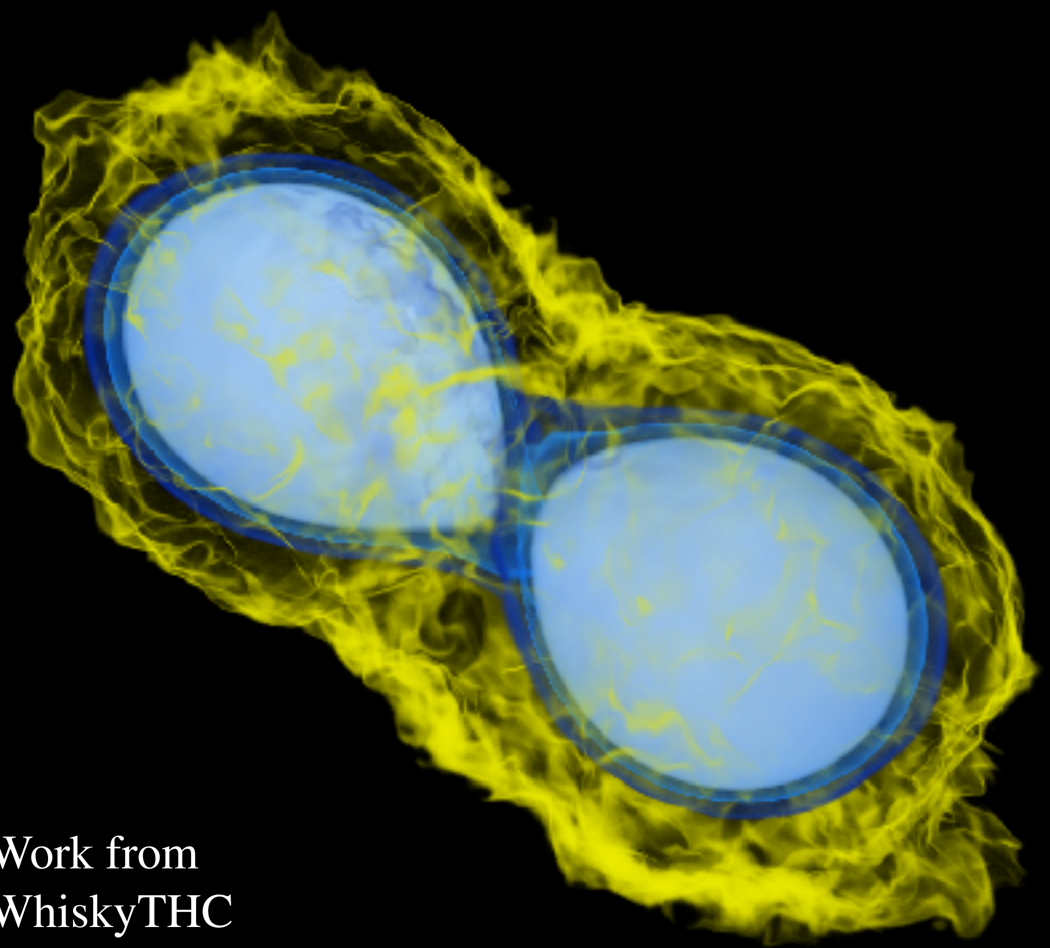
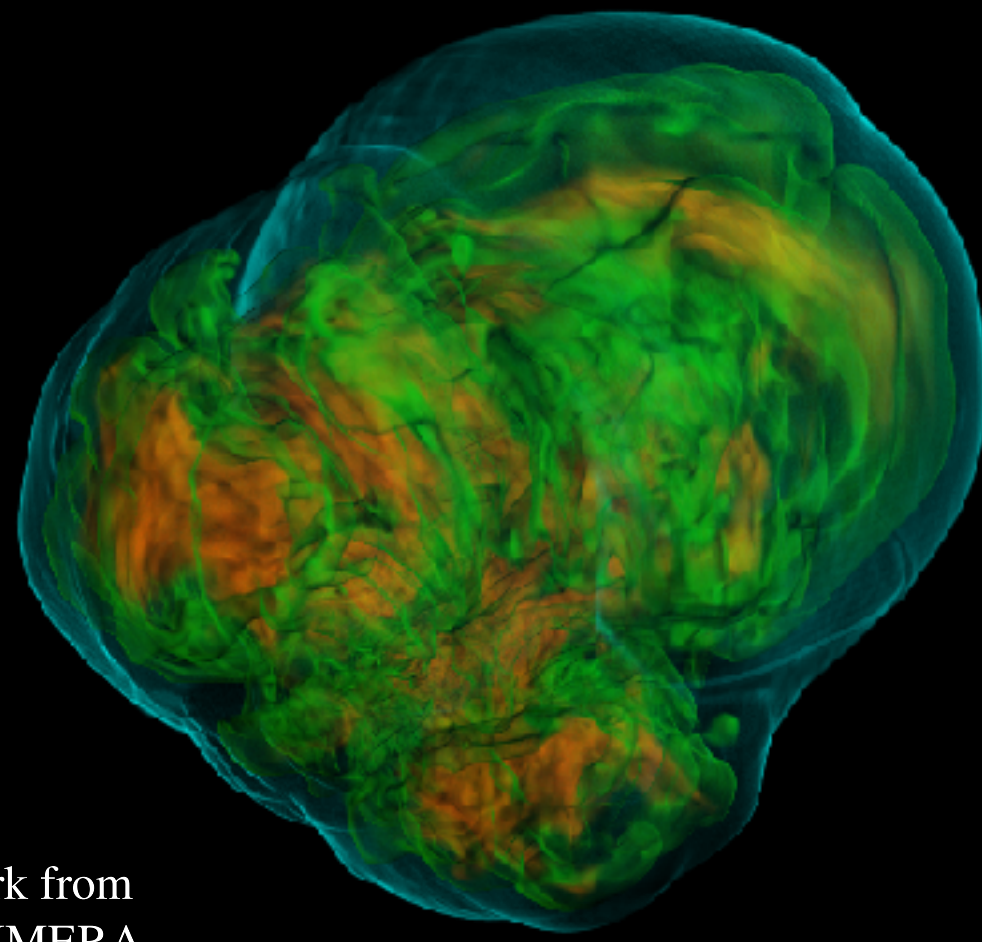
Towards Exascale Astrophysics for



Work from WhiskyTHC



Work from CHIMERA

Mergers and Supernovae

William Raphael Hix (ORNL/U. Tennessee)

