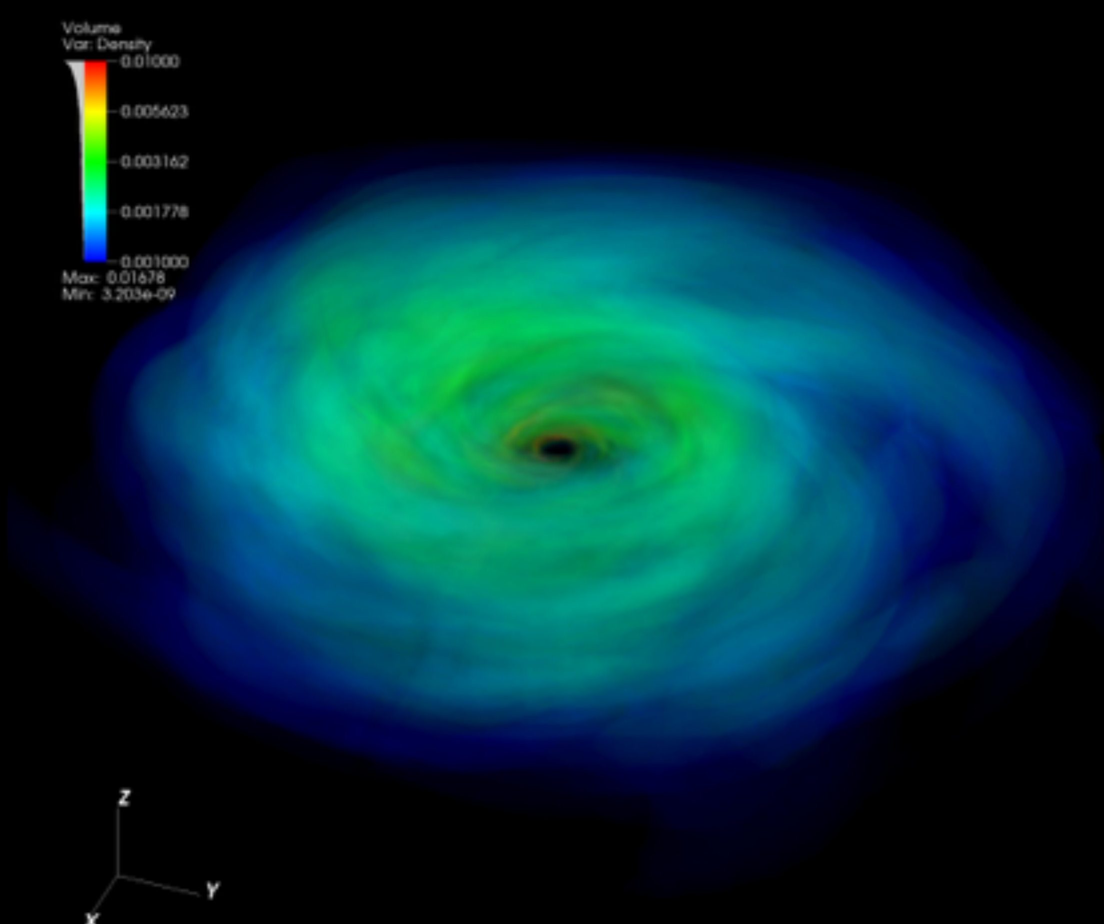
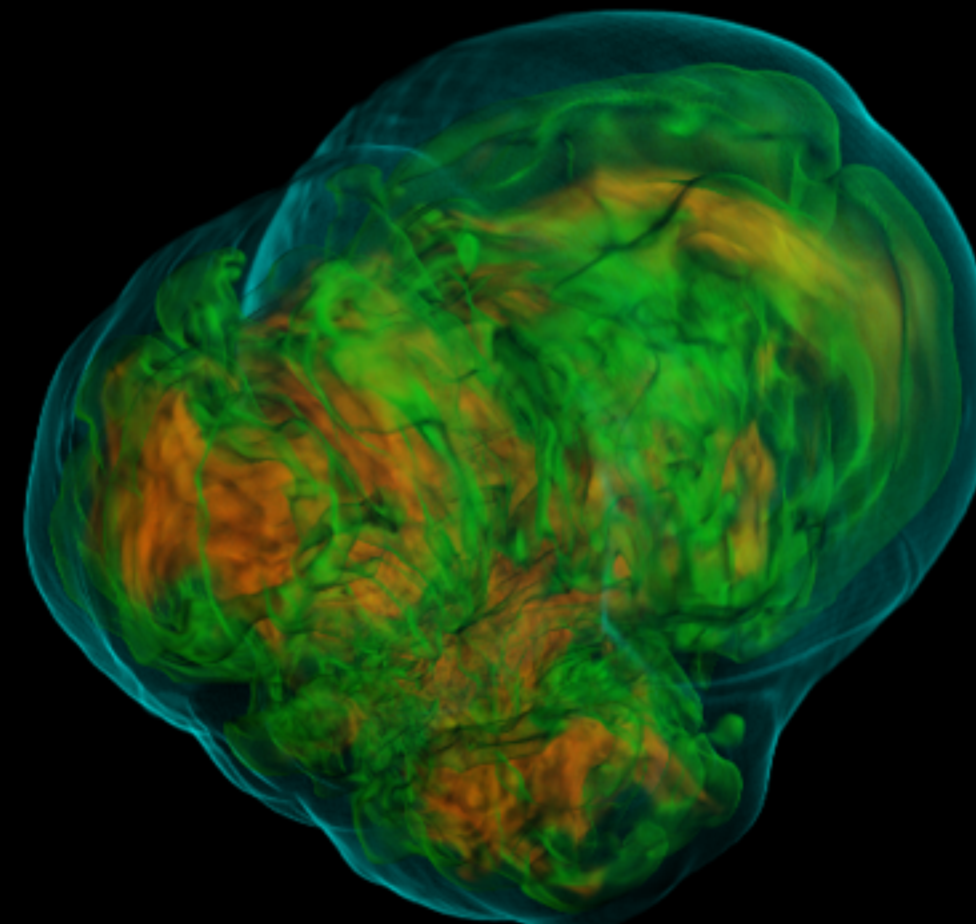
Towards Exascale Astrophysics

