Impact of Community Codes on Astrophysics

Sean M. Couch
Michigan State University

Argonne Training Program in Extreme Scale Computing
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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 (?)
- Learning!

“Community” Astro Codes

FLASH
MESA
Enzo
yt
Gadget
CASTRO
MAESTRO

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

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

Comm. Codes Have Greater Impact

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

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
- …

Multiphysics Complexity

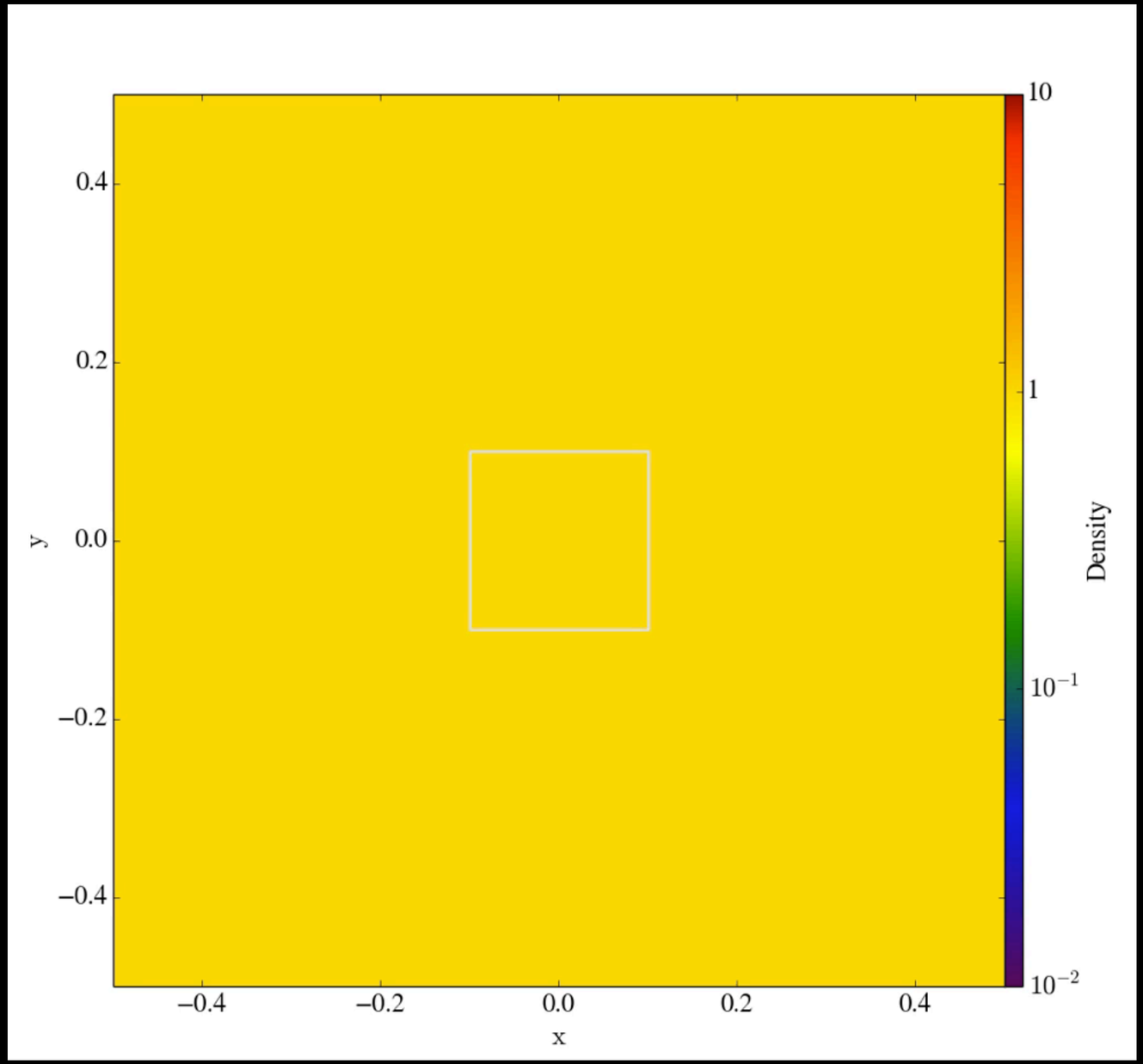
Mathematically…

- 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



I/O

- 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

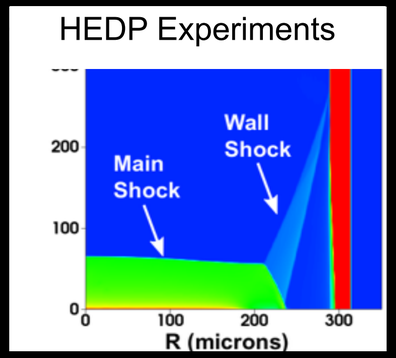
Particles

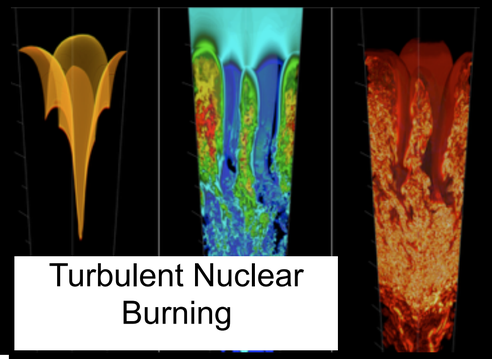
- Lagrangian tracers
- Active (i.e., gravitating, SPH)
- Laser ray tracing
- Fluid-structure interactions

