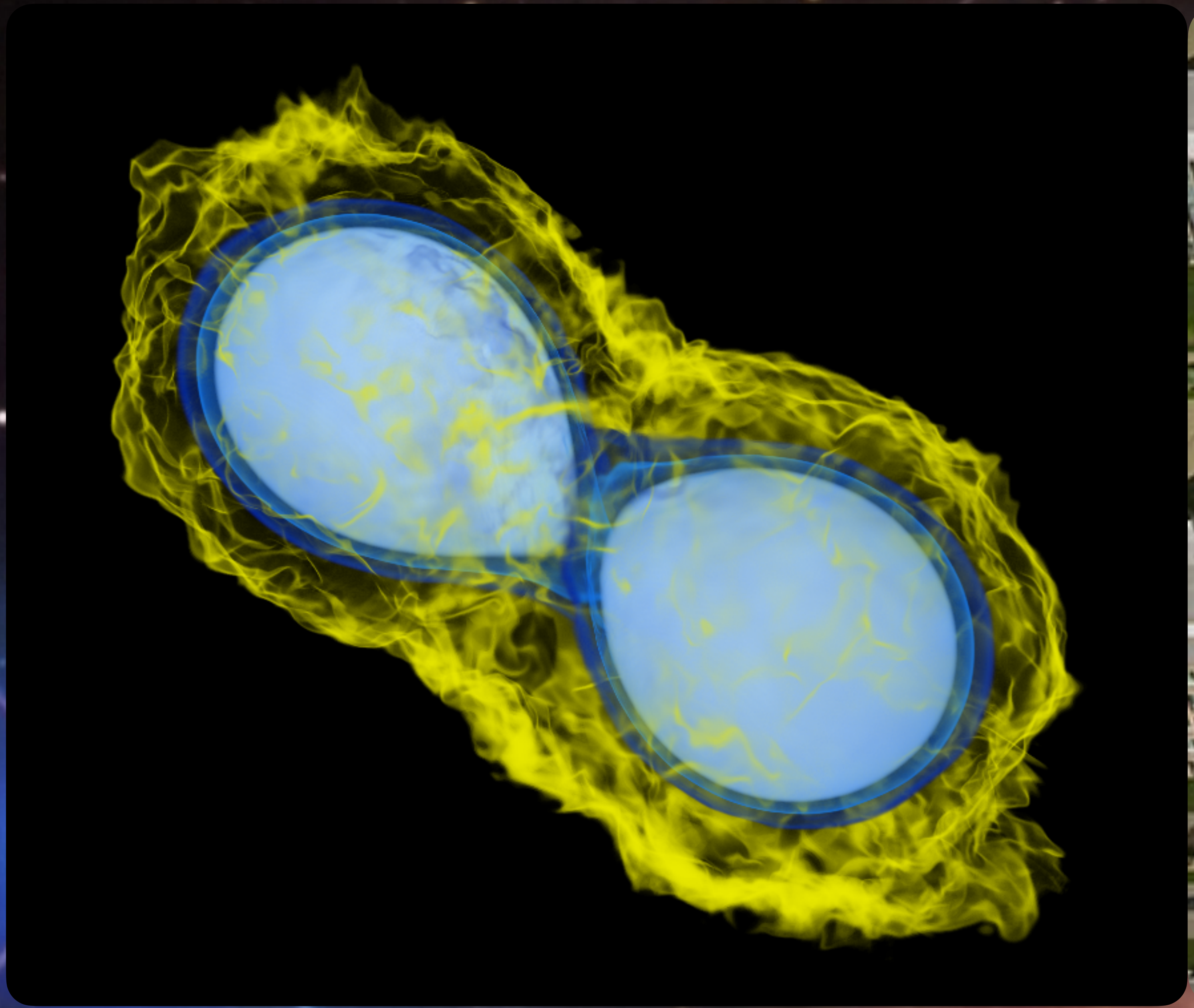
Exascale Nuclear Astrophysics



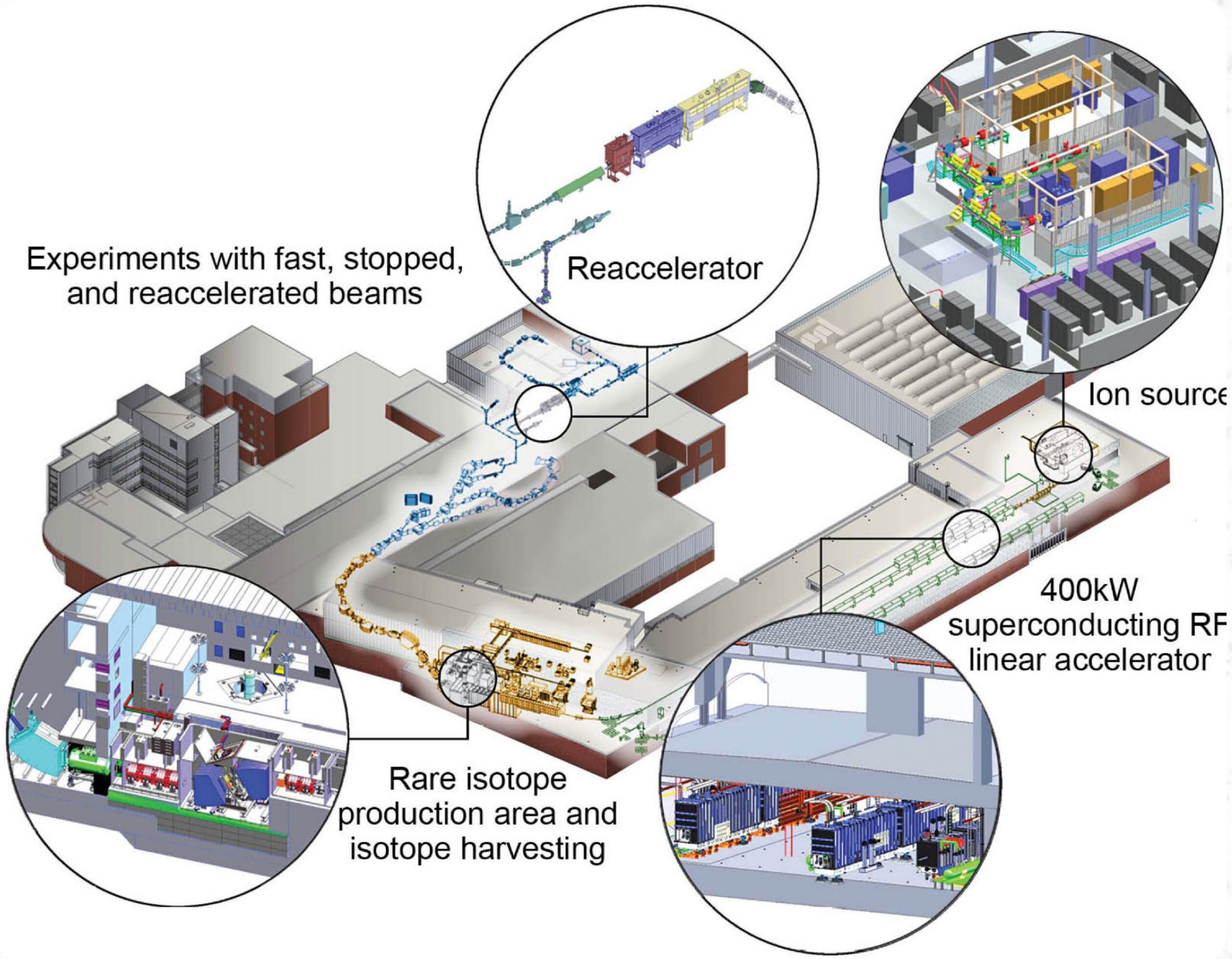
For FRIB (ENAF)

William Raphael Hix (ORNL/U. Tennessee)
for the SciDAC-5 ENAF collaboration

U.S. DEPARTMENT OF ENERGY | Office of Science

Facility for Rare Isotopes

Facility for Rare Isotopes at Michigan State University is a forefront nuclear accelerator facility for the study of short-lived radioactive nuclei.