for the SciDAC-4 TEAMS collaboration

U.S. Department of Energy Office of Science

TEAMS TEAM

Argonne National Laboratory

Saurabh Chawdhary, Anshu Dubey

Los Alamos National Laboratory

Jonah Miller, Chris Fryer, Josh Dolence, Wes Even

Oak Ridge National Laboratory

Leah Huk, Raph Hix, Bronson Messer

Stony Brook University

Alice Harpole, Mike Zingale, Alan Calder

University of California, Berkeley

David Khatami, Dan Kasen

University of Notre Dame

Trevor Sprouse, Rebecca Surman

Lawrence Berkeley National Laboratory

Doreen Fan, Andy Nonaka, Ann Almgren

Michigan State University

Chelsea Harris, Sean Couch, Luke Roberts

Princeton University

Hiroki Nagakura, Adam Burrows David Radice, *Viktoriya Morozova*

University of Tennessee

Xingfu Du, Andrew Steiner, Tony Mezzacappa

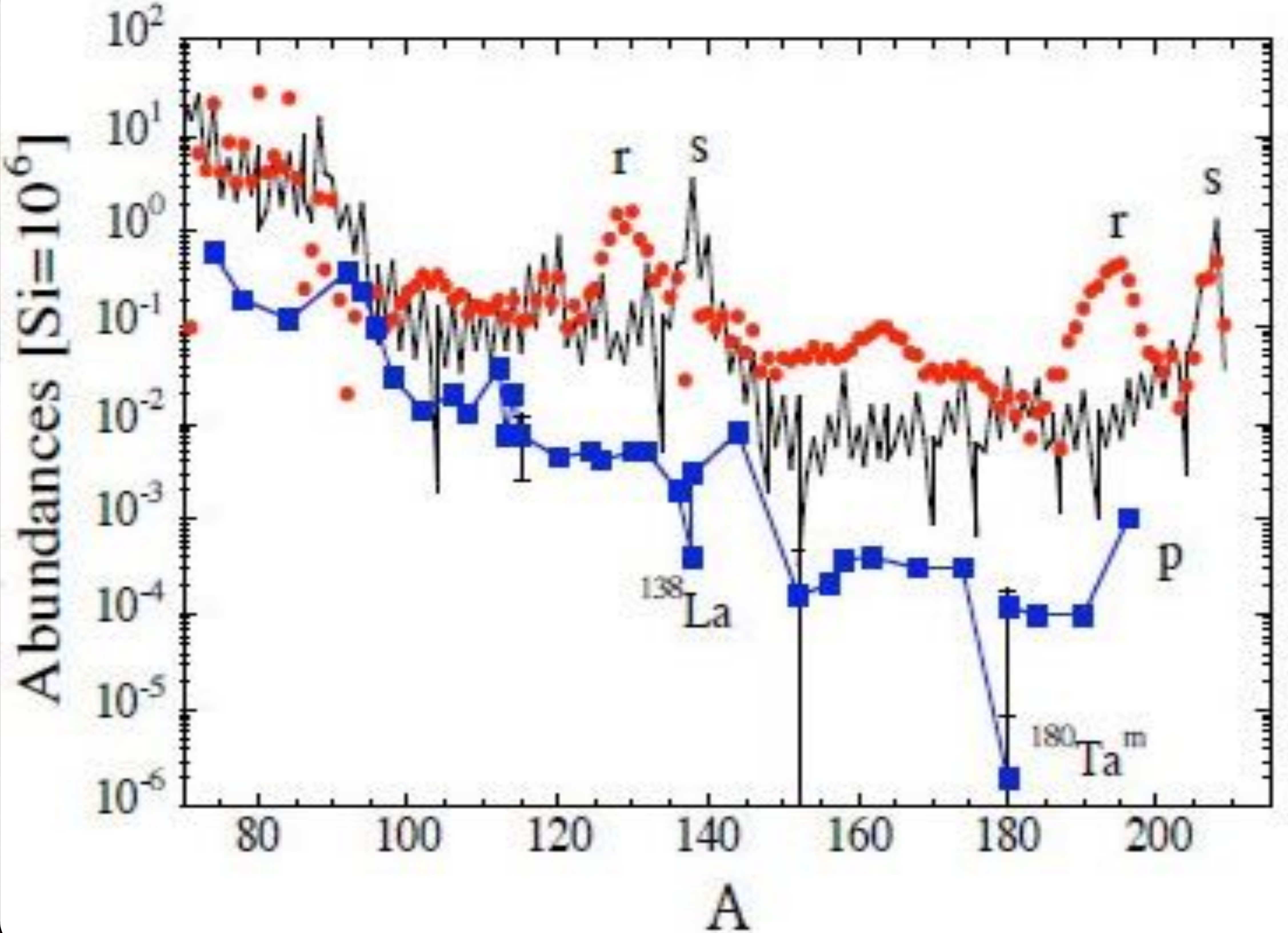
University of California, San Diego

Lucas Johns, George Fuller

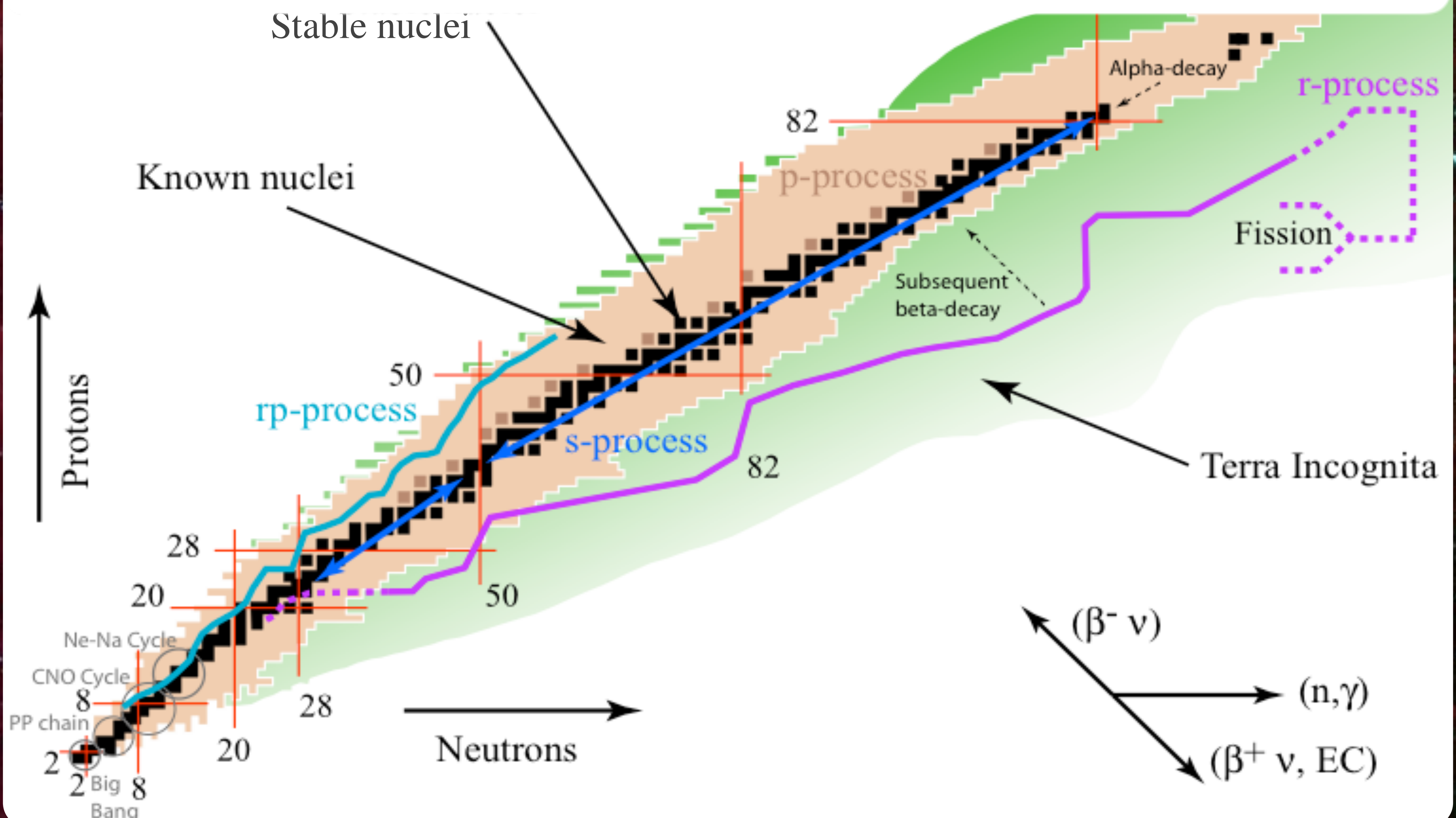
University of Washington

Bryce Fore, Sanjay Reddy

R-PROCESS & P-PROCESS



Processes and Sites

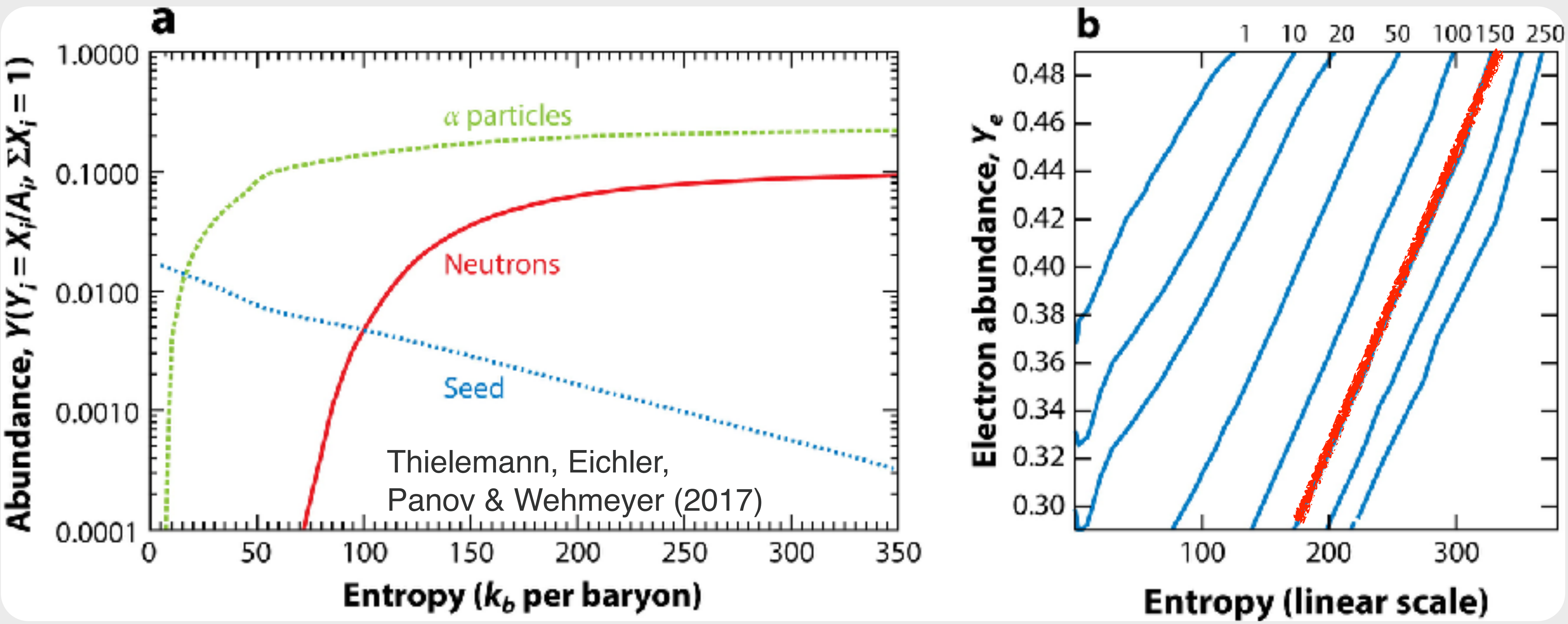


Understanding our nuclear origins means understanding processes that transmute nuclei and the sites where these processes occur.

Recipe for the R-process

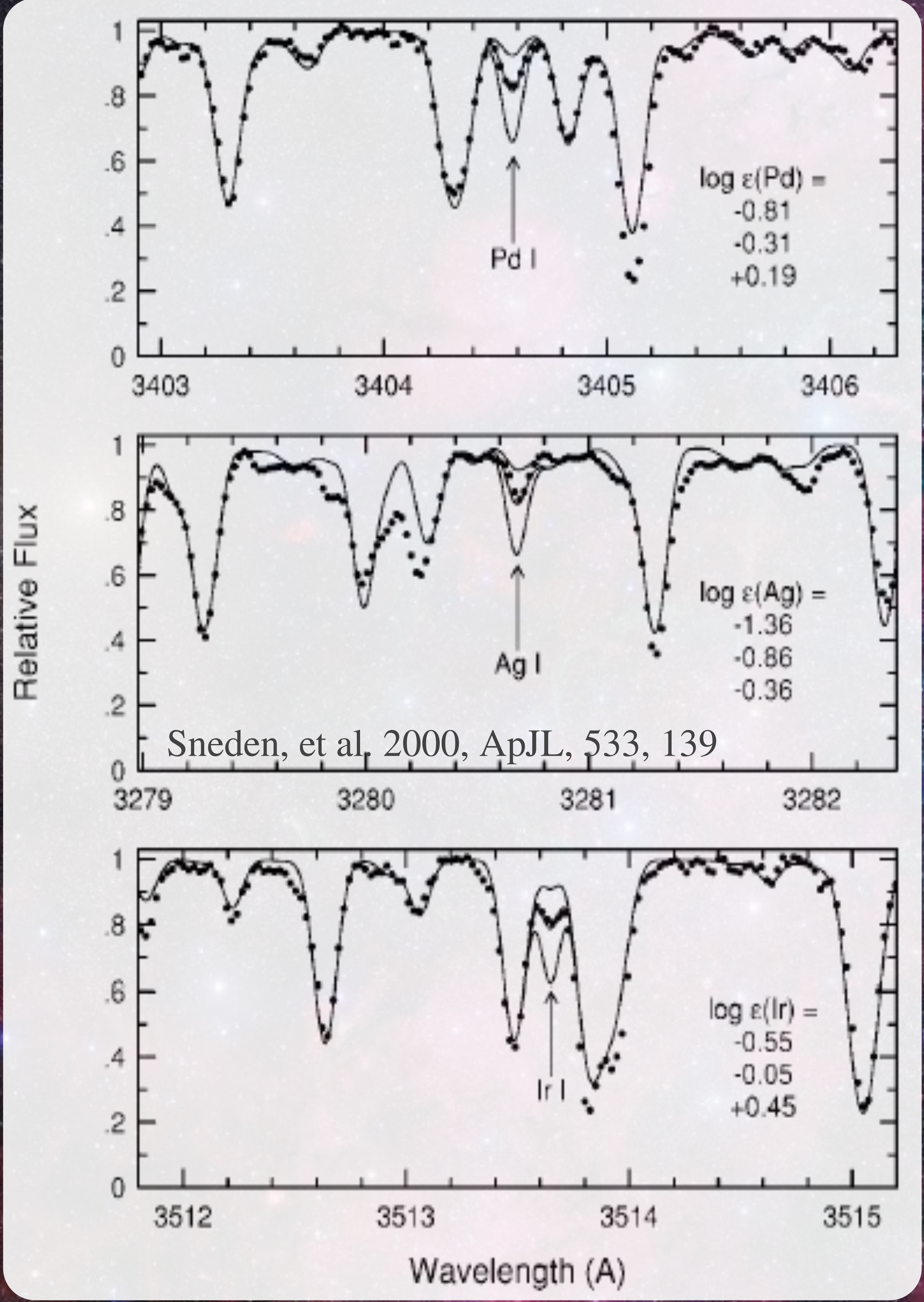
Making the heaviest nuclei via rapid neutron capture requires roughly 150 free neutrons for each *seed* heavy nucleus (typically A > 60).

