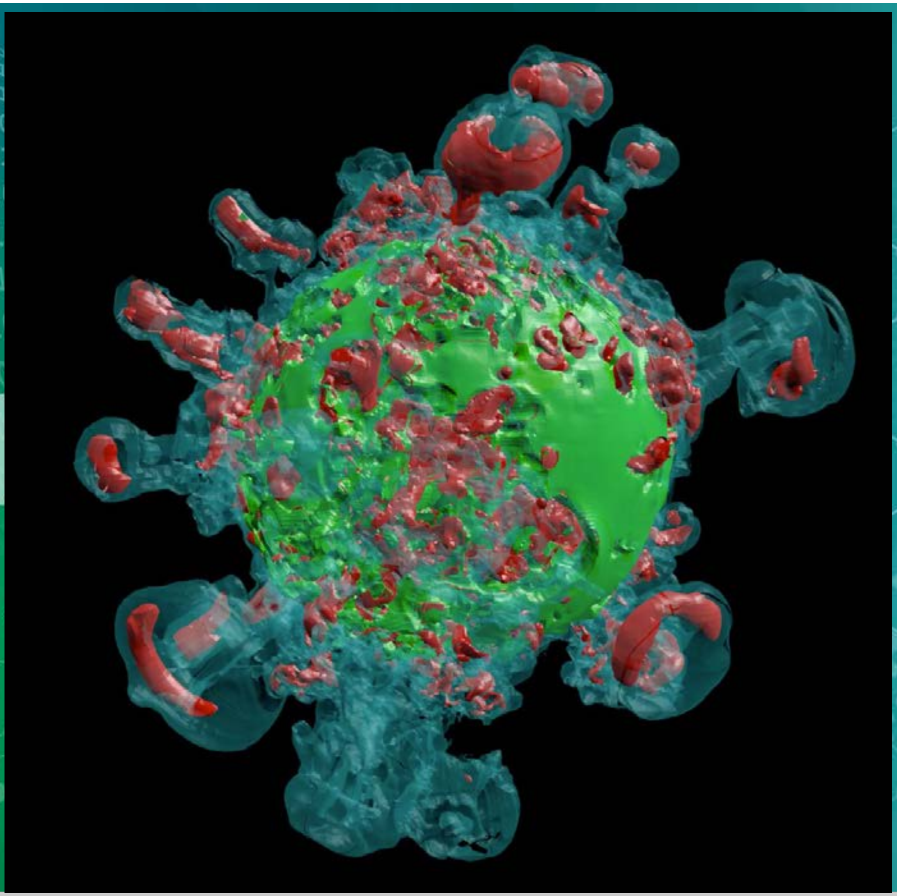
Using High-Performance Computing to Study Explosive Stellar Astrophysics

Bronson Messer

Director of Science
Oak Ridge Leadership Computing Facility
Oak Ridge National Laboratory



ORNL is managed by UT-Battelle LLC for the US Department of Energy

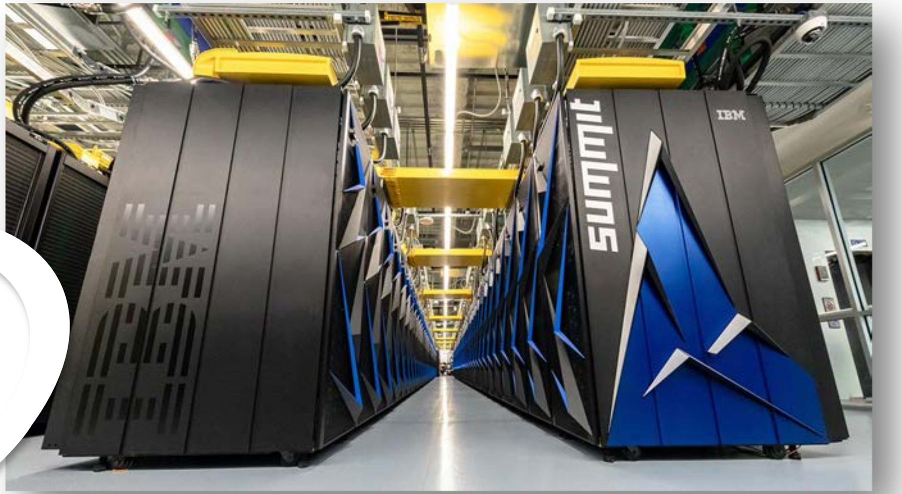
Oak Ridge Leadership Computing Facility (OLCF)

Mission: Deploy and operate the computational and data resources required to tackle global challenges

- Providing the resources to investigate otherwise inaccessible systems at every scale: from galaxy formation to supernovae to earth systems to automobiles to nanomaterials
- With our partners, deliver transforming discoveries in materials, biology, climate, energy technologies, and basic science

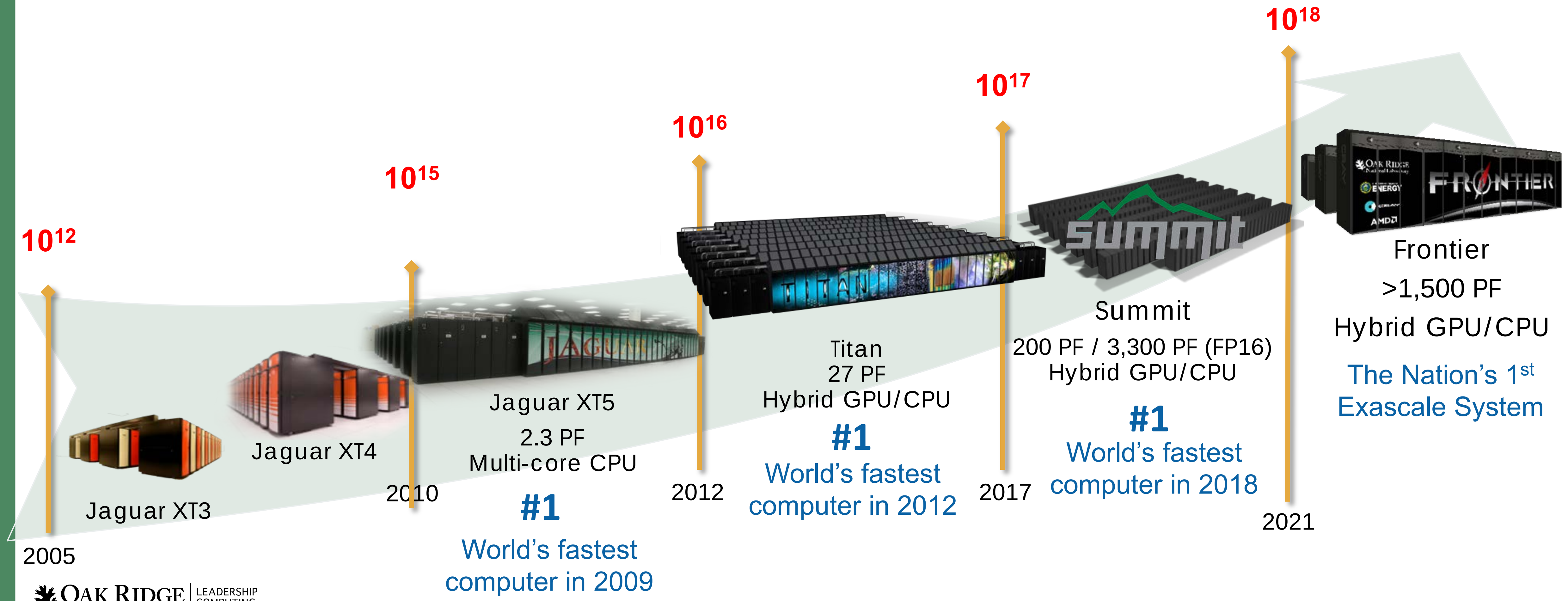
What is the Leadership Computing Facility (LCF)?

- Collaborative DOE Office of Science user-facility program at ORNL and ANL
- Mission: Provide the computational and data resources required to solve the most challenging problems.
- 2 centers/2 architectures to address diverse and growing computational needs of the scientific community
- Highly competitive user allocation programs (INCITE, ALCC).
- Projects receive 10x to 100x more resources than at other generally available centers.
- LCF centers partner with users to enable science and engineering breakthroughs (Liaisons, Catalysts).



Oak Ridge National Laboratory
Argonne National Laboratory

ORNL has had a Top 10 supercomputer in every year since the Leadership Computing Facility was founded in 2005. Jaguar, Titan, and Summit are the only DOE/SC systems to be ranked #1 on the TOP500 list of fastest computers.



ORNL Summit System Overview

System Performance

- Peak of 200 Petaflops (FP_{64}) for modeling and simulation
- Peak of 3.3 ExaOps (FP_{16}) for data analytics and artificial intelligence

The system includes

- 4,608 nodes
- Dual-rail Mellanox EDR InfiniBand network
- 250 PB IBM file system transferring data at 2.5 TB/s

Each node has

- 2 IBM POWER9 processors
- 6 NVIDIA Tesla V100 GPUs
- 608 GB of fast memory (96 GB HBM2 + 512 GB DDR4)
- 1.6 TB of NV memory

