

SIMULATIONS AND
THEORY FOR
MULTI-MESSENGER
ASTRONOMY

WINDOWS ON THE UNIVERSE

With NSF's selection of Windows on the Universe among it's 10 Big Ideas, we are presented with both a tremendous **opportunity** and a tremendous **challenge** to address the science of Multi-Messenger Astronomy.

The goal for this workshop is a wide-ranging discussion among the many constituencies in our community, observational, theoretical, and computational, on what we need to meet this challenge and deliver on this opportunity.

These needs could simply be **organizational**. They could be **financial**. They may already be met by other programs.

These needs certainly **span all of the scientific areas** that touch on MMA; astronomy, gravitational, particle & nuclear physics, and computational science.

OBSERVATIONS OVER TIME

To me, one of the most distinctive features of Multi-Messenger Astronomy is the **long timeline of observations**.

For example, for Supernova 1987a, we have

- 1) progenitor observations of a blue supergiant
- 2) the neutrino signal at neutron star formation
- 3) photospheric and nebular observations of the supernova
- 4) the beginnings of a supernova remnant.

This crosses 35+ years of time and a **tremendous range of physics**.

For GW170817, the range of physics is similar, though the **timeline is compressed**.

Does this range impose additional demands?

EXISTING SUPPORT

There is **already considerable support** for the theory and simulations side of MMA.

- 1) Individual Investigator awards from NSF, NASA & DoE.
- 2) Scientific Discovery through Advanced Computing program (SciDAC) and Exascale Computing Project (ECP)
- 3) Network for Neutrinos, Nuclear Astrophysics and Symmetries (N3AS)
- 4) Focused Research Hubs in Theoretical Physics (FRHTP)
- 5) Software Institutes

Are these not enough? **What is missing?**

How could any gaps be filled?

SciDAC

The Scientific Discovery through Advanced Computing Program is jointly funded by the DoE Office of Advanced Scientific Computing with the other DoE scientific offices to support teams of **Application Scientists** and supporting **Computational Scientists**.

The program has **run since 2001** with some variations in how the Application teams and Computational Scientists are supported.

Under SciDAC-1, support included the *Supernova Science Center* (PI Woosley) and the *Terascale Supernova Initiative* (PI Mezzacappa).

Under SciDAC-2, support included the *Computational Astrophysics Consortium* (PI Woosley)

For SciDAC-3, proposals *Petascale Investigations of our Nuclear Origins* (PI Mezzacappa) and *Supernovae and Neutron Stars as Laboratories for Fundamental Nuclear Physics* (PI Woosley) were unsuccessful.

TOWARD EXASCALE ASTROPHYSICS OF MERGERS & SUPERNOVAE

Argonne National Laboratory

Anshu Dubey

Los Alamos National Laboratory

Chris Fryer

Josh Dolence

Wes Even

Oak Ridge National Laboratory

Raph Hix

Bronson Messer

Stony Brook University

Mike Zingale

Alan Calder

University of California, Berkeley

Dan Kasen

University of Notre Dame

Rebecca Surman

Lawrence Berkeley National Laboratory

Andy Nonaka

Ann Almgren

Michigan State University

Sean Couch

Luke Roberts

Princeton University

Adam Burrows

David Radice

University of Tennessee

Andrew Steiner

Tony Mezzacappa

University of California, San Diego

George Fuller

University of Washington

Sanjay Reddy

TEAMS GOALS

The overall goal of the TEAMS collaboration is to explore as many of the proposed sites of the r-process (and p-process), with **much higher physical fidelity** using the coming generation of exascale computers.

Iron Core-Collapse Supernovae: FORNAX (Princeton), CHIMERA, FLASH

Oxygen-Neon Core-Collapse: CHIMERA (ORNL), FORNAX, FLASH

MHD-driven Supernovae: FLASH (MSU), FORNAX

Neutron Star Decompression: WhiskyTHC (~~Princeton~~), FLASH/CLASH

Black Hole Accretion Disks (NSM or Collapsar): FLASH/CLASH (UCB), bhlight (LANL)

Epstein, Colgate & Haxton Mechanism (in the supernova shocked He layer of stars): CHIMERA (ORNL), FORNAX

Compute **multi-D supernova progenitors**: Maestro (Stony Brook/LBNL).