Because ^{4}He is immune to neutron captures, its presence, even in large quantities, does not diminish the neutron/seed ratio.

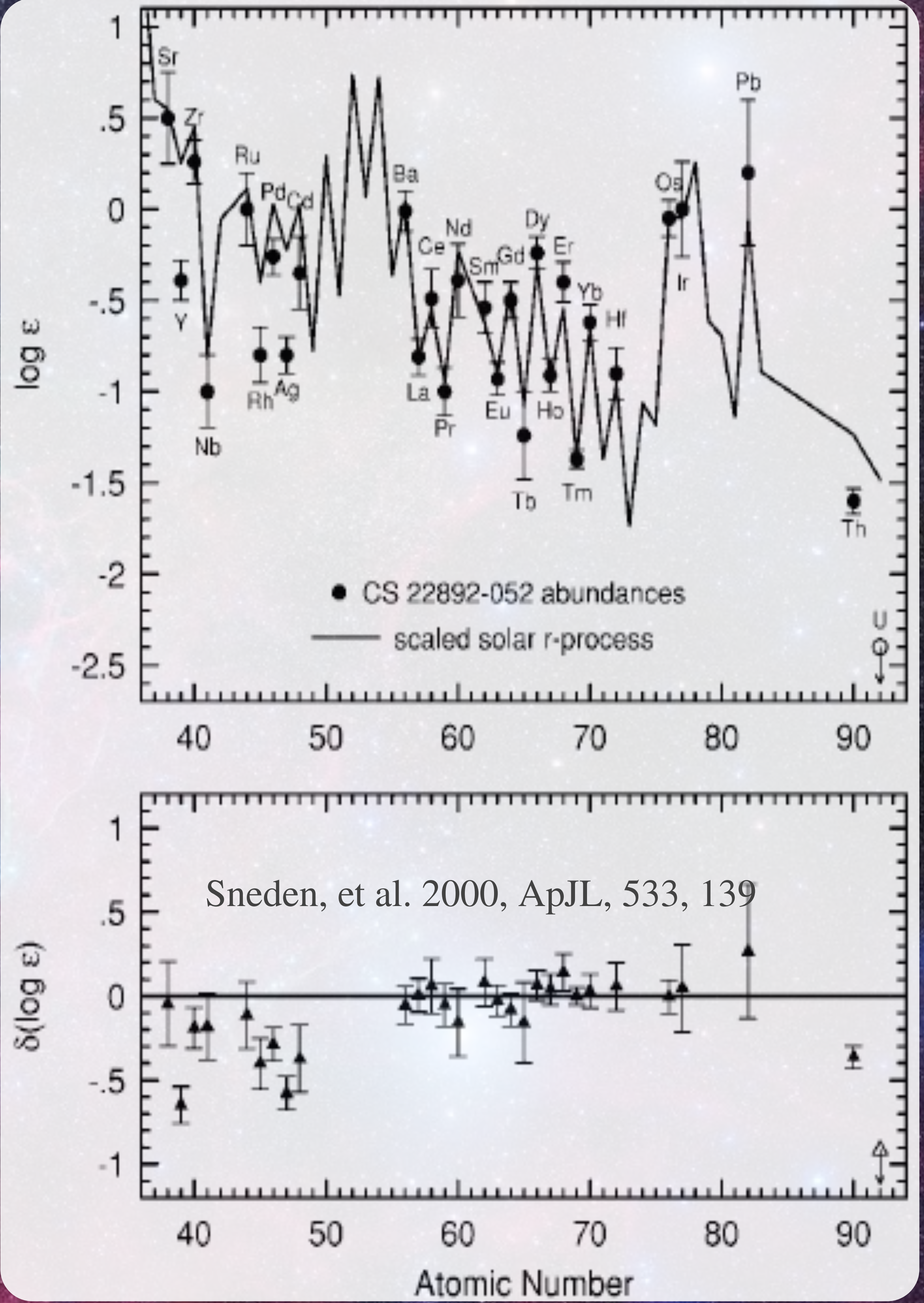


Thus, a similar neutron/seed ratio can be achieved in less neutron-rich conditions by increasing the entropy or otherwise increasing ^{4}He.

r-process Elements in old stars



Sneden, et al. 2000, ApJL, 533, 139



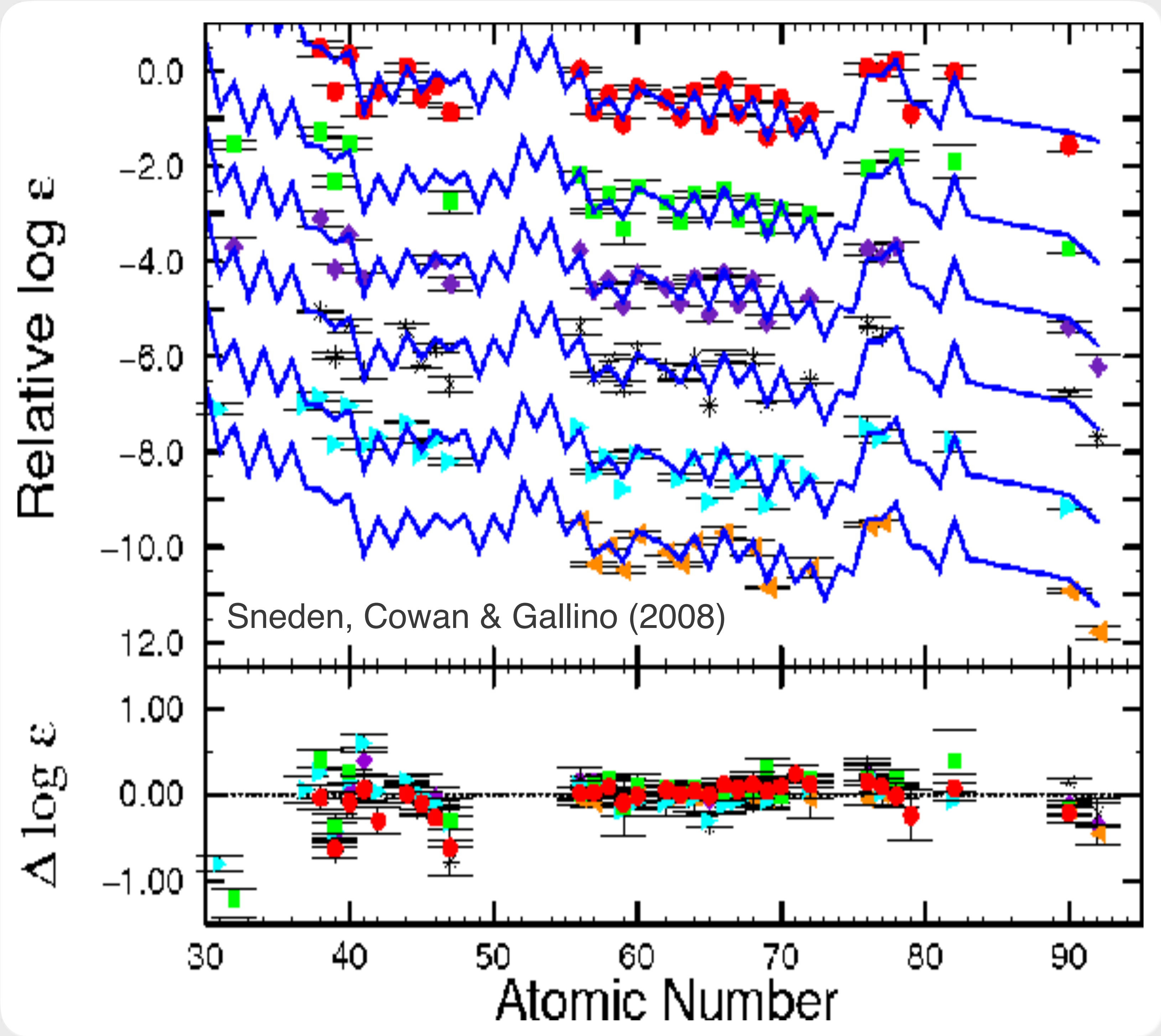
Sneden, et al. 2000, ApJL, 533, 139

Universal R-process?

This similarity between the r-process abundances in the Sun and in some of the Galaxy's oldest stars was not an isolated example.

For Z > 55, the R-process abundances are very similar, whether they come from a single event, like the low metallicity stars, or are the sum of many events over billions of years.