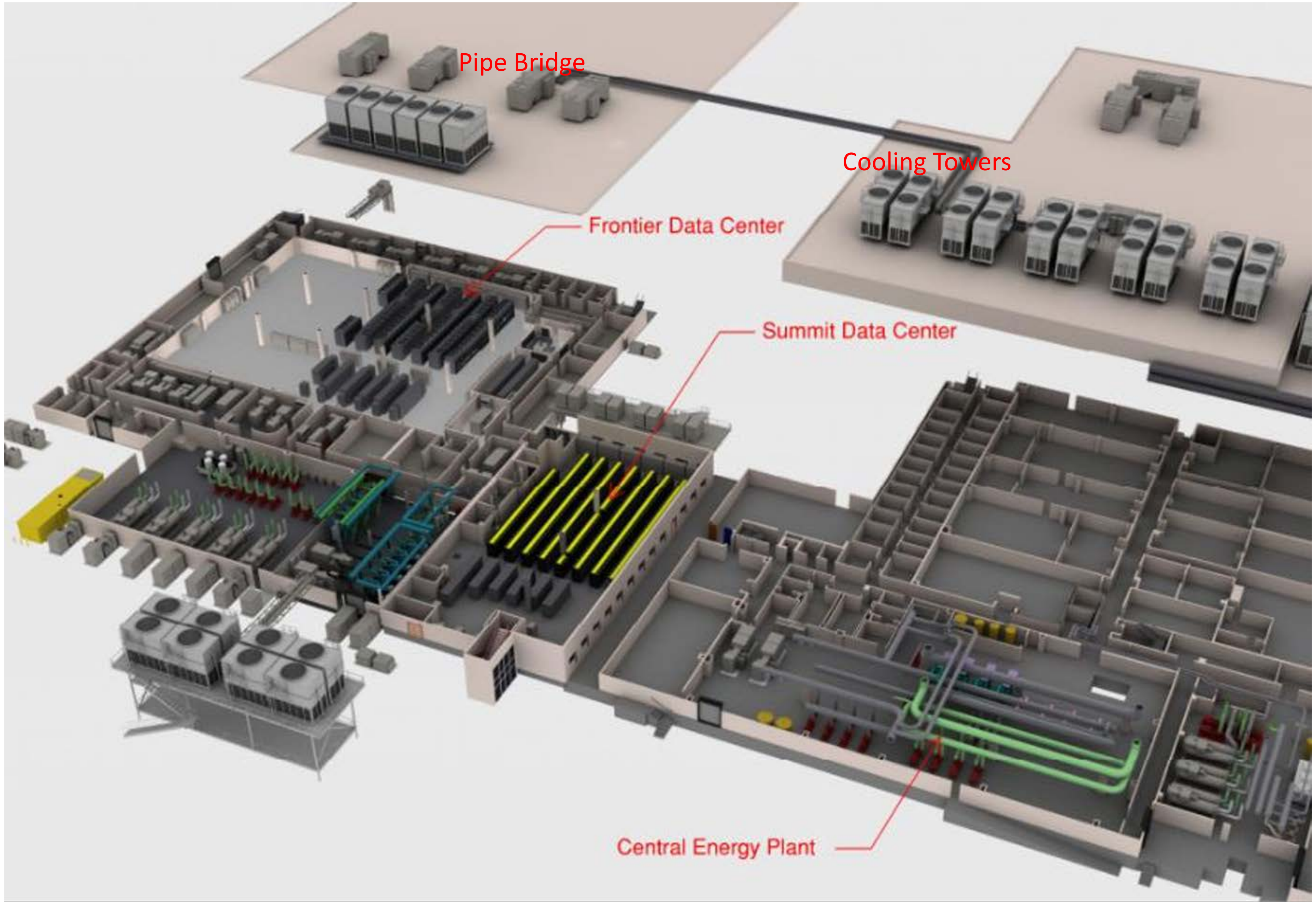
In 2021, Frontier will become the nation's first exascale computer

FRONTIER	
Peak Performance	>1.5 EF
Node	1 HPC and AI-optimized AMD EPYC CPU + 4 purpose-built AMD Radeon Instinct GPU
Memory	Approximately 10 PB of combined high bandwidth and DDR memory
On-node Interconnect	AMD Infinity Fabric Coherent memory across the node
System Interconnect	Cray four-port Slingshot network 100 GB/s
Topology	Dragonfly
Storage	2-4x performance and capacity of Summit's I/O subsystem.
Node-local NVMe	Yes

OLCF Data Centers

OLCF Virtual Tour

https://bit.ly/37bIL8v



1.2 Facility Upgrades Overview

Campus Power Upgrades

- Install new switch outside the ORNL computing complex
- Bring new 13.8kV feeders from a substation to the new switch

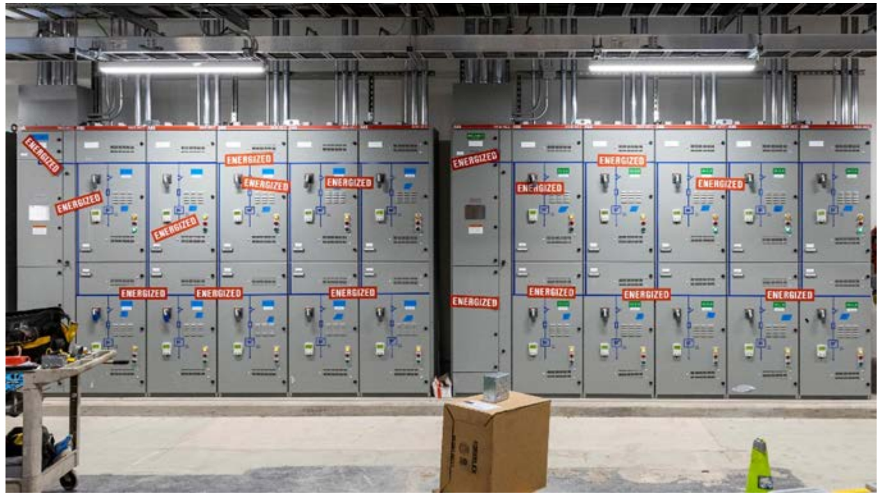
Infrastructure Enhancements

- Demolish existing offices and labs
- Bring power & cooling to the wall of the data center
  - Add 16 MW of new power, reuse 24 MW existing
  - Add 40 MW of new cooling capacity
    - new cooling towers
    - new piping
    - pipe bridge

Data Center Preparations

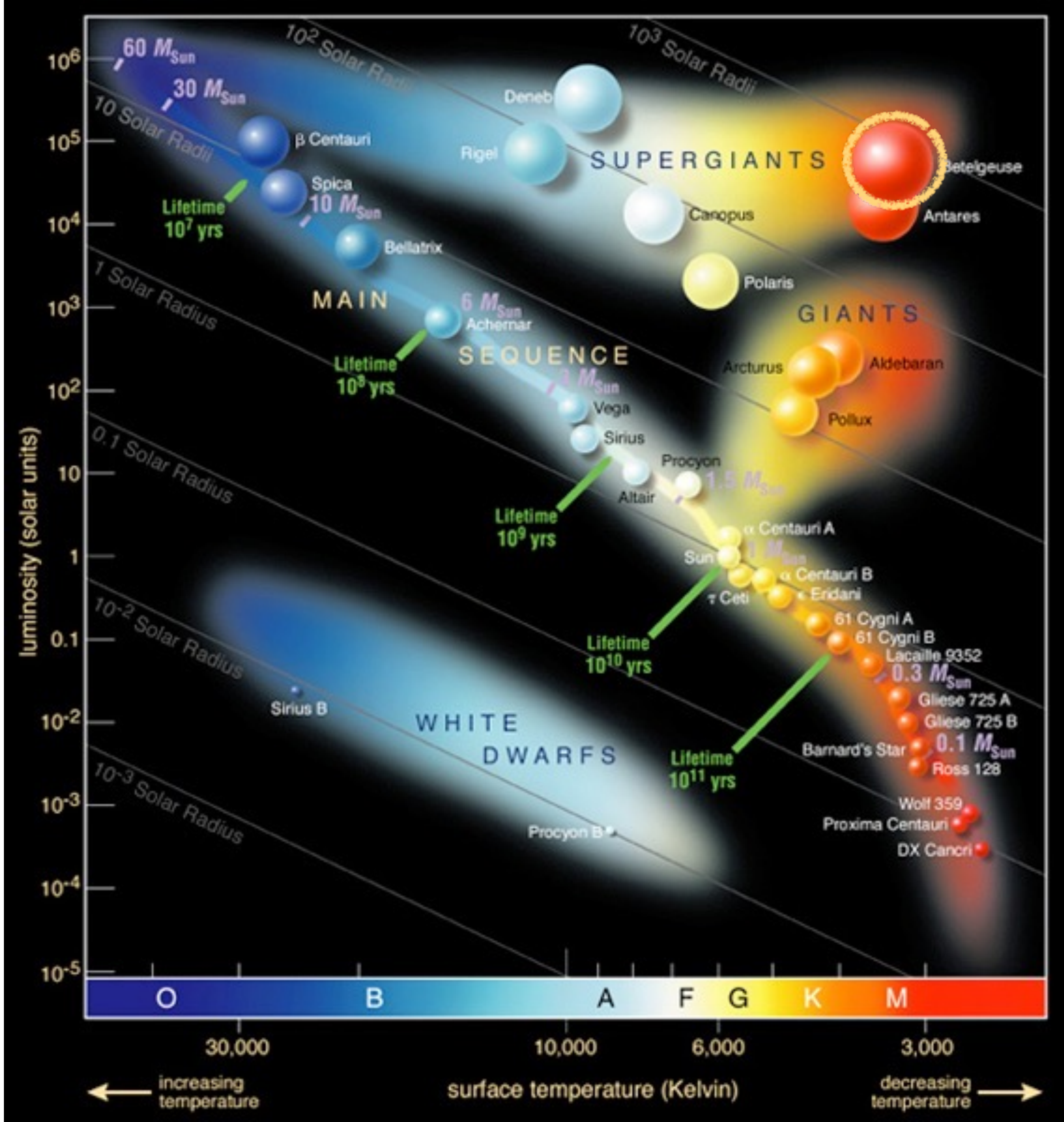
- Upgrade existing Titan room for Frontier
- Distribute power inside the data center
- Distribute cooling water inside the data center
- Fire protection and life safety-systems

Power and cooling are in place for the Frontier computer



Stars die?

- Stars are born, live, and die
- Different stars live very different lives
- Mass is destiny
  - The Sun will live for about 12 billion years
  - A star 15 times the size of the Sun will live for only about 10 million years

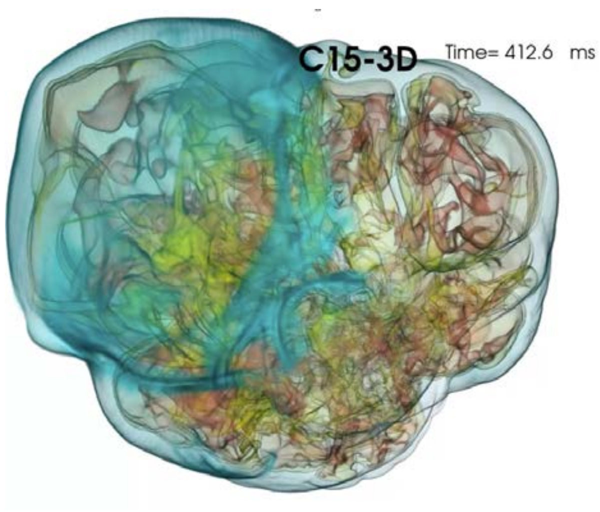


Betelgeuse - The "Martial Star"

- Where?