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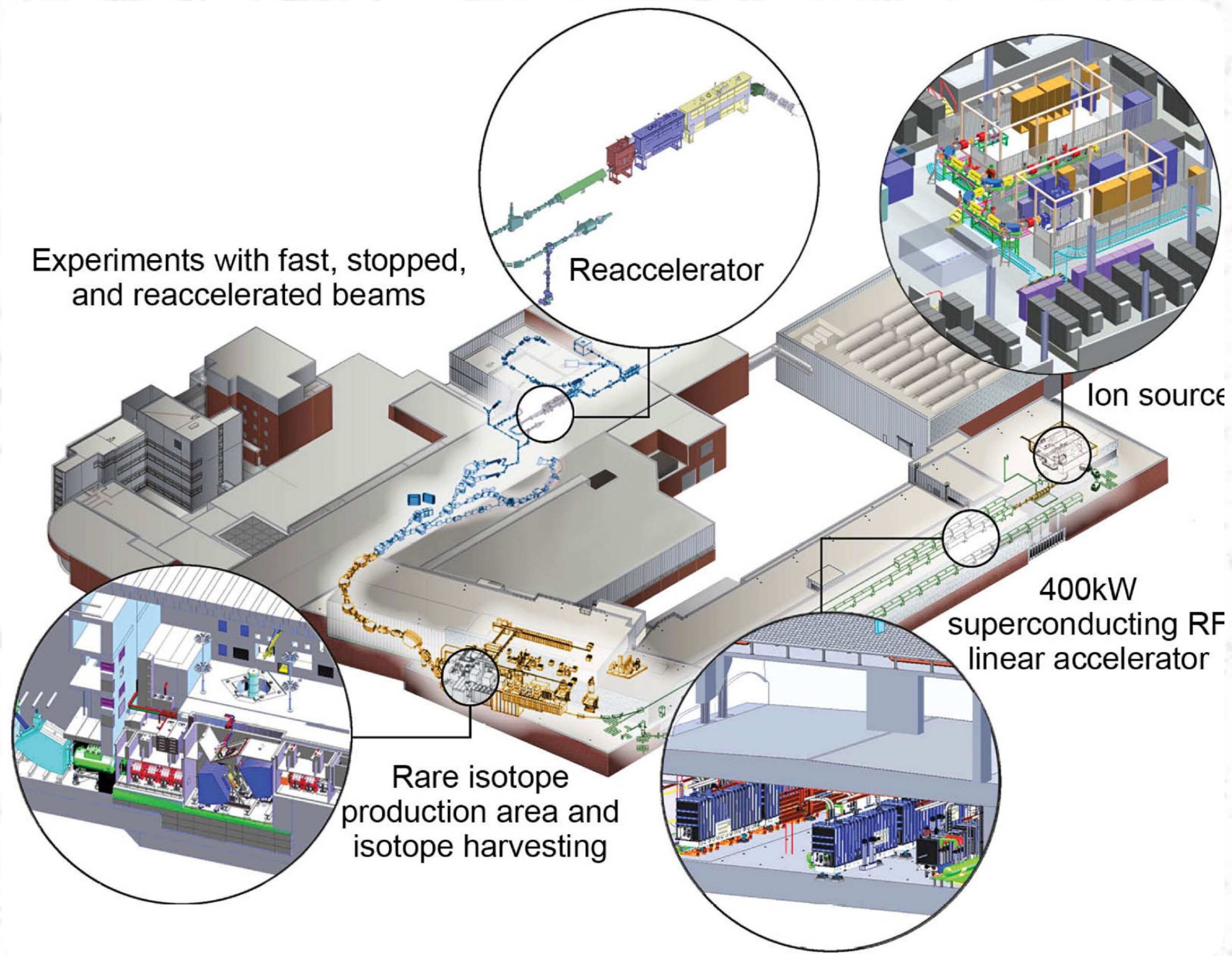
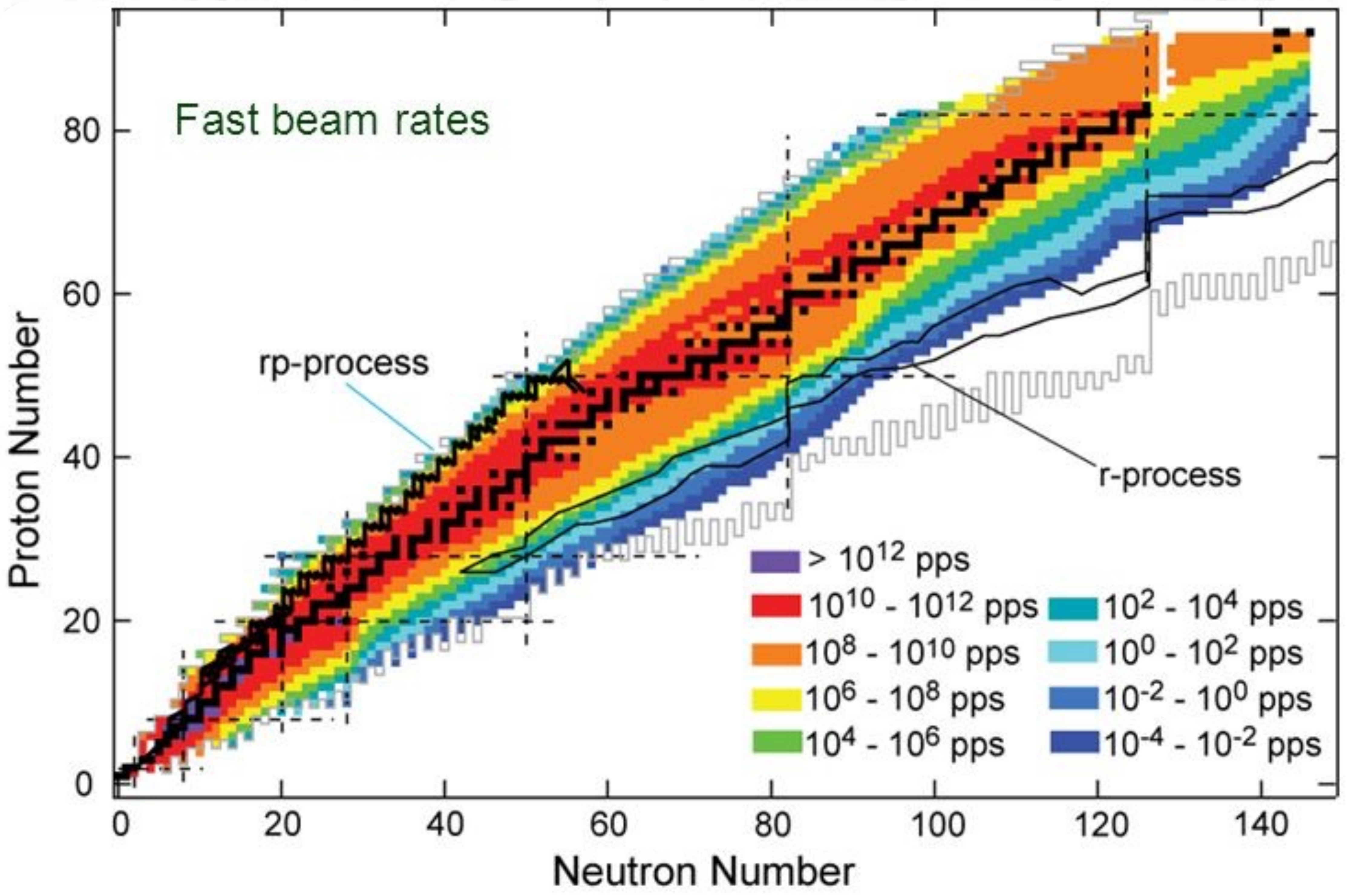
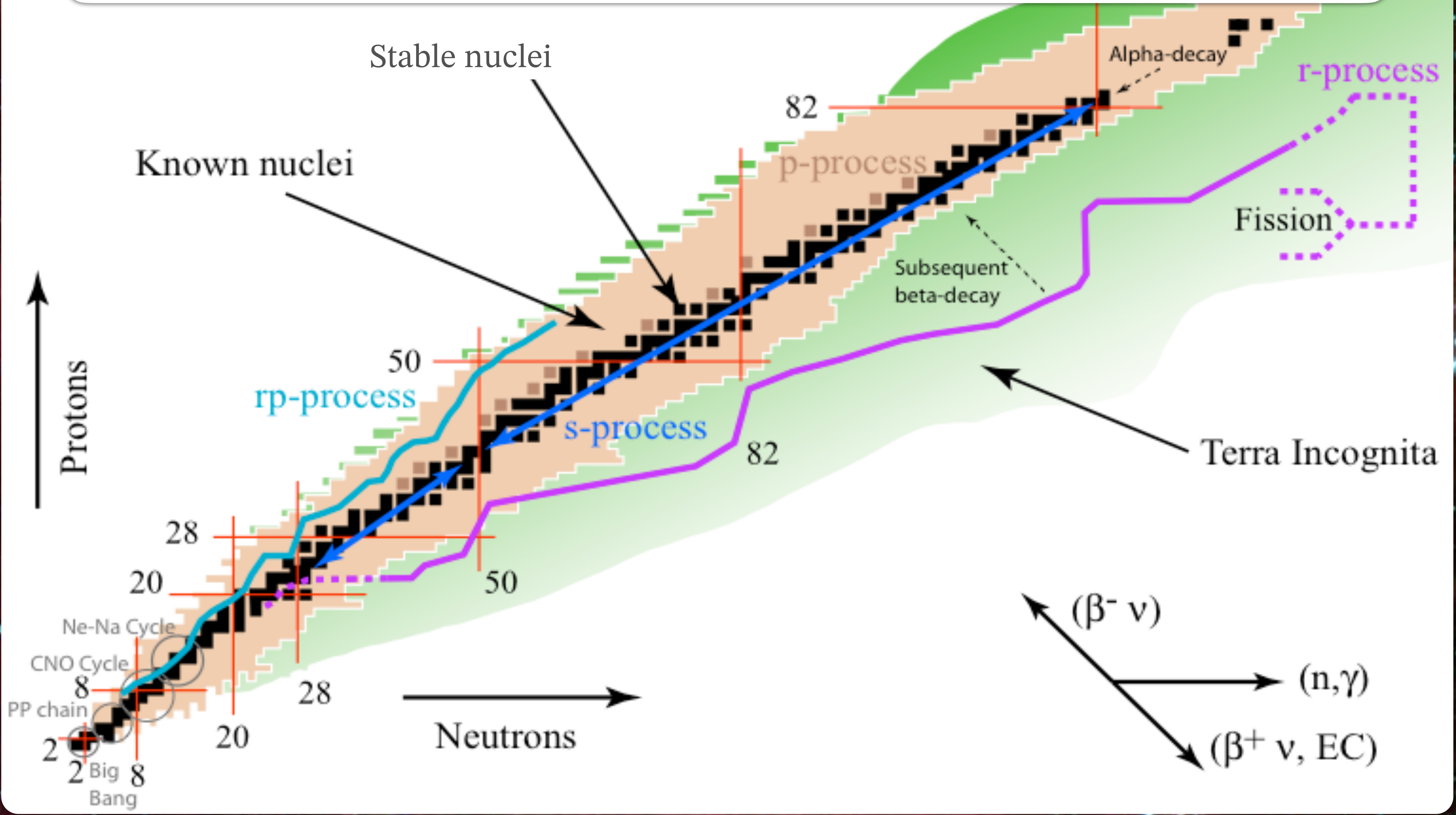




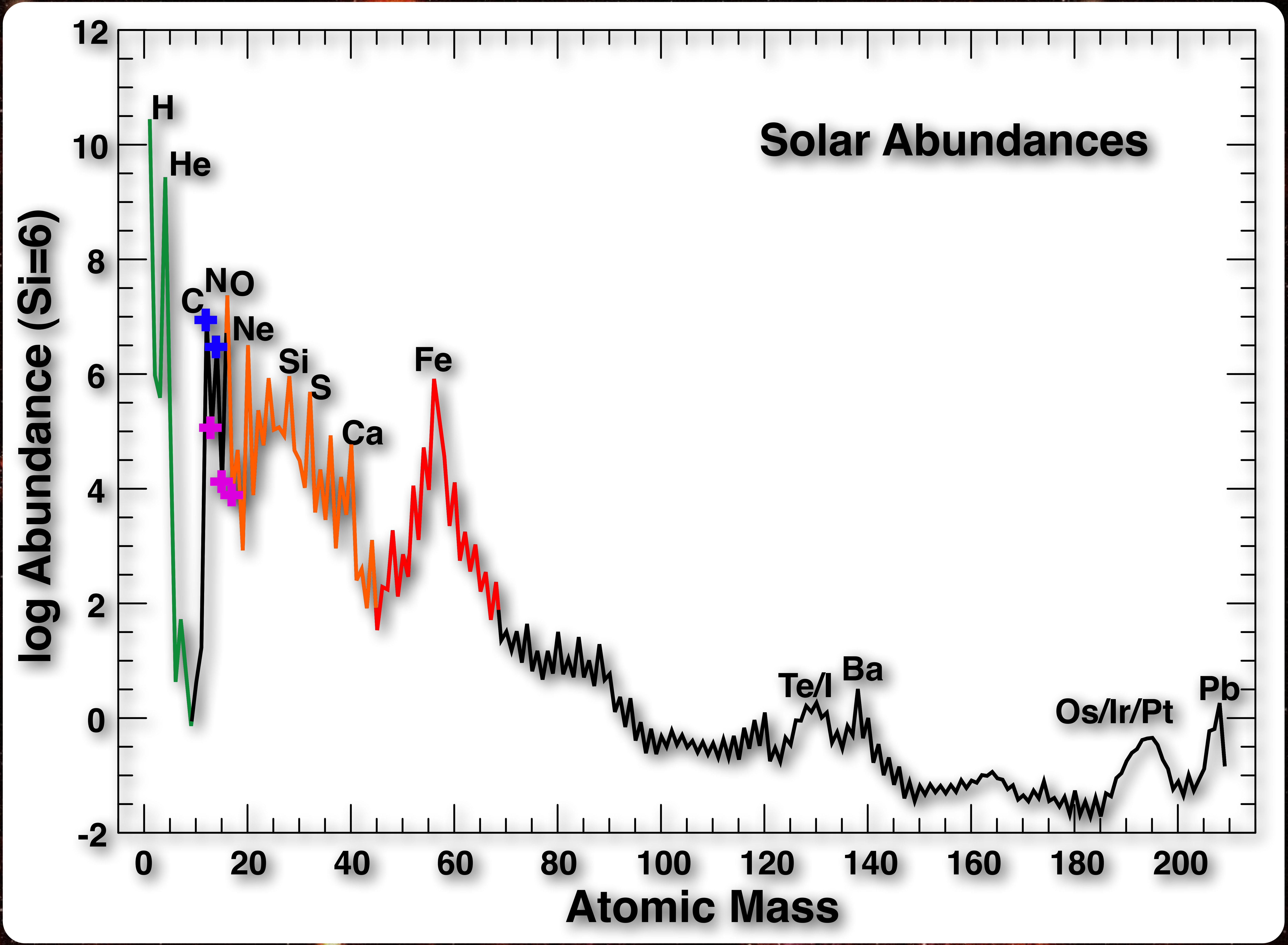
For nuclear astrophysics, FRIB will enable the study of heretofore unreachable species that participate in the rp-process, p-process, and especially the r-process.

Processes and Sites



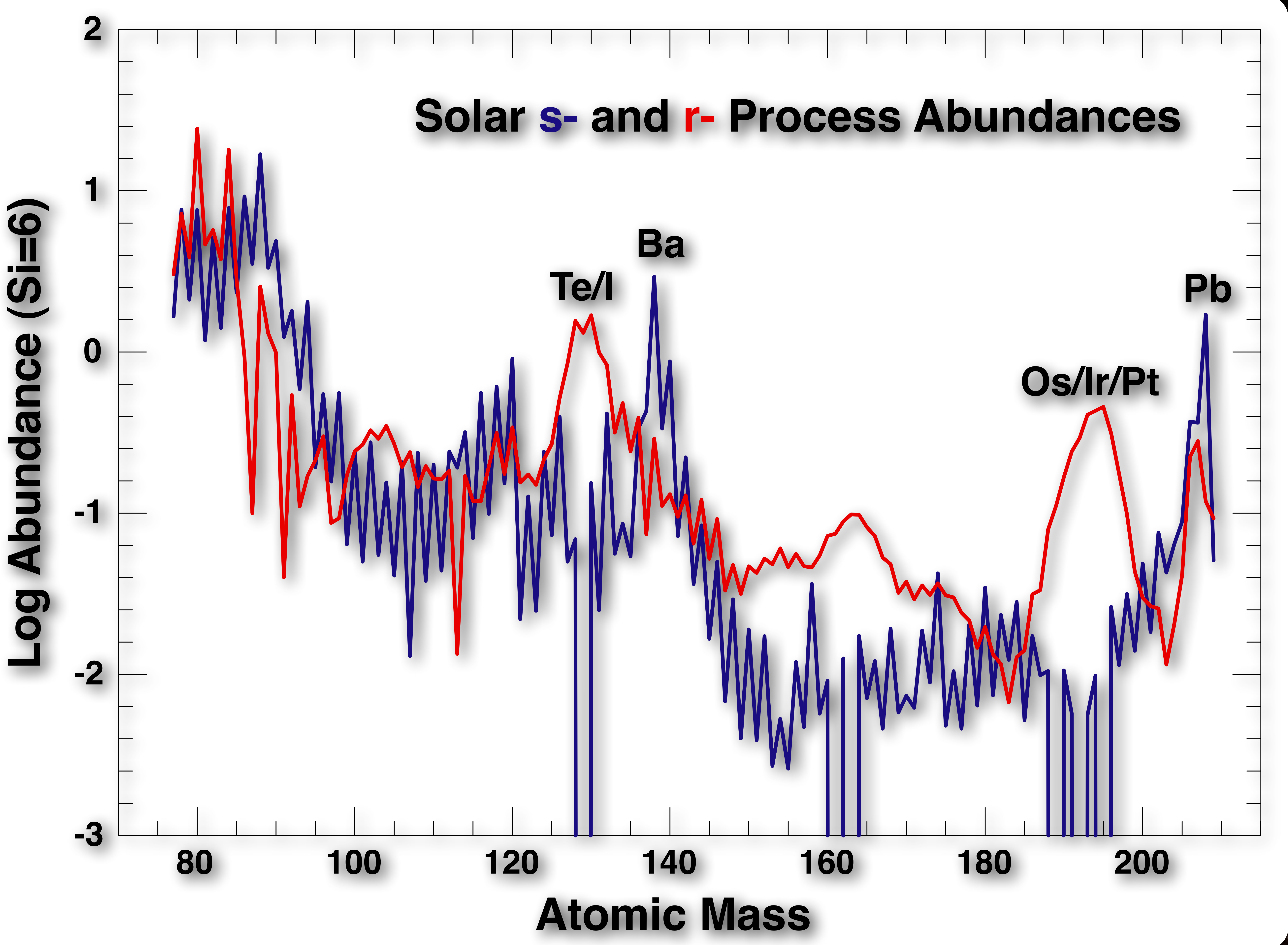
Understanding our nuclear origins means understanding processes that transmute nuclei and the sites where these processes occur.

