Enabling code portability of a parallel & distributed smooth-particle hydrodynamics application, FleCSPH

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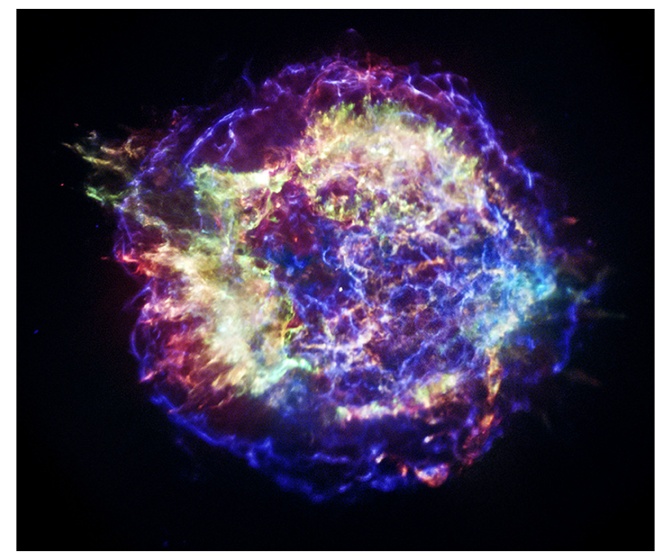
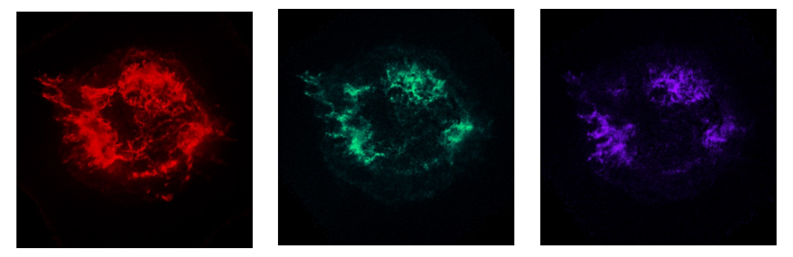
Core-collapse Supernovae (CCSNe): *Nature's grandest explosions*, are a kind of Type II supernovae. These cosmic events are the deaths of massive stars, caused by gravitational collapse that results in a shock-driven explosion. CCSNe are furnaces inside which many elements heavier than carbon are forged.



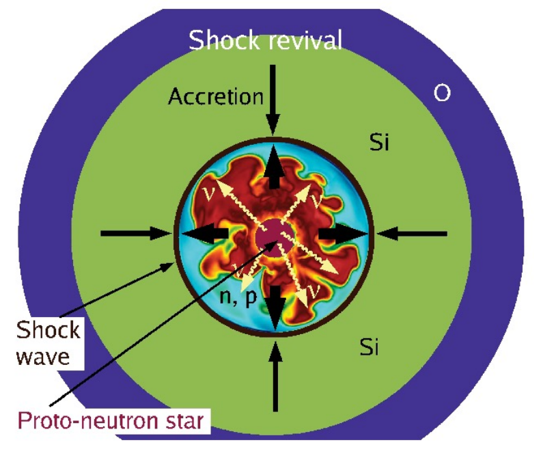
Chandra images of Cassiopeia A (CCSN remnant)
http://chandra.harvard.edu



Mass more than **10x** Sun

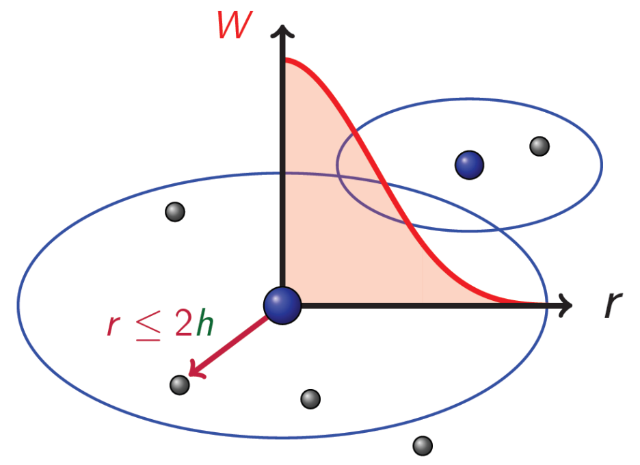
Releases more energy in **1s** than the Sun in its lifetime

Large-scale numerical simulations of CCSNe, can provide a glimpse of hydrodynamic & nucleosynthetic processes that are difficult to observe. However, the CCSNe problem is highly complex and inherently nonlinear: multi-scale, multi-physics, and multi-dimensional. Therefore, to study the impact of various shock structures on CCSNe nucleosynethic yields and distribution of these yields, it is essential to work with numerical tools capable of solving such dynamical systems.



Schematic of shock revival via extreme convection due to neutrino heating, Janka et al., 2012

FleCSPH, a parallel & distributed application, is based on the mesh-free method of Smoothed-Particle Hydrodynamics (SPH). The SPH formulation discretizes the hydrodynamic equations for a set of particles and embeds the properties of the flow onto these particles.



