Perspective from NCSA

Gabrielle Allen
Professor, Department of Astronomy
Associate Director, NCSA
U. Illinois Urbana-Champaign

30 YEARS NCSA
1986–2016

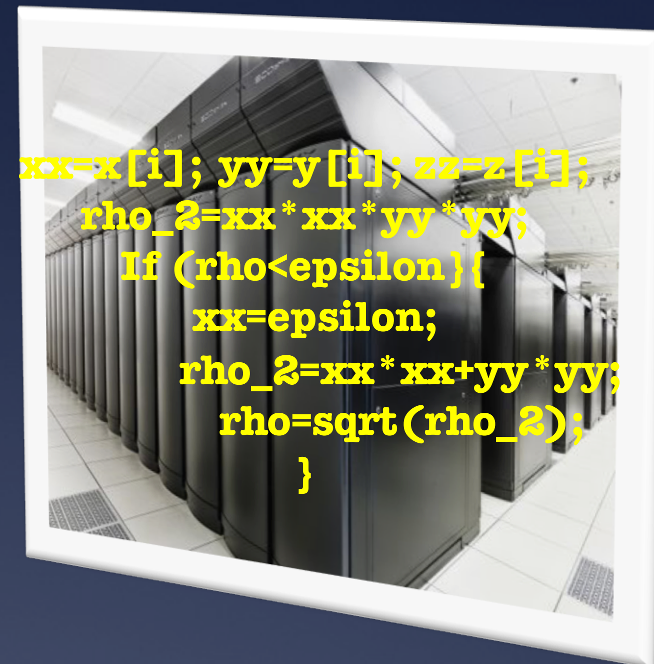
Background

* BSc Mathematics, MS Applied Math, PhD Theoretical physics in UK
* Postdoc/Scientist at Max Planck Institute for Gravitational Physics in Germany
* Professor of Computer Science/Physics at Louisiana State University, Assistant Director at new Center for Computation & Technology
* Led development of scientific software and interdisciplinary science communities – Cactus, GridSphere, Grid Application Toolkit, CyberTools
* NSF Program Director for Scientific Software
* Professor/CIO at new Skolkovo Institute for Science & Technology
* Professor of Astronomy at U. Illinois, Associate Director at National Center for Supercomputing Applications
  * Building interdisciplinary institutional R&E programs
  * Community building in software productivity and sustainability

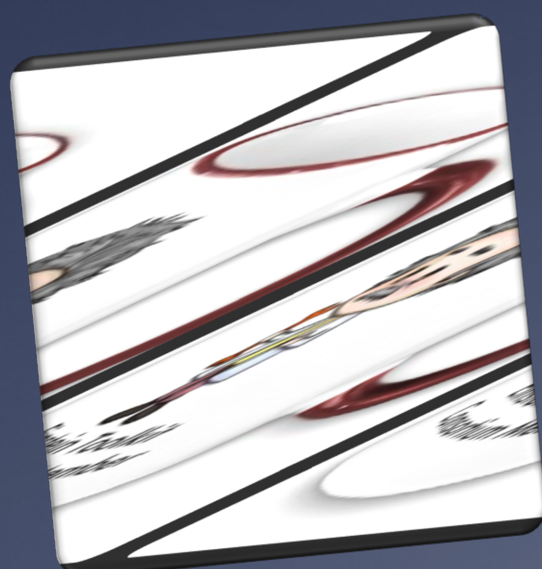
Solving Complex Problems

Science research

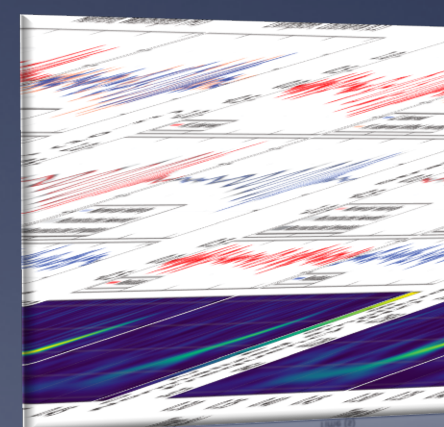
Software (& Hardware)



Community

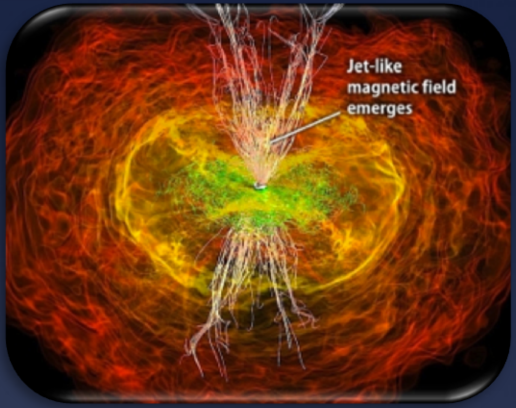


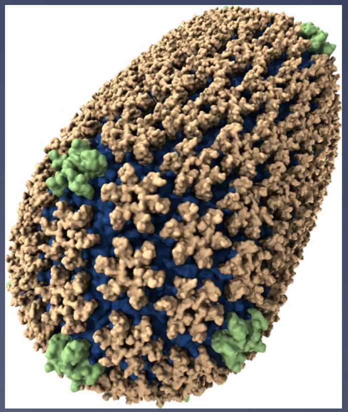
Impact



Complex Problems

* World: multiscale, multiphysics, data-driven
* E.g. Neutron Stars, Plants, Viruses, …
* General Challenges
  * Determine correct scale to describe a physical event and the correct governing equations
  * Determine how different phenomena interact - often at different scales
  * Determine data inputs (experimental, observational, …)
  * Design simple but effective interfaces that can be implemented in software
  * (Find, fund & motivate team)





The Einstein Toolkit: A Community Computational Infrastructure for Relativistic Astrophysics

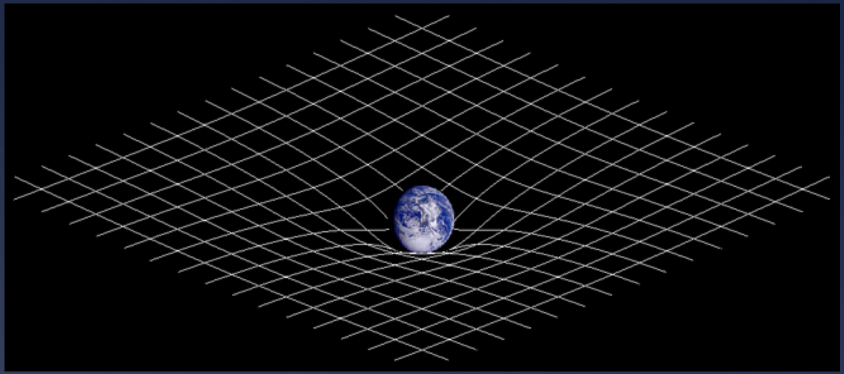
NCSA: An Interdisciplinary Research Environment for Complex Problem Solving Communities

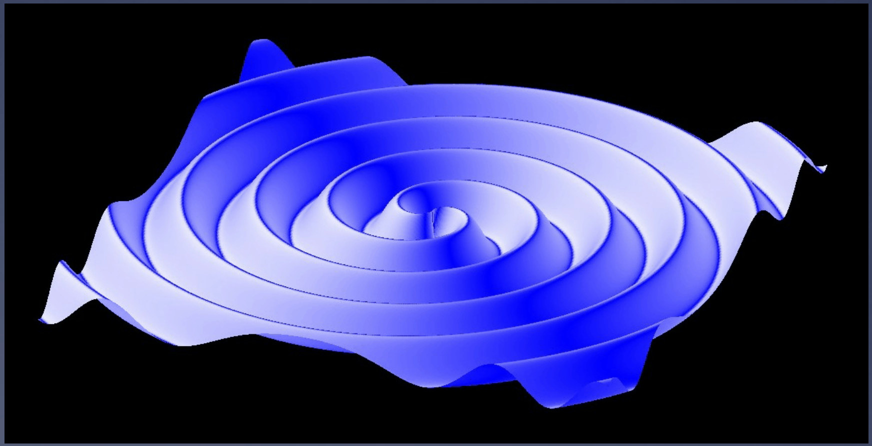
The Einstein Toolkit: A Community Computational Infrastructure for Relativistic Astrophysics

http://www.einsteintoolkit.org

Gravitational Waves

- Changes in the curvature of spacetime that propagate as waves at the speed of light
  - Transport energy as gravitational radiation
- Predicted by Einstein (1916)
  - Theory of General Relativity
- Till recently only *indirectly* observed
- Observations by new gravitational wave detectors have opened a new window on the universe … *gravitational wave astronomy*!





* Changes i
  spacetime
  waves at t
  * Transport
    radiation
* Predicted
  * Theory o
* Till recently
  observed
* Observati
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"All the News That's Fit to Print"

The New York Times

Late Edition

VOL. CLXV . . . No. 57,140 | NEW YORK, FRIDAY, FEBRUARY 12, 2016 | $2.50

Clinton Paints Sanders Plans As Unrealistic

New Lines of Attack at Milwaukee Debate

By AMY CHOZICK and PATRICK HEALY

MILWAUKEE — Hillary Clinton, scrambling to recover from her double-digit defeat in the New Hampshire primary, repeatedly challenged the trillion-dollar policy plans of Bernie Sanders at their presidential debate on Thursday night and portrayed him as a big talker who needed to "level" with voters about the difficulty of accomplishing his agenda.

Foreign affairs also took on unusual prominence as Mrs. Clinton sought to underscore her experience and Mr. Sanders excoriated her judgment on Libya and Iraq, as well as her previous praise of former Secretary of State Henry A. Kissinger. But Mrs. Clinton was frequently on the offensive as well, seizing an opportunity to talk about leaders she admired and turning it against Mr. Sanders by bashing his past criticism of President Obama — a remark that Mr. Sanders called a "low blow."

With tensions between the two Democrats becoming increasingly obvious, the debate was full of new lines of attack from Mrs. Clinton, who faces pressure to puncture Mr. Sanders's growing popularity before the next nominating contests in Nevada and South Carolina.

She is wagering that even voters excited by Mr. Sanders's inspiring message will reconsider their support when they learn of his lack of experience in foreign policy and his vague explanations for how he will pay for his expansive government programs.

Mrs. Clinton pounced from the start, after Mr. Sanders demurred in saying how much his proposals would increase the size of the federal government. She stepped in and said that by economists' estimates, the government would grow 40 percent under Mr. Sanders.

And rather than bashing him as she did at their debate last Thursday, she appeared to try to get under his skin by implying that he had not been transparent about the cost of his programs, such as his proposed expansion of government health care.

"This is not about math. This is

Continued on Page A16

Going Back to Trenton

Gov. Chris Christie has returned to New Jersey to tend to a state he at times abandoned in his run for president. Page A21.

A worker installed a baffle in 2010 to control light in the Laser Interferometer Gravitational-Wave Observatory in Hanford, Wash.

WITH FAINT CHIRP, SCIENTISTS PROVE EINSTEIN CORRECT

A RIPPLE IN SPACE-TIME

An Echo of Black Holes Colliding a Billion Light-Years Away

By DENNIS OVERBYE

A team of scientists announced on Thursday that they had heard and recorded the sound of two black holes colliding a billion light-years away, a fleeting chirp that fulfilled the last prediction of Einstein's general theory of relativity.