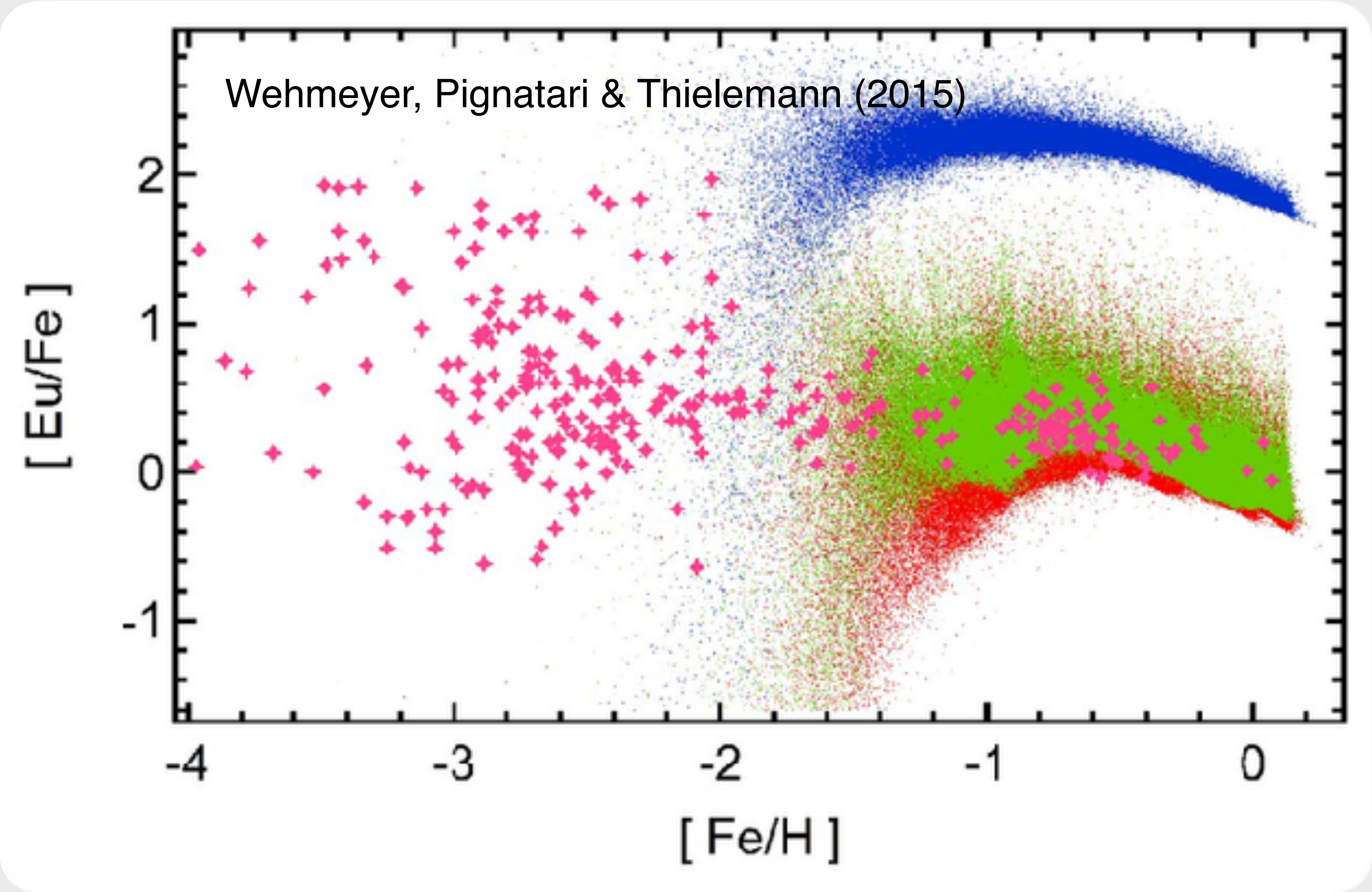
This universality does not seem to apply for Z < 50.



Earliest R-process

With multiple potential r-process sources, there is the possibility that the principle source at the present epoch was not the principle source in the early Galaxy.

This is a particular issue for neutron star mergers, since they necessarily trail the CCSN that marked the birth of those neutron stars.

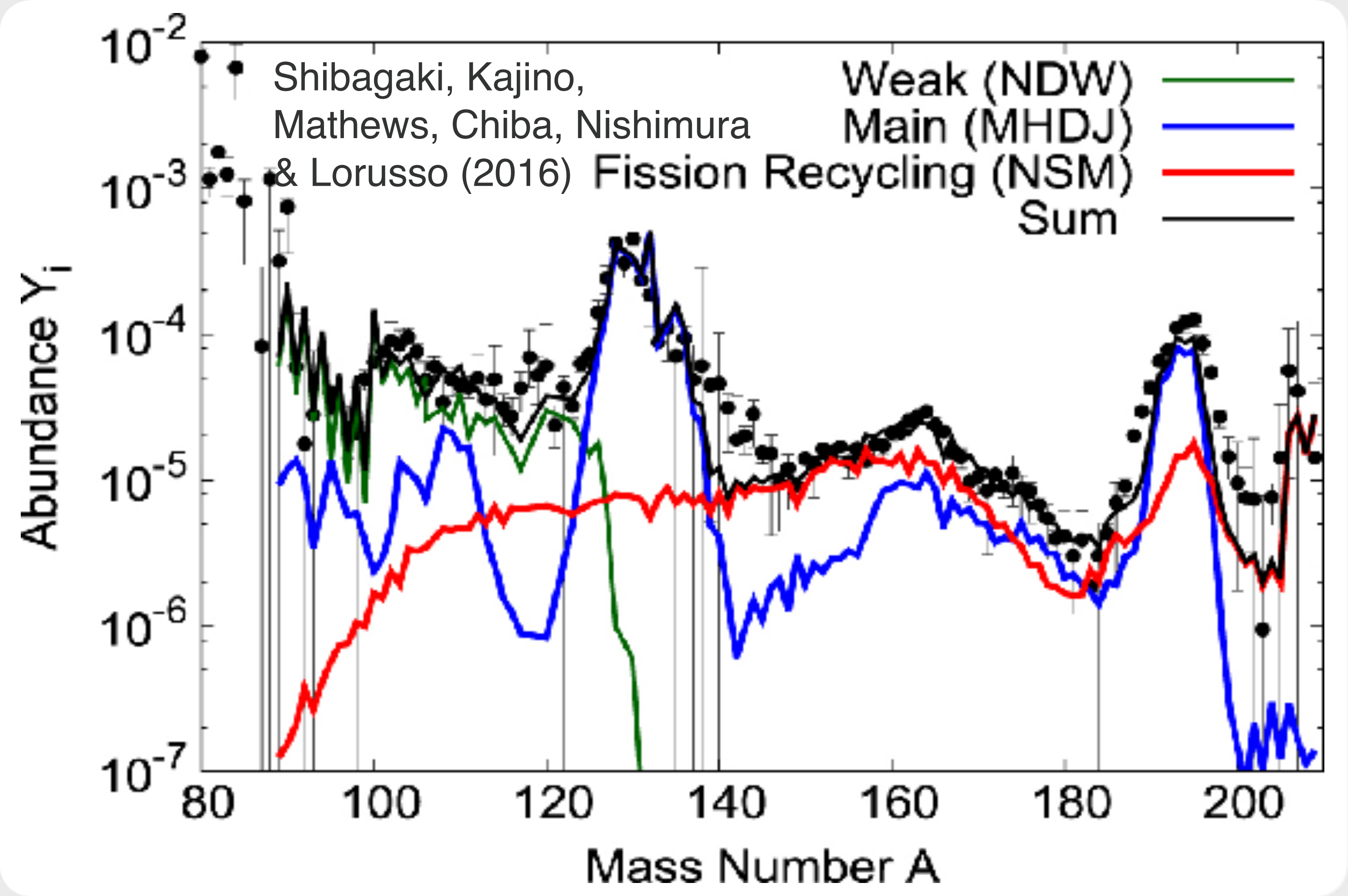


Since there are examples among the oldest stars in the Galaxy with significant r-process abundances, at least one r-process site must be operating very early in the history of the Galaxy.

Multiple sites?

The variability of the weak r-process (Z < 50) in contrast to the universality of the main r-process (Z > 55) suggests to many that more than one r-process site is needed to explain the observations.

With ordinary supernovae struggling to maintain sufficient neutron-richness, because of neutrino interactions, they are generally ruled out for the main r-process.



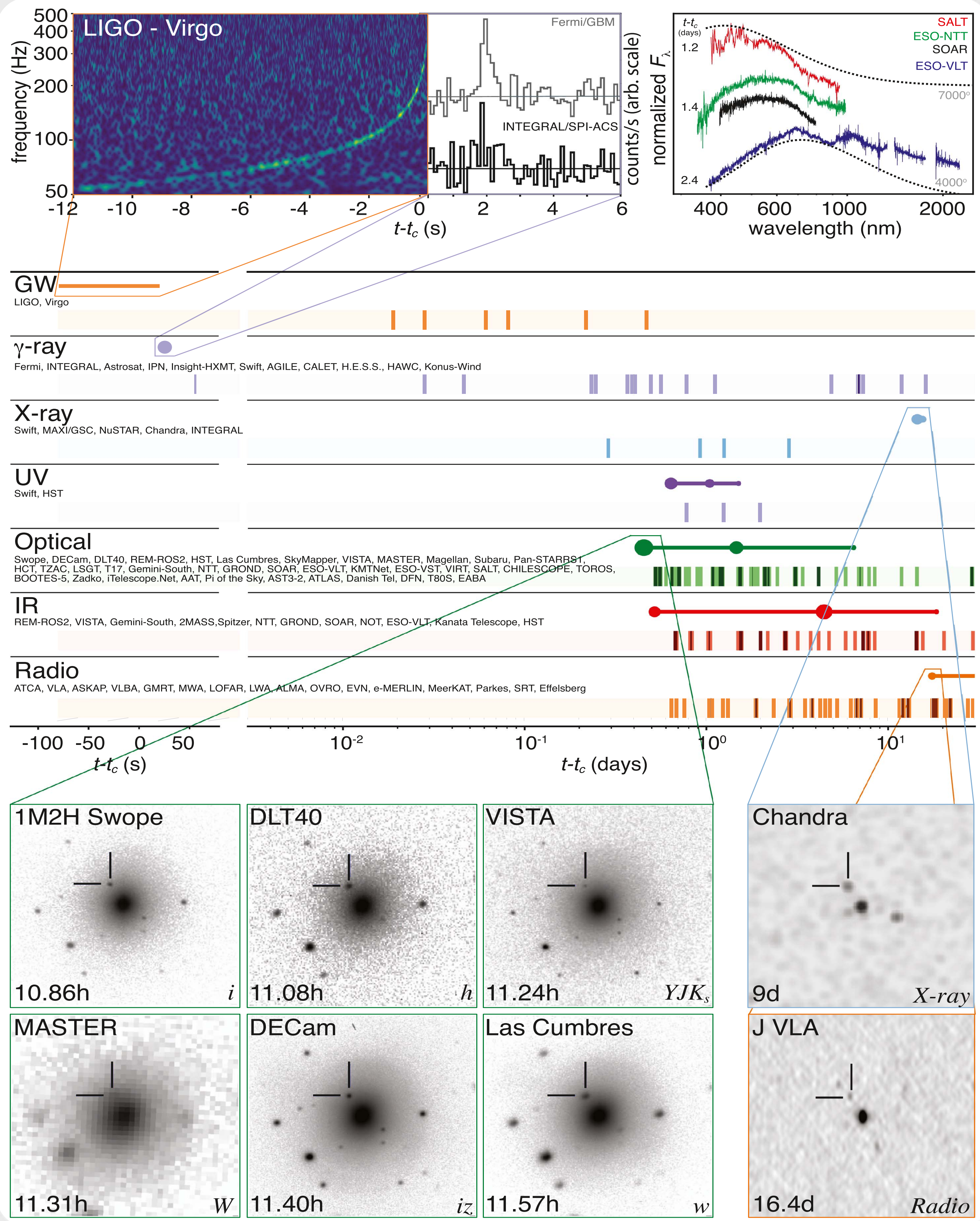
This generally leaves exotic supernovae and neutron star mergers (or both) as the site of the main r-process.

