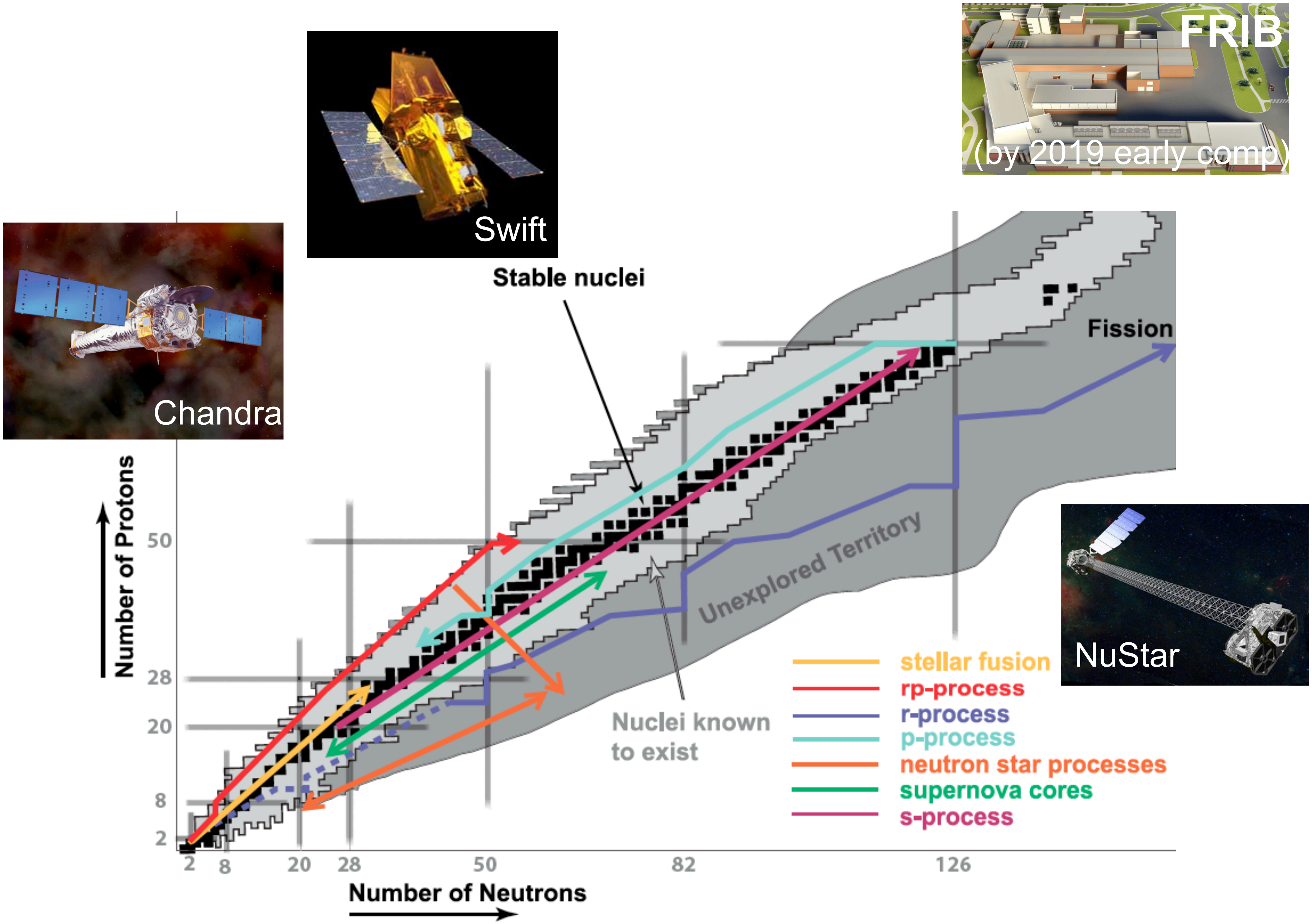
Computational Nuclear Astrophysics

Key Science Drivers of Computational Nuclear Astrophysics

- Primary Goal: Explanation of the Origin of the Elements and Isotopes
- Overwhelmingly, Elements are produced in Stars - quiescently or explosively
- Core-Collapse Supernovae (CCSN) - the Deaths of Massive Stars and Birth of Neutron Stars
- Thermonuclear Supernovae - the Source of much of the Iron Peak
- Novae - source of some light elements
- X-ray bursts - the rp-Process Nuclei
- Merging Neutron stars - with CCSN, the likely source of the r-process Nuclei
- Stellar Evolution involves nuclear reaction rates generated theoretically or experimentally - convective processes and magnetic couplings - multi-dimensional
- Stellar Explosions are always Multi-dimensional, requiring state-of-the-art radiation/hydrodynamic simulations with significant Nuclear Physics input.

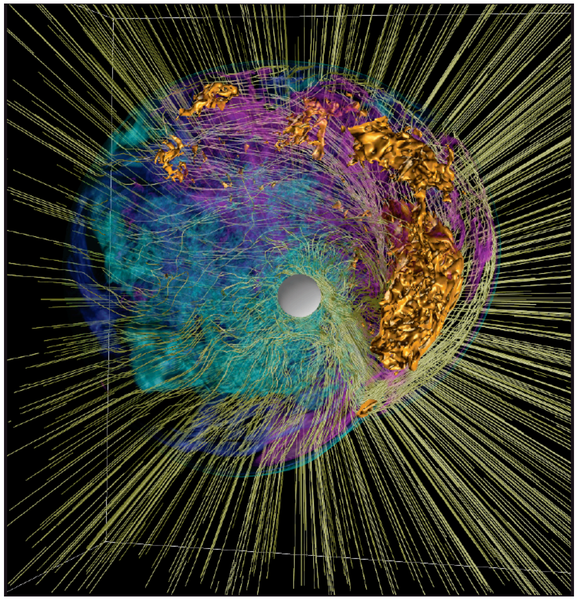
- Nuclear astrophysics entails sophisticated multi-dimensional numerical simulations employing the latest computational tools and the most powerful supercomputers of the DOE complex to address key goals of the Office of Nuclear Physics.

Nuclear Processes in the Cosmos

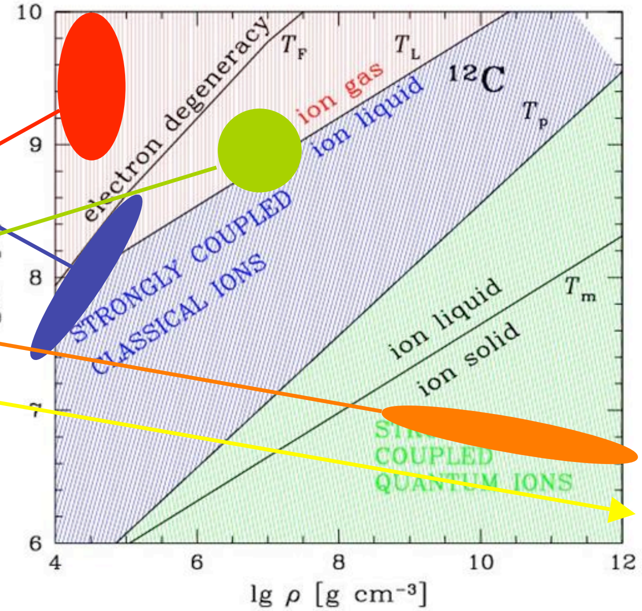


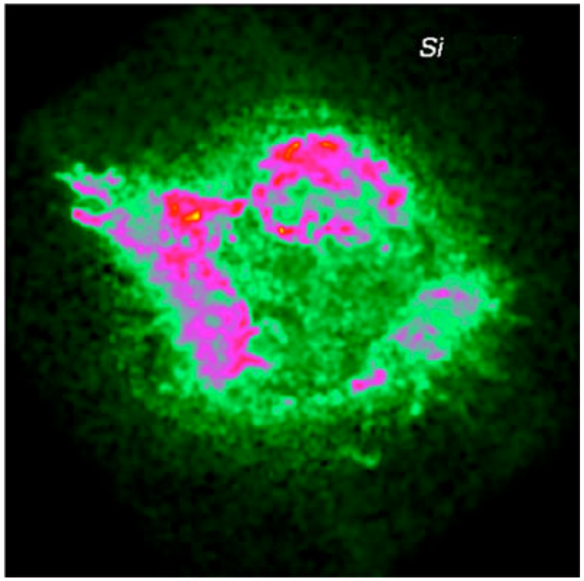
The Cosmic Laboratory;

Understanding nuclear processes at the extreme temperature & density conditions of stellar environments!



- Stellar matter
- Stellar explosions
- White Dwarf matter
- Neutron Star matter
- Quark Star matter
- Big Bang





Field requires close communication between nuclear experimentalists, theorists, stellar modelers and stellar observers (astronomers)

Core-Collapse Supernova Explosions

A 7(+) dimensional problem;
Nuclear EOS;
Nucleosynthesis

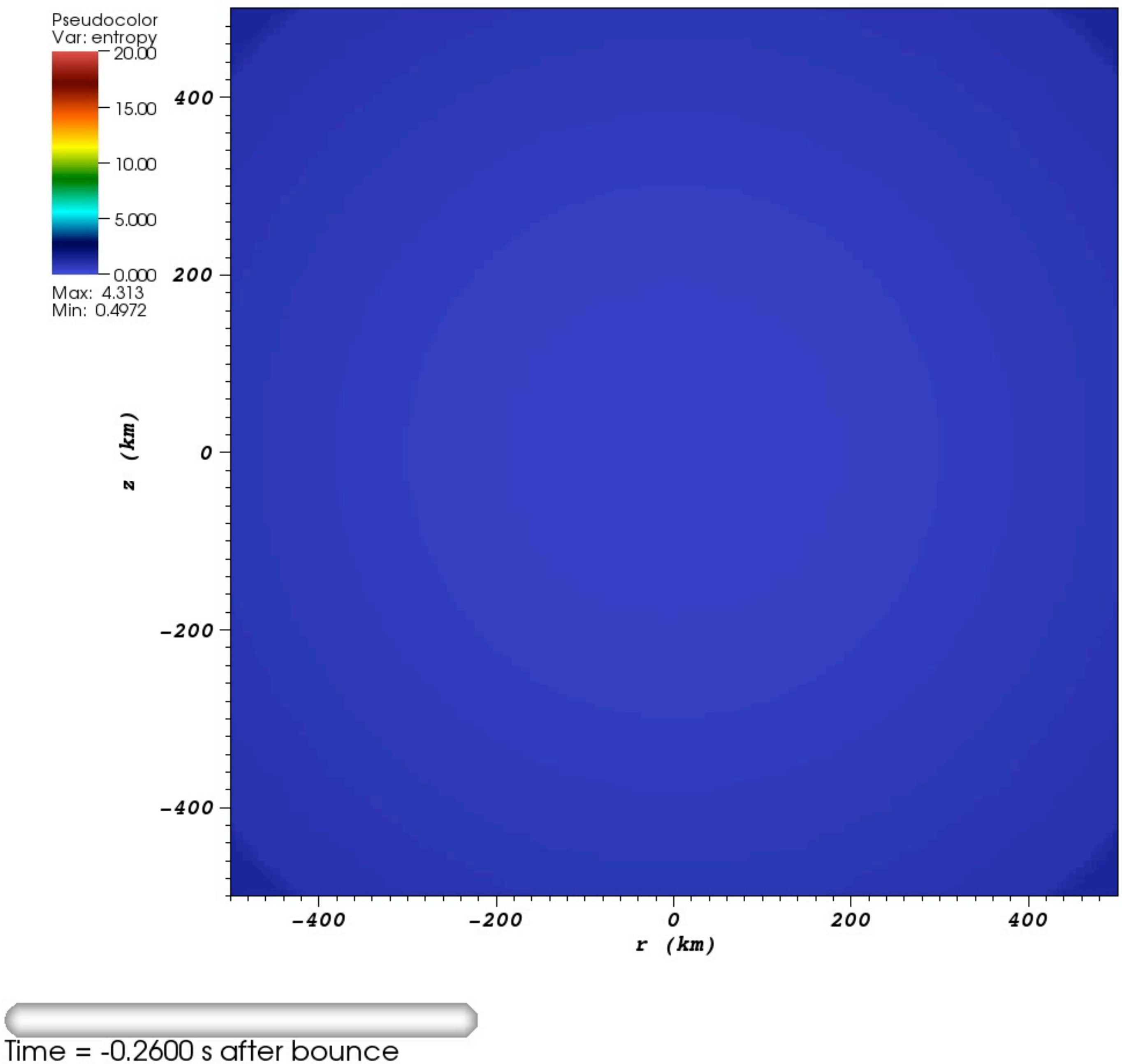
Partnership between Nuclear Astrophysicists and Applied Mathematicians to Create State-of-the-Art Computational Capabilities

- 2nd-order, Eulerian, unsplit, compressible hydro
- PPM and piecewise-linear methodologies
- Multi-grid Poisson solver for gravity
- Multi-component advection scheme with reactions
- Adaptive Mesh Refinement (AMR) - flow control, memory management, grid generation
- Block-structured hierarchical grids
- Subcycles in time (multiple timestepping - coarse, fine)
- Sophisticated synchronization algorithm
- BoxLib software infrastructure, with functionality for serial distributed and shared memory architectures
- 1D (cartestian, cylindrical, spherical); 2D (Cartesian, cylindrical); 3D (Cartesian)
- Multigroup Transport with v/c terms and inelastic scattering
- Uses scalable linear solvers (e.g., hypre) with high-performance preconditioners that feature parallel multi-grid and Krylov-based iterative methods - challenging!
- Example partnership: John Bell, Ann Almgren, Weiqun Zhang, Louis Howell, Adam Burrows, Jason Nordhaus - LBNL, LLNL, Princeton

