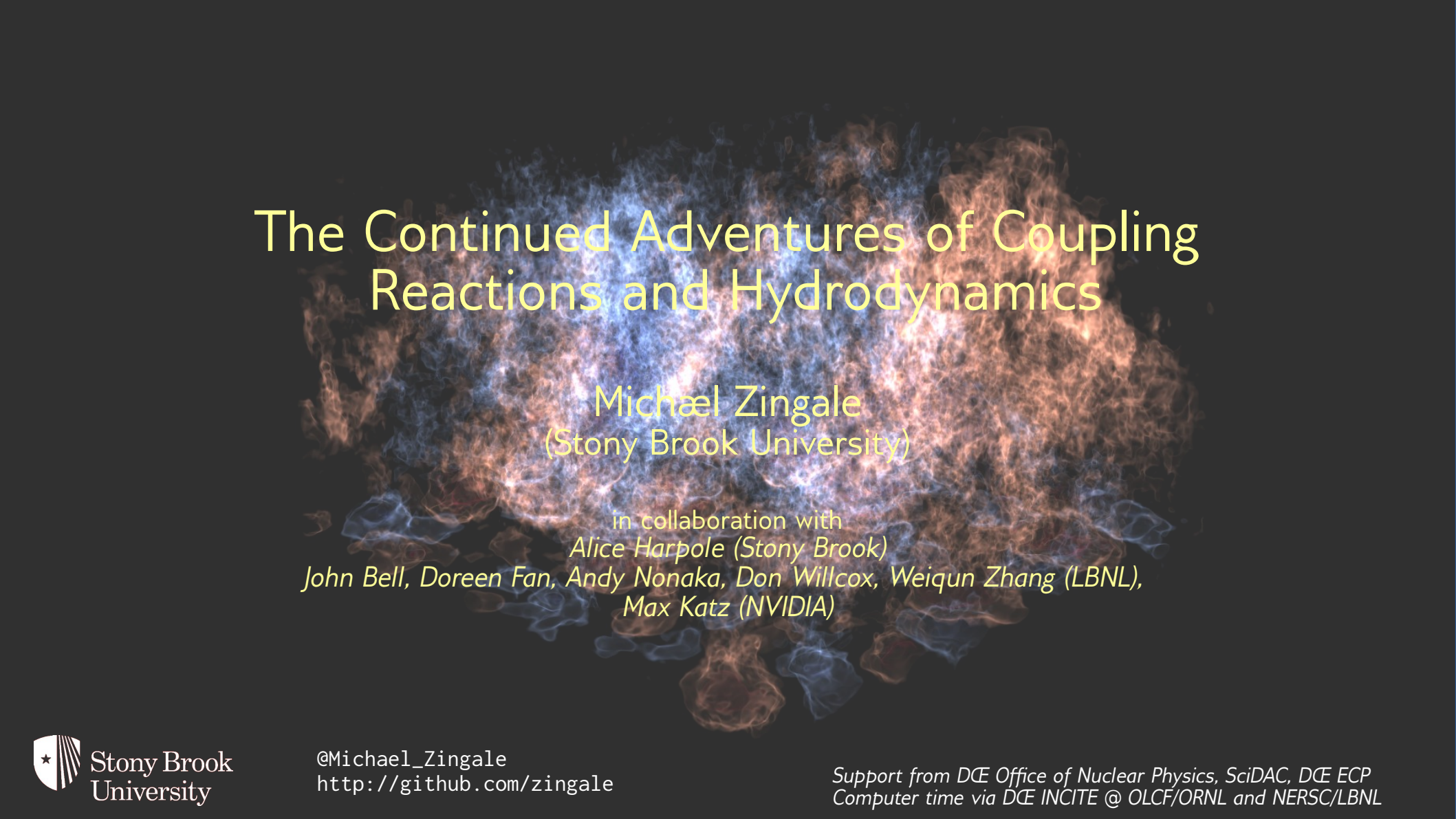

The Continued Adventures of Coupling Reactions and Hydrodynamics

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Convective Flows in Massive Stars

- *Original goal*: MAESTROeX models of late stages of massive star convection
- *Difficulty*: nuclear timescale is much smaller than advective CFL
- *New goal*: how close to the CFL can we get while keeping hydro + reactions coupled?
- *Algorithmic effort*: SDC
  - Working in Castro to start