FLASH: A Multiphysics Simulation Framework

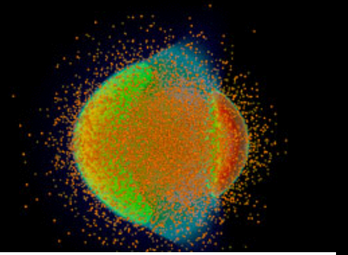
Type Ia SNe

Intracluster interactions



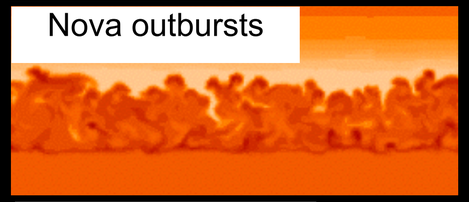


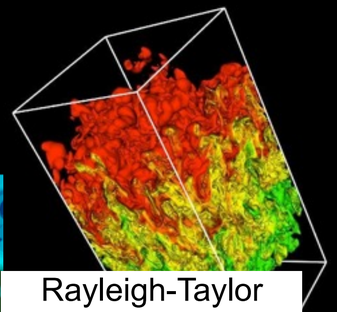
Turbulent Nuclear Burning



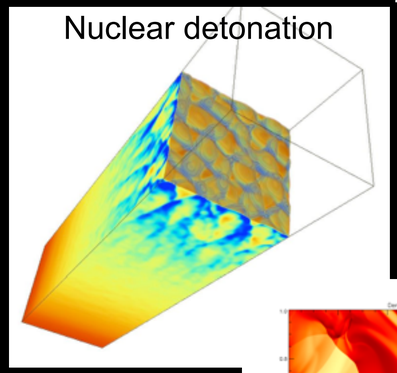
Galaxy Clusters

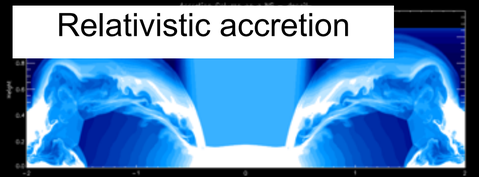
Nova outbursts



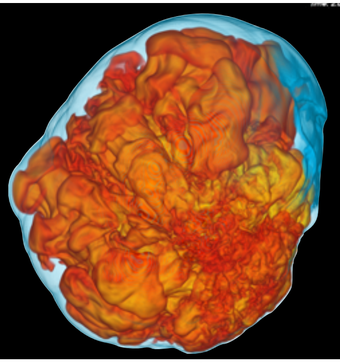


Rayleigh-Taylor instability



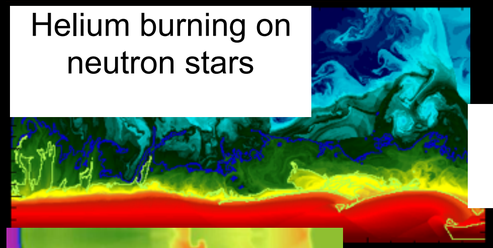


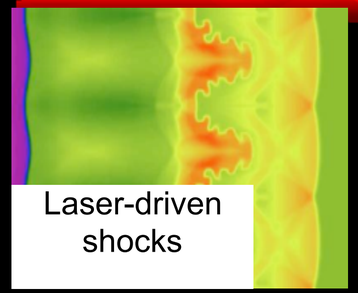
Relativistic accretion



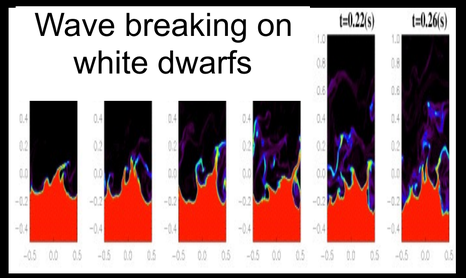
Core-collapse Supernovae

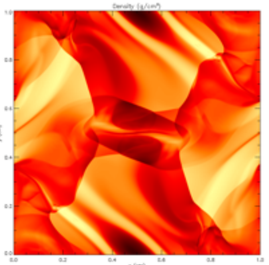
Helium burning on neutron stars