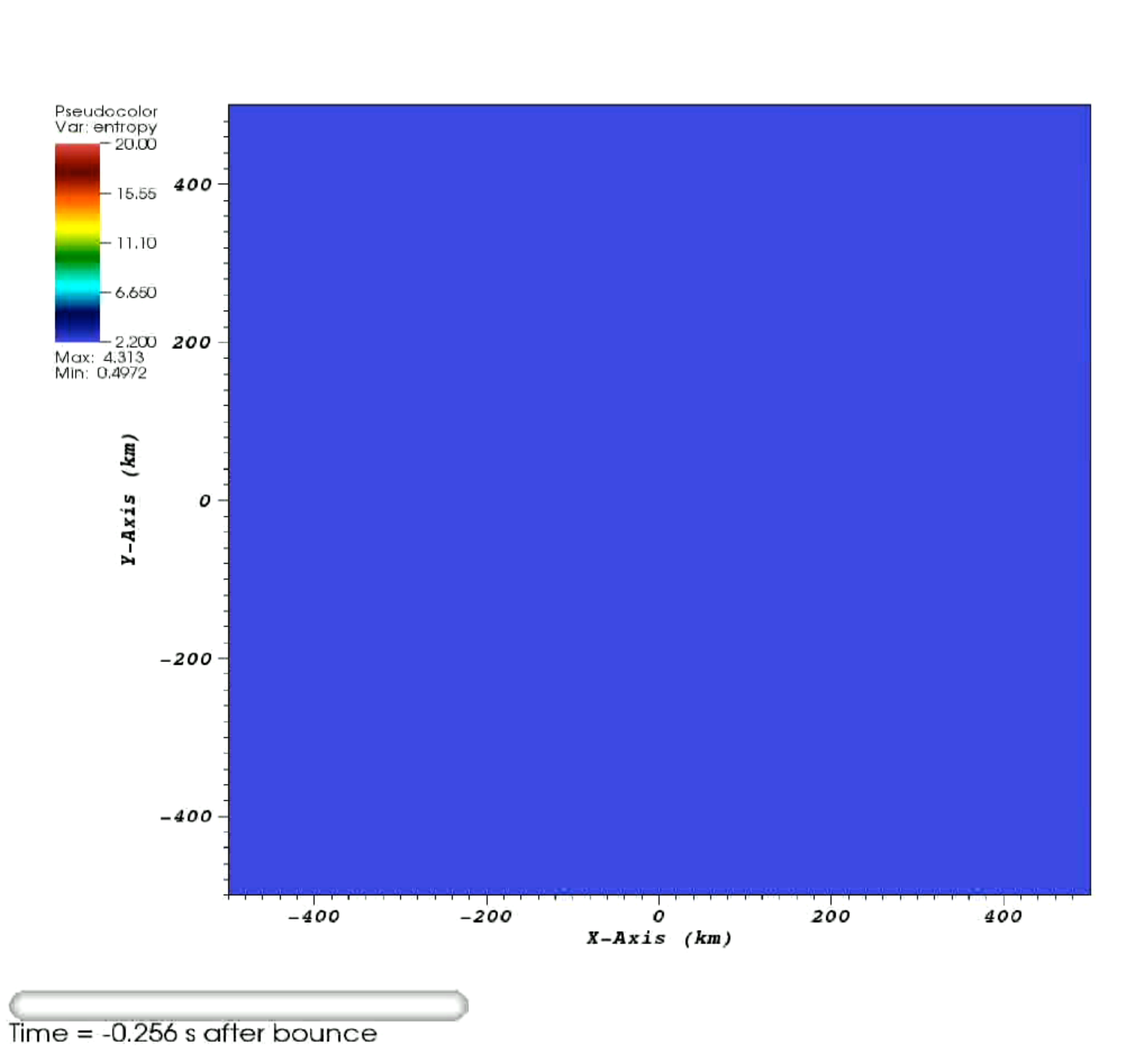
2D:2.3

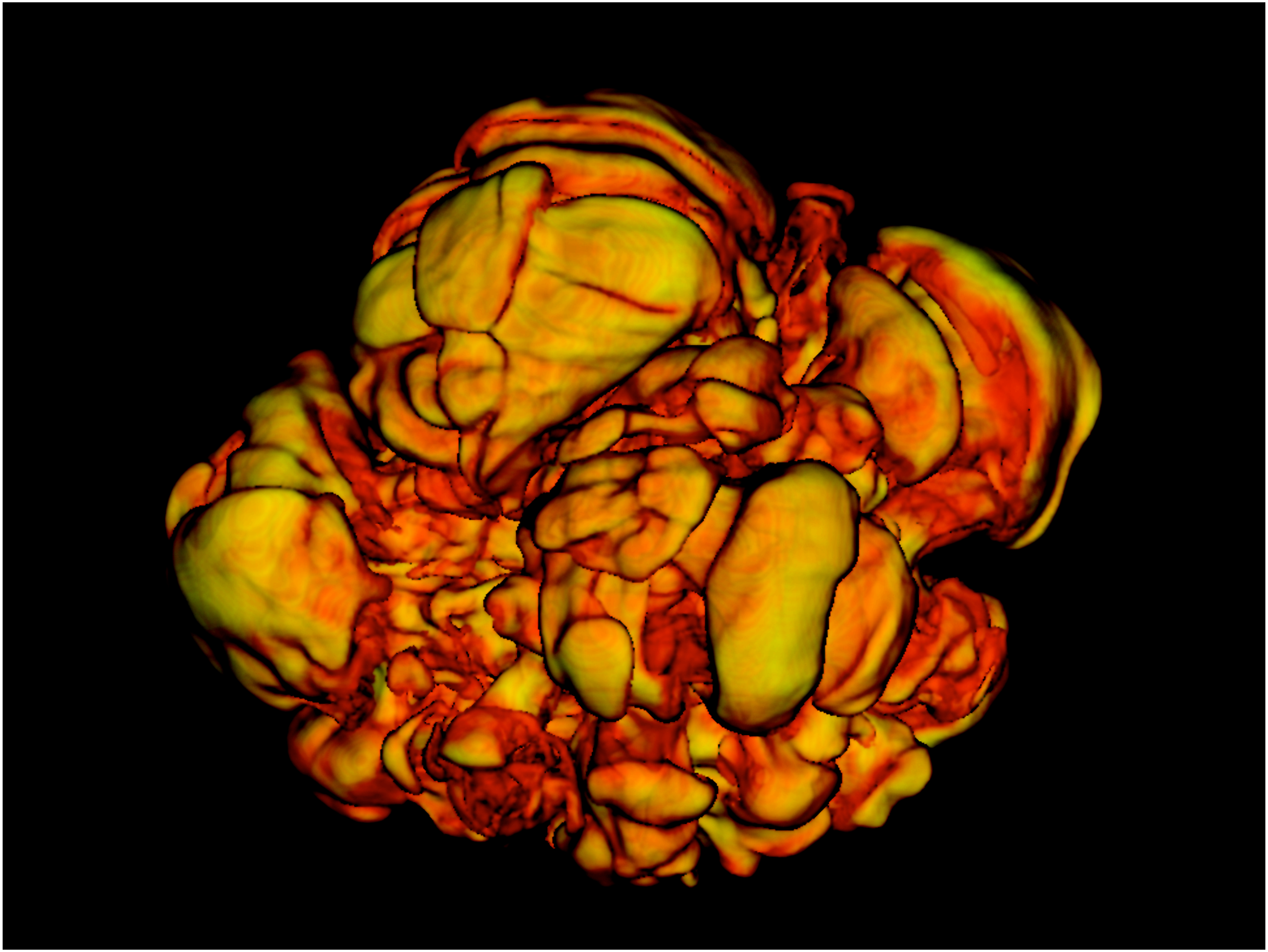
"Inverse" Energy Cascade in 2D -

Buoyancy-Driven Convection has (anomalously) a lot of large-scale power - Often confused for the SASI

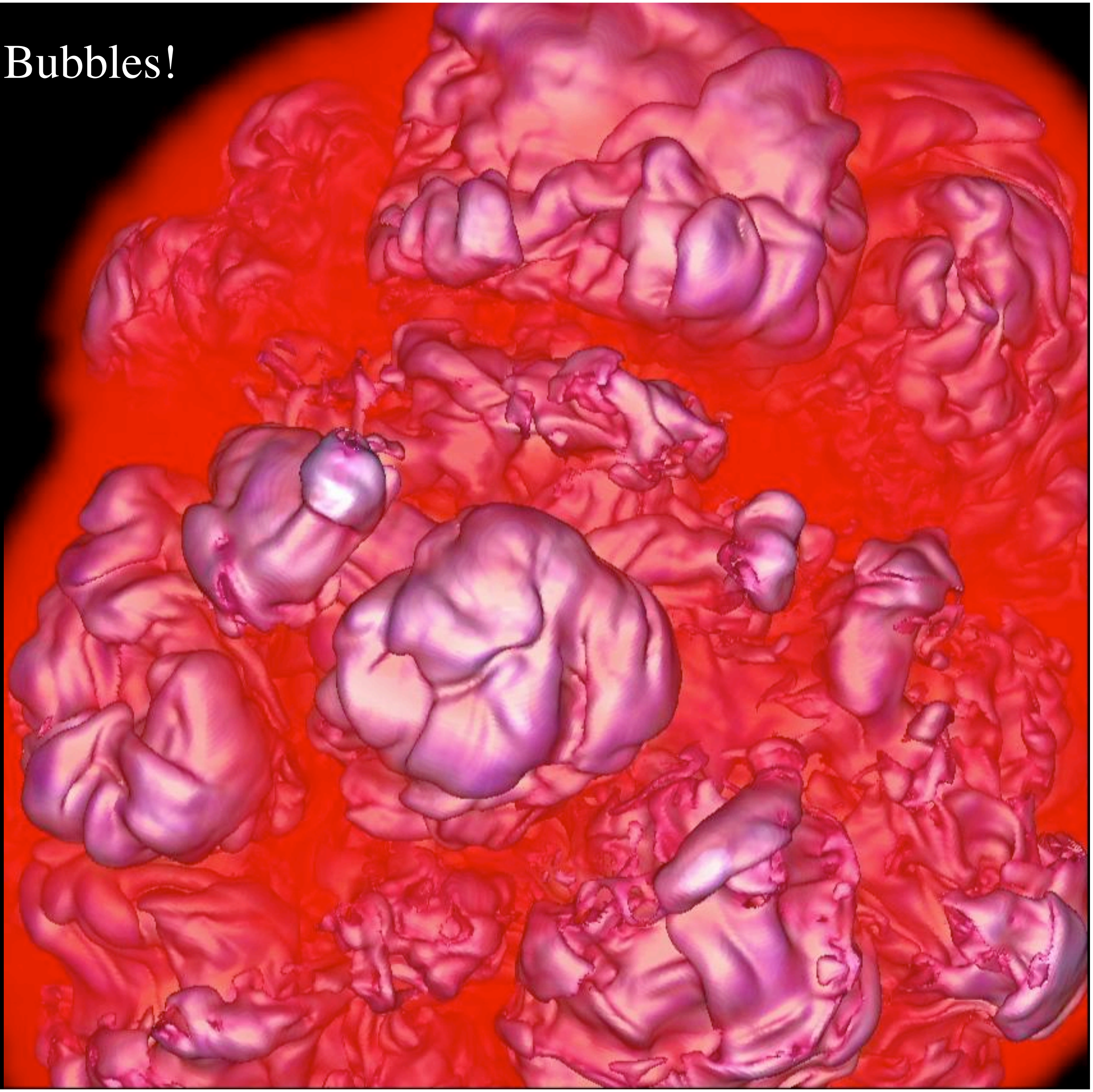


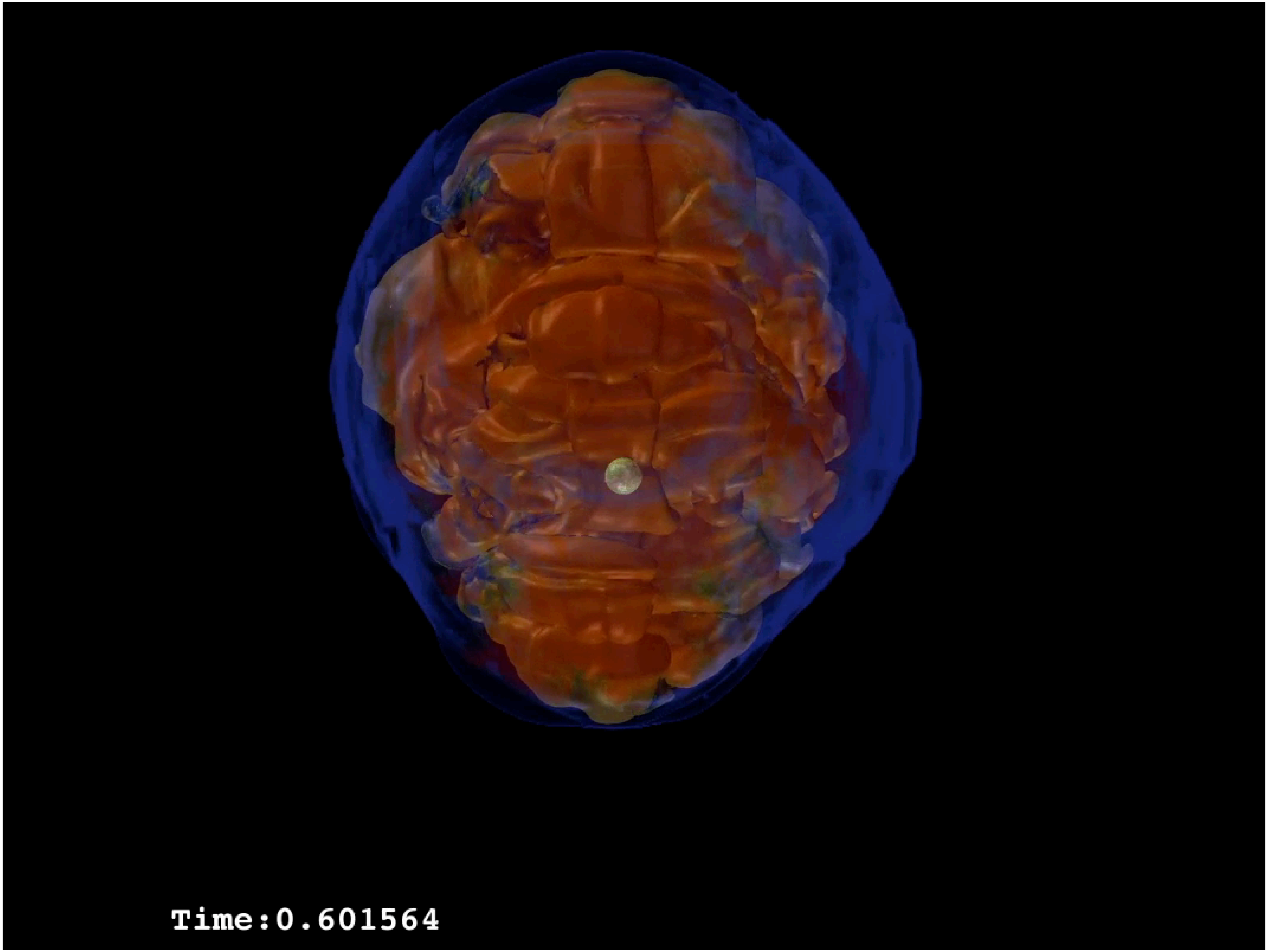
Character of 3D turbulence and Explosion Very Different from those in 2D

