AMReX-Astro: Developments and Science

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Overview

- CASTRO and MAESTROeX
  - Compressible and low Mach number hydrodynamic solvers.
  - Structured grid, finite volume, adaptive mesh refinement codes based on AMReX framework.
  - Both suitable for wide range of problems: full starts down to resolved flames
  - CASTRO:
    - Mike Zingale talk tomorrow with CASTRO algorithmic (and more science) updates
  - MAESTROeX:
    - Efficient for low speed flows (compared to the sound speed).
    - Time steps O(100)+ larger, overall efficiency O(10)+ over compressible.
  - Both codes share data structures / infrastructure - can restart CASTRO simulations with MAESTROeX data.

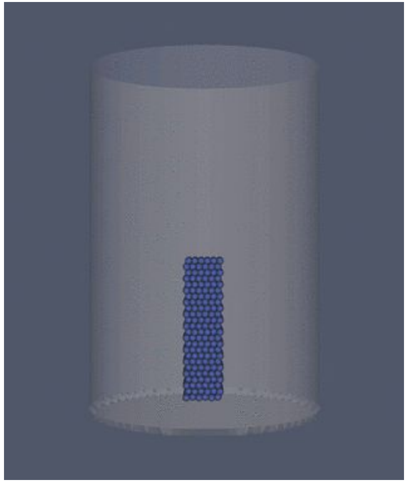
- Starkiller Microphysics
  - Common astrophysical microphysics routines with interfaces for AMReX codes

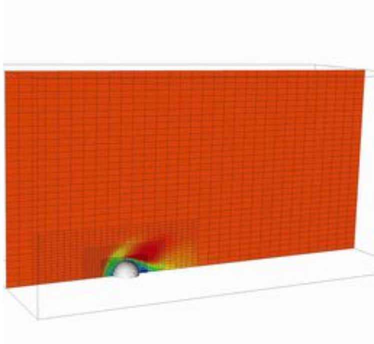
Overview

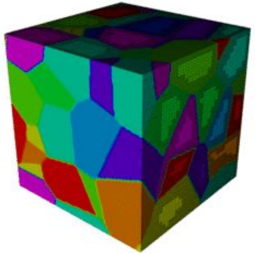
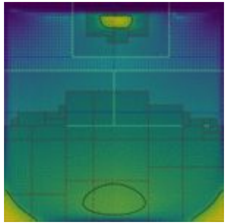
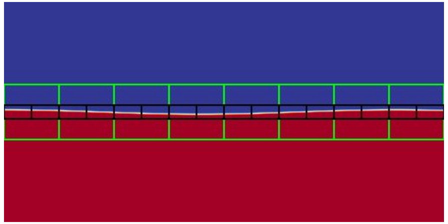
- Focus last year: “modernizing” code by
  - Eliminate Fortran -> pure C++ implementation
  - Use AMReX-based GPU implementation strategy
- Previous Science
  - MAESTRO: single-degenerate WD, sub-Chandra WD, massive star convection
  - CASTRO: core collapse, exoplanet atmospheres, low-energy SN, magnetar supernovae, pair-instability SN
- New Science (summary slides today)
  - Rotating massive stars (with Sean Couch; Mike talk tomorrow)
  - X-ray bursts
  - Merging white dwarfs
  - Rotating star convection
  - Electron capture supernovae
  - Convective Urca process

AMReX Updates

- Exascale Computing Project co-design center software framework
  - Block structured adaptive mesh refinement (no parent-child relationship)
  - Performant on current/next-gen multicore/GPU platforms.
  - Support for grid data, particles, linear solvers, subcycling in time, embedded boundaries
  - Supports numerous mature SciDAC/ECP, plus industrial / lab / university collaborations
    - Astrophysics (TEAMS), cosmology, combustion, multiphase flow, accelerators, microelectronics, solid mechanics, wind plants, rheology, mesoscale fluids, …





AMReX Updates

- All general infrastructure improvements driven by needs of individual applications are inherited by AMReX-Astro.