That faint rising tone, physicists say, is the first direct evidence of gravitational waves, the ripples in the fabric of space-time that Einstein predicted a century ago. It completes his vision of a universe in which space and time are interwoven and dynamic, able to stretch, shrink and jiggle. And it is a ringing confirmation of the nature of black holes, the bottomless gravitational pits from which not even light can escape, which were the most foreboding (and unwelcome) part of his theory.

More generally, it means that a century of innovation, testing, questioning and plain hard work after Einstein imagined it on paper, scientists have tapped into the deepest register of physical reality, where the weirdest and wildest implications of Einstein's universe become manifest.

Conveyed by these gravitational waves, power 50 times greater than the output of all the stars in the universe combined vibrated a pair of L-shaped antennas in Washington State and Louisiana known as LIGO on Sept. 14.

If replicated by future experiments, that simple chirp, which rose to the note of middle C before abruptly stopping, seems destined to take its place among the great sound bites of science, ranking with Alexander Graham Bell's "Mr. Watson — come here" and Sputnik's first beeps from orbit.

"We are all over the moon and back," said Gabriela González of Louisiana State University, a spokeswoman for the LIGO Scientific Collaboration, short for Laser Interferometer Gravitational-Wave Observatory. "Einstein would be very happy, I think."

Members of the LIGO group, a

Continued on Page A12

Long in Clinton's Corner, Blacks Notice Sanders

Courted Hard in South Carolina, Loyalists Listen Closely

By RICHARD FAUSSET

ORANGEBURG, S.C. — When Helen Duley was asked whom she would vote for in the South Carolina primary, she answered as if the very question were absurd.

"What I'm seeing is a bunch of confusion, hearsay and foolishness," said Ms. Duley, 60, a retired nursing assistant who is African-American, shortly after finishing breakfast at the downtown McDonald's. "What I also see is a veteran who's already been in the White House eight years. A veteran: Hillary Clinton."

But that was late January. Interviewed again Tuesday as Mrs. Clinton's rival, Senator Bernie Sanders of Vermont, was surging toward an overwhelming victory in the New Hampshire Democratic primary, Ms. Duley found herself suddenly intrigued by a candidate she barely knew. "It makes me feel good," she said, chuckling, "that young people are listening to the elderly people." She now said she was an undecided voter and planned to do some homework on Mr. Sanders.

Mrs. Clinton has long looked forward to the Feb. 27 Democratic contest in South Carolina, the first state where blacks will make up a dominant part of the primary vote. African-Americans accounted for more than half the voters in the 2008 Democratic primary, and she has been counting on them as a bulwark, not just

Continued on Page A18

Reginald Abraham, left, an organizer for Hillary Clinton, at a barbershop in Orangeburg, S.C.

Last Occupier In Rural Oregon Is Coaxed Out

This article is by ***Dave Seminara, Richard Pérez-Peña*** *and* ***Kirk Johnson.***

PRINCETON, Ore. — They implored the last holdout in the armed occupation of a wildlife refuge here to think about the Holy Spirit. They explained that the First Amendment was about freedom of speech and the Second was about the right to bear arms, and said that they were in that order for a reason. They asked him what he thought Jesus would have done in his situation.

He, in turn, asked for pizza and marijuana, criticized a government that condoned abortion and drone strikes, and talked about U.F.O.s and dying rather than going to prison.

In the final moments, a standoff fed by big ideas about the role of government came down Thursday morning to the grievances and fears of one troubled young man, and the tense but successful efforts of his sympathizers and F.B.I. agents to coax him to surrender, ending the occupation of Malheur National Wildlife Refuge in southeastern Oregon.

"I'm actually feeling suicidal right now," said David Fry, 27, of Blanchester, Ohio, the last of the

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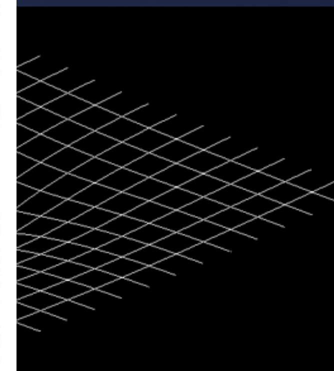
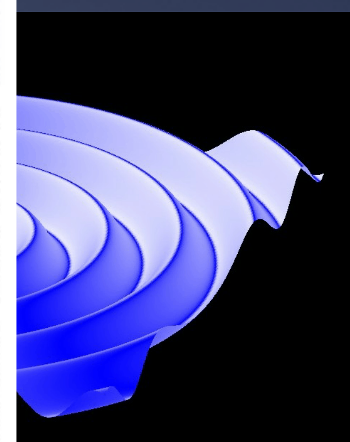
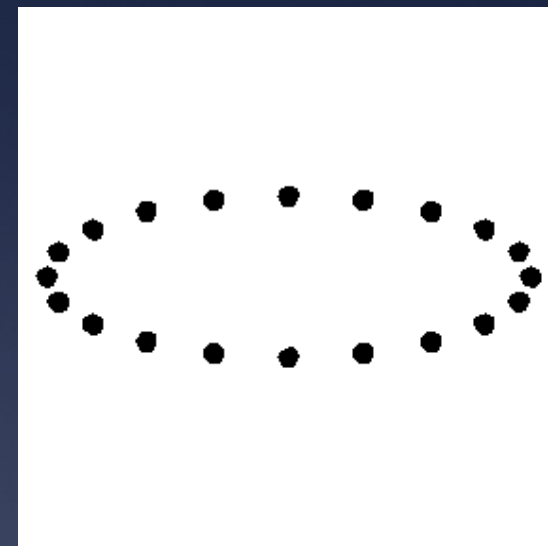
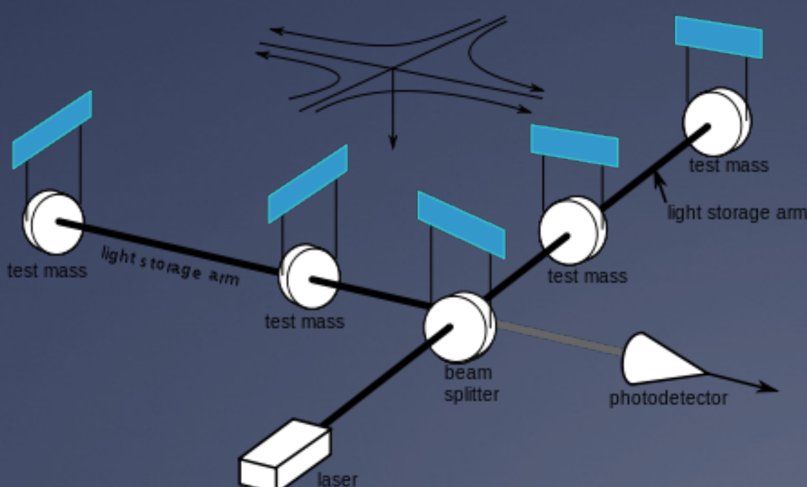
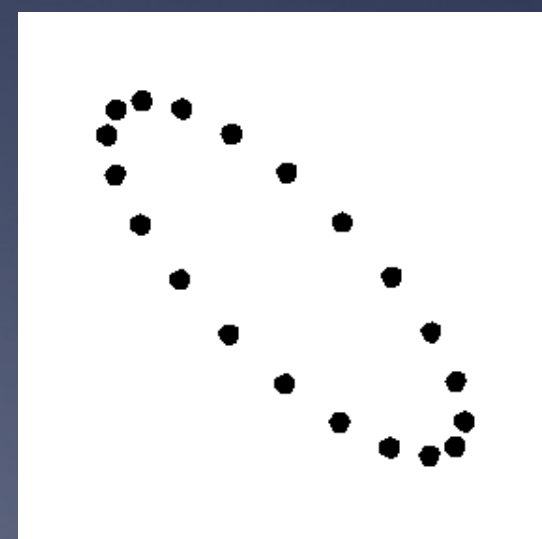




Laser Interferometer Gravitational Wave Observatory (LIGO)

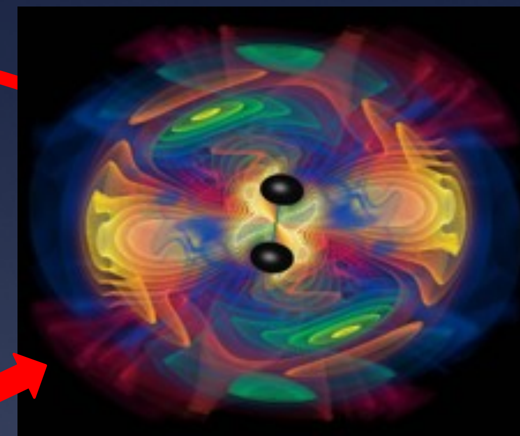






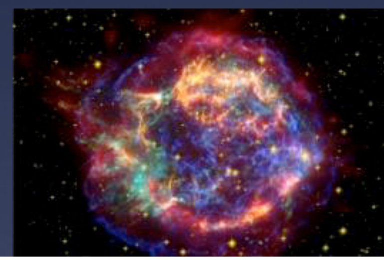
Gravitational Wave Physics

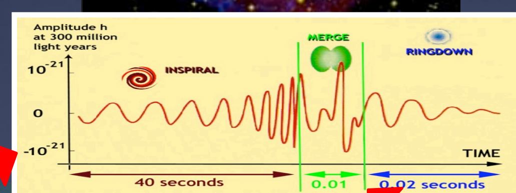
Models & Simulation



Observations

Scientific Discovery!