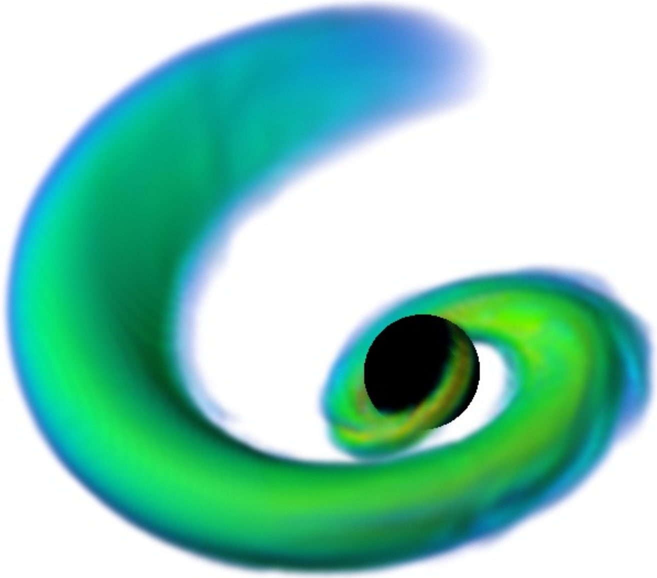
  The shoulder of Orion
- 8th brightest star in the night sky
- ~640 light years away --> one of largest and most luminous stars known
- ~20 $M_\odot$
- ~10 million(!) years old
- Betelgeuse will die in a supernova explosion. You'll know when it happens...

Stellar explosions - cosmic laboratories of physics



Core-collapse
supernova simulations

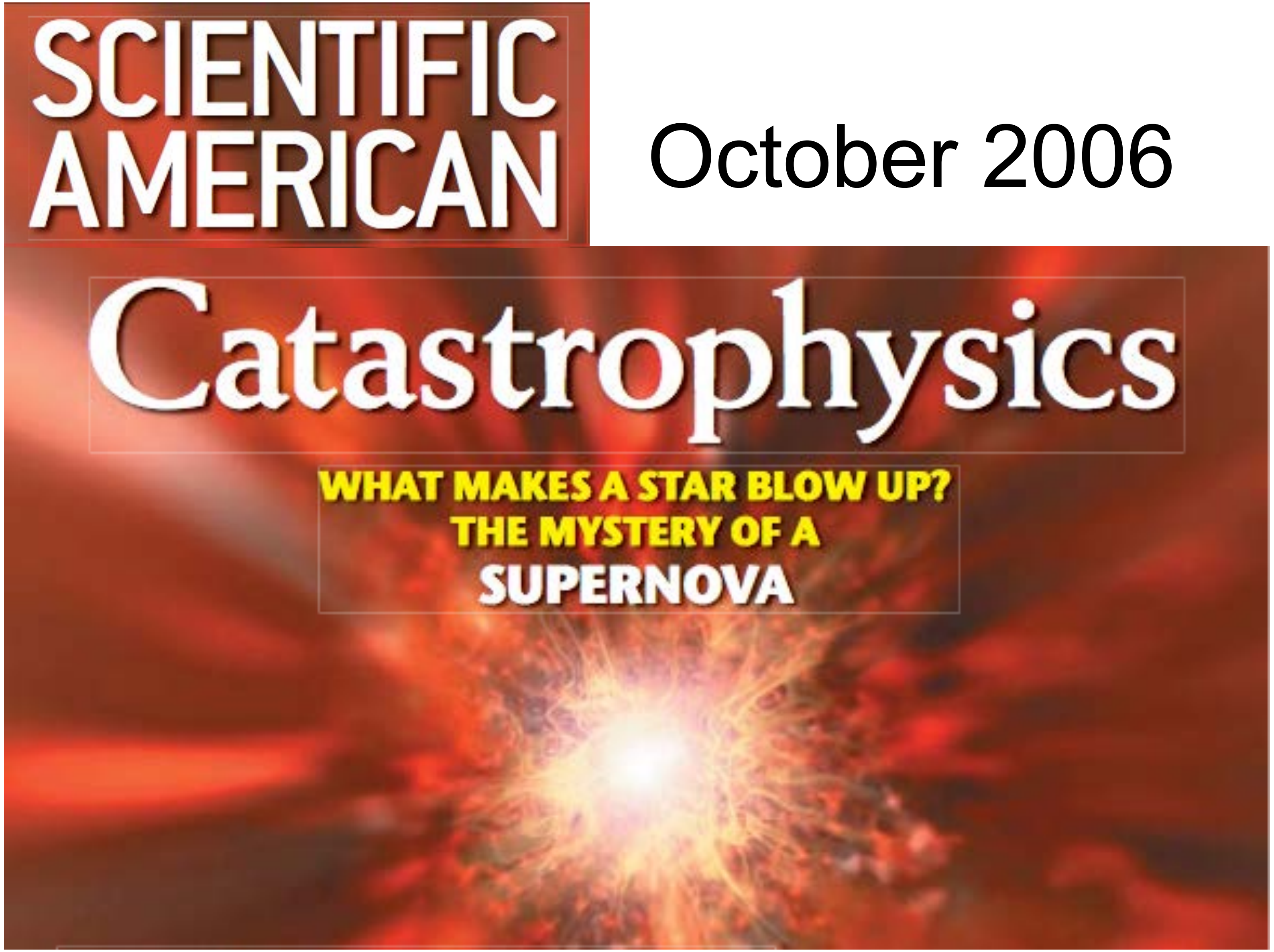
- What is the cosmic origin of the elements?
- What are the sources of gravitational waves?
- What is the nature of matter at extreme densities?
- How can we use stellar explosions to map out the expansion of the Universe (dark energy)?



neutron star mergers

And related phenomena:

Thermonuclear (Type Ia) supernovae
X-ray bursts (neutron star eruptions)
Gamma-ray bursts
Magnetar powered supernovae
Black hole formation + accretion



October 2006

How to Blow Up a Star

By Wolfgang Hillebrandt,
Hans-Thomas Janka
and Ewald Müller

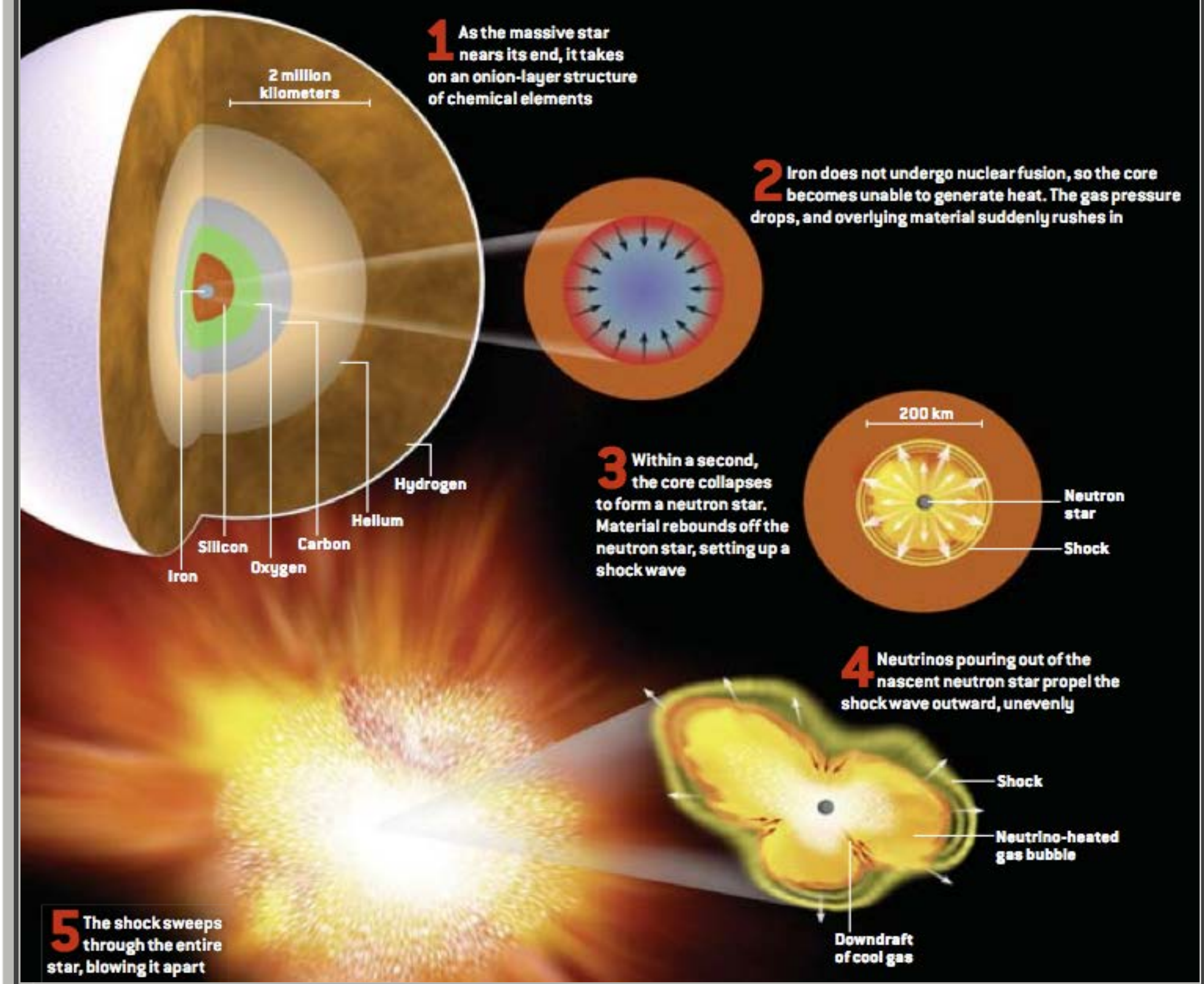
It is not as easy as you would think.