Compressible Reactive Flow

- Reactive-hydro system:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{U}) = 0$$

$$\frac{\partial (\rho \mathbf{U})}{\partial t} + \nabla \cdot (\rho \mathbf{U}\mathbf{U} + p) = \rho \mathbf{g}$$

$$\frac{\partial (\rho E)}{\partial t} + \nabla \cdot [(\rho E + p)\mathbf{U}] = \rho \mathbf{U} \cdot \mathbf{g} + H_{\mathrm{nuc}}$$

$$\frac{\partial (\rho X_k)}{\partial t} + \nabla \cdot (\rho \mathbf{U} X_k) = \rho \dot{\omega}_k$$

- Species creation rates found via system of ODEs:

$$\dot{\omega}_k = \dot{\omega}_k(\rho, T, X_j)$$

- Reactions and hydrodynamics change on different timescales
  - Use different integration techniques for these two processes
  - But they need to remain coupled together.

Strang Splitting

- Treat each process independent of the others
- Ex: advection-reaction:

$$\phi^{n+1} = R_{\Delta t/2} A_{\Delta t} R_{\Delta t/2} \phi^n$$

  - Hydro and burning can decouple when $t_{\text{hydro}} \sim t_{\text{burn}}$
  - Limited to 2nd order

Assumes constant density in the evolution, for low Mach you might assume constant p and evolve enthalpy

- Reaction rate sensitivity ~T^{40}
  - Some codes ignore this in rate evaluation
- Operator split energy equation

$$\frac{dX_k}{dt} = \dot{\omega}(X_k, \rho, T(\rho, e, X_k))$$

$$\frac{de}{dt} = H_{\text{nuc}}$$

- Misses effects of advection; density doesn't evolve

Castro Retry Functionality

- Reaction-based timestep limiters are popular:

$$\Delta t = \texttt{dtnuc\_e} \min_{i,j,k} \left\{ \frac{e_{i,j,k}}{\dot{e}_{i,j,k}} \right\}$$

$$\Delta t = \texttt{dtnuc\_X} \min_{i,j,k} \left\{ \min_{n} \frac{X^n_{i,j,k}}{\dot{X}^n_{i,j,k}} \right\}$$

  - Important for Strang, when reactions and hydro decouple
  - Might not be needed with SDC

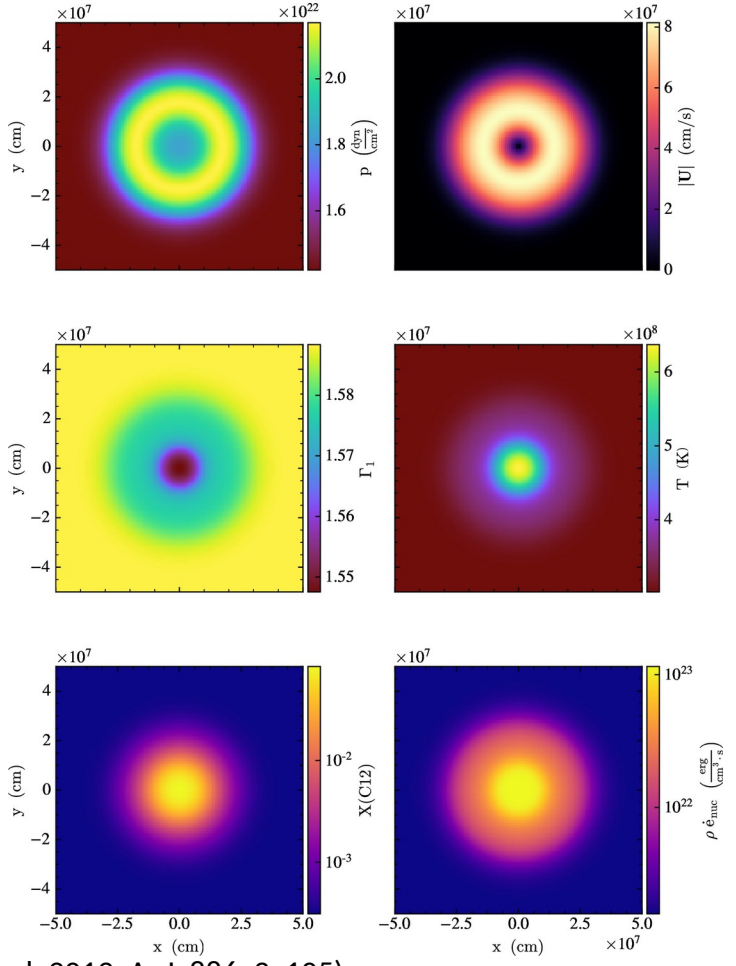
- Castro retries:
  - Advance is thrown out if:
    - CFL is exceeded on a level
    - Negative density encountered
    - Integration failure in burner
    - Reaction timestep constraints not met (e.g. tol not met)
  - Level advance restarted with a smaller timestep
    - subcycle in subcycle

Reacting Hydro Convergence

- Reacting version of acoustic pulse (3-α + $^{12}C(\alpha,\gamma)^{16}O$ network)
  - Strang + CTU has trouble with species

Table 6. Convergence (L_1 norm) for the reacting convergence problem with the Strang CTU solver.