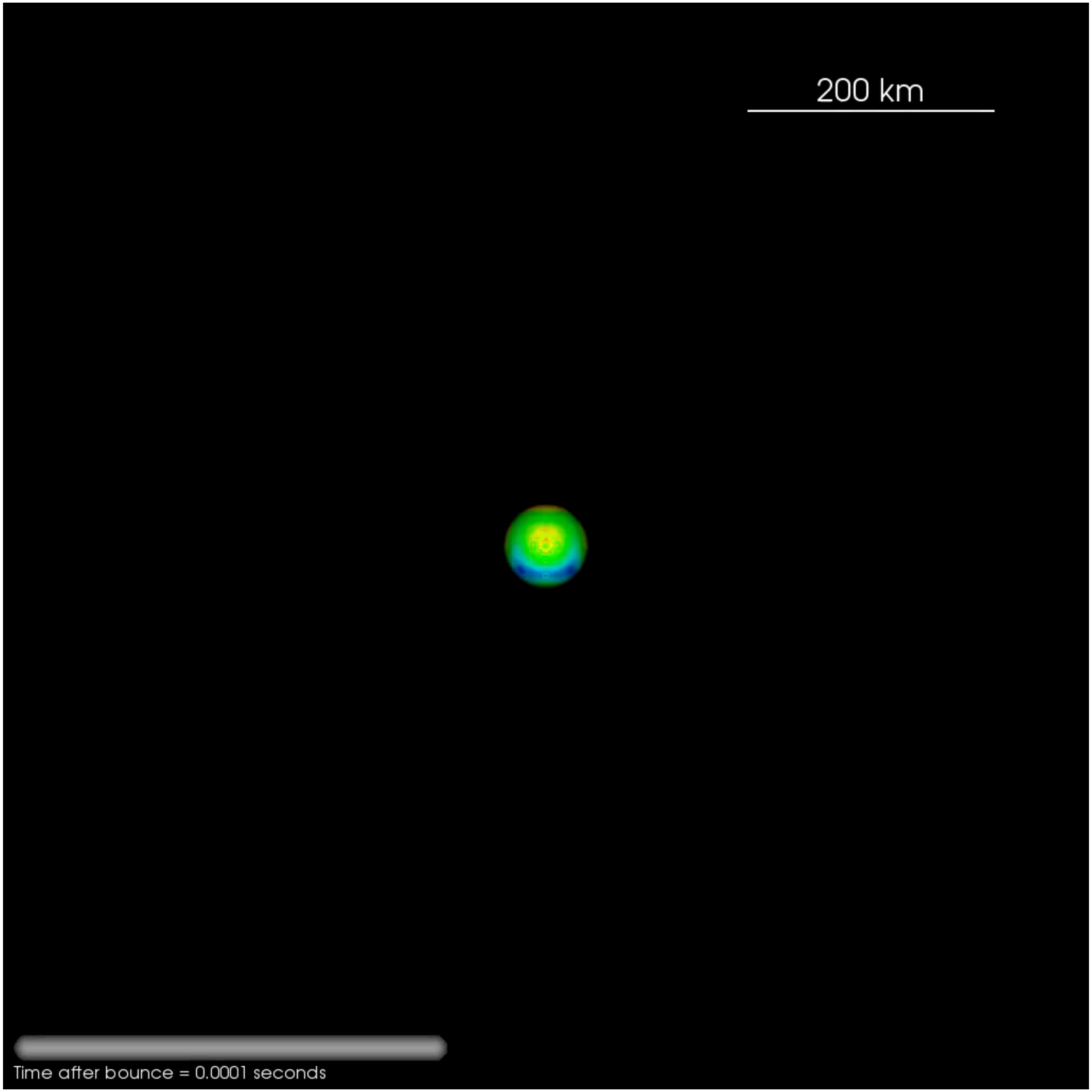




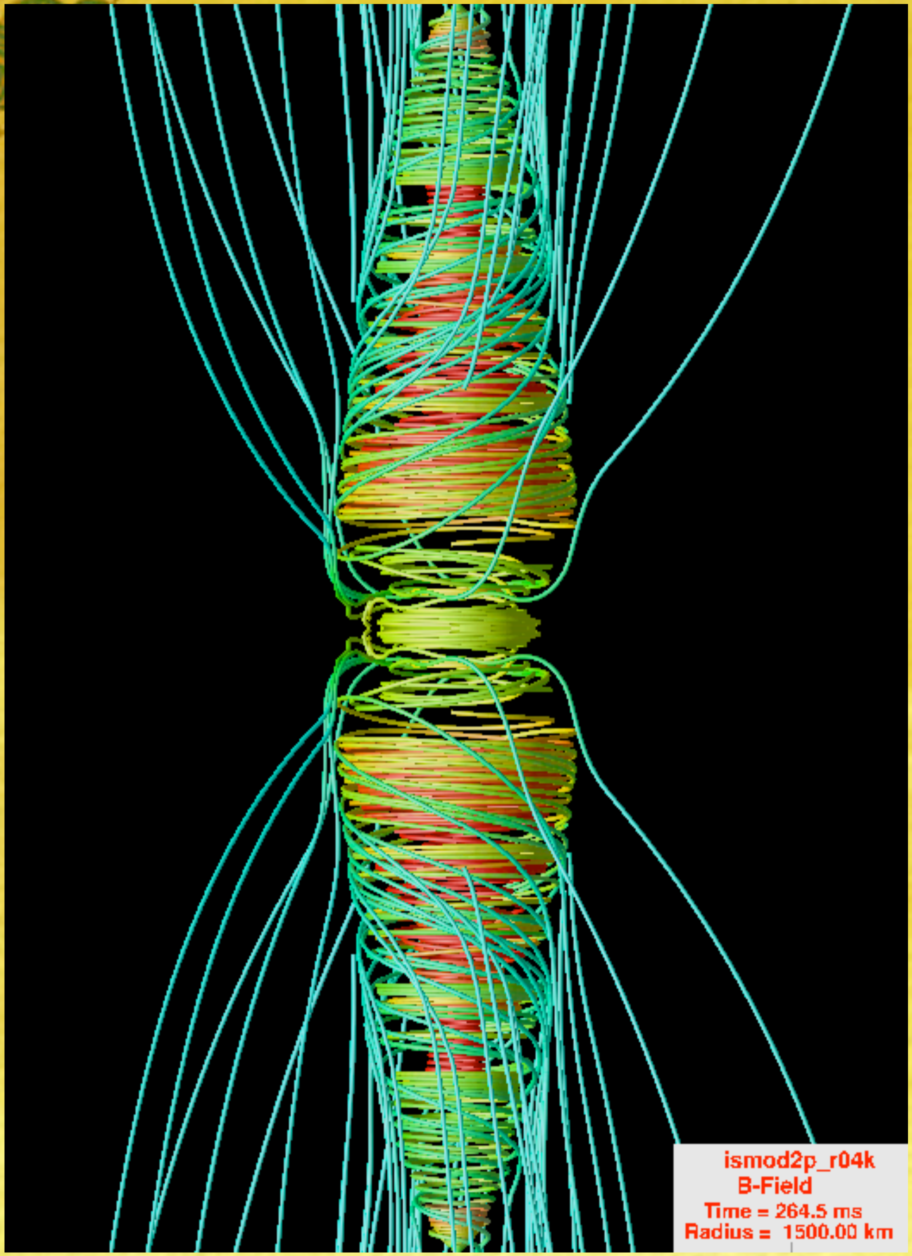
Buoyancy-driven Bubbles!

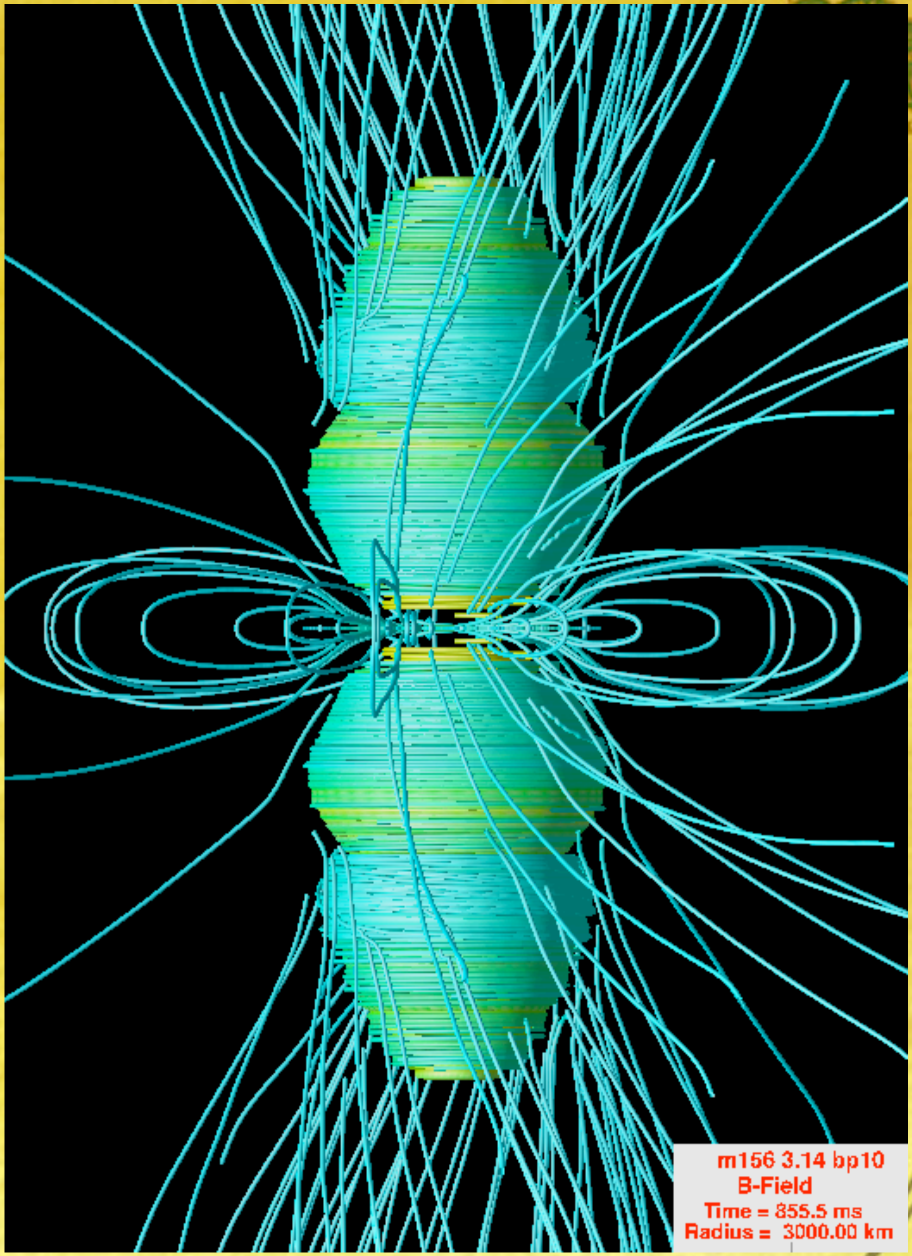



Time:0.601564

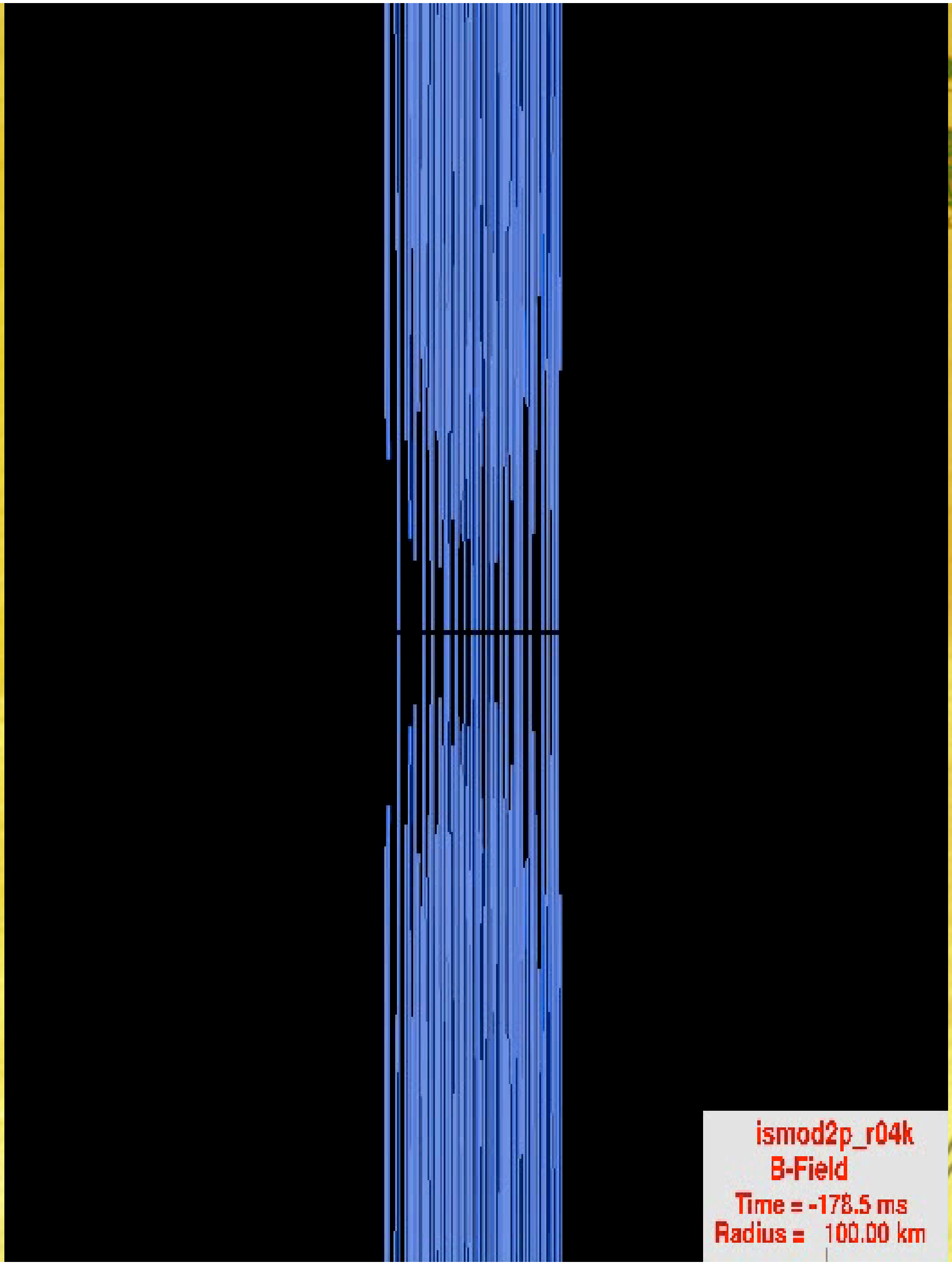

200 km
Time after bounce = 0.0001 seconds

Magnetic CCSN Explosions: Might be the Source of Some R-Process





Multi-group “2 1/2”-D Radiation-Magneto-Hydrodynamic (RMHD) simulations of Core-Collapse Supernovae