- C++ macros and CUDA extended lambdas
  - Macros support multicore (MPI+OpenMP) as well as GPU (MPI+CUDA)
  - Flexible enough to support CUDA Fortran and OpenACC in individual codes.
- CUDA managed memory to handle data movement
  - Goal: run and store everything on the GPU; stay away from the host.
  - AMReX libraries have been rewritten to keep data on GPU

- Open source: github.com/AMReX-Codes

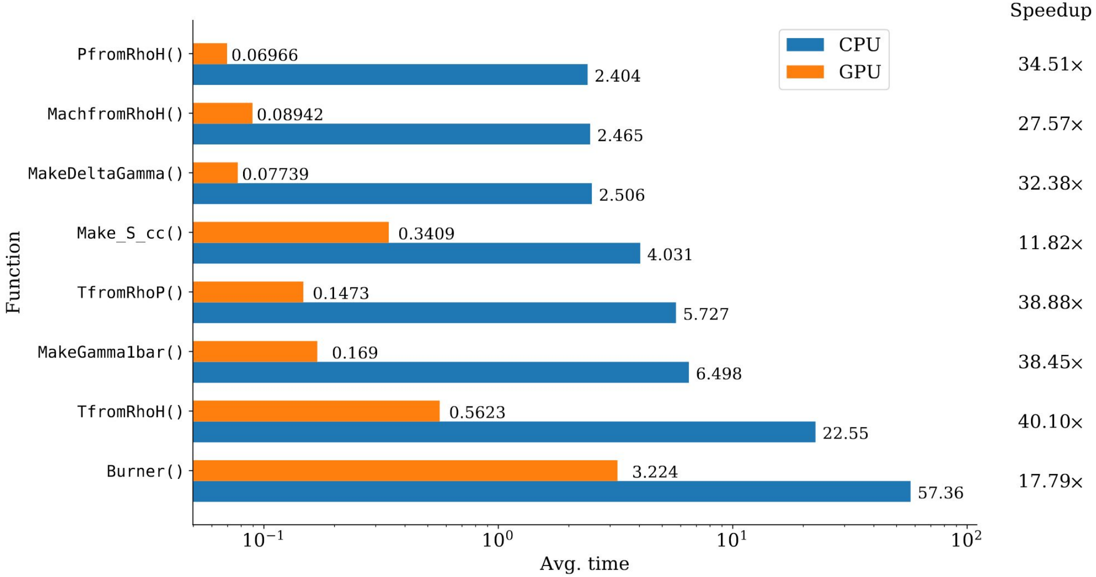
```
// Computes divergence at cell center from face-centered data
void ComputeDiv(MultiFab& divergence,
                const std::array<MultiFab, AMREX_SPACEDIM>& phi)
{
    for ( MFIter mfi(divergence); mfi.isValid(); ++mfi ) {

        const Box& bx = mfi.tilebox();

        const Array4<Real> & div = divergence.array(mfi);

        Array4<Real const> const& phix = phi[0].array(mfi);
        Array4<Real const> const& phiy = phi[1].array(mfi);
        Array4<Real const> const& phiz = phi[2].array(mfi);

            amrex::ParallelFor(bx, [=] AMREX_GPU_DEVICE (int i, int j, int k) noexcept
            {
                div(i,j,k) = (  phix(i+1,j,k) - phix(i,j,k)
                              + phiy(i,j+1,k) - phiy(i,j,k)
                              + phiz(i,j,k+1) - phiz(i,j,k) ) / dx;
            });
        }
    }
}
```