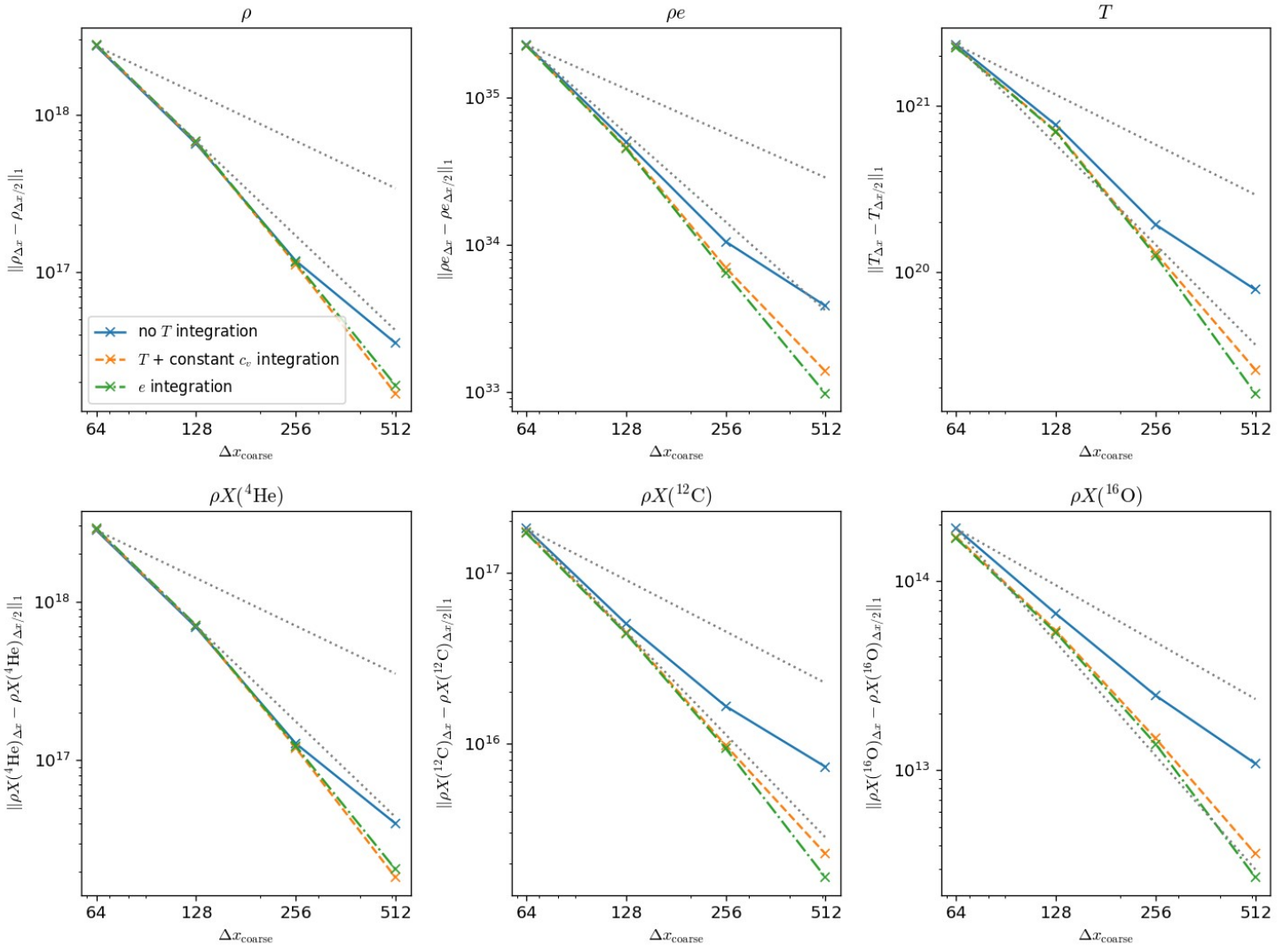
field	$\epsilon_{64\to128}$	rate	$\epsilon_{128\to256}$	rate	$\epsilon_{256\to512}$
ρ	2.780×10^{18}	2.051	6.706×10^{17}	2.580	1.121×10^{17}
ρu	6.780×10^{26}	2.446	1.245×10^{26}	2.907	1.659×10^{25}
ρv	6.780×10^{26}	2.446	1.245×10^{26}	2.907	1.659×10^{25}
ρE	2.465×10^{35}	2.333	4.893×10^{34}	2.650	7.797×10^{33}
ρe	2.268×10^{35}	2.298	4.611×10^{34}	2.721	6.991×10^{33}
T	2.245×10^{21}	1.682	6.995×10^{20}	2.439	1.290×10^{20}
$\rho X(^4\mathrm{He})$	2.861×10^{18}	2.027	7.018×10^{17}	2.553	1.195×10^{17}
$\rho X(^{12}\mathrm{C})$	1.717×10^{17}	1.945	4.458×10^{16}	2.194	9.745×10^{15}
$\rho X(^{16}\mathrm{O})$	1.717×10^{14}	1.648	5.479×10^{13}	1.898	1.471×10^{13}
$\rho X(^{56}\mathrm{Fe})$	2.780×10^{-12}	2.051	6.706×10^{-13}	2.580	1.121×10^{-13}