Compute **photon signatures** using Sedona (UCB), Cassio & SUPERNU (LANL).

TEAMS GOALS II

Reaching our goals for improved physical fidelity with near-exascale simulations requires improvements not just in our astrophysics, but also in our nuclear physics.

To this end, TEAMS includes expertise in nuclear physics and nucleosynthesis.

Nuclear Equation of State for Supernovae and Neutron Stars:
Steiner (UTK)

Consistent Neutrino Opacities:
Reddy(UW) and Roberts (MSU)

Nuclear Physics Uncertainty Quantification for the r-process:
Surman (Notre Dame)

Astrophysical Uncertainty Quantification for Nucleosynthesis:
Surman (Notre Dame), Hix (ORNL), and Fryer (LANL).

EXASTAR

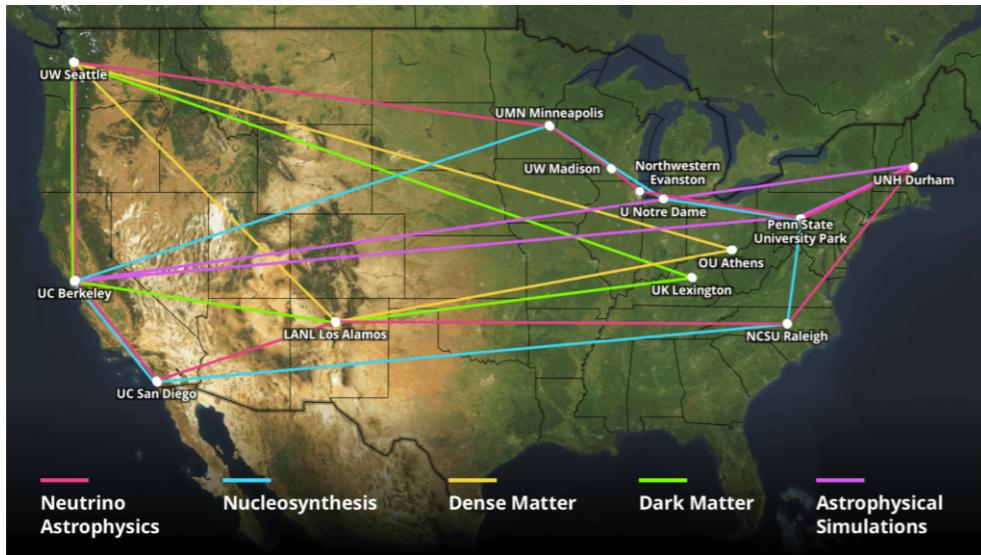
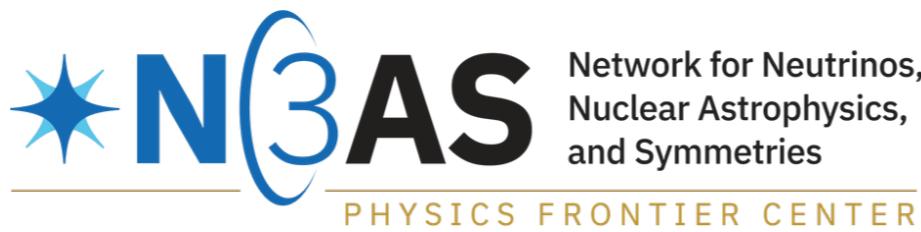
The Exascale Computing Project, part of the National Strategic Computing Initiative, is a collaboration of DoE-SC and NNSA to deploy exaflop computing hardware and the software to take advantage of it by 2021.

ExaStar is an application development focus area for nuclear astrophysics. The collaboration of LBNL, ORNL, ANL and Stony Brook is working on what we originally called CLASH framework.

CLASH unites exascale adaptive mesh refinement package AMReX, with block level physics from Castro, FLASH and CHIMERA.

CLASH also includes new radiation transport developments, a implicit/explicit moment method neutrino transport solver (thornado) and improvements to Monte Carlo transport (Sedona).

