MAESTROeX: Applications and Future Developments

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in collaboration with

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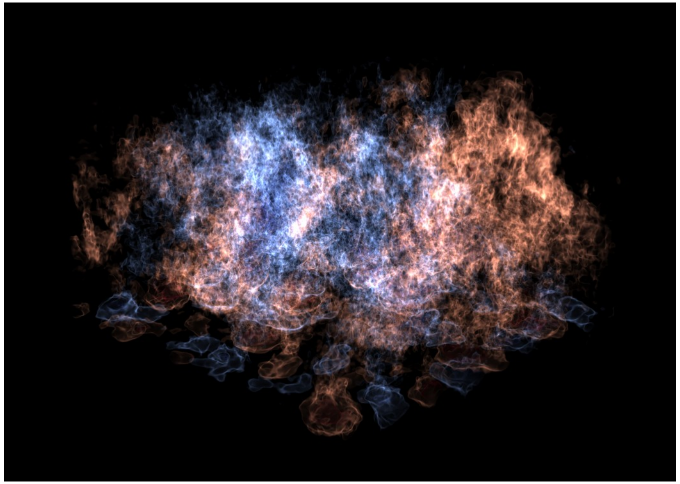
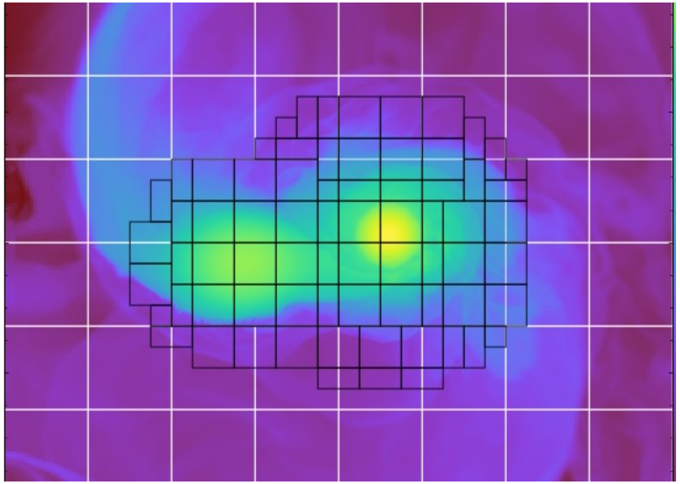
Computer time via DŒ INCITE @ OLCF/ORNL and NERSC/LBNL

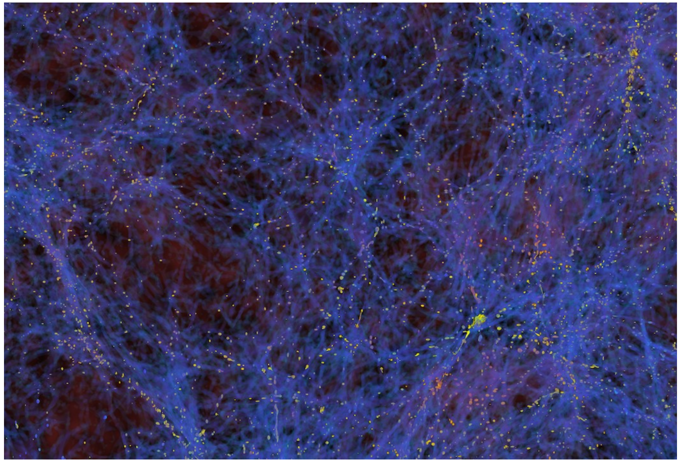
AMReX Astrophysics Suite



MAESTROeX: low Mach number stratified flows



Castro: compressible (radiation-) hydrodynamics



Nyx: cosmological hydrodynamics + N-body

https://github.com/amrex-astro

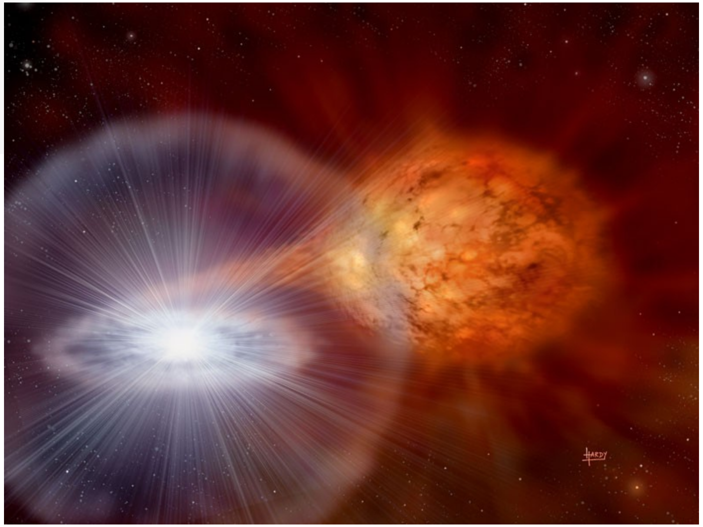
Open Science

Every line of code needed to rerun the simulations shown (SN Ia convection, sub-Ch convection, WD mergers, & XRB) is in our public github repos