Sample Computational Requirements for Future Core-Collapse Supernova Simulations

Platform	Space	Neutrino	$\#f_\nu$	Matrix	Ops./Δt
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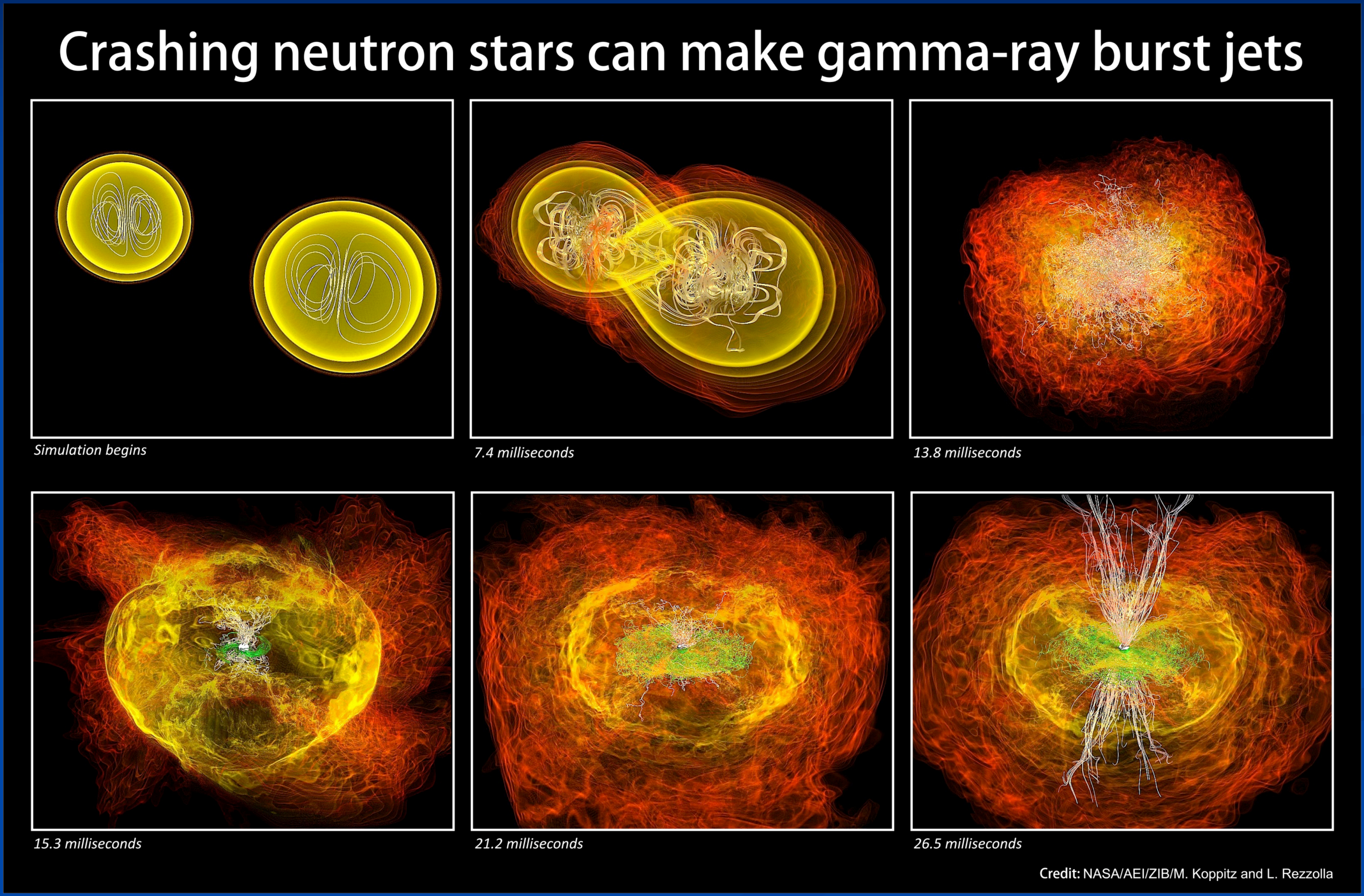
Near-Term	512x64x128	12x24x20	600 GB	200 TB	2×10^{15}
Exa-Scale	512x128x256	24x24x24	6 TB	3 PB	8×10^{16}
"Full Coupling"	512x128x256	24x24x24	6 TB	80 PB	4×10^{19}

Kotake et al. 2012

Cycle and Memory Requirements for Supernova Simulations

- 1985 (1D) - ~10^{2-3} CPU-hours per run; 10 Gbytes memory
- 1995 (low 2D) - ~10^{5-6} CPU-hours per run; 100 Gbytes memory
- 2005 (medium 2D) - ~10^{6} CPU-hours per run; 10^{2} cores; Tbytes memory
- 2010 (low 3D) - ~10^{6-7} CPU-hours per run; 10^{3-4} cores; Tbytes memory
- 2015 (medium 3D) - ~10^{7-8} CPU-hours per run; 10^{5} cores; 0.2-1 Pbytes memory
- 2020 (heroic 3D) - ~10^{8-9} CPU-hours per run; 10^{5-6} cores; >10 Pbytes memory

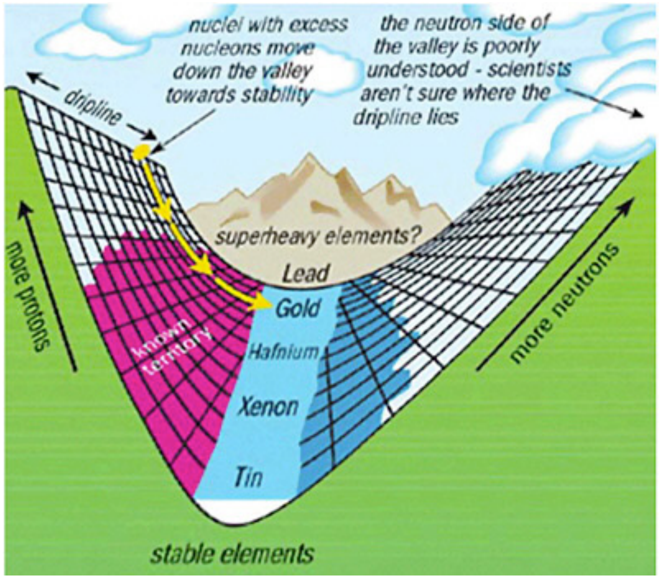
Short-Hard GRB Model: Merger of Neutron Stars - Site of the R-Process?



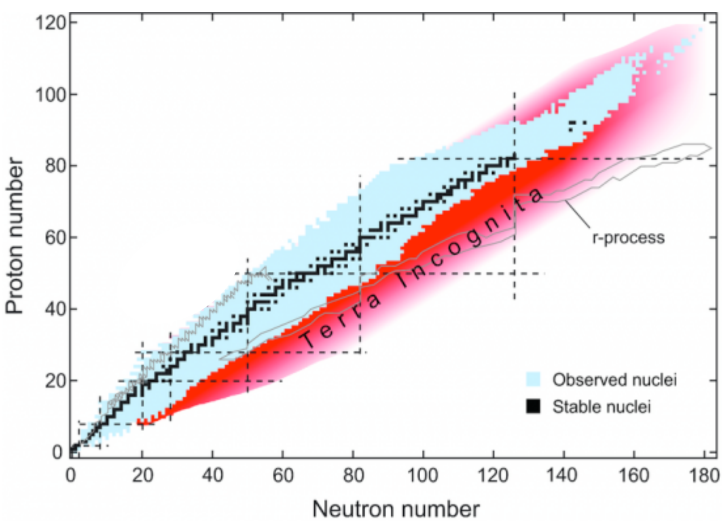
The R-Process:

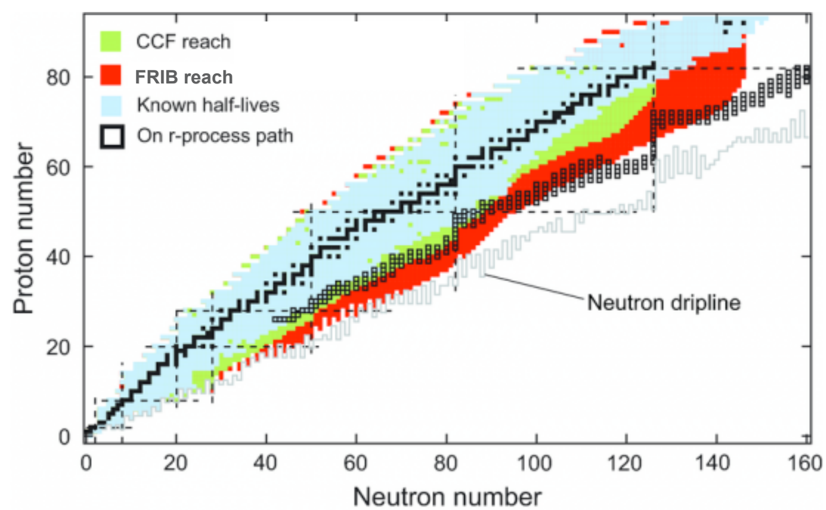
Core-Collapse Supernovae, Merging Neutron Stars, or Hypernovae - Multiple Sites?

Reach of FRIB - Link to Nuclear Astrophysics

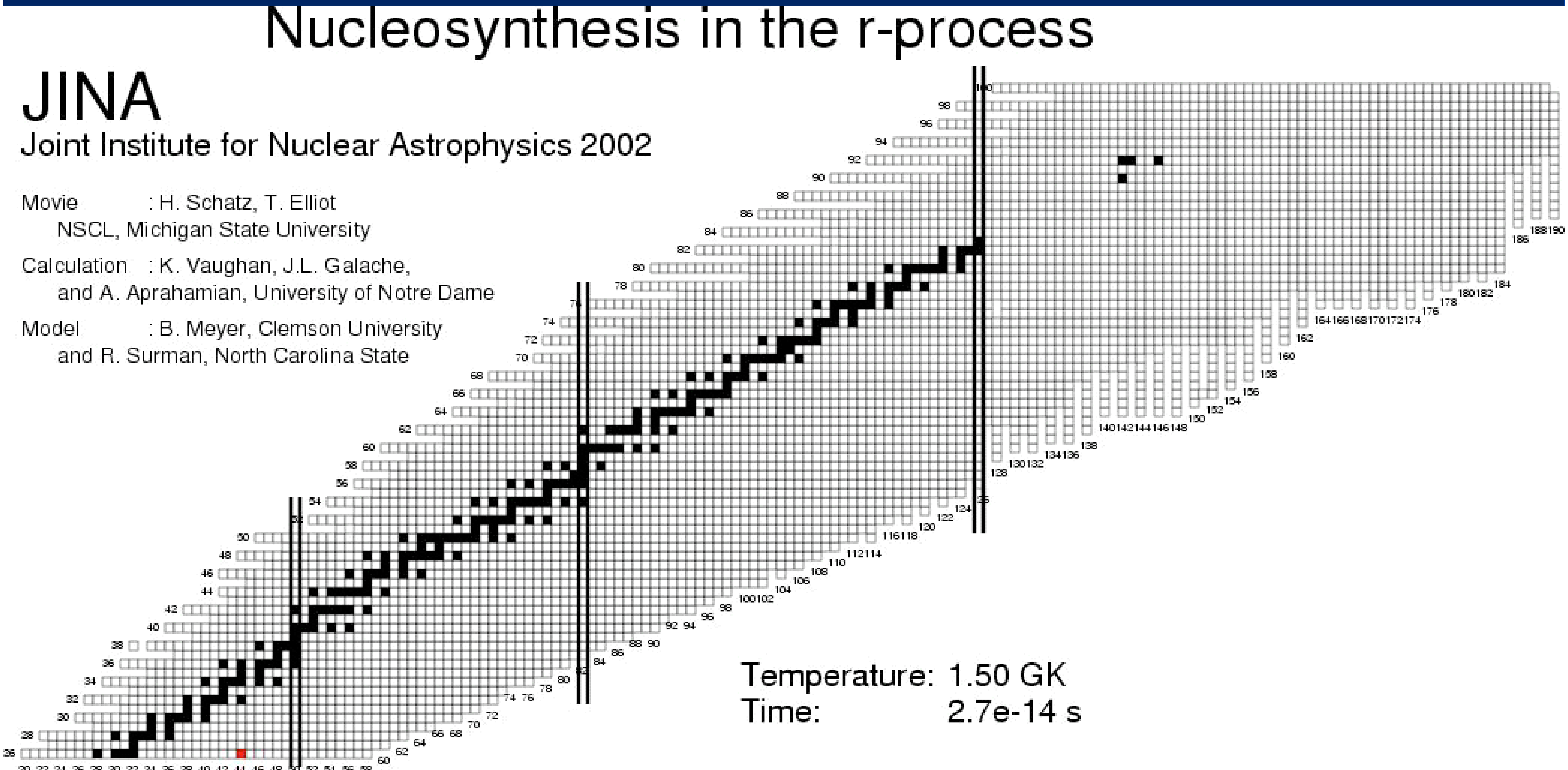


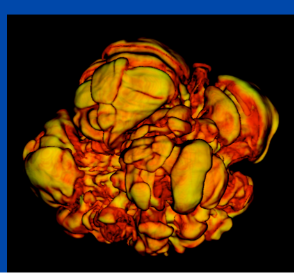
- Nuclear Masses & decay properties
- Neutron halos
- Disappearance of shell structure
- Emergence of new shapes,
- New collective modes of excitation
- Mapping the driplines
- Islands of stability

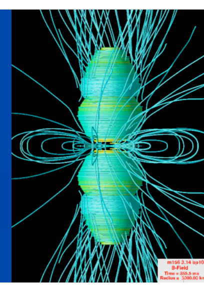


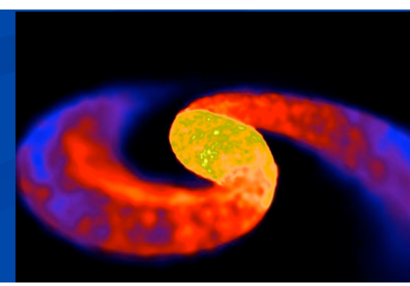


R-Process Nucleosynthesis









Neutrino Oscillations in Core-Collapse Supernovae: A Computational Challenge

Neutrino Oscillations and Self-Coupling- Coherent Neutrino Flavor Evolution

- Wigner density matrix, ensemble-averaging →

$$\mathcal{F} = \langle n_i|\rho|n_j\rangle = \begin{pmatrix} f_{\nu_e} & f_{e\mu} \\ f^*_{e\mu} & f_{\nu_\mu} \end{pmatrix}$$

→ Diagonal elements: real numbers: Phase-Space densities

→ Off-diagonal elements: complex numbers: Macroscopic Overlap densities

$$f_r = \frac{1}{2}\left(f_{e\mu} + f^*_{e\mu}\right)$$ (Real part)

$$f_i = \frac{1}{2i}\left(f_{e\mu} - f^*_{e\mu}\right)$$ (Imaginary part)

Neutrino Oscillations and Collective Self-interactions

$$\frac{\partial f_{\nu_e}}{\partial t} + \mathbf{v}\cdot\frac{\partial f_{\nu_e}}{\partial \mathbf{r}} + \dot{\mathbf{p}}\cdot\frac{\partial f_{\nu_e}}{\partial \mathbf{p}} = -f_i\left(\frac{2\pi c}{L}\sin 2\theta + 2\beta\int(1-\cos\theta^{\mathbf{pq}})\left(f_r+\tilde{f}_r\right)d^3\mathbf{q}\right) + 2\beta f_r\int(1-\cos\theta^{\mathbf{pq}})\left(f_i+\tilde{f}_i\right)d^3\mathbf{q} + C_{\nu_e}$$

$$\frac{\partial f_{\nu_\mu}}{\partial t} + \mathbf{v}\cdot\frac{\partial f_{\nu_\mu}}{\partial \mathbf{r}} + \dot{\mathbf{p}}\cdot\frac{\partial f_{\nu_\mu}}{\partial \mathbf{p}} = f_i\left(\frac{2\pi c}{L}\sin 2\theta + 2\beta\int(1-\cos\theta^{\mathbf{pq}})\left(f_r+\tilde{f}_r\right)d^3\mathbf{q}\right) - 2\beta f_r\int(1-\cos\theta^{\mathbf{pq}})\left(f_i+\tilde{f}_i\right)d^3\mathbf{q} + C_{\nu_\mu}$$

$$\frac{\partial f_r}{\partial t} + \mathbf{v}\cdot\frac{\partial f_r}{\partial \mathbf{r}} + \dot{\mathbf{p}}\cdot\frac{\partial f_r}{\partial \mathbf{p}} = f_i\Big[\frac{2\pi c}{L}(A-\cos 2\theta) + \beta\int(1-\cos^{\mathbf{pq}})\left(f_{\nu_e}-\tilde{f}_{\nu_e}-f_{\nu_\mu}+\tilde{f}_{\nu_\mu}\right)d^3\mathbf{q}\Big] + \left(f_{\nu_e}-f_{\nu_\mu}\right)\beta\int(1-\cos\theta^{\mathbf{pq}})\left(\tilde{f}_i-f_i\right)d^3\mathbf{q}$$