(Zingale et al. 2019, ApJ, 886, 2, 105)

Strang

- Not integrating “energy” converges first order



(Zingale et al. 2021, RNAAS)

High-order SDC

- General finite-volume method + SDC time integration

$$\begin{aligned}\langle \boldsymbol{\mathcal{U}} \rangle_i^{m+1,(k+1)} = \langle \boldsymbol{\mathcal{U}} \rangle_i^{m,(k+1)} &+ \Delta t_m \left[\langle \boldsymbol{\mathcal{A}}(\boldsymbol{\mathcal{U}}) \rangle_i^{m,(k+1)} - \langle \boldsymbol{\mathcal{A}}(\boldsymbol{\mathcal{U}}) \rangle_i^{m,(k)} \right] \\ &+ \Delta t_m \left[\langle \mathbf{R}(\boldsymbol{\mathcal{U}}) \rangle_i^{m+1,(k+1)} - \langle \mathbf{R}(\boldsymbol{\mathcal{U}}) \rangle_i^{m+1,(k)} \right] \\ &+ \mathcal{I}_m^{m+1} \left(\langle \boldsymbol{\mathcal{A}}(\boldsymbol{\mathcal{U}}) \rangle_i^{(k)} + \langle \mathbf{R}(\boldsymbol{\mathcal{U}}) \rangle_i^{(k)} \right)\end{aligned}$$

  - Last term is integral over temporal nodes

$$\mathcal{I}_m^{m+1} \left(\langle \boldsymbol{\mathcal{A}}(\boldsymbol{\mathcal{U}}) \rangle_i^{(k)} + \langle \mathbf{R}(\boldsymbol{\mathcal{U}}) \rangle_i^{(k)} \right) = \int_{t^m}^{t^{m+1}} \mathrm{d}t \left(\langle \boldsymbol{\mathcal{A}}(\boldsymbol{\mathcal{U}}) \rangle_i^{(k)} + \langle \mathbf{R}(\boldsymbol{\mathcal{U}}) \rangle_i^{(k)} \right)$$

- Integral evaluated with either Gauss-Lobatto or Radau quadrature

Reacting Hydro Convergence

- SDC-2 and SDC-4 converge as expected

Table 7. Convergence (L_1 norm) for the reacting convergence problem with the SDC-2 solver.

field	$\epsilon_{64\to128}$	rate	$\epsilon_{128\to256}$	rate	$\epsilon_{256\to512}$
ρ	2.024×10^{18}	2.011	5.022×10^{17}	2.021	1.238×10^{17}
ρu	3.720×10^{26}	2.063	8.901×10^{25}	2.030	2.180×10^{25}
ρv	3.720×10^{26}	2.063	8.901×10^{25}	2.030	2.180×10^{25}
ρE	2.302×10^{35}	2.030	5.635×10^{34}	2.014	1.395×10^{34}
ρe	2.053×10^{35}	2.025	5.043×10^{34}	2.013	1.249×10^{34}
T	1.643×10^{21}	2.060	3.939×10^{20}	2.026	9.676×10^{19}
$\rho X(^4\mathrm{He})$	2.002×10^{18}	2.015	4.951×10^{17}	2.027	1.215×10^{17}
$\rho X(^{12}\mathrm{C})$	1.042×10^{17}	2.032	2.546×10^{16}	2.019	6.281×10^{15}
$\rho X(^{16}\mathrm{O})$	1.564×10^{14}	1.935	4.090×10^{13}	2.003	1.020×10^{13}
$\rho X(^{56}\mathrm{Fe})$	2.024×10^{-12}	2.011	5.022×10^{-13}	2.021	1.238×10^{-13}

