Modeling Astrophysical Thermonuclear Explosions

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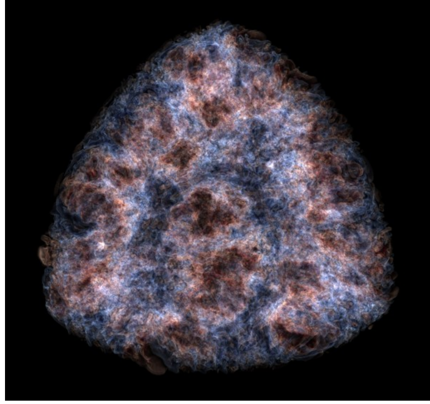
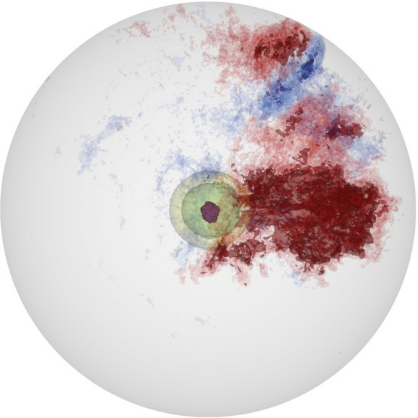
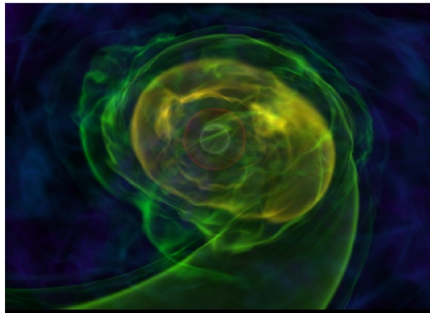
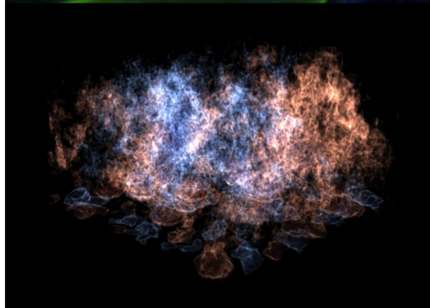
What can we learn from modeling stellar environments?

- What is the mechanism behind supernovae?
- How does each event contribute to nucleosynthesis?
- What is the dense matter equation of state?
- What is the site of R-process?

Challenges of stellar simulations

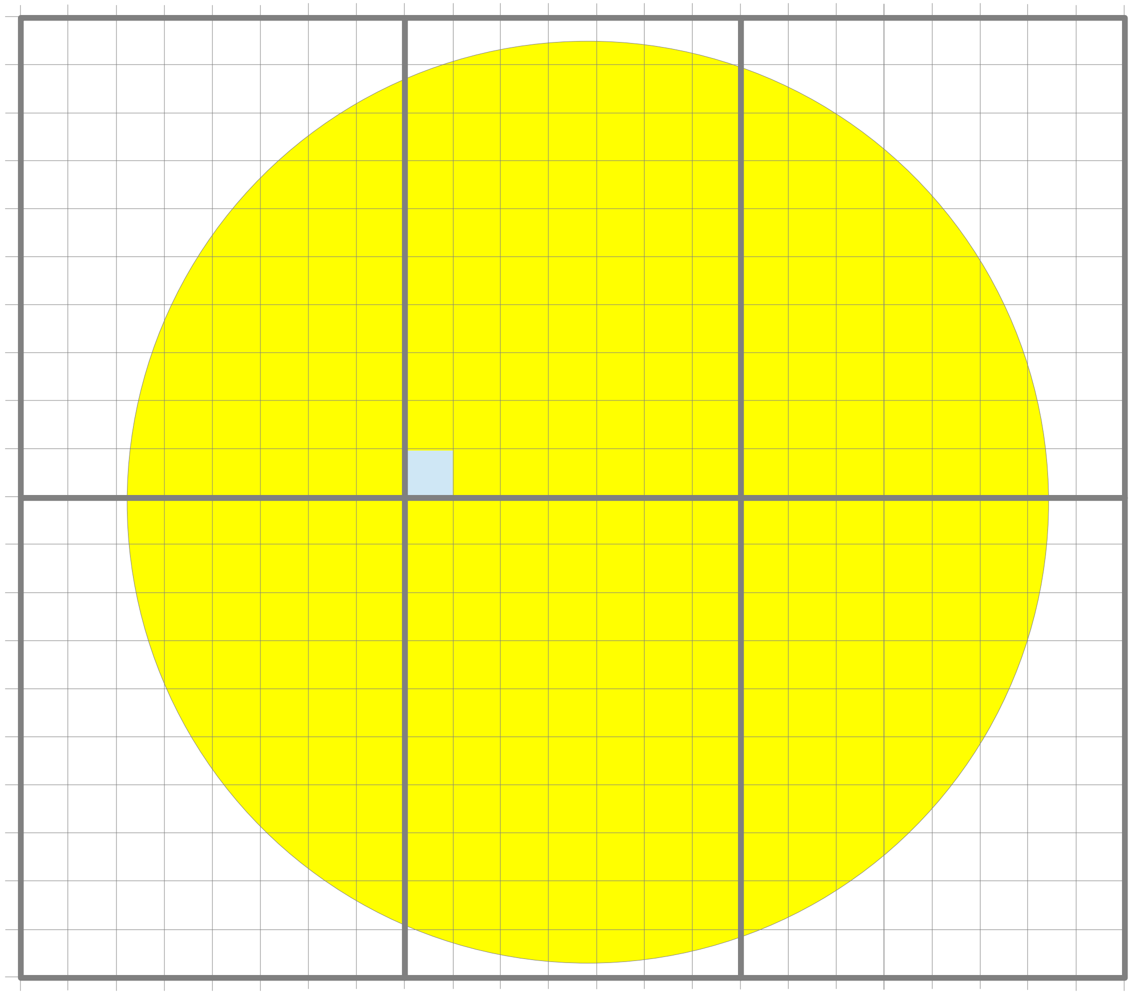
- Stars involve:
  - Hydrodynamics (including turbulence and instabilities)
  - Combustion / nuclear reactions
  - Self-gravity
  - Radiation / diffusion
  - Magnetic fields
- *We need to write the laws of physics in a form that a computer can solve*
- Most of stellar evolution is done in 1D
  - But convection, binary interactions, magnetic fields, … are all inherently 3D

Computational modeling

- Solve conservation laws:

$$\mathcal{U}_t + \nabla \cdot \mathbf{F}(\mathcal{U}) = \mathbf{S}$$

- Discretize by star on a grid
- Cell update depends its surroundings
  - Complexity is in computing the fluxes through boundaries
- Parallelism achieved by dividing domain across nodes