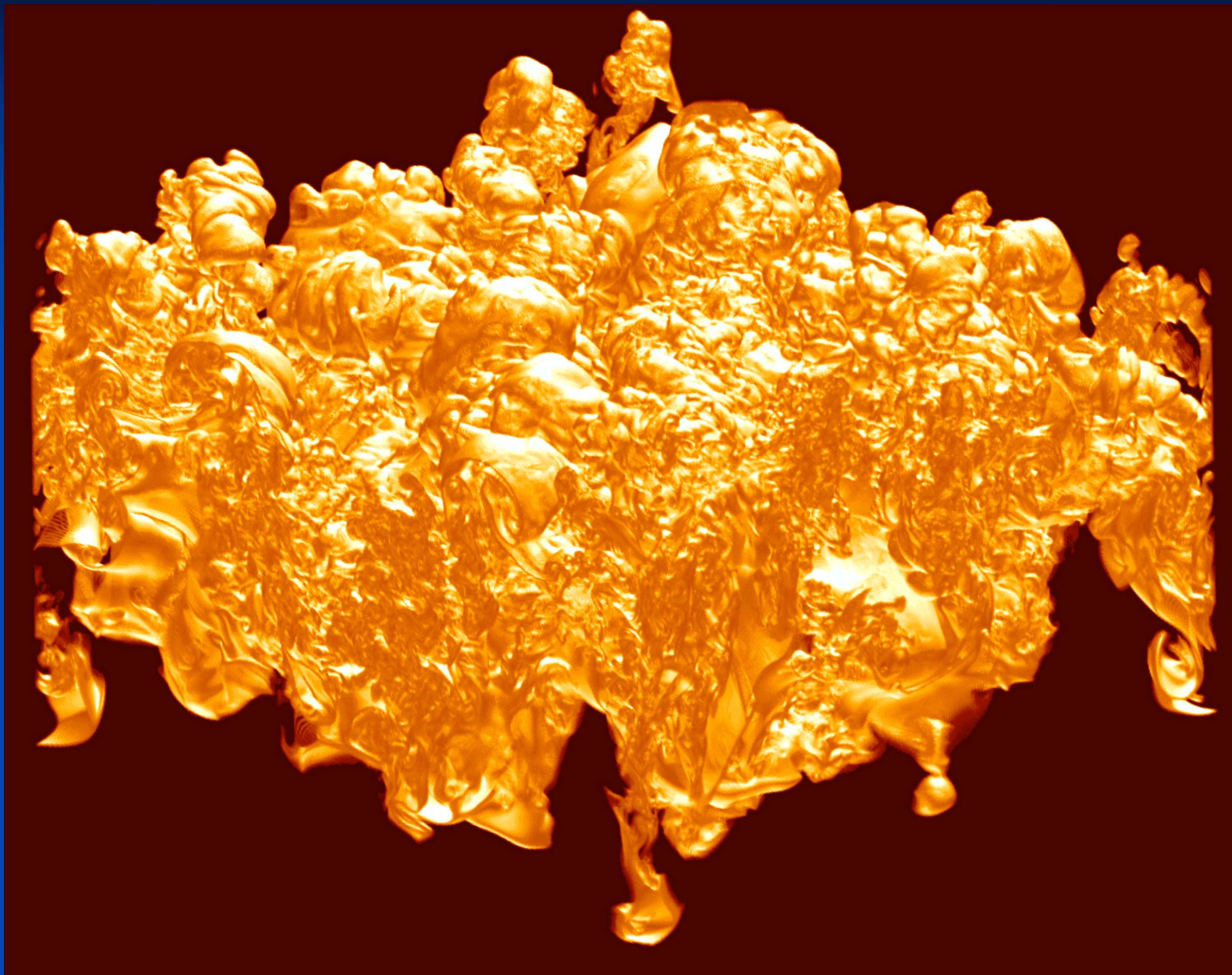
$$\frac{\partial f_i}{\partial t} + \mathbf{v}\cdot\frac{\partial f_i}{\partial \mathbf{r}} + \dot{\mathbf{p}}\cdot\frac{\partial f_i}{\partial \mathbf{p}} = \left(f_{\nu_e}-f_{\nu_\mu}\right)\left[\frac{\pi c}{L}\sin 2\theta + \beta\int(1-\cos^{\mathbf{pq}})\left(f_r-\tilde{f}_r\right)d^3\mathbf{q}\right] - f_r\Big[\frac{2\pi c}{L}(A-\cos 2\theta) + \beta\int(1-\cos^{\mathbf{pq}})\left(f_{\nu_e}-\tilde{f}_{\nu_e}-f_{\nu_\mu}+\tilde{f}_{\nu_\mu}\right)d^3\mathbf{q}\Big]$$

6 species x 6 species = 36
transport densities/variables!

$$L = \frac{4\pi\hbar c\varepsilon}{\Delta m^2 c^4} \qquad A = \left(\frac{L}{\pi c}\right)\frac{2\sqrt{2}G_F}{\hbar}n_e(\mathbf{r})$$

Type Ia (Thermonuclear) Supernova Explosions

Turbulent Thermonuclear Flame Front



White Dwarf Deflagration

Resolution: 6 km

Initial Bubble Radius: 25 km

Ignition Offset: 100 km

Variable 1: Density [1.5e+07 - 2.0e+07]

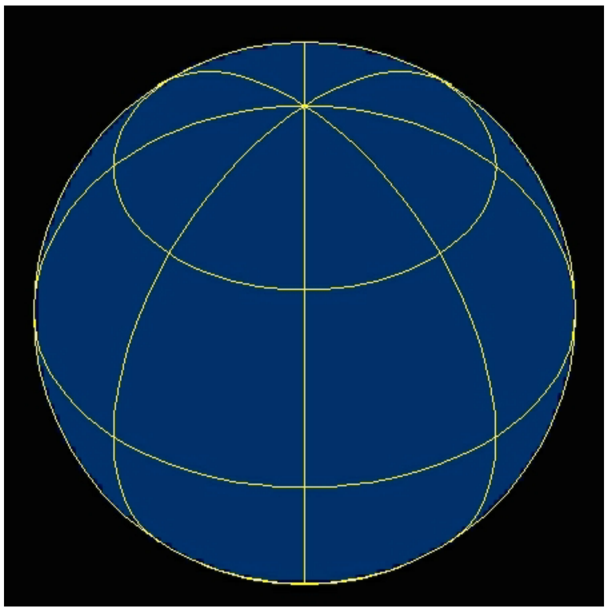
Variable 2: Reaction Progress [0.0 - 1.0]

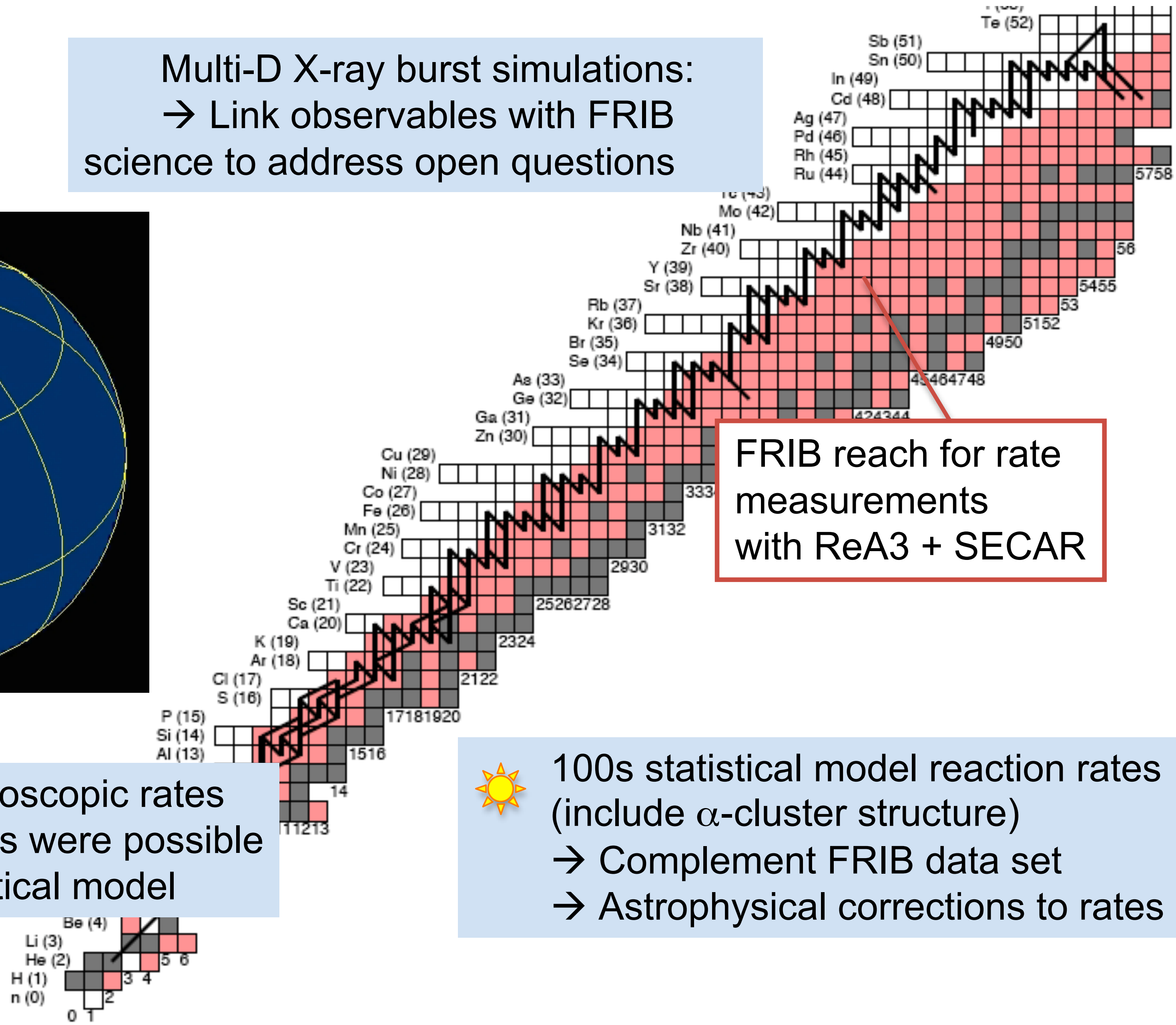
X-Ray Bursts - The rp-Process

Understanding the X-ray sky: rp-process in X-ray bursts

Multi-D X-ray burst simulations:
→ Link observables with FRIB science to address open questions

A. Spitkovsky



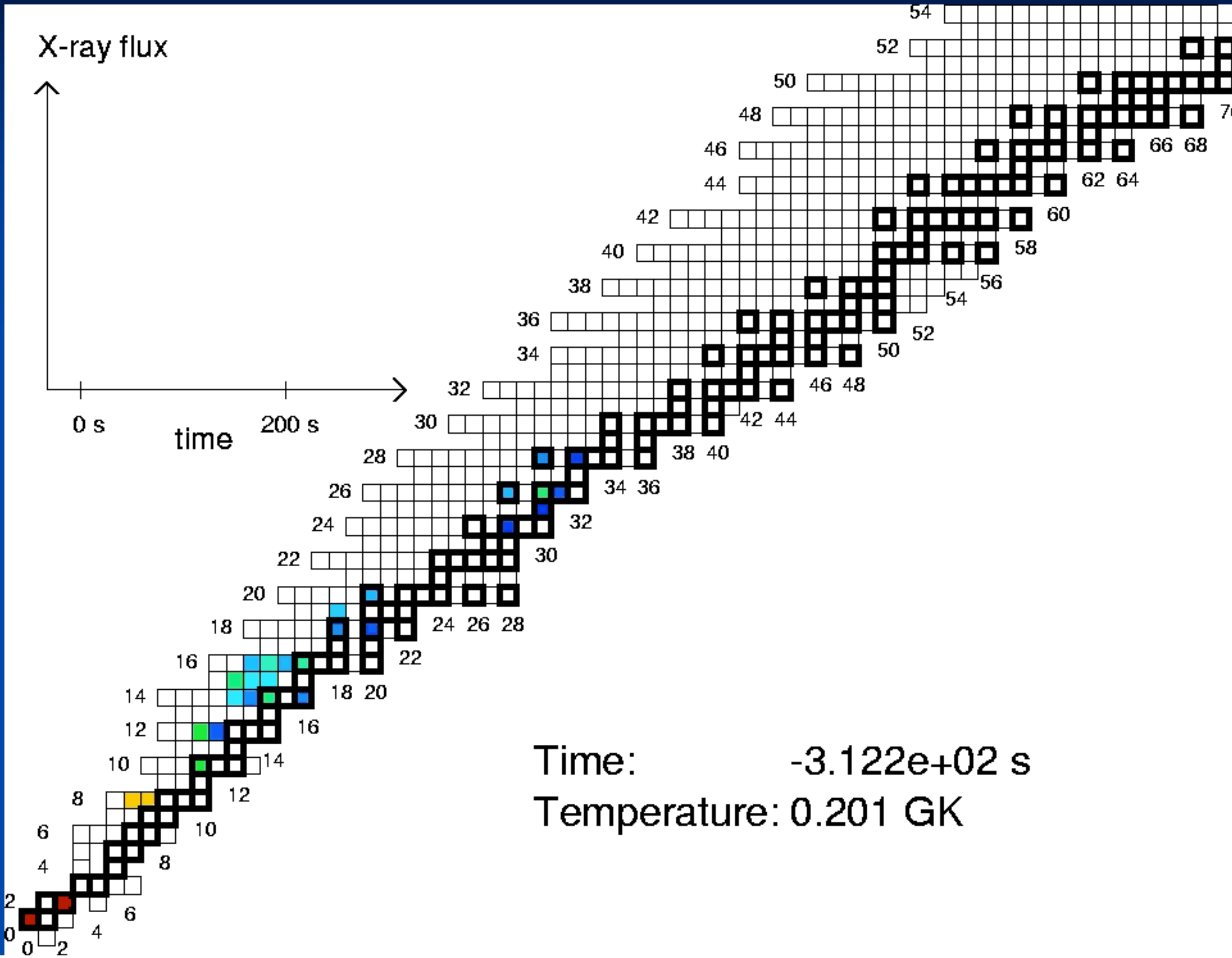


FRIB reach for rate measurements with ReA3 + SECAR

ab-initio or microscopic rates
→ Reliable rates were possible
→ Inform statistical model

100s statistical model reaction rates (include α-cluster structure)
→ Complement FRIB data set
→ Astrophysical corrections to rates

