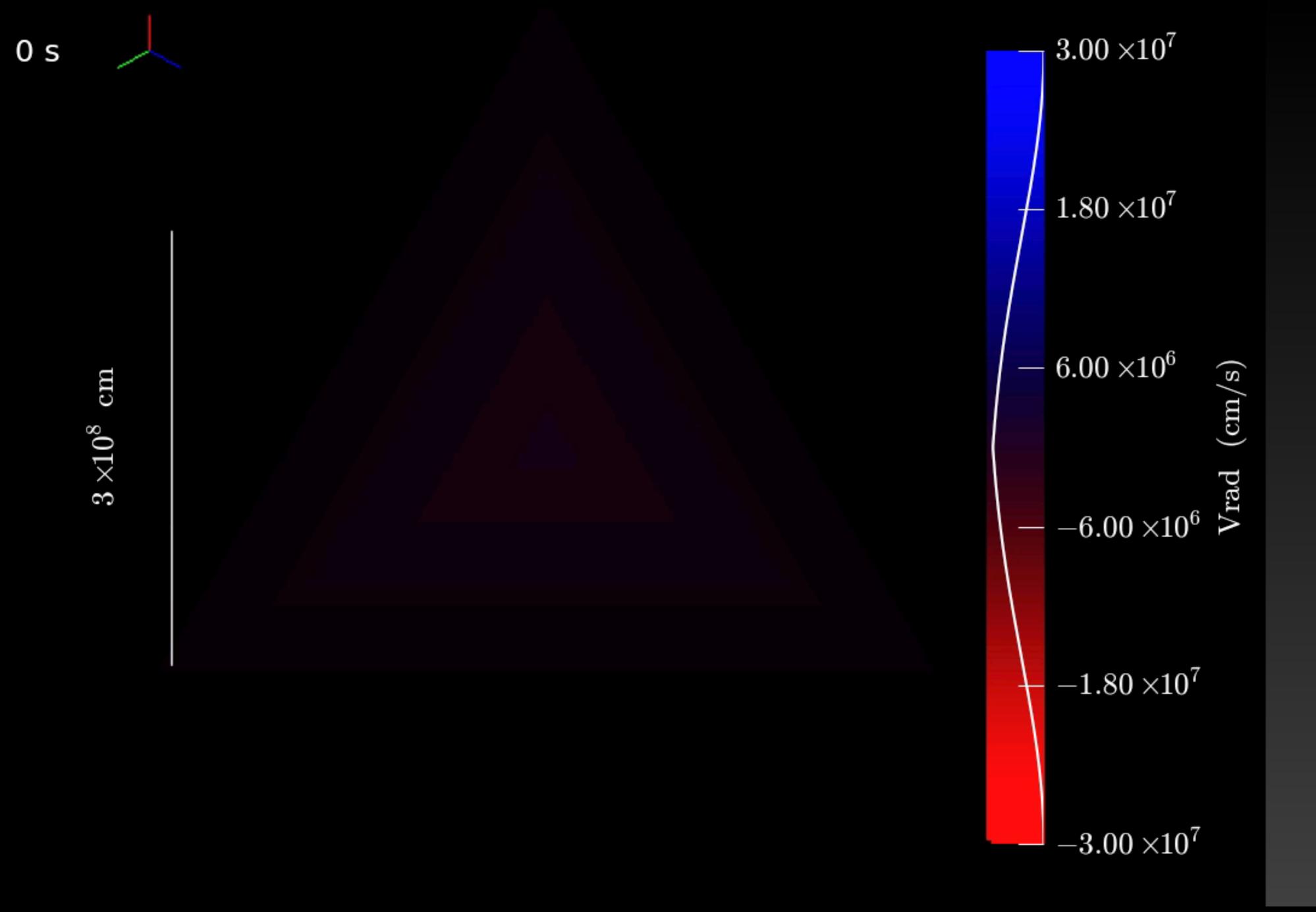
MESA Enabling New Science



SMC et al. 2015, ApJL, 808, L21

- Combine two different community codes: FLASH + MESA
- Can address new problems!