Schematic of SPH kernel and the smoothing length N. de Brye et al., 2016

$$< f(\mathbf{r}) > \approx \sum_b \frac{m_b}{\rho_b} f(\mathbf{r_b}) W(|\mathbf{r} - \mathbf{r_b}|, h)$$

W : Kernel
h : Smoothing-length
r_b : Position vector of particle b
m_b : Mass of particle b
ρ_b : Density of particle b

2nd order accuracy

Conservation properties

Easy to solve gravity interactions

Modelling CCSNe with FleCSPH required expansion, modification, and adaptation of FleCSPH and its functionality.

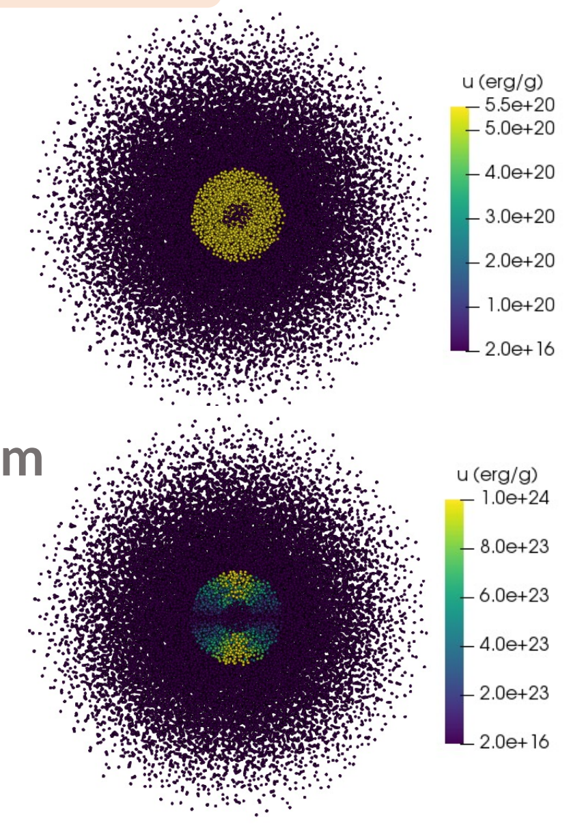
① Shock energy injection

Trigger shock-driven explosion

Artificial injection of energy **1e51 erg**

Spherical shock shell of specified radius **200 km** and width **0.1 M$_\odot$**

Uniform & polar-nonuniform energy distribution schemes