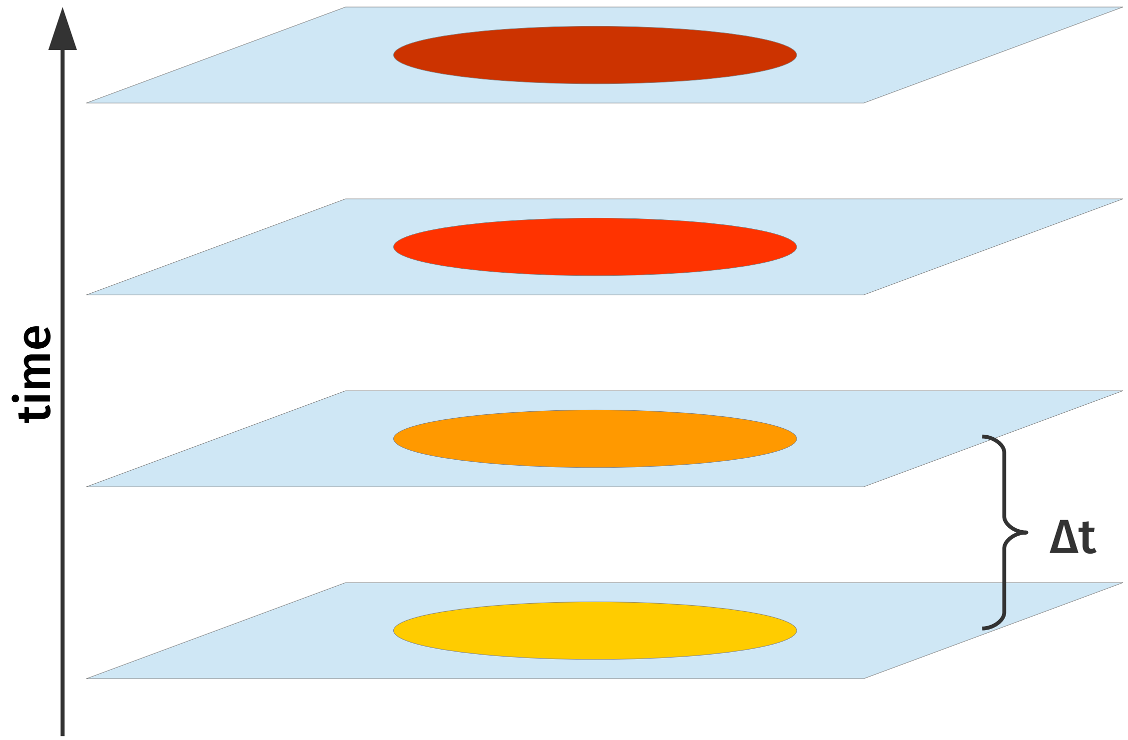


Computational modeling

- Mathematical constraint on size of timestep
  - Information cannot move more than one zone per timestep
- Compressible hydro:

$$\Delta t \leq \frac{\Delta x}{|\mathbf{U}| + c_s}$$

- Multiphysics integration is more complex



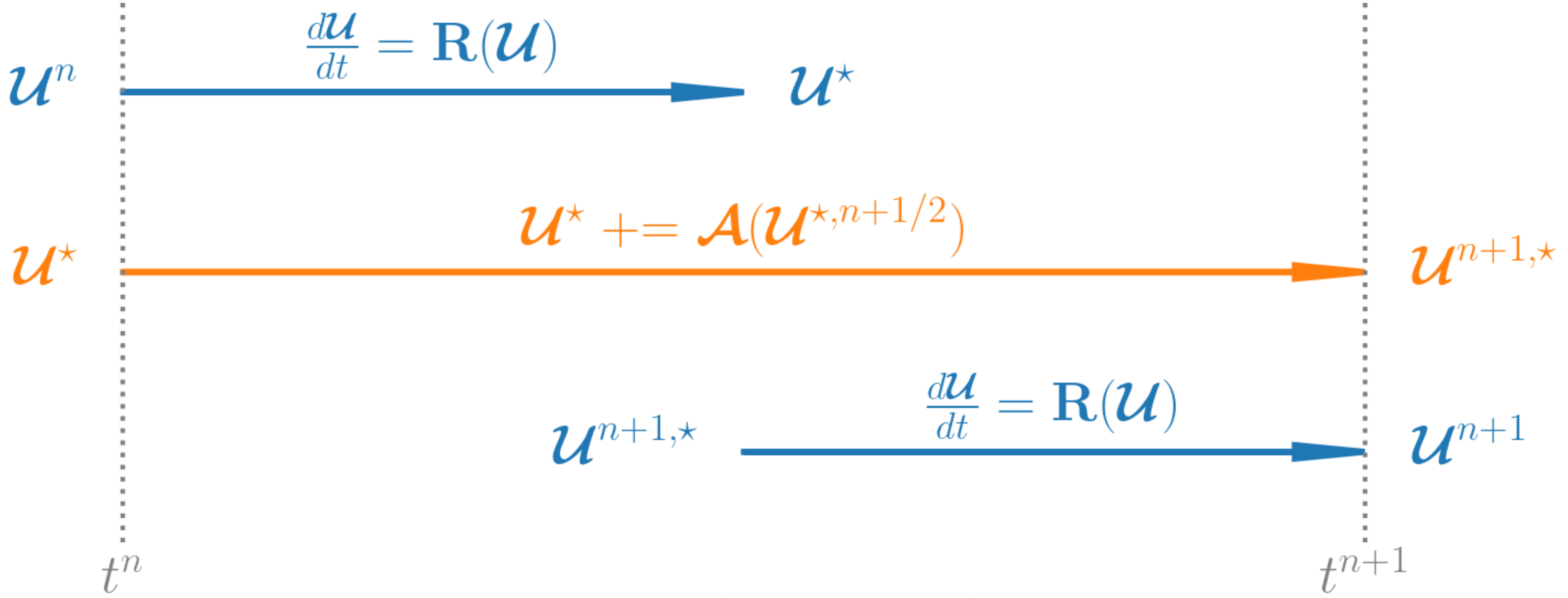
Reaction + hydro coupling

- Hydro: conservation of mass, momentum, and energy
- Reactions change composition + inject energy
- Express system as:

$$\frac{\partial \mathcal{U}}{\partial t} = \mathcal{A}(\mathcal{U}) + \mathbf{R}(\mathcal{U})$$

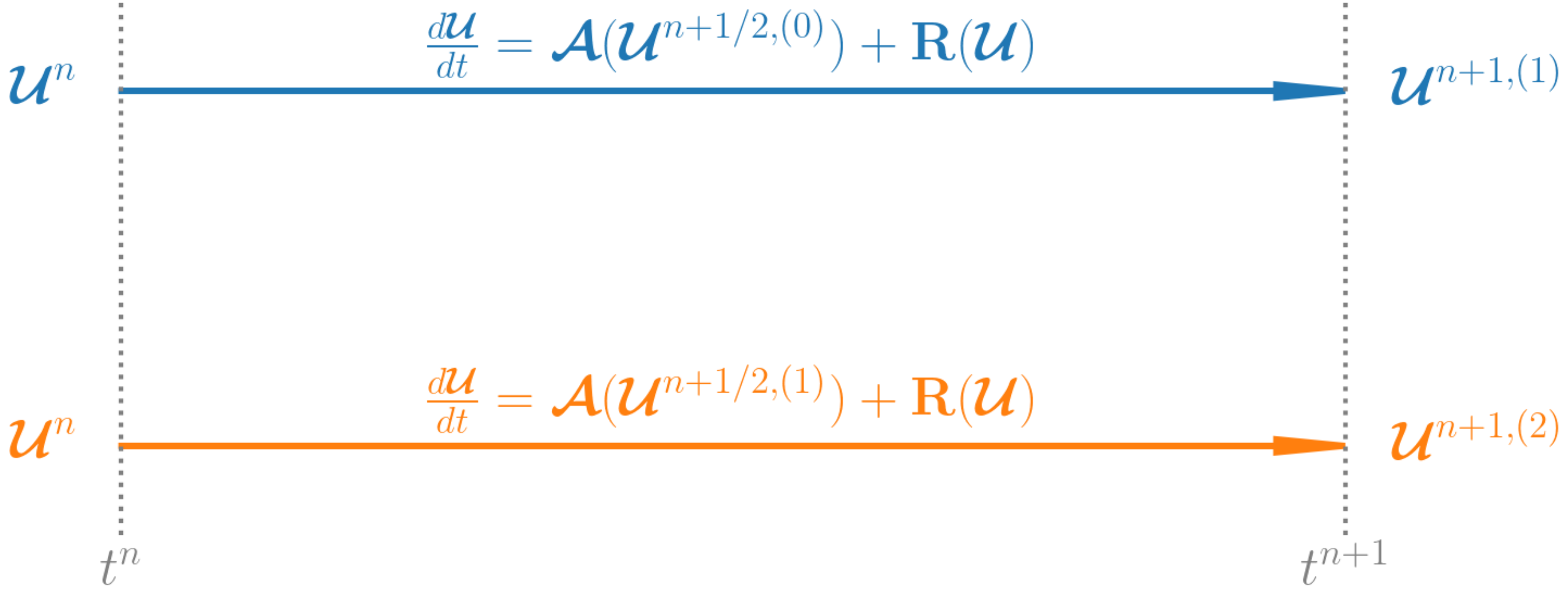
- Reaction challenges
  - Reaction rates are *strongly* T dependent
  - Burning and hydrodynamics can decouple
- Reaction-based timestep limiters popular