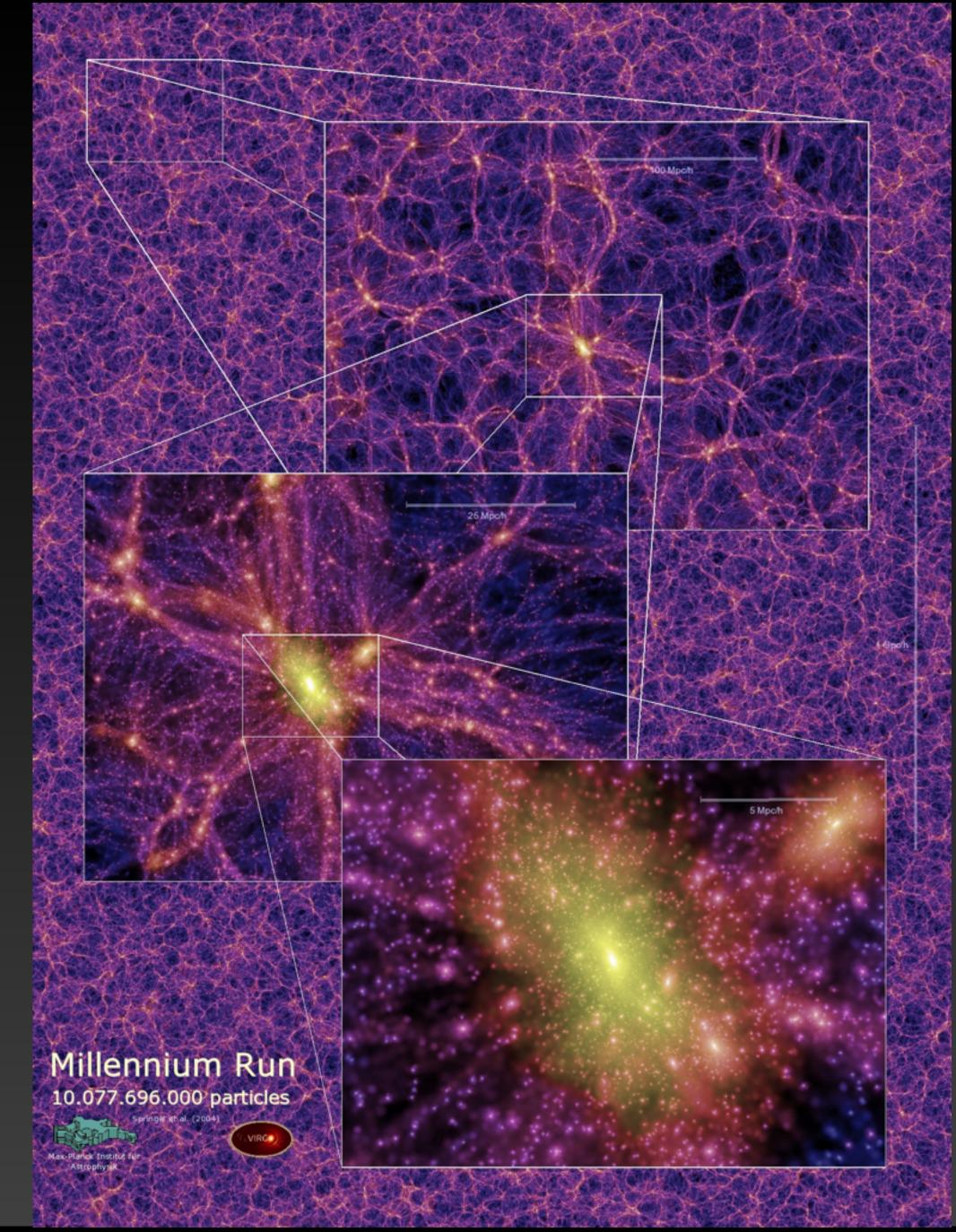


Some pitfalls

• If you make it too easy to use, or too stable, everybody will use it.