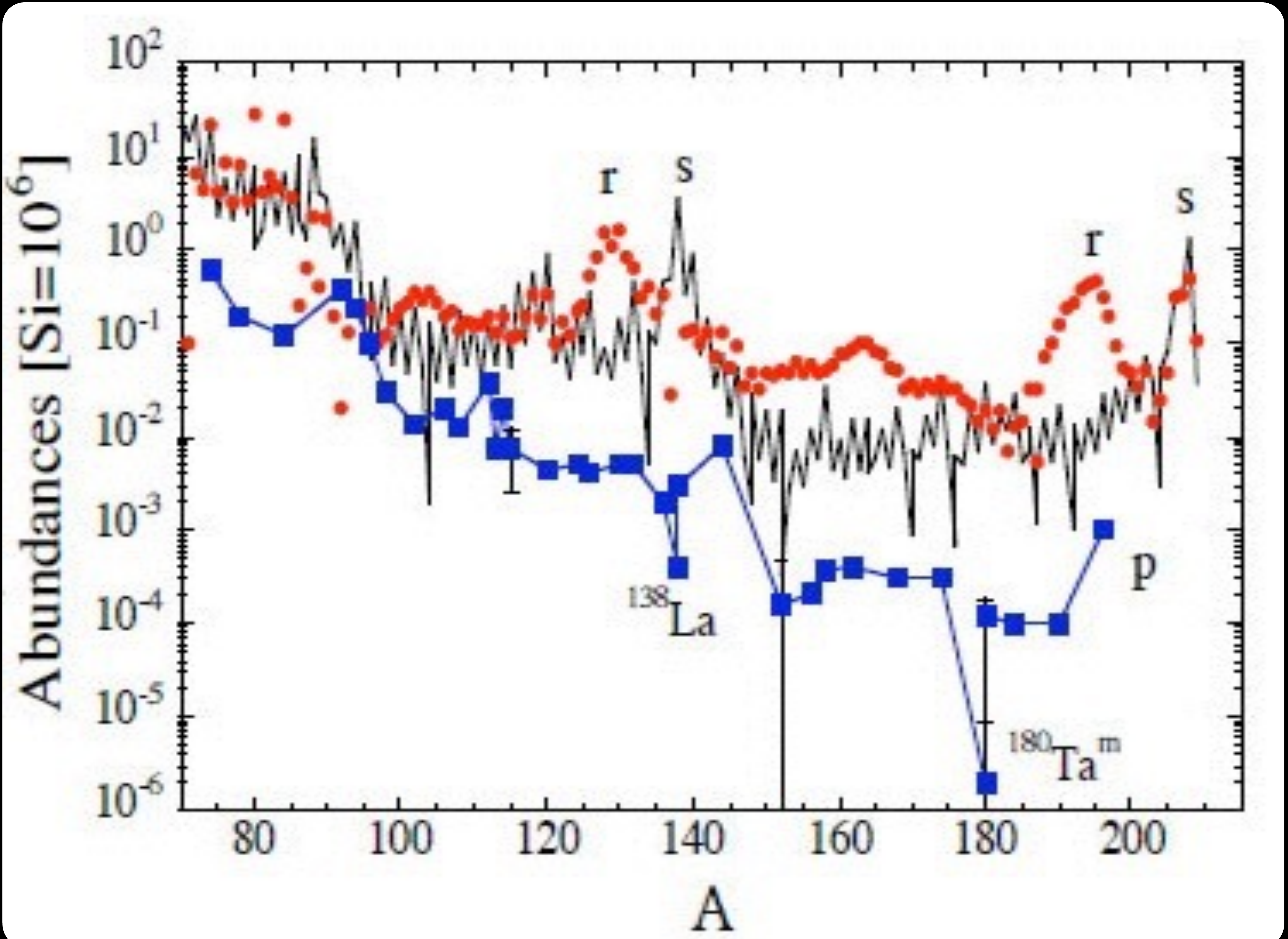




for Mergers and Supernovae

William Raphael Hix (ORNL/U. Tennessee)
for the SciDAC-4 TEAMS collaboration

Our Isotopes



2 Essential Questions of Nuclear Astrophysics

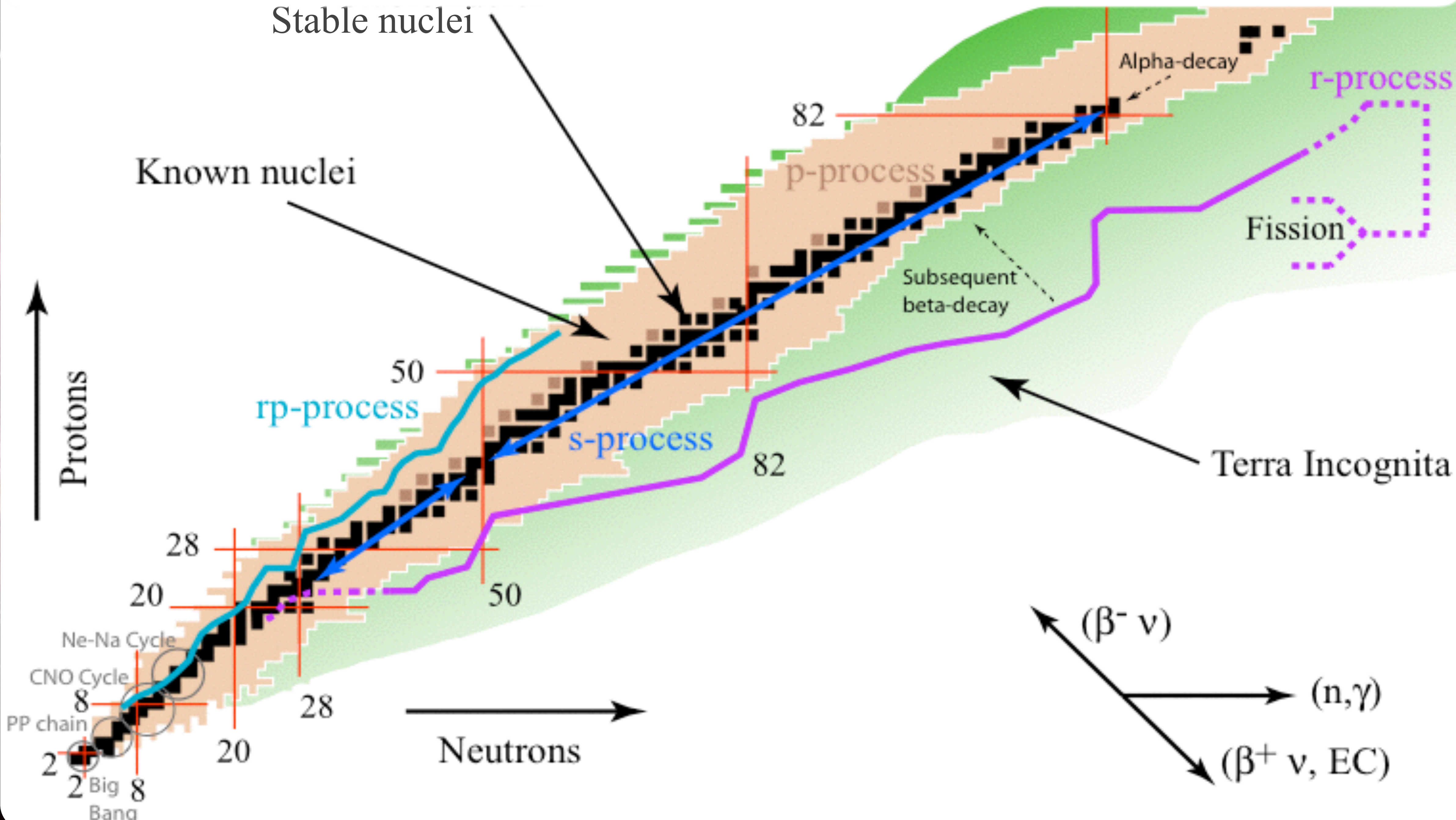
1) How do nuclei get made?

When? Where? Is it an ongoing process?

2) How does making nuclei affect the stellar environment?

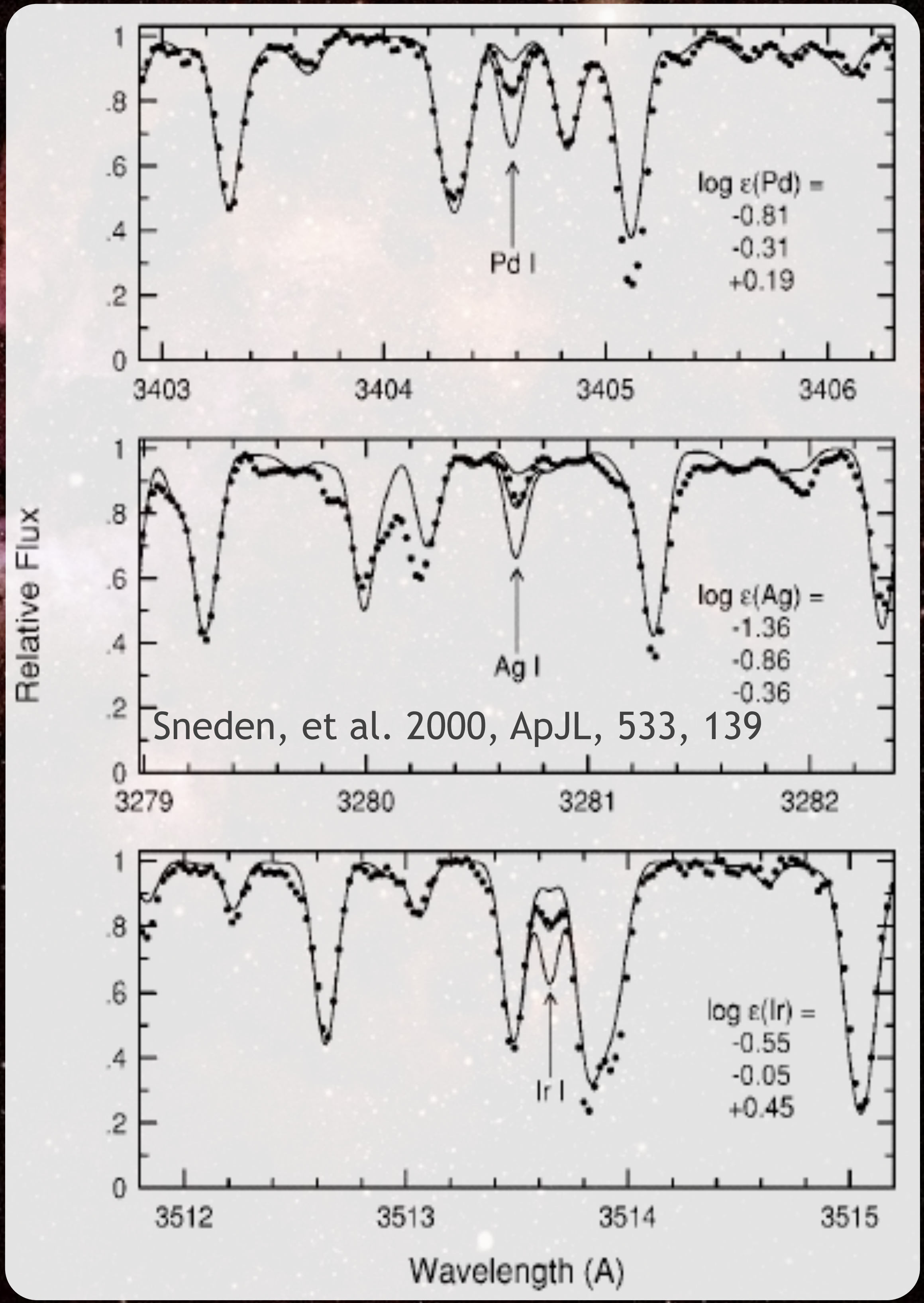
Quiescent or Explosive? Exothermic or Endothermic?

