An introduction to the Einstein Toolkit

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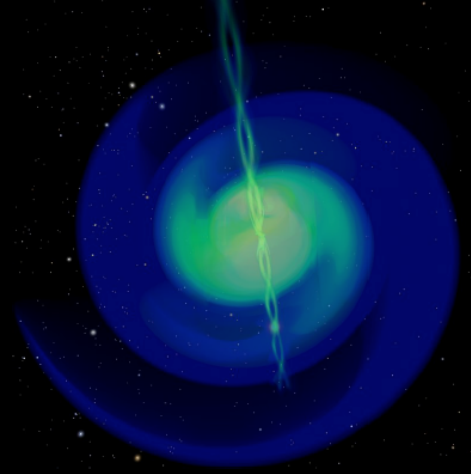
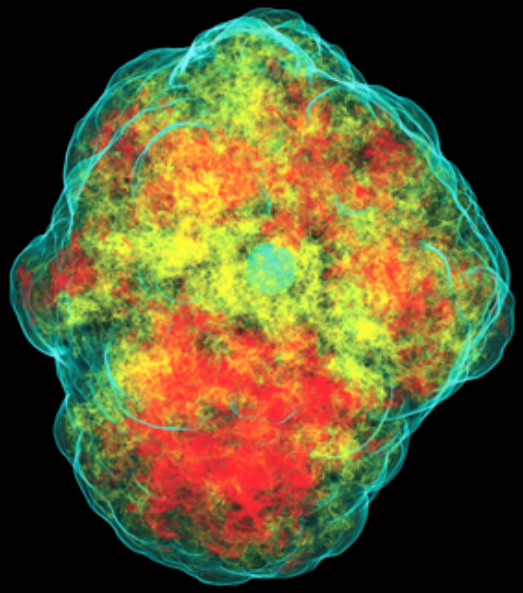
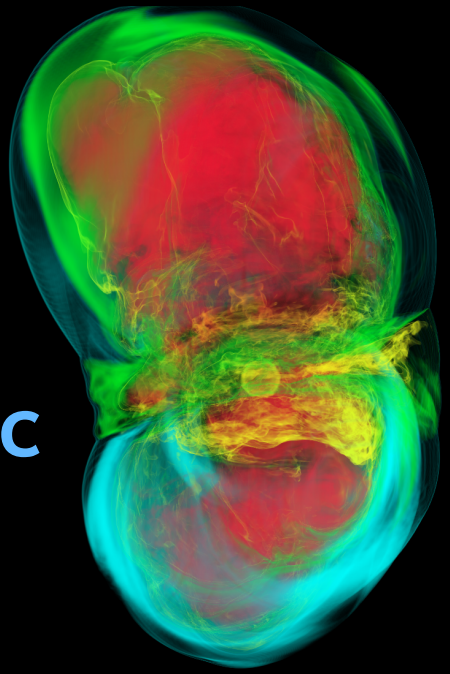
Open Digital Infrastructure in Astrophysics
KITP, Jun 5 2019