X-Ray Burst rp-Process Nucleosynthesis



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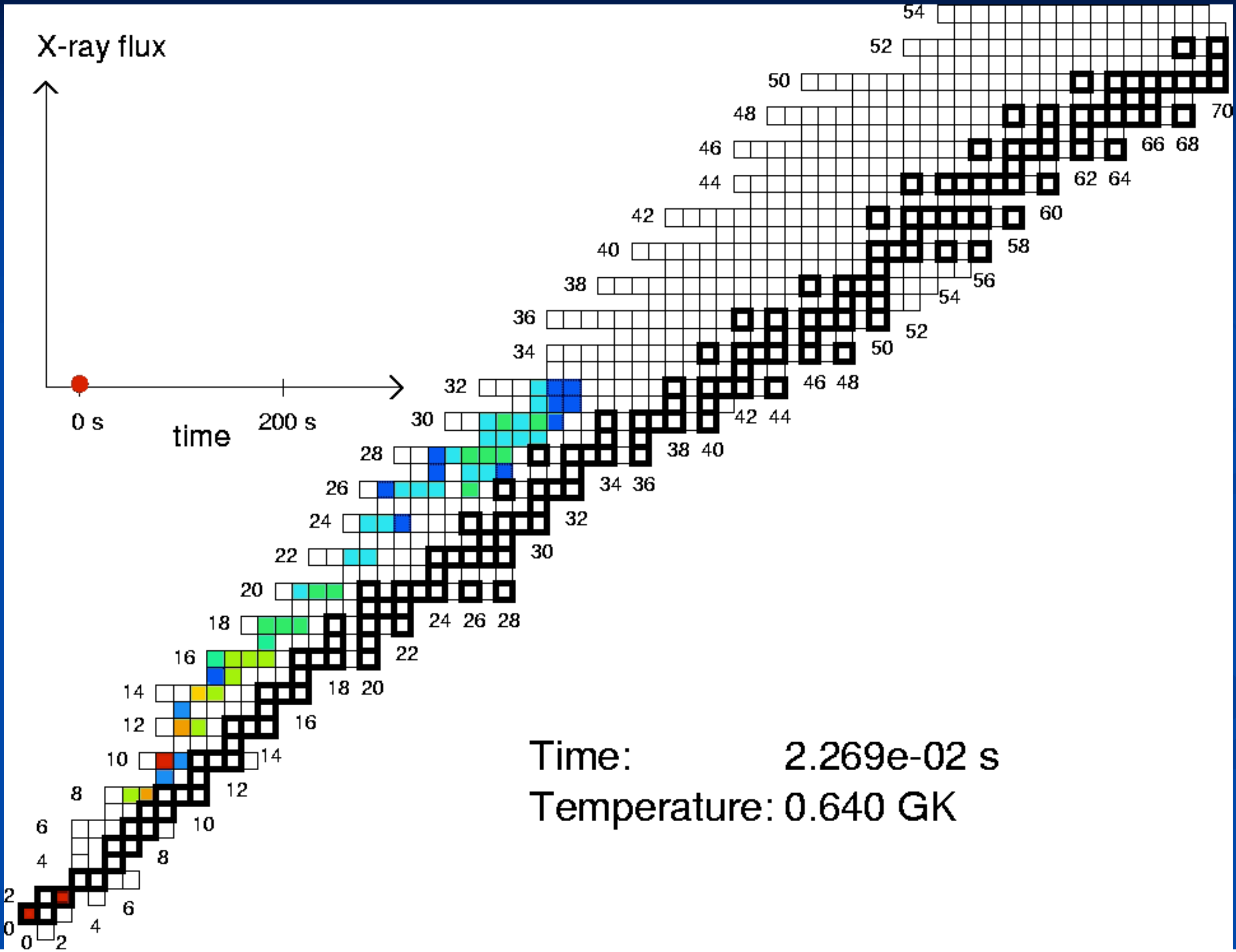

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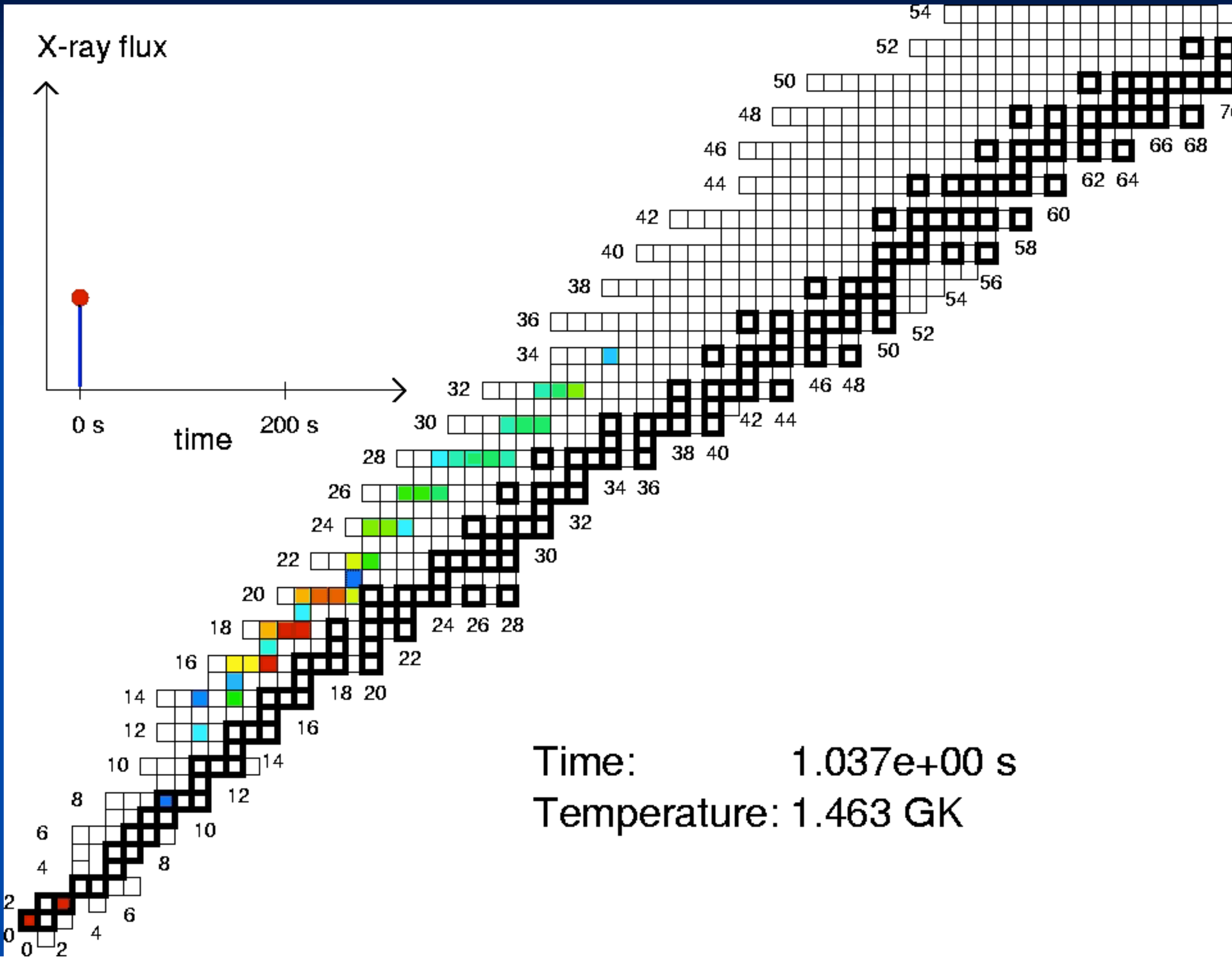

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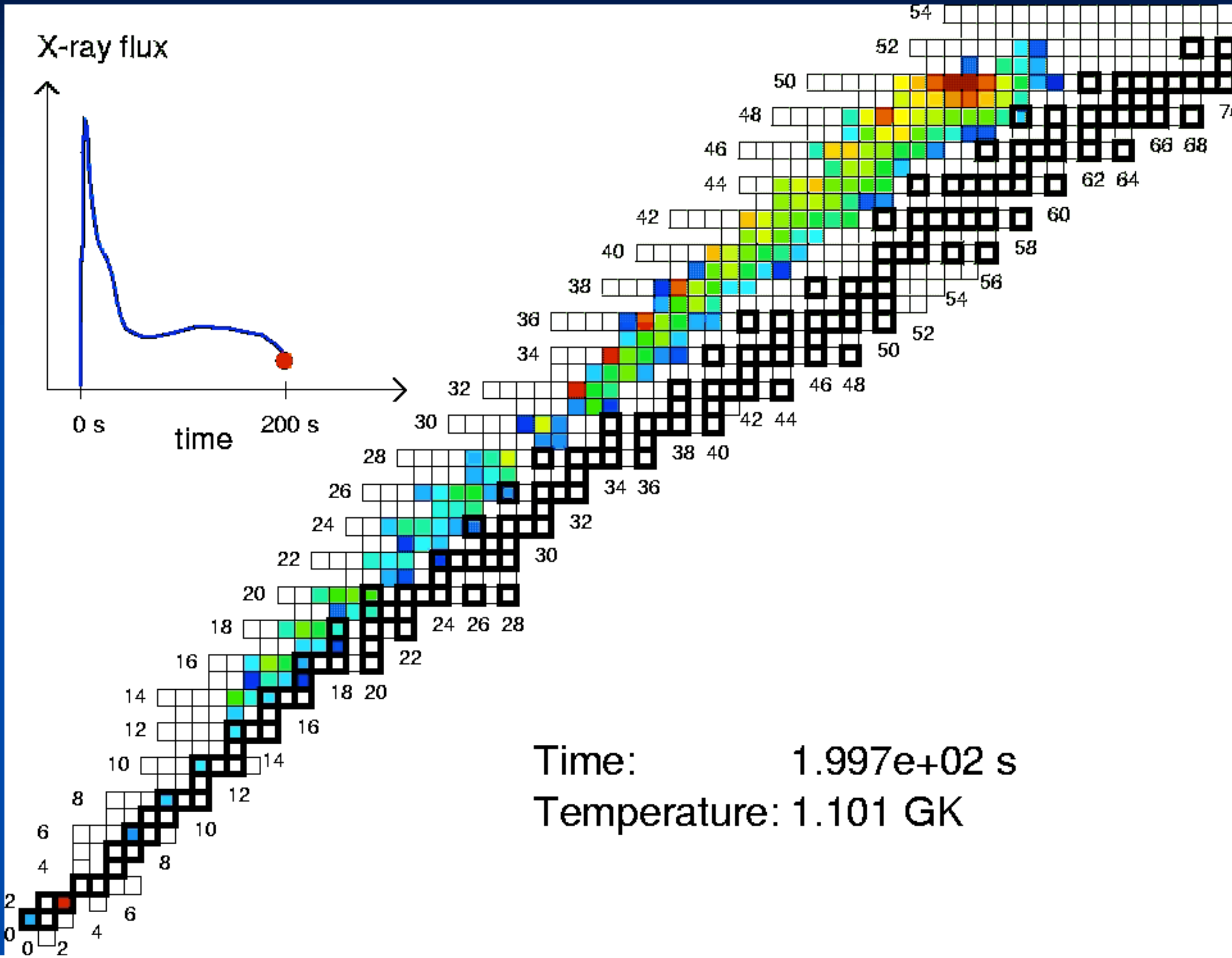

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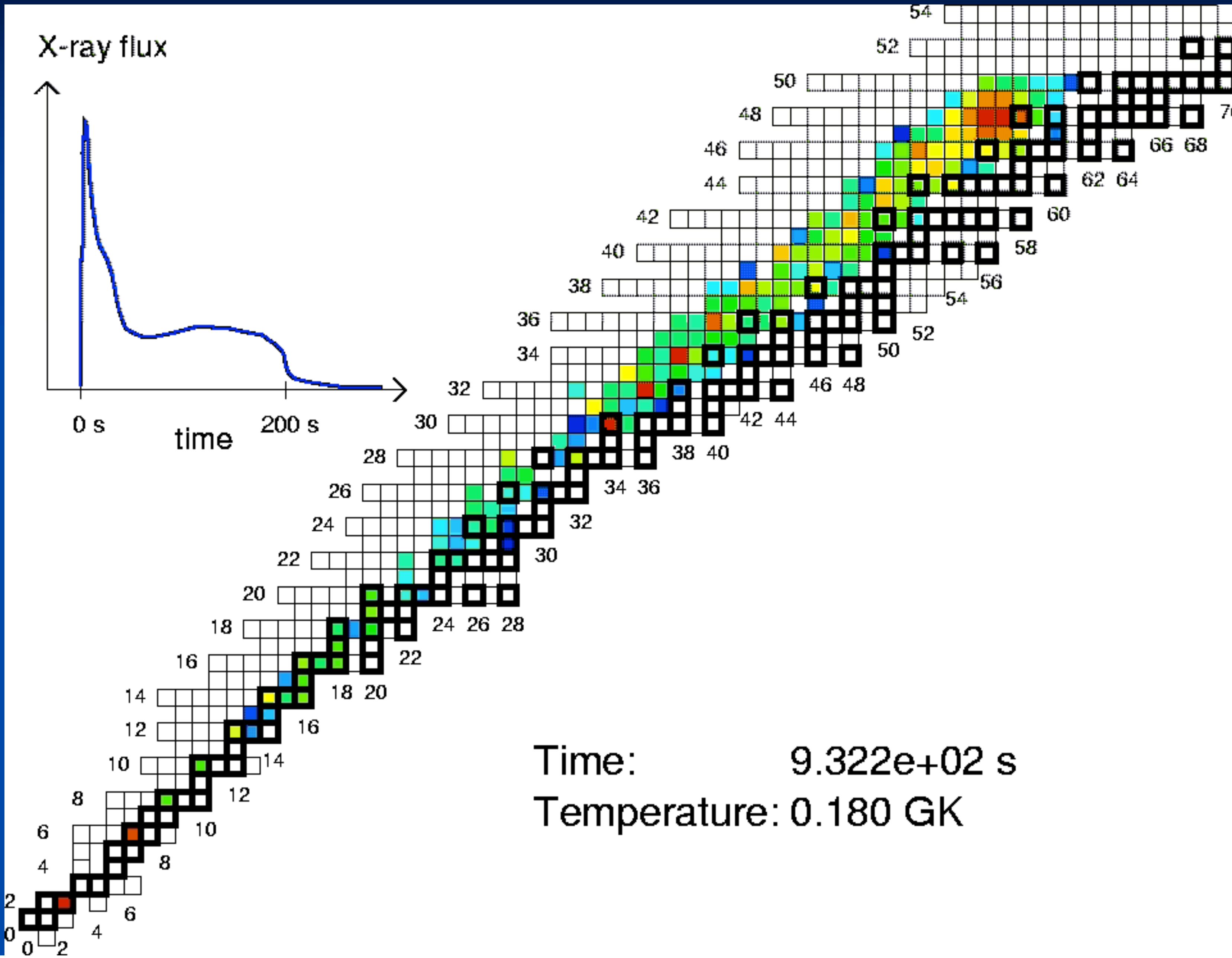


Nuclear Reaction Rate Calculations

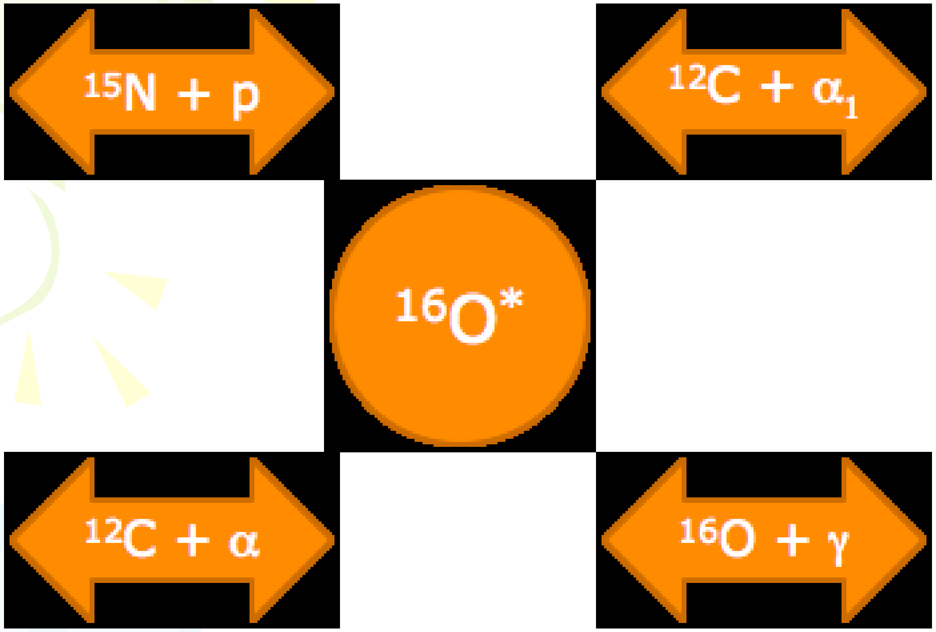
- General mathematical formalism for characterizing low-energy reaction cross sections