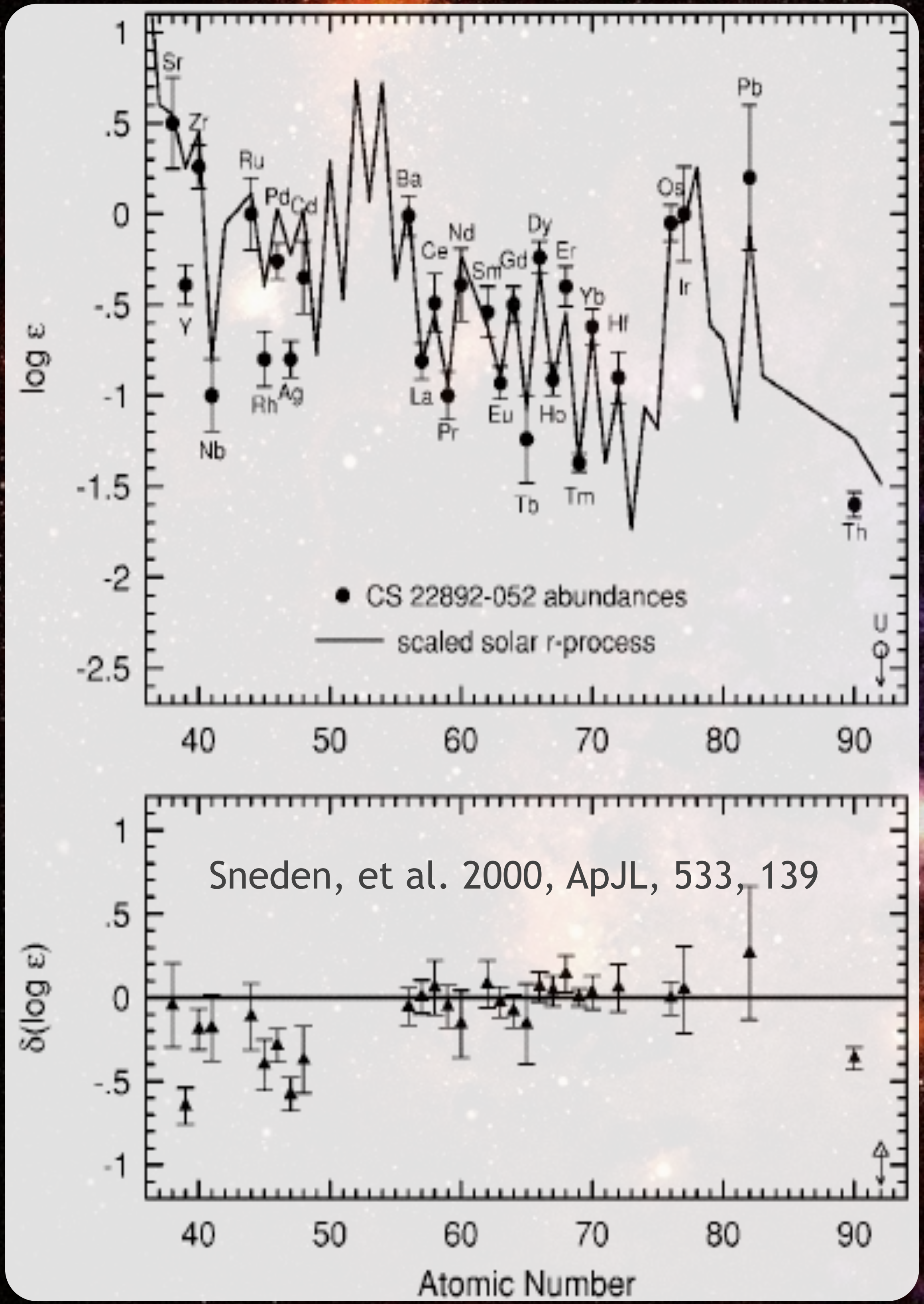
Processes and Sites



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

r-process Elements in old stars



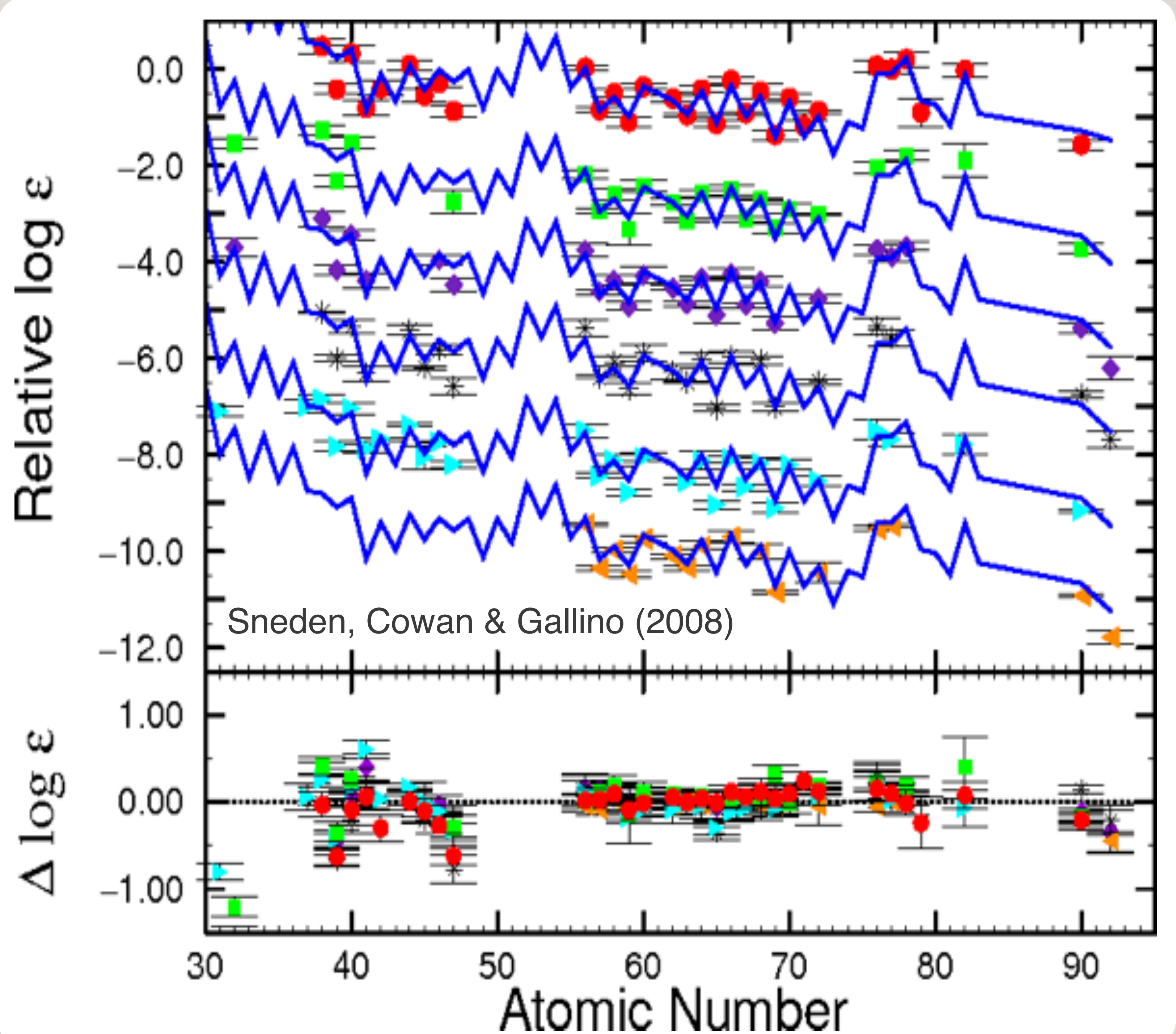


Universal R-process?

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.

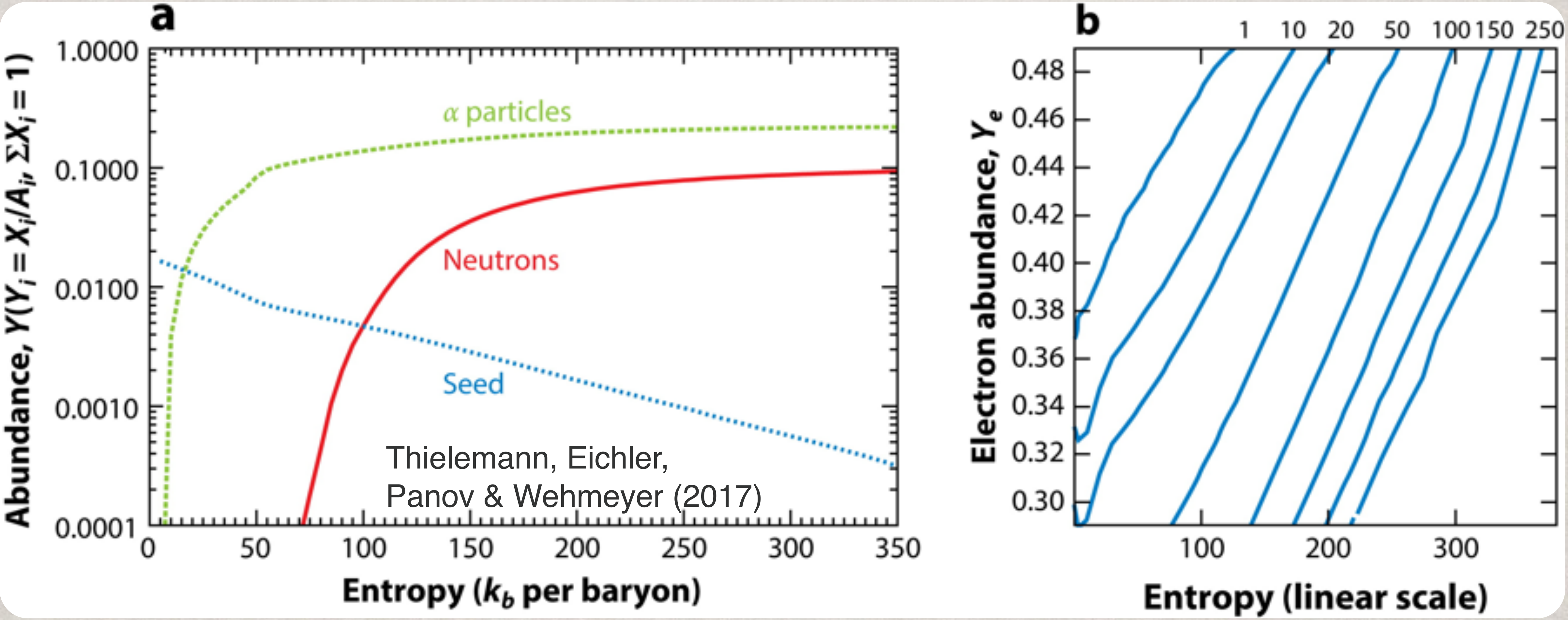
This universality does not seem to apply for $Z < 50$.



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.