R-PROCESS



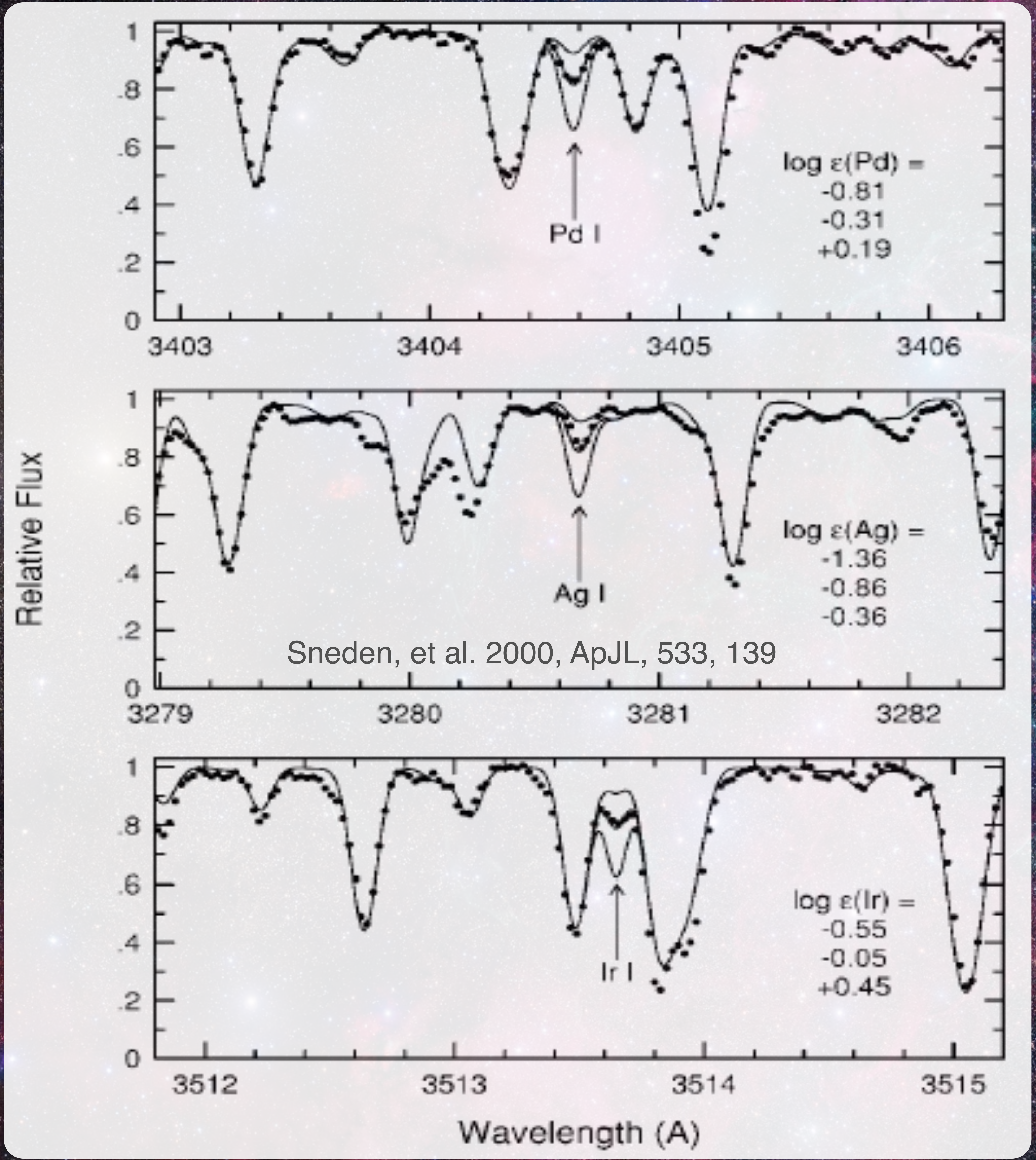
Solar Abundances
log Abundance (Si=6)
Atomic Mass
H
He
C
N
O
Ne
Si
S
Ca
Fe
Te/I
Ba
Os/Ir/Pt
Pb
12
10
8
6
4
2
0
-2
0
20
40
60
80
100
120
140
160
180
200

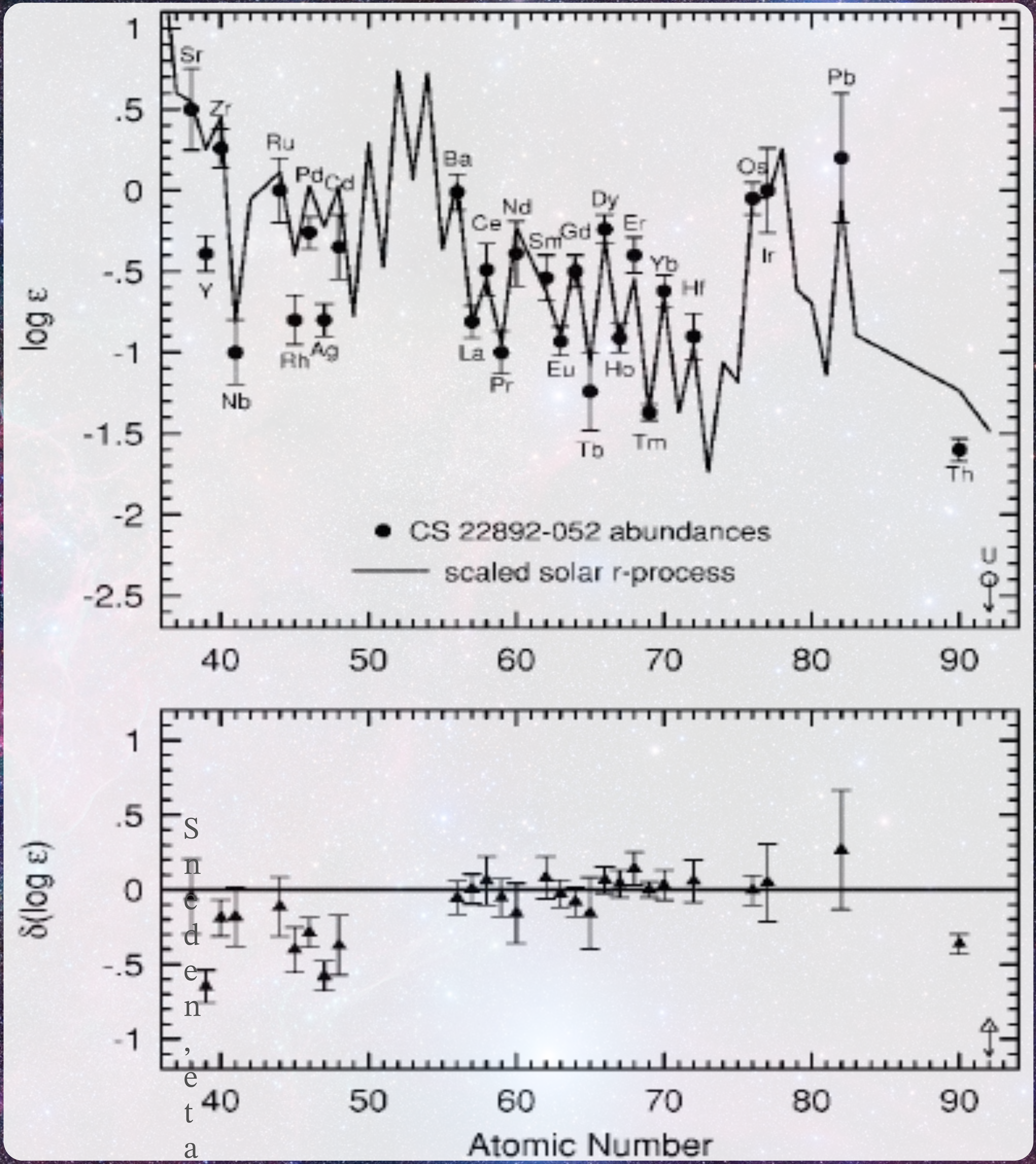
R-PROCESS



Solar s- and r- Process Abundances
Te/I
Ba
Os/Ir/Pt
Pb
Log Abundance (Si=6)
2
1
0
-1
-2
-3
80
100
120
140
160
180
200
Atomic Mass

r-process Elements in old stars



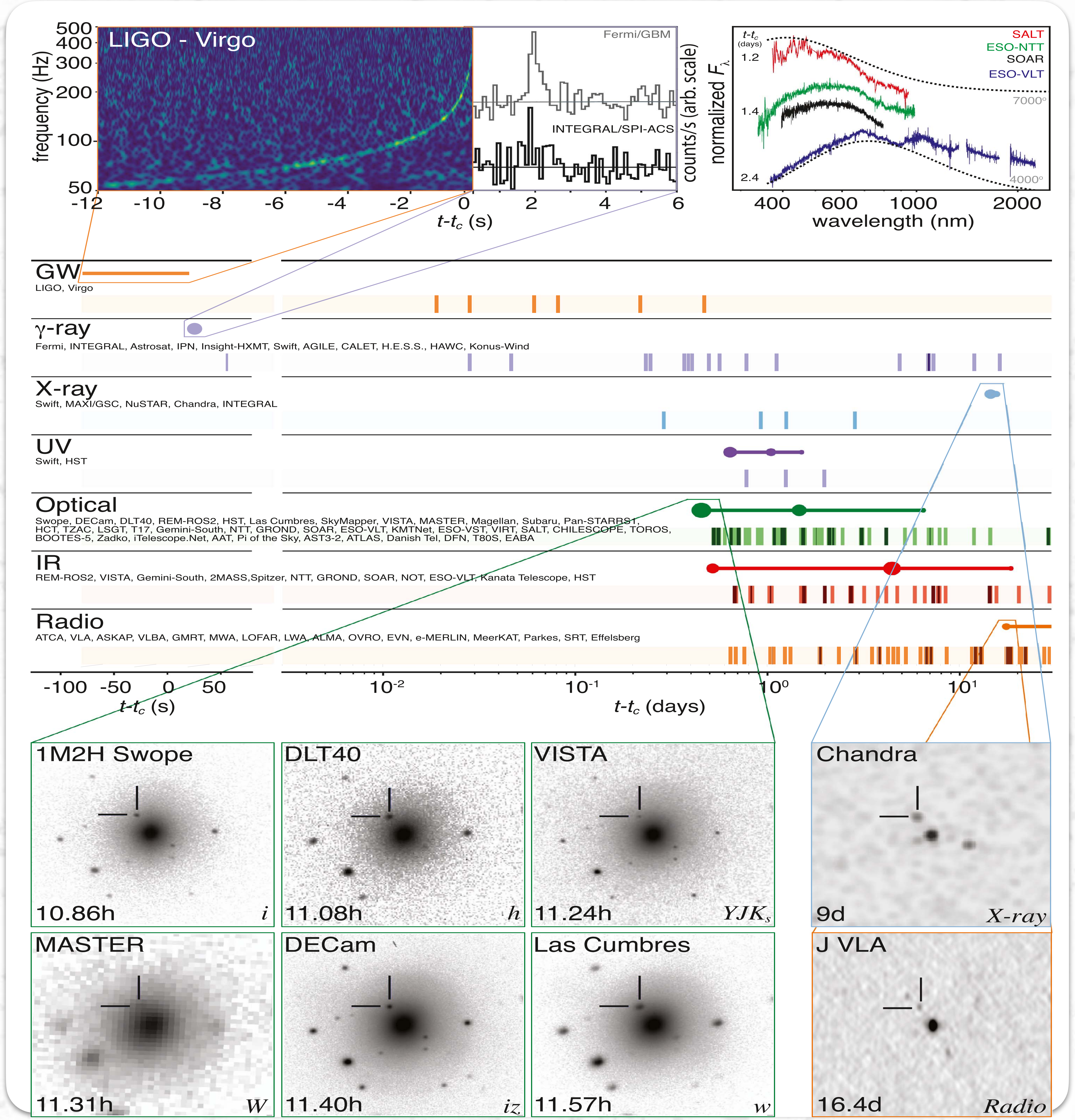


Seeing the r-process?