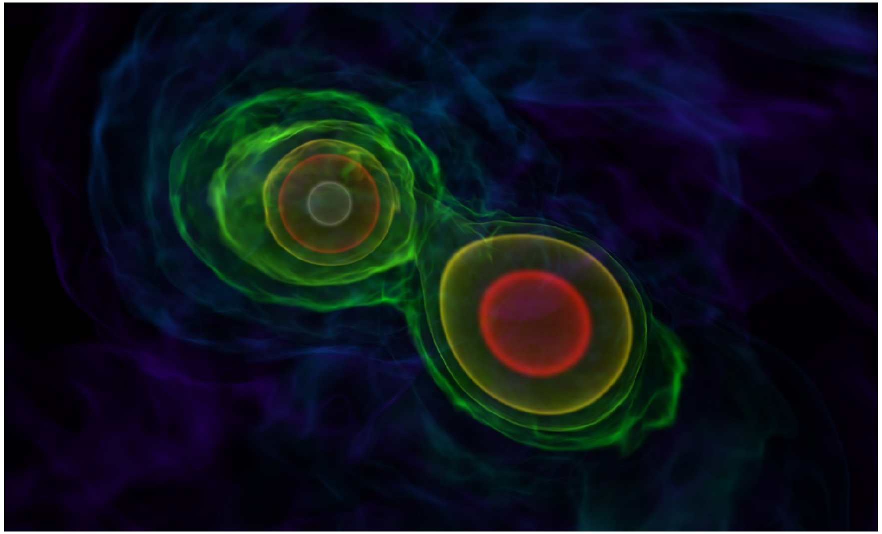
- http://github.com/AMReX-Astro
  - Includes inputs files, analysis scripts, submission scripts, etc…
  - User contributions via PRs and issues
  - repos: MAESTRO, Castro, …
- These are our actual development repos
- Reproducibility:
  - Output files store the git hash of the source, the machine name, compiler versions and flags, values of all runtime parameter, …
  - Most papers include the github hash of the repos used for simulations
- Nightly regression tests

Type Ia Supernovæ

- 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)

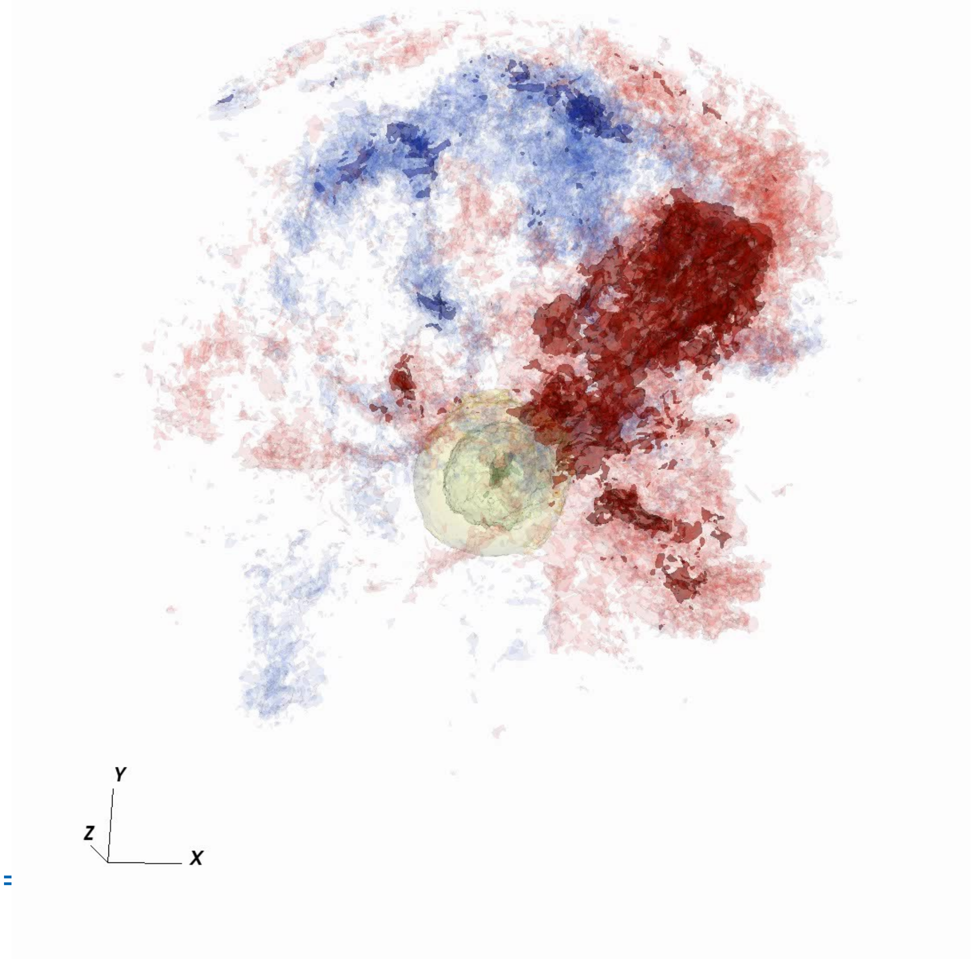


Variations in SNe Ia

- Chandra model:
  - Burning front begins near center
  - Does nature make massive WDs?
  - Does the burning remain subsonic?
- Mergers (double degenerates):
  - Two WDs inspiral, explosion either prompt or after (long term?) accretion
  - Can we avoid the accretion induced collapse?
  - Does the explosion looks like an SNe Ia?
- Sub-Chandra model:
  - Double detonation: ignite in He layer on surface of WD, shock converges at center of underlying C/O WD and detonates inside out
  - Can we hide the He?
  - Can we make normal SNe Ia?
- What does nature do?