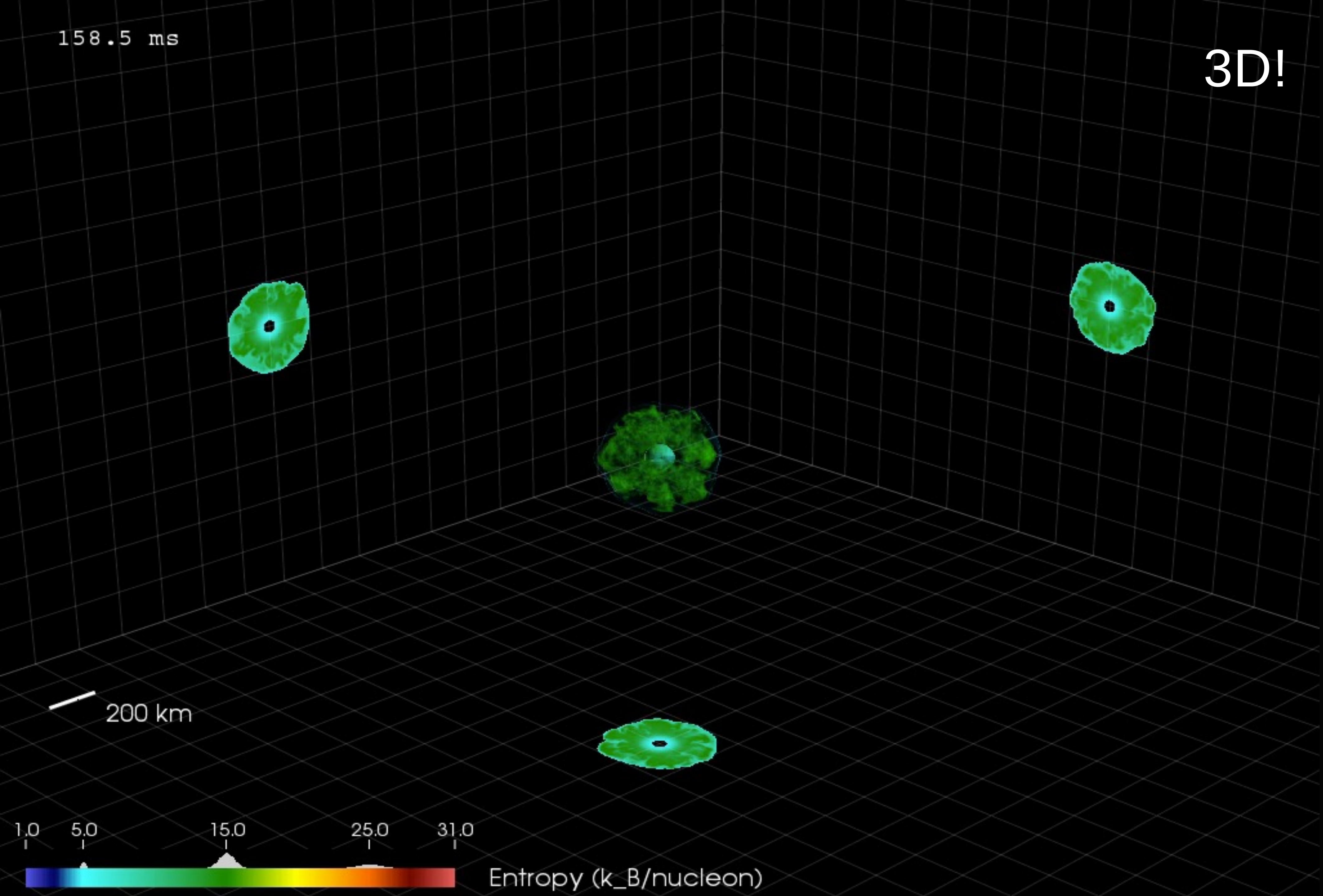
TEN SECONDS AFTER IGNITION, a thermonuclear flame has almost completed its incineration of a white dwarf star in this recent simulation. Sweeping outward from the deep interior (*cutaway*), the nuclear chain reaction has transformed carbon and oxygen (*lilac, red*) to silicon (*orange*) and iron (*yellow*). Earlier simulations, which were unable to track the turbulent motions, could not explain why stars exploded rather than dying quietly.

On November 11, 1572, Danish astronomer and nobleman Tycho Brahe saw a new star in the constellation Cassiopeia, blazing as bright as Jupiter. In many ways, it was the birth of modern astronomy—a shining disproof of the belief that the heavens were fixed and unchanging. Such "new stars" have not ceased to surprise. Some 400 years later astronomers realized that they briefly outshine billions of ordinary stars and must therefore be spectacular explosions. In 1934 Fritz Zwicky of the California Institute of Technology coined the name "supernovae" for them. Quite apart from being among the most dramatic events known to science, supernovae play a special role in the universe and in the work of astronomers: seeding space with heavy elements, regulating galaxy formation and evolution, even serving as markers of cosmic expansion.

Zwicky and his colleague Walter Baade speculated that the explosive energy comes from gravity. Their idea was that

Hillebrandt & Janka 2006 (Sci Am)




158.5 ms
3D!
200 km
1.0
5.0
15.0
25.0
31.0
Entropy (k_B/nucleon)

hydrodynamics

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

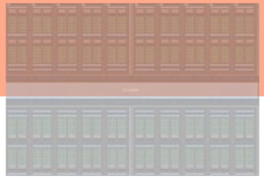
Methods: *Finite volume Godunov methods*

Extensions: GR magnetohydrodynamics

nuclear reactions

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

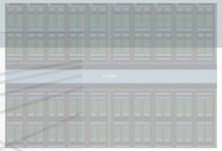
Methods: *Accelerated stiff ODE solvers with spectral deferred correction coupling to dynamics*



radiation transport

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

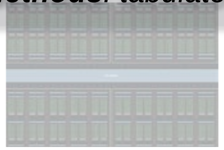
Methods: *implicit-explicit time integration w/ discontinuous Galerkin descritization of two-moment formulation. Monte Carlo methods for post-processing and refined closures.*



EoS

Requirements: nuclear high density equation of state

Methods: *tabulated*

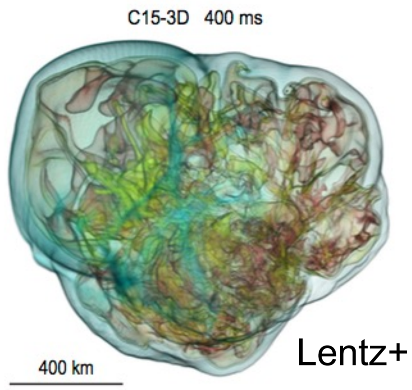


Gravity

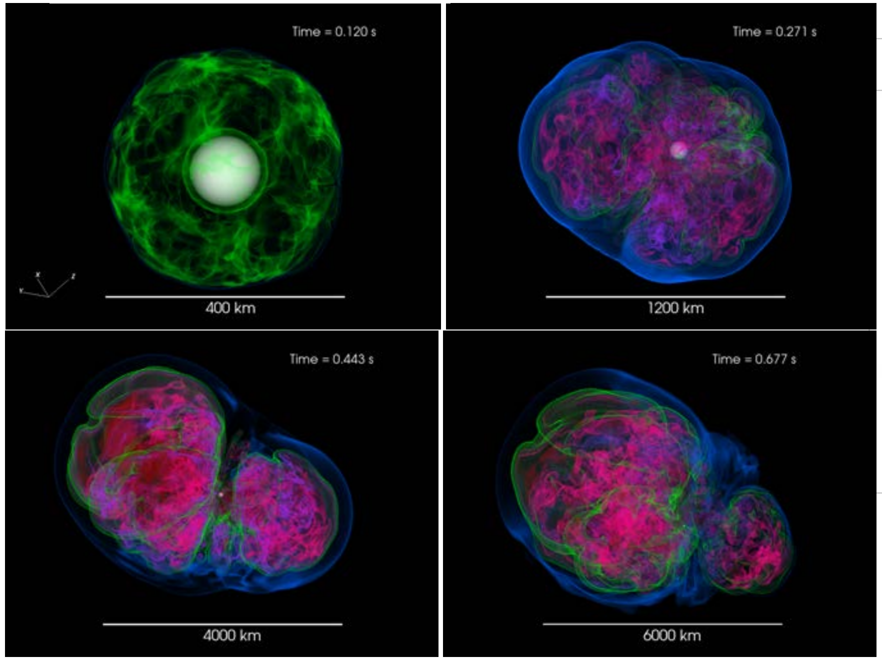
Requirements: Solution of Poisson equation with post-Newtonian corrections
Methods: *Asynchronous multipole/mutli-grid solvers of elliptic PDE*
Extensions: Dynamical spacetime solver

block-structured adaptive mesh (AMReX)

Little details matter…

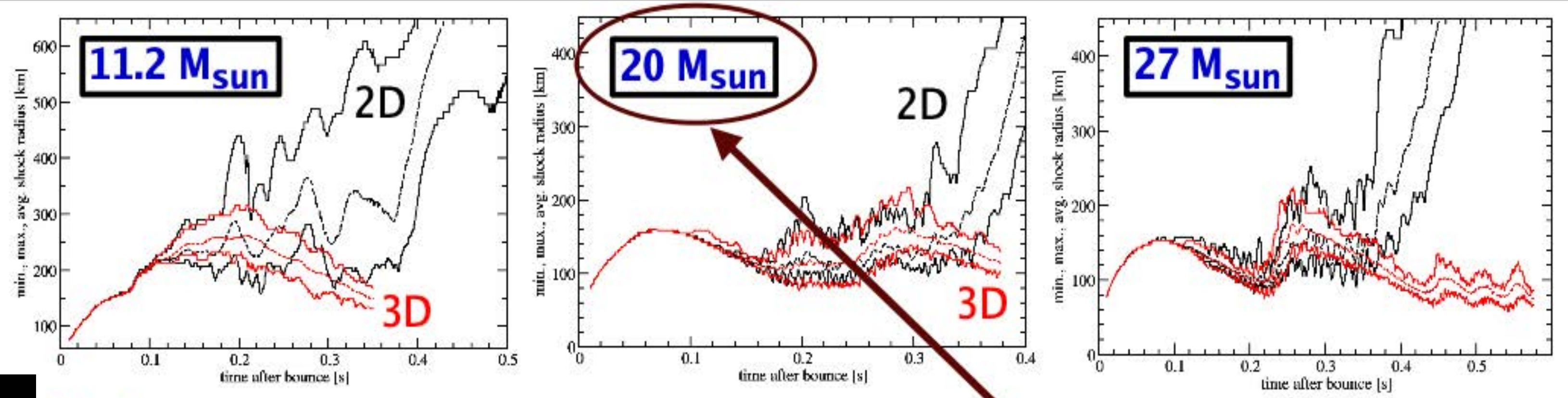


Lentz+ (2015)