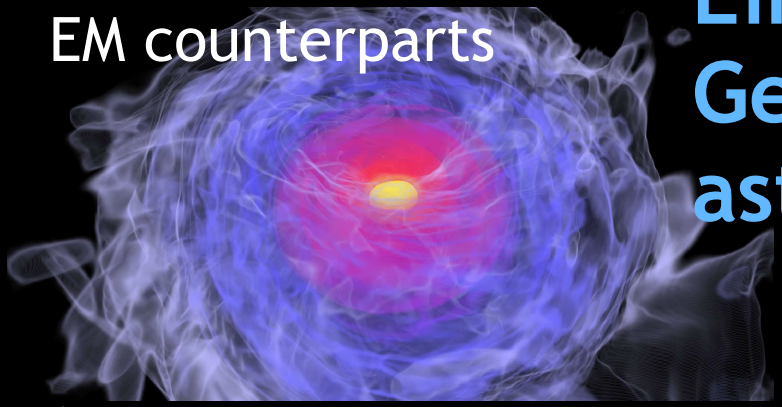




Core-collapse supernovae
neutrinos
turbulence

(Binary) black holes
accretion disks
EM counterparts





Einstein Toolkit: General-relativistic astrophysics

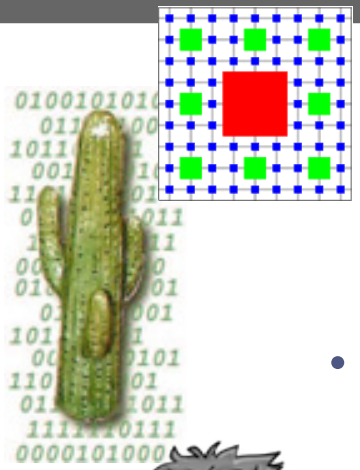
Binary neutron stars
gravitational waves +EM
sGRBs
heavy elements

Extreme core-collapse
hyperenergetic/superluminous
lGRBs
heavy elements

Radice, Bernuzzi, **PM+ 16**

Einstein Toolkit

Einstein Toolkit



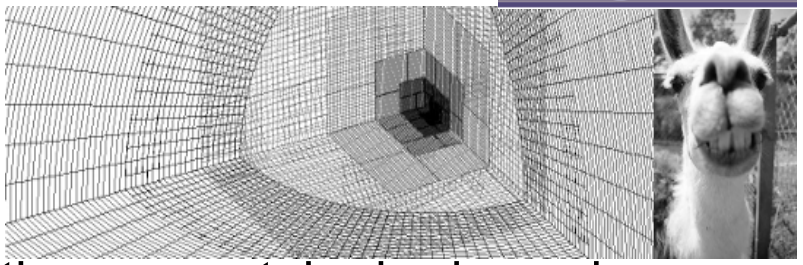
einstein toolkit

- Open source framework
  - Decentralized code development
  - Active and friendly user community
  - Online tutorials and workshops
- Infrastructure modules
  - Parameter file handling
  - Parallelization (MPI + OpenMP)
  - Mesh refinement
  - IO and checkpointing
- Physics modules
  - Spacetime evolution
  - General relativistic radiation magnetohydrodynamics
  - Multigrid elliptic solver

NumPy

HDF

VisIt



Einstein Toolkit

Einstein Toolkit - software

- Goals
  - community-driven
    - mailing list
    - wiki, bug tracker
  - core computational tools for relativistic astrophysics and gravitational physics
- Components
  - Cactus thorns for GW science
  - Simulation factory
  - GetComponents component retrieval tool
  - Kranc
  - Waveform analysis

- Guiding principles
  - Open, community-driven software development
  - Well thought out and stable interfaces
  - Separation of physics software from computational science infrastructure
  - complete working production codes
- does not itself develop codes
  - codes are proposed for inclusion, then reviewed
  - must be of current interest for the community

Einstein Toolkit

Cactus framework (http://cactuscode.org)

basic APIs, high-level data structures and functions, mixed language integration

Carpet grid driver: Cartesian/Multi-Block AMR, memory management, I/O, communication, scheduling, load