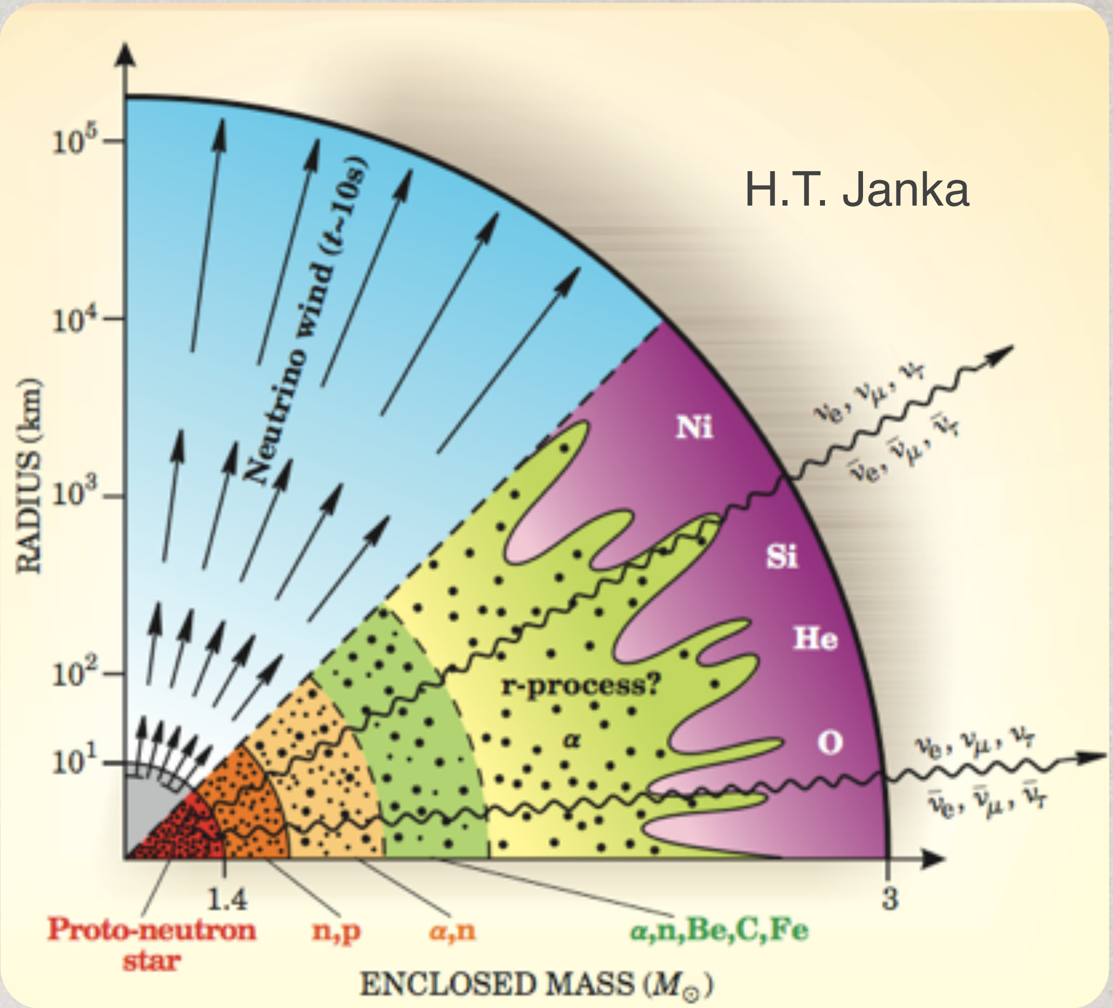
Site of the r-process

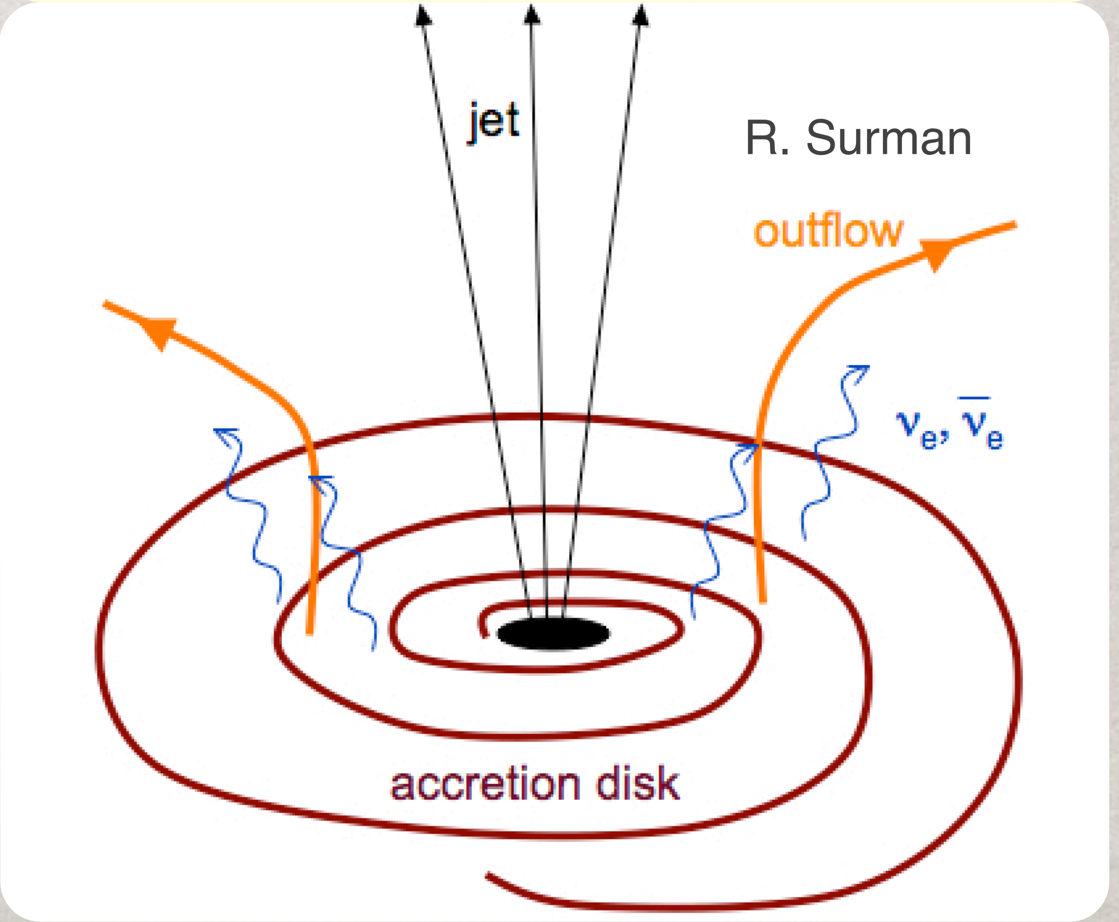
Formation of r-process requires neutron-rich, high entropy matter such as may occur in

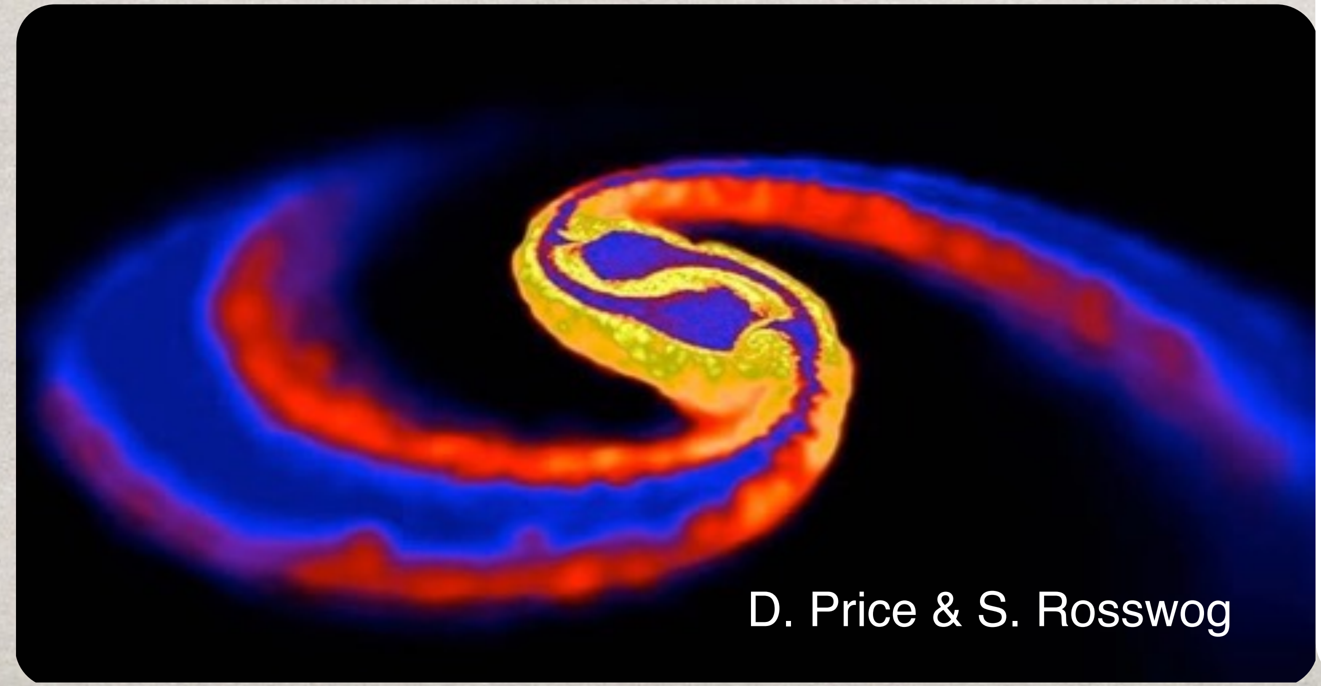
1) PNS wind in an SN,

2) in a wind from an accretion disk around a black hole,

3) or in a neutron star merger.