Table 8. Convergence (L_1 norm) for the reacting convergence problem with the SDC-4 solver.

field	$\epsilon_{64\to128}$	rate	$\epsilon_{128\to256}$	rate	$\epsilon_{256\to512}$
ρ	2.127×10^{17}	3.855	1.470×10^{16}	3.972	9.369×10^{14}
ρu	3.401×10^{25}	3.856	2.349×10^{24}	3.958	1.511×10^{23}
ρv	3.401×10^{25}	3.856	2.349×10^{24}	3.958	1.511×10^{23}
ρE	1.945×10^{34}	3.891	1.311×10^{33}	3.953	8.463×10^{31}
ρe	1.672×10^{34}	3.899	1.120×10^{33}	3.955	7.223×10^{31}
T	1.236×10^{20}	3.708	9.463×10^{18}	3.949	6.125×10^{17}
$\rho X(^4\mathrm{He})$	2.147×10^{17}	3.858	1.481×10^{16}	3.969	9.458×10^{14}
$\rho X(^{12}\mathrm{C})$	8.789×10^{15}	3.798	6.319×10^{14}	3.911	4.201×10^{13}
$\rho X(^{16}\mathrm{O})$	1.294×10^{13}	3.765	9.518×10^{11}	3.872	6.501×10^{10}
$\rho X(^{56}\mathrm{Fe})$	2.127×10^{-13}	3.855	1.470×10^{-14}	3.972	9.369×10^{-16}

(Zingale et al. 2019, ApJ, 886, 2, 105)

SDC Complexity

- 4^{th} order is slow
  - Maybe we only need to do parts to 4^{th} order, like the burn?
- Ghost cell fills at intermediate time nodes are tricky
- Code path is completely separate from Strang, so additional burden to maintain

- Simplified SDC
  - Reuse CTU PPM + (mostly) the Strang ODE integration
  - Still explicitly couple reactions and hydro
  - Benefits from larger CFL of CTU

Simplified-SDC

- Simple methodology that uses the CTU PPM hydro solver
  - Implemented in both MAESTROeX and Castro
- Consider our system as:

$$\frac{\partial \mathcal{U}}{\partial t} = -\nabla \cdot \mathbf{F}(\mathcal{U}) + \mathbf{S}(\mathcal{U}) + \mathbf{R}(\mathcal{U})$$

  - Grouping hydro sources:

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

- Do sdc iteration k:
  - Predict advective update $\mathcal{A}$ using iteratively lagged reaction source
  - Solve reaction ODE system with piecewise-constant-in-time advective source :

$$\frac{d\mathcal{U}_i}{dt} = [\boldsymbol{\mathcal{A}}(\mathcal{U})]_i^{n+1/2} + \mathbf{R}(\mathcal{U}_i)$$

  - Defines $\mathcal{U}^{(k+1)}$
  - Construct new reaction source term for next iteration

Simplified SDC Implementation

- Advective term:
  - Standard CTU PPM algorithm
  - Add reactive source term to primitive variable interface states
- Final update
  - Only subsystem directly integrated:

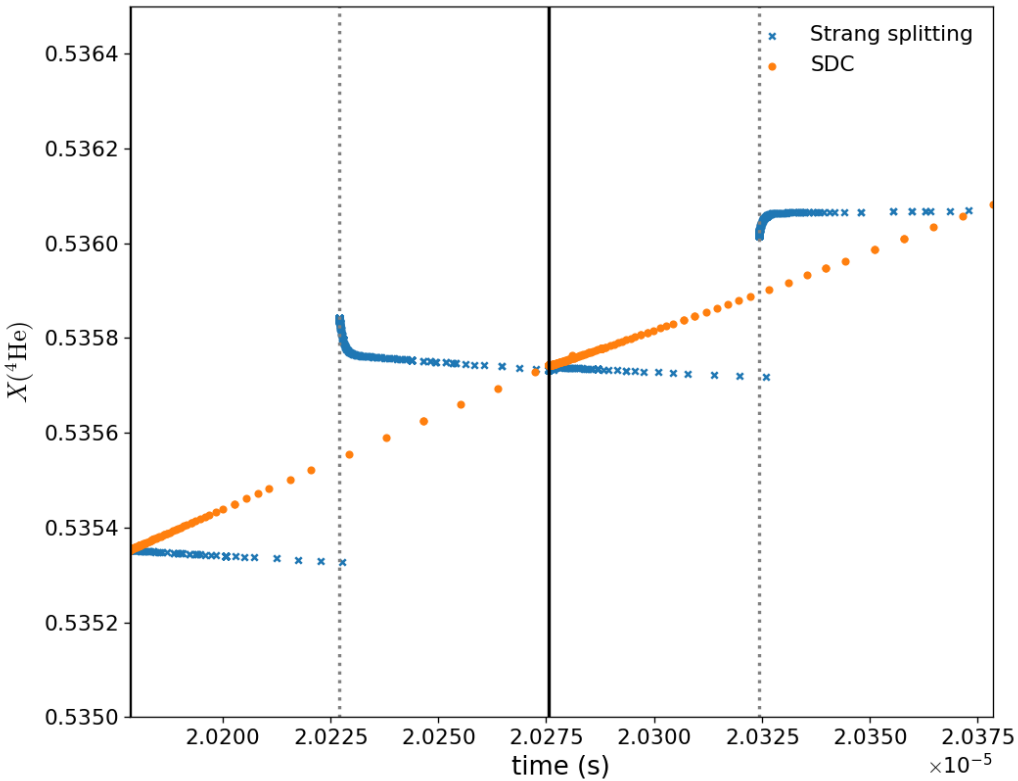
$$\boldsymbol{\mathcal{U}} = (\rho X_k, \rho e)^\intercal$$

  - Density and momentum algebraically updated
  - Total energy conservatively updated after integration

- Implementation:
  - We use VODE integrator
    - Our version is a C++ “de-goto-ized” version
    - Additional step-rejection logic
  - Species equations gain piecewise-constant-in-time advective term
  - Runs completely on GPUs

SDC Costs?

- We essentially do hydro twice
- But reactions are less stiff when advection included, so VODE works less hard



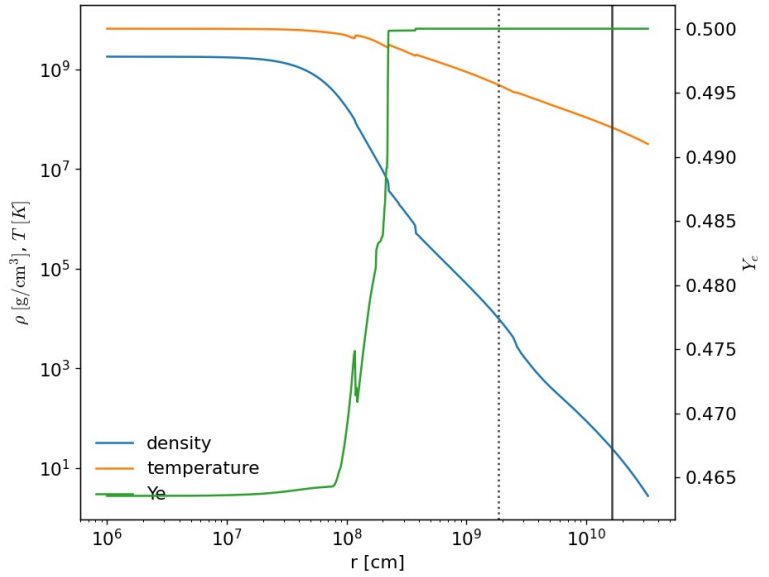
(Zingale et al. 2019, JPCS, 1225, 012005)