Exastar will deliver code (e.g. next version of Castro and FLASH), but not science.

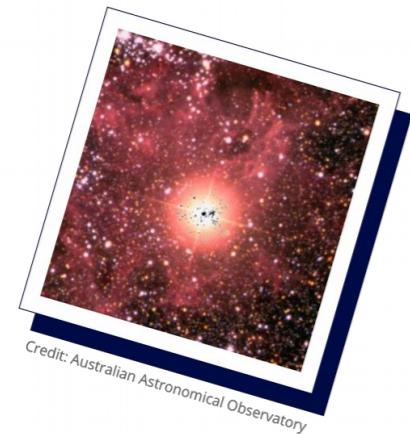


Multi-institutional
network of senior
investigators and
postdoctoral fellows.

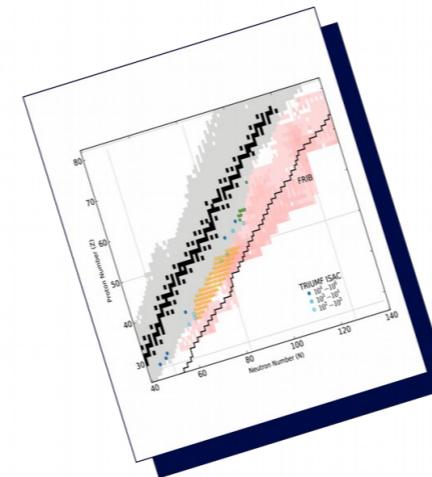


Focus areas

Neutrinos



Nucleosynthesis



Dark Matter



Astrophysical simulation



Credit: National Science Foundation/LIGO/
Sonoma State University/A. Simonnet.