- Extrapolate cross sections to nearby energies but REQUIRES experimental data for constraint

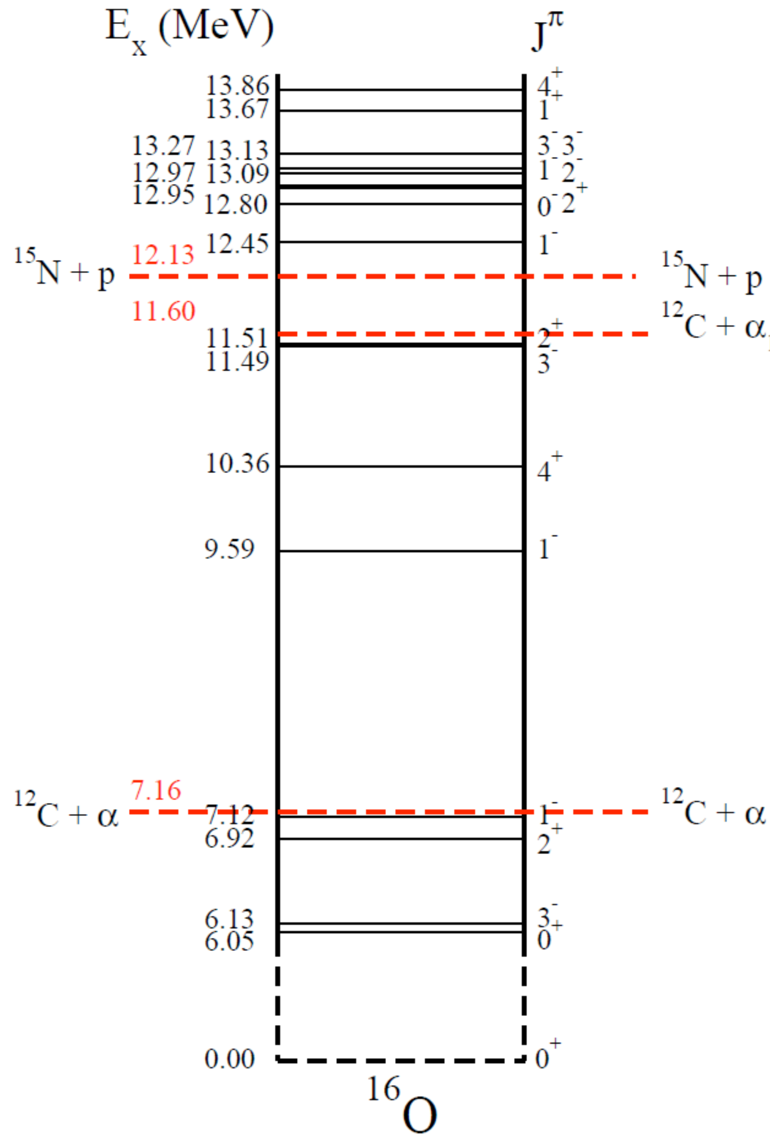
- Most straightforward for Compound Nucleus type reactions

- May be applied to other reaction types using approximations:

a) Radiative Capture
b) Beta-delayed particle emission



$^{15}N(p,\gamma)^{16}O$
$^{12}C(\alpha,\alpha)^{12}C$
$^{12}C(\alpha,\alpha)^{12}C$
$^{12}C(\alpha,p)^{15}N$
$^{12}C(\alpha,\gamma)^{16}O$
$^{15}N(p,p)^{15}N$
$^{15}N(p,\alpha)^{12}C$
$^{15}N(p,\alpha)^{12}C$



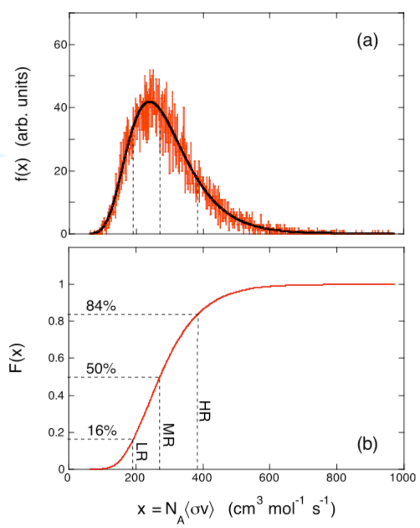
Multiple Channel Example

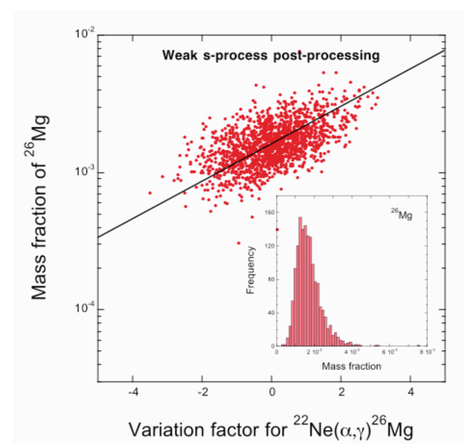
Nuclear Rate Calculations

Thermonuclear reaction rates are an essential ingredient for any stellar model.

A major obstacle in providing defensible uncertainties is that the rates are highly complex quantities derived from a multitude of nuclear properties extracted from laboratory measurements.

A solution to this challenge, devised recently by Iliadis and collaborators, is STARLIB which contains Monte Carlo sampled probability densities of each rate at each temperature.



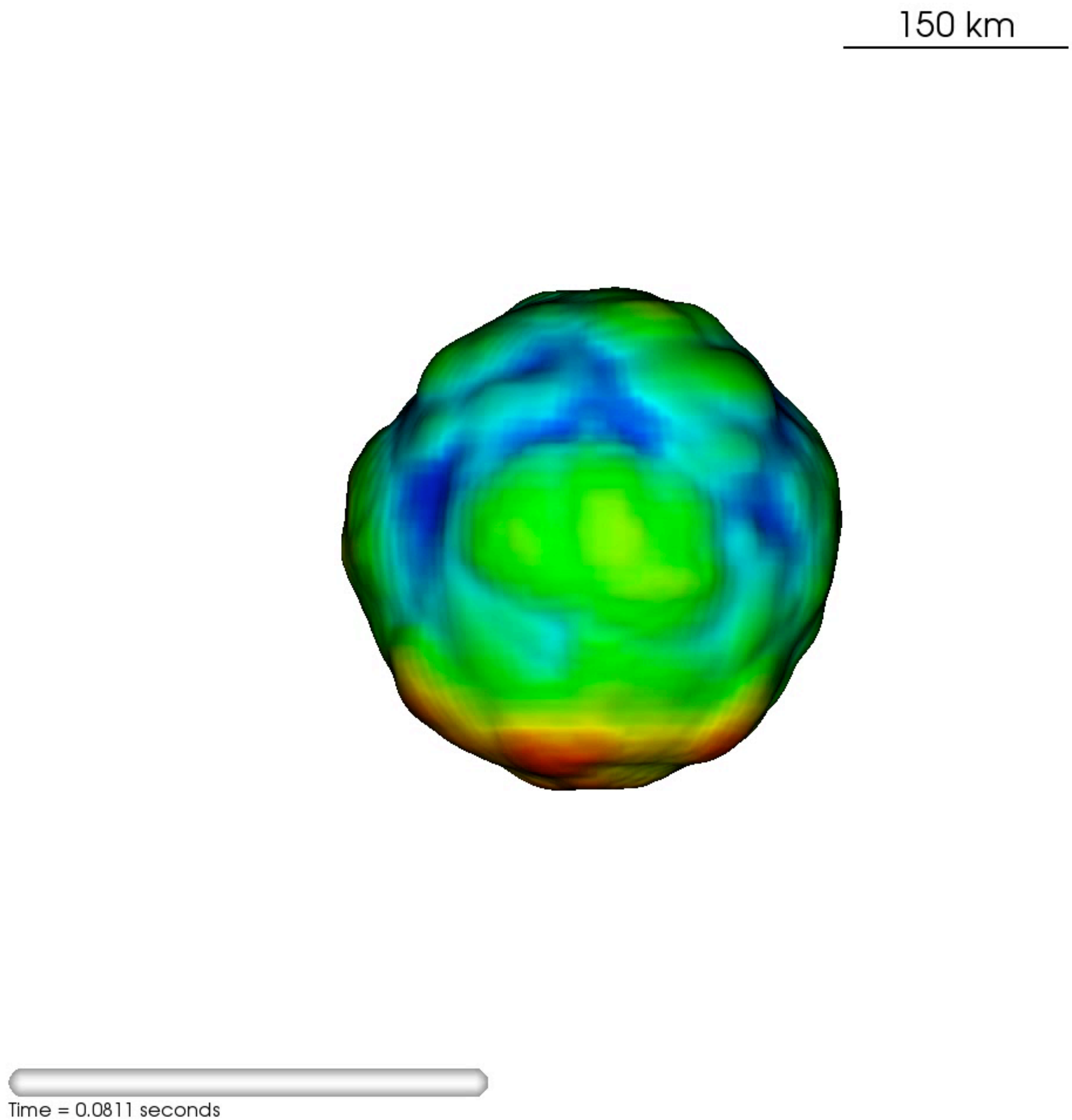


The MESA Stellar Evolution Code currently has over 400 registered users across the globe, with many users at D.O.E nuclear physics sponsored programs.

MESA employs modern numerical approaches and is written with present and future shared-memory, multi-core, multi-thread and possibly hybrid architectures.

Computational Nuclear Astrophysics Addresses Key Experimental and Theoretical Goals of the Office of Nuclear Physics

- Computational nuclear astrophysics also supports important components of the DOE Office of Nuclear Physics Experimental program:
  - The astrophysics of neutron-rich nuclei is one of four scientific ``legs" of the Facility for Rare Isotope Beams (FRIB).
  - Supernova modeling efforts are important to the DOE's experimental Neutrino Physics program. The flagship experimental program in DOE's Intensity Frontier program includes a megadetector that could follow neutrino light curve of a CCSN
  - The Nuclear equation of state is a third intersection with the DOE experimental program: JLab measurements constrain the nuclear symmetry energy, and, thus, the EOS for neutron-rich matter
- Nuclear astrophysics entails sophisticated multi-dimensional numerical simulations employing the latest computational tools and the most powerful supercomputers of the DOE complex to address key goals of the Office of Nuclear Physics.



150 km
Time = 0.0811 seconds

Sample Computational Requirements for Future Core-Collapse Supernova Simulations

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Kotake et al. 2012

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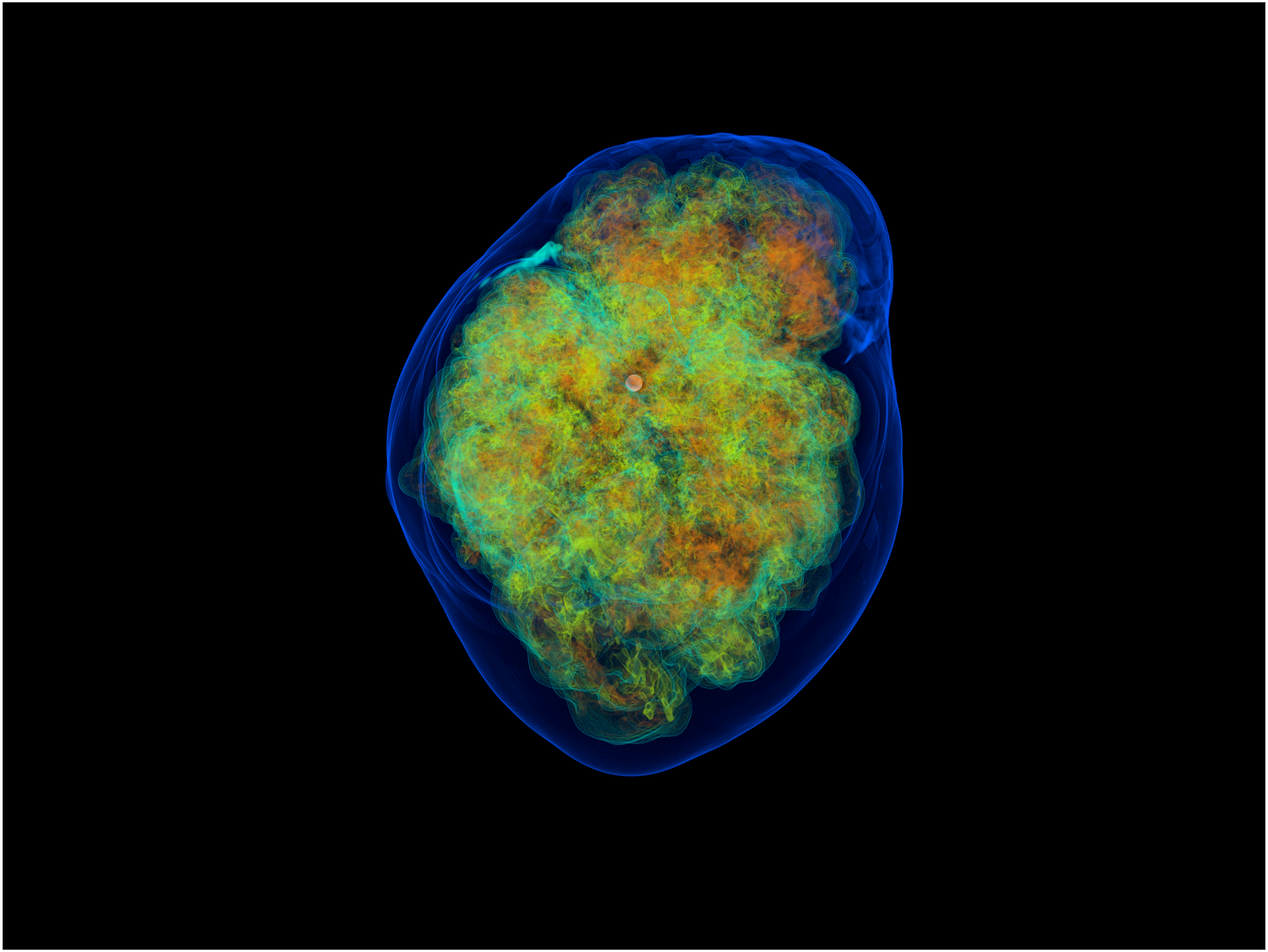
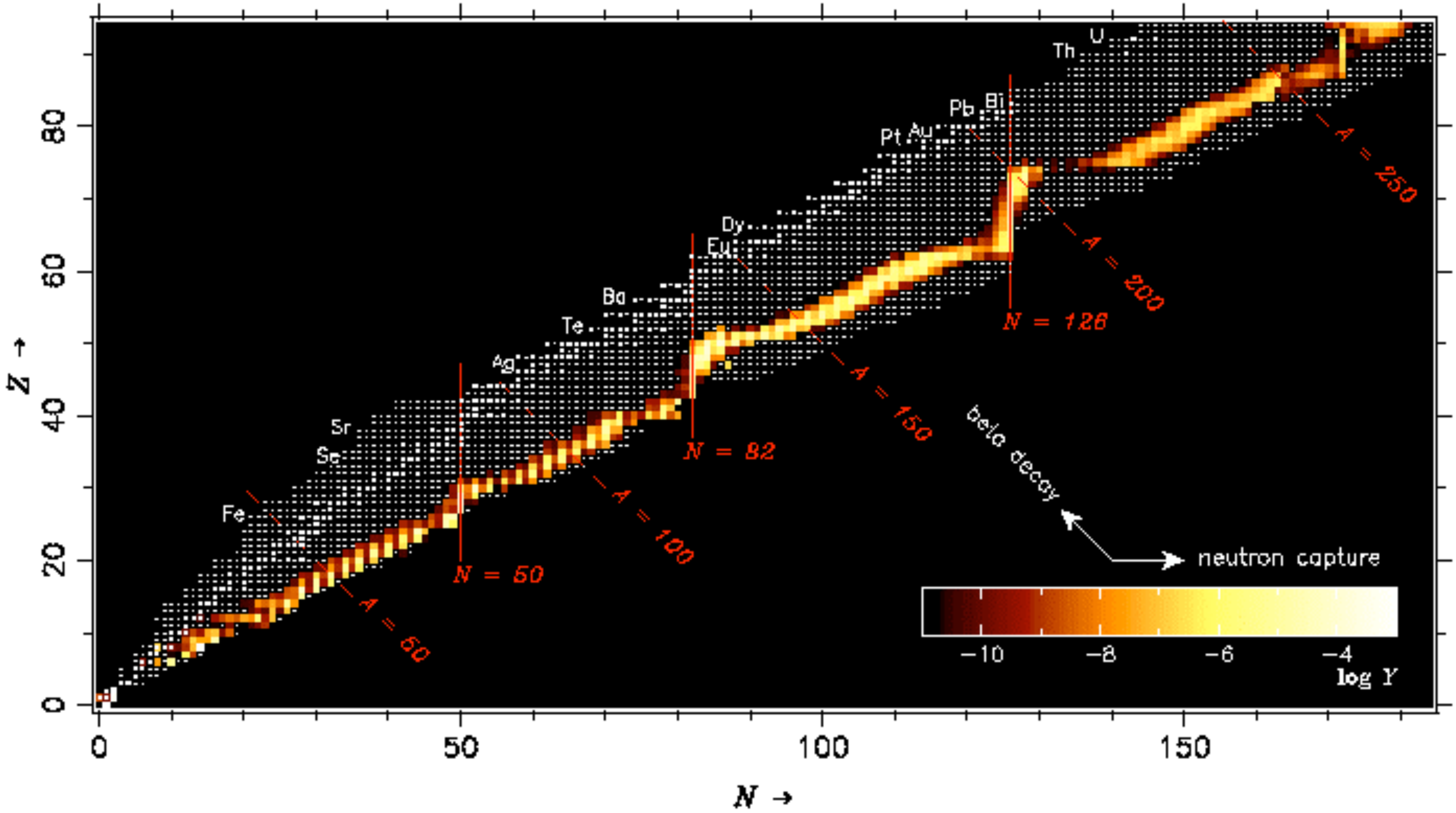
- 2020 (heroic 3D) - ~$10^{8\text{-}9}$ CPU-hours per run; $10^{5\text{-}6}$ cores; >10 Pbytes memory