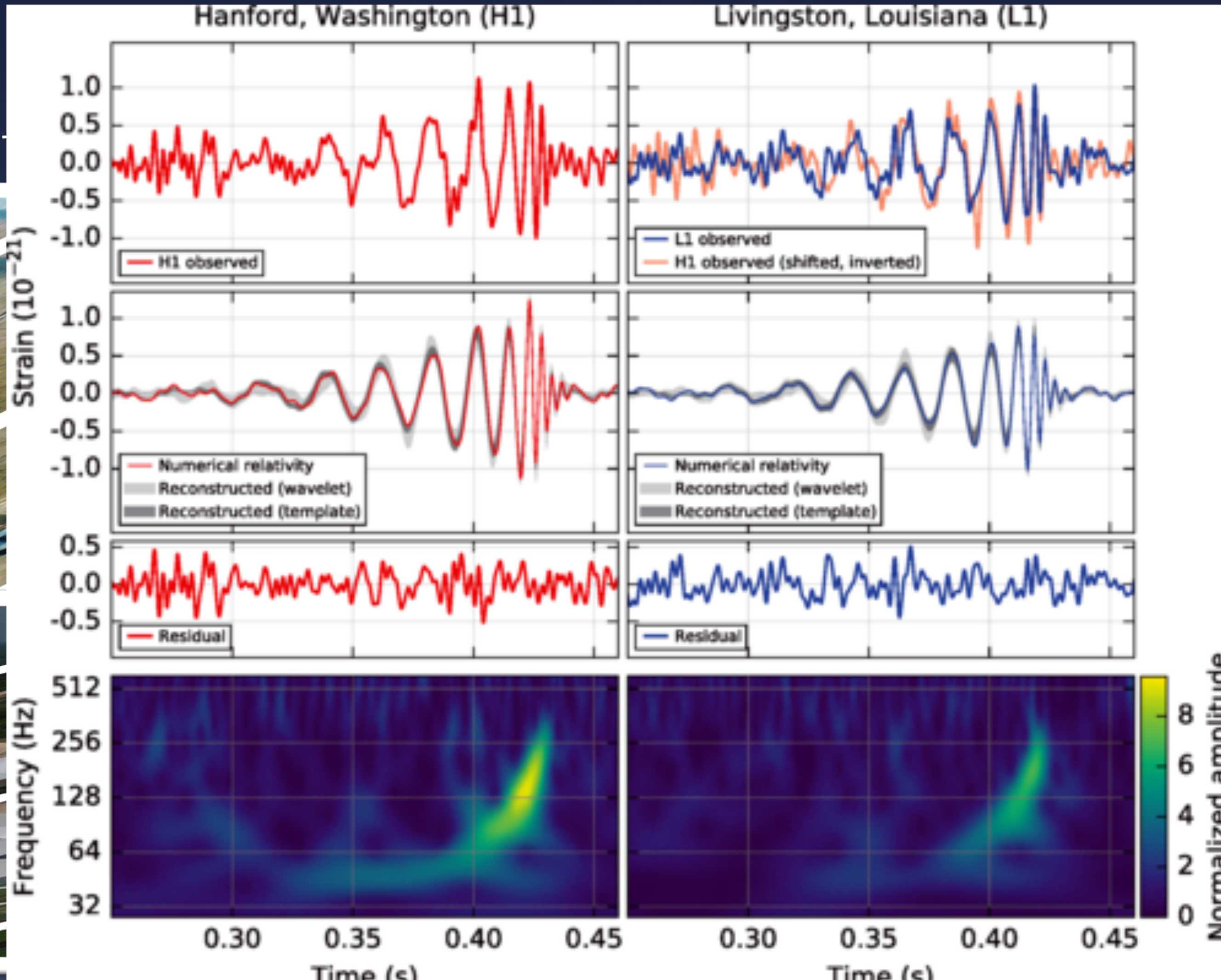
Theory

$$G_{\mu\nu} = 8\pi T_{\mu\nu}$$

Compact binaries, supernovae collapse, gamma-ray bursts, oscillating NSs, gravitational waves, …

Gravitational Wave Physics

Inst



ory

neutron

ollapse,

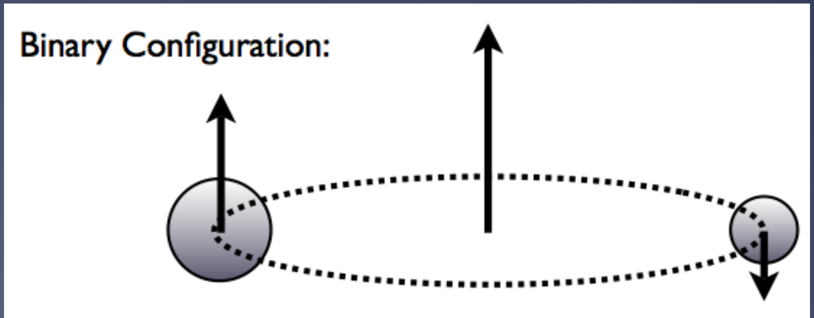
bang, …

Numerical Relativity

- Using numerical methods and algorithms to solve problems governed by General Relativity
  - Black holes, neutron stars, gamma-ray bursts, gravitational waves, stellar core collapse, cosmology
  - Complex equations, tensors, non-linear, 1000's of terms

$$R_{\mu\nu} - \frac{1}{2} g_{\mu\nu} R + g_{\mu\nu} \Lambda = \frac{8\pi G}{c^4} T_{\mu\nu}$$

- Binary black holes:
  - Simple system (no matter)
  - Two body problem: just a few parameters
  - Important for gravitational wave detection
  - Precursor for problems with matter

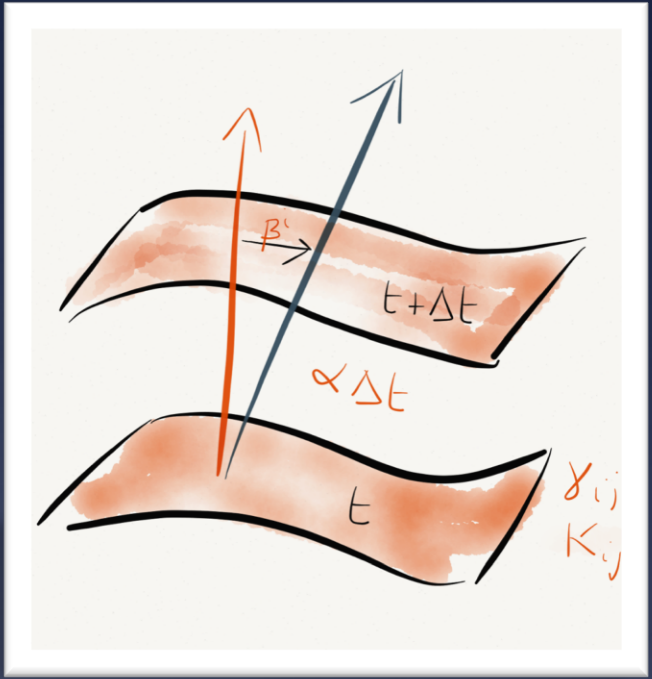


Basic Formalism: ADM

1. Choose initial spacelike surface and provide initial data (3-metric, extrinsic curvature)

2. Choose coordinates:
   * Construct timelike unit normal to surface, choose lapse function
   * Choose time axis at each point on next surface (shift vector)

3. Evolve 3-metric, extrinsic curvature



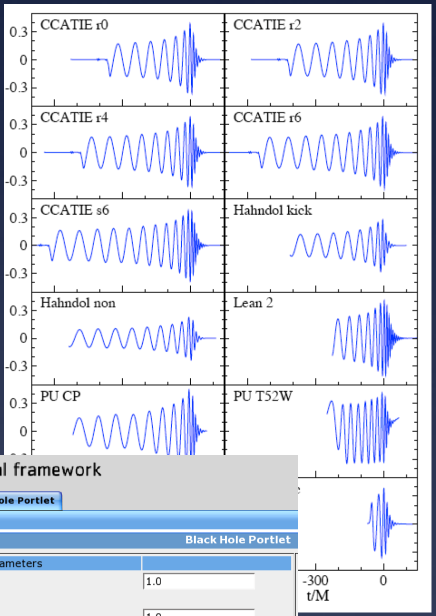
Usual numerical methods:

* Structured meshes (including multi-patch), finite differences (finite volumes for matter), adaptive mesh refinement (since ~2003). High order methods.

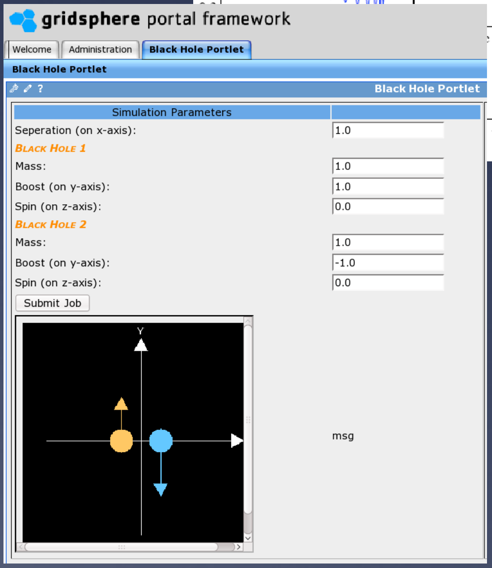
* Some groups use high accuracy spectral methods for vacuum space times

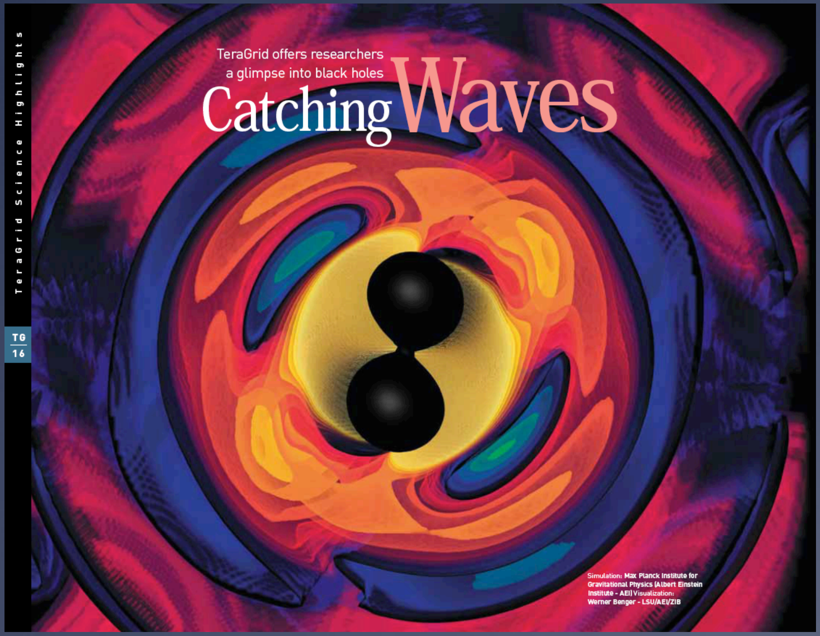
Black Holes & Vacuum Spacetimes

- 40+ year effort to model … big advance in 2005
- Now: Accurate waveforms for nearly arbitrary masses, spins, momentum
- Numerically generated waveforms now used with gravitational wave data analysis, theoretical relativity



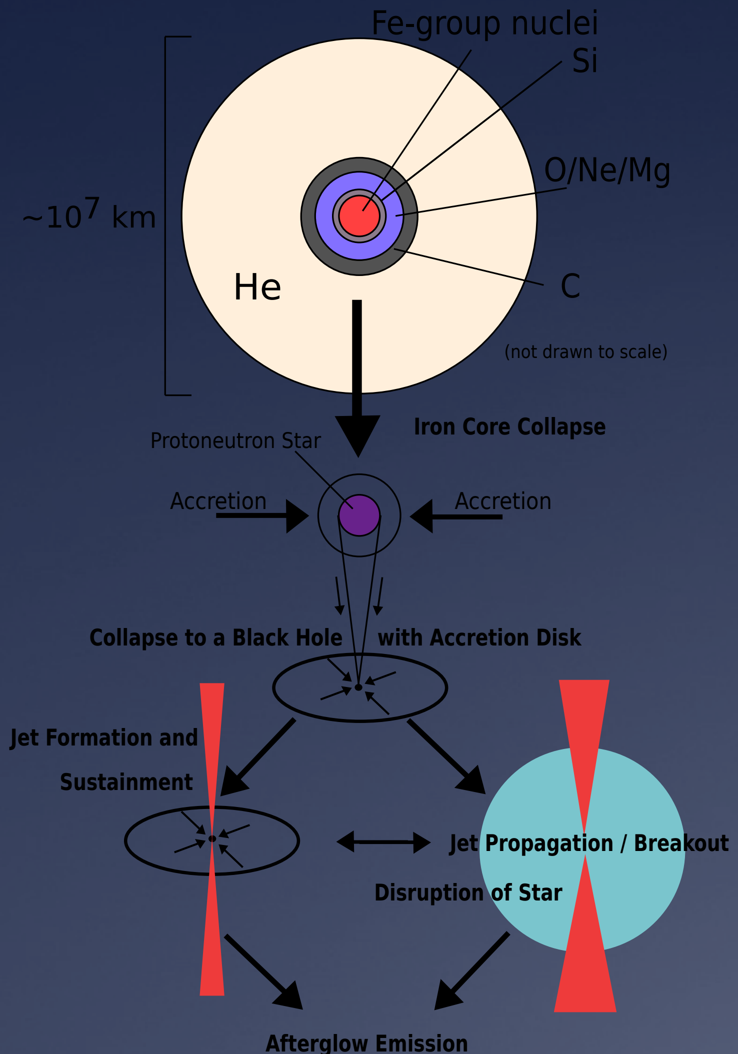
B.Aylott *et al* 2009 Clas. Quantum Grav. 26 1650