Vartanyan+ (2019)

Florian Hanke, PhD project (2014), MPA



Melson et al., ApJL 808 (2015) L42

but…

$$\frac{d\sigma_0}{d\Omega} = \frac{G_F^2\epsilon^2}{4\pi^2}\left[c_v^2(1+\cos\theta) + c_a^2(3-\cos\theta)\right], \quad (1)$$

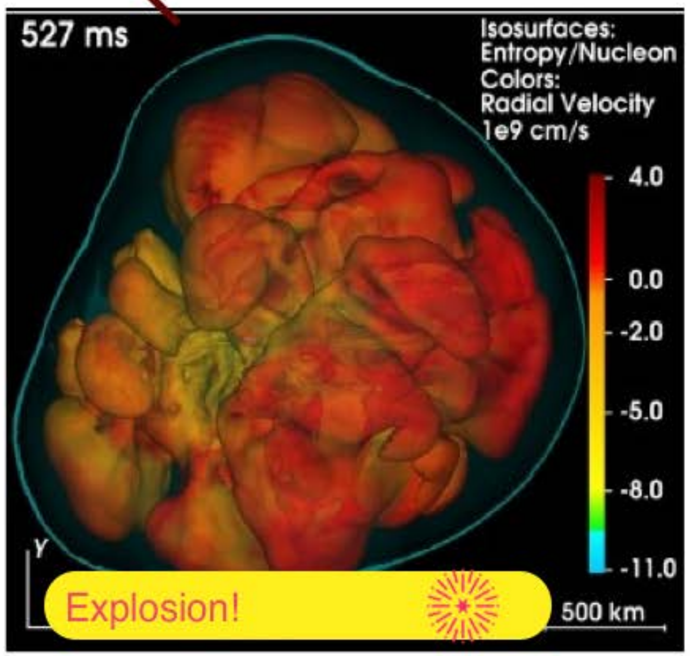
$$\sigma_0^t = \int_{4\pi} d\Omega \frac{d\sigma_0}{d\Omega}(1-\cos\theta) = \frac{2G_F^2\epsilon^2}{3\pi}\left(c_v^2 + 5c_a^2\right). \quad (2)$$

$$c_a = \frac{1}{2}(\pm g_a - g_a^s), \quad (3)$$

$g_a = 1.26$

$g_a^s = -0.2$

Effective reduction of neutral-current neutrino-nucleon scattering by ~15%



General Relativity: Code generators allow for precise unpacking of equations

- Useful for expressing symbolic tensor formulations in executable forms
- Data structures written to easily access information like derivative terms, e.g. a metric structure that holds equations for curvature tensors etc.
- Developing “Spacetime Variable” (STvAR or stVar) project in python for generating executable code for AMReX applications
- Inspired by the NRPy+ project and the Einstein Toolkit, STvAR project aims to perform code gen for AMReX C++ applications for spacetime evolution and PDEs in general

$$R_{\mu\nu} - \frac{1}{2} g_{\mu\nu} R = 8\pi T_{\mu\nu}$$

Ricci tensor — metric tensor — Ricci scalar — stress-energy tensor

$$\partial_0 \bar{\gamma}_{ij} = -\frac{2}{3}\bar{\gamma}_{ij}\bar{\mathcal{D}}_k\beta^k - 2\alpha\bar{A}_{ij} + \frac{2}{3}\alpha\bar{\gamma}_{ij}\bar{A},$$

$$\partial_0\phi = \frac{1}{6}\bar{\mathcal{D}}_i\beta^i - \frac{1}{6}\alpha K,$$

$$\partial_0\bar{A}_{ij} = -\frac{2}{3}\bar{A}_{ij}\bar{\mathcal{D}}_k\beta^k - 2\alpha\bar{A}_{ik}\bar{A}^k_j + \alpha\bar{A}_{ij}(K - 2\Theta)$$
$$+e^{-4\phi}[-2\alpha\bar{\mathcal{D}}_i\bar{\mathcal{D}}_j\phi + 4\alpha\bar{\mathcal{D}}_i\phi\bar{\mathcal{D}}_j\phi + 4\bar{\mathcal{D}}_{(i}\alpha\bar{\mathcal{D}}_{j)}\phi - \bar{\mathcal{D}}_i\bar{\mathcal{D}}_j\alpha + \alpha(\bar{R}^{Z4}_{ij} - 8\pi S_{ij})]^{\mathrm{TF}},$$

$$\partial_0 K = e^{-4\phi}[\alpha(\bar{R}^{Z4} - 8\bar{\mathcal{D}}^i\bar{\mathcal{D}}_i\phi - 8\bar{\mathcal{D}}^2\phi) - (2\bar{\mathcal{D}}^i\alpha\bar{\mathcal{D}}_i\phi + \bar{\mathcal{D}}^2\alpha)] + \alpha(K^2 - 2\Theta K)$$
$$-3\kappa_1(1+\kappa_2)\Theta + 4\pi\alpha(S - 3E),$$

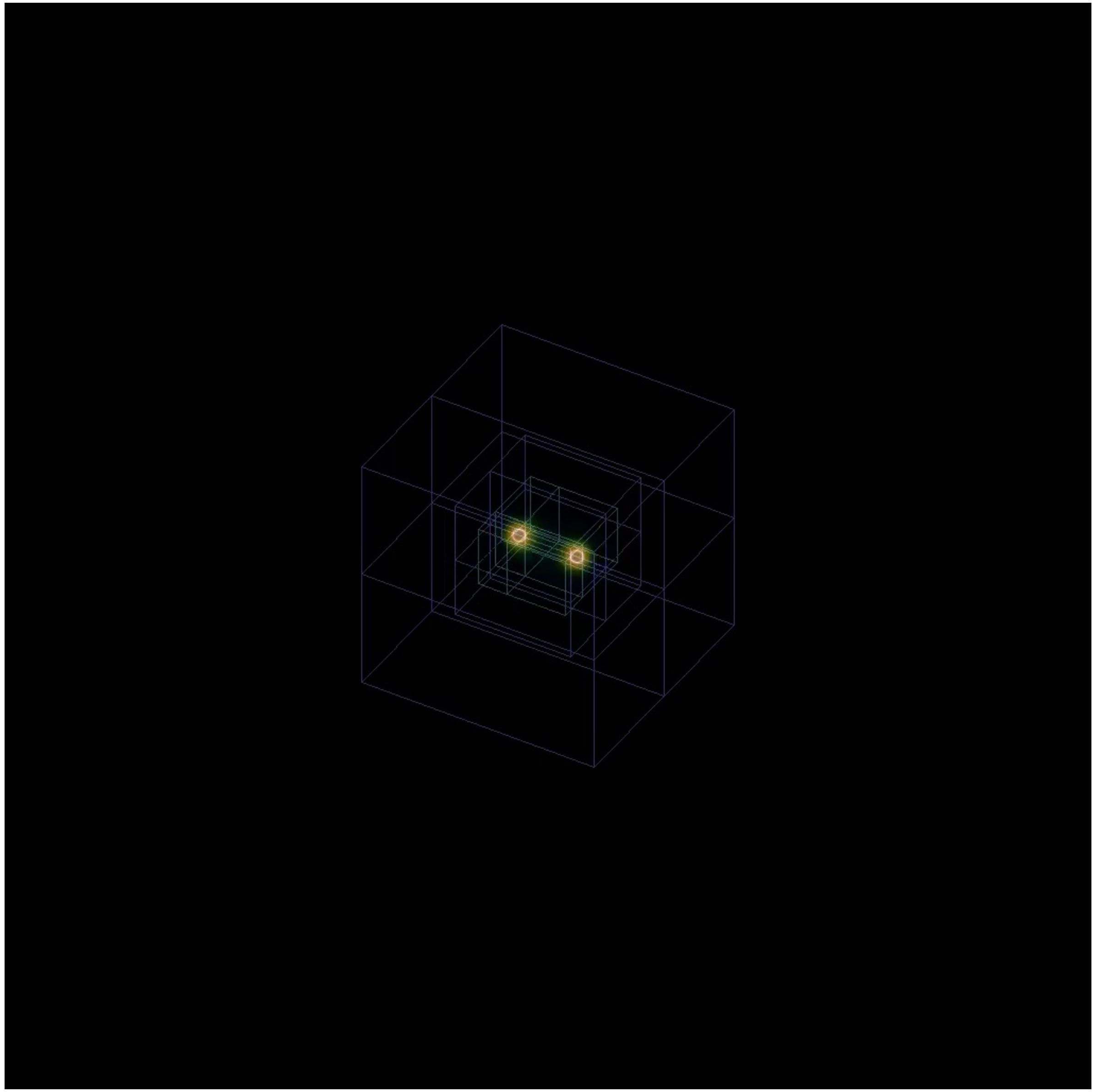
$$\partial_0\Theta = \frac{1}{2}\alpha[e^{-4\phi}(\bar{R}^{Z4} - 8\bar{\mathcal{D}}^i\phi\bar{\mathcal{D}}_i\phi - 8\bar{\mathcal{D}}^2\phi) - \bar{A}^{ij}\bar{A}_{ij} + \frac{2}{3}K^2 - 2\Theta K]$$
$$-Z^i\partial_i\alpha - \kappa_1(2+\kappa_2)\Theta - 8\pi\alpha E,$$