Observations of GW170817 and GRB 170817a confirmed the long suspected connection between short GRBs and neutron star mergers.

They also launched a extensive multi-wavelength observational campaign, which provided observations of the second ever *kilonova*, with expected red (high opacity) and unexpected blue (low-opacity) components.

This high opacity component is consistent with heavy r-process production, but interpretation of the quantity and composition of the ejecta are model-dependent.



ENAF(LITE) TEAM

Argonne National Laboratory
Anshu Dubey

University of California, Berkeley
Dan Kasen

University of Notre Dame
Rebecca Surman

Oak Ridge National Laboratory
Raph Hix,
Bronson Messer

North Carolina State University
Gail McLaughlin

Pennsylvania State University
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ASCR supports continued development of the community Flash-X code, including portable performance and GPU-enabling of important computational kernels.

NP supports a chain of investigations including neutrino flavor transformations, neutron star mergers and the resulting kilonovae and the r-process.

TEAMS TEAM

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

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Rebecca Surman

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Andy Nonaka, Ann Almgren

Michigan State University
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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 was 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

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

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

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

Improve EOS (UTK), Neutrino Opacities (UW, MSU).

Quantify Nuclear (Notre Dame) & Astrophysics (LANL, ORNL) nucleosynthesis uncertainties.

ExaStar team

University of California, Berkeley
Dan Kasen
Ann Almgren

Argonne National Laboratory
Anshu Dubey

Stony Brooke University
Mike Zingale

Oak Ridge National Laboratory
Raph Hix,
Bronson Messer

Michigan State University
Sean Couch

Part of the Exascale Computing Project, ExaStar developed Flash-X, uniting exascale adaptive mesh refinement package AMReX, with existing block level physics from Castro, FLASH and CHIMERA.

Exastar also included development of a new MHD solver (Spark), a new implicit/explicit moment method neutrino transport solver (thornado), GR spacetime solver, and improvements to Monte Carlo transport (Sedona).

Exastar's goal was exascale-ready code, not science.

FLASH-X

Exascale development of the community FLASH code, supported by ECP and SciDAC-4

hydrodynamics

Requirements: 3D AMR hydro w/ effective resolution of ~100's meters

Methods: *Finite volume Godunov methods*

Extensions: GR magnetohydrodynamics

nuclear reactions

Requirements: sizable in-situ reaction networks (~150 isotopes)

Methods: *Accelerated stiff ODE solvers with spectral deferred correction coupling to dynamics*

radiation transport

Requirements: Spectral (~ 30 groups) neutrino transport with key microphysics (frame-dependent terms, relativistic effects, non-isoenergetic scattering).

Methods: *implicit-explicit time integration w/ discontinuous Galerkin descritization of two-moment formulation. Monte Carlo methods for post-processing and refined closures.*

EoS

Requirements: nuclear high density equation of state

Methods: *tabulated*

Gravity

Requirements: Solution of Poisson equation with post-Newtonian corrections

Methods: *Asynchronous multipole/mutli-grid solvers of elliptic PDE*

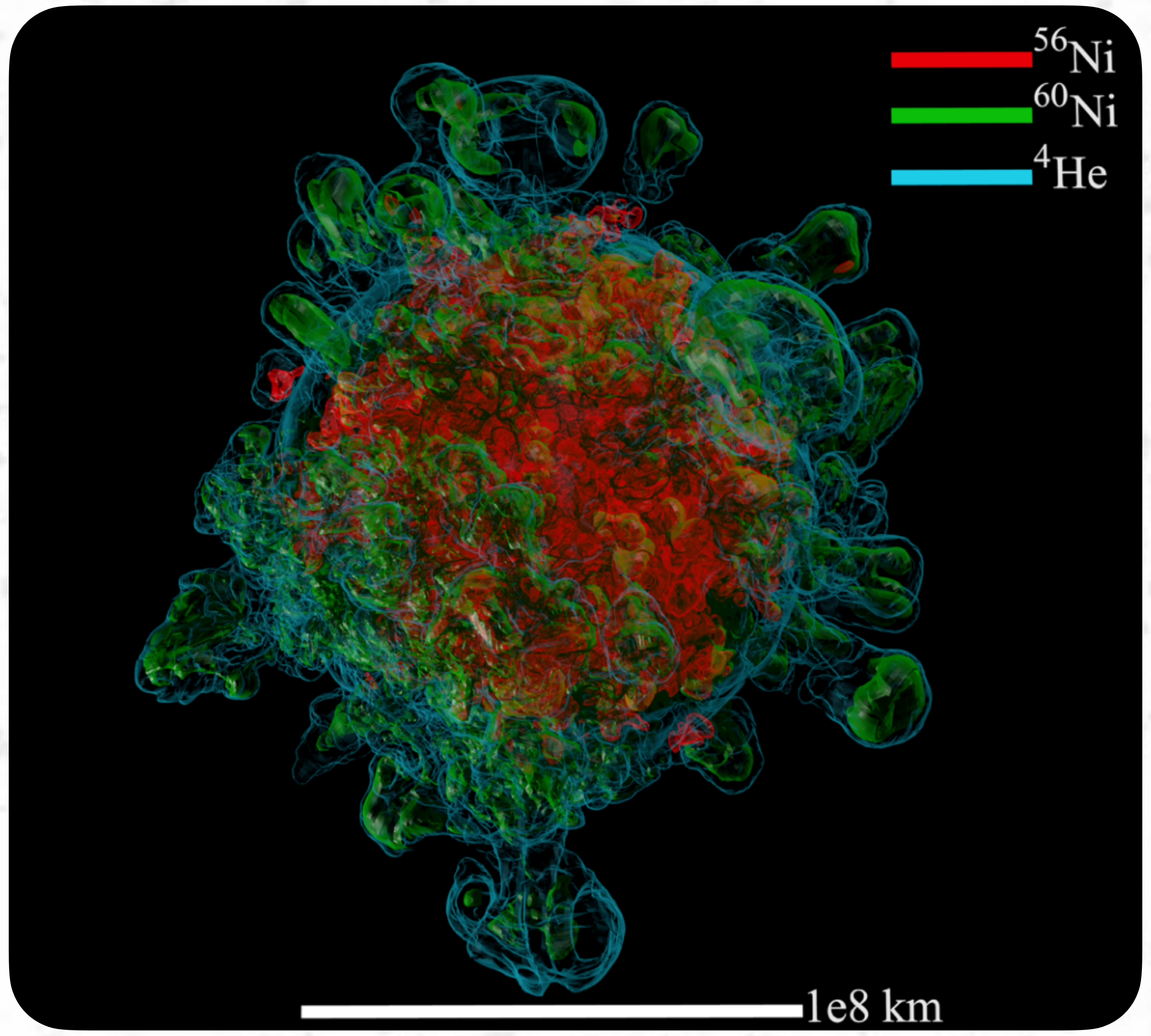
Extensions: Dynamical spacetime solver

block-structured adaptive mesh (AMReX or PARAMESH)

Flash-X development at ORNL

Development work at ORNL will concentrate on high-performance GPU-based implementations of several important computational kernels necessary to advance the state-of-the-art in various nuclear astrophysics settings.

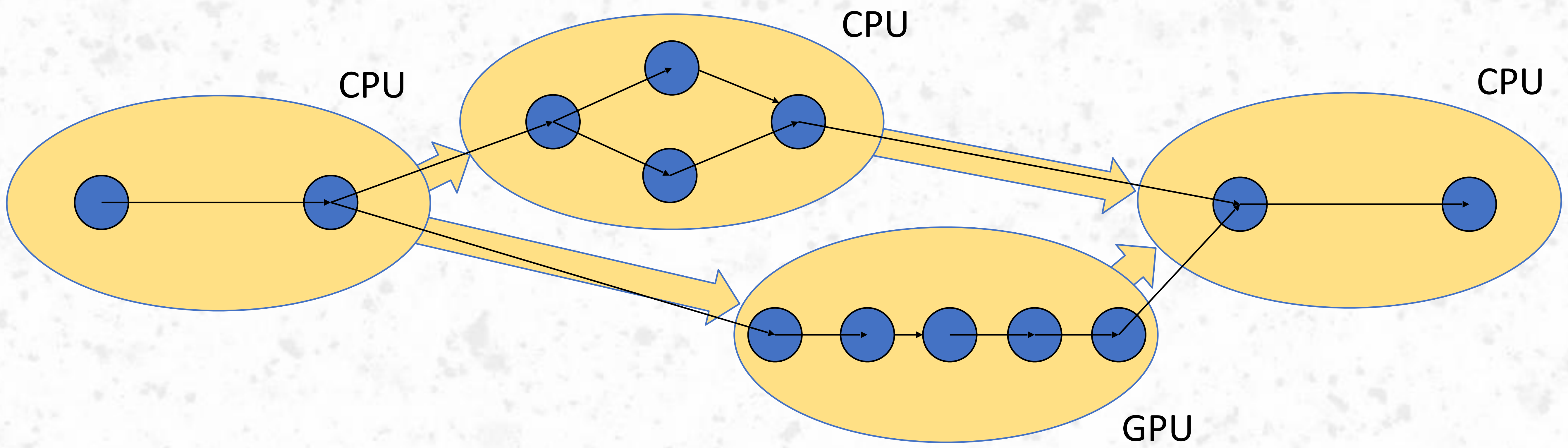
- We will build robust ML-based inference engines designed to replace simpler interpolation schemes for various physical quantities typically included in simulations as tabular data.
- We will continue to work on implementations intended to maximize the computational intensity of GPU-enabled kernels for radiation transport.
- We will develop a new set of preconditioners for the larger, more dense linear systems encountered when additional leptonic degrees of freedom are introduced into our transport codes (i.e., when we include the effects of muons in hot, dense environments).



CGKIT

The problems of achieving high performance on ever-changing architectures is magnified for multi-physics codes. CGKit is a tool to help achieve this portable performance, started under SciDAC-4 (TEAMS).

- User expresses time-stepping control flow in a pseudocode-like recipe
- CGkit converts it to a graph, figures our the map of computation to devices
- Create a (flat) **control flow graph** where nodes (blue) represent computational work (i.e., kernels) and edges represent dependencies between kernels and data flow
- Assign attributes to nodes representing which device it will execute on (e.g., CPU, GPU)



- Generate device specific apply routines for aggregated device specific kernels
- Traversal of graph yields the call sequence of device specific apply routines

CGKit Plan for ENAF

CGKit relies on platform specific templates to emit code.

Recipes can also differ depending upon included physics.

We are creating a library of templates for all flavors of recipes on target platforms.

We have created a performance model for Flash-X.

Using recipes, it is possible to explore the performance possibilities.

We will do this analysis and create a database of parameters to performance map.