Convection in Chandra Model

- Explosion in Chandra model for SN Ia preceded by centuries of simmering / convection
  - Sets explosion initial conditions
- Dipole / jet feature seen (as in previous calculations)
  - Asymmetry in radial velocity field
  - Direction changes rapidly
- Ignition is localized
  - Single point, off-center favored

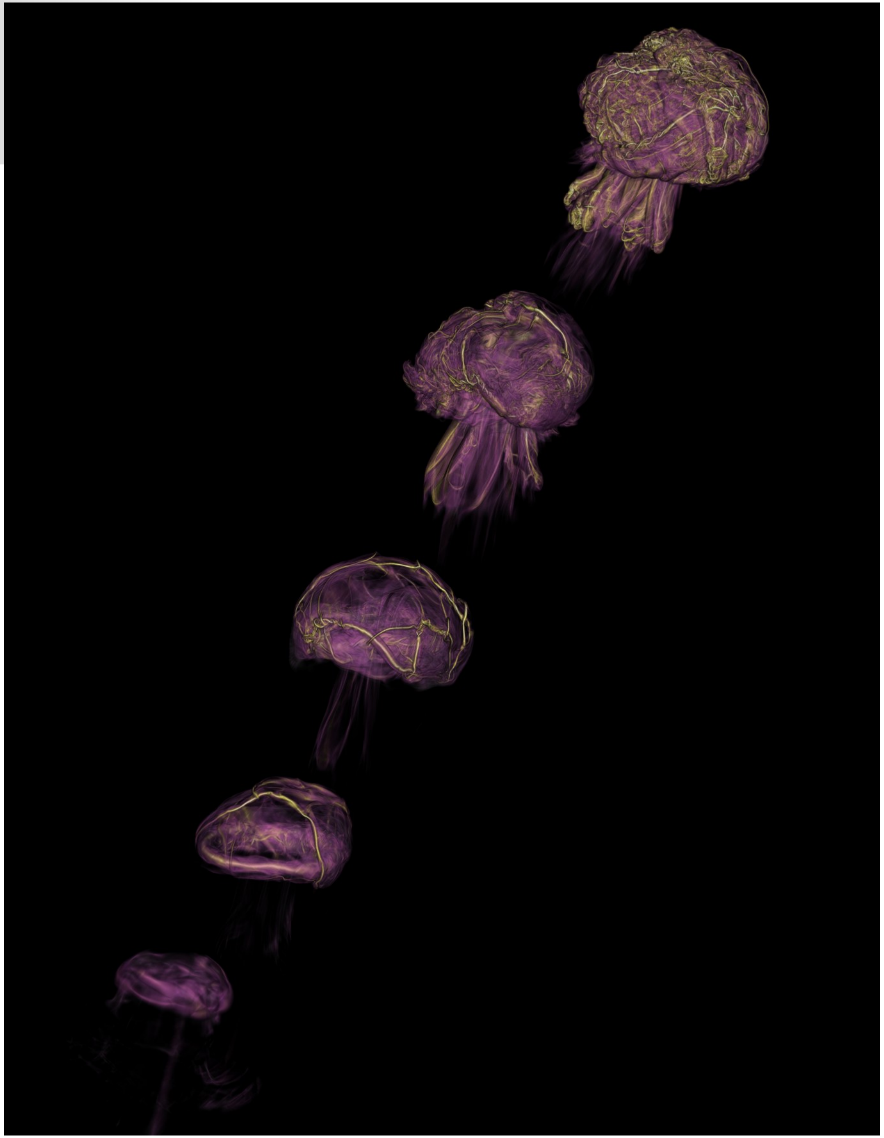


refs:
Zingale et al. 2009
Zingale et al. 2011
Nonaka et al. 2012

Radial velocity field (red = outflow; blue = inflow) in an 1152^3 non-rotating WD simulation.

On To Explosion...

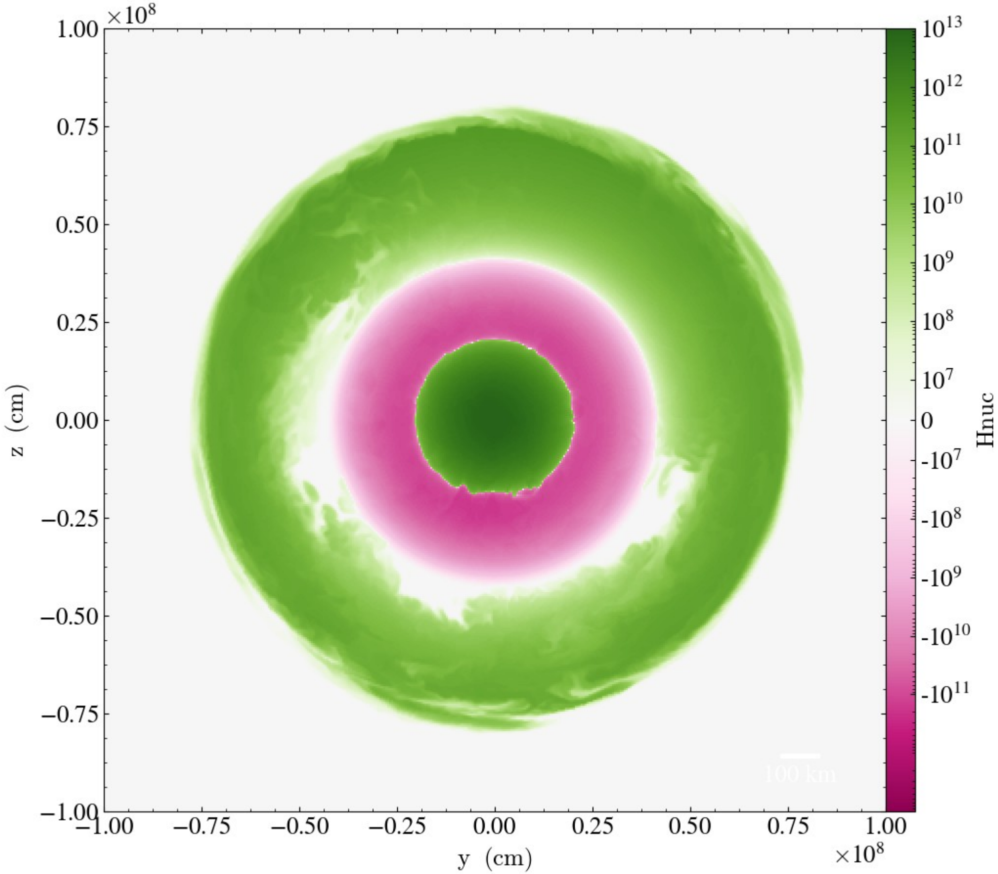
- Mach number gets large (ignition): restart in our compressible code, Castro
  - Same underlying AMReX discretization
  - Same Microphysics
- Basic findings:
  - Off-center ignition: background turbulence doesn't strongly affect flame propagation.
  - Central ignition: convective turbulence can push the flame off-center.
  - Single-degenerate model almost always produces an asymmetric explosion
  - Single spot = small amount of burned mass = less expansion = higher density when DDT occurs