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.



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: MAESTROeX (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.

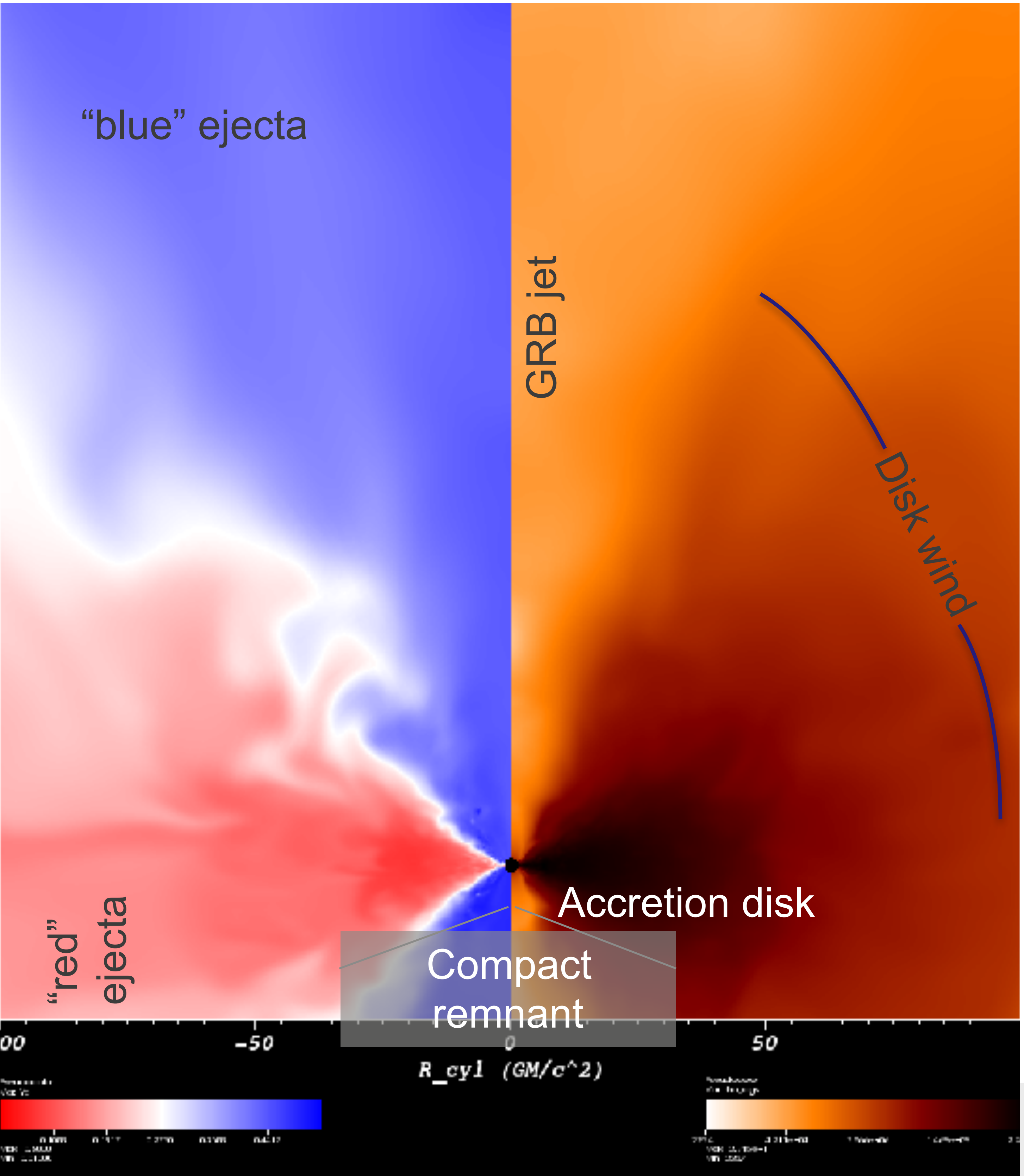
Nuclear Equation of State for Supernovae and Neutron Stars:
Steiner (UTK)

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).