Radiation transport: two-moment analytic closure (M1) / "leakage" approximation

GRMHD solvers: Finite volume, HLLE/HLLC, ePPM/PPM/WENO5, constrained transport

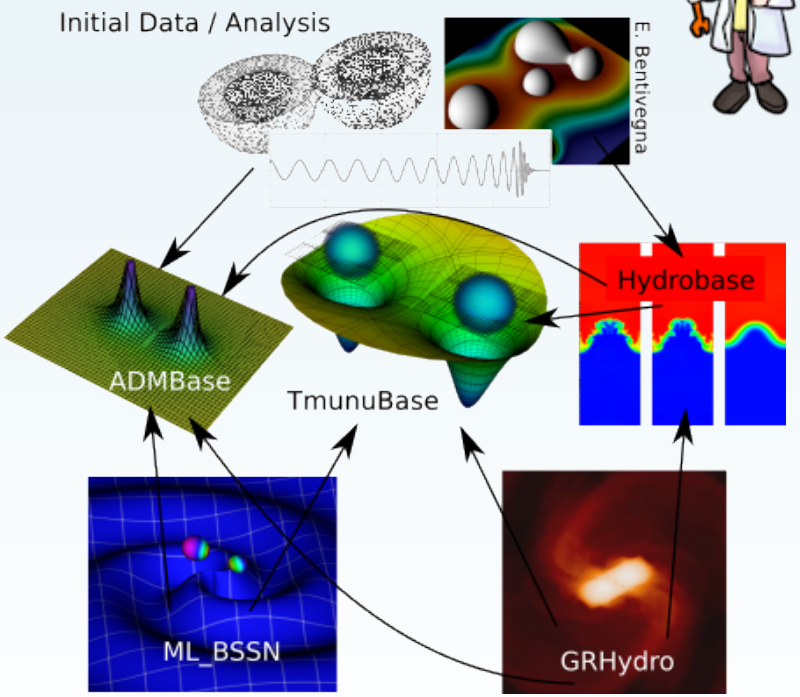
Coupling: Method of Lines, RK2/RK4

Analysis: horizon finders, wave extraction

Spacetime solvers

Main Einstein Toolkit Cactus modules

- Einstein Toolkit defines **base** thorns that contain no code but declare hooks for thorns to interact:
  - ADMBase: metric, lapse, shift. ...
  - HydroBase: rest mass density, pressure, …
  - TmunuBase: stress-energy-tensor
- “default” evolution thorns
  - McLachlan
  - GRHydro or IllinoisGRMHD
  - PITTNull code



Einstein Toolkit: Background

- Background: Offspring of numerical relativity efforts started in 1990s at NCSA -> Max Planck -> LSU (Ed Seidel/Gabrielle Allen)
- Used by major numerical relativity groups in the US/Europe (total ~240 users & ~50 groups; main users from ~10 groups).
- Users/Groups use framework + some application/analysis thorns; generally have their own proprietary thorns for applications.
- Funding: NSF Physics at the Information Frontier Grant, 2006-2015 (renewed twice); GA Tech, Caltech, LSU, RIT; level: $160k/yr (~1.5 postdocs) -> partial postdocs/staff at sites; TCAN centered at RIT

Einstein Toolkit: Background

- 206 citations to the original Einstein Toolkit paper (2012)
- Many more for individual components
- Official suggested papers citation policy
- Likely move to software DOI for citation in future

But: This doesn't tell the full story!

Einstein Toolkit: Community

Einstein Toolkit

http://www.einsteintoolkit.org

1998-09-25

einstein
toolkit

Einstein Toolkit: User base

- Online tutorials / examples

- Workshops and schools

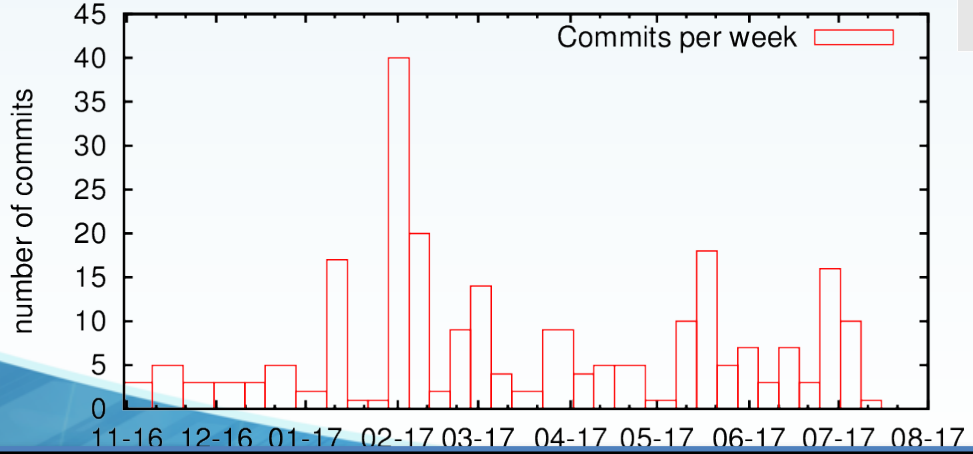
- Email list / bug tracking / ticket system