(Malone et al. 2014)

Convective Urca

- Extending this simulation methodology to model convective Urca in white dwarfs
- Competition between electron captures and β-decays
    - e^- captures at higher densities, β-decays at lower
- Understanding of how Urca affects WD structure requires multi-d simulations



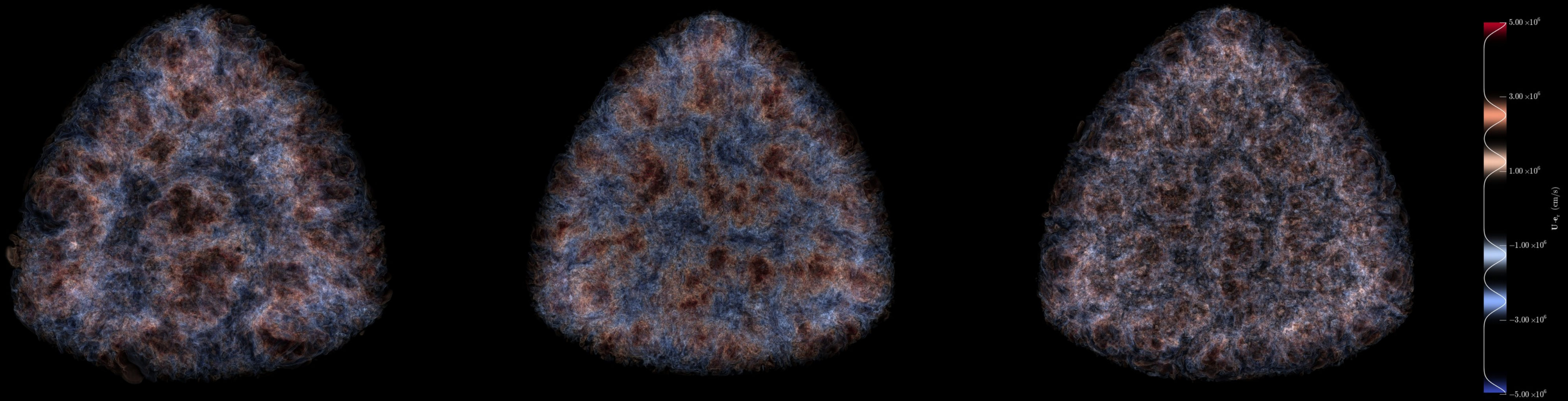
Convective Urca process in a WD with a resolution of 5 km, showing the energy generation from nuclear rest masses and (thermal + A=23 Urca) neutrino losses. We see the effects of carbon burning and neutrino energy losses in the core and β-decays in the upper region of the convection zone. These regions are separated by the A=23 Urca shell.

Don Willcox PhD thesis

sub-Chandra SNe Ia Models

- Basic idea:
  - Burning begins in an accreted helium layer on WD surface
  - Detonation
- How does the burning transfer to the C/O core?
  - Edge lit: direct propagation of detonation across interface. May require ignition at altitude
  - Double detonation: compression wave converges at core, ignites second detonation at WD center
- Main problem: how much surface He is too much?
- Our focus:
  - *What does the ignition in the He layer look like?*
  - *What variety of outcomes can we expect for different masses?*