AMReX macros provide simple implementation C++ CUDA extended lambda functions

AMReX-Astro Updates

- MAESTROeX
  - RIP Fortran
  - Completed porting to AMReX C++ lambda functions.
- CASTRO
  - Porting to pure C++ lambda GPU underway
- Microphysics
  - Porting of additional reactions networks and EOS underway
- All codes fully open source on github:

  github.com/AMReX-Astro
  github.com/starkiller-astro

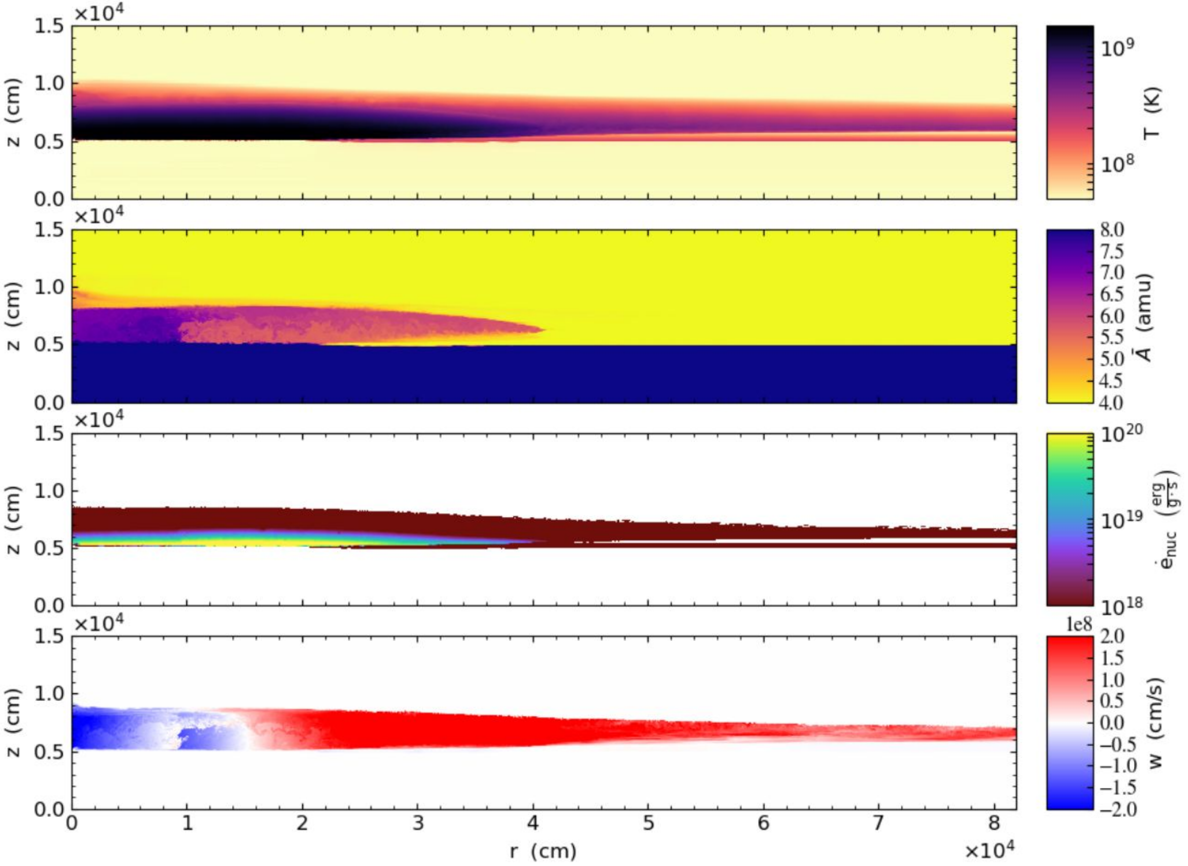


GPU speedup on a summit node.
“CPU” = 42 MPI x 4 OMP
“GPU” = 6 x (MPI+GPU)

Applications

X-ray Bursts

- Previously: 3D Convection in mixed H/He atmosphere with MAESTROeX
- New: Resolved flame structure with CASTRO
  - 2D Model flame spreading on the He surface (why 2D? Δt factor of 700 smaller)
  - L ~ 100m; ~5cm resolution, 10-20ms evolution
- Timmes' conductivity + 13-isotopic alpha-chain reaction network
  - Flame proceeds mainly via conduction as a deflagration
- Rotation model: Coriolis terms at 2000Hz
- Simplified SDC approach to couple hydrodynamics + reactions.
- Result: Inclined flame with small angle from the horizontal, a function of the pressure scale height and Rossby radius (Coriolis force, gravity, pressure gradient)