Dense matter and neutron stars

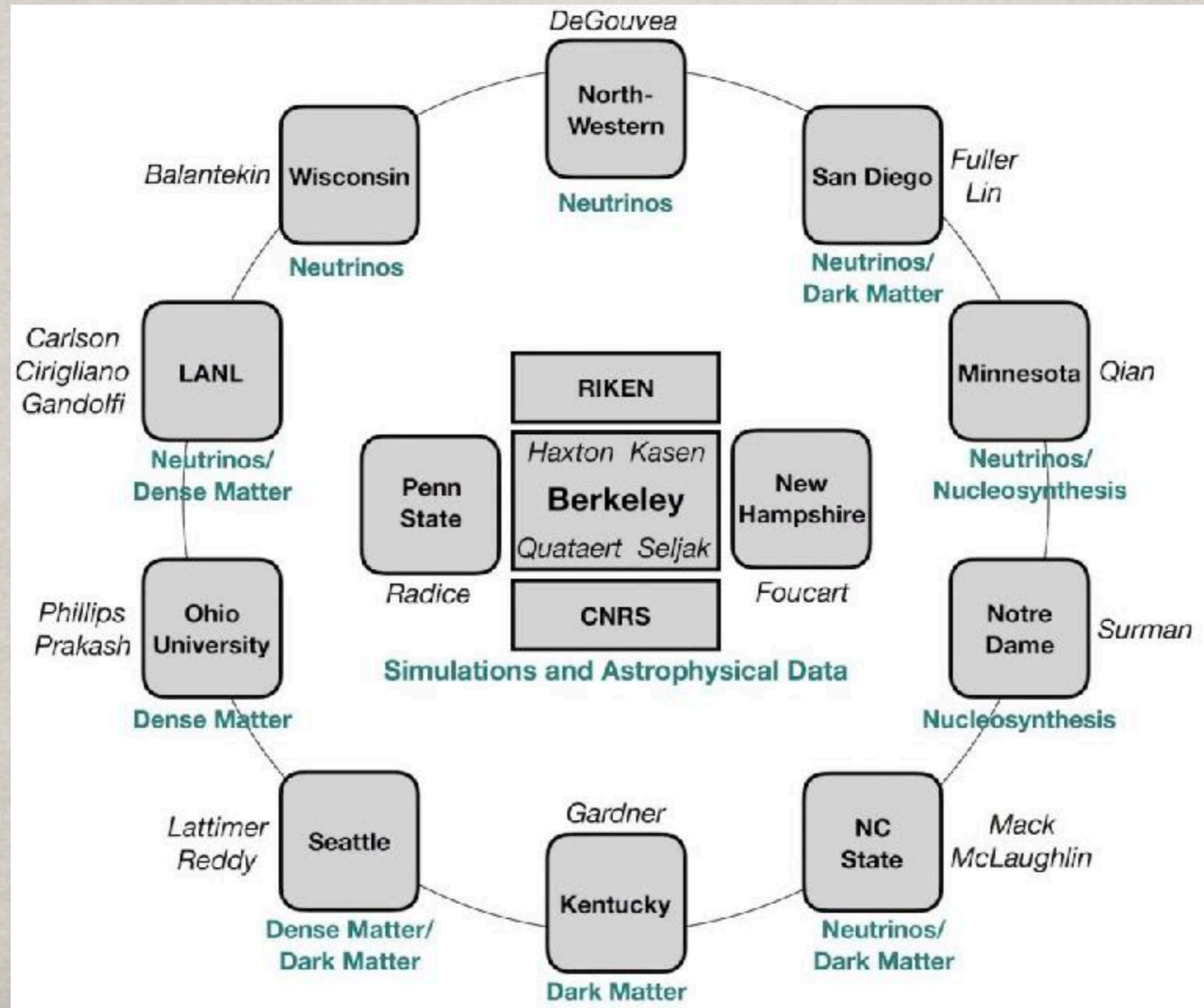


Credit: NASA and STScI

Postdoctoral training:

collaborations across the network, seminars, journal clubs, scientific writing, teaching certificates, outreach

N3AS SENIOR INVESTIGATORS



FOCUSED RESEARCH HUBS IN THEORETICAL PHYSICS

N3AS began life as a FRHTP in 2016, before becoming a PFC in 2020.

In the FY2021 FRHTP call, Theoretical Nuclear Physics solicited a new hub in the area of **Models and Simulations for Nuclear Astrophysics**. Award will be 5 years, less than \$4.3 million.

There are probably several proposal teams at this workshop planning to respond to the call.

NSF SOFTWARE INSTITUTE

Office of Advanced Cyberinfrastructure has a program of **Software Institutes**, bring together domain application scientists with computational science and applied mathematics experts.

A recent example is the [Institute for Research and Innovation in Software for High-Energy Physics \(IRIS-HEP\)](#), a \$25 million, 5 year effort to tackle the unprecedented amount of data that will come from the High-Luminosity Hadron Collider, the world's most powerful particle accelerator.

Our community submitted an unsuccessful proposal to that program in 2019.

Would something like this be a useful vehicle to meet our MMA challenges?

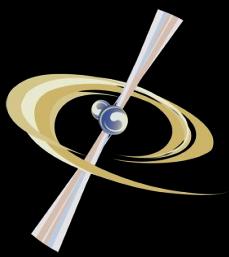
OTHER EFFORTS?

What have I missed?

TCAN

SciMMA

DoE Topical Collaborations



The TCAN on BNS simulation

Manuela Campanelli

RIT | College of Science
Center for Computational Relativity and Gravitation



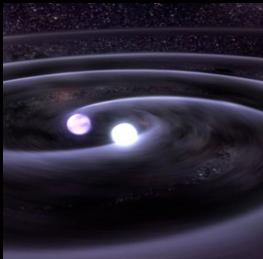
ASPIRE - Astrophysics and Space
Physics Institute for Research
Excellence



S4MMA 2020
9-10 2020 – zoom

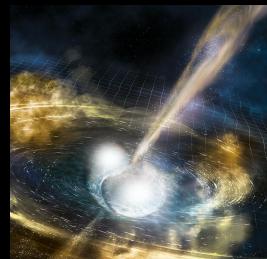


About BNS simulations ...



GW170817

+



GRB

170817A

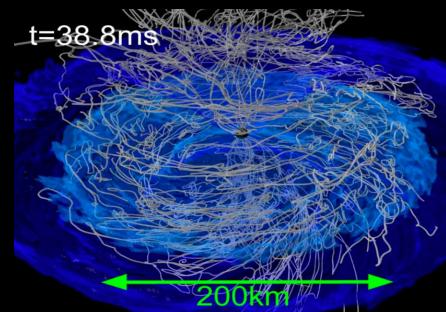
What is the central engine of a sGRB?
How is the jet launched?
What is the nature of the remnant?