A new Hydro/MHD solver based on Gaussian Process is will also be added

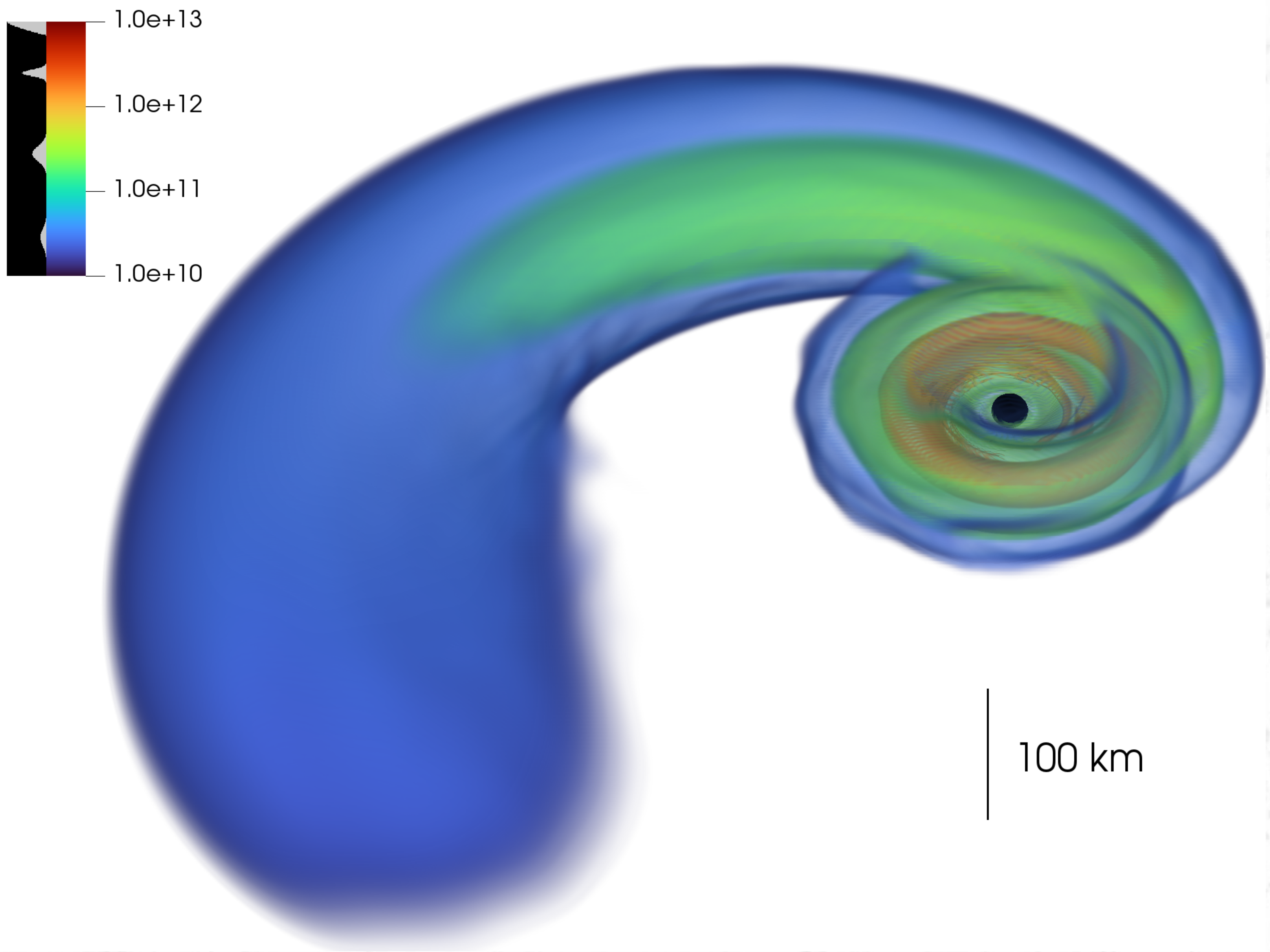
Neutron star merger simulations

Explore diversity of merger outcomes and how they depend on the binary parameters with M1 neutrino-transport

Perform long-term postmerger simulations of selected configurations

Explore impact of magnetic fields on the nucleosynthesis yields from mergers

Include neutrino quantum-kinetic effects (PSU and NCSU teams)



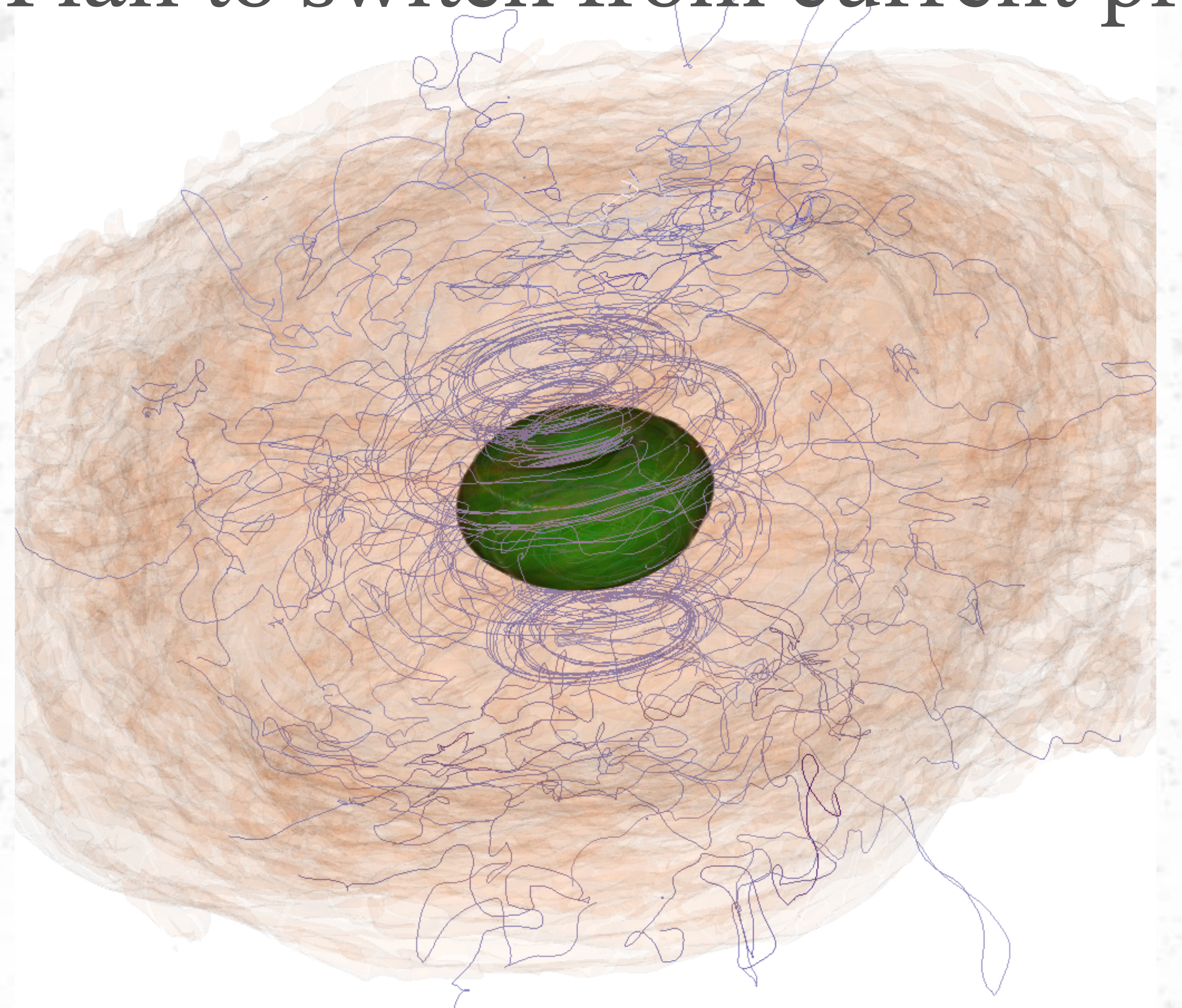
Tidal disruption and black hole formation in a high mass-ratio binary neutron star merger simulation

PSU Code development efforts

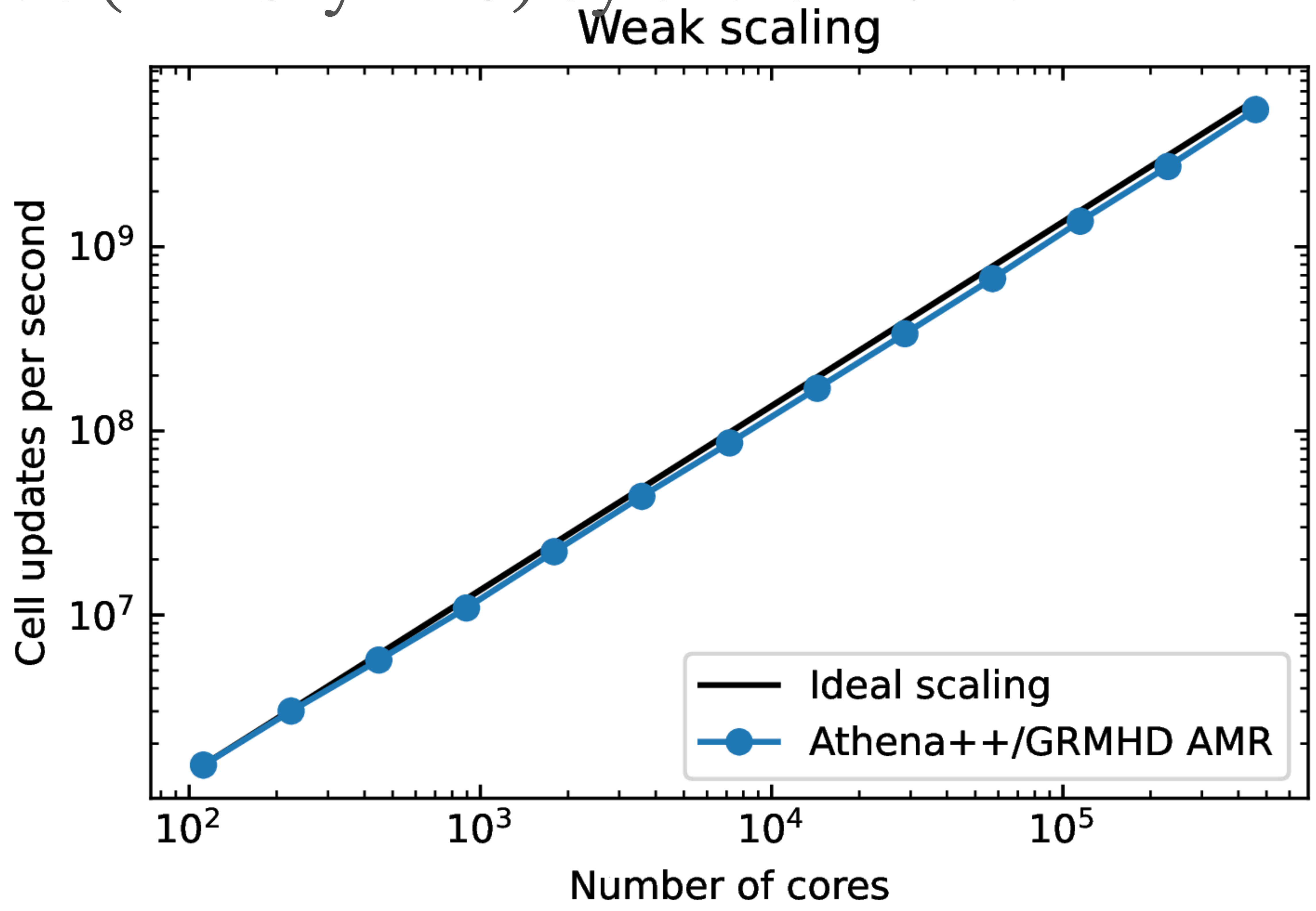
Complete Kokkos version of our new GRMHD code (GR-Athena++)

Include spectral Boltzmann neutrino transport, important to neutronization of ejecta

Plan to switch from current production code (WhiskyTHC) by end of 2024.



Magnetic field lines in a NS merger remnant simulated with GR-Athena++

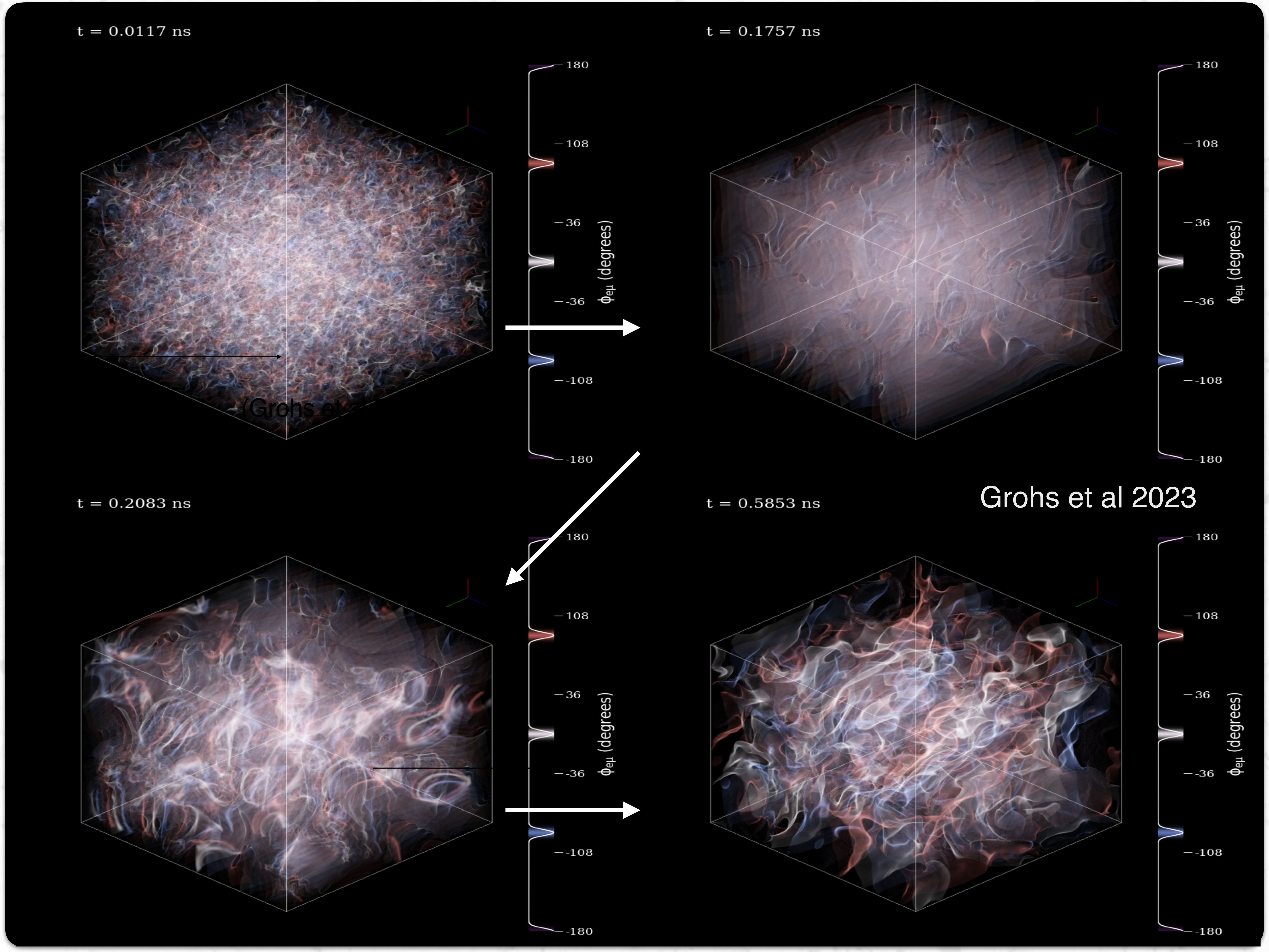


Neutrino oscillations above a NS merger

The oscillation of neutrinos between the electron, mu, and tau flavors changes their interactions with matter.