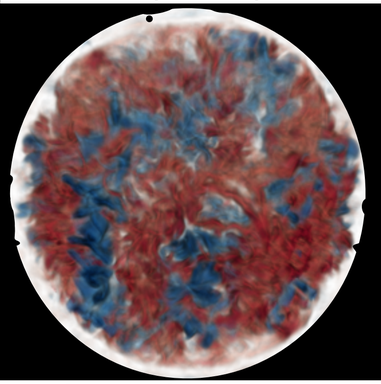


Laser-driven shocks





Orzag/Tang MHD vortex



Stellar Convection

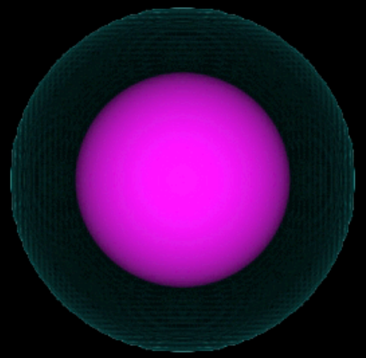
Adaptability: FLASH

- 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, transport,…

Time = 2 ms



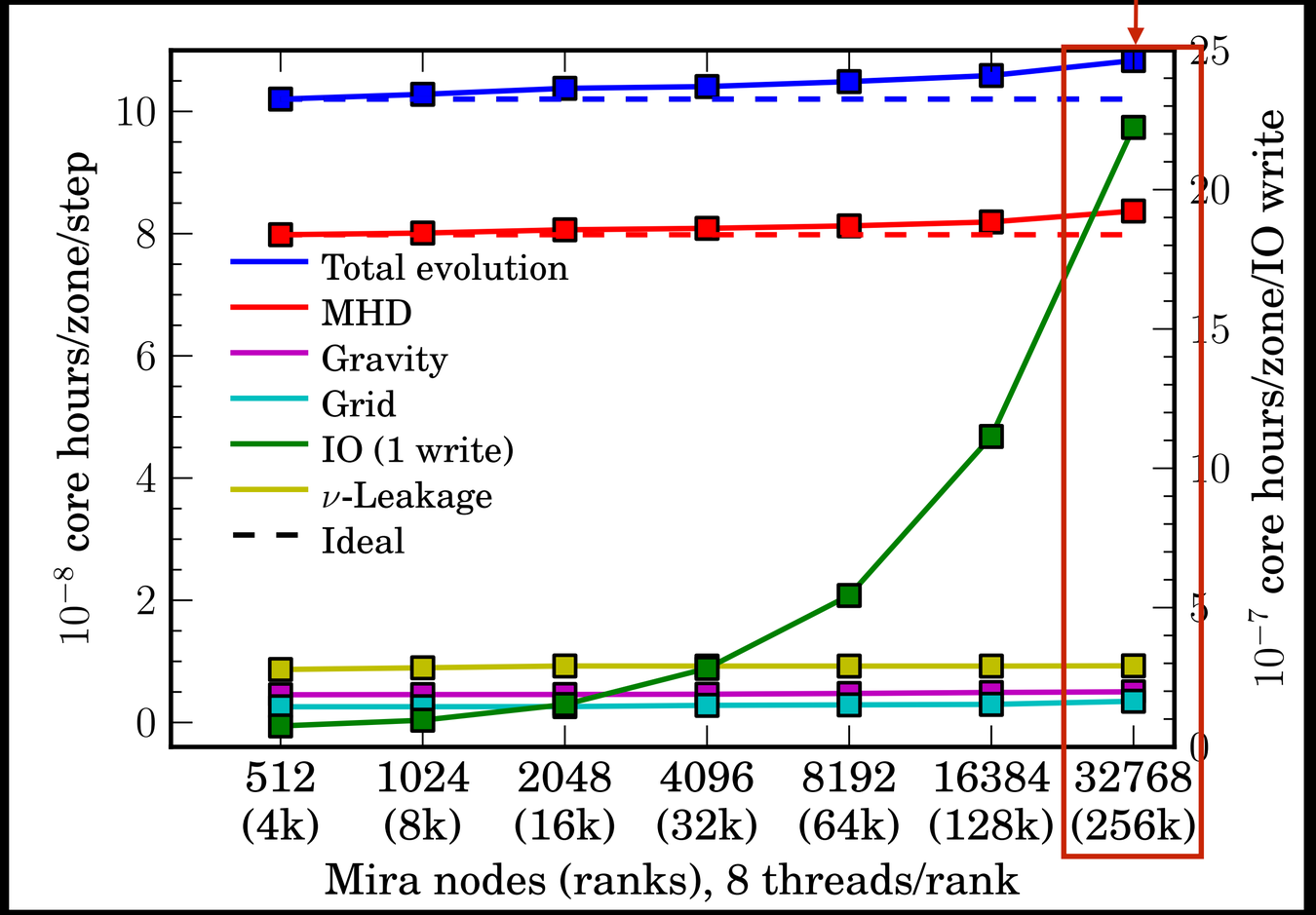
200 km

SMC & Ott 2013, ApJL, 778, L7

E.g. FLASH Scaling

524k cores!
>2 Million threads!

CCSN 3D sims cost upwards of 100 Million core-hours!

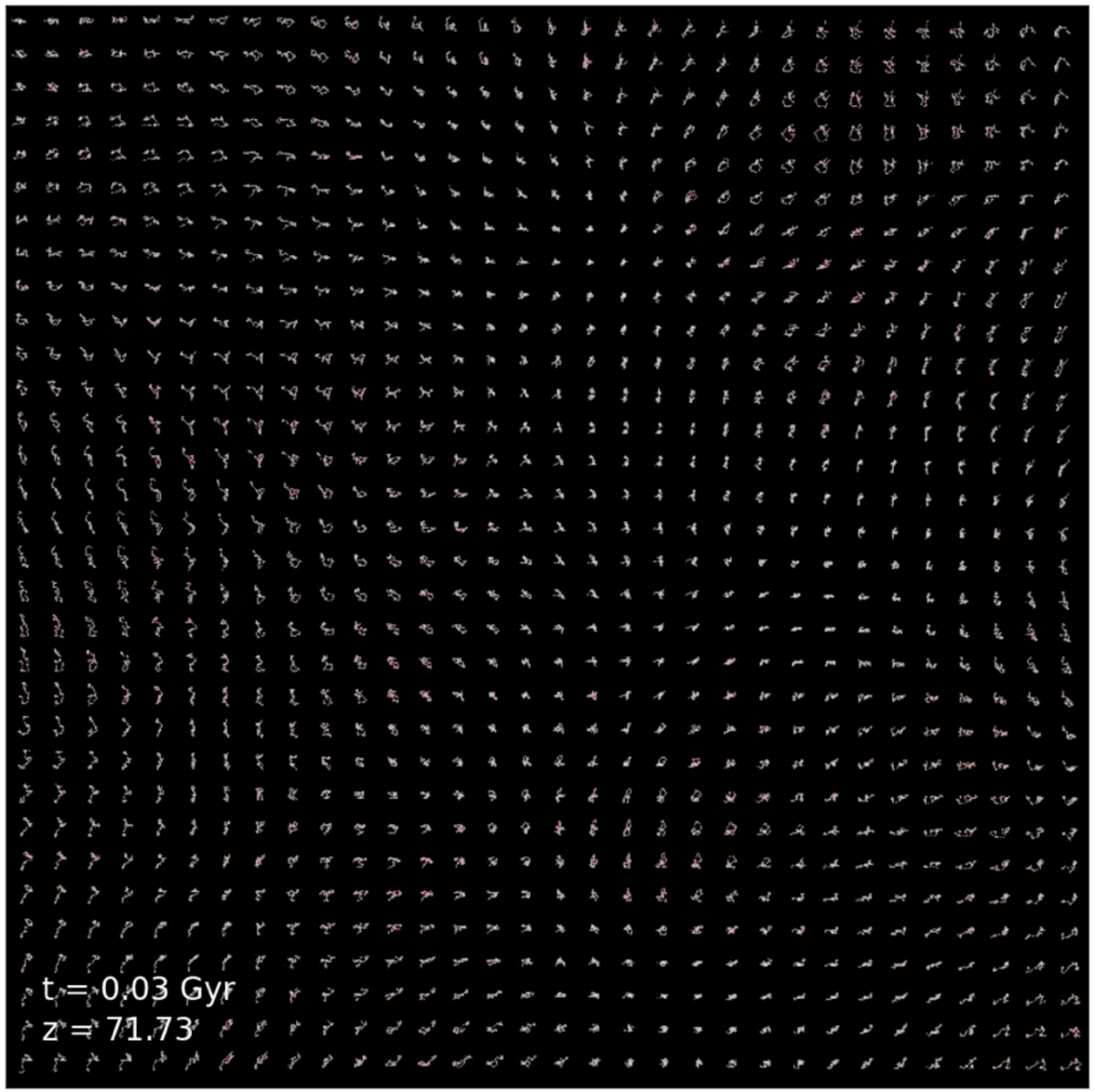


FLASH is Special

- 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

Enzo



AMR
N-body particle dynamics
Gas dynamics (MHD)
Complex gas chemistry
Radiative cooling
Sub-grid feedback schemes