Temperature

Mean molecular weight of ash

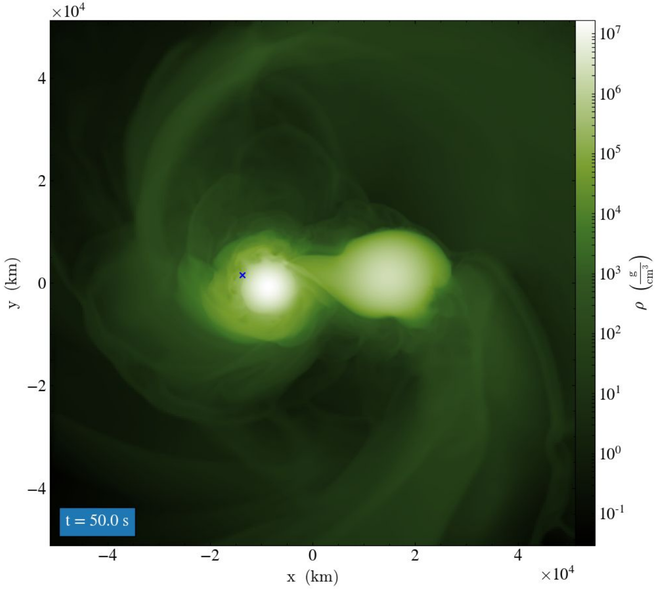
Energy generation rate

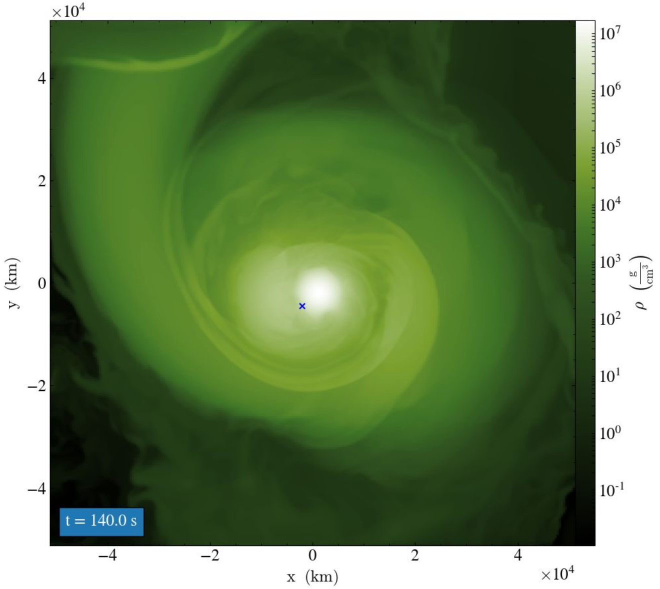
Velocity out of simulation plane

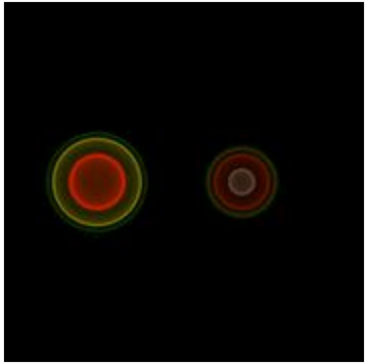
Helium flame spreading across the surface of a neutron star.