sub-Chandra He Convection



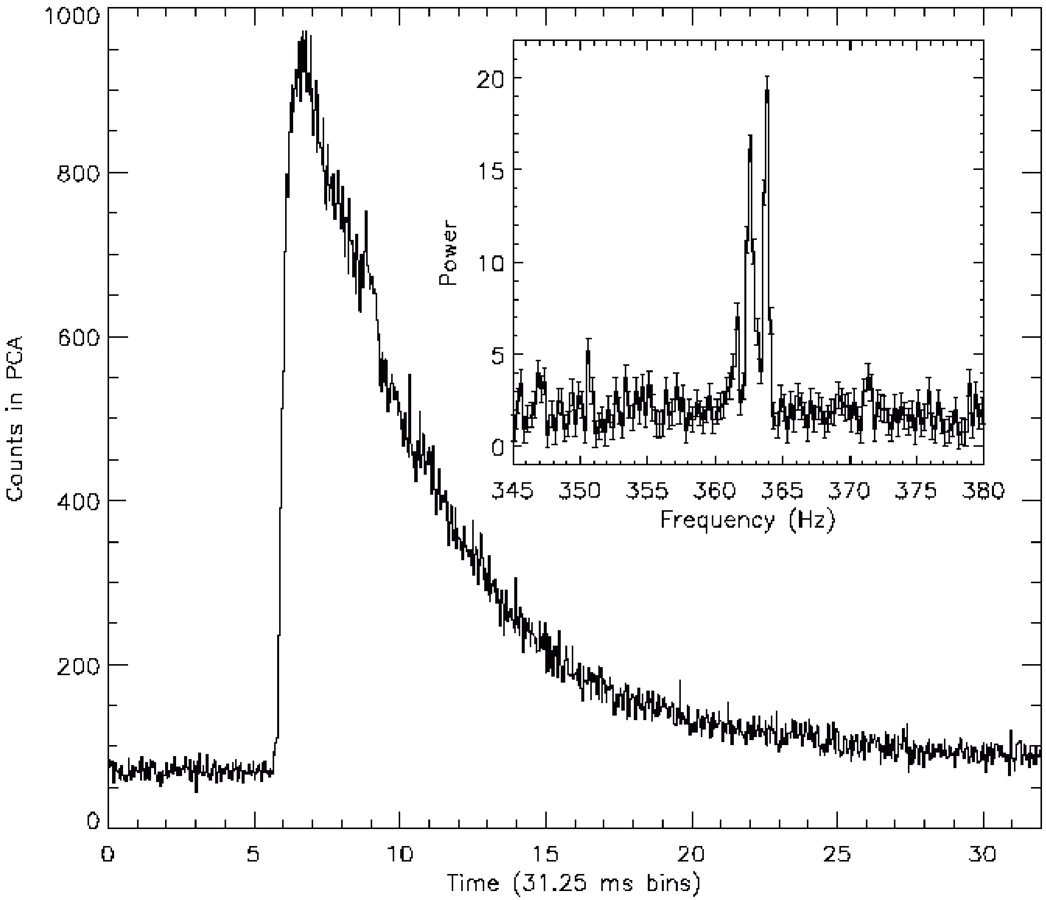
Adam Jacobs thesis

- Variations for WD/He layer masses
- Cellular pattern forums
  - Length scale converged with resolution
  - Hot spots rise up and expand
- Three types of outcomes
  - Localize runaway on short timescale
  - Nova-like convective burning
  - Quasi-equilibrium (?)

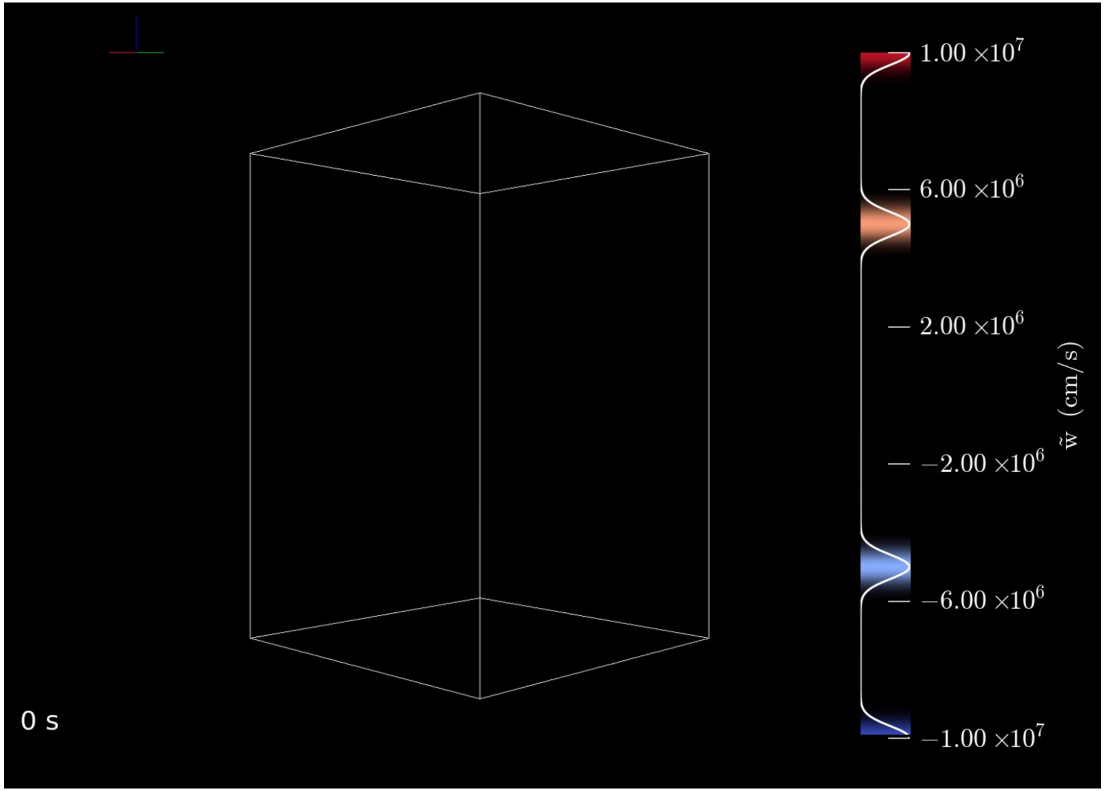
refs: Zingale et al. 2013; Jacobs et al. 2016

X-ray Bursts

- Thermonuclear runaway in thin accreted H/He layer on surface of a neutron star
- Accretion timescale ~ hours to days
- Runaway timescale ~ seconds
- > 70 sources known, some with 10s or more individual bursts.
- Potential site for rp-process nucleosynthesis