Enzo

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

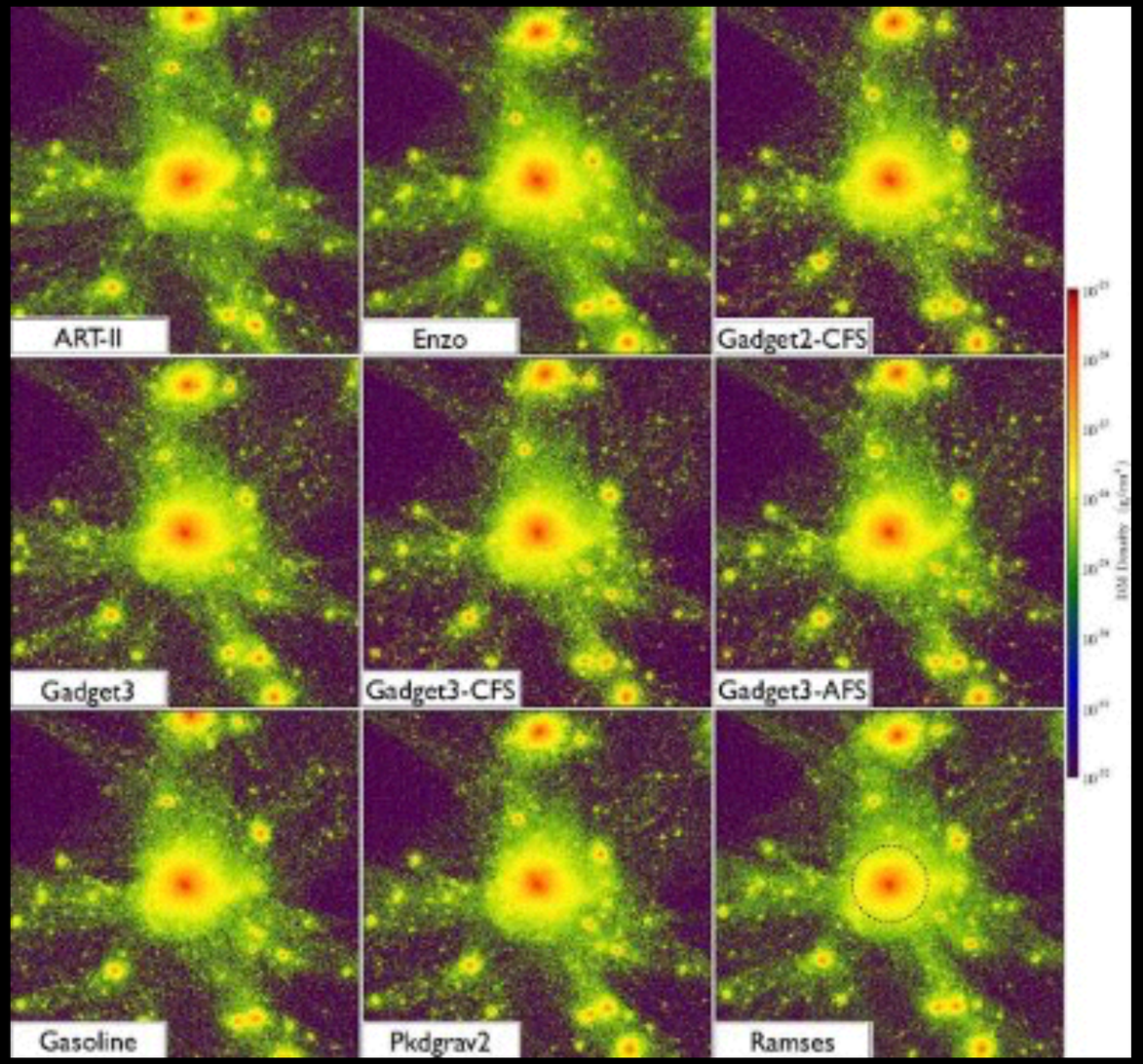
Einstein Toolkit

- Annual workshop
- Rules for merging, contributing, etc.
- Governance and official maintainers

yt

yt-project.org

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



Not all areas of Astro

- Stellar evolution
- Radiation transport

Massive Stars

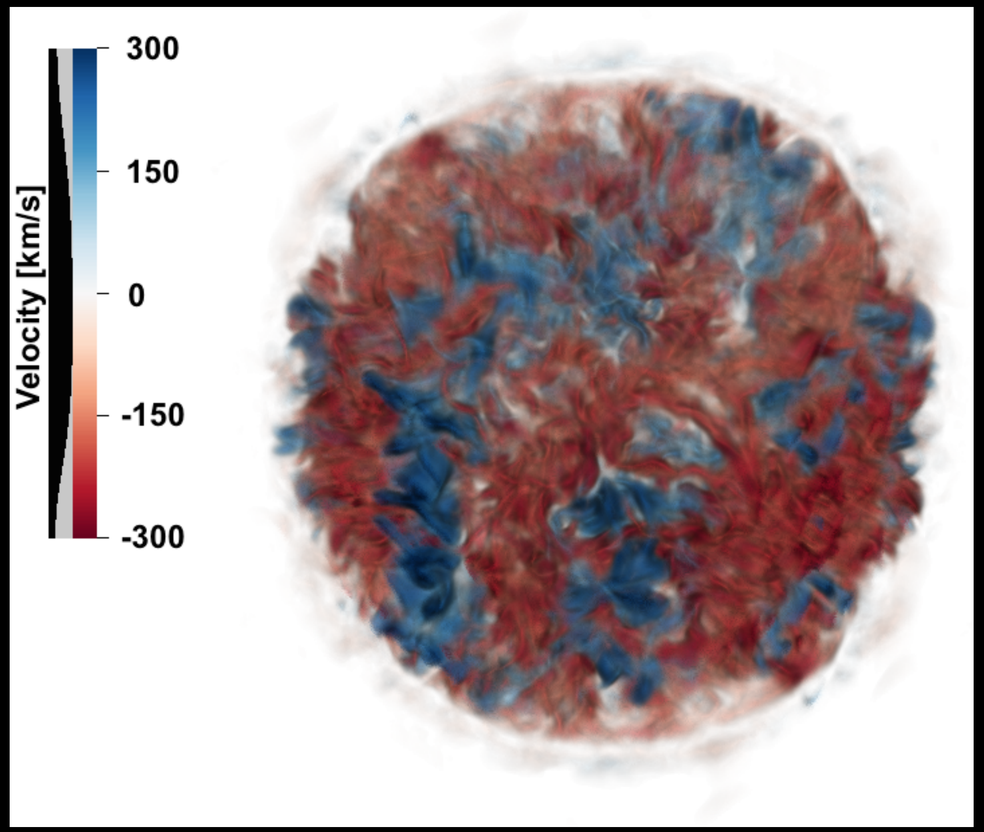
- Core-collapse supernova progenitors
- One code, one group for decades!
- New community code: MESA