Merging White Dwarfs (Maria G. (Lupe) Barrios, Stony Brook)

- Study the merger of two White Dwarfs as possible progenitor of Type Ia Supernovae using CASTRO
- Hydrodynamics + gravity only, Helmholtz EOS
- Setup: Initial binary separation with mass transfer about to start.
- So far: Different mass combinations, with primary $0.9M_\odot$ and secondaries ranging from 0.9-0.6 $M_\odot$. ~200 km resolution
- Exploratory studies:
  - More accurate initial conditions by including a relaxation phase.
  - Use of co-rotating frame.
  - Larger initial separation, ensuring no immediate mass transfer.
  - MHD



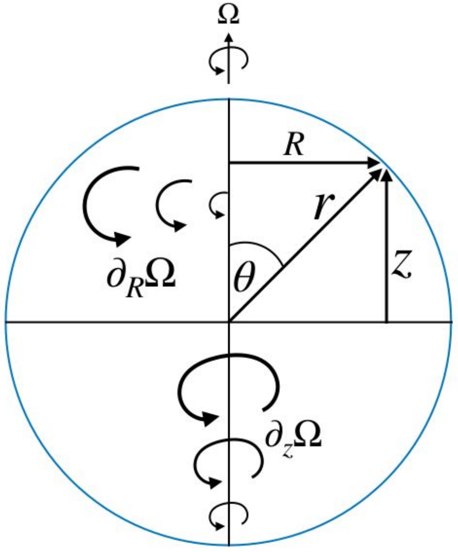


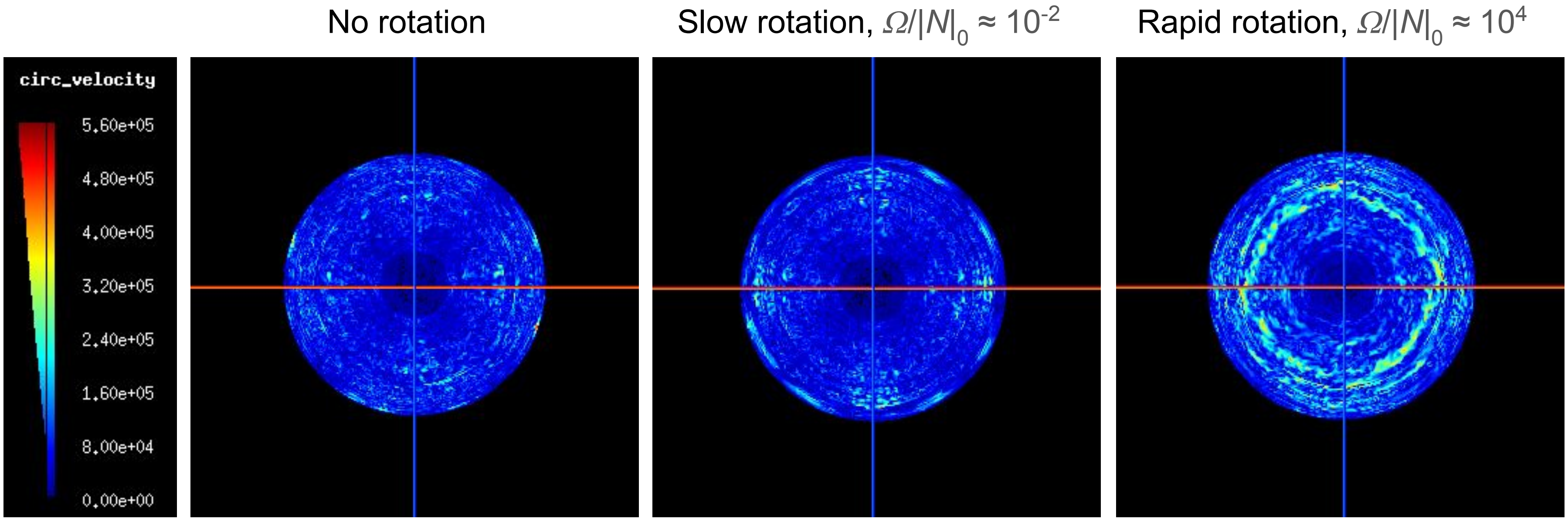


Density slices of a 0.9 + 0.6 $M_\odot$ WDs system at different times of the evolution. The crosses mark the point of maximum temperature.