Time:-0.282

R-Process Nucleosynthesis

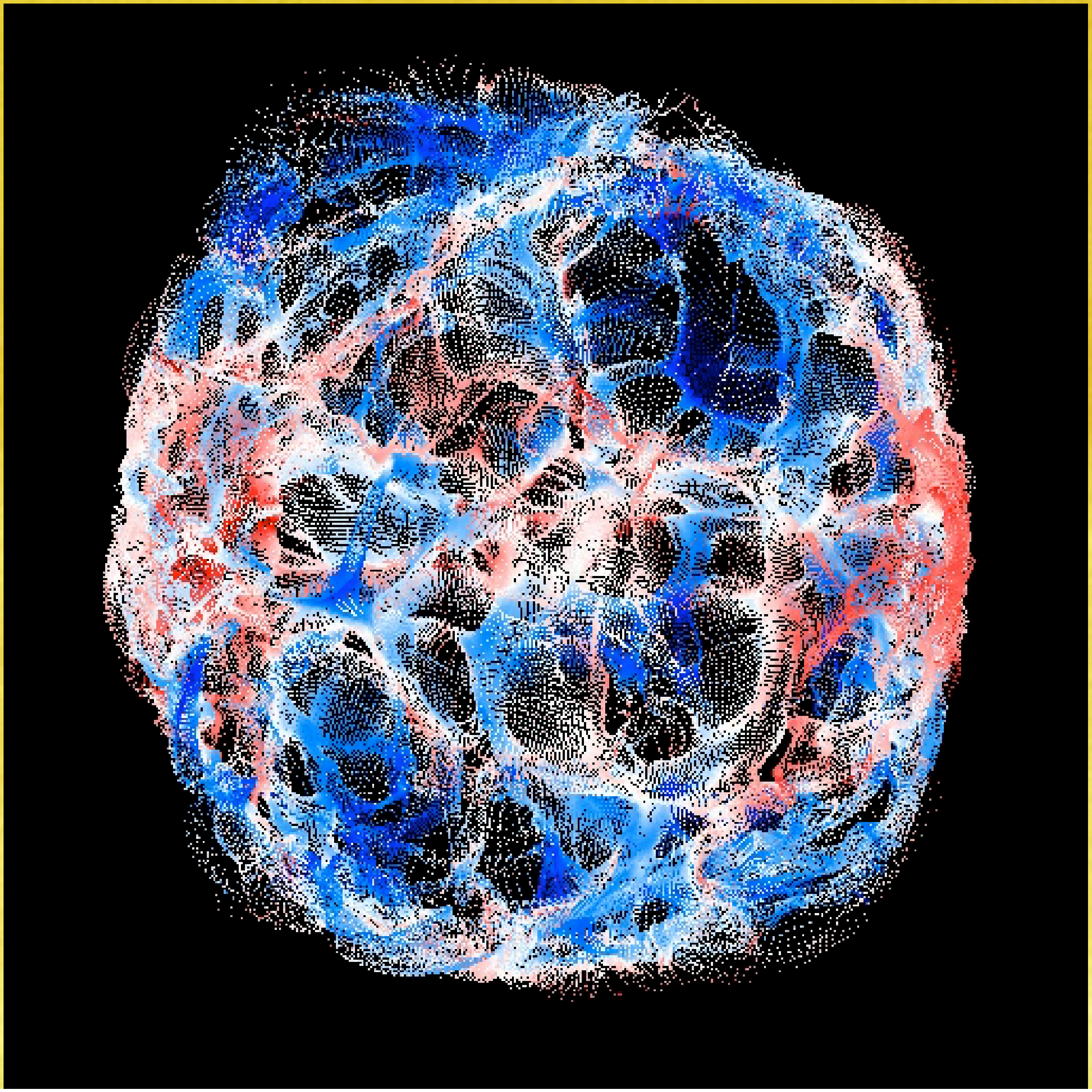


Compare calculated results with abundance observations ?

→ Masses, half-lives, n-capture rates of very unstable, exotic nuclei need to be known

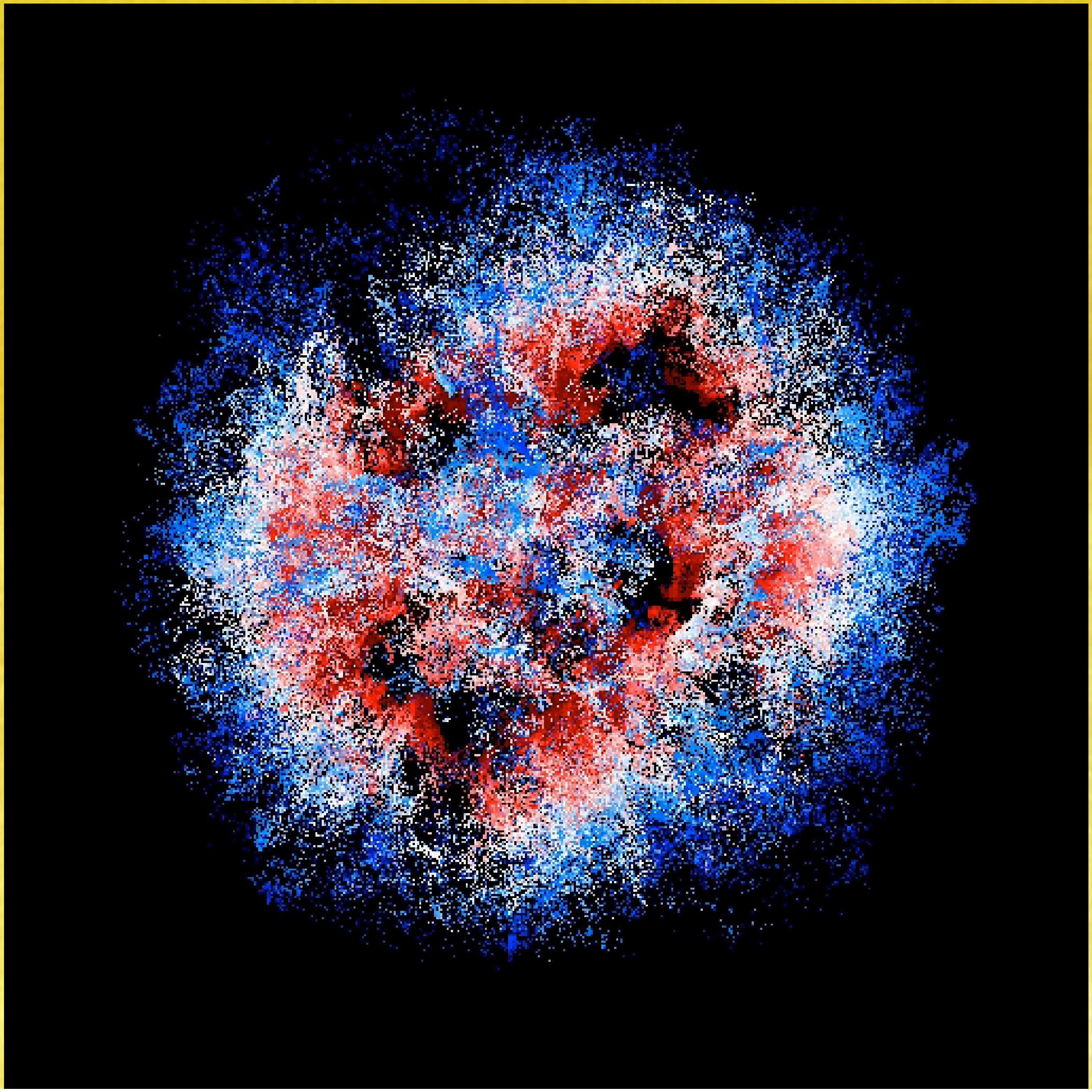
→ Need experiments and nuclear theory

Lagrangian Particle Advection Through the Shock - Heating Distribution in 3D - Early advection



Lagrangian Particle Advection Through the Shock - Heating Distribution in 3D

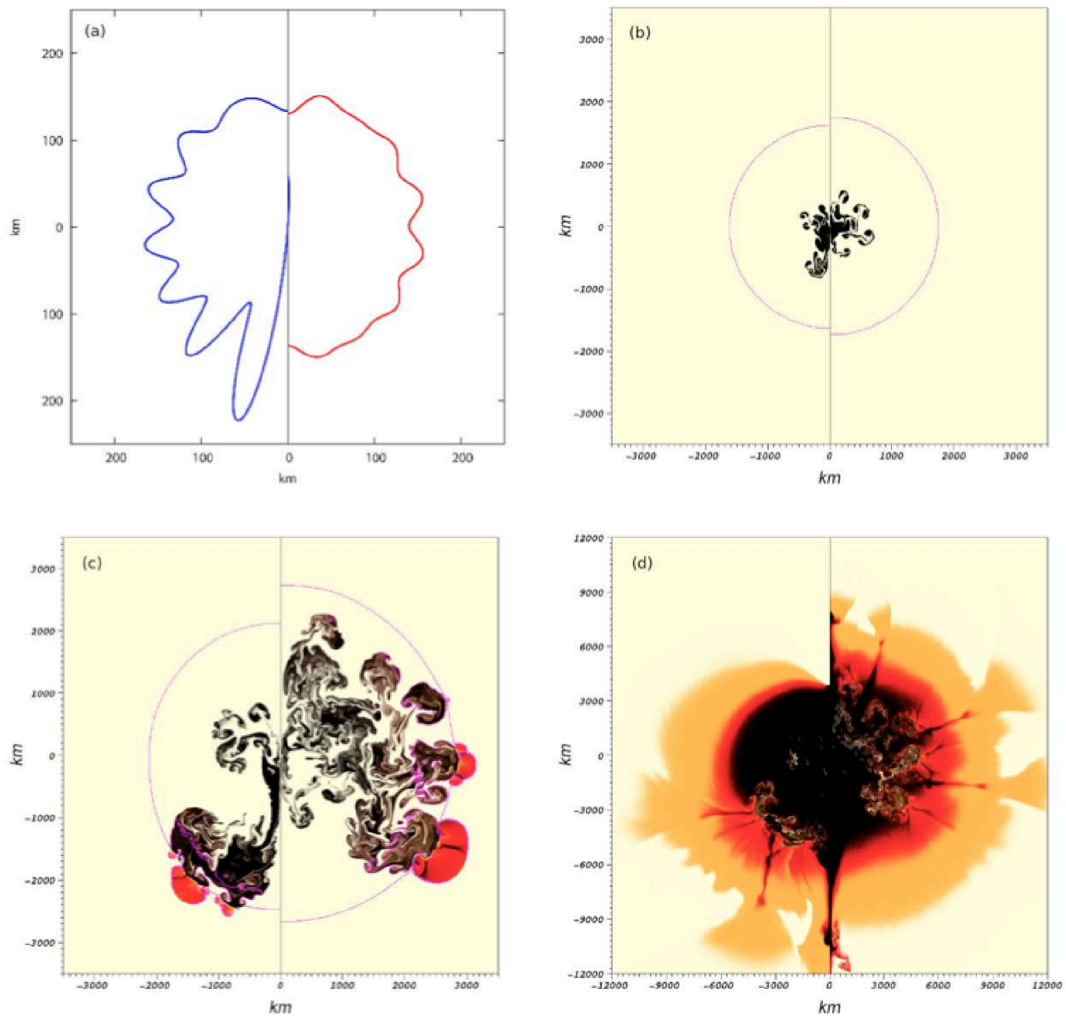
FRAME 3:



Type Ia Supernova Facts

- Thermonuclear Explosion of the entire accreting C/O White Dwarf; Explosion lasts ~1 second
- Emits mostly Optical and Infrared light
- Used as a primary yardstick for the Cosmology. Can be seen across the Universe: Indicates the Universe is Accelerating - Nobel Prize
- Significant element production and ejection: Iron (radioactive Nickel), Ca, Si, S, Ar, …
- Light lasts months; Peak Luminosity ~ 10^{21} Megatonnes of TNT/second (very bright)
- Complete disassembly; Energy > 10^{28} Mtonnes of TNT

The Progenitors of Type Ia supernovae, whose use as an empirical tool won this year’s Nobel Prize, are unknown. Identifying the nucleosynthetic signatures in their spectra of different progenitors channels is needed to reduce the uncertainty in the distance measurements, and quantify the nature of the dark energy with increased precision.



X-Ray Burst rp-Process Nucleosynthesis