MESA

Modules for Experiments in Stellar Astrophysics

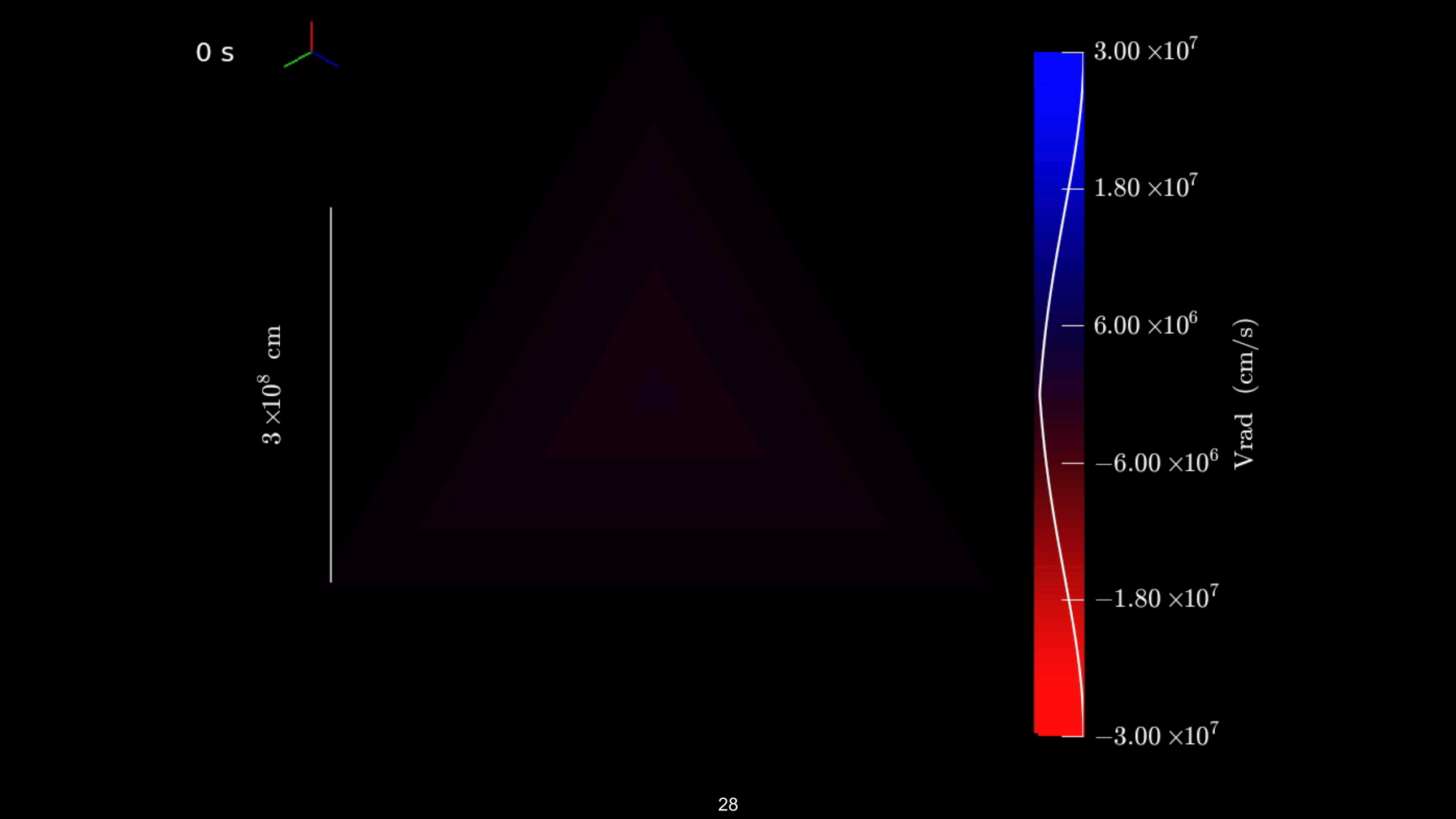
- mesa.sourceforge.net
- Started with one principal dev (Bill Paxton)
- Grown into large, active community
- Distributed development
- Contributions generally go through Bill

