

Impact of Community Codes on Astrophysics Sean M. Couch Michigan State University

Argonne Training Program in Extreme Scale Computing St. Charles, IL - 9 August 2016



FACILITY FOR RARE ISOTOPE BEAMS



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, <u>ascl.net</u> >800 codes listed!

Comm. Codes Have Greater Impact

Code

Gadget

Zeus

FLASH

Enzo

MESA

Approx. Publications
3000
1000
1000
400
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?

- found...
- Testing more rigorous

More eyes on the code means more bugs

Multiphysics Complexity Astrophysics Has It!

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

- Nuclear burning
- Multifluids
- Detailed EOS
- Relativity

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









- 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

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

Particles

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

- analysis/viz tools
- transport,...

• FLASH had: Hydro, gravity, AMR, I/O, data

 I could focus on just new stuff: nuclear equation of state, neutrino physics,





200 km

SMC & Ott 2013, ApJL, 778, L7

Time = 2 ms

E.g. FLASH Scaling

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



524k cores! >2 Million threads!



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

FLASH is Special

B.W. O'Shea

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Enzo

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



- ~12 core developers in very different locales
- distributed version control (!)

Enzo

Heavy use of online collaboration tools

Einstein Toolkit

- Annual workshop
- Rules for merging, contributing, etc.

Governance and official maintainers



- 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

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MESA importante Stallar Actrop

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



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SMC et al. 2015, ApJL, 808, L21

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





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Repository for the Astropy core p	ackage http://www.astropy.org		
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astropy	Merge pull request #4760 from mirca/fit-with-sigmaclip	a day ago
🖀 astropy_helpers @ 3e044eb	Update astropy-helpers to v1.2	2 months ago
i cextern	undoing ERFA changes	2 months ago
i docs	Merge pull request #4760 from mirca/fit-with-sigmaclip	a day ago
in examples	Deprecate angles.rotation_matrix/angle_axis in favour of matrix_utili	9 days ago
icenses	Move Numdisplay's license to its own file in the licenses directory	3 months ago
i static	Fixed support on Python 3, and got rid of .astropy-root per astropy/a	2 years ago
astropy-root	Don't rely on .git to enable auto-build when importing from source tr	a year ago
i .gitattributes	Use union merge for changelog	2 years ago
.gitignore	change to putting the sphinx gallery build products in docs/generated	3 months ago
gitmodules	Update the astropy_helpers URL to the real astropy-helpers.	2 years ago
i .mailmap	updated contributor list	2 months ago
i .rtd-environment.yml	try yml way of specifying pip dependencies	3 months ago
.travis.yml	Changing pep8 tool to pycodestyle to follow their change of name. The	6 days ago
CHANGES.rst	Merge pull request #4760 from mirca/fit-with-sigmaclip	a day ago
CITATION	remove the "do not require" part	a year ago
CONTRIBUTING.md	Add a clarification that a changelog entry shouldn't be added right a	7 months ago
MANIFEST.in	rename as suggested by @astrofrog	2 months ago
README.rst	Added Gitter Badge	4 months ago
ah_bootstrap.py	Update astropy_helpers to its current masterthis includes astropy/a	10 months ago
appveyor.yml	Changing temporary workaround for VS version, using Update 2 directly	24 days ago
i ez_setup.py	Update ez_setup.py to latest version	2 months ago
pip-requirements	Updated pip-requirements to numpy 1.7.0	2 months ago
pip-requirements-dev	references to doc-pip-requirements -> pip-requirements-doc	2 months ago
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Not just simulation

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 Bourgue
- Larry Bradley
- Gustavo Bragança
- Erik M. Bray
- Eli Bressert
- Hannes Breytenbach
- Hugo Buddelmeijer

Kaylea Nelson for designing this web site.

- Doug Burke
- Mihai Cara
- Patti Carroll

Other Credits

29

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

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!

- Karan Grover
- Kevin Gullikson
- Hans Moritz Günther

Joe Lyman

Curtis McCully

Vinayak Mehta

Aaron Meisner

Brett Morris

Michael Mueller

Stuart Mumford

Demitri Muna

Prasanth Nair

Bogdan Nicula

Joe Philip Ninan

Bryce Nordgren

Miruna Oprescu

Carl Osterwisch

Madhura Parikh

Sergio Pascual

David Perez-Suarez

Adrian Price-Whelan

J. Xavier Prochaska

David Pérez-Suárez

QuanTakeuchi

 Tanuj Rastogi Iuan Luis Cano

Rodríguez

Orion Poplawski

Luigi Paioro

Asish Panda

Neil Parley

Rohit Patil

Ray Plante

Asra Nizami

Serge Montagnac

José Sabater Montes

Francesco Montesano

- 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

Roban Hultman

 Dominik Klaes Kacper Kowalik

Kramer

Arne de Laat

Antony Lee

Daniel Lenz

Simon Liedtke

Stuart Littlefair

Pey Lian Lim

Joseph Long



Evert Rol

Alex Rudy

Joseph Ryan

Eloy Salinas

David Shiga

Albert Y. Shih

David Shupe

Jonathan Sick

Brigitta Sipocz

 Ole Streicher Matej Stuchlik

James Taylor

Víctor Terrón

Scott Thomas

James Turner

Julien Woillez

Lisa Walter

Julien Woillez

Víctor Zabalza

Jake VanderPlas

Jake VanderPlas

Jeff Taylor

Leo Singer

Some pitfalls

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

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

Gadget





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
- Proliferation of proprietary versions



Some pitfalls

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

models

Some pitfalls

- Assigning credit
- deserve credit
- Traditional academic mechanisms

Codes are "instruments" and builders

(publications, citations, etc.) often don't fit

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



- 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	С	
Castro	BSD	Distributed*	GitHub	F90/C++	
Cactus	~GPL	open/devs	tarball	C++/F90	
Zeus	?	disparate	tarball	С	
MESA	GPL	contributory	SourceForge	F90	
Athena	GPL	central	tarball	C/F90	
yt	BSD	community	BitBucket	Python/C	
Pluto	GPL	central	tarball	C++	