Operator splitting



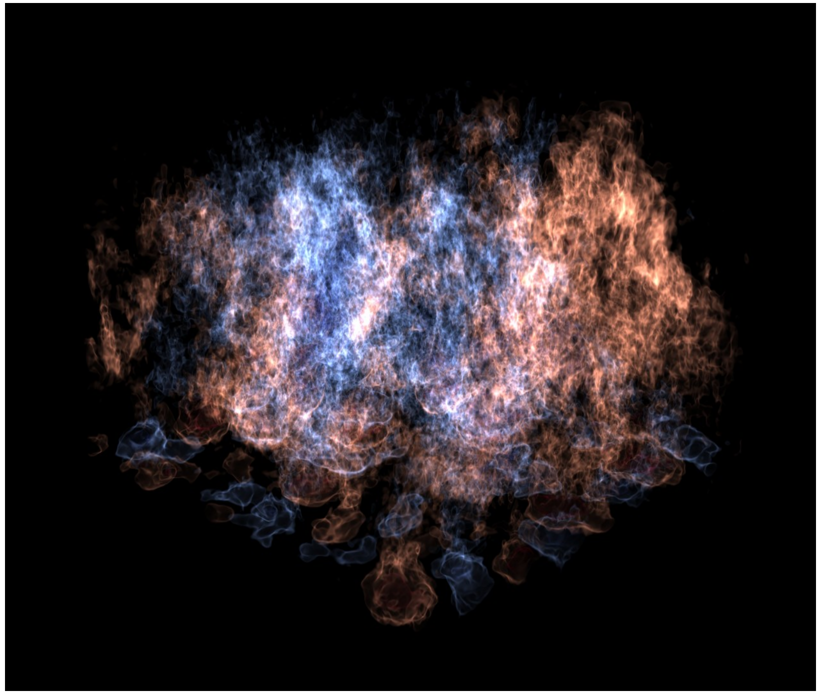
- **Traditional method: operator (Strang) splitting**
  - Alternate burning and hydro
  - Each process is independent of the other
  - 2^{nd} order accurate

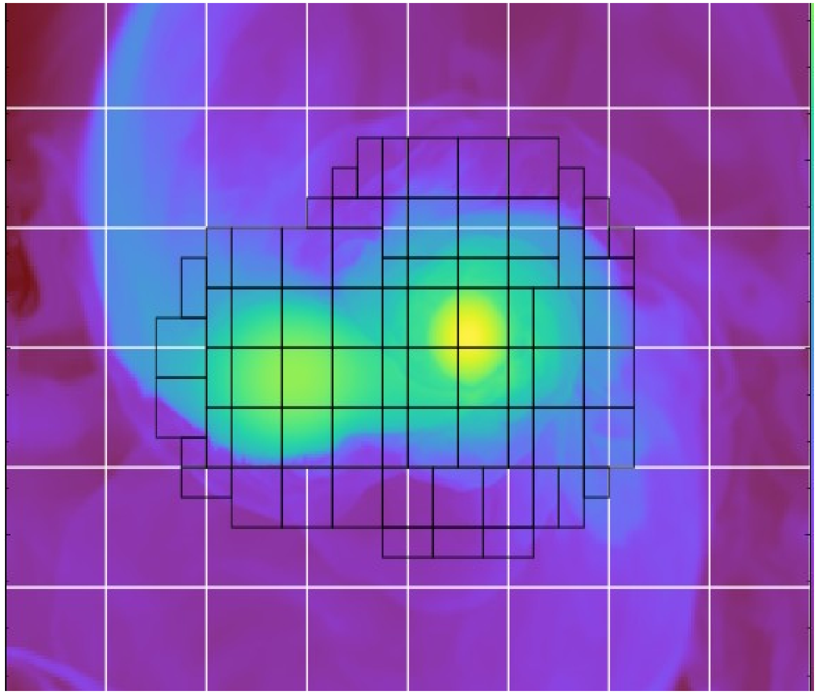
Simplified-SDC

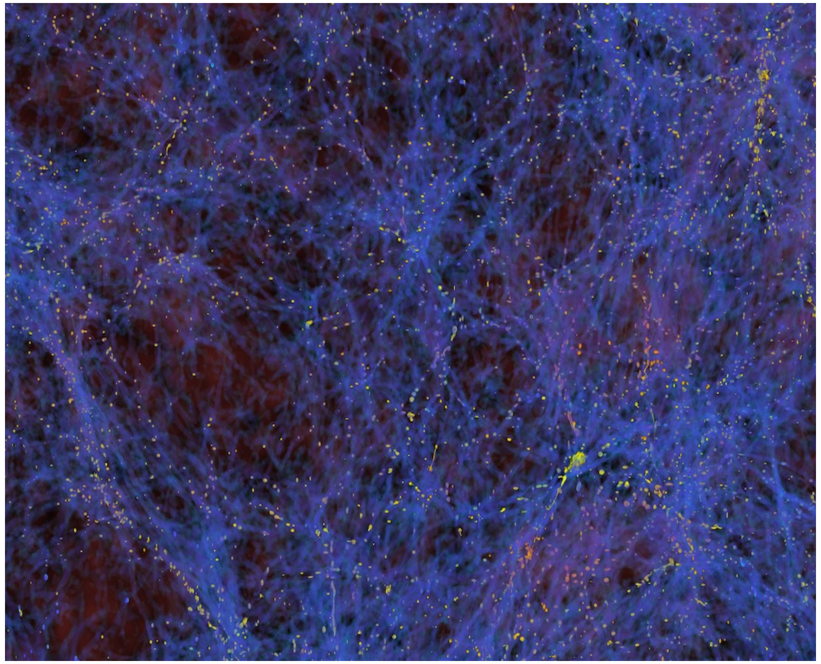


- **Iteratively couples hydro and reactions:**
  - Reactive update knows that advection is taking place
  - Burn responds to flow
- **Based off of spectral deferred corrections (SDC)**