MESA Enabling New Science



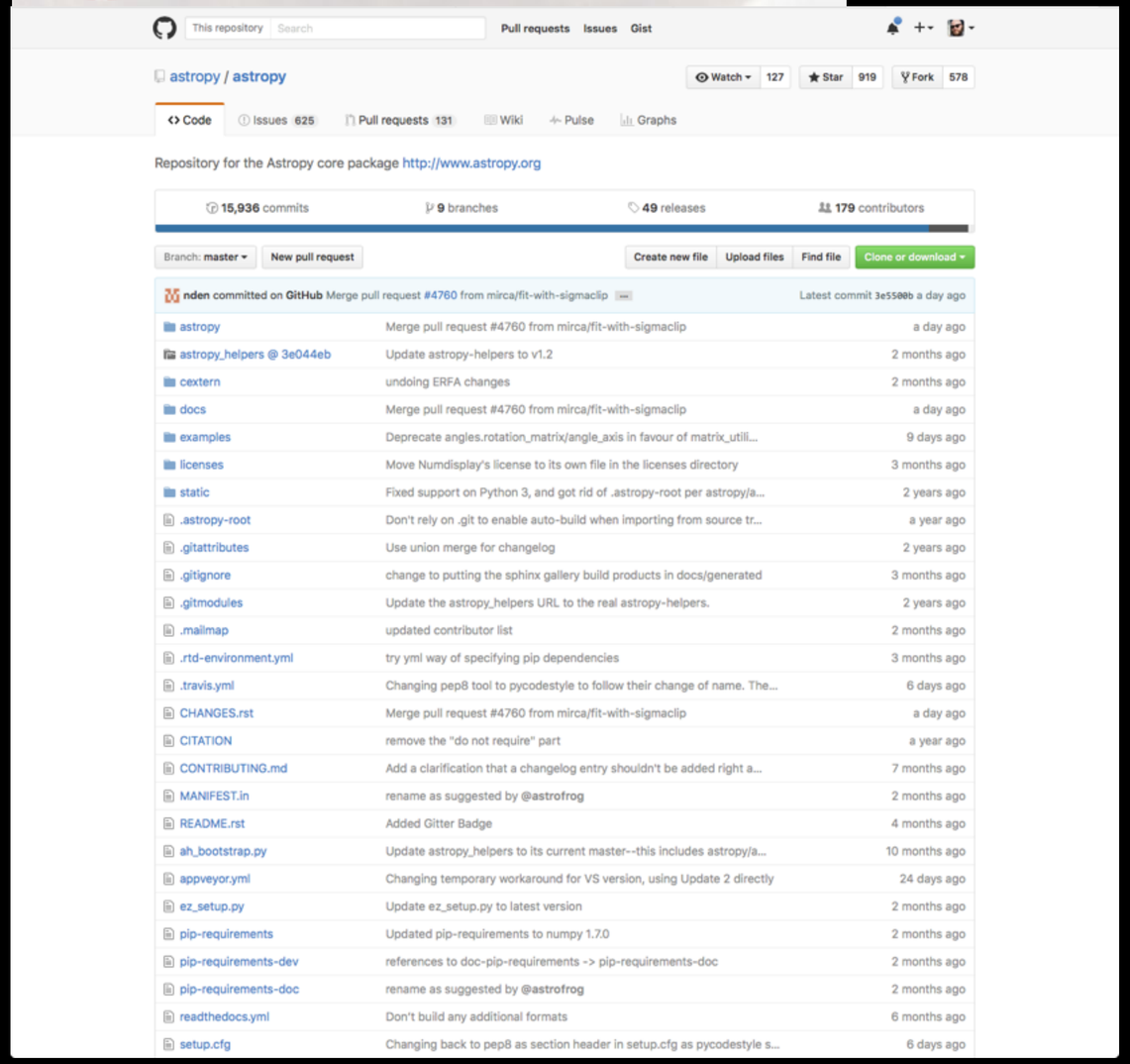
SMC et al. 2015, ApJL, 808, L21

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


0 s
3×10^{8} cm
3.00×10^{7}
1.80×10^{7}
6.00×10^{6}
-6.00×10^{6}
-1.80×10^{7}
-3.00×10^{7}
Vrad (cm/s)

Not just simulation

astropy
A Community Python Library for Astronomy



The Team

Astropy is under continuous development by a group of professional astronomers and software developers from around the world. The Project is community-driven, with decisions generally made by consensus, but with oversight and organization provided be a three-person coordinating committee.

Astropy Project Coordinators

- Tom Aldcroft
- Kelle Cruz
- Thomas Robitaille
- Erik Tollerud

Core Package Contributors

- Ryan Abernathey
- Shailesh Ahuja
- Tom Aldcroft
- Anthony Horton
- Anne Archibald
- Cristian Ardelean
- Matteo Bachetti
- Kyle Barbary
- Geert Barentsen
- Pauline Barmby
- Paul Barrett
- Andreas Baumbach
- Chris Beaumont
- Daniel Bell
- Elijah Bernstein-Cooper
- Kristin Berry
- Francesco Biscani
- Thompson Le Blanc
- Christopher Bonnett
- Joseph Jon Booker
- Médéric Boquien
- Azalee Bostroem
- Matthew Bourque
- Larry Bradley
- Gustavo Bragança
- Erik M. Bray
- Eli Bressert
- Hannes Breytenbach
- Hugo Buddelmeijer
- Doug Burke
- Mihai Cara
- Patti Carroll
- Mabry Cervin
- Pritish Chakraborty
- Alex Conley
- Jean Connelly
- Simon Conseil
- Ryan Cooke
- Yannick Copin
- Matthew Craig
- Steven Crawford
- Neil Crighton
- Robert Cross
- Kelle Cruz
- Dan P. Cunningham
- Daniel Datsev
- Matt Davis
- Christoph Deil
- Nadia Dencheva
- Jörg Dietrich
- Axel Donath
- Michael Droettboom
- Zach Edwards
- Jonathan Eisenhamer
- Thomas Erben
- Henry Ferguson
- Jonathan Foster
- Ryan Fox
- Lehman Garrison
- Simon Gibbons
- Adam Ginsburg
- Christoph Gohlke
- Danny Goldstein
- Perry Greenfield
- Dylan Gregersen
- Austen Groener
- Frédéric Grollier
- Karan Grover
- Kevin Gullikson
- Hans Moritz Günther
- Chris Hanley
- Alex Hagen
- Paul Hirst
- Moataz Hisham
- Michael Hoenig
- Emma Hogan
- Derek Homeier
- Anthony Horton
- JC Hsu
- Lingyi Hu
- Eric Jeschke
- Eric Depagne
- Joseph Jon Booker
- Sarah Kendrew
- Marten van Kerkwijk
- Wolfgang Kerzendorf
- Lennard Kiehl
- Rashid Khan
- Aleh Khvalko
- David Kirkby
- Dominik Klaes
- Kacper Kowalik
- Roban Hultman Kramer
- Arne de Laat
- Antony Lee
- Daniel Lenz
- Simon Liedtke
- Pey Lian Lim
- Stuart Littlefair
- Joseph Long
- Joe Lyman
- Curtis McCully
- Vinayak Mehta
- Aaron Meisner
- Serge Montagnac
- José Sabater Montes
- Francesco Montesano
- Brett Morris
- Michael Mueller
- Stuart Mumford
- Demitri Muna
- Prasanth Nair
- Bogdan Nicula
- Joe Philip Ninan
- Asra Nizami
- Bryce Nordgren
- Miruna Oprescu
- Carl Osterwisch
- Luigi Paioro
- Asish Panda
- Madhura Parikh
- Neil Parley
- Sergio Pascual
- Rohit Patil
- David Perez-Suarez
- Ray Plante
- Orion Poplawski
- Adrian Price-Whelan
- J. Xavier Prochaska
- David Pérez-Suárez
- QuanTakeuchi
- Tanuj Rastogi
- Juan Luis Cano Rodríguez
- Evert Rol
- Alex Rudy
- Joseph Ryan
- Eloy Salinas
- Gerrit Schellenberger
- David Shiga
- Albert Y. Shih
- David Shupe
- Jonathan Sick
- Leo Singer
- Brigitta Sipocz
- Shivan Sornarajah
- Shantanu Srivastava
- Ole Streicher
- Matej Stuchlik
- Bernardo Sulzbach
- James Taylor
- Jeff Taylor
- Kirill Tchernyshyov
- Víctor Terrón
- Scott Thomas
- James Turner
- Jake VanderPlas
- Miguel de Val-Borro
- Jonathan Whitmore
- Julien Woillez
- Jake VanderPlas
- Lisa Walter
- Benjamin Alan Weaver
- Jonathan Whitmore
- Julien Woillez
- Víctor Zabalza