Stellar Convection with Rotation (w / Adam Jermyn, CCA Flatiron)

- Explore effects of rotation in convection zones of stars with MAESTROeX
- m = 0.3 M_{sun}, 70%/30% X(H^1/He^4)
- Determine/verify scaling between the rotation frequency w.r.t. non-rotating Brünt-Väisälä frequency, $\Omega/|N|_0$, and the differential rotation, $(\partial_R\Omega, \partial_z\Omega)$
    - Two regimes of interest: $\Omega \ll |N|_0$ (slow rotation) and $\Omega \gg |N|_0$ (hydrodynamic rapid rotation)
- Rotation model includes Coriolis terms only; no burning
- Initial tests: 512^3 resolution (1400 km resolution), over ~90 hours (10-30 nodes, for 1-4 hours)
    - AMR + GPU scaling should allow us at least 2048^3 effective resolution



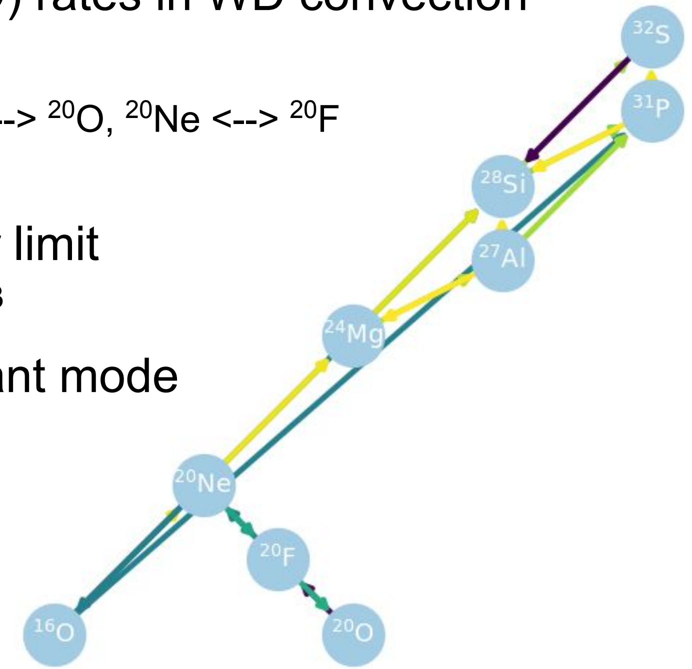


Circumferential velocity in the z=0 plane for various rotation rates.