$$\partial_0\tilde{\Lambda}^i = \bar{\gamma}^{jk}\hat{\mathcal{D}}_j\hat{\mathcal{D}}_k\beta^i + \frac{2}{3}\Delta\Gamma^i\bar{\mathcal{D}}_j\beta^j + \frac{1}{3}\bar{\mathcal{D}}^i\bar{\mathcal{D}}_j\beta^j - 2\bar{A}^{jk}(\delta^i_j\partial_k\alpha - 6\alpha\delta^i_j\partial_k\phi - \alpha\Delta\Gamma^i_{jk})$$
$$-\frac{4}{3}\alpha\bar{\gamma}^{ij}\partial_j K + 2\bar{\gamma}^{ij}(\alpha\partial_j\Theta - \Theta\partial_j\alpha - \frac{2}{3}\alpha K Z_j) - 2\kappa_1\bar{\gamma}^{ij}Z_j + 2\kappa_3(\frac{2}{3}\bar{\gamma}^{ij}Z_j\hat{\mathcal{D}}_k\beta^k - \bar{\gamma}^{jk}Z_j\hat{\mathcal{D}}_k\beta^i)$$
$$-16\pi\alpha\bar{\gamma}^{ij}S_j.$$

```
gfs_rhs[THETA][idx] = fCCZ4*(ThetadD0*tmp116 + ThetadD1*tmp82 + ThetadD2*tmp112 -
alphadD0*tmp276 - alphadD1*tmp301 - alphadD2*tmp319 - tmp457*tmp651 - tmp459*tmp65
1 - tmp460*tmp650 - tmp461*tmp650 - tmp462*tmp652 - tmp464*tmp652 - tmp465*tmp653
- tmp467*tmp653 - tmp468*tmp650 - tmp493*tmp617 - tmp568*(kappa2 + 2) + tmp650*((2
.0/3.0)*tmp454 + tmp569 + tmp596));
```

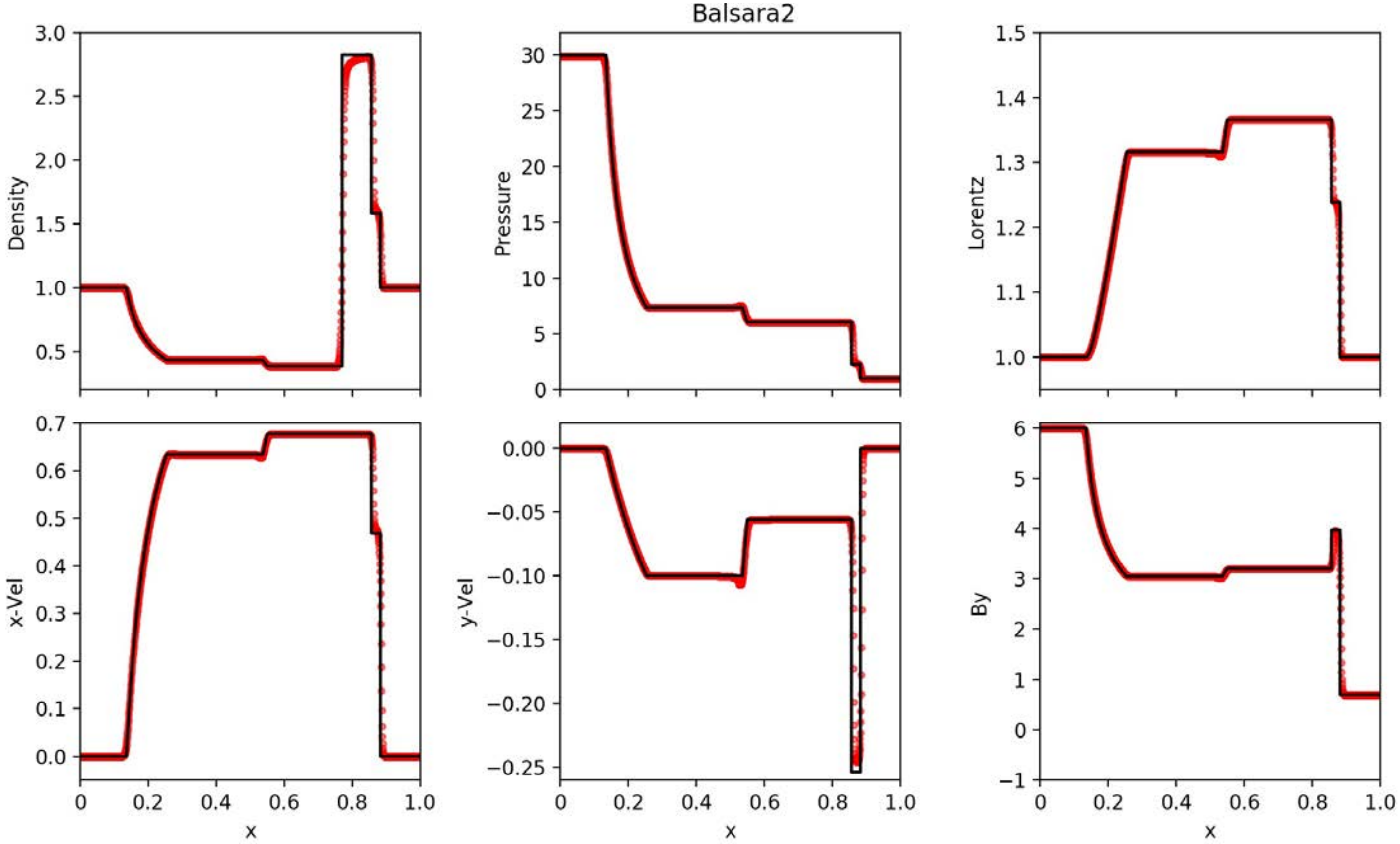
Black hole merger produced from Z4c code generator

- Black hole merger simulated using AMReX
- General relativity equations evolved in the 3+1 Z4c formulation
- STvAR code generator used to translate symbolic tensor equations into AMReX executable code
- 3D render of black hole merger simulation



General Relativistic Magneto-Hydrodynamics

- Generalized conservative variables & fluxes for magnetic field contributions
- Robust 3D Newton-Raphson conservative to primitive (con2prim) root finder for generalized equation of state
  - 1D Brent’s method fallback
- Numeric benchmarks for 5 relativistic shock tube tests (Balsara 2001)