Fast flavor conversion is the fastest of the neutrino flavor instabilities that can occur in neutron star mergers.

Currently, we can follow the evolution of quantum phase of neutrinos in 8 cm box under neutron star merger conditions with the angular moment method.



Plans for the Flavor future

Current capability for direct numerical simulations of the fast flavor transformations do not reach the km scale needed for simulations of the neutron star mergers. Therefore, sub-grid representations of this important physics are needed.

Future plans for the NC State team include:

(1) global predictions of instability using neutron star merger models from Penn State

(2) estimates of flavor transformation saturation throughout system

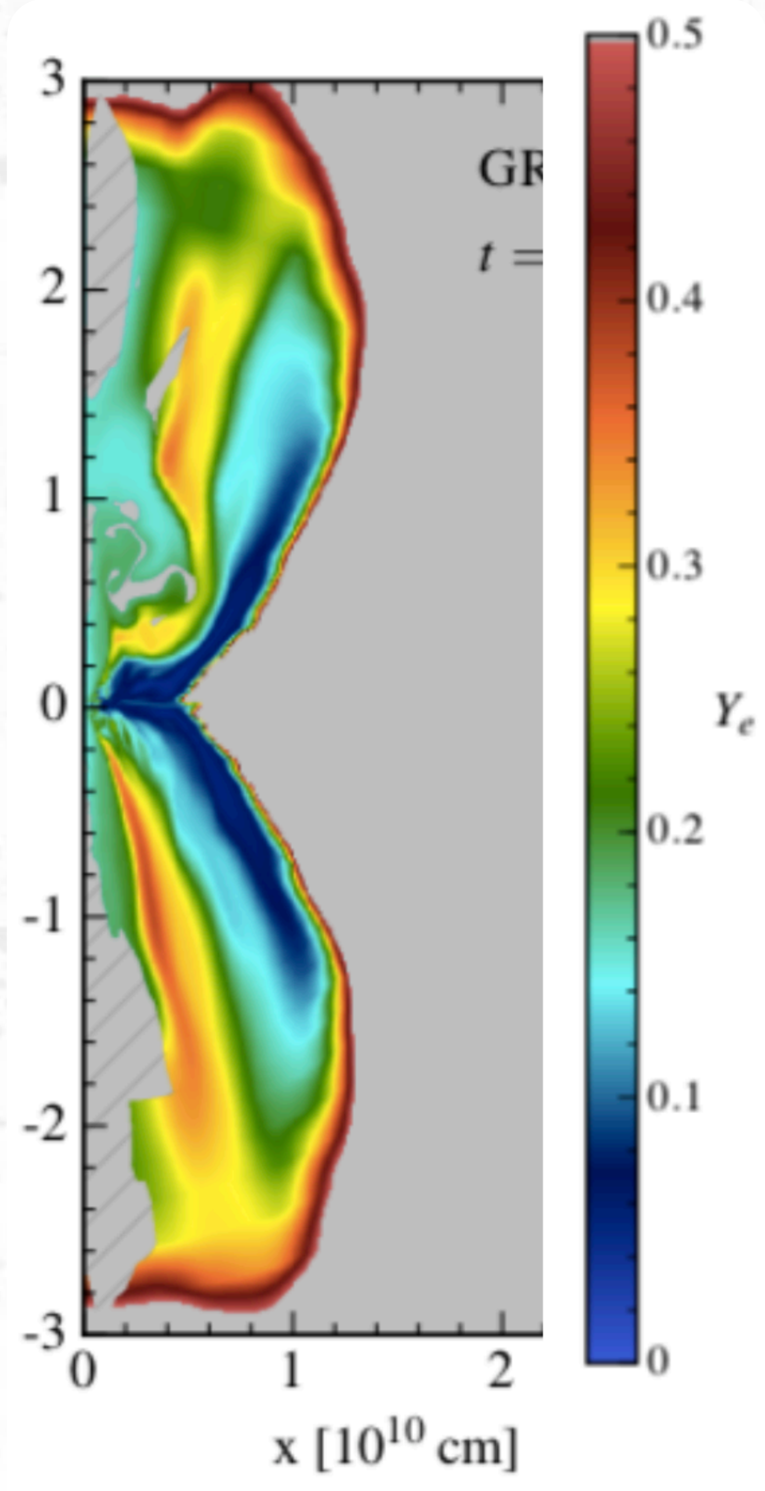
(3) inclusion of neutrino mass to predict slow modes

(4) working with Penn State to include effective saturation outcomes in dynamical neutron star merger simulation

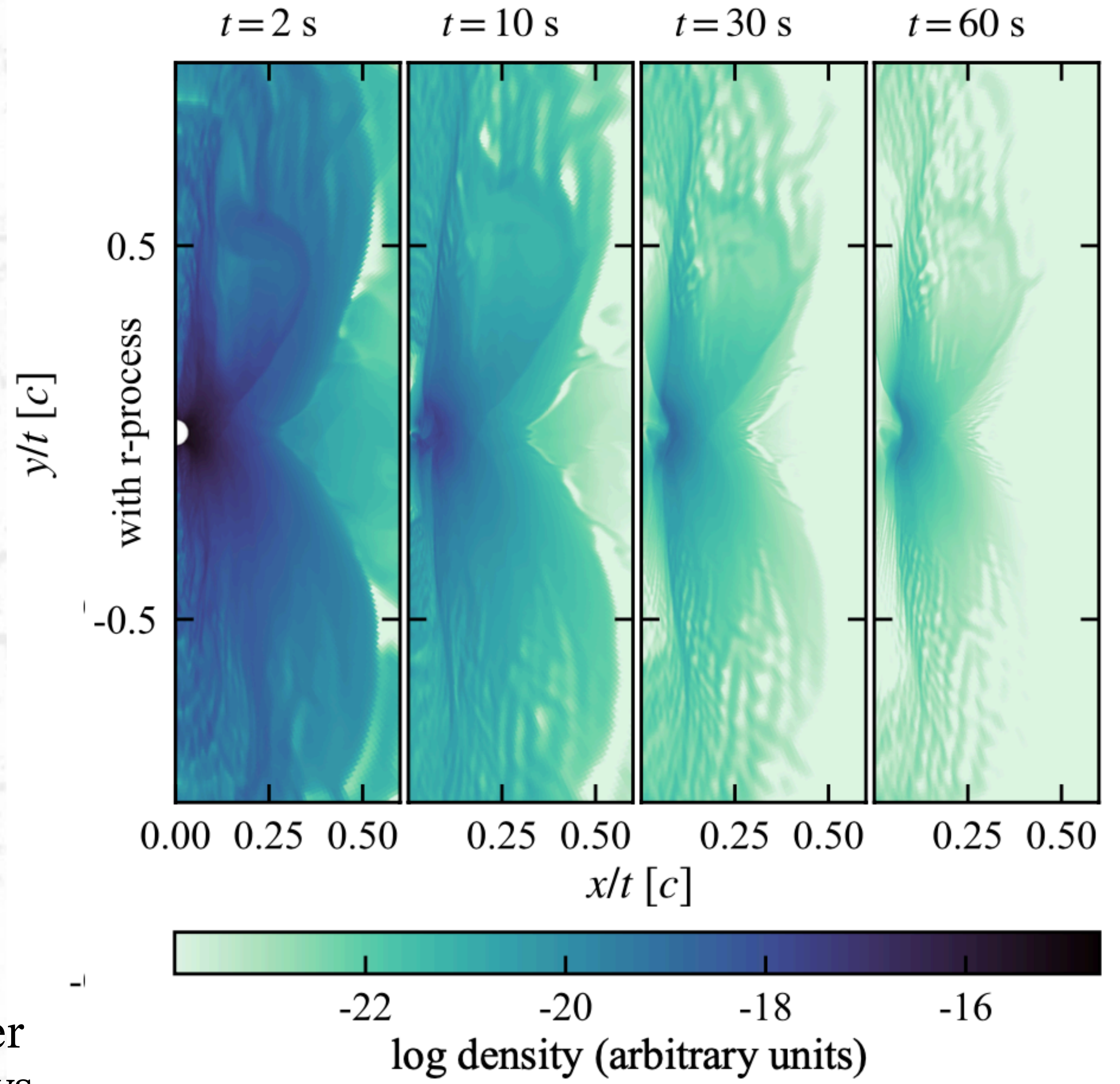
(5) inclusion of neutrino collisions

Probing heavy r-process nucleosynthesis in Mergers

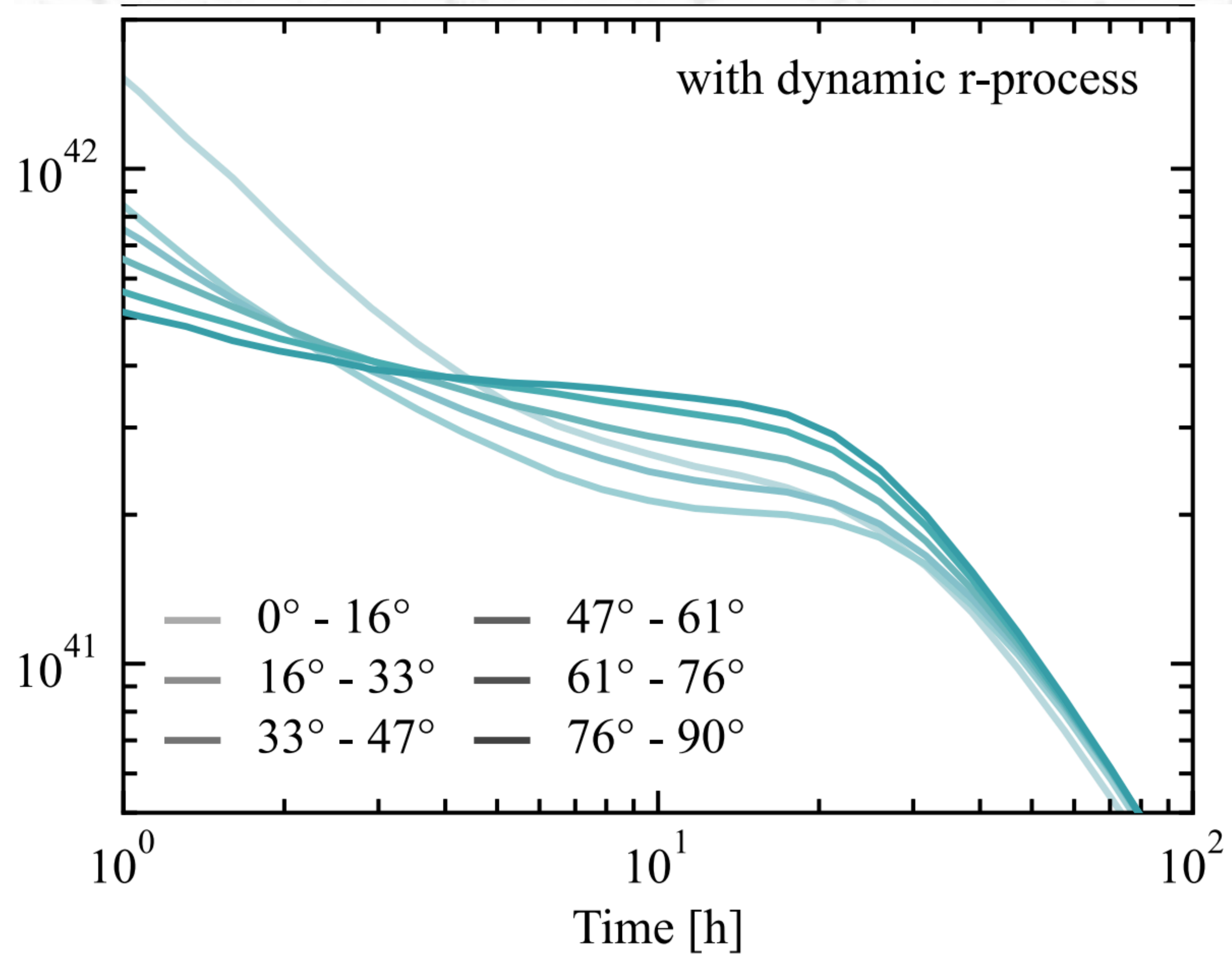
Connecting multi-physics simulations to thermal emission due to radioactive isotopes.