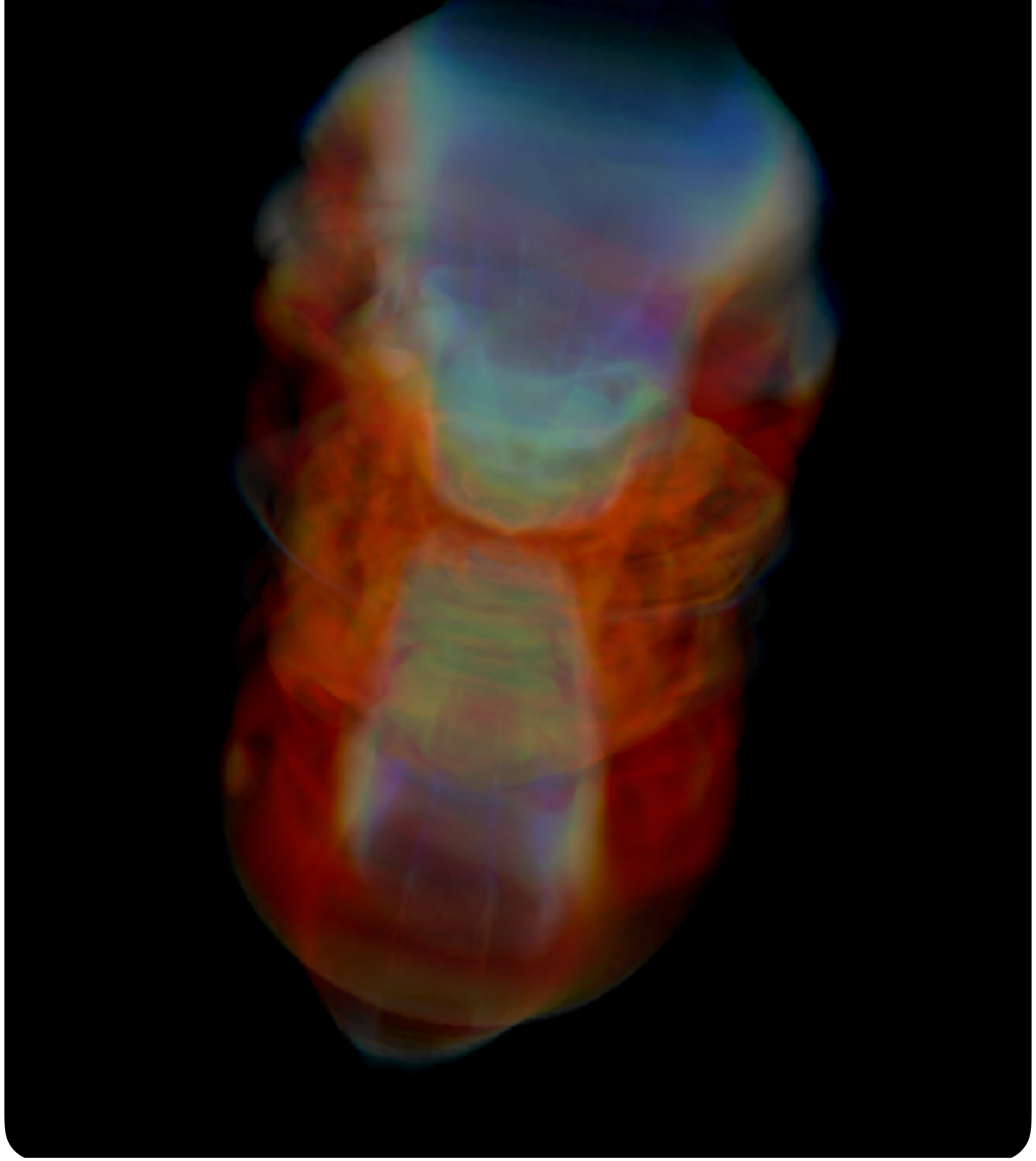
THE AFTERMATH OF GW170817

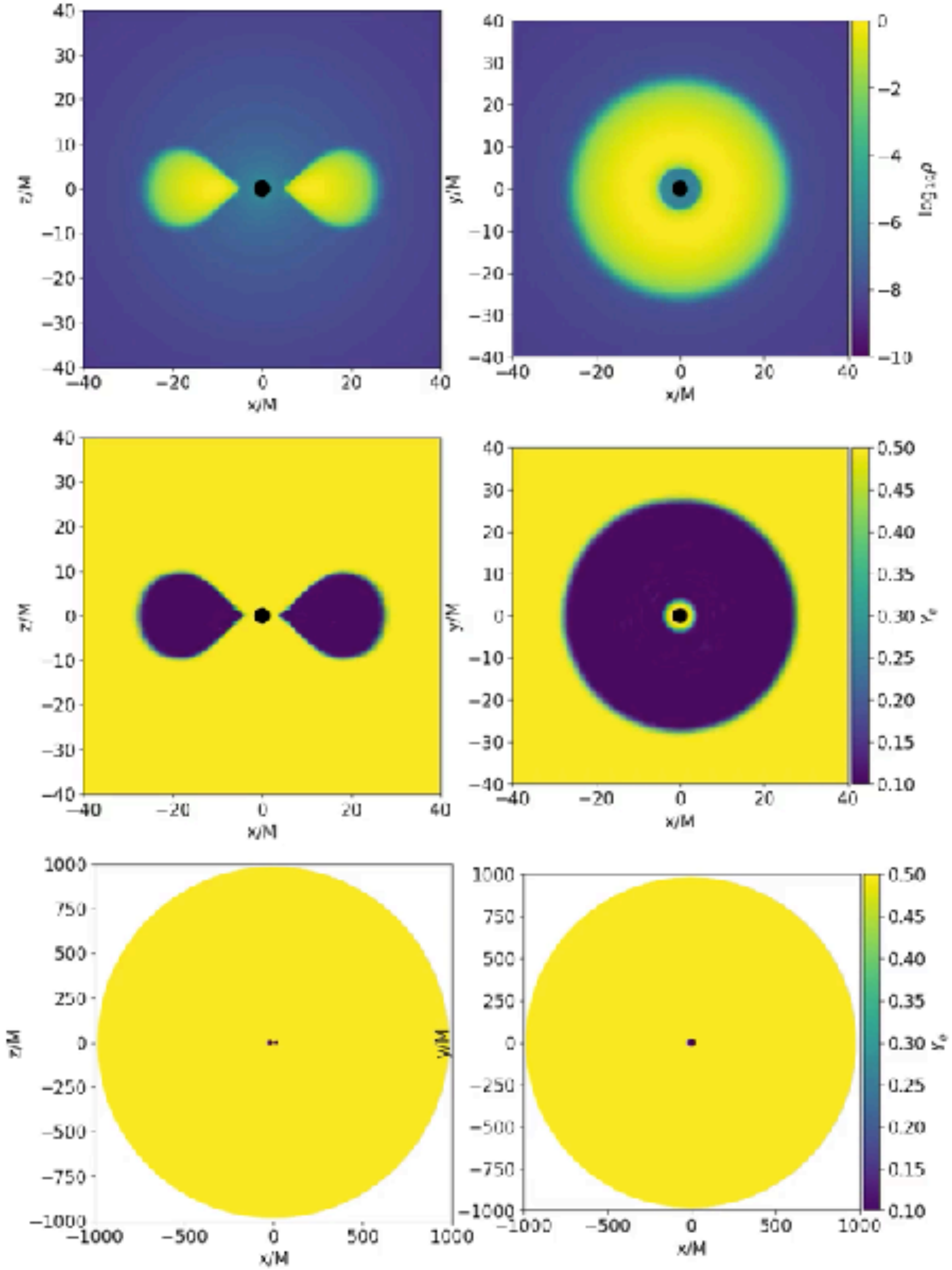


- Both dynamical and light curve modeling suggest merger events produce multiple components of outflow with different masses, velocities, and compositions
- Necessary physics:
  - General relativity
  - Magnetohydrodynamics
  - "Realistic" EOS
  - Neutrino transfer with appropriate weak interactions
  - Nuclear reactions to determine nucleosynthesis in ejecta
  - Photon radiation transport to compute light curves and spectra

Full 3D neutrino radiation MHD disk modeling

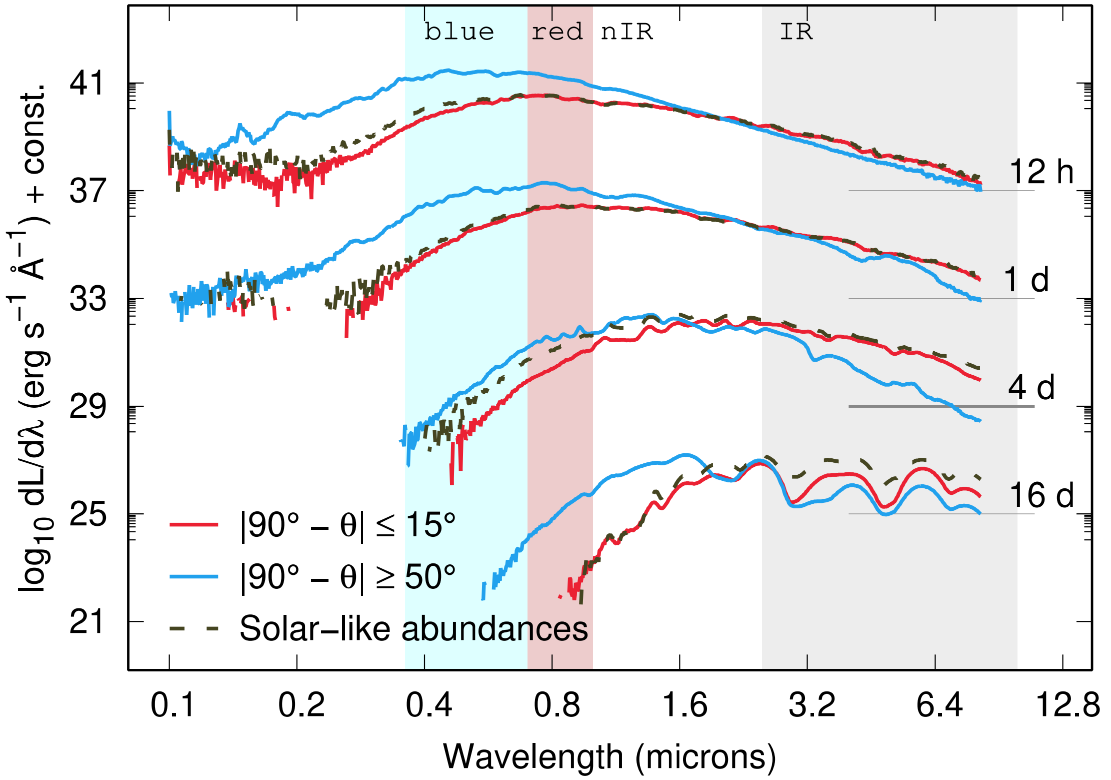
is now possible

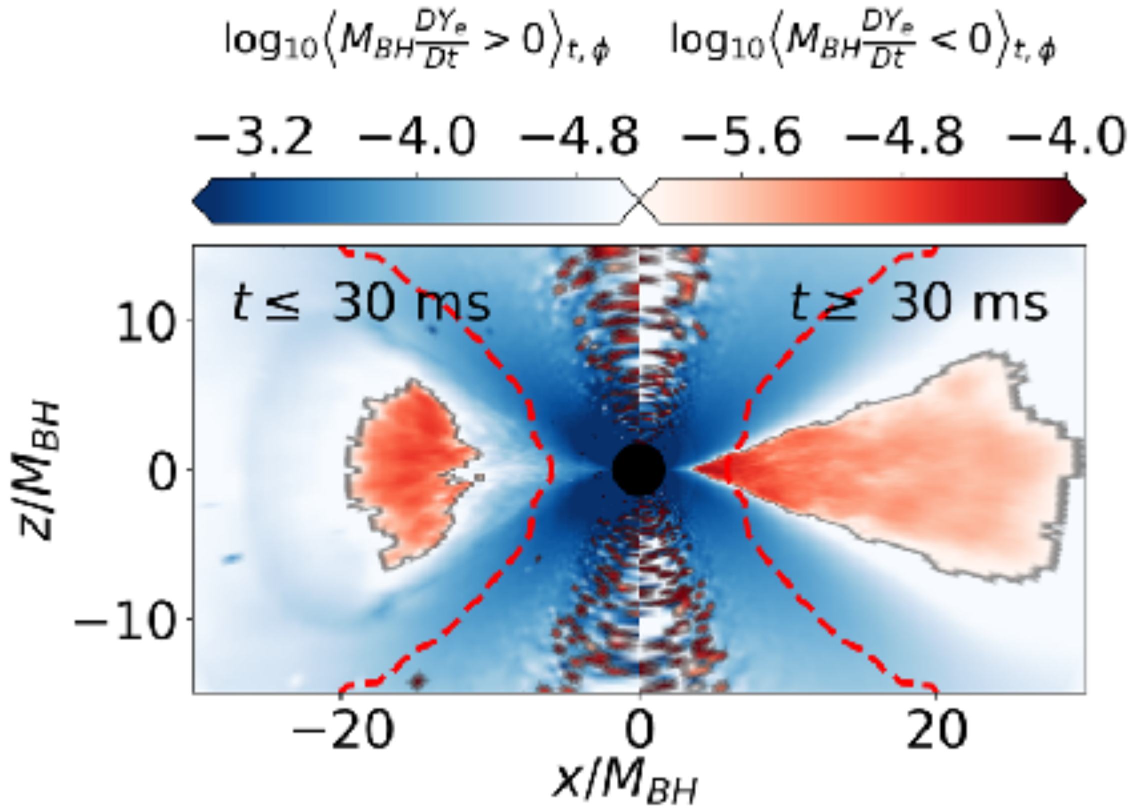




Full Transport Model of GW170817-Like Disk Produces a Blue Kilonova

- Simulation using newly developed νbhlight code (Miller, Ryan, Dolence, ApJS, 2019)
  - Ideal GRMHD
  - Full general-relativistic Monte Carlo transport
  - Full suite of microphysics including neutrinos and nuclear EOS
- Simulation tied to full nucleosynthesis and photon transport pipeline; from first principals to observables
- Major conclusions
  - Blue kilonova emerges naturally; does not require tuning, a long-lived neutron star, or unreasonable initial conditions
  - BH-NS mergers may also produce a blue kilonova
  - The fidelity of the neutrino treatment matters





(See poster by Miller)

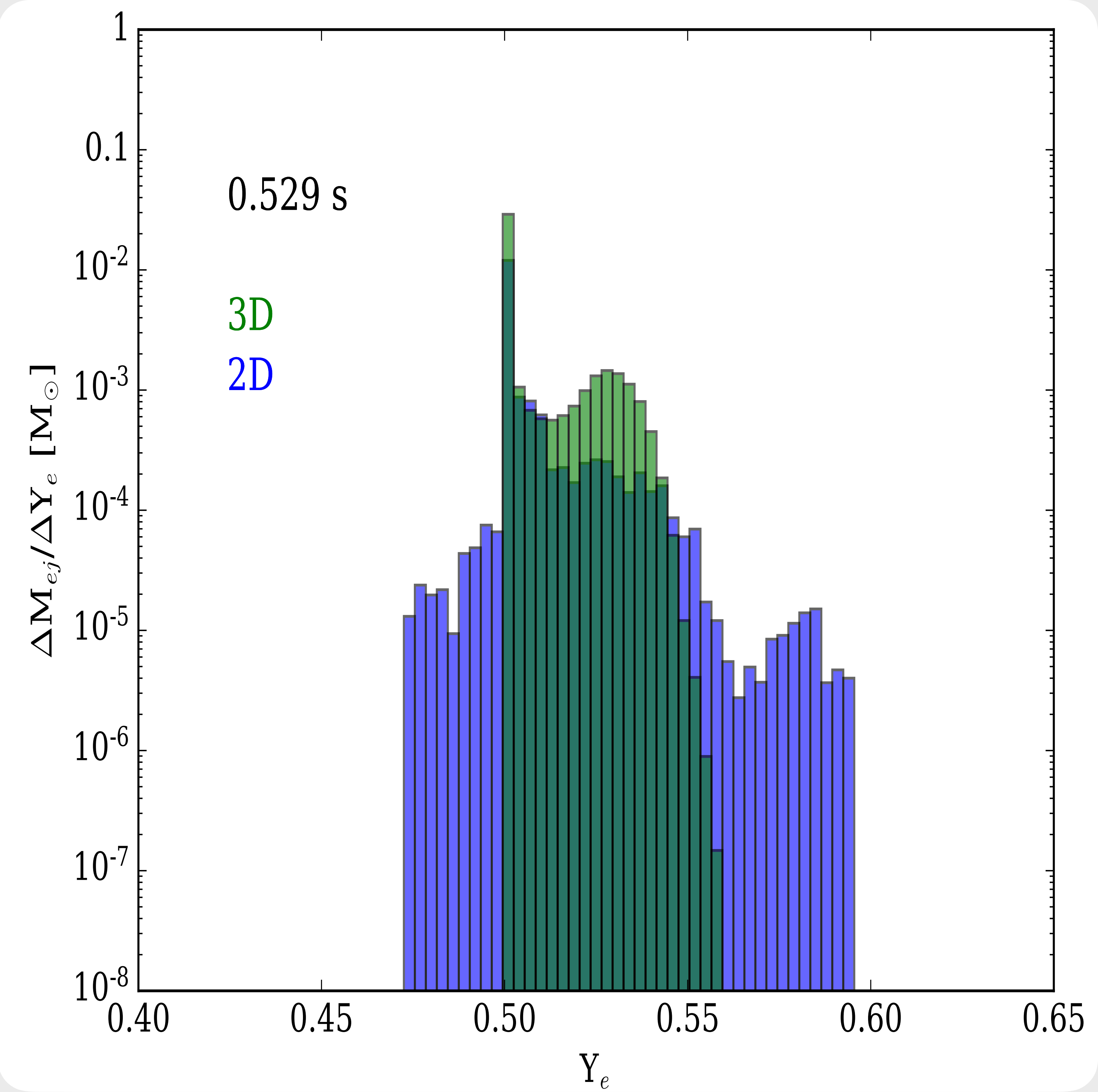
Miller, Ryan, Dolence+19

Fornax Supernova Models

Fornax is the supernova modeling code under development at Princeton. It includes multi-group neutrino transport employing the M1 two-moment closure scheme with approximate GR.