Gadget

- N-body (active particles)
- Smoothed particle hydro (SPH)
- Various heating/cooling
- Very centralized development: V. Springel



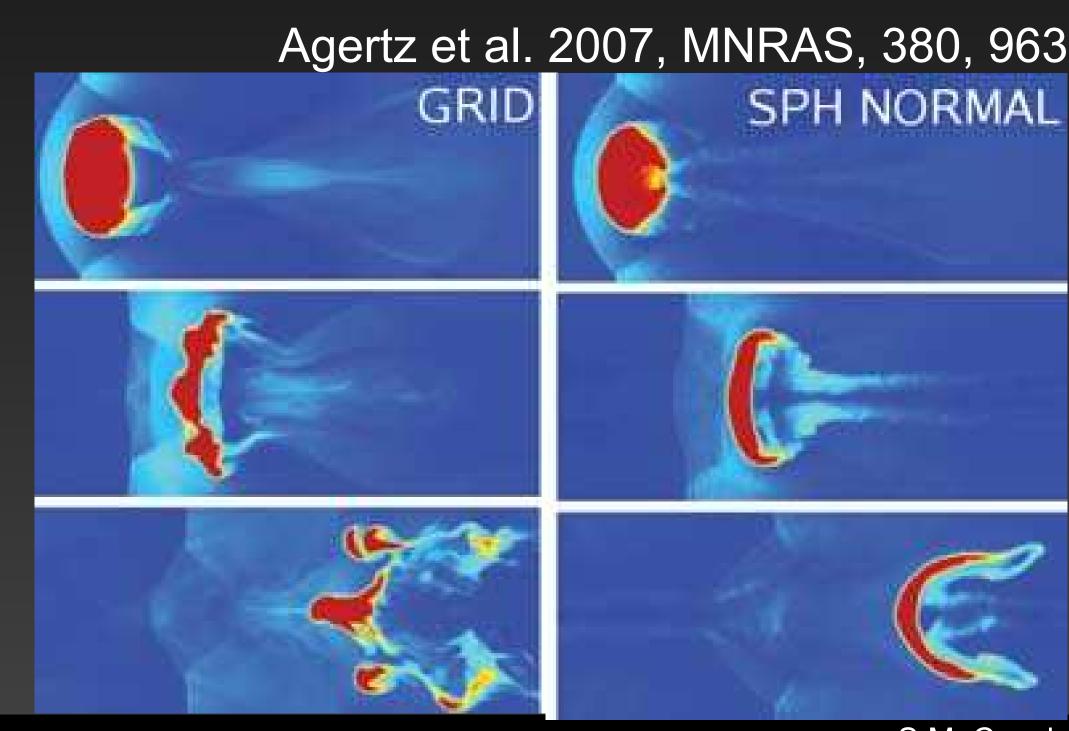
Cautionary Tale: Gadget

- Easy to use, stable, open =>
- Enormous impact on galaxy formation!
- But.... Problem with original implementation of SPH

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Cautionary Tale: Gadget

- Easy to use, stable, open =>
- Enormous impact on galaxy formation!
- But.... Problem with original implementation of SPH
- Distribution model meant slow adoption of fix (a la Stagefright)
- Proliferation of proprietary versions



Some pitfalls

- Code divergence (balkanization)
- Can be a problem in all development models

Some pitfalls

- Assigning credit
- Codes are "instruments" and builders deserve credit
- Traditional academic mechanisms
 (publications, citations, etc.) often don't fit