AMReX astrophysics suite







MAESTROeX: low Mach number stratified flows

Castro: compressible (magneto-, radiation-) hydrodynamics

Nyx: cosmological hydrodynamics + N-body

https://github.com/amrex-astro

pynucastro

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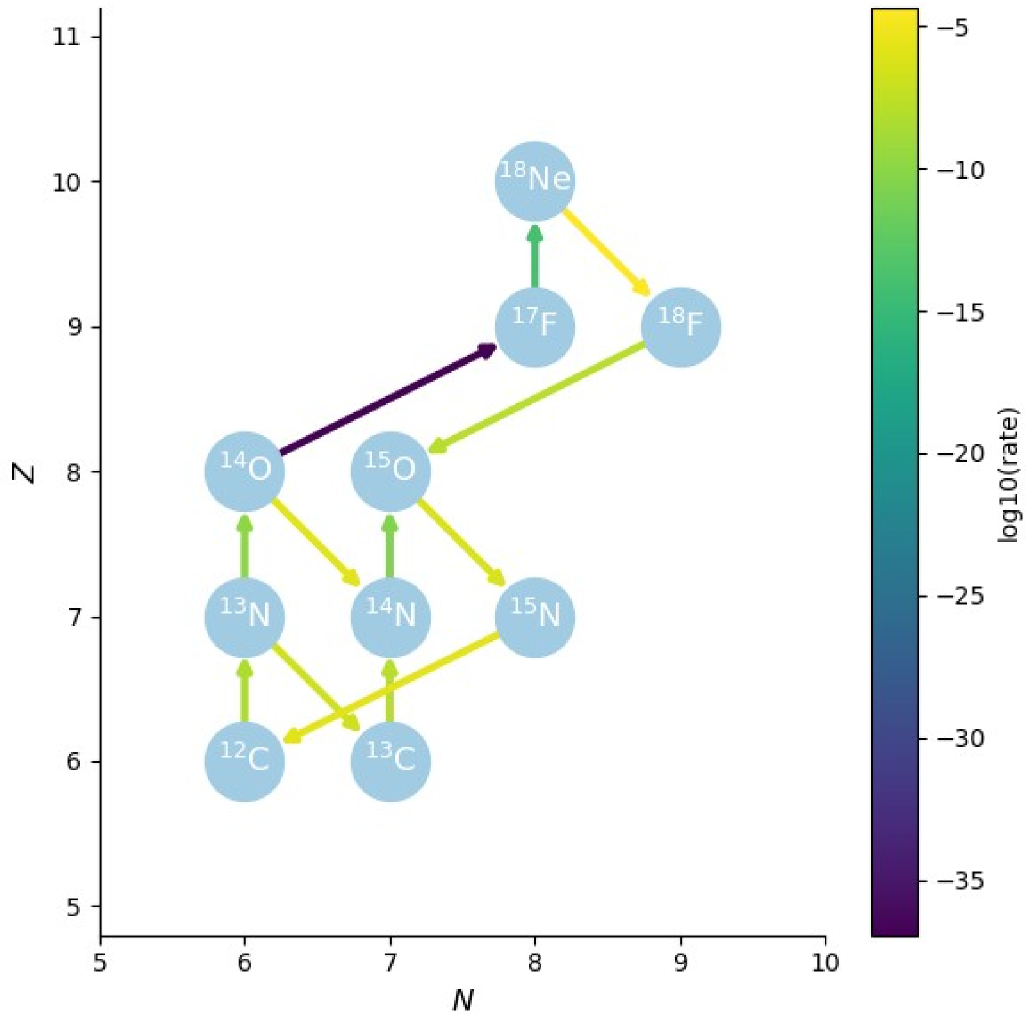
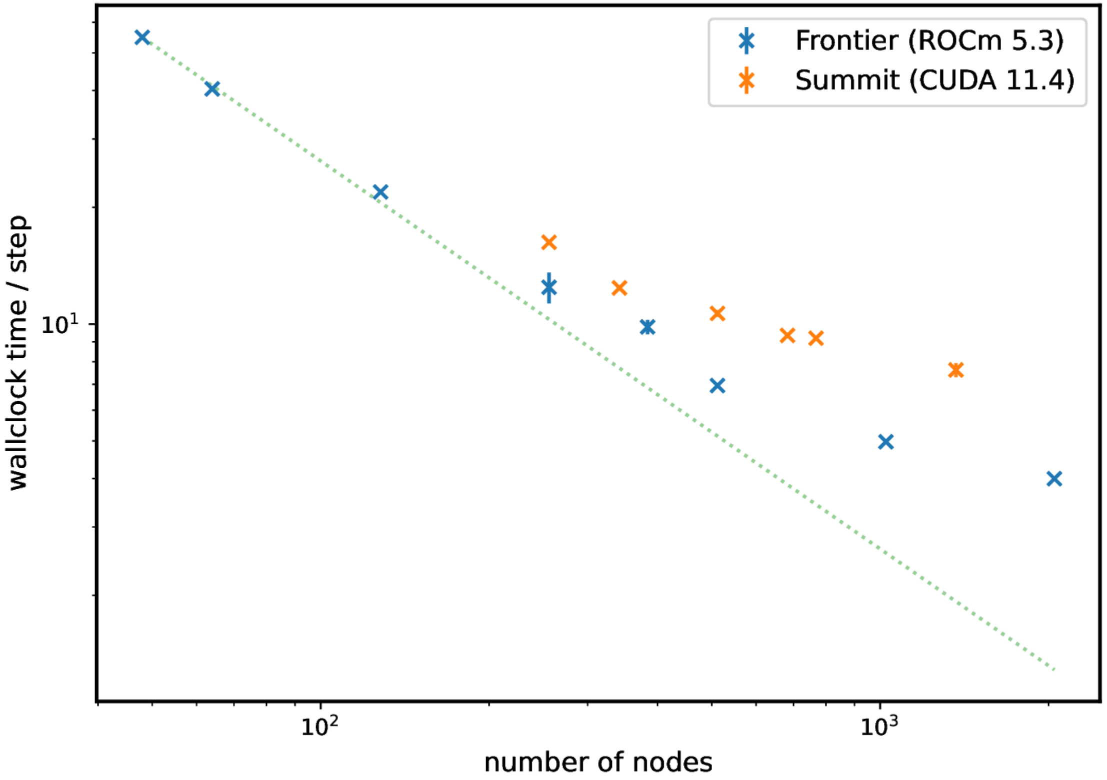


- **pynucastro: python framework for working with reaction databases**
  - Interfaces reaction rate libraries
  - Allows for interactive exploration of rates and networks in Jupyter
- **Outputs the full righthand side routine in python or C++**

(Smith Clark et al. 2023)

Modern supercomputers

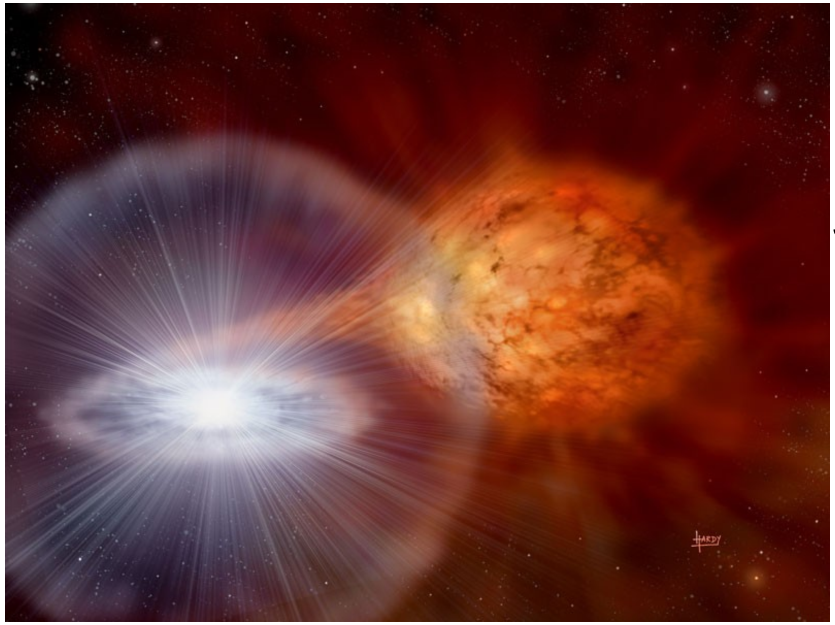
- OLCF Frontier
  - 9408 nodes, each with
    - 1 AMD CPU with 64 cores
    - 4 AMD MI250X GPUs (x2 graphics compute dies)
  - 1 exaflop performance
- GPU offloadng:
  - Move data to GPUs at the start and do all computation there
  - Leverage AMReX “ParallelFor”



How does coupling / time-integration affect our science?

Type Ia supernovae

- No H; strong Si, Ca, Fe lines
- Occur in old populations
- Bright as host galaxy, L ~10^{43} erg s^{-1}
- ^{56}Ni powers the lightcurve
- Act as standard candles
- *General consensus: thermonuclear explosion of a carbon/oxygen white dwarf*
  - What progenitor?