Under SciDAC-4, FORNAX has been used to model a number of developing supernovae in 3D, running as much as ¾ second after bounce with maximum shock radius reaching 5000 km.

Proton-rich ejecta is evident, suggesting a potential contribution to the p-process, though the development of the PNS wind is likely several seconds in the future.



t = 0.010 s

Fornax Simulation

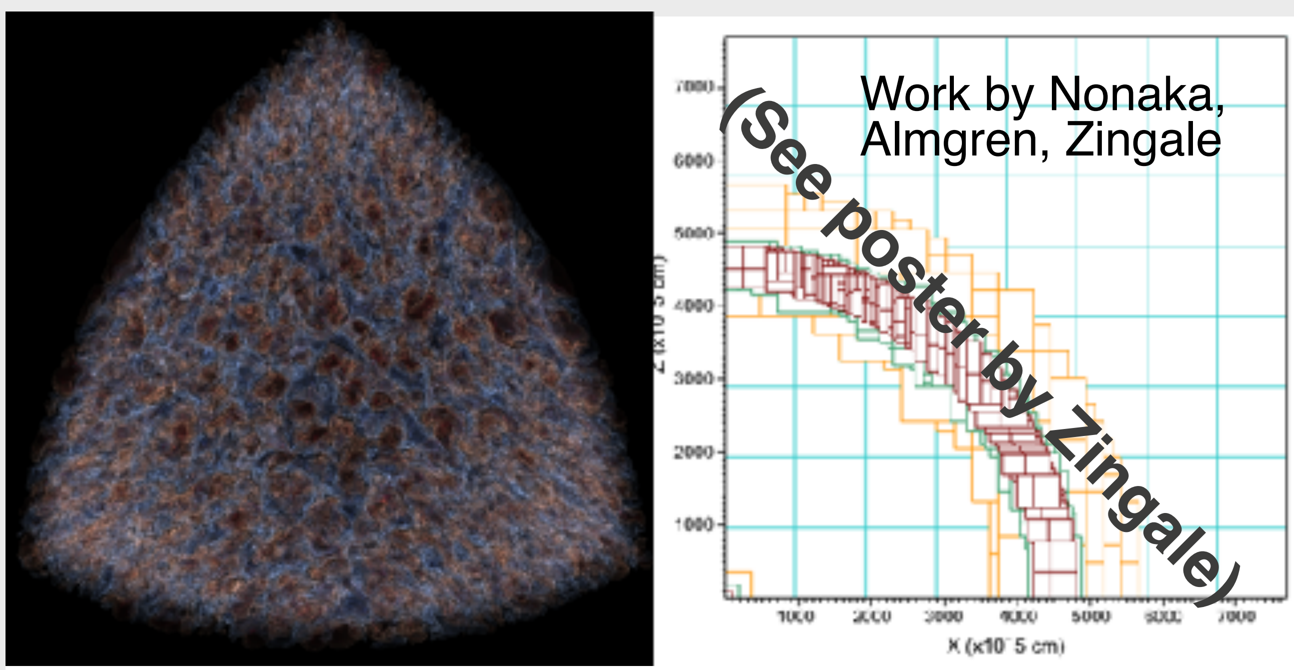
Entropy; 25 $M_\odot$ Progenitor

Low Mach Number Methods for Astrophysical Phenomena

Many astrophysical phenomena are characterized by subsonic flow in a stratified atmosphere. By combining low Mach number modeling techniques with adaptive mesh refinement (AMR), researchers can efficiently integrate long-time dynamics that are too expensive for compressible solvers.

The existing MAESTRO code was migrated to use the exascale-ready software framework AMReX, forming MAESTROeX, in order to enable detailed high-resolution simulations on high-performance architectures.

With the AMReX software framework, researchers are now able to study low Mach number, stratified astrophysical phenomena using state-of-the art linear solvers, grid hierarchy management, load balancing and intra-node optimization. AMReX uses a hybrid approach to parallelism.



(Left) Convective plumes driven by nuclear burning in a helium layer on the surface of a sub-Chandra white dwarf. (Right) AMR focuses computational resources in regions of interest.

Current algorithmic developments including improved hydrostatic mapping, rotating stars, and efficient coupling to a compressible code framework for post-ignition studies.

Transpilation -

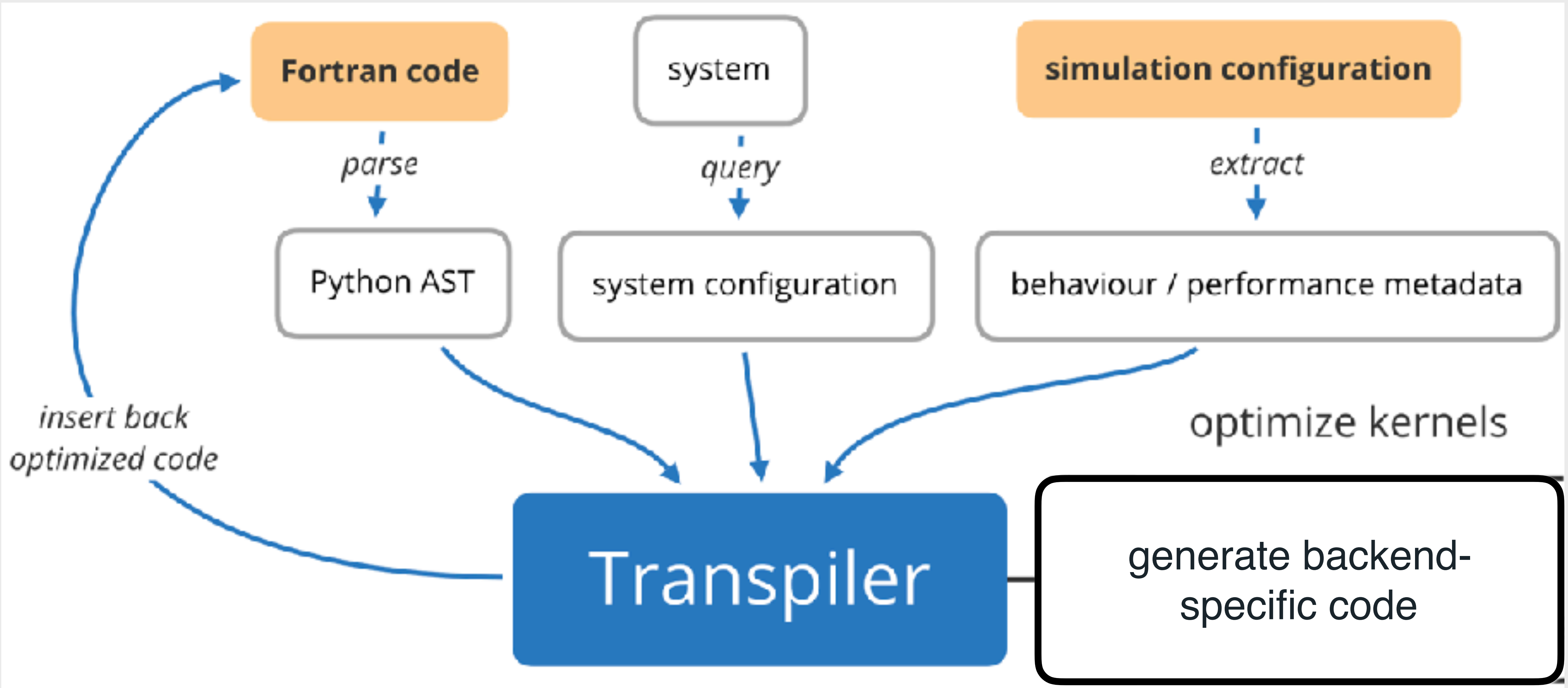
Code Transformation for Performance Portability

- **Compilation**:
  combining information from many sources into single entity
- **Translation**:
  converting information from one language to another
- Translation + Compilation:
  Transpilation

- AST of CPython
  - accessible, modifiable and synthesizable at runtime
- High-level syntactic structures
- Python originally designed for dynamic typing
  - No type information
- Recently: type hints

- At FLASH end
  - Convert code to fine-grained kernels – better exposure for optimization possibilities
  - Code still in Fortran
- Transpiler inlines functions – avoid overhead of function calls
- Inserts OpenMP, OpenACC pragmas as needed

FLASH transpilation



Transpiler exercised with hydrodynamics only (Sod) and hydrodynamics + thermonuclear kinetics (Cellular)