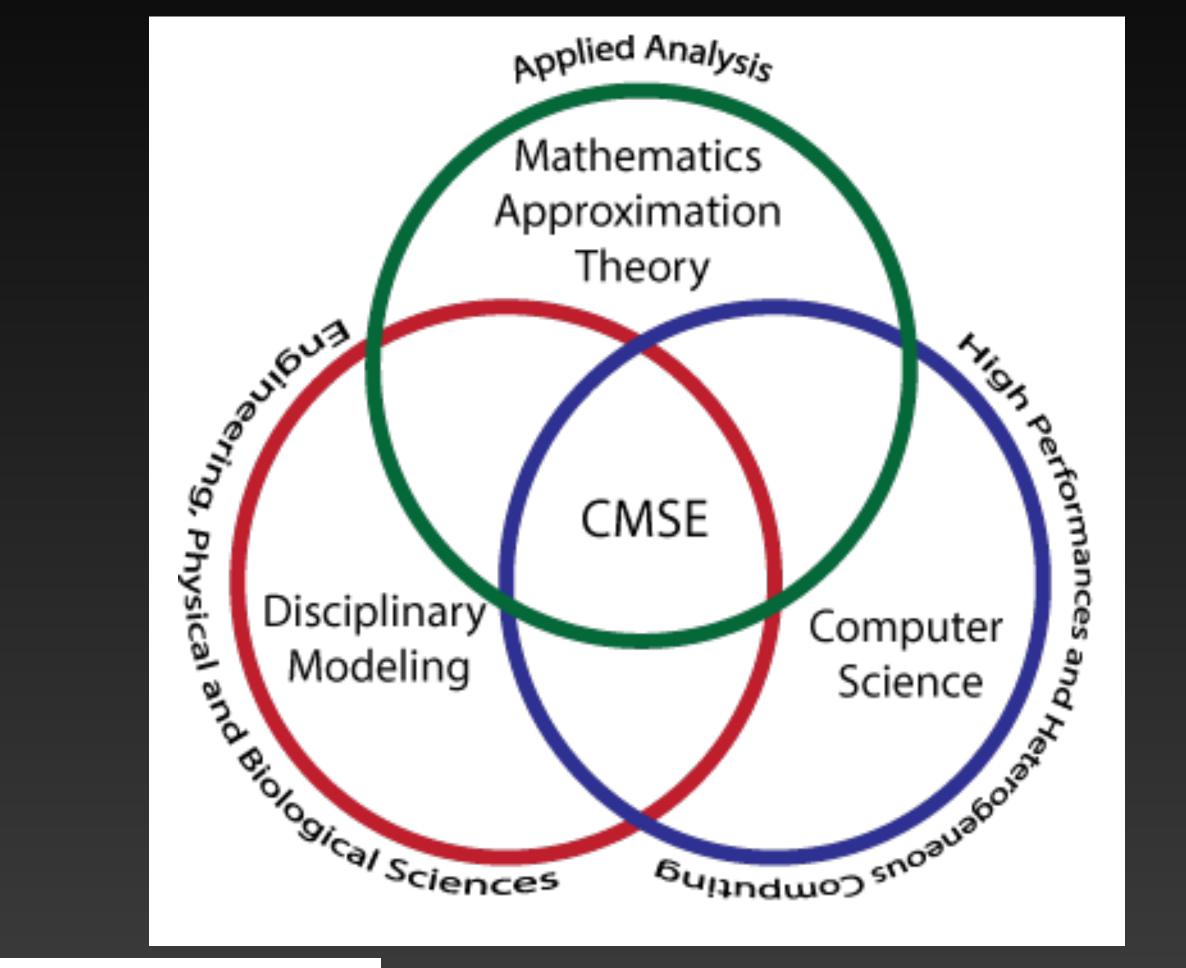
The Future

- Hardware complexity increasing...
- Today's codes may be living on borrowed time
- Need portability
- Abstraction of tasks may be critical!
- Need professional architecture and design

The Future

- But... funding for professional development of astrophysics codes has DECREASED
- No way to exascale without it.
- May be no way to 100 petaflops without it!

Computational Math, Science, Engineering at MSU



Overview

| Code | License | Dev Model | Distribution | Language | |
|--------|-----------|--------------|--------------|----------|--|
| FLASH | Custom* | Central | tarball | F90/C | |
| Enzo | UofI/NCSA | Distributed | hg | F90/C++ | |
| Gadget | GPL | Central? | tarball | C | |
| CASTRO | BSD | Distributed* | git | F90/C++ | |
| Cactus | ~GPL | open/devs | tarball | C++/F90 | |
| Zeus | ? | disparate | tarball | C | |
| MESA | GPL | open* | svn | F90 | |
| Athena | GPL | open* | tarball | C/F90 | |
| yt | BSD | open | hg | Python/C | |
| Pluto | GPL | open | tarball | C++ | |