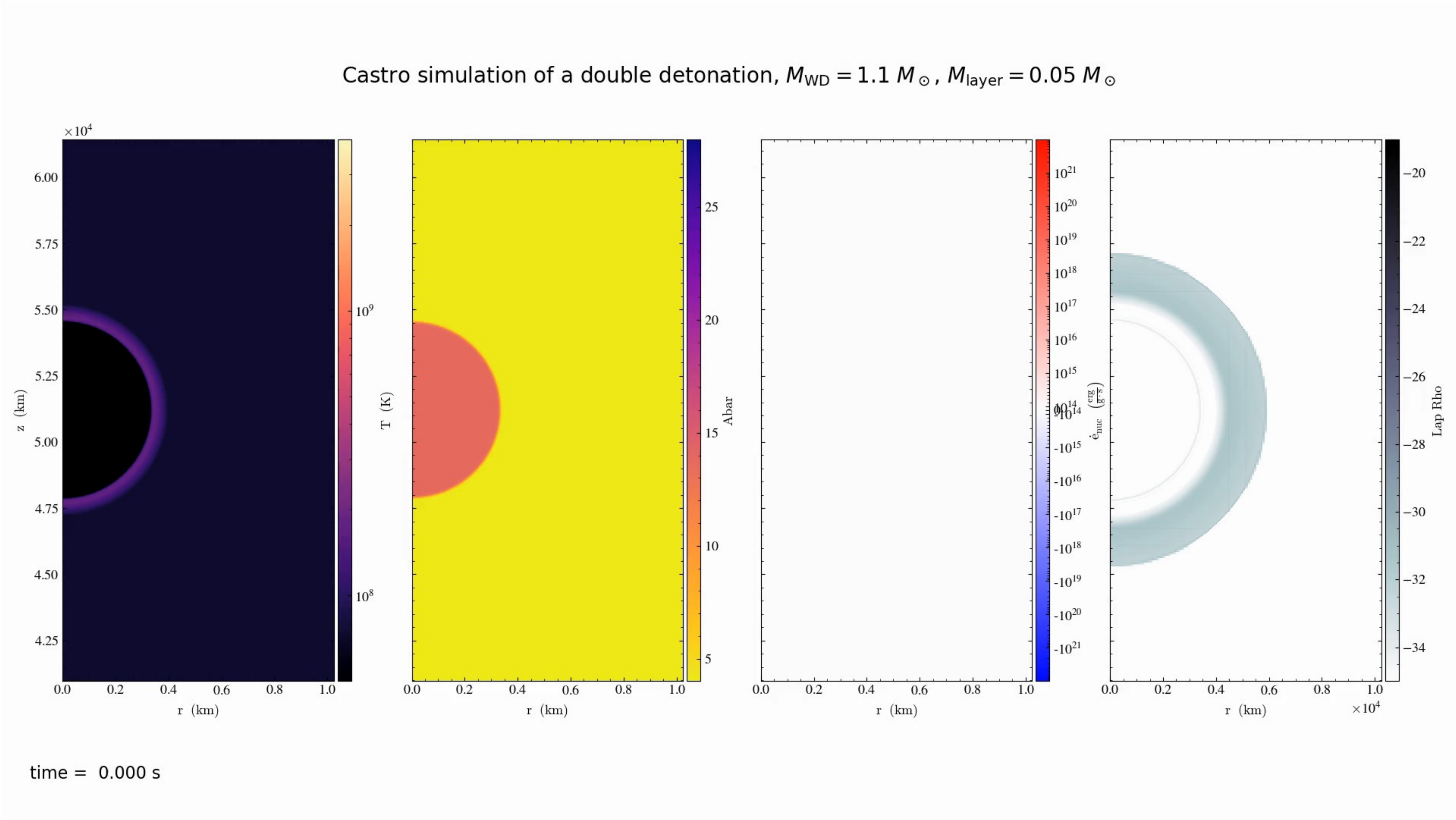
(David A. Hardy & PPARC)

SN 1994D (High-Z SN Search team)

Double detonations

- Several competing SN Ia models currently
- Double detonation:
  - Sub-Chandra WD builds He layer
  - Detonation in He layer triggers detonation in underlying CO WD
- Challenge: avoid numerically-seeded detonations
  - Some artificially limit the reactions
  - High resolution is needed to avoid entirely (Katz & Zingale 2019)
- Can SDC integration help?

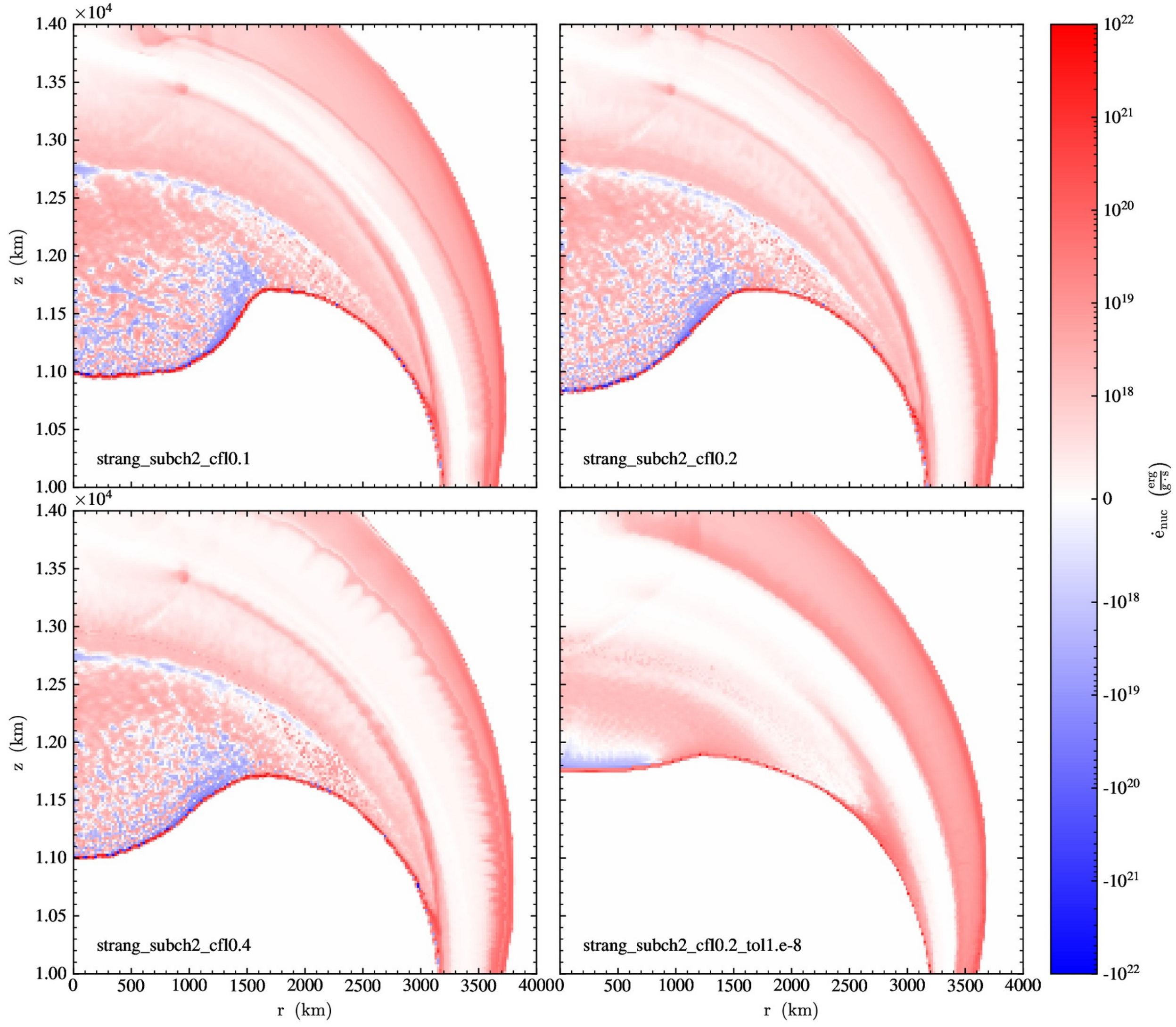
Double detonation



Double detonations

- Integration test:
  - Kick the He layer hard and see what happens
- Strang has difficulty compared to SDC
  - Converges to SDC with tighter network tols
- Simplified-SDC is no more expensive, despite doing both operations twice

Strang split



(Zingale et al. 2022, ApJ, 936, 6)