X-ray Bursts

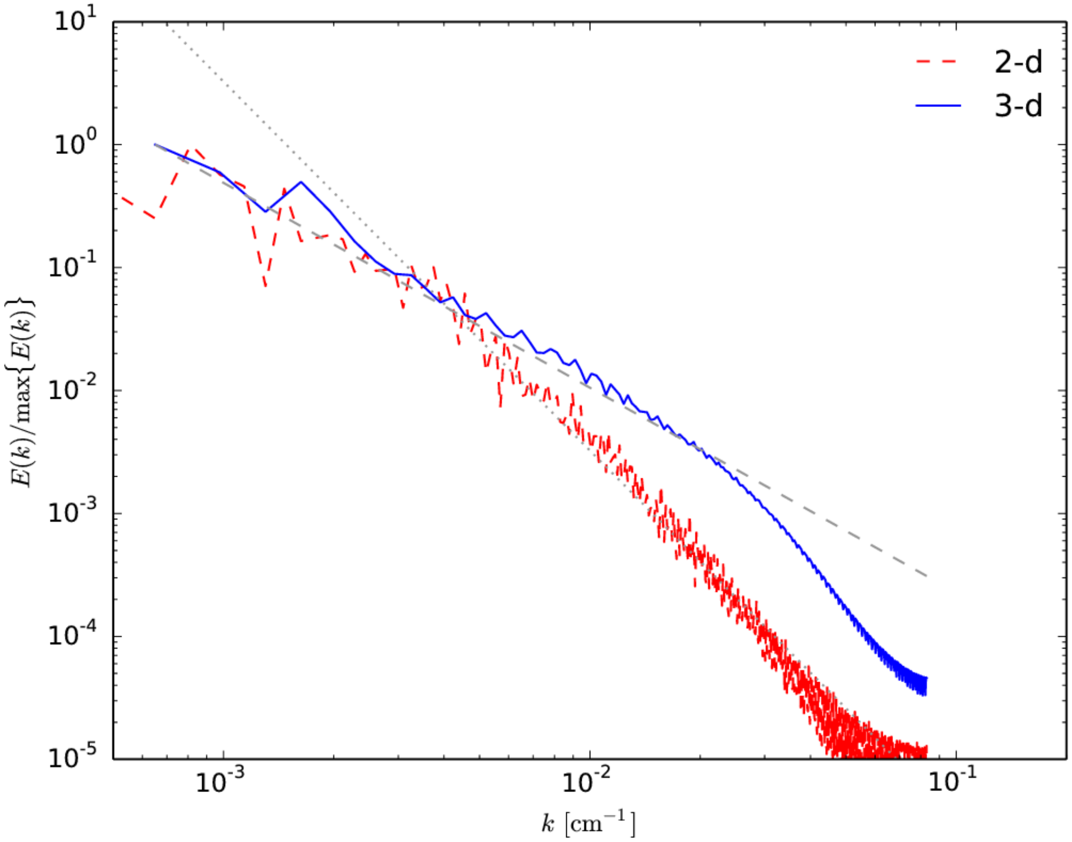


- Convection:
  - 512 × 512 × 768 zones
  - 6 cm resolution
  - 11 nuclei network
    - Captures H burning (hot CNO), 3-α, rp-process breakout
  - T increase over 10^9 K, evolve for 0.02 s
- Next steps:
  - Bigger domains
  - Variety of initial models

refs:
Malone et al. 2011
Malone et al. 2014
Zingale et al. 2015

We Need 3-d!

- Convection requires 3-d
- Turbulence and instabilities are only properly realized in 3-d
    - We'll never resolve dissipation scale—Re ~ 10^{14} for some of these systems



Note that capturing turbulence requires a minimum of 512 zones across in our experience. If turbulence is important to your problem, you really need to do high resolution.

Modeling Reacting Flow

- 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 $t_{\mathrm{hydro}} \sim t_{\mathrm{burn}}$
  - Limited to 2nd order

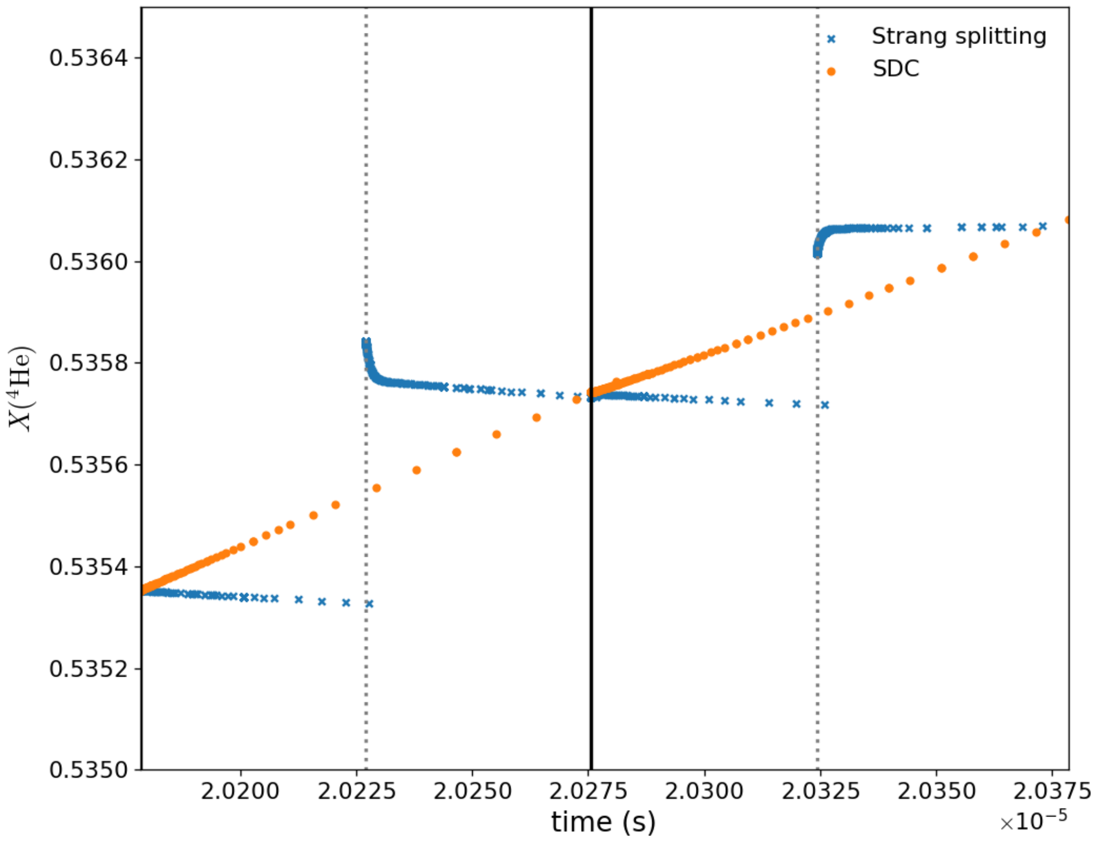
- Spectral deferred corrections
  - Reactions and hydro coupled via explicit source terms
  - Can remove stiffness from system
  - Simple second order method:

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

  - More general, fully 4th order method implemented in Castro

Issues / Difficulties

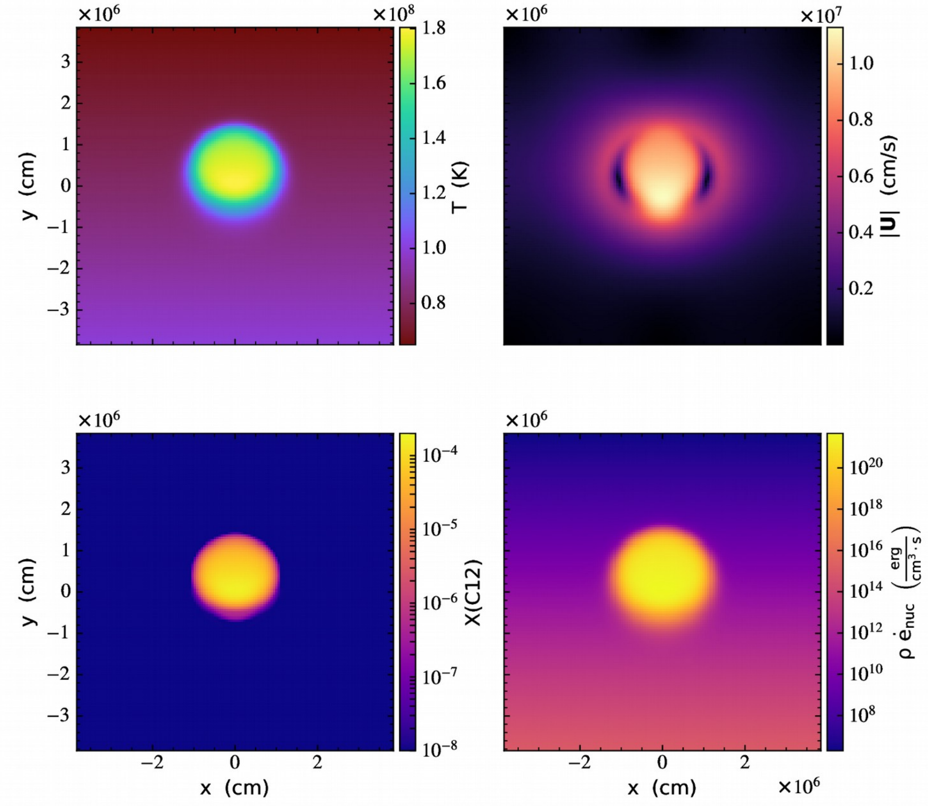
- SDC can remove some stiffness from the system
- Splitting can require smaller timesteps to improve coupling
- For intense burning stages and NSE, SDC should help reduce the cost of reaction networks
- Expected to be important for MAESTROeX massive star calculations



(Zingale et al., 2019, J Phys Conf Series, 1225, 012005)