- BH + accretion disk
- Hypermassive long-lived NS + torus – delayed collapse to a BH
- Stable NS

Long, accurate, GRMHD BNS and BH/NS simulations are required in full 3d:

- NR + GRMHD
- Nuclear and Neutrino Physics, EOS
- Neutrino/photon transport
- R-processes/nucleosynthesis

And they are inherently **multi-physics, multi-scale!**



resolution of 17.5 m for 4--5 ms after the onset of the merger

Kenta Kiuchi+
2015

Need to simulate
~1 sec after the
onset of the
merger with
resolutions of the
scale of the MRI!



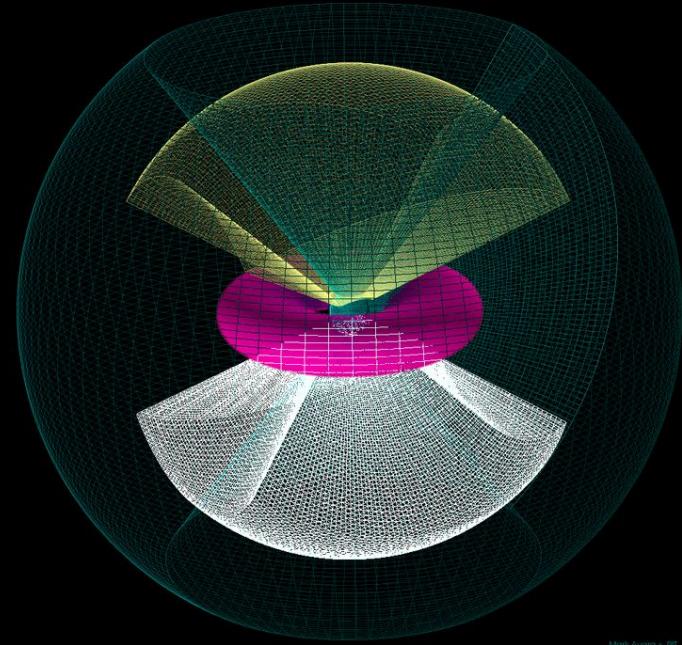
TCAN: Building an Integrated set of Computational Tools for the entire BNS merger

Advancing Computational Methods to Understand the Dynamics of Ejection, Accretion, Winds and Jets in Neutron Star Mergers

- initial data for both neutron stars' structures + surrounding spacetime
- merger proper: gravitational wave radiation + MHD
- prompt ejecta dynamics
- orbiting bound matter dynamics and radial profile
- jet-launching and propagation through ejecta
- nuclear evolution in ejecta and disk
- outflows: thermodynamics, nuclear evolution, photon spectrum