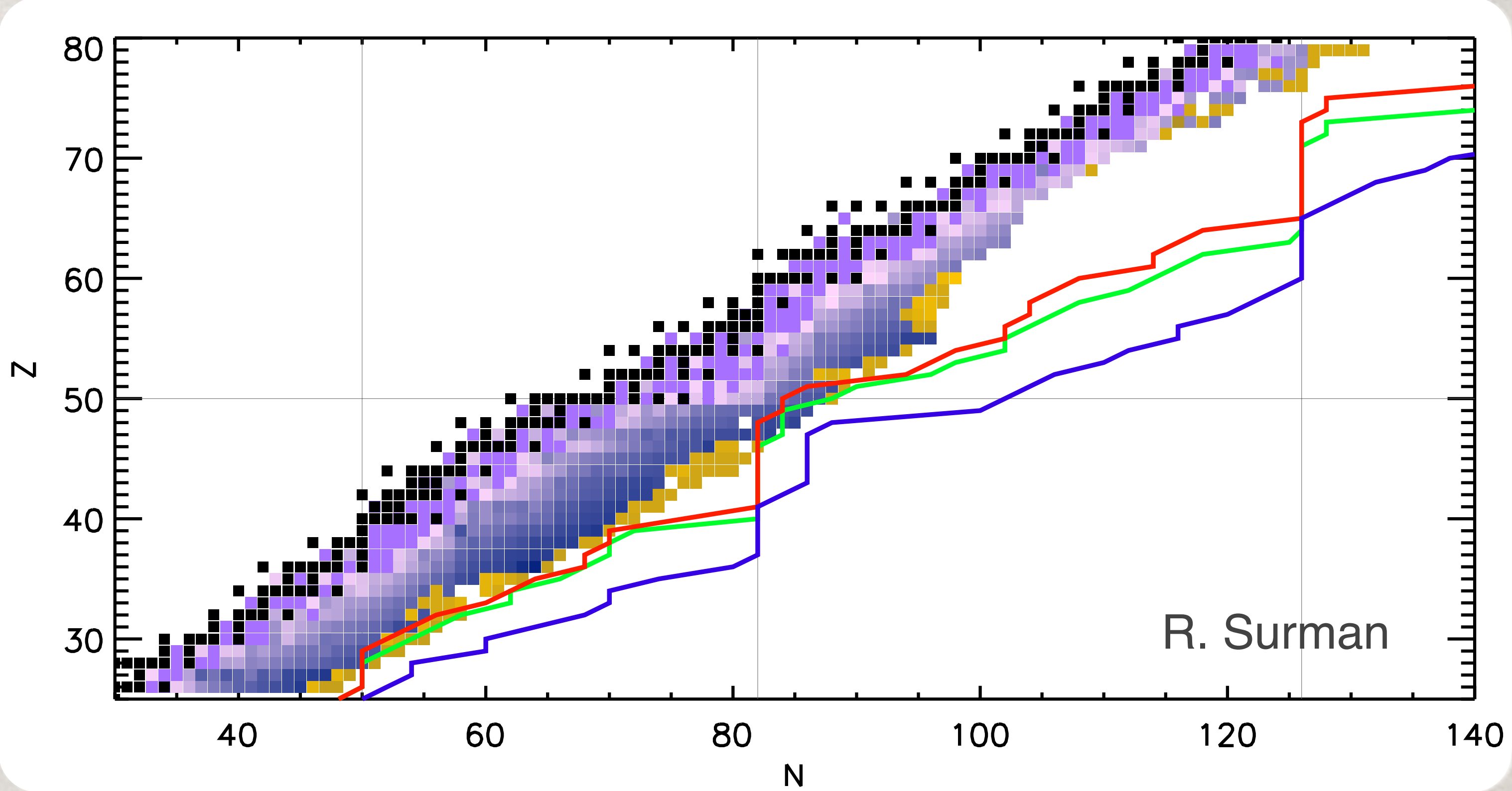




Site dependence?

As a result, the clean distinction between process and site is muddied for the r-process, with the r-process reaction path having a noticeable dependence on the site.

For example, the paths for neutrino-driven wind scenarios with greater and lesser neutronization, are distinctly different from those due to the decompression of neutron star matter.



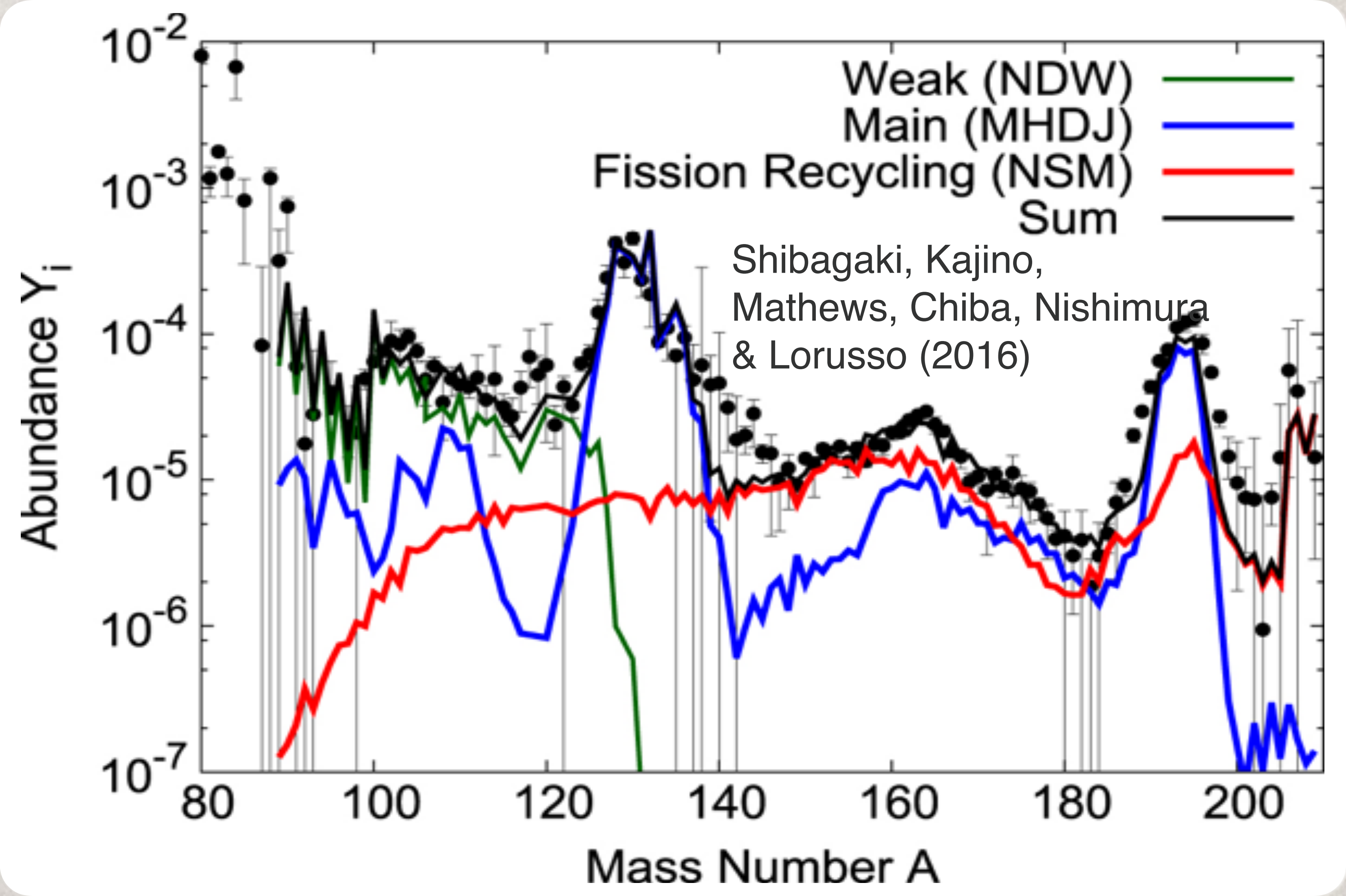
For reference, stable species are shown as black squares, currently measured half-lives are shown in purple.

Thus understanding the nuclear physics needs of the r-process requires knowing the site or sites of the r-process.

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.