- Opens the door to general relativistic hydrodynamics

New Frontiers: Relativistic Matter



Schnetter et al, PetaScale Computing: Algorithms and Applications, 2007

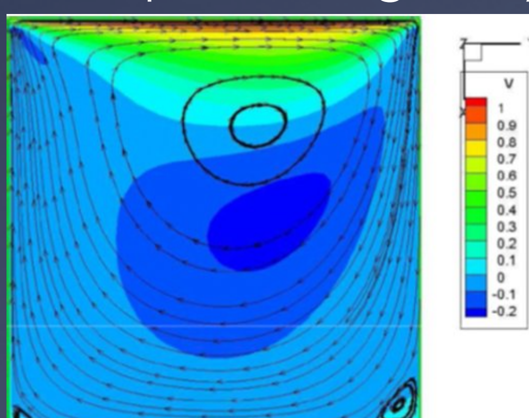
- General relativity
- Nuclear equations of state
- Relativistic magnetohydrodynamics (GRMHD)
- Radiation Transport (neutrinos/photons)
  - Expensive and complicated!
  - Requires opacities/emissivities
- Chemical reactions (thermonuclear, chemical)
- Computation:
  - Multiphysics!!
  - GRMHD: petascale problem
  - Radiation transport beyond this
- Resolve 10^2m to 10^{10}m, 500 grid variables

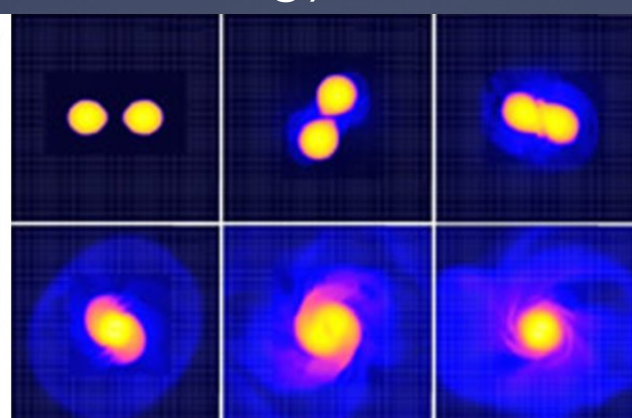
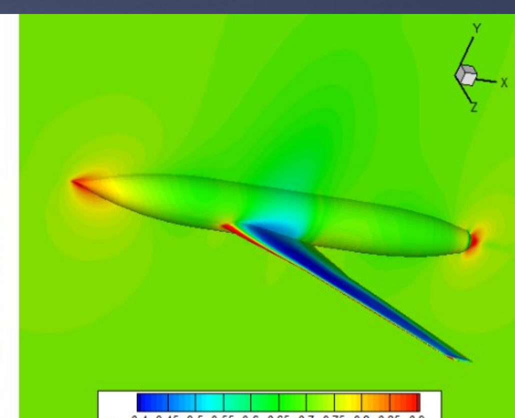
Software
Platform

Cactus Framework

Cactus: www.CactusCode.org

- Open source component framework for HPC
- Modular system with **high level abstractions**
  - Components ("thorns") defined by parameters, variables, methods
  - Cactus "flesh" binds together
  - Cactus Computational Toolkit: general thorns
- Different application areas
  - Numerical relativity, CFD, coastal science, petroleum, quantum gravity, cosmology, …



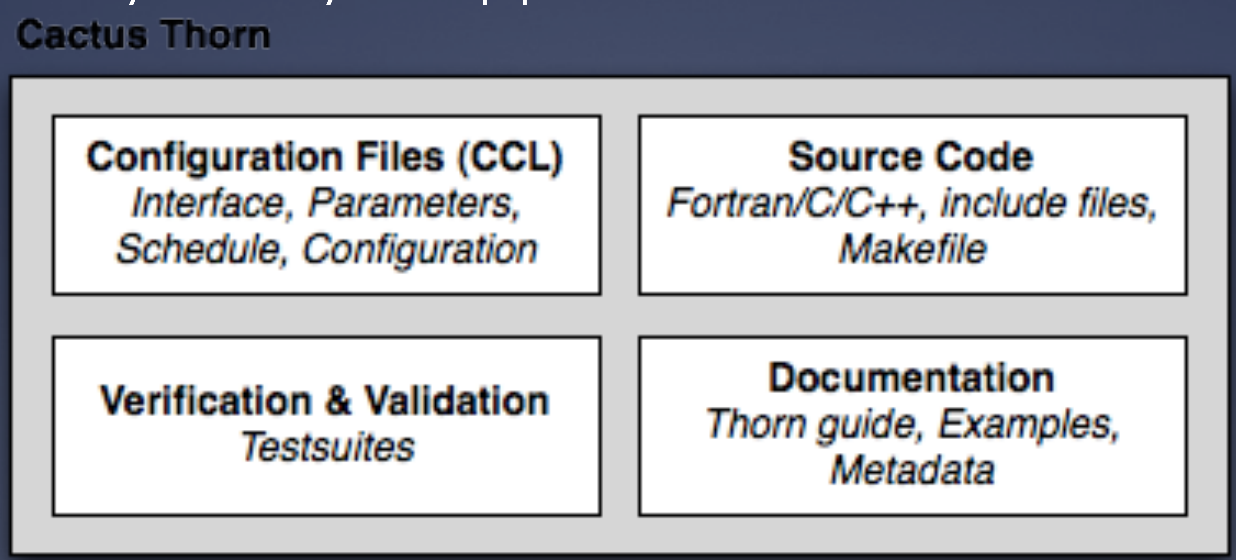
Building a Computational Numerical Relativity Community

- Cactus came from the relativity community
- European project with 10 sites developed community open code base
- Each group had different expertise
- Cactus allowed developing shared interfaces/standards
- Easy to add a component, share components
- Supports both collaboration and competition

EU Network for Gravitational Wave Sources: 2001

Key Features

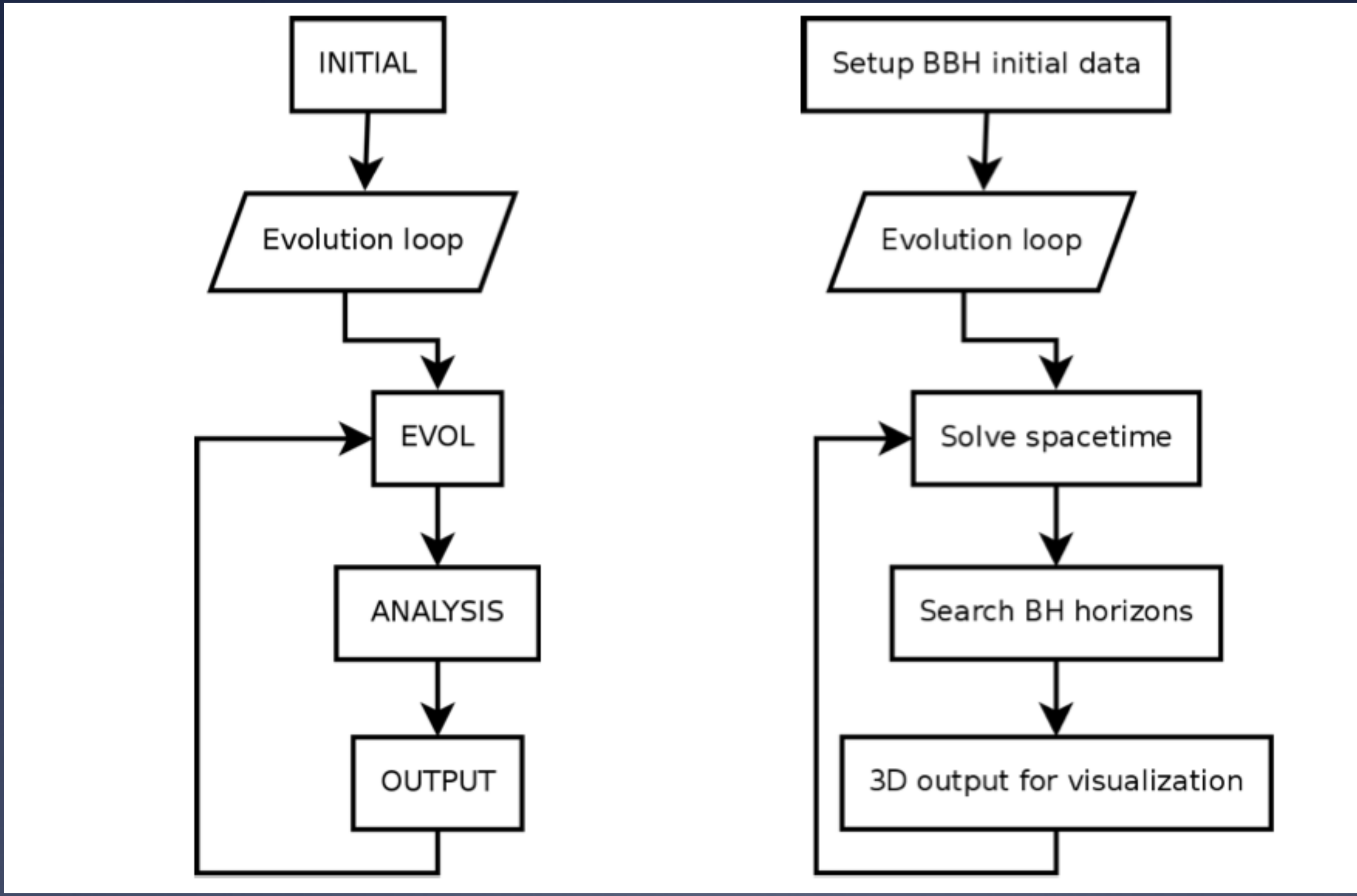
- Cactus framework provides scheduling, application APIs for parallel operations
- Driver thorn provides scheduling, load balancing, parallelization
- Application thorns deal only with local part of parallel mesh
- Different thorns can be used to provide the same functionality, easily swapped.