Double detonations

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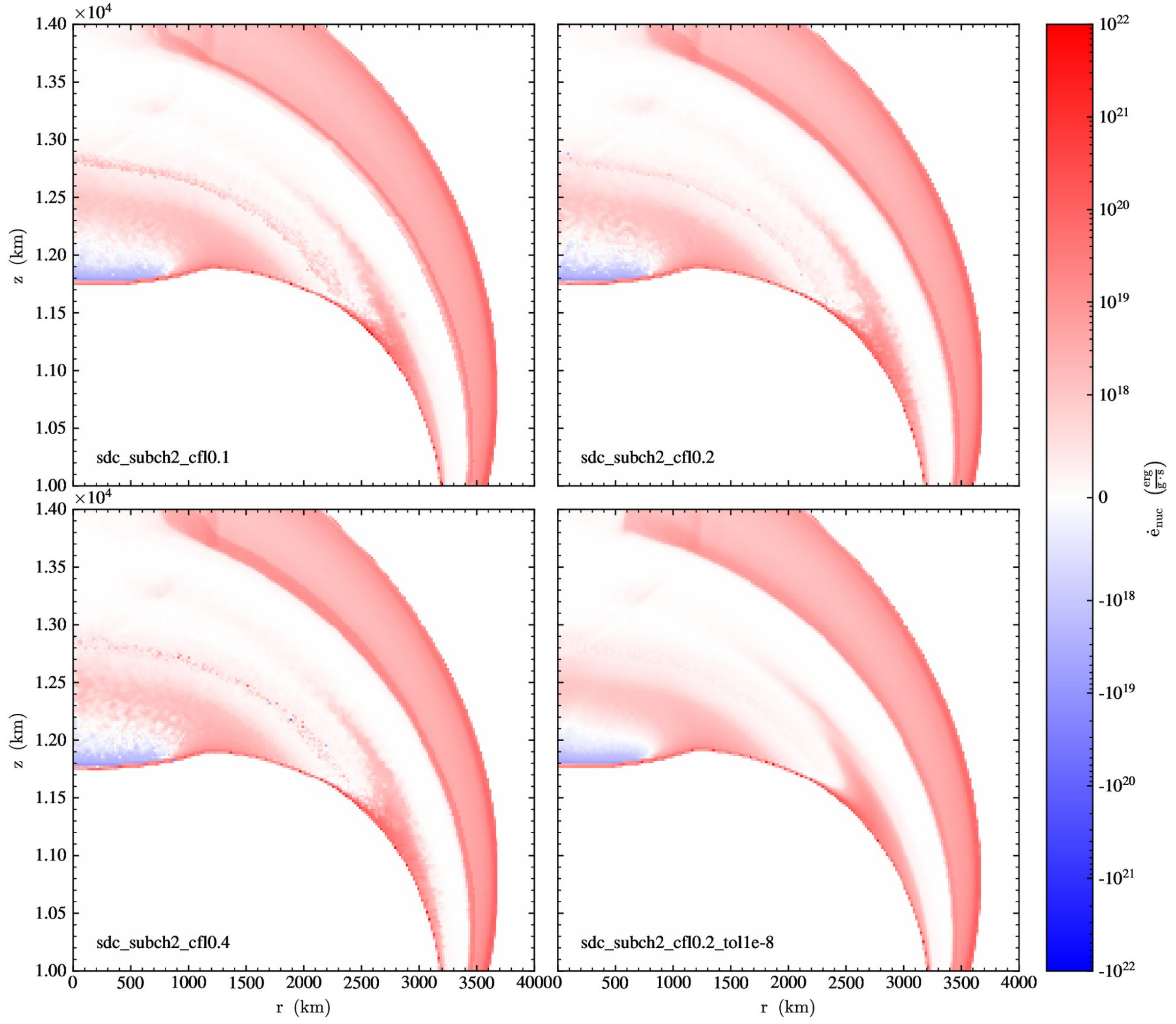
simplified-SDC



(Zingale et al. 2022, ApJ, 936, 6)

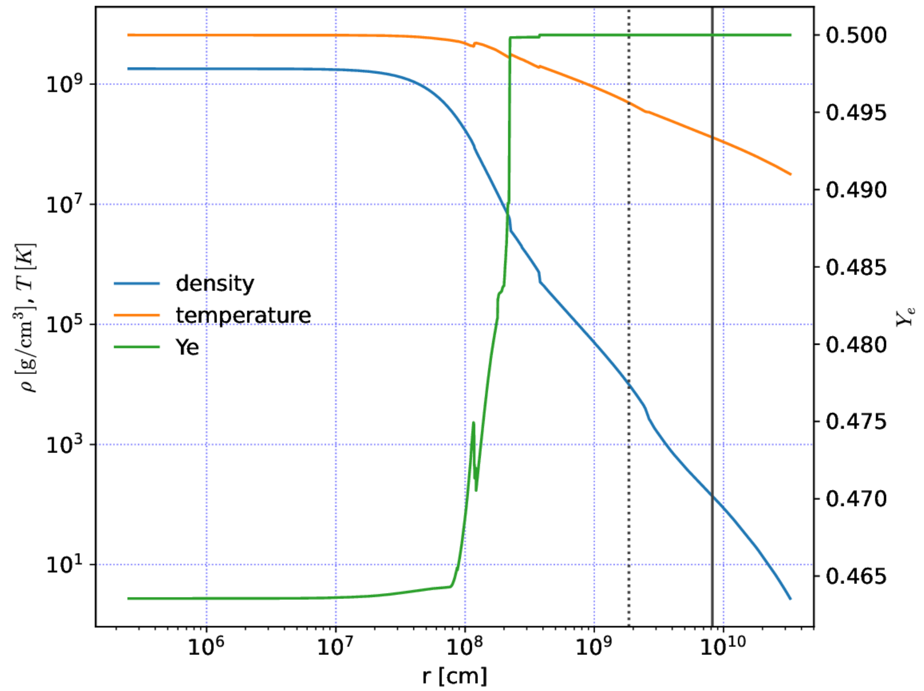
Massive stars

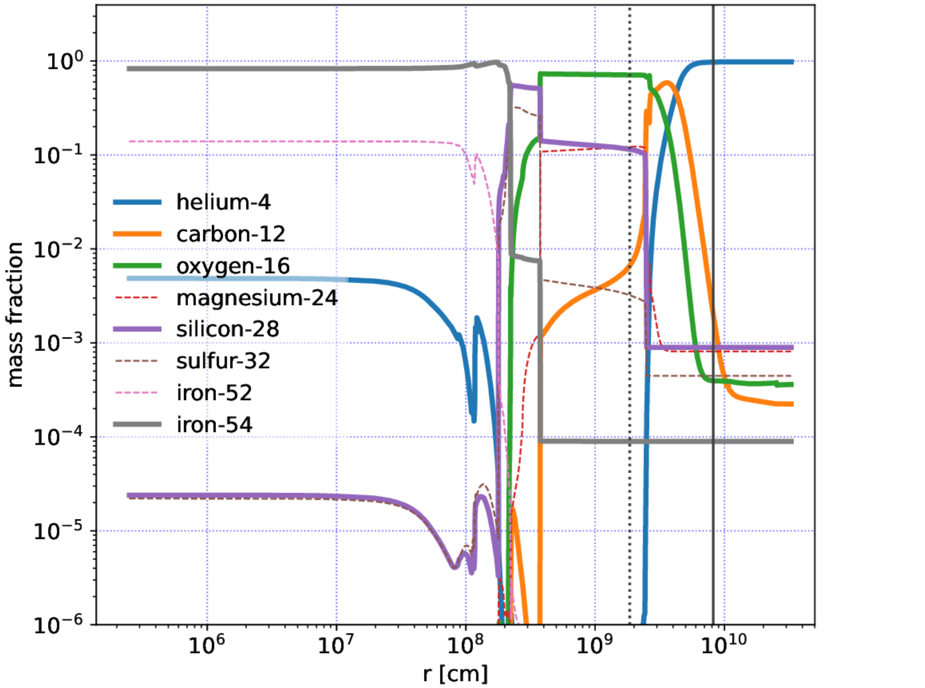
- Goal: evolution of massive star leading to core-collapse
- Challenge:
  - e^- captures + NSE in core
  - Si burning is hard
- *Can we avoid cutting the timestep harshly?*

- Our approach:
  - NSE table (with Y_e fraction evolution) + traditional net
  - Energy evolution with reactions is critical
  - NSE "bailout" during ODE solve
- SDC formalism allows for 2nd-order accurate integration