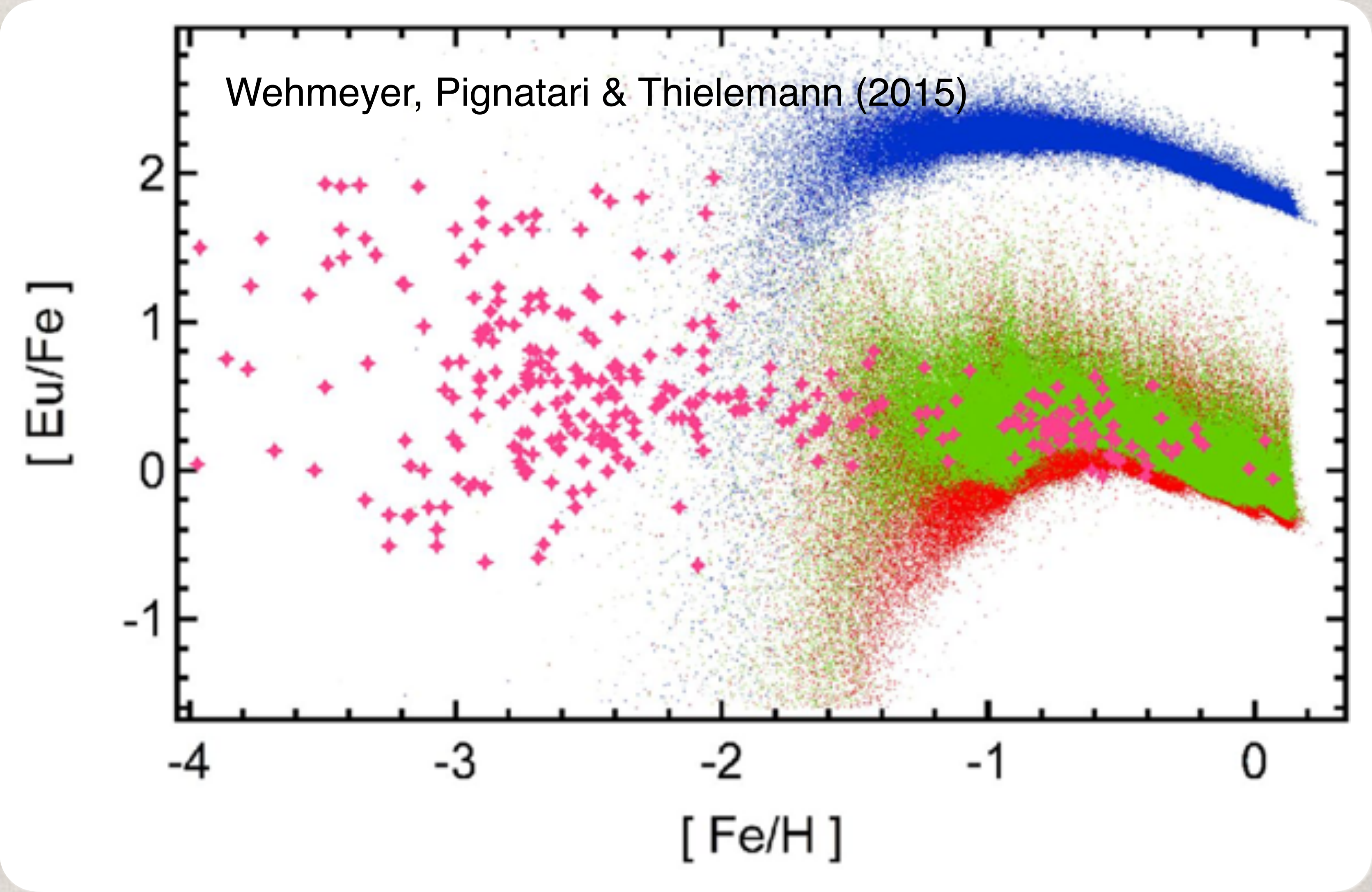


This generally leaves exotic supernovae and neutron star mergers (or both) as the site of the main r-process.

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 supernovae 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.

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)

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

We will compute multi-dimensional supernova progenitors: Maestro (Stony Brook/LBNL).

We will also compute observable signatures using SedonaBox (UCB), Cassio & SUPERNU (LANL).

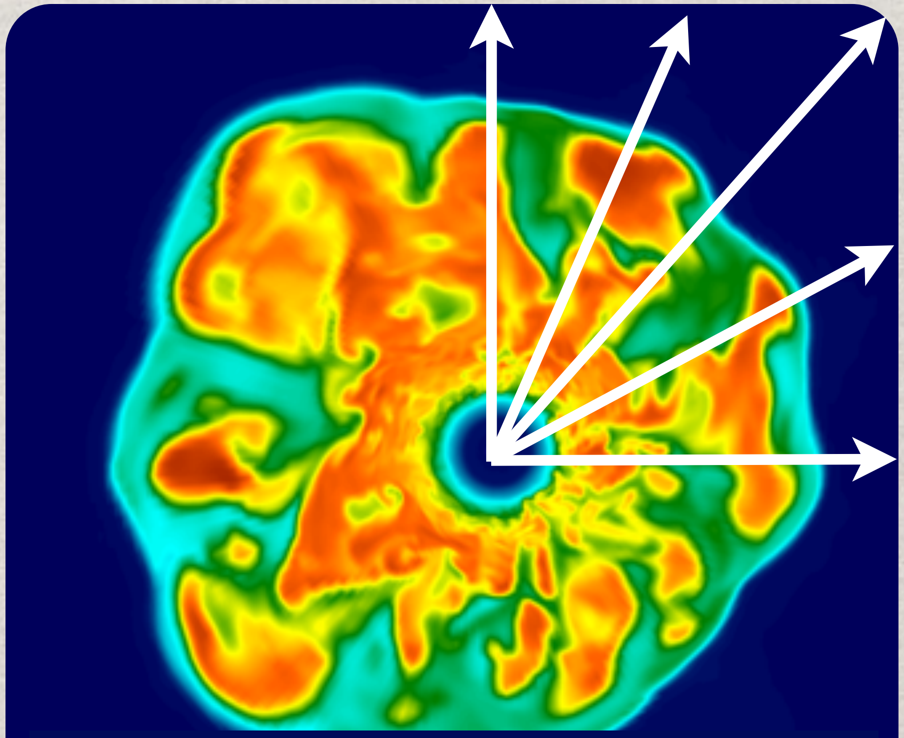
CHIMERA

CHIMERA has 3 “heads”

- Spectral Neutrino Transport (MGFLD-TRANS, Bruenn) in Ray-by-Ray Approximation
- Shock-capturing Hydrodynamics (VH1, Blondin)
- Nuclear Kinetics (XNet, Hix & Thielemann)
- Plus Realistic Equations of State, Newtonian Gravity with Spherical GR Corrections.

Models use a variety of approximations

- Self-consistent models use full physics to the center.
- Leakage & IDSA models simplify the transport.
- Parameterized models replace the core with a specified neutrino luminosity.



Ray-by-Ray Approximation

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)

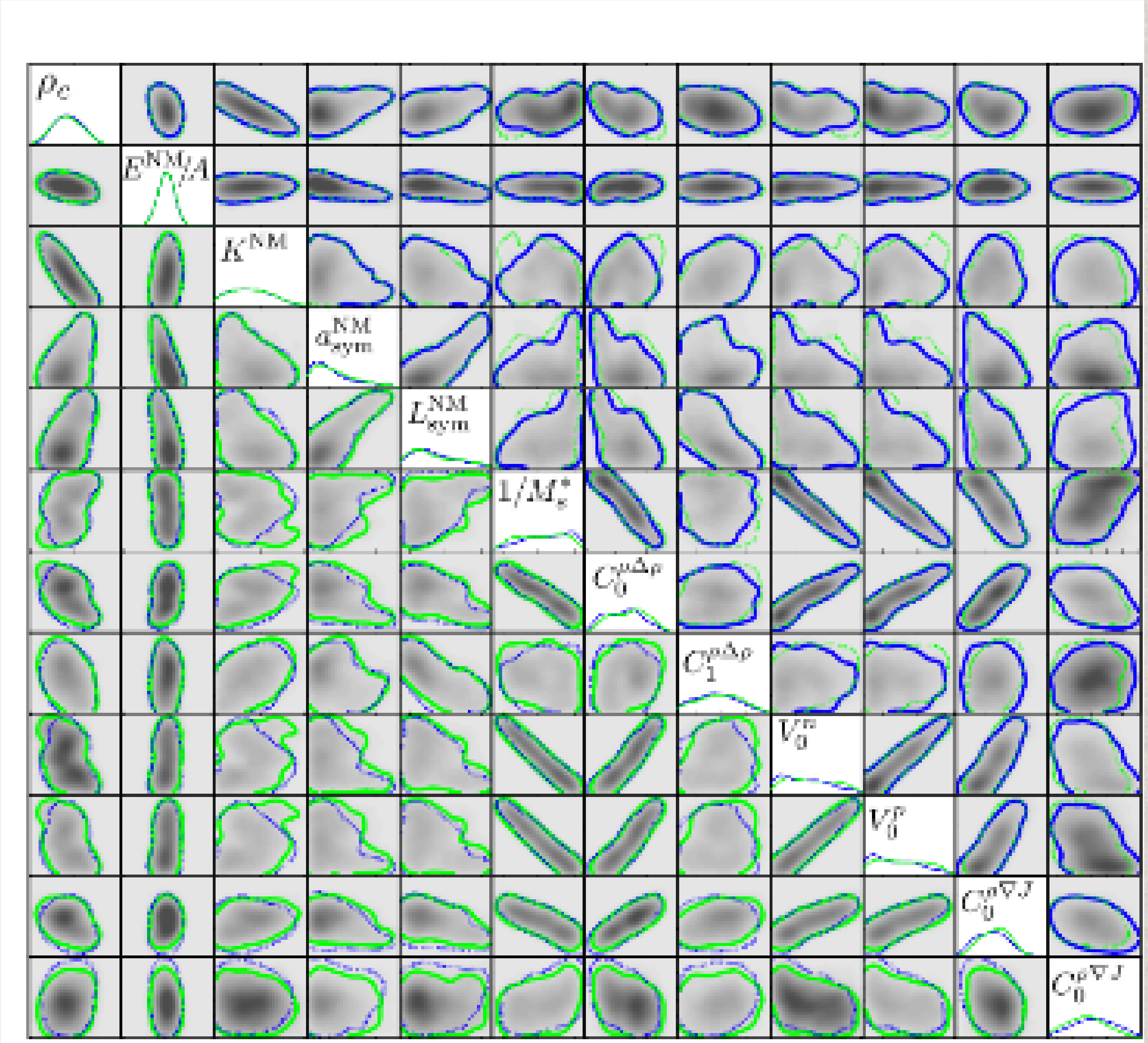
Astrophysical Uncertainty Quantification for Nucleosynthesis: Surman (Notre Dame), Hix (ORNL), and Fryer (LANL).