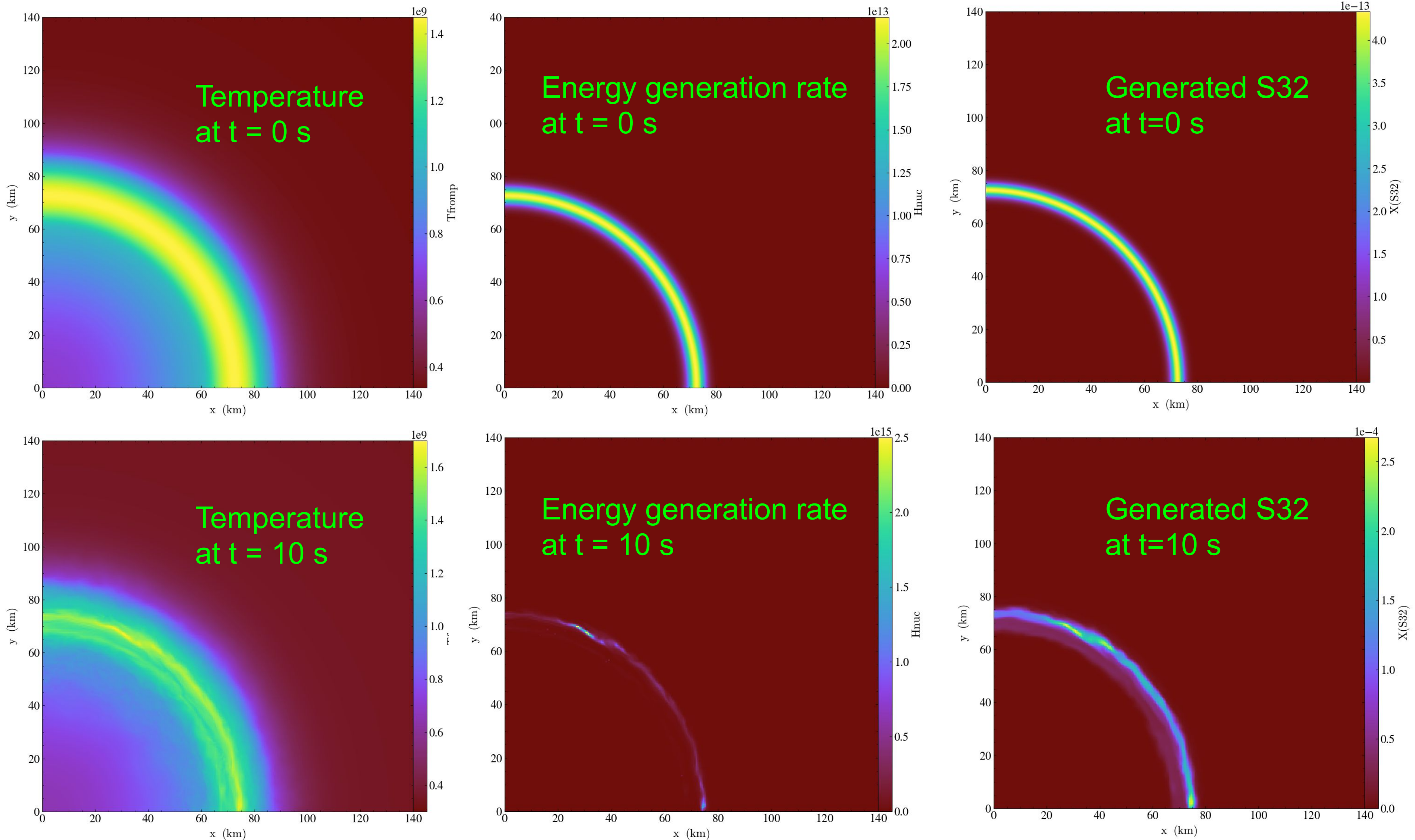
- Additional runs: $1 \lesssim \Omega/|N|_0 \ll 10^4$
- Instrument diagnostics to compare to Adam Jermyn's theories, differential rotation kinetic energy, convective kinetic energy, meridional circulation, convection speed, ...

Electron Capture Supernovae (Xinlong Li, Stony Brook)

- Explore electron-capture (EC) and beta-decay (BD) rates in WD convection zones with MAESTROeX
  - 11 species, 19 reactions, main EC and BD reactions: ^{20}F <--> ^{20}O, ^{20}Ne <--> ^{20}F
- Initial composition: ^{20}Ne 40% and ^{16}O 60%
- Initial state: fully convective star at Chandrasekhar limit
- Convection area: T ~ 1.4e9 K, density ~ 7e9 g/cm^3
- Initial runs: 4 levels of AMR, 0.8km resolution, octant mode
  - Model inner ~140km of star