Massive stars

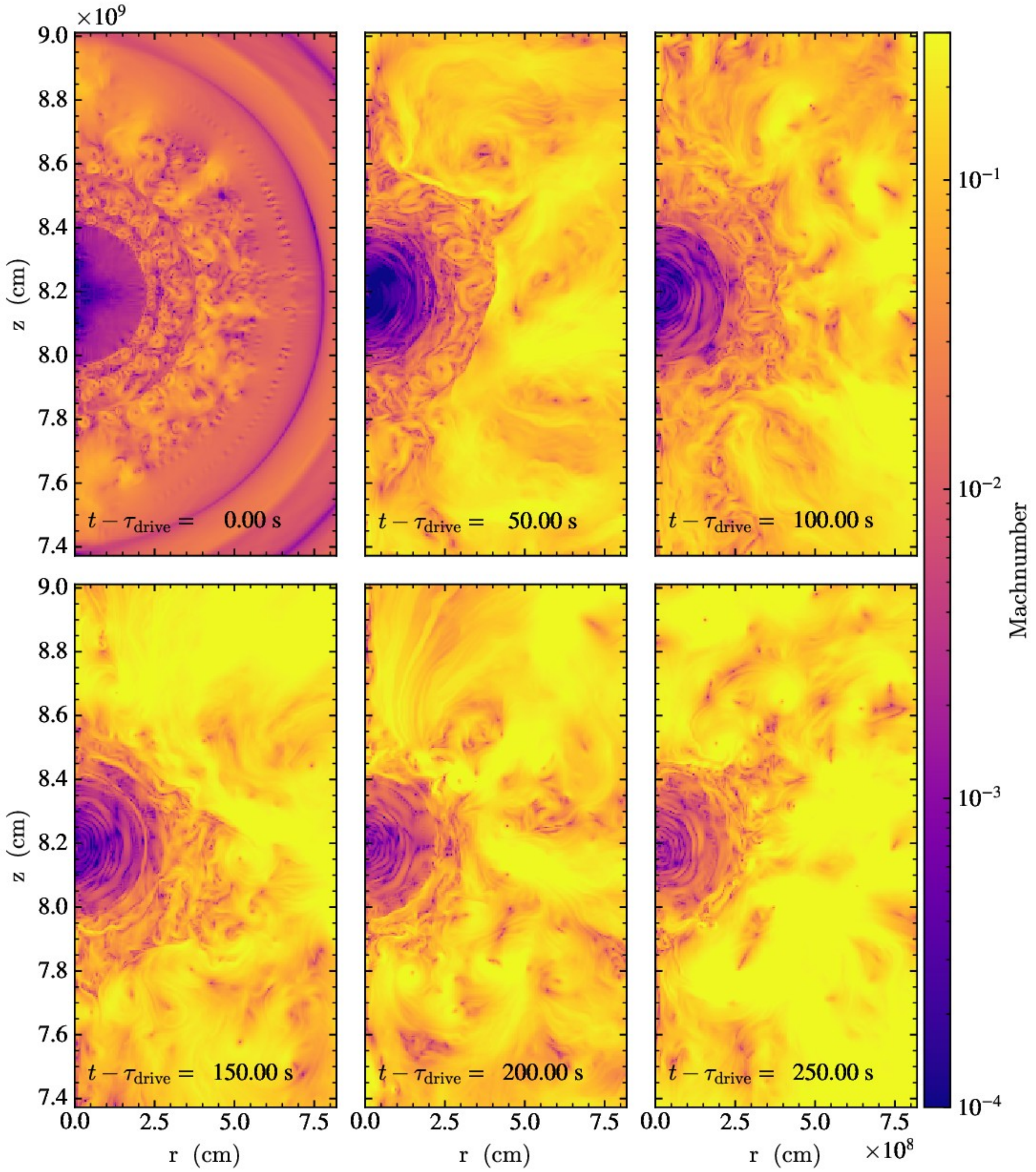
- 15 M$_\odot$ progenitor
- Capture Fe core, Si, O, C shells on grid
- Use 2D axisymmetry with 20 km maximum resolution
  - We are interested in the time-integration strategy, so 2D is fine