Merger simulations need accurate EOSs

- EOS microphysics
  - Connection to the scattering length in dilute nucleonic matter
  - Reproduce nuclear masses and charge radii
  - Ab-initio theory provides the best description of
    - Neutron matter "near" the saturation density
    - Finite-temperature properties of nucleonic matter
  - Matter beyond the saturation density
  - Nuclear structure in dense matter environment

Using NUCLEI Posterior Distributions

- Bayesian inference applied to
  - nuclear masses (deformed and spherical)
  - charge radii
  - Odd-even staggering
  - Fission isomer energies
- Generates a posterior distribution of Skyrme parameters



Kortelainen et al. (2014); McDonnell et al. (2015)

- We ignore the isovector parts of the interaction because they are poorly constrained (e.g. violates Tews, Lattimer, Ohnishi, and Kolmeitsev (2017) limit)
- Many models must be removed because nucleon effective masses diverge at a density inside neutron stars
- Recent work by Bogner et al. (2018) goes beyond Skyrme

Merger simulations need accurate EOSs

- EOS microphysics

  Pure phenomenology; Du, Steiner, and Holt (2018)

  - Connection to the scattering length in dilute nucleonic matter

    Virial expansion (Horowitz and Schwenk)

  - Reproduce nuclear masses and charge radii

    Skyrme models with parameters described by a posterior distribution determined by a fit to nuclear masses and charge radii (NUCLEI)

  - Ab-initio theory provides the best description of

    - Neutron matter "near" the saturation density

      QMC results from S. Gandolfi

    - Finite-temperature properties of nucleonic matter

      Chiral interaction + Kohn-Luttinger-Ward perturbation series from J.W. Holt

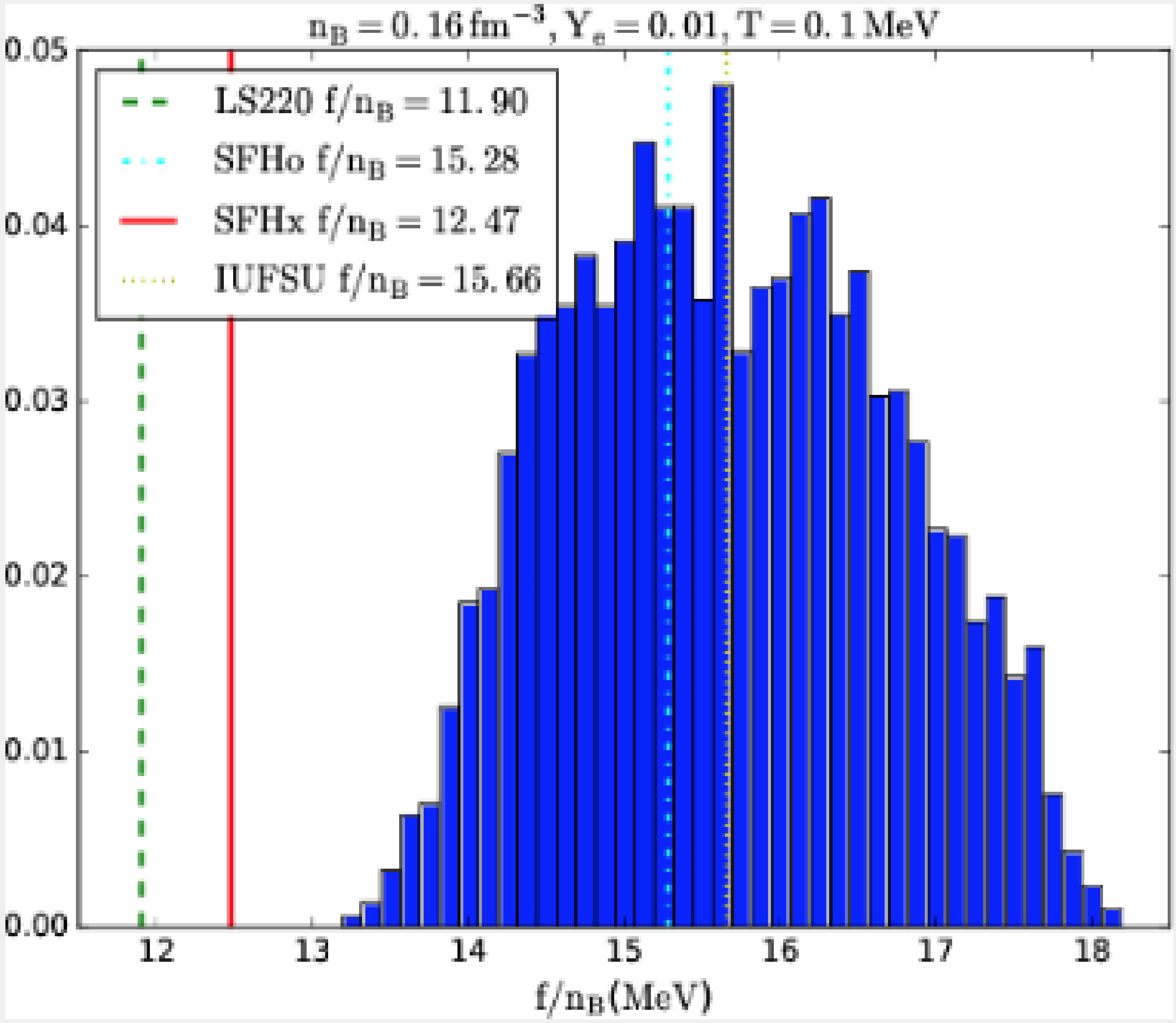
  - Matter beyond the saturation density

    Neutron star observations from Steiner et al. (add heavy-ion collisions later)?

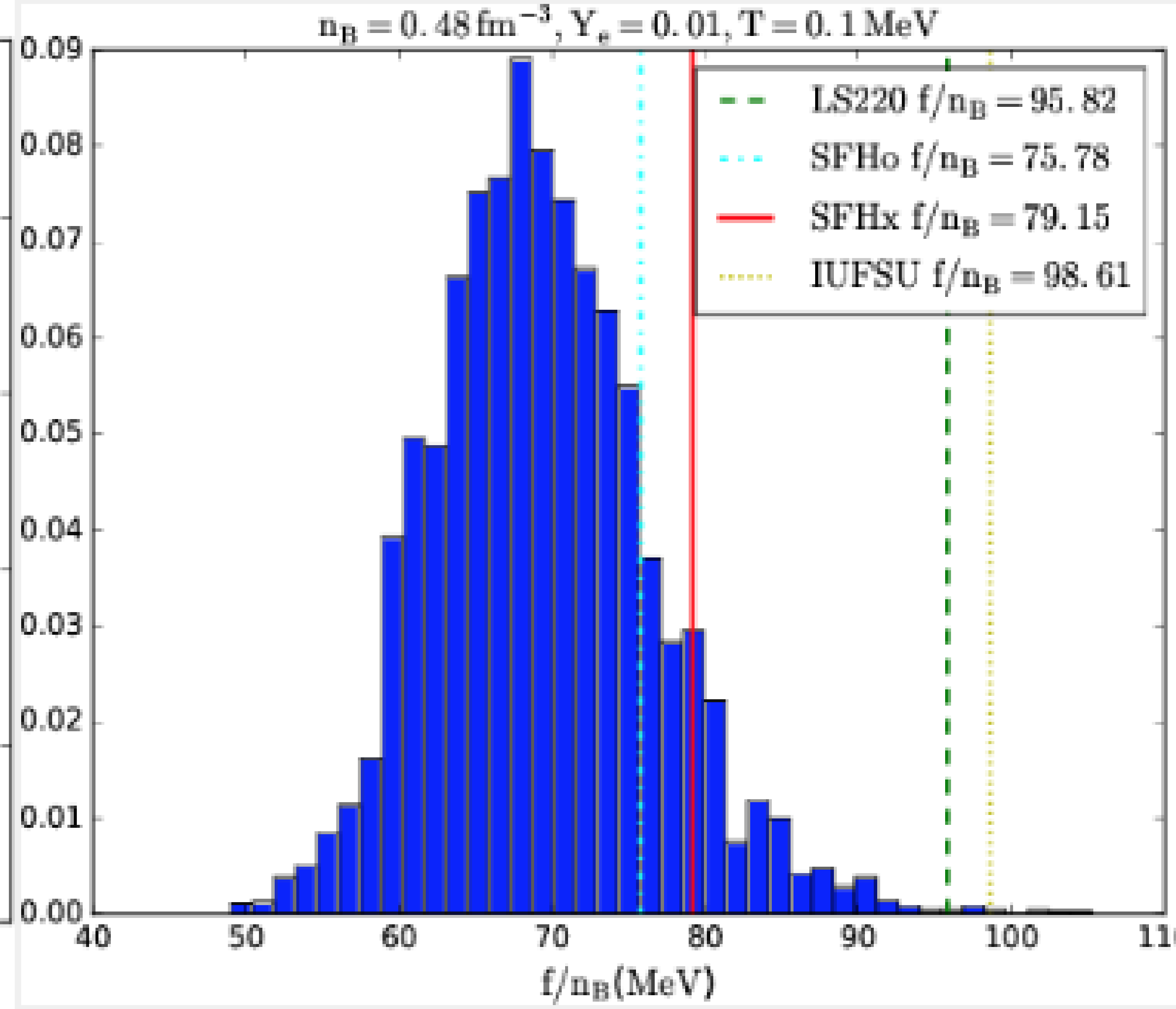
  - Nuclear structure in a hot and dense environment

    In progress...