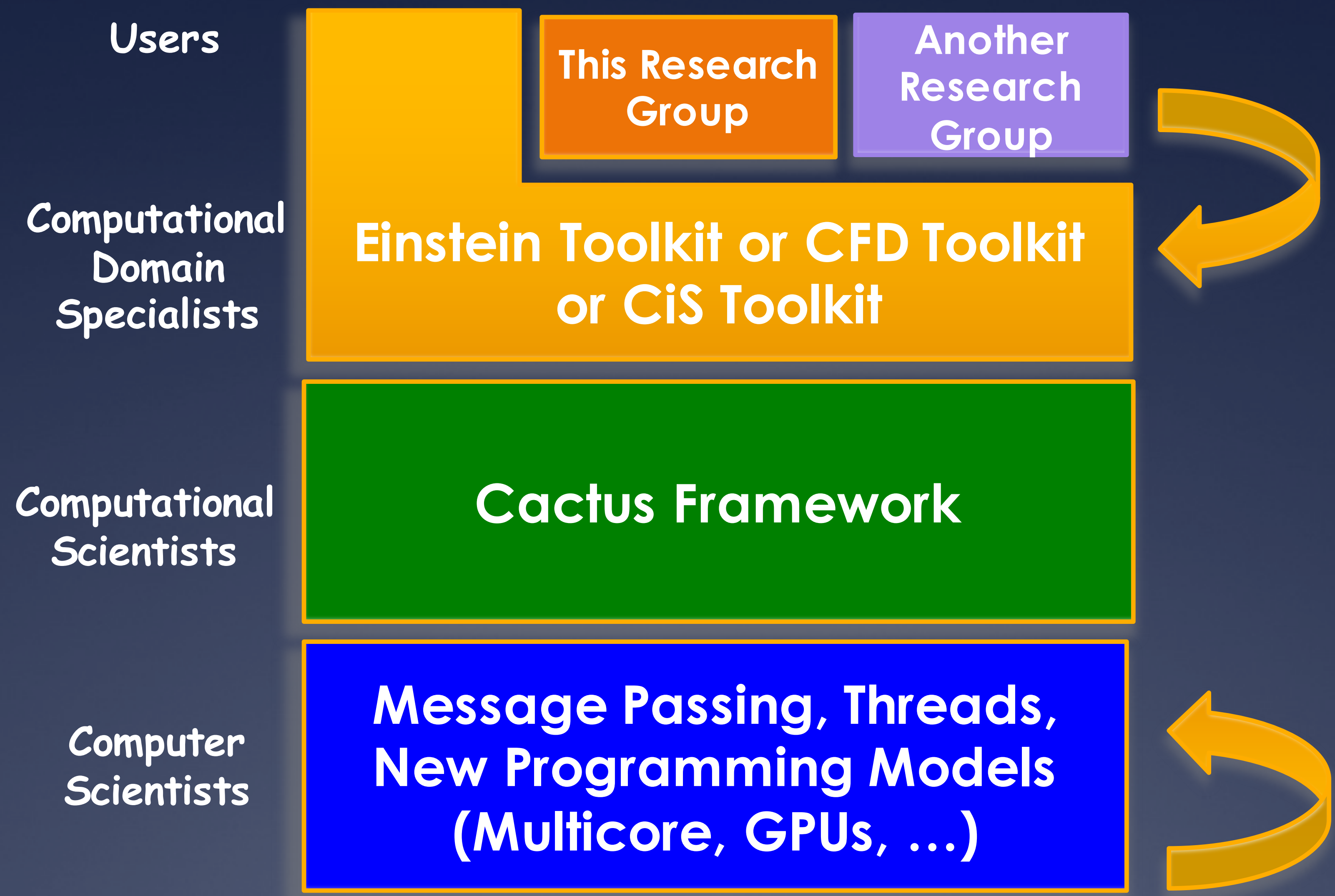
Thorn (Components)

- Several configuration files (called CCL files) that define interface of a thorn with the Flesh and other thorns
  - Implementation name and inheritance relations
  - Variables
  - Runtime parameters
  - Scheduled methods and storage, synchronization
  - Any configuration details
- Much information, defined by thorn writer
  - E.g. For a parameter, name, type, allowed values, defaults, steerable

Example scheduling tree

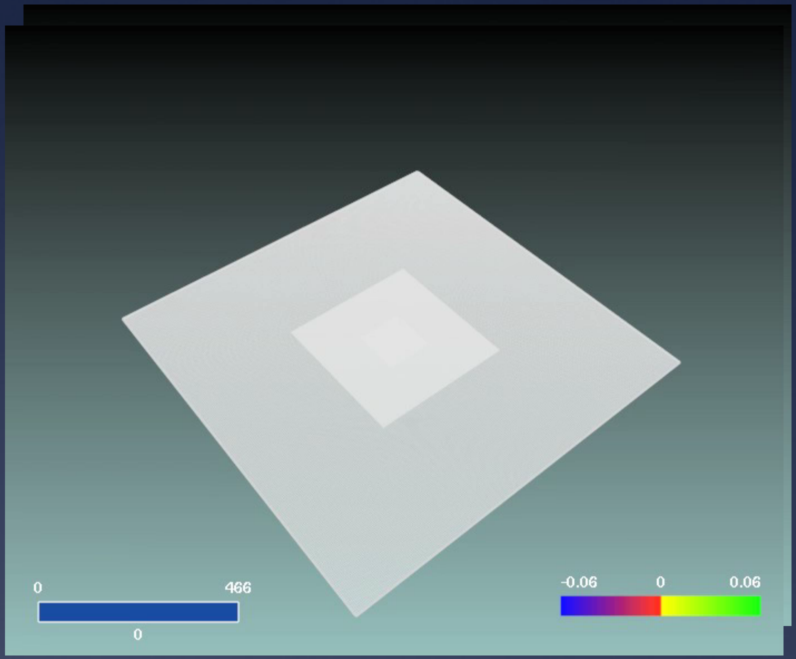


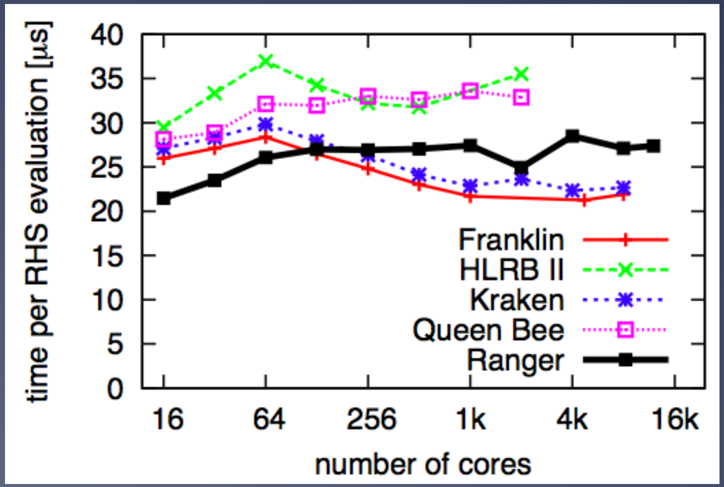
Component Toolkit Ecosystem



AMR: Carpet

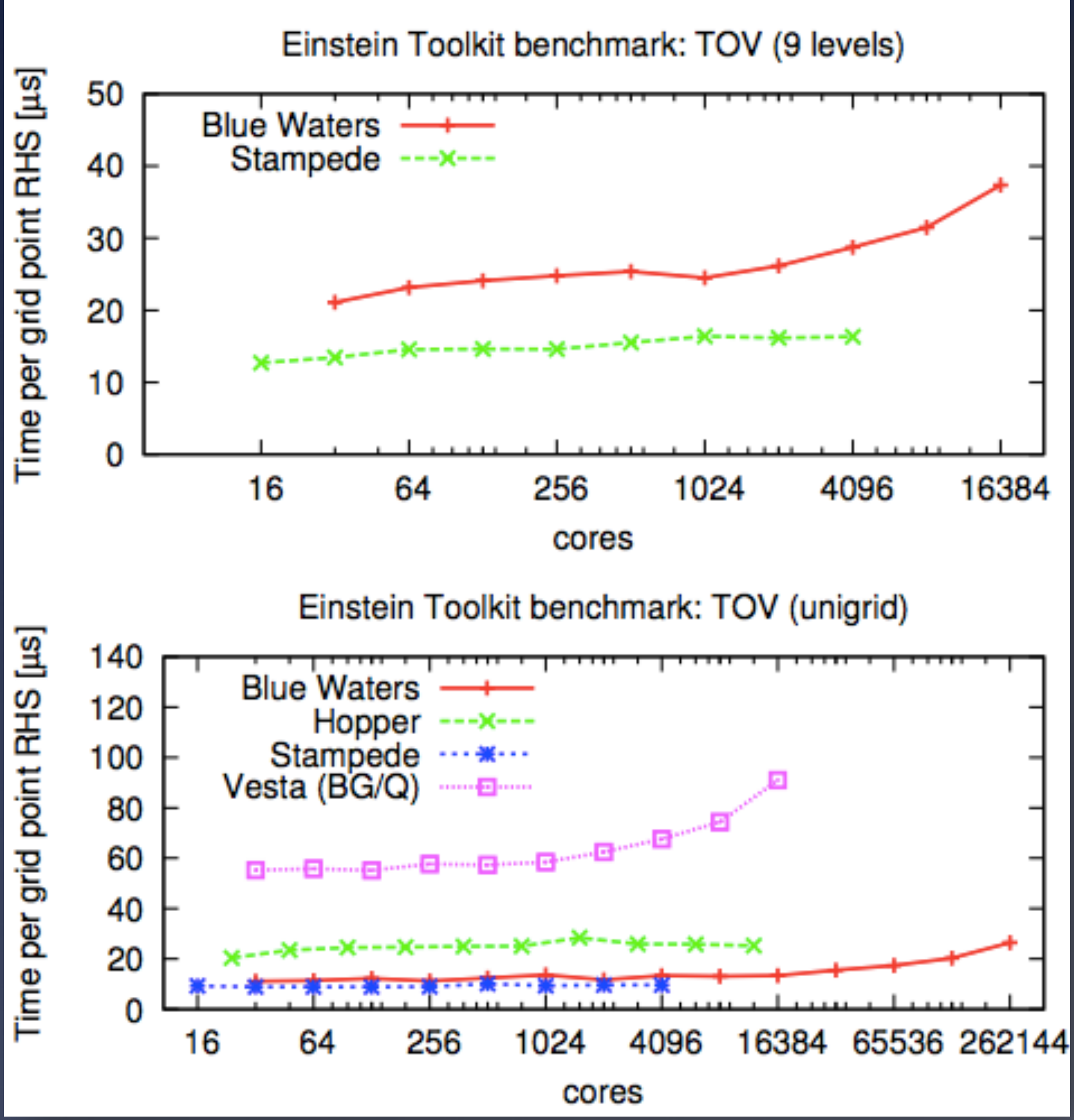
* Set of Cactus thorns
  * Developed by Erik Schnetter
* Berger-Oliger style adaptive mesh refinement with sub-cycling in time
  * High order differencing (4,6,8)
  * Domain decomposition
  * Hybrid MPI-OpenMP
* 2002-03: Design of Cactus means many groups, even competing ones, suddenly had AMR with little code change





E. Schnetter

Cactus/Carpet Scaling



Schnetter, 2013, arXiv:1308.1343

- Single core performance
  - Strategies for better cache use
  - Understanding performance data
- Node scaling
  - Memory bandwidth limitations
  - OpenMP/MPI
  - Accelerators
- MPI scaling
  - Load balancing