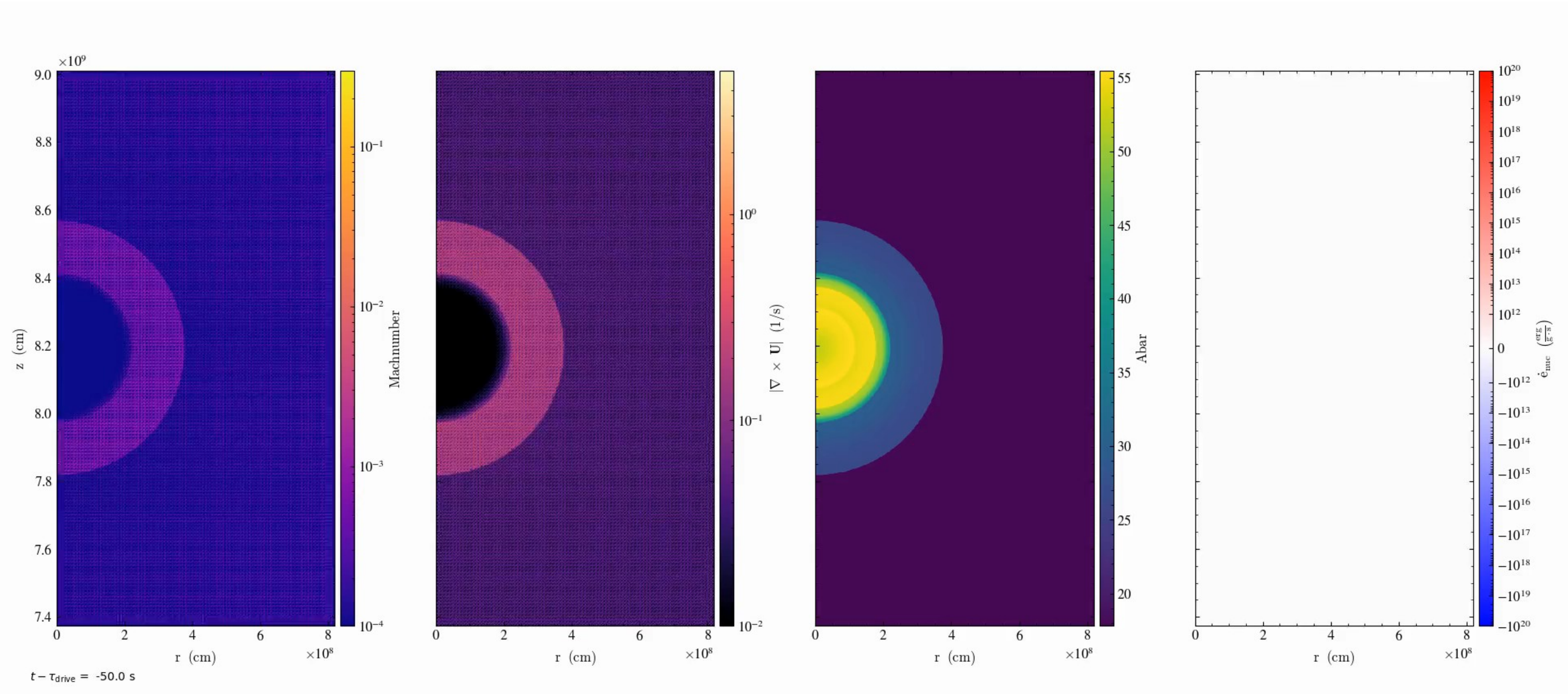


Massive stars

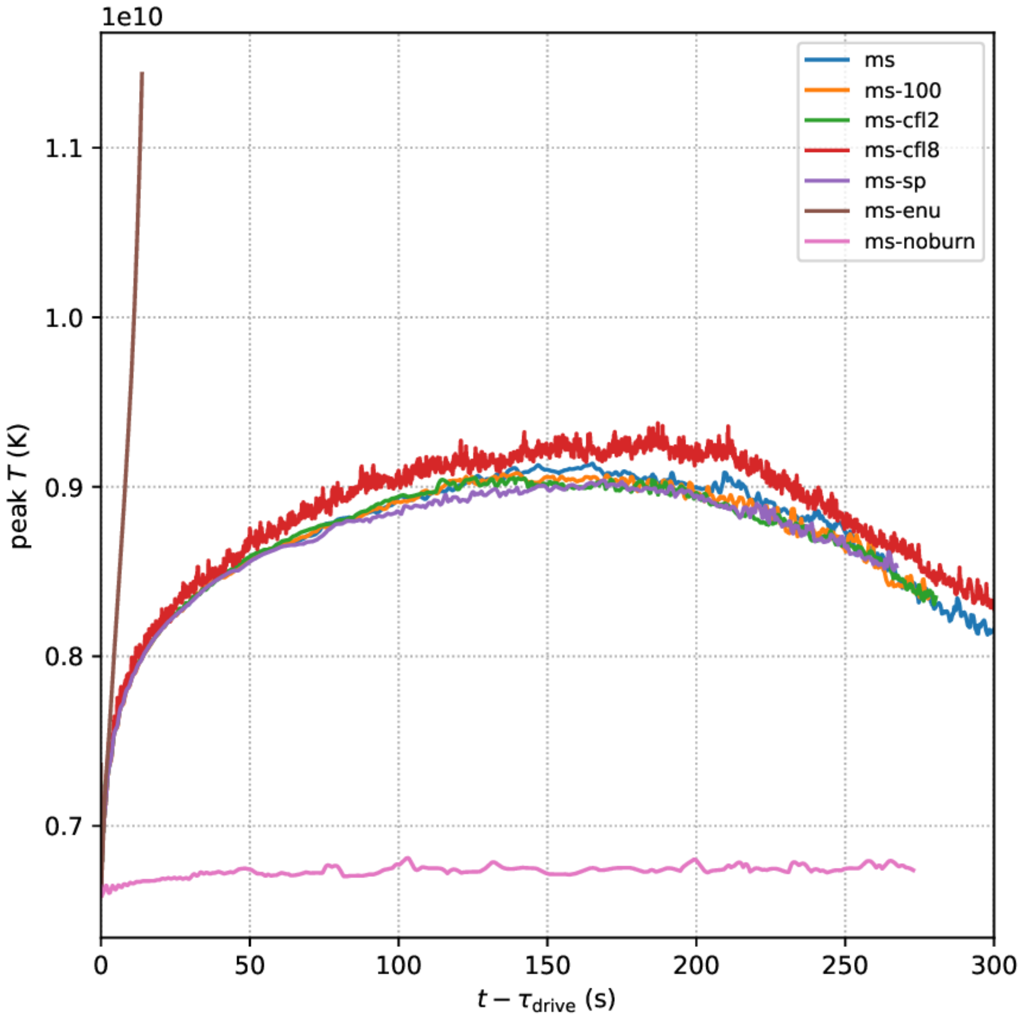
- Fe core modeled self-consistently on the grid
- Strong convection builds up in O layer
- 2D convection is not “real”, erodes Si layer



Massive stars



Sensitivity of results



- Solution is robust to:
  - Timestep (CFL #)
  - Domain size
  - Initialization process
- Evolution can take place on hydro timescale

How do we train students to do computational science?

How do we train students?

- Introduction to programming
  - We have UG and grad versions of this
- Class on numerical methods
  - We have a regular grad class
  - UG level is as “special topics”
- Training on software engineering
  - Generally learned via working in a research group

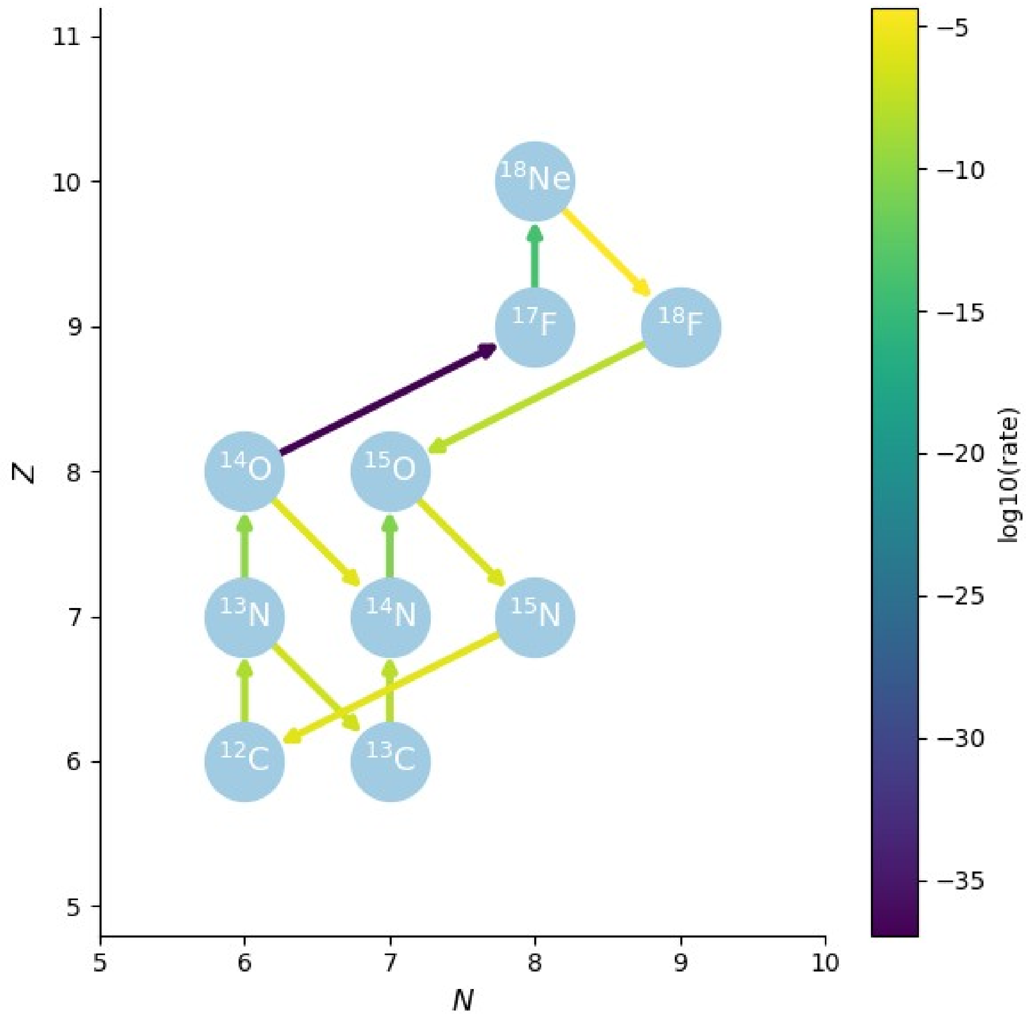
What has worked in the classroom?

- Jupyter-book for organizing content
  - combines a collection of notebooks into a webpage
  - Allow for easy running in the cloud
- Github classroom for assignments
  - Builds comfort with git
- General goals:
  - Write all methods from scratch before using libraries
  - Teach testing (e.g. convergence, unit tests, …)
  - Learn when not to use a particular method
- Classes are usually language agnostic

A tour

- Finished product: https://zingale.github.io/computational_astrophysics/

Classroom ↔ Research https://github.com/pynucastro



- HW from grad Stars class:
  - Download rates for nuclear reactions involved in CNO burning and integrate
  - No students did it
- My solutions became the pynucastro library
- All students in our group contribute to its development

(Smith Clark et al. 2023)

Open astrophysics bookshelf

- Hosted on github:
  https://github.com/Open-Astrophysics-Bookshelf
- Open licensed texts:
  - Contributions accepted from community
- Current texts on stellar physics, star formation, astrophysical processes, computational astro

- Introduction to Computational Astrophysical Hydrodynamics
  - Works through the derivation of all the methods used in our code
  - Every figure has a hyperlink to the code used to generate it
  - Used by many students to learn these methods

Summary

- New algorithms can improve efficiency / accuracy
- Multiphysics integration requires new techniques
  - Operator splitting can lead to breakdowns in coupling
  - We've developed new techniques to strongly couple hydro + reactions
- Simulations of SN Ia and massive stars benefit
  - No need to cut the timestep to reactive timescale
- Training students in computation is critical
- Everything is open: https://github.com/AMReX-Astro