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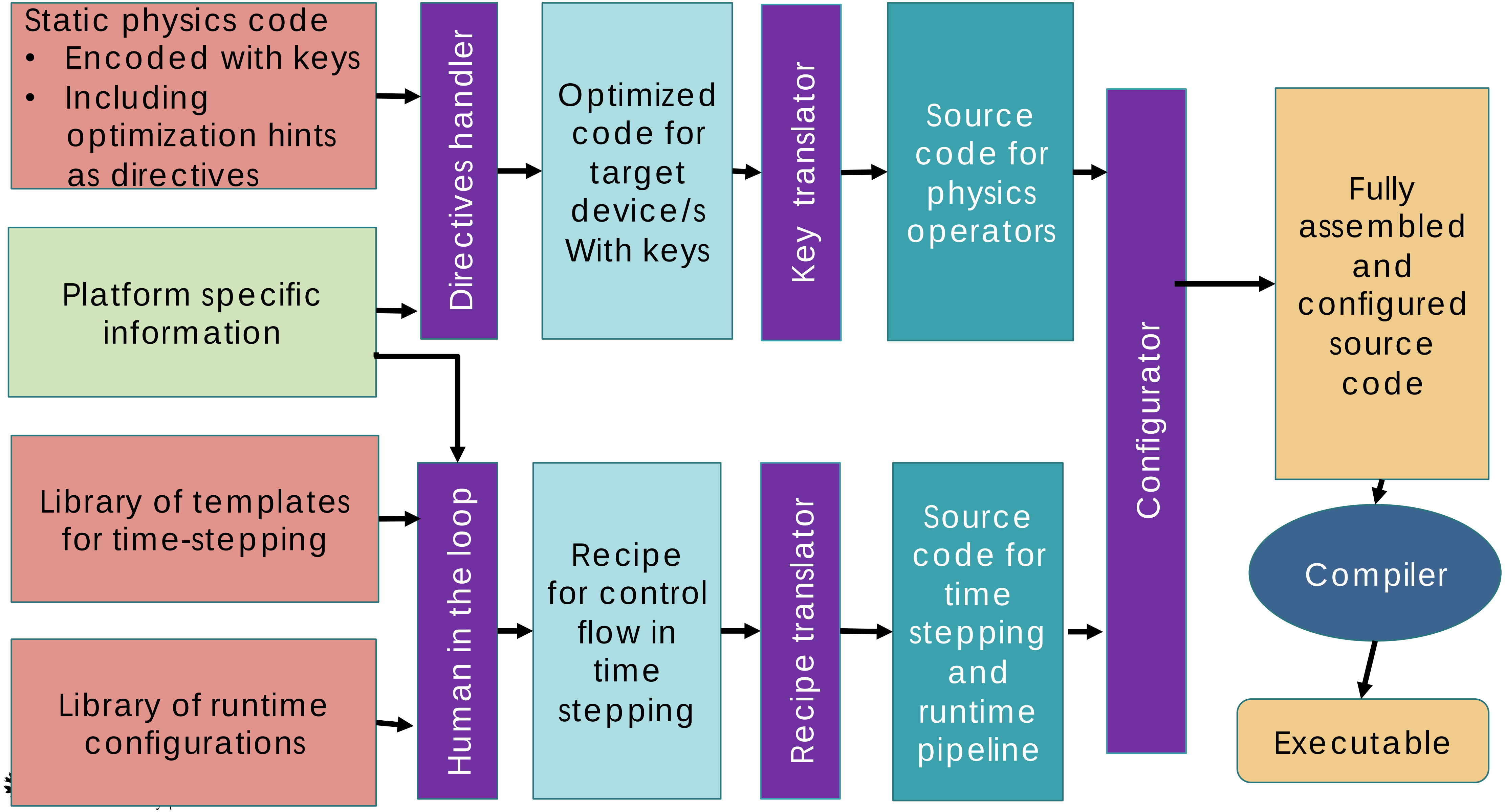
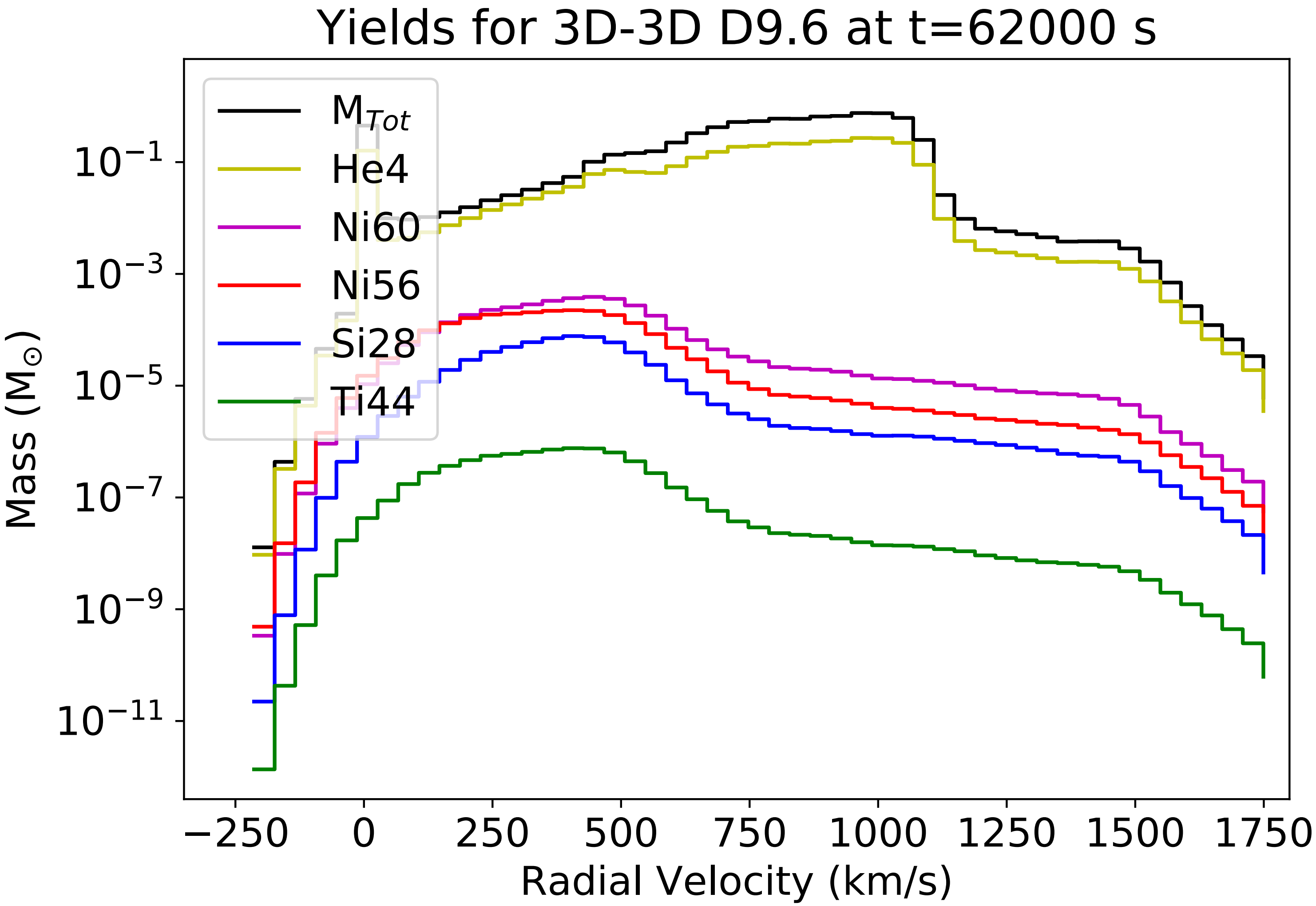
Beyond just Multiphysics Coupling: Orchestration



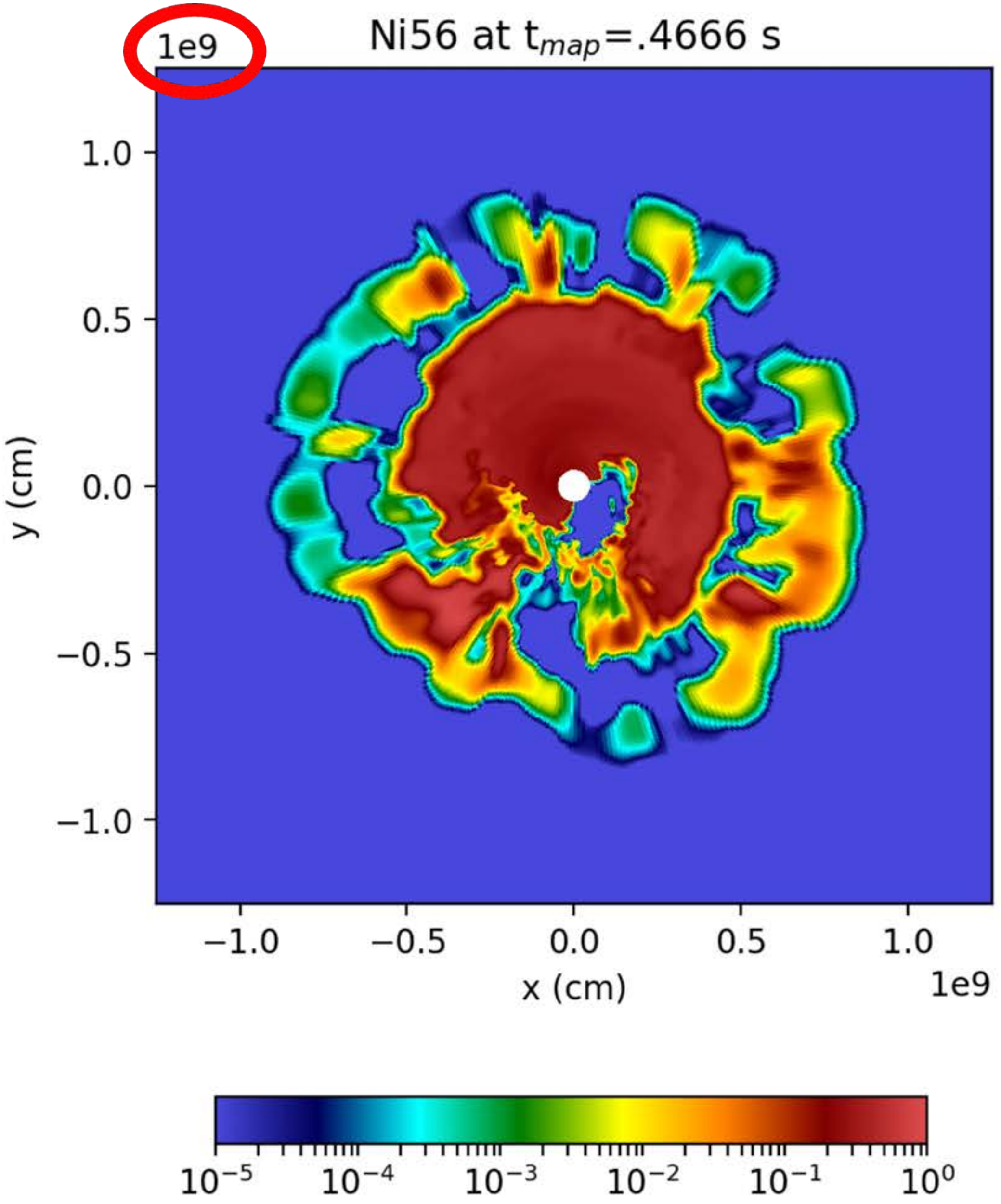
Sandoval et al. (accepted)