GRMHD simulations of post-merger disk winds find asymmetric outflows, with more neutron-rich material ejected only at the equator. Post-processing nucleosynthesis indicates the production of the range of light (1st -2nd peak) and heavy (3rd peak) r-process isotopes (Christie et al 2020)



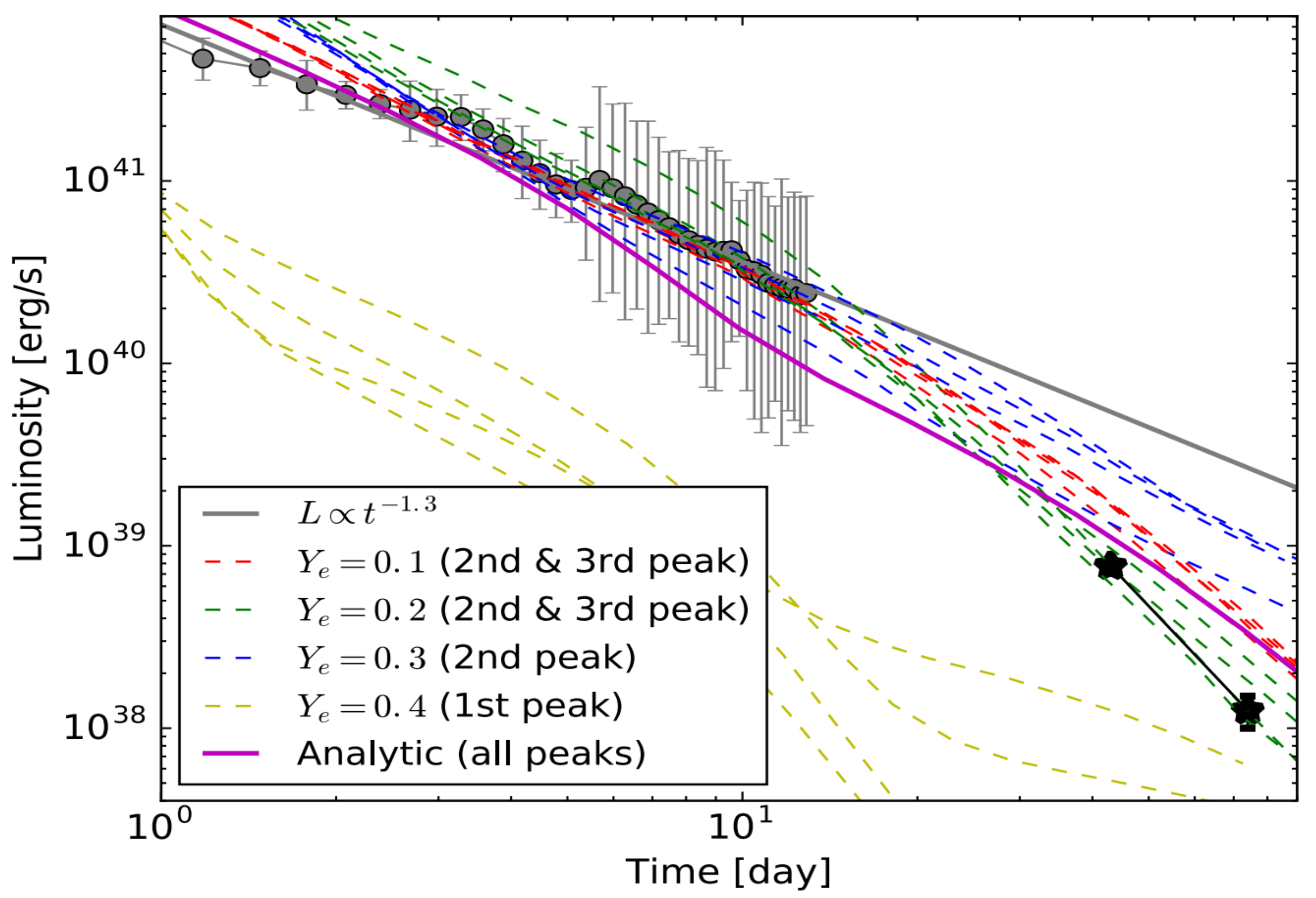
Longer term hydrodynamical models including the dynamical effect of nuclear reactions and radioactive decay determine the final ejecta kinematics, compositional structure and multi-dimensional geometry (Klion et al 2022, Darbha et al 2021)



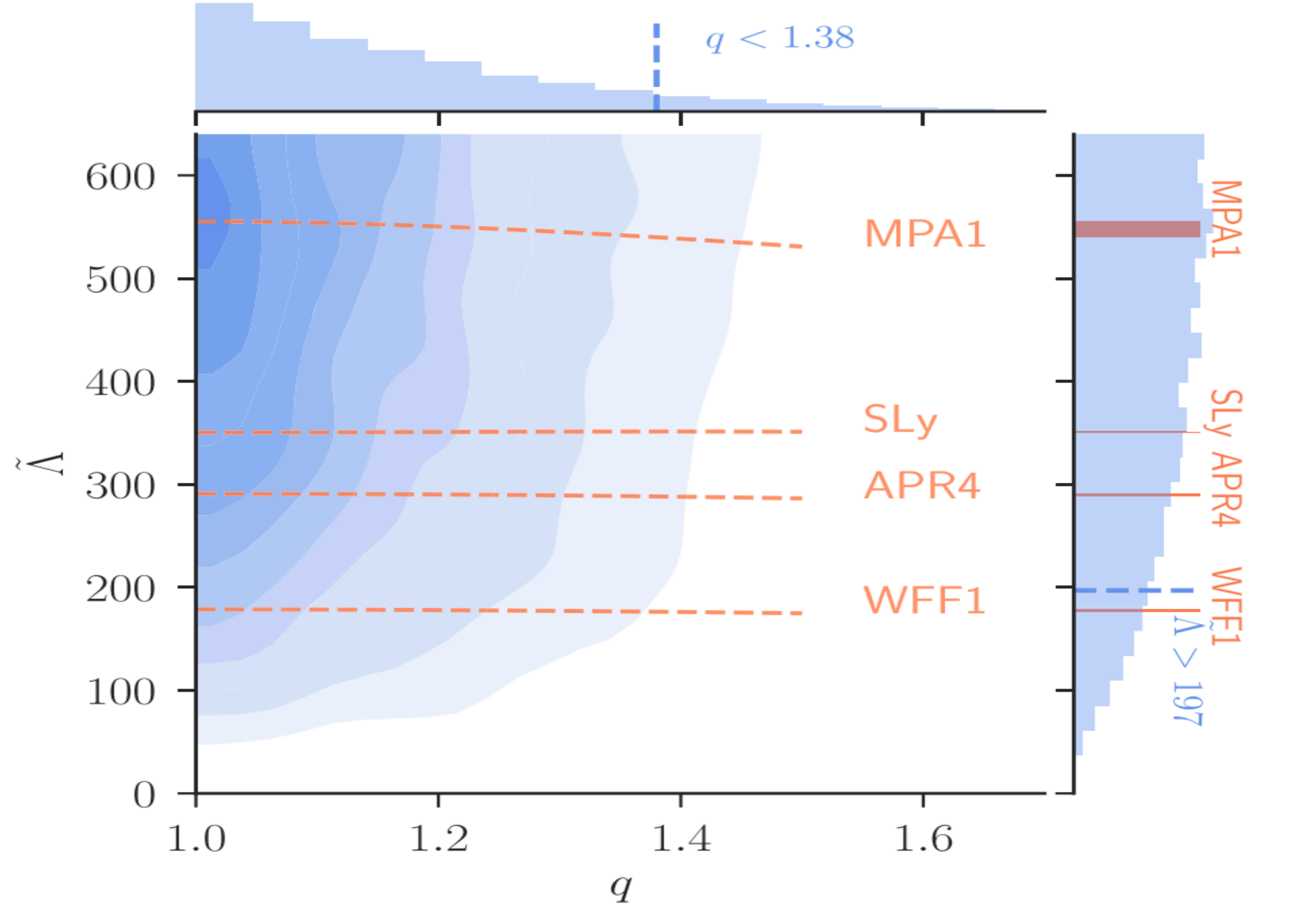
Finally, multi-dimensional radiation transport calculations synthesize the observable optical/infrared light curves and spectra. Comparison to observed events (e.g., the counterpart to gravitational wave source GW170817) provide a direct probe of the r-process yields, helping to address the origin of the heavy elements (Klion et al 2021, 2022).

Impact of Nuclear Physics & Equation of State

Simulating electromagnetic (EM) signals reveal the importance of nuclear inputs (of relevance to FRIB) and can test theoretical nuclear models of the equation of state of dense matter.

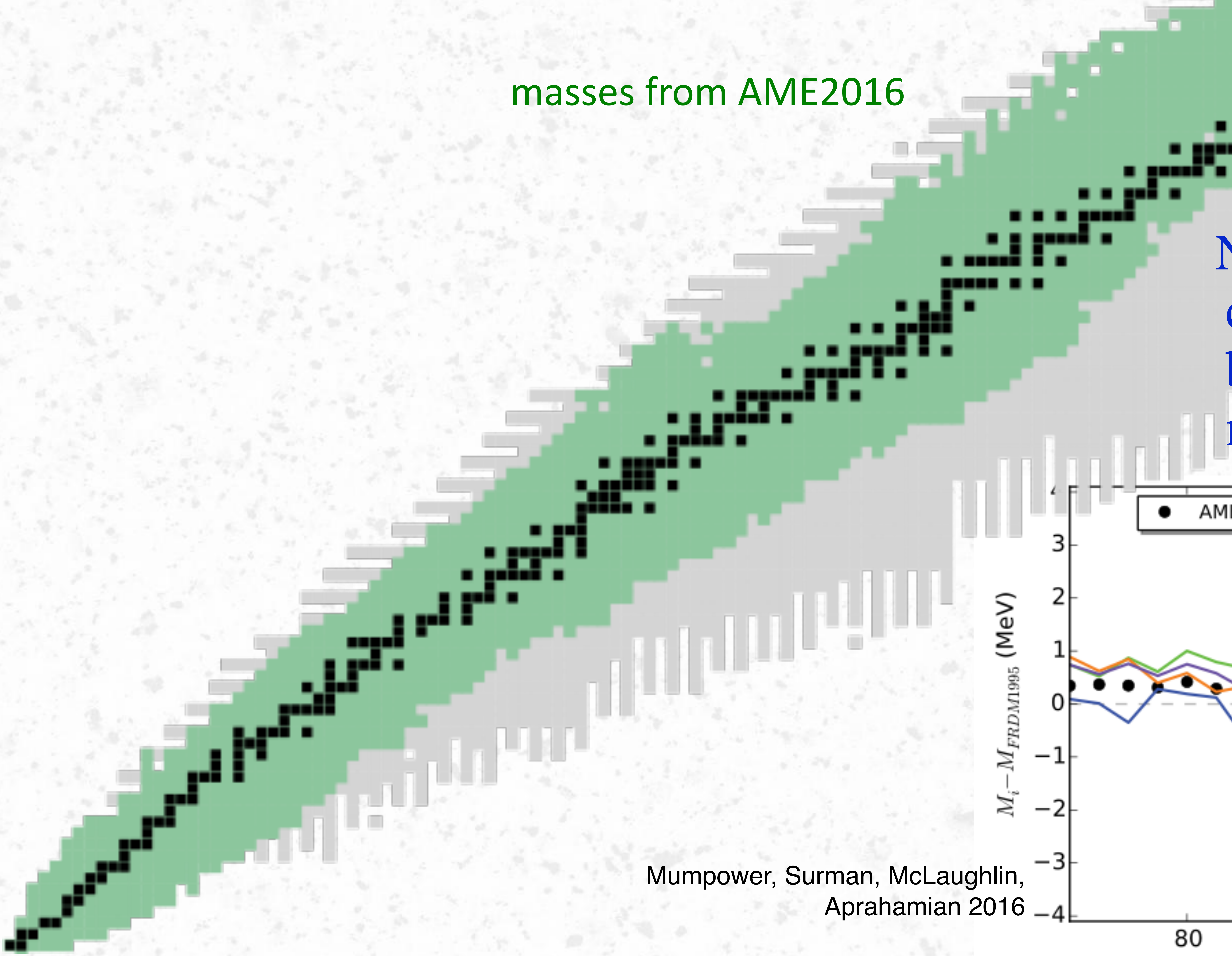


The r-process yields depend on the physical conditions in the ejecta (e.g., electron fraction) and the nuclear properties of isotopes far from stability (of relevance to FRIB). EM data — especially late time infrared observations with Spitzer and JWST — probe the thermalization of beta/alpha/fission decay of select isotopes with longer half-lives (Kasen & Barnes 2019, Kasliwal, Kasen, et al 2022).