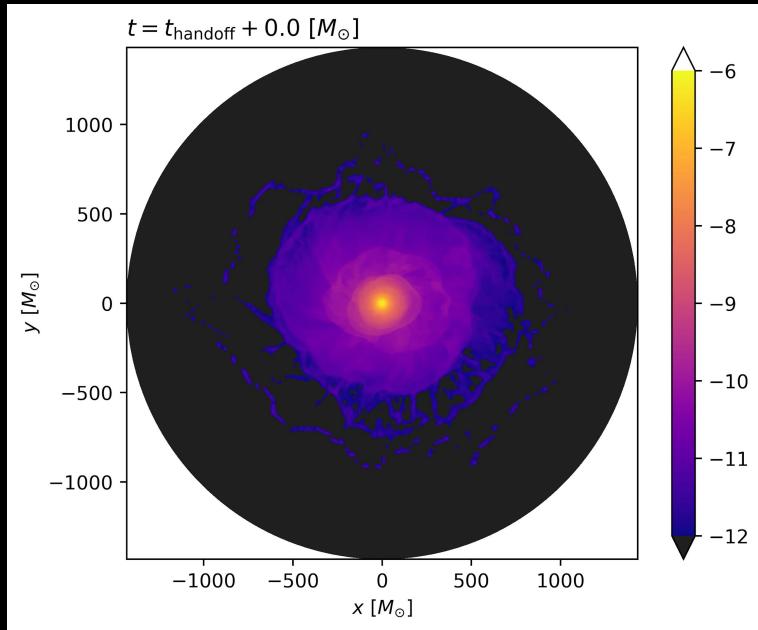
TCAN: Computational Strategy

- Provide pipeline of BNS and BH/NS initial data sets from Lorene.
- General tabulated EOS using neutrino-matter interaction rates from NuLib, Helmholtz EOS compatible with SkyNet for follow-up nucleosynthesis, and neutrino leakage/neutrino transport.
- AMR NR + GRMHD for the merger proper (Cartesian, vector-potential: e.g., IGM and Spritz)
- After collapse to BH or stable NS, handoff data to post-merger code using spherical grids: e.g. HARM3D/PWMHD, SphericalNR (requires good treatment of polar axis for jets)
- Evolve for ~1s: jet formation and kilonovae emission.
- Multiple codes to validate simulations via comparisons with collaborators.
- Make the ecosystem of codes and data sets publicly available.



PatchworkMHD – Avara+ 2020 in prep,
Shiokawa+ 2018
New software infrastructure for problems
of discrepant physical, temporal, scales
and multiple geometries.

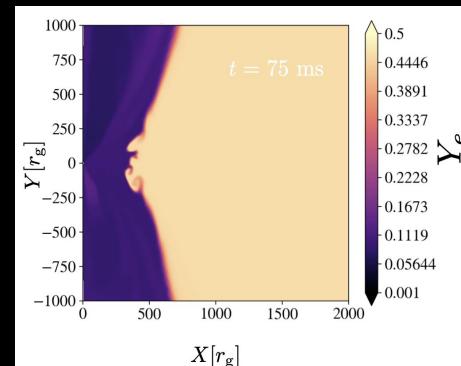
TCAN: Status Update



Handoff of BNS from IGM/Spritz to Harm3D postmerger evolution – Lopez-Armengol+ 2020

Using tabulated EOS SLy4 and grey neutrino leakage scheme– Murguia-Berthier+ 2020 in prep

- Pipeline of BNS initial data sets from Lorene, now available in compact-binaries.org
- The Handoff was very challenging due to algorithmic differences e.g. atmosphere treatment, common EOS, neutrino physics, and treatment of MHD.
- But now complete and postmerger simulations are underway on TACC's Frontera.



TCAN: Pioneering a new approach to complex Simulations

- Divide problem according to physical characteristics; different codes for different regimes
- Large (few dozen member) team structured by working groups
- Physical consistency for stable data hand-off from one code to another
- Coordinated scheduling to avoid development bottlenecks
- Weekly group video conferences to keep everyone informed and on-schedule
- Annual (when possible, in-person) all-team + external workshop
- Recruit new team members for additional expertise, larger workforce

ALL PEOPLE



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Campapelli, Manuela
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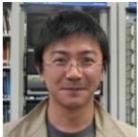
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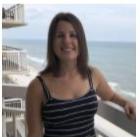
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Yosef Zlochower
Associate Professor of Mathematical Sciences at Rochester Institute of Technology

Discussion:

- Theory and simulations are key to the interpretation of observations of binary compact MMA sources.
- The demand for high-fidelity physical models will only increase as more exciting discoveries are made.
- The promise of MMA can be realized only if sufficient, sustained and community cyberinfrastructure is available!
 - Multi-domain expertise of astrophysicists, physicists and software engineers.
 - Sustained ecosystem of collaborative software.
 - Public, coordinated, data and code repositories and common portal /hub to share simulation products with the larger scientific community and observers.
 - Scalable software Infrastructure and access to Peta/Exascale Supercomputers
 - Workforce training and retention

White Papers: [Kollmeier+2020](#), [Allen+2020](#), [Chang+2020](#),
[Kavli-IAU white paper by Cenko+2020](#),
S4MMA coming soon!