Higher-order

- SDC provides a path to higher-order coupling in time



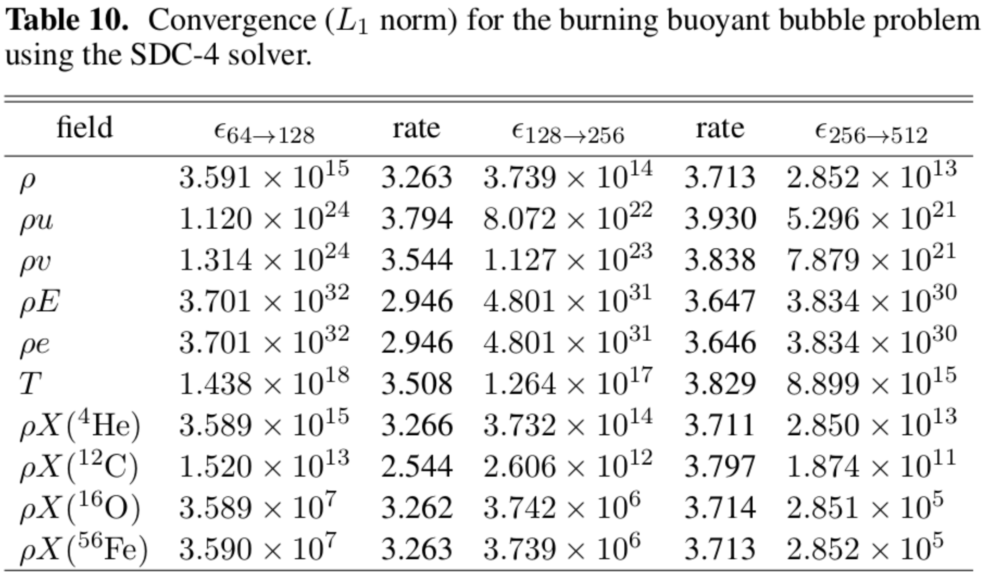


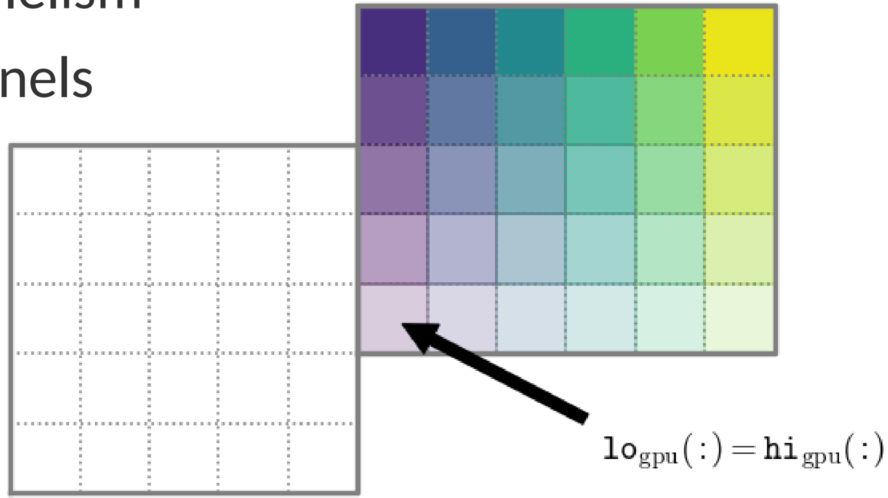
Table 10. Convergence (L_1 norm) for the burning buoyant bubble problem using the SDC-4 solver.

field	$\epsilon_{64\to128}$	rate	$\epsilon_{128\to256}$	rate	$\epsilon_{256\to512}$
ρ	3.591×10^{15}	3.263	3.739×10^{14}	3.713	2.852×10^{13}
ρu	1.120×10^{24}	3.794	8.072×10^{22}	3.930	5.296×10^{21}
ρv	1.314×10^{24}	3.544	1.127×10^{23}	3.838	7.879×10^{21}
ρE	3.701×10^{32}	2.946	4.801×10^{31}	3.647	3.834×10^{30}
ρe	3.701×10^{32}	2.946	4.801×10^{31}	3.646	3.834×10^{30}
T	1.438×10^{18}	3.508	1.264×10^{17}	3.829	8.899×10^{15}
$\rho X(^{4}\mathrm{He})$	3.589×10^{15}	3.266	3.732×10^{14}	3.711	2.850×10^{13}
$\rho X(^{12}\mathrm{C})$	1.520×10^{13}	2.544	2.606×10^{12}	3.797	1.874×10^{11}
$\rho X(^{16}\mathrm{O})$	3.589×10^{7}	3.262	3.742×10^{6}	3.714	2.851×10^{5}
$\rho X(^{56}\mathrm{Fe})$	3.590×10^{7}	3.263	3.739×10^{6}	3.713	2.852×10^{5}

(Zingale et al., 2019, submitted to ApJ)

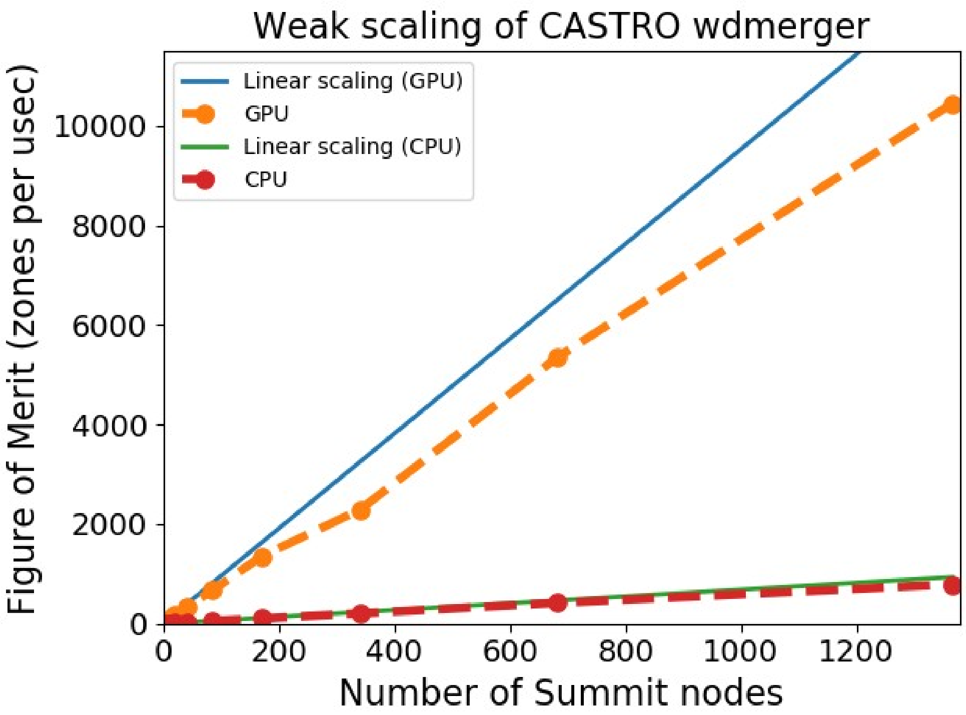
Performance Portability (GPUs)

- General design:
  - Grid management, memory allocation, parallelism in C++
  - Computational kernels written in Fortran
- Fortran kernels take a box (`lo`, `hi`) and operates on it
  - MPI + X approach for finer grained parallelism
  - Approach reuses the same compute kernels
- MPI distributes boxes to tasks
- *Each zone assigned to separate CUDA core*



GPUs

- Castro has been ported to GPUs
- Same compute kernels used with MPI+OpenMP as with MPI+CUDA
- Reactions follow the same prescription
- MAESTROeX GPU port well underway



Performance OLCF Summit (6 GPUs + 42 CPU cores / node)

Summary/Future

- Chandra SNe Ia:
  - Single-point, off-center ignition
  - Urca process calculations are starting
- Sub-Ch SNe Ia: variety, likely single-point…
- XRBs: we are resolving laterally propagating flames to understand dynamics

- Astrophysical modeling requires the cooperation of many different domain scientists
- MAESTROeX development directions:
  - Rotation
  - Higher-order / SDC
  - MHD
- *Releasing simulation codes / problem files is part of scientific reproducibility*