Community

Einstein Toolkit

Einstein Toolkit Consortium

- developing and supporting open software for relativistic astrophysics.
- provide the core computational tools to enable new science, broaden community, facilitate interdisciplinary research and take advantage of emerging petascale computers and advanced cyberinfrastructure."
- Consortium: 100 members, 51 sites, 14 countries
- Sustainable community model:
  - 9 Maintainers from 6 sites: oversee technical developments, quality control, V&V, distributions /releases
  - Whole consortium engaged in directions, support, development
  - Open development meetings
  - Thirteen releases (Brahe)

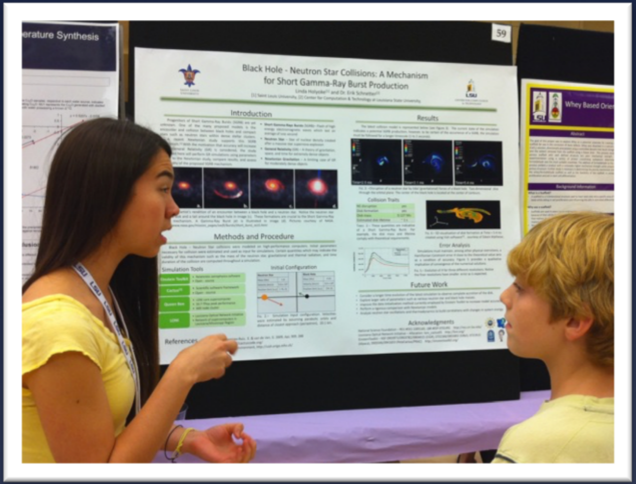
http://www.einsteintoolkit.org

Components

* Software
  * Around 200 Cactus thorns: Initial data, evolution, analysis, AMR, …
  * 3100 files, 1M LOC (C, C++, Perl, Fortran)
  * Tools, viz, etc
* Provide extensible standard interface for general relativity variables (e.g. variables, parameters, data model for output, tests, language)
* Examples and tutorials
  * Complete ***production*** codes for black holes, neutron stars, cosmology
  * New users: Test account on supercomputer
* Community support: active mail list, ticket system

http://www.einsteintoolkit.org

Community Building



Distributed & Inclusive

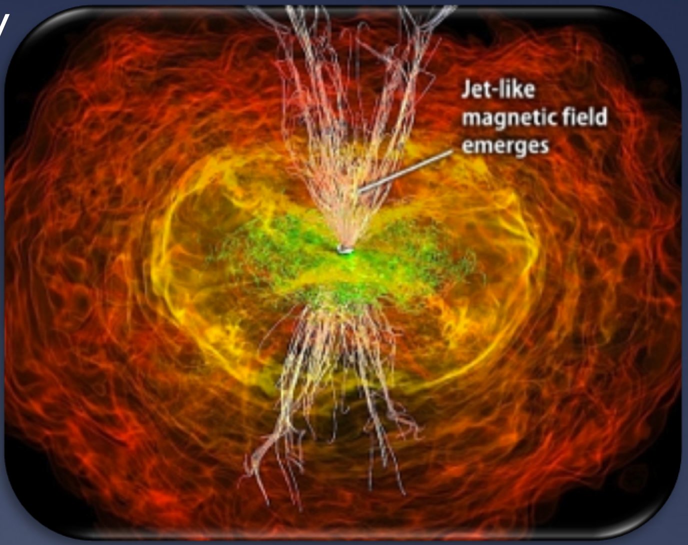
Hayley McPherson, PhD student, U. Melbourne

Distributed & Inclusive

Hayley McPherson, PhD student, U. Melbourne

GRHydro ET Thorn

- Base: GRHD public version of Whisky code (EU 5th Framework)
  - Much development plus new MHD
  - Caltech, LSU, AEI, GATECH, Perimeter, RIT (NSF CIGR Award)
- Full 3D and dynamic general relativity
- Valencia formalism of GRMHD: Relativistic magnetized fluids in ideal MHD limit
- Published text results, convergence
  - arXiv: 1304.5544 (Moesta et al, 2013)
- All code, input files etc part of Einstein Toolkit
- User support



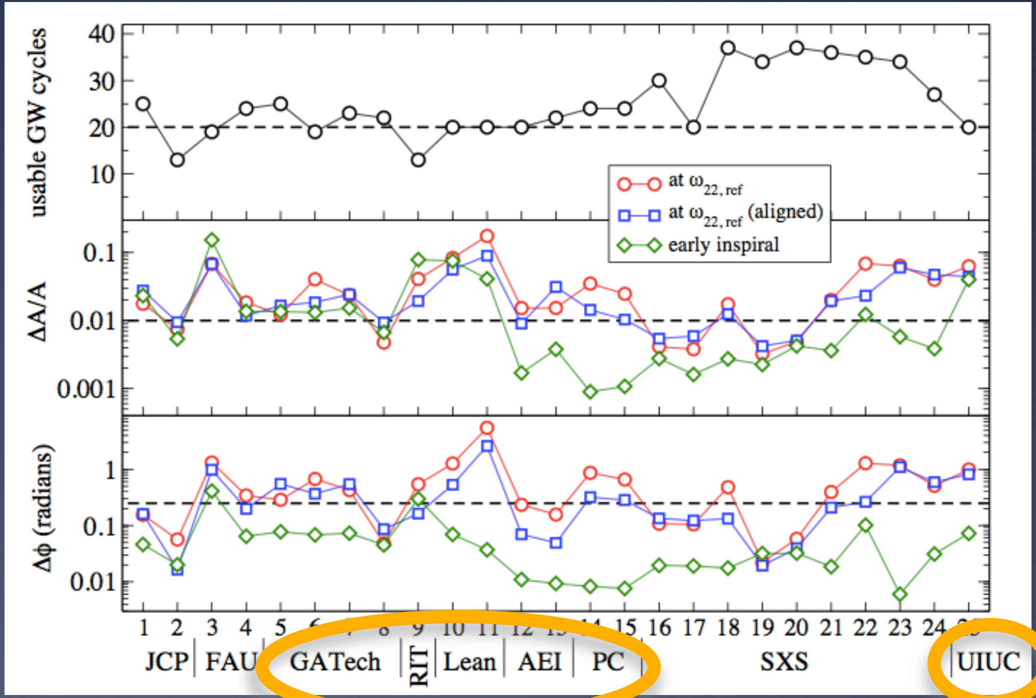
GRHydro:
A new open source general-relativistic magnetohydrodynamics code for the Einstein Toolkit

Philipp Mösta[1], Bruno C. Mundim[2,3], Joshua A. Faber[3], Roland Haas[1,4], Scott C. Noble[3], Tanja Bode[8,4], Frank Löffler[5], Christian D. Ott[1,5], Christian Reisswig[1], Erik Schnetter[6,7,5]

Example: Codes in Analytical Relativity Collaboration (NRAR)

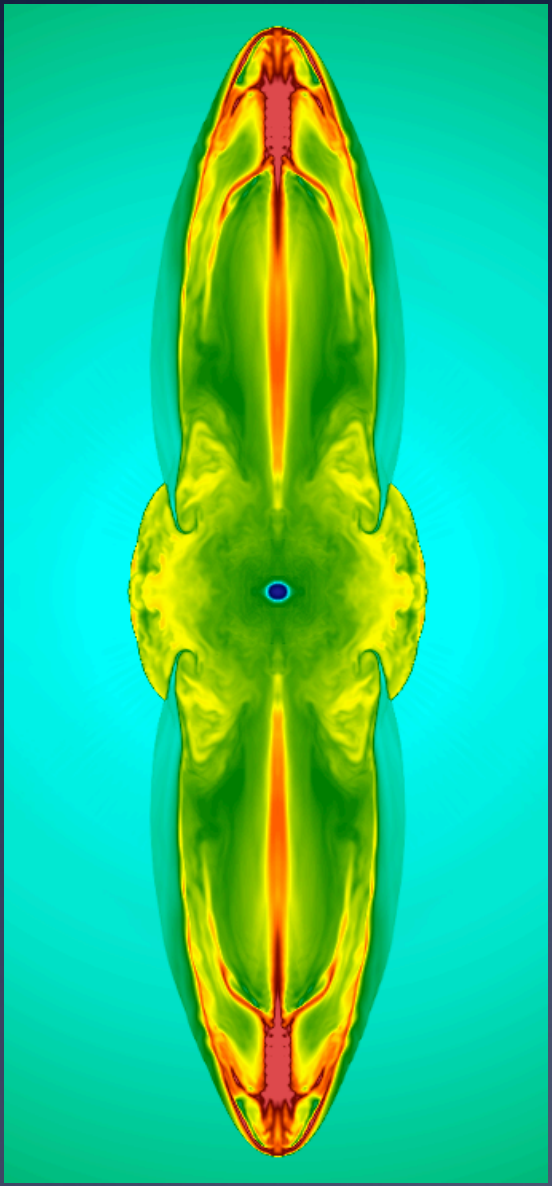
Error-analysis and comparison to analytical models of numerical waveforms produced by the NRAR Collaboration

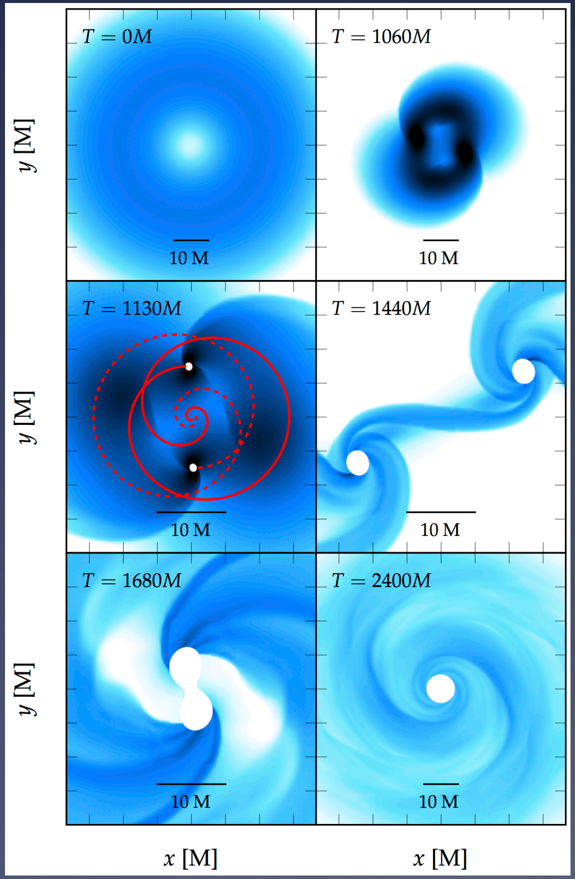
Ian Hinder[1], Alessandra Buonanno[2], Michael Boyle[3], Zachariah B. Etienne[4], James Healy[5], Nathan K. Johnson-McDaniel[6], Alessandro Nagar[8], Hiroyuki Nakano[7,9], Yi Pan[2], Harald P. Pfeiffer[10,11], Michael Pürrer[12], Christian Reisswig[13], Mark A. Scheel[13], Erik Schnetter[14,15,16], Ulrich Sperhake[13,17,18,19], Bela Szilágyi[13], Wolfgang Tichy[20], Barry Wardell[1,21], Anıl Zenginoğlu[13], Daniela Alic[1], Sebastiano Bernuzzi[6], Tanja Bode[5], Bernd Brügmann[6], Luisa T. Buchman[13], Manuela Campanelli[7], Tony Chu[10,13], Thibault Damour[8], Jason D. Grigsby[6], Mark Hannam[12], Roland Haas[5], Daniel A. Hemberger[3], Sascha Husa[26], Lawrence E. Kidder[3], Pablo Laguna[5], Lionel London[5], Geoffrey Lovelace[3,13,22], Carlos O. Lousto[7], Pedro Marronetti[20,23], Richard A. Matzner[24], Philipp Mösta[1,13], Abdul Mroué[10], Doreen Müller[6], Bruno C. Mundim[1,7], Andrea Nerozzi[25], Vasileios Paschalidis[4], Denis Pollney[26,27], George Reifenberger[20], Luciano Rezzolla[1], Stuart L. Shapiro[4,28], Deirdre Shoemaker[5], Andrea Taracchini[2], Nicholas W. Taylor[13], Saul A. Teukolsky[3], Marcus Thierfelder[6], Helvi Witek[17,25], Yosef Zlochower[7]