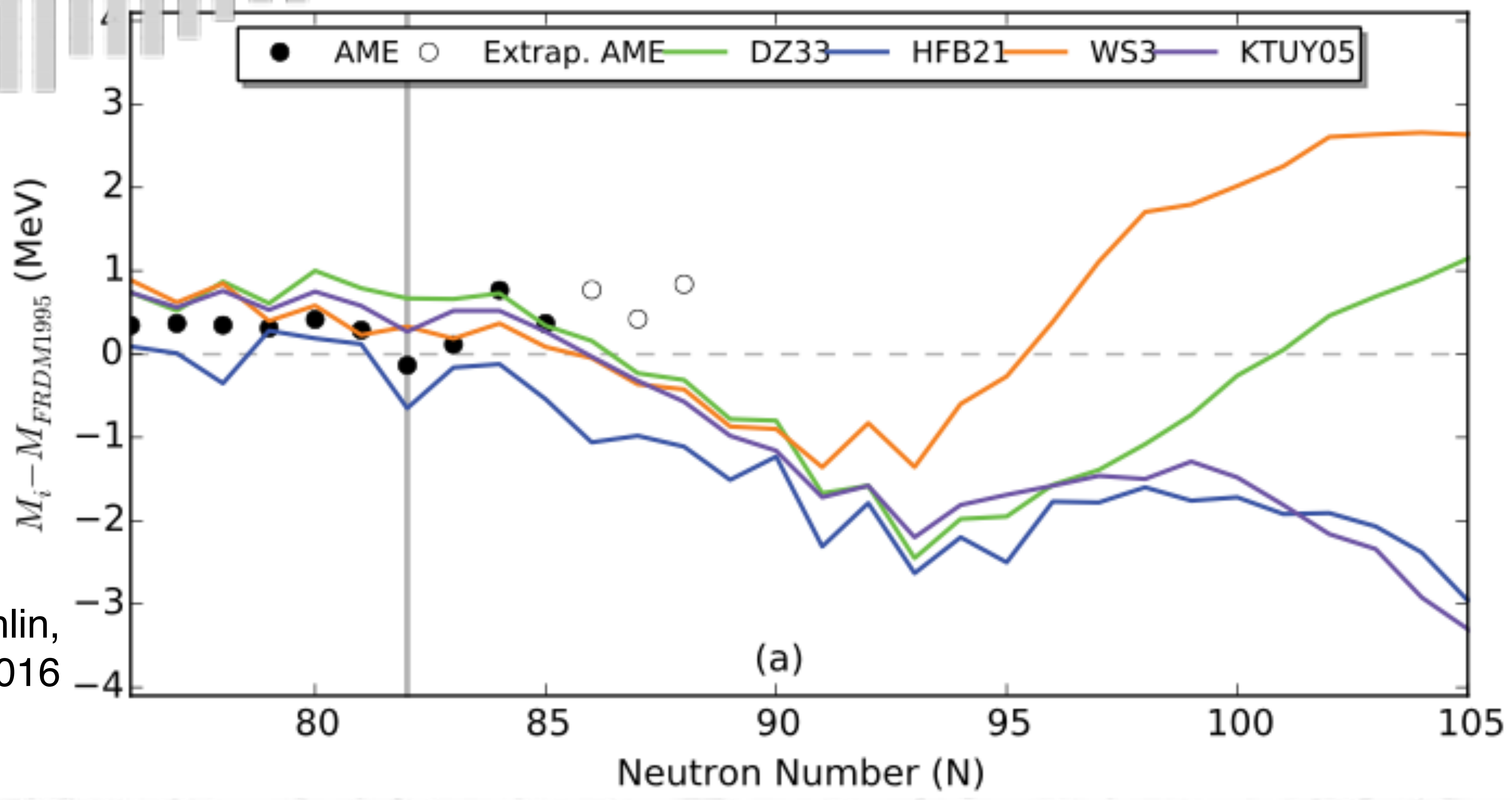
Systematically fitting EM observations with radiative transfer models of merger counterparts (via machine-learning techniques) constrains the ejected mass and in turn the deformability of the neutron star. Such estimates can be used to constrain theoretical models of the dense matter equation of state, in a way complementary to gravitational wave signals (Coughlin, et al 2018).

Nuclear data for r-process simulations

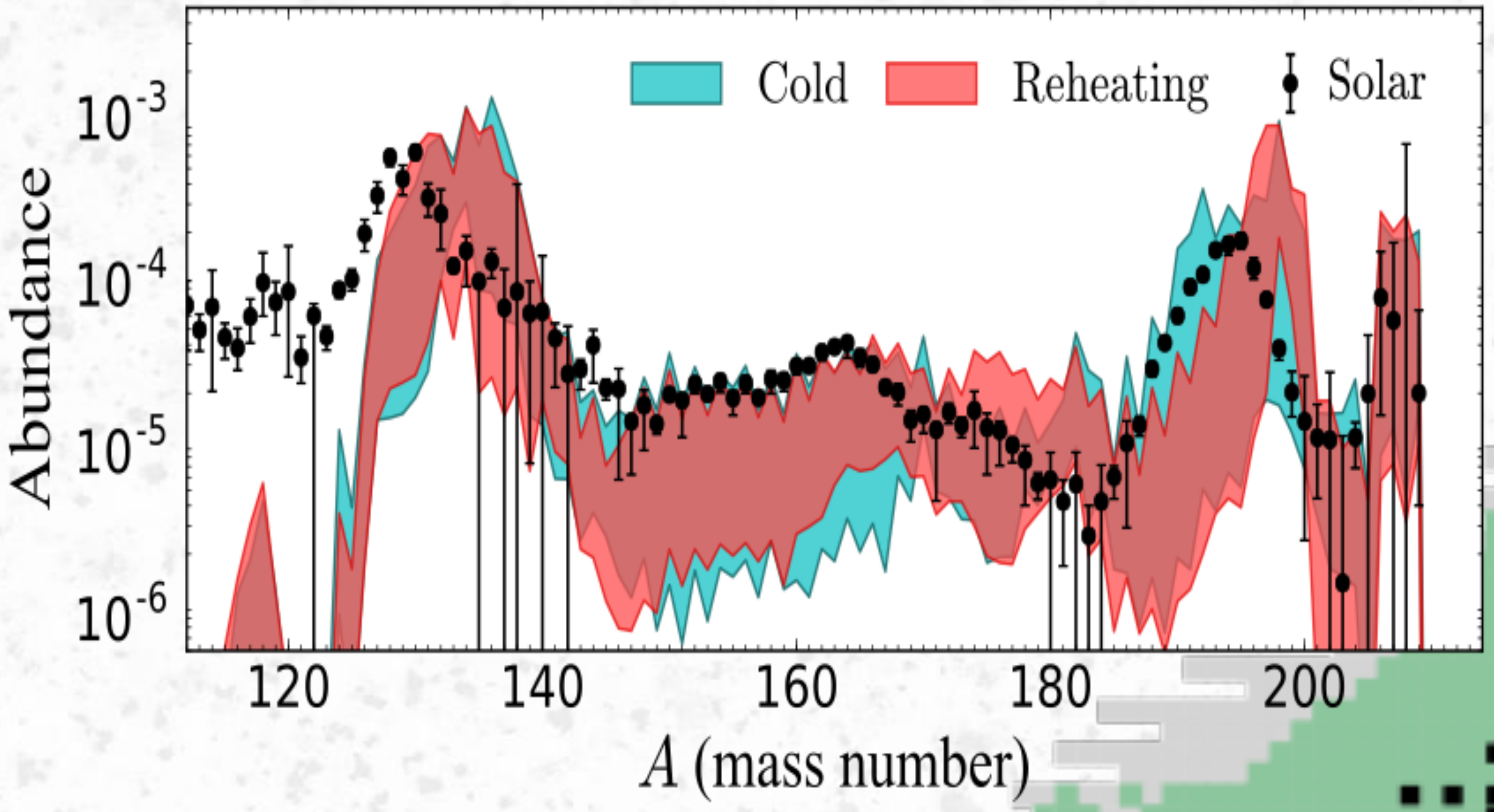


masses from AME2016

Nuclear models are generally consistent with available data, but extrapolations into neutron-rich regions diverge sharply

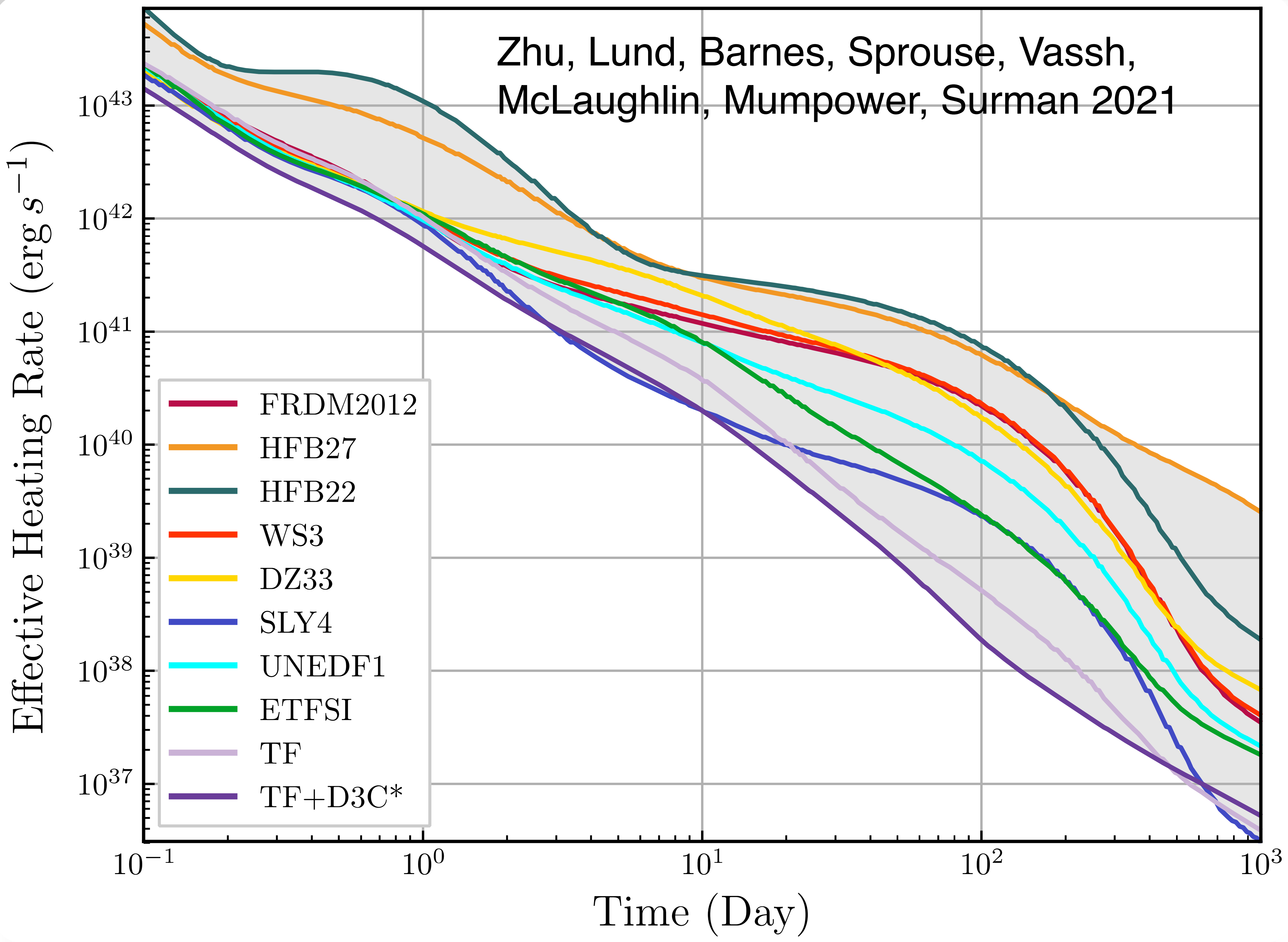


Mumpower, Surman, McLaughlin, Aprahamian 2016



Côté, Fryer, Belczynski, Korobkin, Chruślińska, Vassh, Mumpower, Lippuner, Sprouse, Surman, Wollaeger 2018

This translates into large uncertainties in predictions of r-process observables



ENAF WILL …

- … compute models of world-class physical fidelity for Neutron Star Mergers and the subsequent kilonovae, taking advantage of advances in HPC.
- … build world-class implementations of the neutrino flavor oscillations.
- … investigate the r-process predictions of these merger and kilonova simulations, taking advantage of nuclear data provided by FRIB.
- … quantify the nuclear and astrophysical uncertainties in our nucleosynthesis predictions.
- … compute observable signatures of these models in photons, neutrinos and gravitational waves.
- … continue to exploit advances made by our computational science colleagues to improve the speed and fidelity of our simulations.
- … request astronomical amounts of **supercomputer time**.