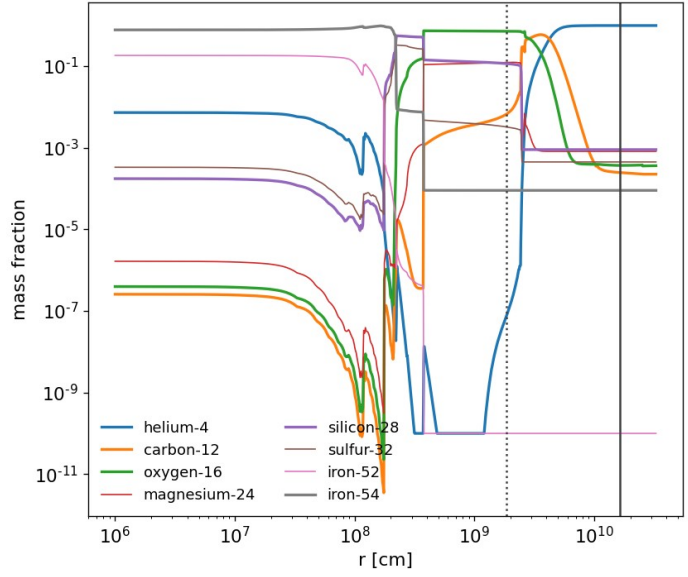
Massive Star

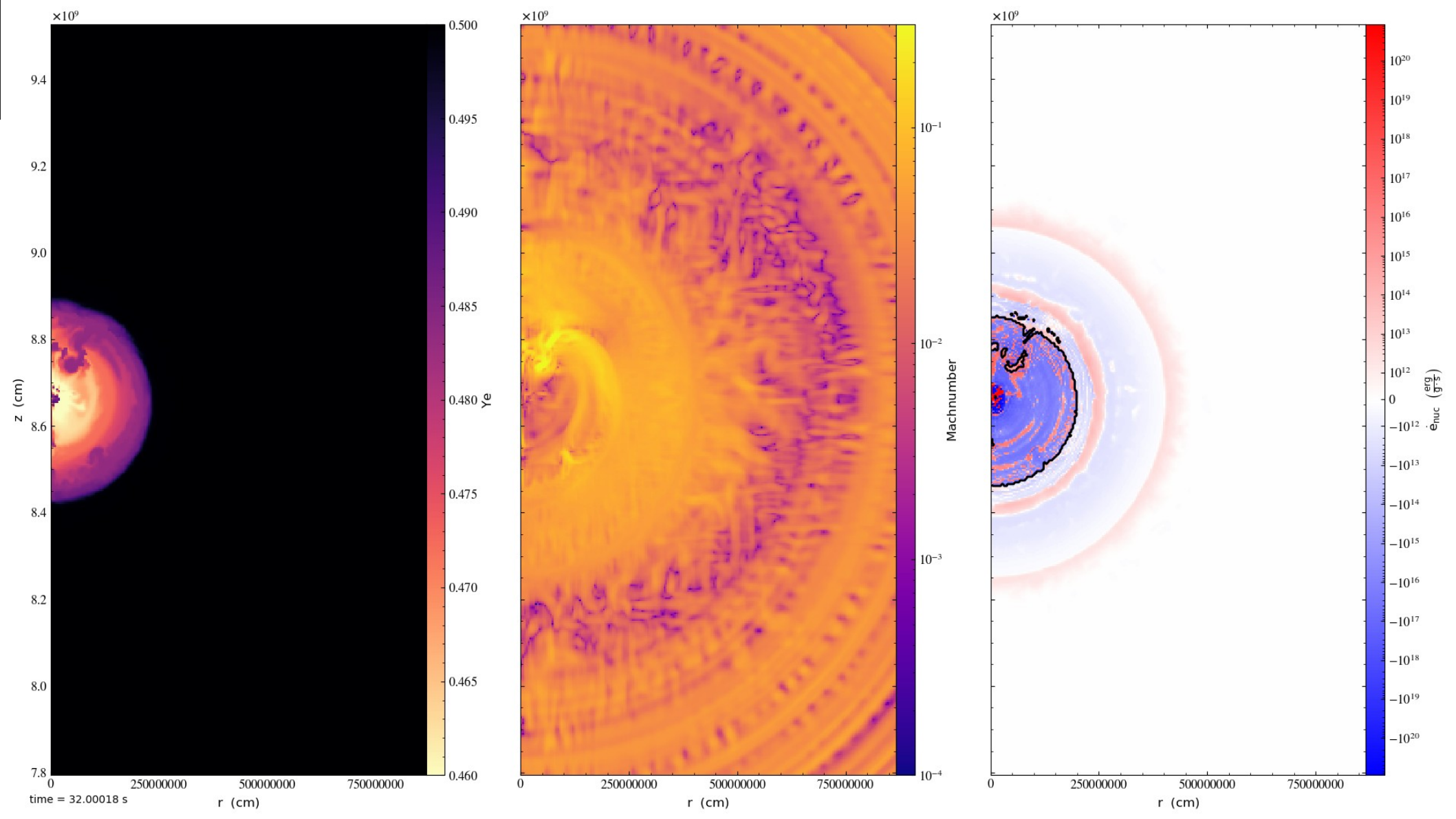
- We use a model from Sean
- Hybrid 19 isotope net + NSE table from 125 species network (from Stan)
  - SDC now needs to predict sources for:

$$Y_e, \bar{A}, (B/A)$$

  - NSE test problem shows close to 2nd order convergence for SDC+NSE
    - Strang is not as good
- NSE bailout if integration enters NSE during burn
- We model hydro + reactions in the core as well as shells