Other Credits

- Kaylea Nelson for designing this web site.
- Kyle Barbary for designing the Astropy logos and documentation themes.
- Andrew Pontzen and the pynbody team (For code that grew into astropy.units)
- Everyone on astropy-dev and the astropy mailing list for contributing to many discussions and decisions!

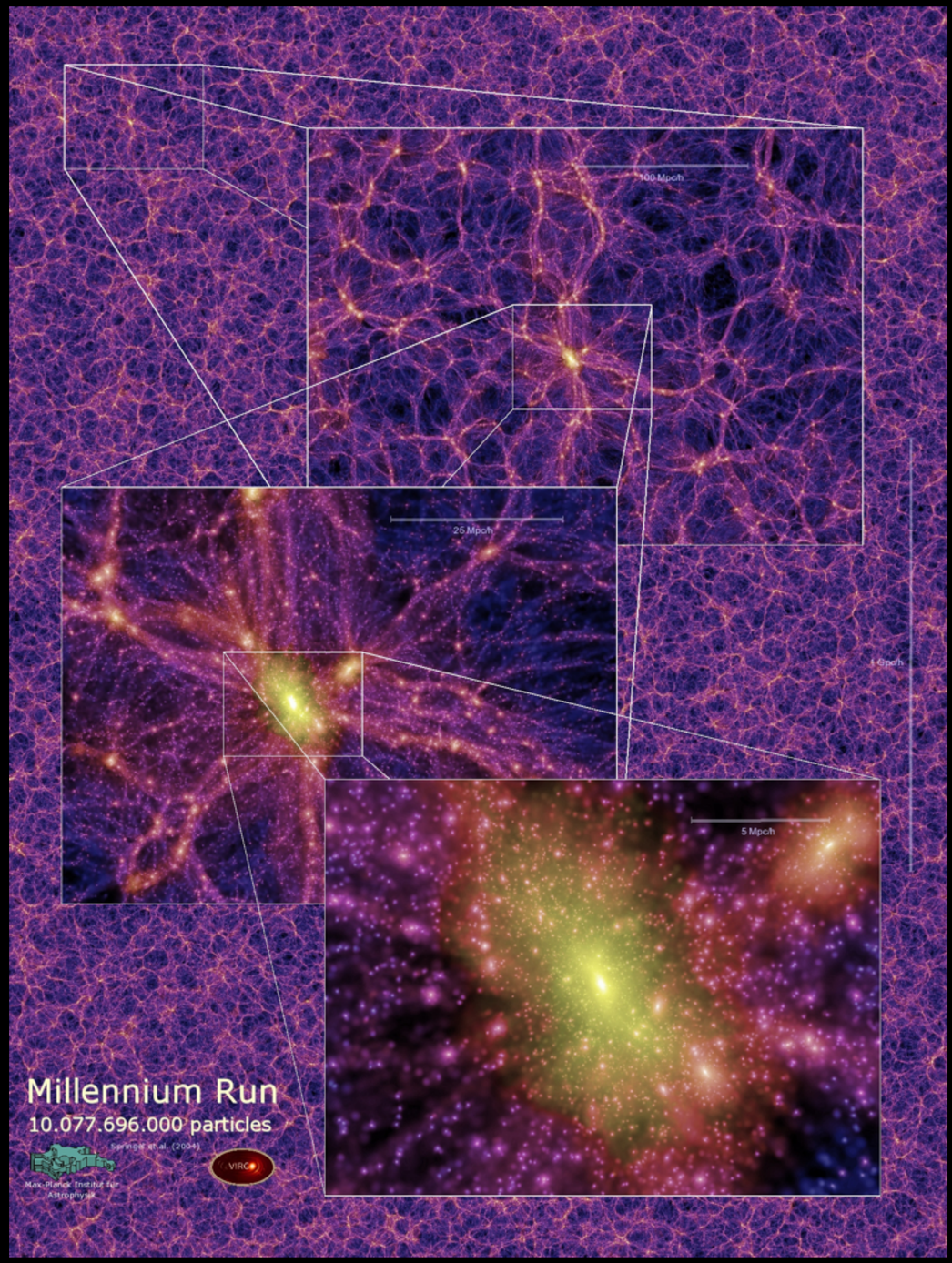
If you have contributed to the Astropy project and your name is missing, please send an email to the coordinators, or open a pull request for the

Some pitfalls

- If you make it too easy to use, people will use it.