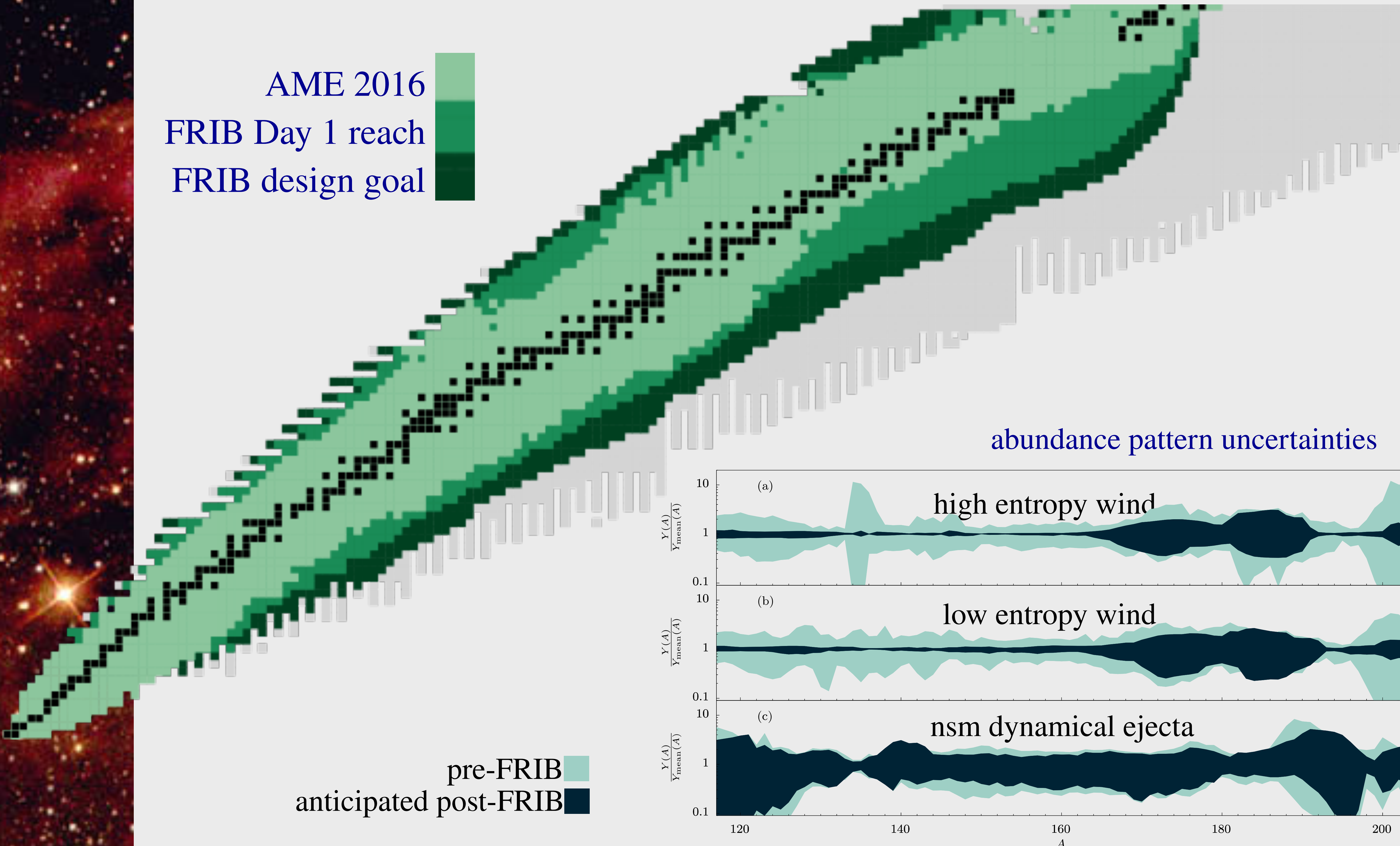
Code generated for CPU and GPU performance is still suboptimal

(See poster by Dubey)

Chawdhary, Dubey, Wahib & Bysiek

Future prospects at FRIB: masses

Sprouse, Navarro Perez, Surman, McLaughlin, Mumpower, Schunk arXiv:1901.10337



Sprouse, Navarro Perez, Surman, McLaughlin, Mumpower, Schunk
arXiv:1901.10337

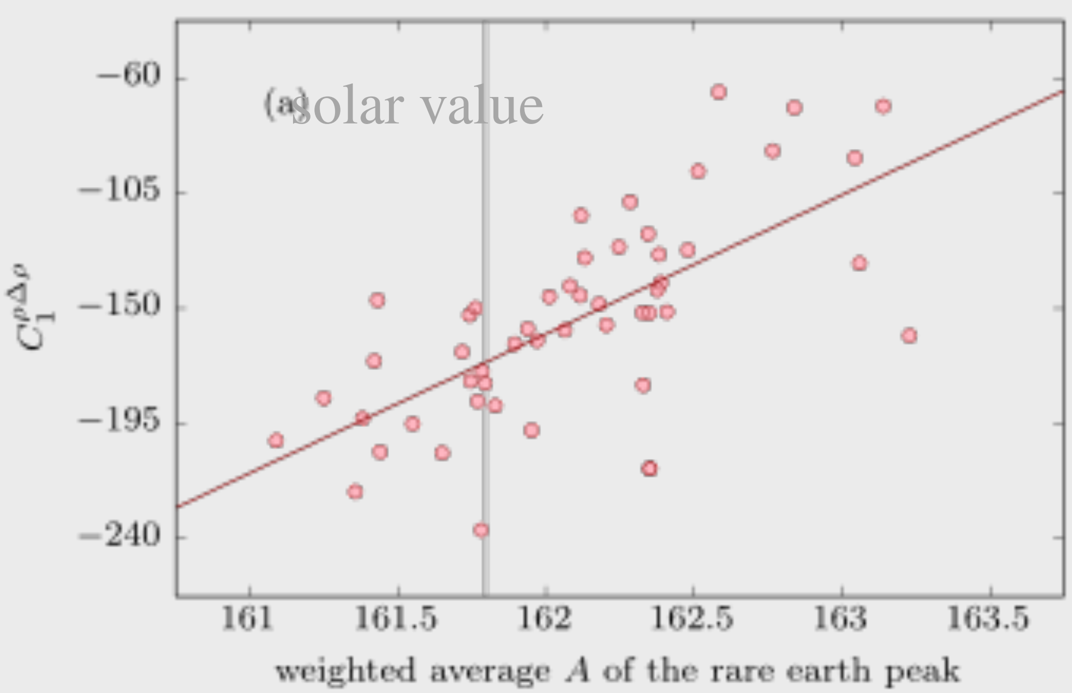
Impact of Nuclear Uncertainties

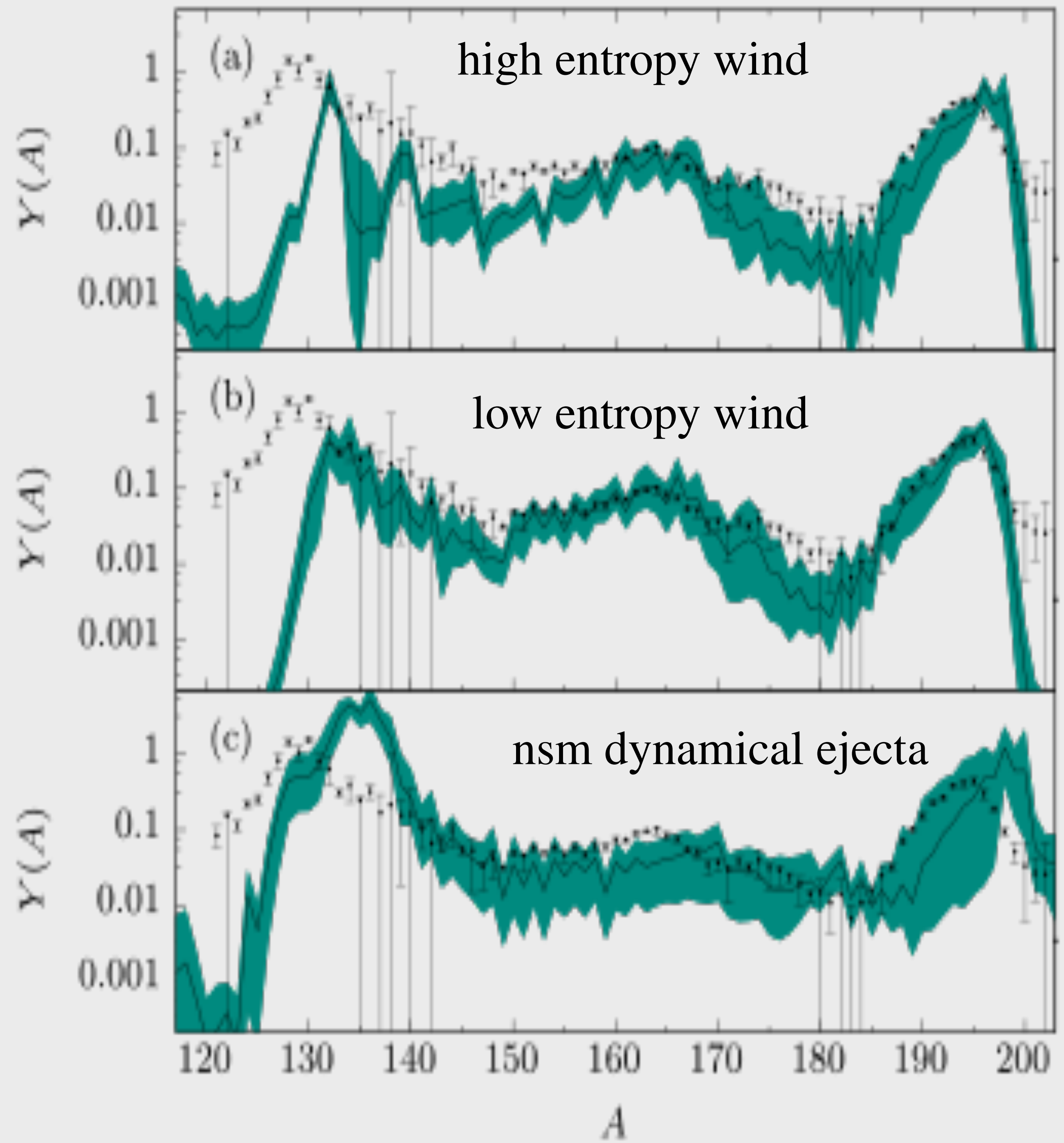
Examined the impact of variations of UNEDF1 functional within model uncertainties on *r*-process nucleosynthesis.

Abundance pattern ranges for 50 sets of masses calculated with UNEDF1 are shown at right.

Potential correlations between UNEDF1 functional parameters and *r*-process abundance pattern features were also examined.

(See poster by Sprouse)





TEAMS WILL …

… compute models of world-class physical fidelity for the majority of potential r-process and p-process sites, including Neutrino-driven Iron and Oxygen-Neon Core Collapse, Magneto-Hydrodynamic-Driven Supernovae, Neutron Star Mergers and Accreting Black Holes, and their progenitors, taking advantage of advances in HPC.

… compute observable signatures of these models in photons, neutrinos and gravitational waves.

… build world-class implementations of the essential nuclear microphysics.

… quantify the nuclear and astrophysical uncertainties in our nucleosynthesis predictions.

… continue to exploit advances made by our computational science colleagues to improve the simulations.

… request astronomical amounts of **supercomputer time**.