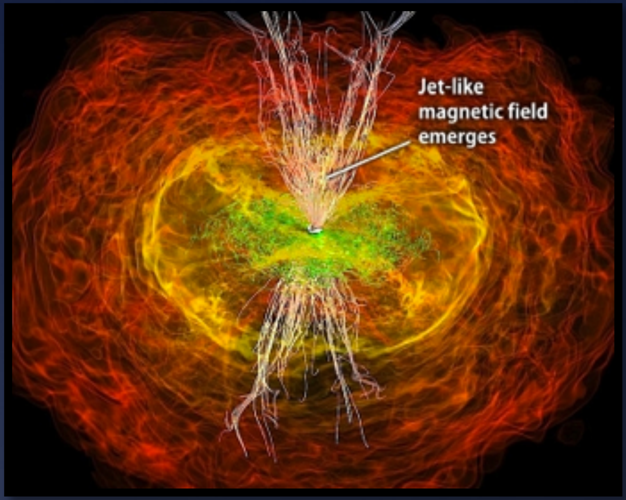


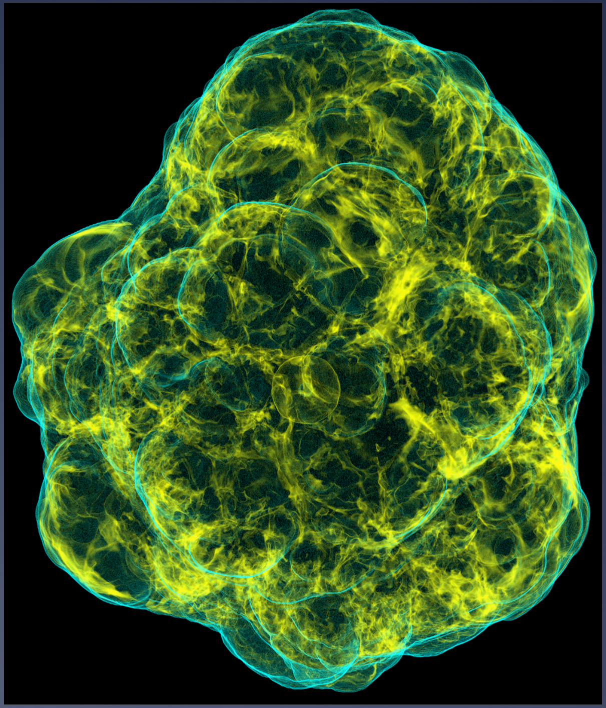
Hinder et al (2013), arXiv:1307.5307

Discovery



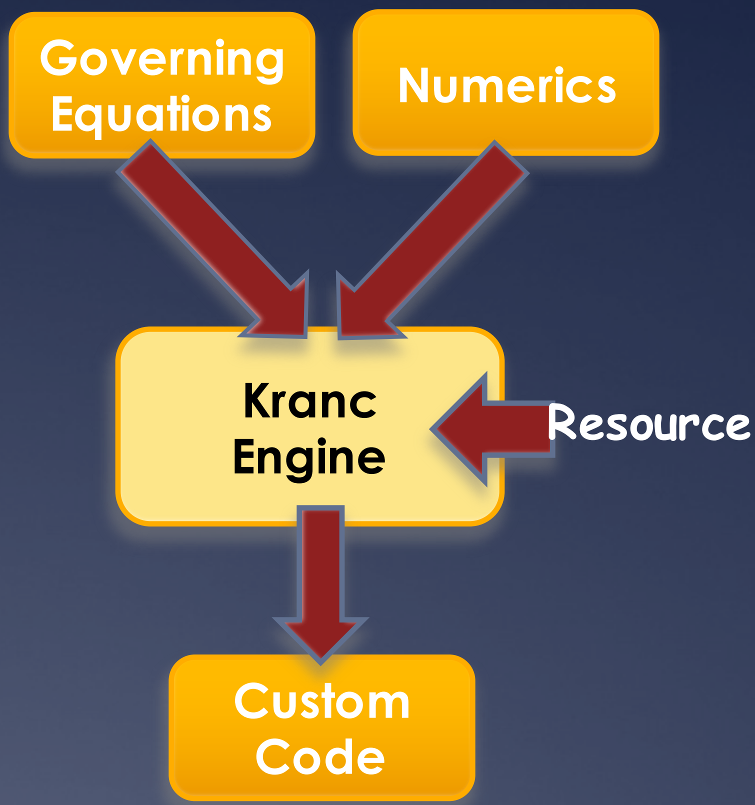

T = 0M
10 M
T = 1060M
10 M
T = 1130M
10 M
T = 1440M
10 M
T = 1680M
10 M
T = 2400M
10 M
y [M]
y [M]
y [M]
x [M]
x [M]


Jet-like
magnetic field
emerges



Automatic Code Generation

- Einstein equations very complex
  - Coding cumbersome, error prone
  - Deters experimentation
- Kranc: Mathematica tool to generate Cactus thorns from PDEs, specify differencing methods
- Vision: Generate entire codes from underlying equations/problem specification, optimize codes for target architectures
  - Opportunity to integrate verification/validation/data description

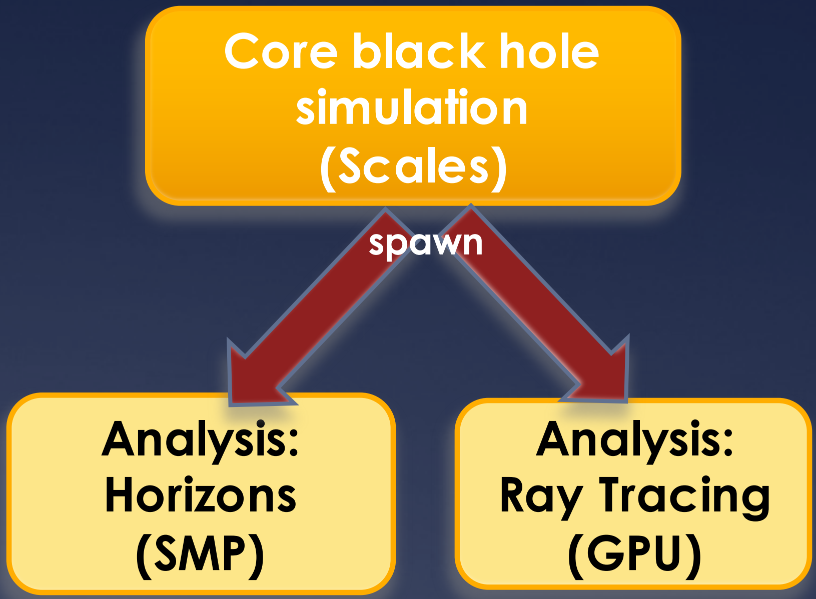


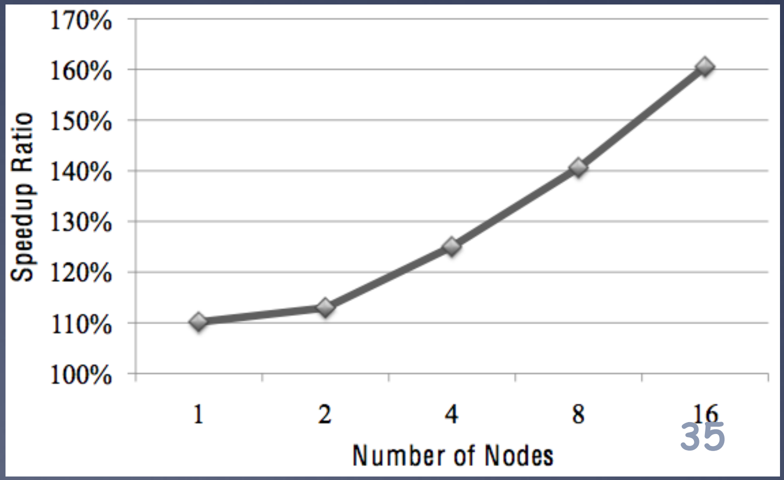
Kranc

Kranc Assembles Numerical Code

Autonomous Simulations

* Simulations have components using different algorithms/methods (e.g. analysis)
  * Different scaling properties
* Issues will get more severe
  * Multi-physics
  * Petascale/Exascale
* Simulations intelligently redirect work to other resources, architectures
* Cactus "spawning" thorn
  * Uses SAGA API for remote operations