Window on the Universe



Mid-scale Research Infrastructure



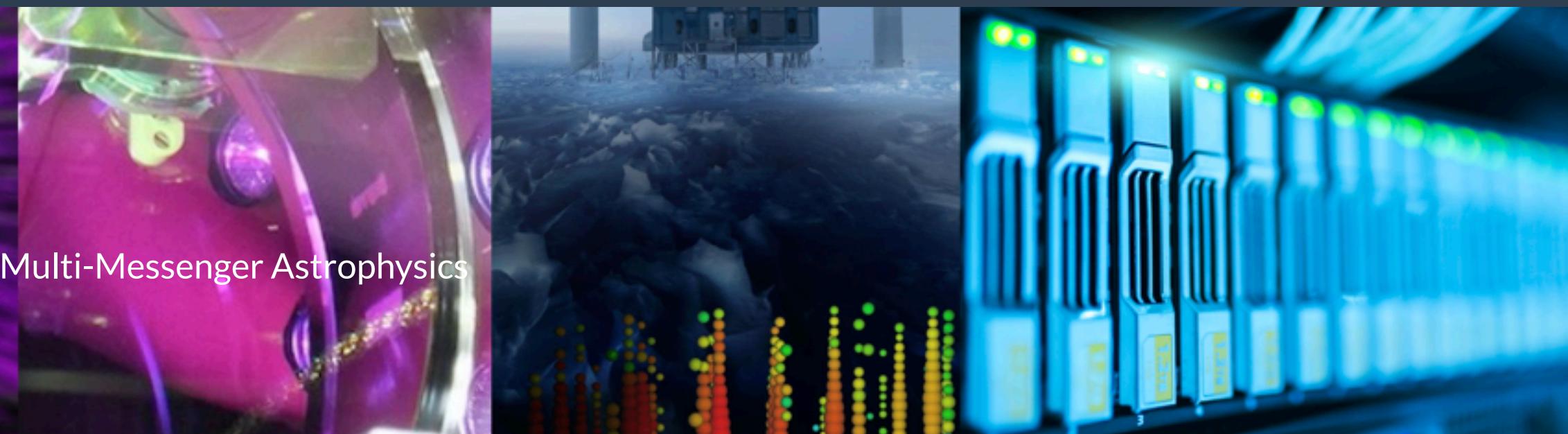
Growing Convergence Research





SCiMMA

Scalable Cyberinfrastructure to support Multi-Messenger Astrophysics



Multi-Messenger Astrophysics (MMA) is an exciting new field of science that combines traditional astronomy with the brand new ability to measure phenomena such as gravitational waves and high-energy neutrino particles that originate from celestial objects.

The promise of Multi-Messenger Astrophysics can be realized only if sufficient cyberinfrastructure is available to rapidly handle, combine, and analyze the very large-scale distributed data from all the types of astronomical measurements. This project is to carry out community planning for scalable cyberinfrastructure to support MMA. The primary goal is to identify the key questions and cyberinfrastructure projects required by the community to take full advantage of current facilities and imminent next-generation projects for MMA. Two products of the project will be: 1) a community white paper that presents an in-depth analysis of the cyberinfrastructure needs and the opportunities for collaborations among astronomers, computer scientists, and data scientists; and 2) a strategic plan for a scalable cyberinfrastructure institute for multi-messenger astrophysics laying out its proposed mission, identifying the highest priority areas for cyberinfrastructure research and development for the US-based multi-messenger astrophysics community, and presenting a strategy for managing and evolving a set of services that benefits and engages the entire community.

In this context, cyberinfrastructure consists of the distributed data-handling, computing, analysis, and collaboration services/systems to enable discovery, education, and innovation.

Participate

- [SCiMMA GitHub](#)
- [SCiMMA YouTube Channel](#)
- Join the [SCiMMA Google Group](#) by logging into Google or sign up with any email account by sending an email to scimma+subscribe (at) googlegroups.com with the subject "subscribe"

This project is supported by National Science Foundation grants [OAC-1841625](#), [OAC-1934752](#). Any opinions, findings, conclusions or recommendations expressed in this material are those of the developers and do not necessarily reflect the views of the National Science Foundation.