Gadget

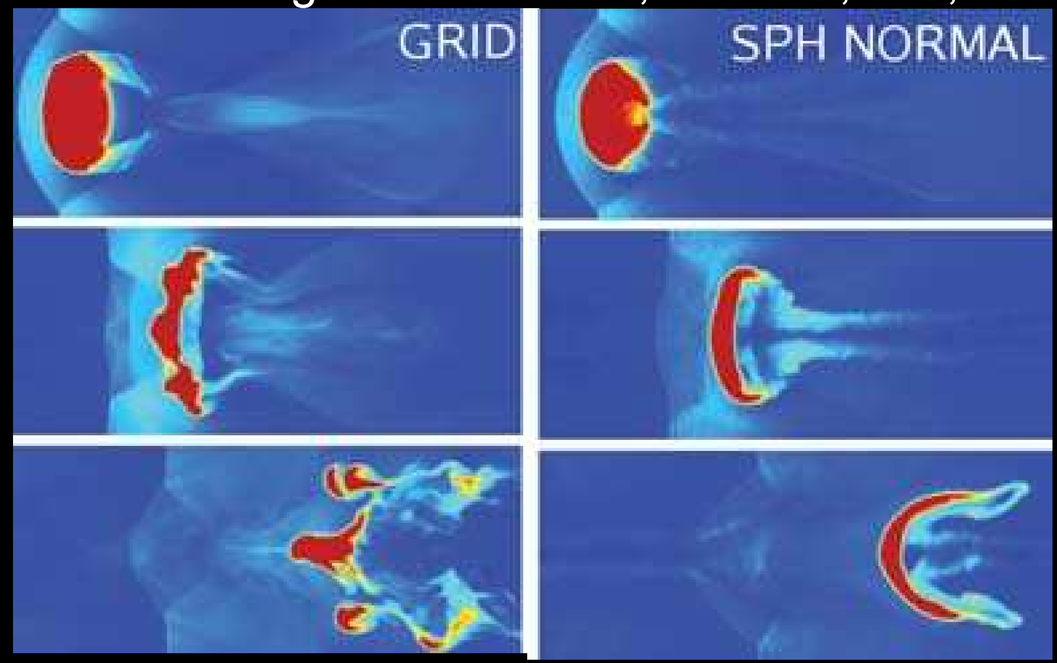
- N-body (active particles)
- Smoothed particle hydro (SPH)
- Various heating/cooling
- Very centralized development:
  V. Springel



Cautionary Tale: Gadget

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

Agertz et al. 2007, MNRAS, 380, 963



- Distribution model meant slow adoption of fix
- 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

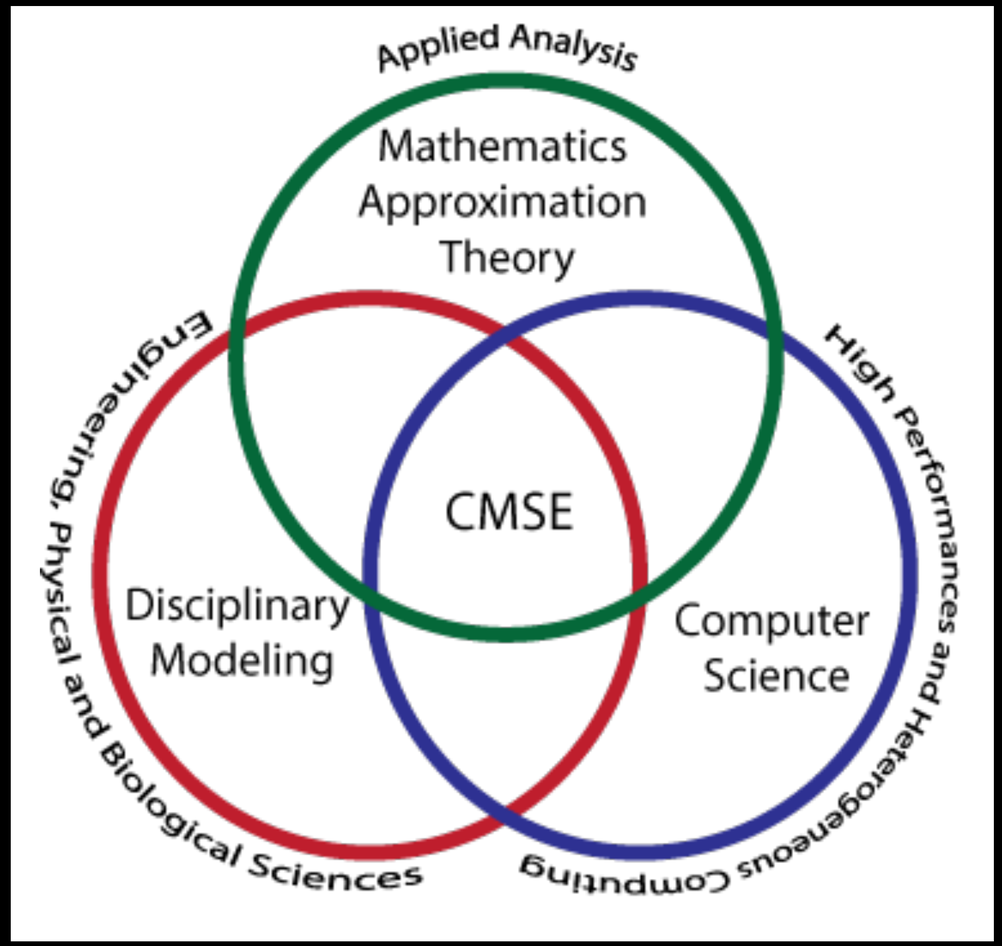
- Hardware complexity increasing…
- Today’s codes may be living on borrowed time
- Need portability
- Abstraction of tasks may be critical!
- Need professional architecture and design

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

- >10 faculty in A&A
- #1 Nuclear Physics graduate program
- Joint Institute for Nuclear Astrophysics
- Major nuclear physics experiment/theory facility (NSCL/FRIB)
- Brand New Department of Computational Math, Science, & Engineering
- MSU High-Performance Computing Center



MICHIGAN STATE UNIVERSITY

Overview

Code	License	Dev Model	Distribution	Language	
FLASH	Custom*	Central	tarball	F90/C	
Enzo	Uofl/NCSA	Distributed	BitBucket	F90/C++	
Gadget	GPL	Central?	tarball	C	
Castro	BSD	Distributed*	GitHub	F90/C++	
Cactus	~GPL	open/devs	tarball	C++/F90	
Zeus	?	disparate	tarball	C	
MESA	GPL	contributory	SourceForge	F90	
Athena	GPL	central	tarball	C/F90	
yt	BSD	community	BitBucket	Python/C	
Pluto	GPL	central	tarball	C++	