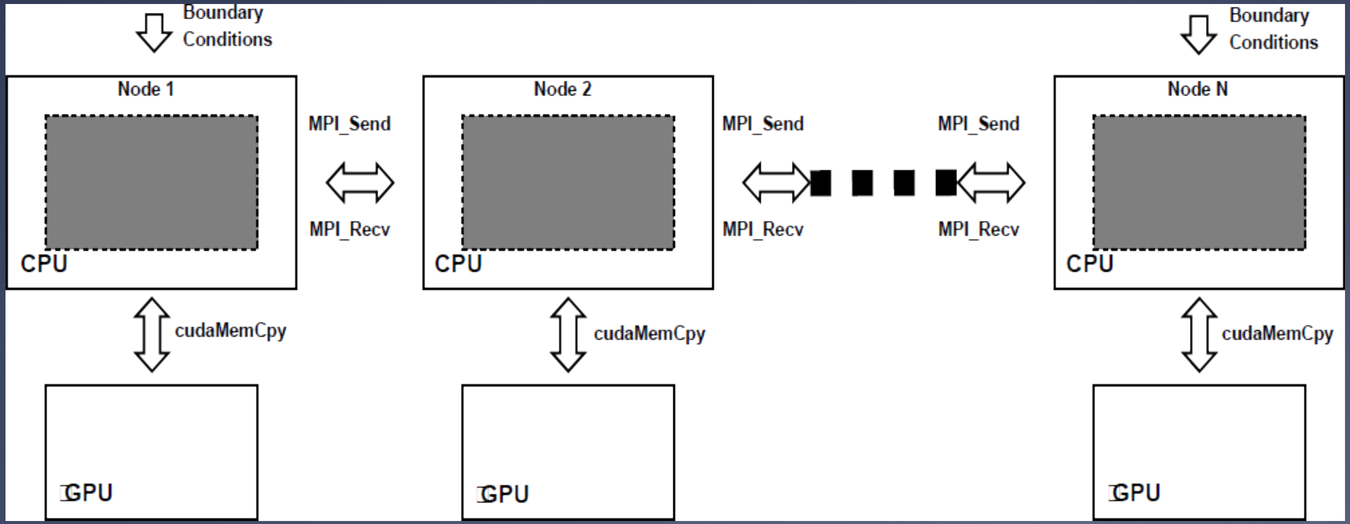




Chimora

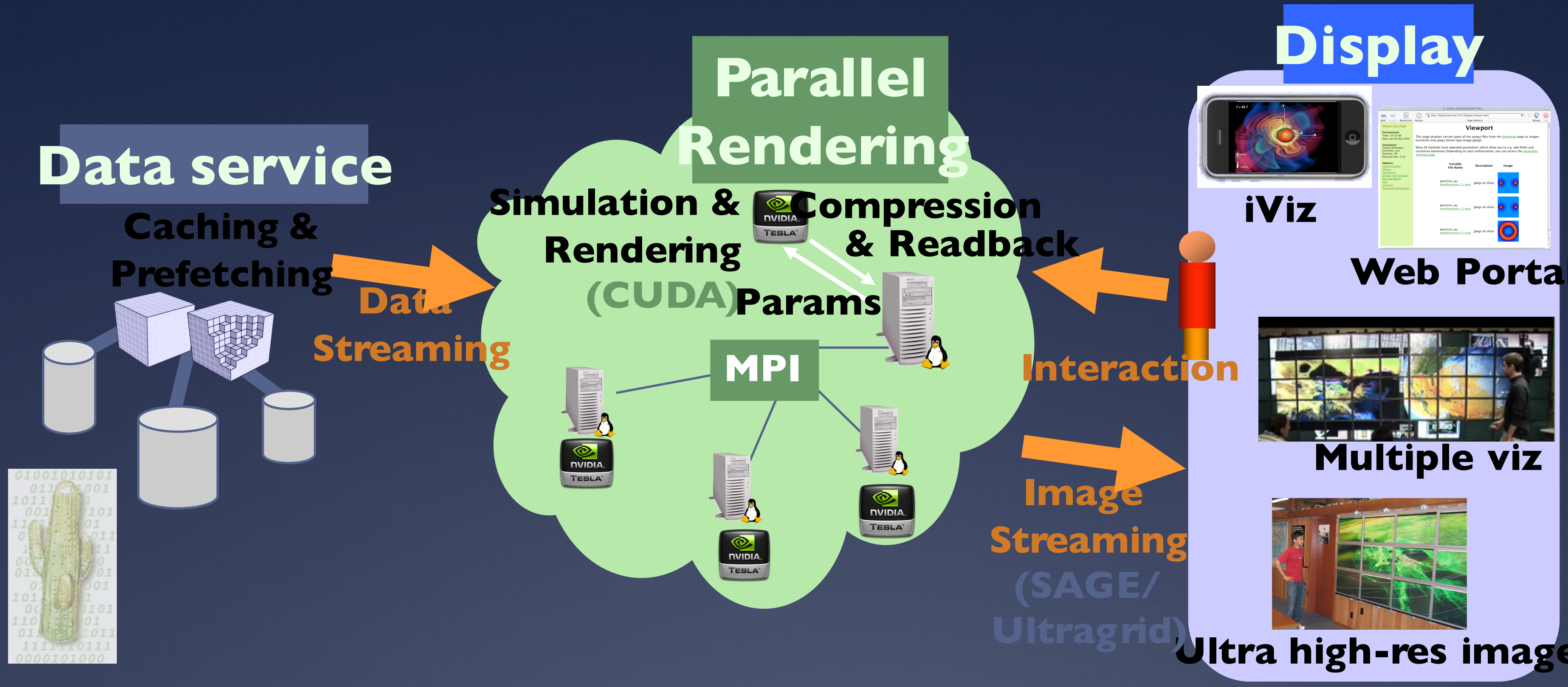
* Use large scale CPU/GPU systems efficiently for complex applications
* Reduce code rewrite, new programming paradigms
* Strategy uses:
  * High level code transformations
  * Loop traversal strategies
  * Dynamically selected data/instruction cache
  * JIT compiler tailored to application

1265449



Blazewicz et al (2013), arXiv:1307.6488

Remote Visualization, Interaction



Memory hierarchy

GPU texture cache →GPU DRAM→RAM→Net→Disk

Viz specific workload distribution & resource selection

eg frame-rate, resolution

Some Challenges for Petascale and Beyond

* New physics: neutrino transport, photon radiation transport
* Massive scalability
  * Local metadata, remove global operations
  * Extend Cactus abstractions for new programming models
  * Robust automatically generated code
  * Multithreading, accelerators
  * Multi-physics modules have different optimization/scaling
* Tools: real time debuggers, profilers, more intelligent application-specific tools
* Data, visualization, provenance information, archive results, …
* Growing complexity of application, programming models, architectures.
* Social: how to develop sustainable software for astrophysics? CDSE and supporting career paths? Education and training?

NCSA: An Interdisciplinary Research Environment for Complex Problem Solving Communities

National Center for Supercomputing Applications (NCSA)

- Part of U. Illinois Urbana-Champaign
  - 2.5 hrs South of here
- Established 1986; one of five original centers of NSF's supercomputer centers program
  - ~200 staff
- Create & operate national cyberinfrastructure driven by and enabling diverse real world applications (national, regional, campus)
- Interdisciplinary research institute building on strong campus partnerships and computation & data platform

30 YEARS NCSA 1986–2016

NSF Blue Waters

Largest U.S. system for open science and engineering research

- 13 PF peak performance
- 1.5 PB memory
- 1 TB/sec bandwidth
- 26 PB disk
- 380+ PB near-line tape storage
- World’s largest HPSS
- 400 Gpbs network

- 7% (~1PF) for Illinois use
- NPCF: 90,000sqft, 400 Gbits

NCSA Vision 2020:

http://www.ncsa.illinois.edu/about/ncsa2020

"NCSA will be a home for addressing complex research problems in science and society, powered by the development and application of advanced and comprehensive digital environments."

NCSA Vision 2020:

http://www.ncsa.illinois.edu/about/ncsa2020

Goal 1: Transform NCSA into world-class center for transdisciplinary research, education and innovation

Goal 2: Create the world's most advanced digital environment that integrates large-scale computing, instrumentation, and data services.

Goal 3: Drive innovation, and economic, and societal impact for Illinois and the nation.

NCSA Directorates

- Research & Education
- Integrated Cyberinfrastructure
- Economic & Societal Impact
- Major Projects: Blue Waters, XSEDE, National Data Service, LSST

R&E Directorate at NCSA

* 6 thematic areas
* 100 affiliate faculty
* 20 Blue Waters professors
* 30 postdoctoral scholars with a postdoc program
* House two academic programs, two student groups
* Weekly colloquia program bringing in thought leaders
* Graduate and undergraduate students in interdisciplinary, theme based offices

Thematic Areas at NCSA

Astronomy and Physics

Led by Athol Kemball
NCSA, Astronomy

Culture and Society

Led by Donna Cox
NCSA, Art and Design

Bioinformatics and Health Science

Led by C. Victor Jongeneel
NCSA, Woese Institute for Genomic Biology, Bioengineering

Earth and Environment

Led by Shaowen Wang
NCSA, Geography and GIS

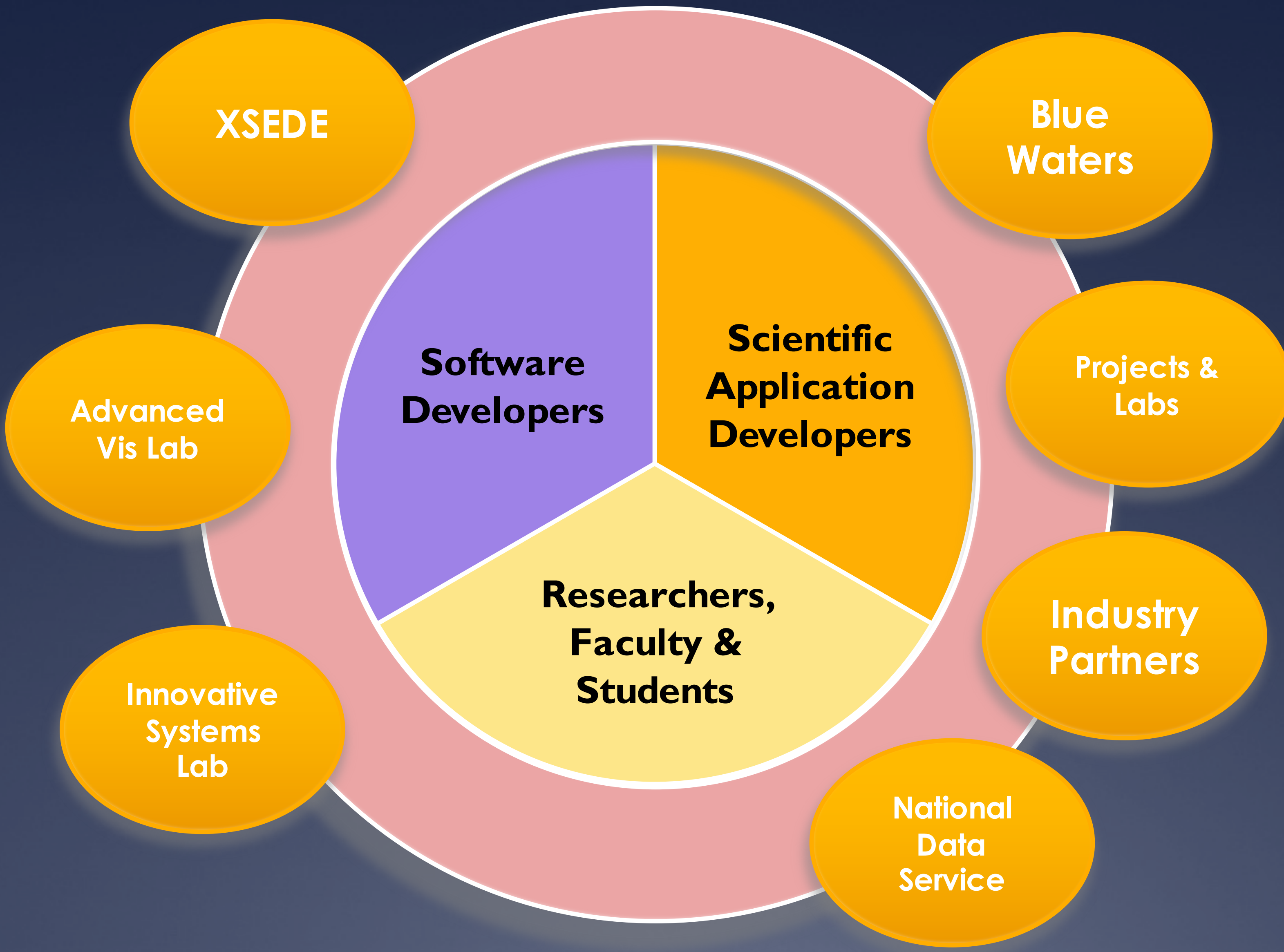
Computational and Data-enabled Science

Led by Gabrielle Allen
NCSA, Astronomy

Materials and Manufacturing

Led by Narayana Aluru
NCSA, Mechanical Science and Engineering

Complex Problem Solving at NCSA



Questions?