- weekly user / developer calls

Einstein Toolkit: Releases

“Hack” statistics

- 240 thorns
- 1 new thorn (LORENE2)
- 344 individual commits by 20 authors



Language	files	blank	comment	code
C	779	26899	66223	229427
C++	538	47160	18089	213773
Fortran	574	15924	14574	105525
C/C++ header	655	11512	14731	50395

Einstein Toolkit: Schools/workshops

"Hack" workshops

- School and workshop at NCSA in August 2017
  - 51 school participants
  - 48 workshop participants
  - mostly from American continent
- 3 days of school
  - 6 lectures, 2 hands on tutorials
- 2 days of workshop
  - 12 lightning talks
- ad-hoc MHD workshop
  - code specific to MHD and task-based parallelism
  - at Columbia University (Daniel Siegel)
  - kickstarter for projects
- ET workshop and EdFest 2017
  - this meeting
  - 64 participants
  - 13 countries.

Einstein Toolkit: Development

- 7 maintainers

- Focused working groups

- Workshops / development calls

- Official stable releases every 6 months

- Regression testing / standard tests run daily

Einstein Toolkit: Development

HydroToyOpenMP – a new hydro code

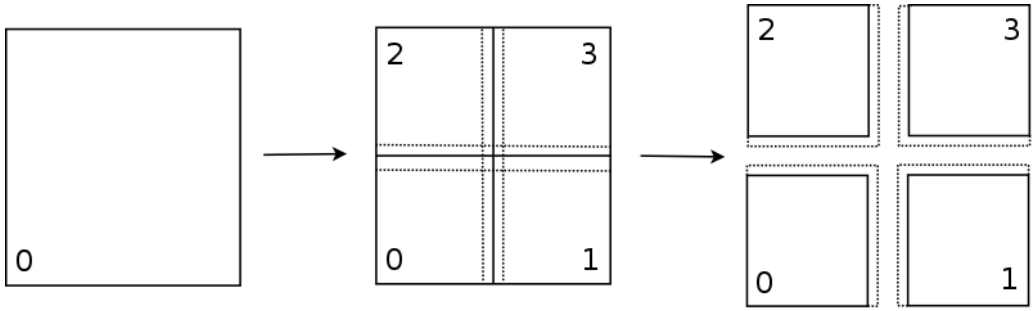
- Work with Erik Schnetter (PI), Hannah Klion, Aashrita Mangu (UCB)
- proof of concept hydro code for modern CPUs
- no options or complex methods, keep it simple
- achieve good per-node performance

- single scheduled routine with a pointwise kernel
- C++14 lambda function for looping, tile handling
- OpenMP “task” for parallelism
- re-use inner code from GRHydro where possible
- allow for overlap between computation and communication

```
git clone -b eschnett/hydrotoy https://bitbucket.org/cactuscode/cactusexamples
```

Einstein Toolkit: Development

HydroToyOpenMP scheduling



(c) BrokenSphere / Wikimedia Commons

- subdivide data into tiles that fit into L2
- first operation copies from grid to tile
- later operations read from cache
- tile looping construct via λ function that takes a λ function as a science kernel that takes a λ function to loop over points. . .
- . . . wrap in λ to use OpenMP task construct for parallelism

Einstein Toolkit: Issues

Structural challenges:

- Code curation/maintenance vs. innovation

- Fragmented approach does not work well

- Involvement of user base / steep learning curve

- Longevity/sustainability: postdocs move on

Einstein Toolkit: Issues

Expand/diversify userbase:

- Schools good for local students

- Library/functional requirement

- Online tutorials / webpage / documentation

Einstein Toolkit: Issues

Funding:

"Easy" to fund new things. Difficult to fund maintenance and community support. TCAN/Einstein Toolkit funding innovation driven

Need dedicated "instrument" scientist(s) in future!

Funding for verification purposes?

Einstein Toolkit: Issues

Where is the Einstein Toolkit going to be in 10/20 years?

- Community-driven development vs large-scale managed efforts
- How to stay relevant on modern HPC infracstructure ?
- Where do we move as a community: Single vs multiple codes / verification / … ?