Equation of State with Uncertainty Quantification



Probability distribution for the energy of the neutron matter at saturation



Probability distribution for the energy of the neutron matter at three times saturation

Du, Steiner, and Holt (2018)

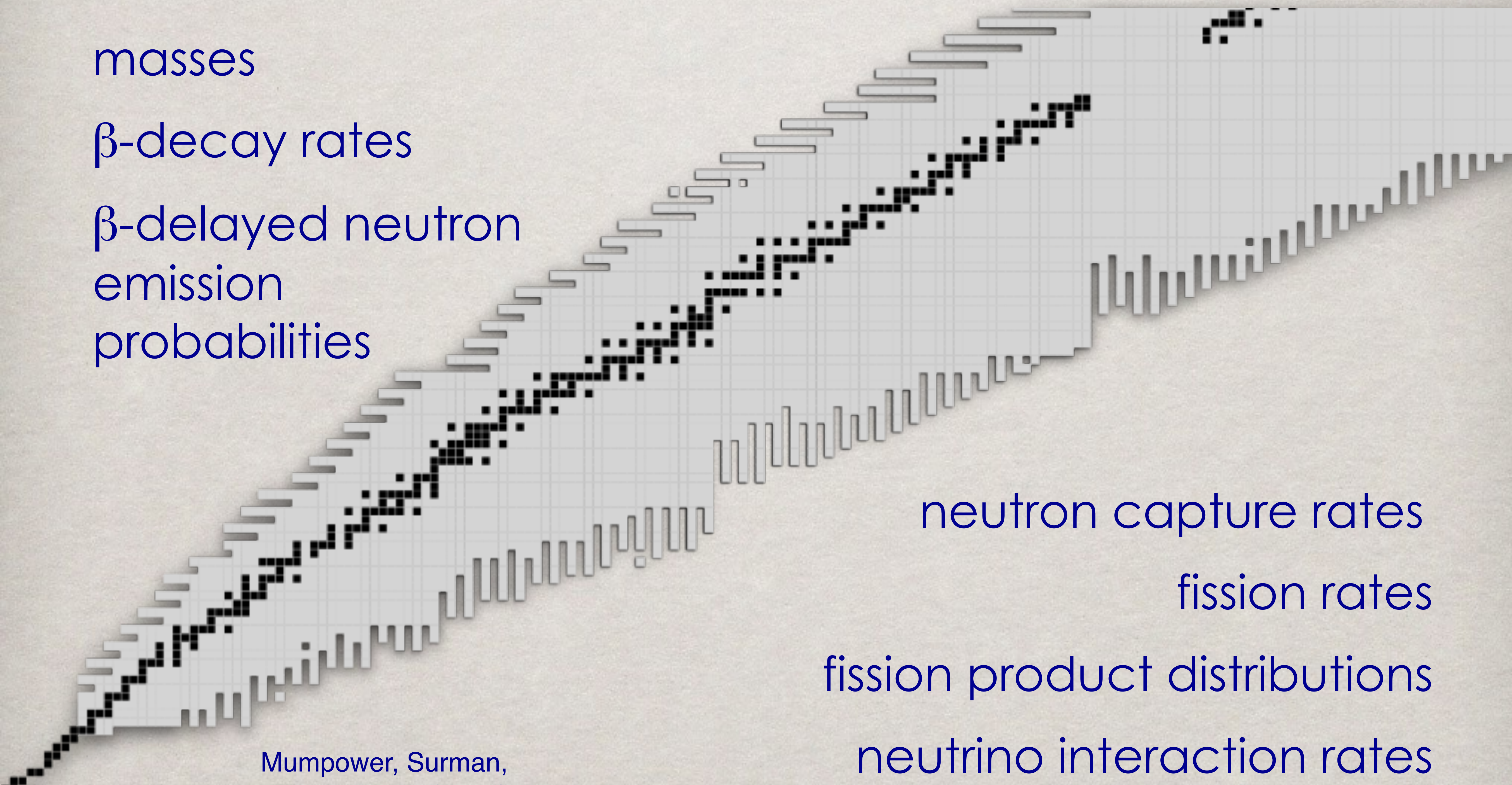
- Give up self-consistency in order to match experimental and observational data
- Generate a full posterior distribution of equations of state
- Full range of (n_B, Y_e, T)

NUCLEAR PHYSICS NEEDS FOR SUPERNOVA & MERGER ELEMENT SYNTHESIS

masses

β-decay rates

β-delayed neutron emission probabilities



Mumpower, Surman, McLaughlin, Aprahamian (2016)

neutron capture rates

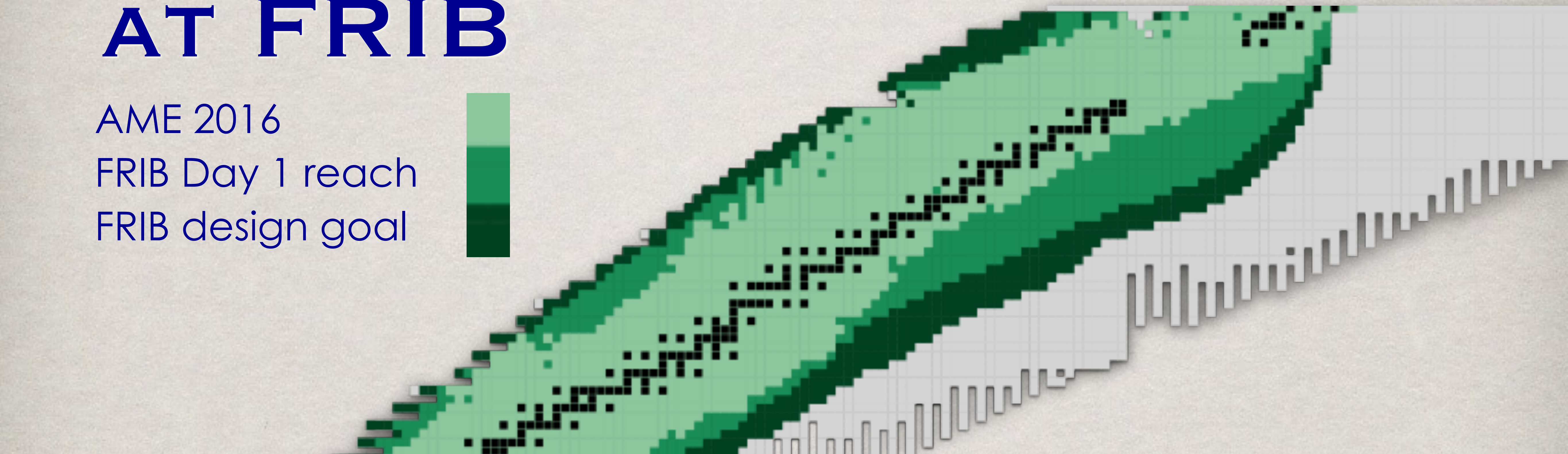
fission rates

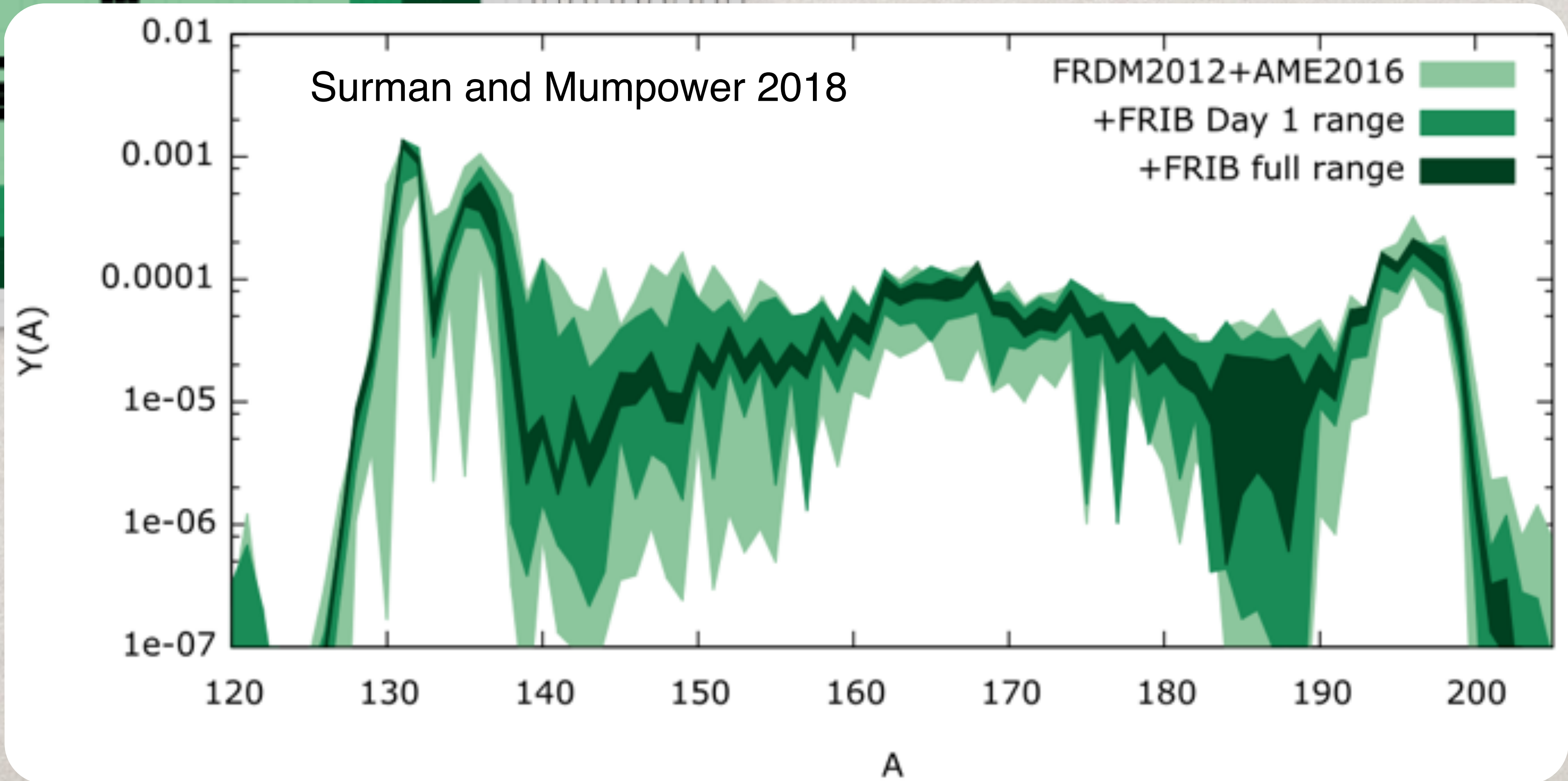
fission product distributions

neutrino interaction rates

EXPERIMENTAL PROSPECTS AT FRIB

AME 2016
FRIB Day 1 reach
FRIB design goal





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 nuclear Equation of State and neutrino opacities.

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

… exploit advances made by our nuclear theory and nuclear experimental colleagues to improve

… request an astronomical amount of **supercomputer time**.