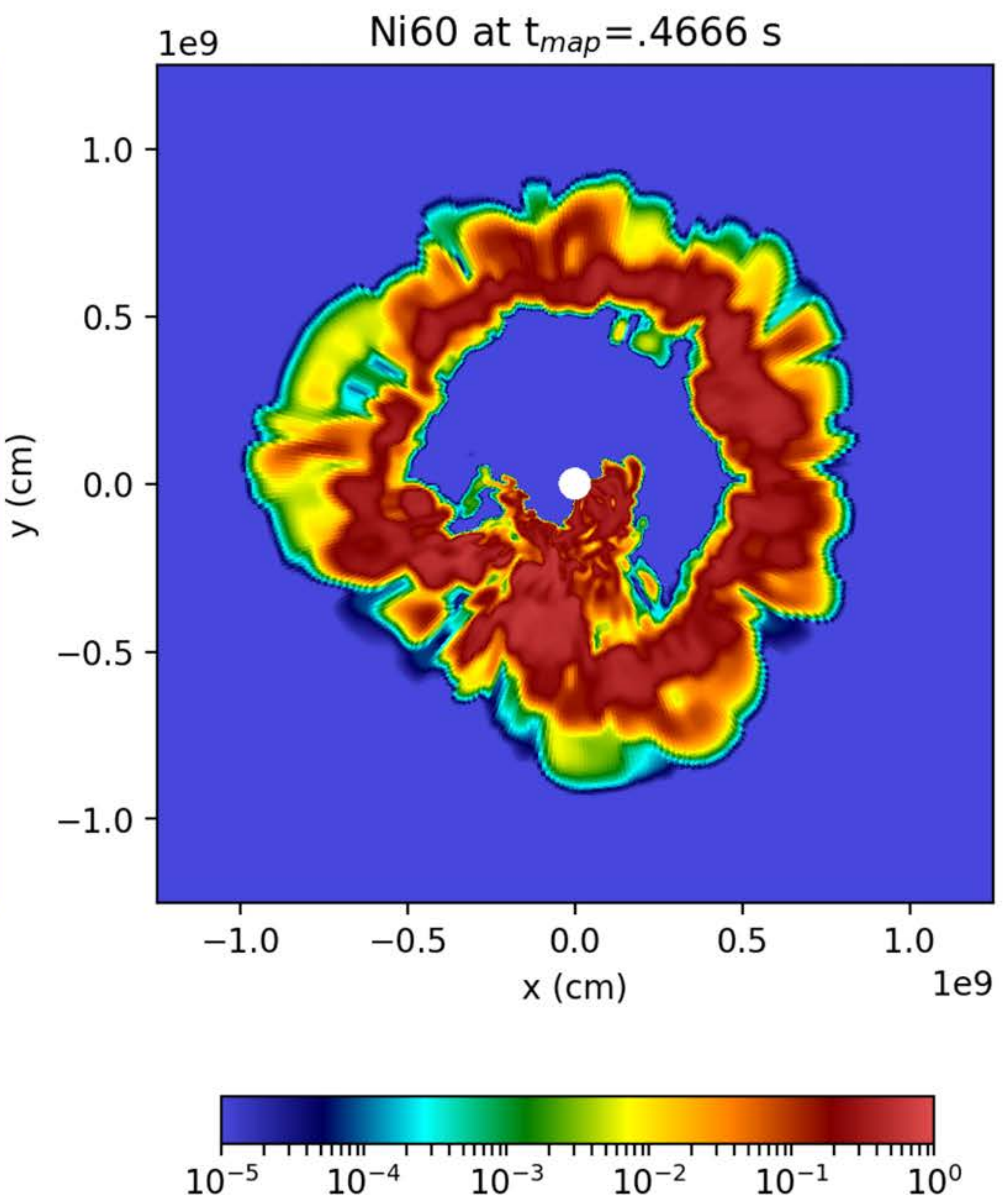
Hot off Summit: Extended CCSNe sims

- SN160 network
  - Full RadHydro simulation(Chimera) remapped at 0.466 s to FLASH AMR grid
    - GPU-accelerated burner back-ported from FLASH to Chimera
  - Burning while any appreciable energy release present on the grid
  - Composition carried for the full 17 hours



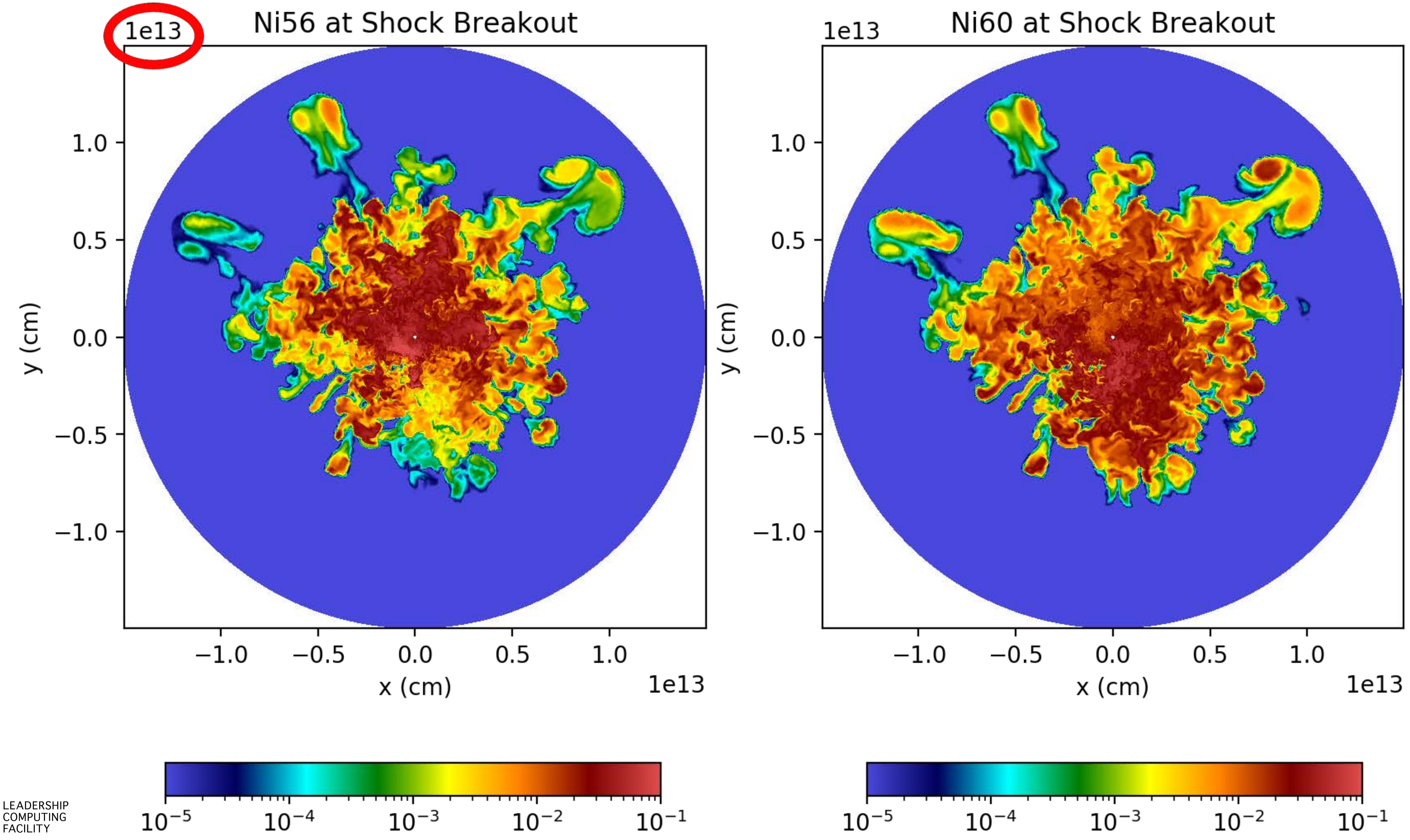
Sandoval et al. (accepted)

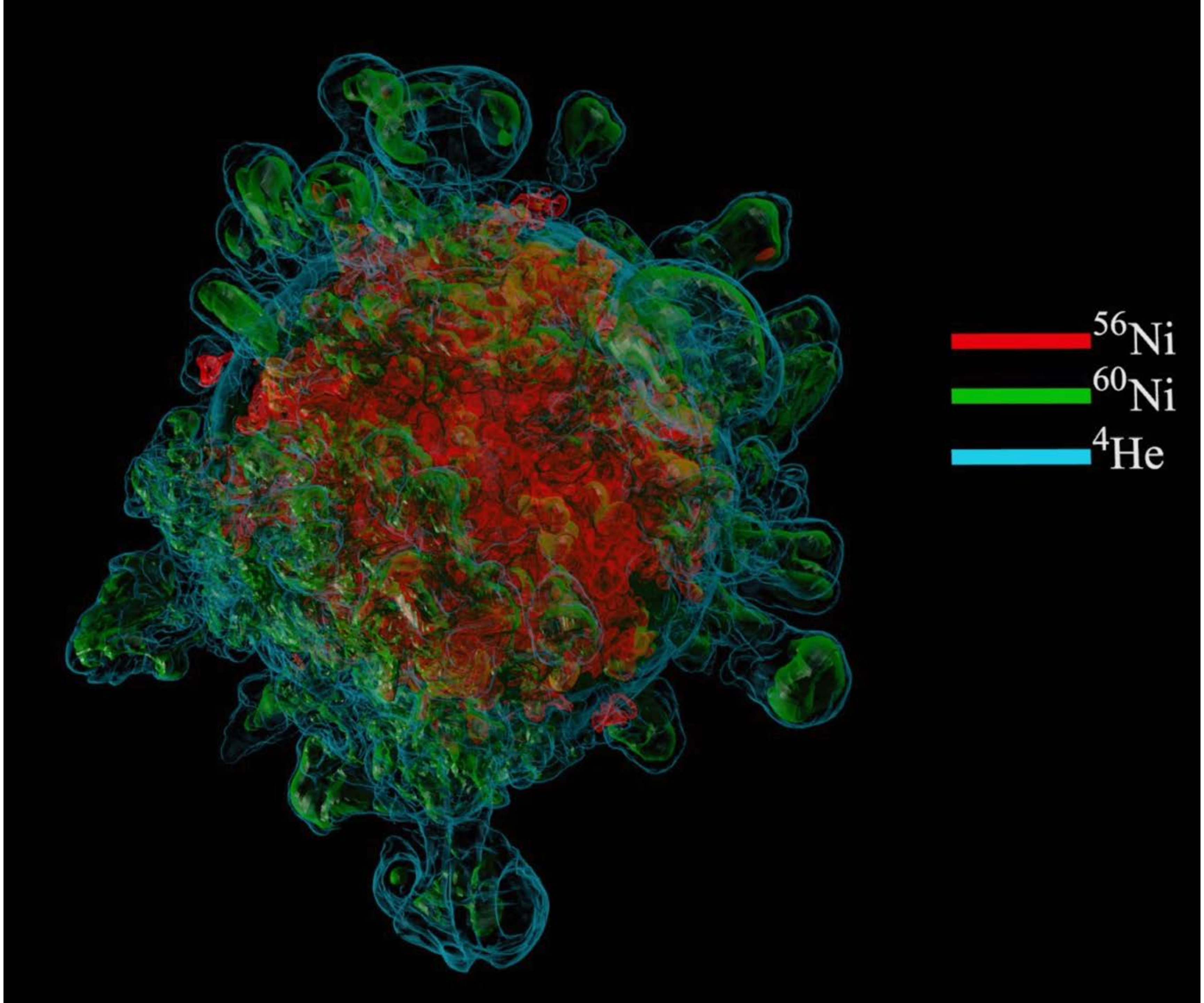




Sandoval et al. (accepted)

17 hours later, 10,000 times bigger




^{56}Ni
^{60}Ni
^{4}He

Summary

- Supernova modeling is as close to being a Renaissance physicist as you can get!
- Necessary realism: Multifrequency neutrino transport with relativistic effects and a state-of-the-art weak interaction set, and general relativity
    - Better gravity+better resolution+better nuclear physics (neutrino oscilllations!) will require **exascale**!
- 2D CHIMERA models confirm successful prolate explosions across a range of progenitors driven by neutrino heating and SASI with outcomes consistent with observations.
- 3D CCSN simulations are very expensive! But, necessary to answer questions definitively.