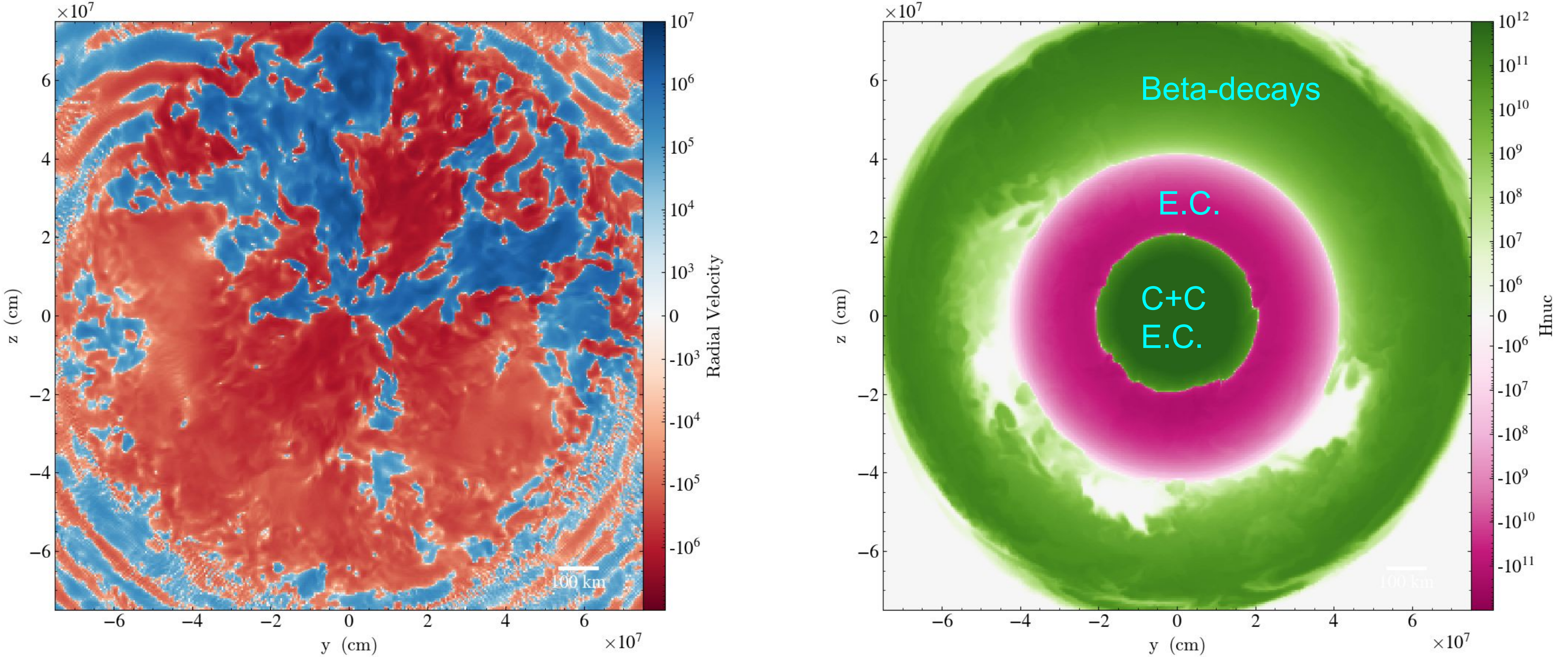
- Future work: evolve the WD for a longer time, and explore the evolution of the composition in the convection area



Temperature
at t = 0 s
Energy generation rate
at t = 0 s
Generated S32
at t=0 s
Temperature
at t = 10 s
Energy generation rate
at t = 10 s
Generated S32
at t=10 s

Convective Urca Process (Don Willcox, LBL)

- Study the role of Urca weak reactions in setting the composition of convective WD cores using MAESTROeX.
- *Setup*: convective 1.4 $M_\odot$ WD in equilibrium w/ Urca weak rates.
  - Reactions module accounts for Urca neutrino energy losses.
  - Internal energy changes accounted for via electron fraction.
- *Current:* 3D simulations covering ~10 convective turnover times. C/O WD with Urca reactions involving ^{23}Na and ^{23}Ne.
  - Suite of models with central densities - 4.5e9, 5.5e9 g/cm^3; central T - 0.6 GK.
- *Next:* Longer timescale simulations for current models, addition of Urca pair reactions involving ^{25}Na and ^{25}Mg, assess effects on ignition hotspot statistics.



Slices showing convective WD core radial velocity (left) with nuclear energy generation (right), showing regions with carbon burning (C+C), Urca electron captures (E.C.), and Urca beta decays.

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  - X-ray bursts
  - Merging white dwarfs
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