×10^9
9.4
9.2
9.0
8.8
8.6
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8.0
7.8
z (cm)
0
250000000
500000000
750000000
r (cm)
time = 32.00018 s
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0.495
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0.485
0.480
0.475
0.470
0.465
0.460
Ye
×10^9
0
250000000
500000000
750000000
r (cm)
10^-1
10^-2
10^-3
10^-4
Machnumber
×10^9
0
250000000
500000000
750000000
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10^20
10^19
10^18
10^17
10^16
10^15
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10^13
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0
−10^12
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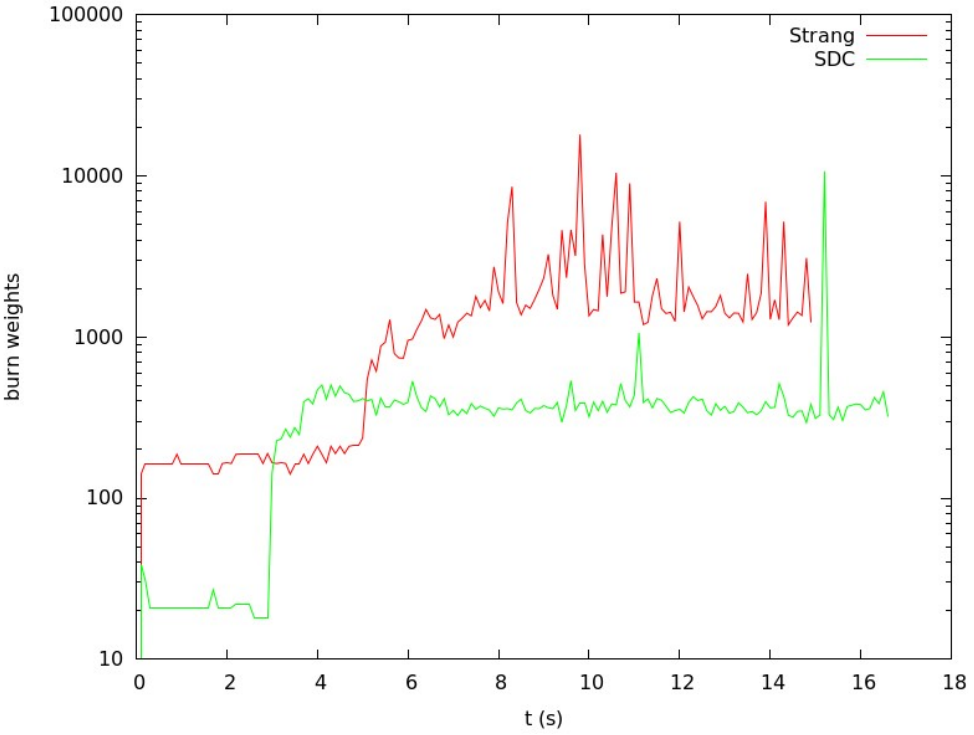
−10^15
−10^16
−10^17
−10^18
−10^19
−10^20
ė_nuc (erg/g-s)

Massive Star

- Still assessing how the solution compares between SDC and Strang
- Preliminary findings:
  - SDC takes many fewer RHS calls than Strang
  - Note: this is second half of Strang compared to second iter of SDC
- Possibilities for further optimization of SDC not yet explored



Summary

- SDC + NSE method seems to (mostly) work for massive star
  - Writing it up now (and have been for the last 3 years…)
- Runs are fast on GPUs (~ 100s of Summit node hours)
- Rotation is implemented and ready to go for Castro
- Everything shown here is up on github: https://github.com/amrex-astro/
- We believe SDC is the path forward
  - LBL combustion code does this by default now
  - All of the developments here can be used in MAESTROeX
- If you do Strang, please integrate T / e !
  - We have convergence test problems you can run to see how you do currently

Fun with Neutron Stars

- Castro modeling of flame's on NS / XRBs
  - Two 2D studies published
    (Eiden et al. 2020, Harpole et al. 2021)
  - 3D run cooking now on Summit
  - Mixed H/He bursts running now
  - Doubled GPU performance over last year