Uniform vs. nonuniform energy distribution

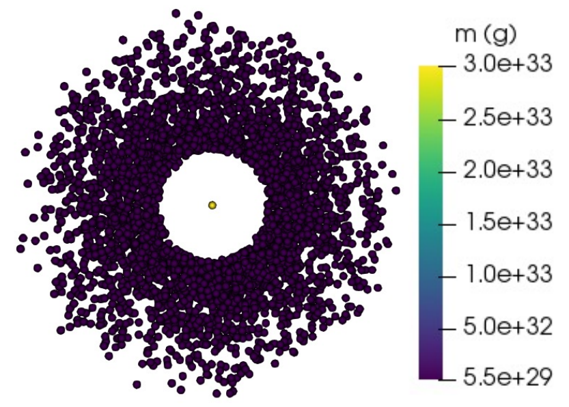
② Freeze radius

Remove region interior to shock radius

1 central particle of equivalent mass

Mitigates the need to resolve highest densities

Particles entering the region set with **0** velocity



Freeze radius implementation

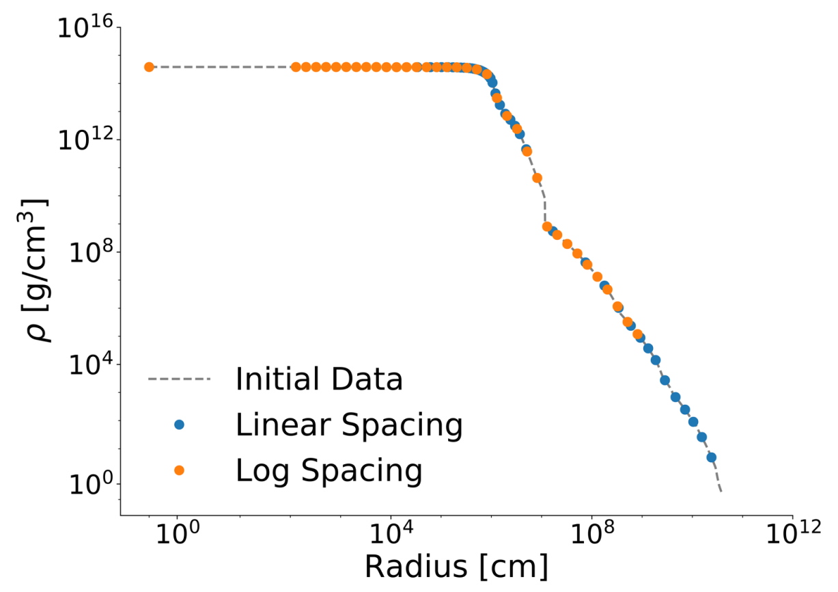
③ Particle generator

Extreme ranges in density and radius

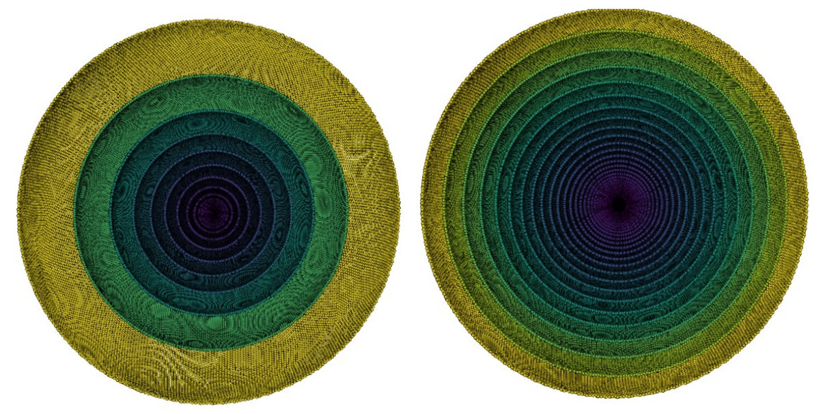
15+ orders of magnitude

Logarithmic instead of linear shell spacing

Varying particle masses between shells



Density profile of the two lattice models



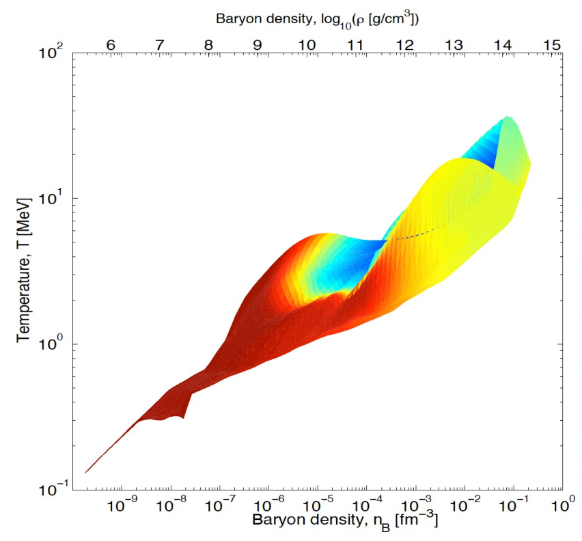
Linear (left) vs. log (right) spacing

④ Equation of state (EOS)

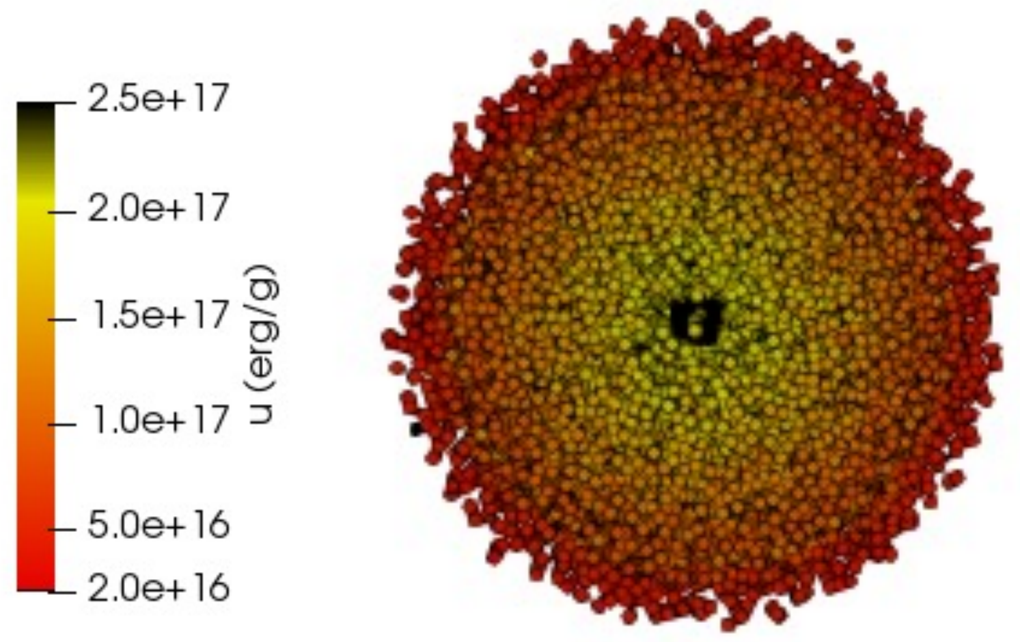
No analytical EOS for CCSNe

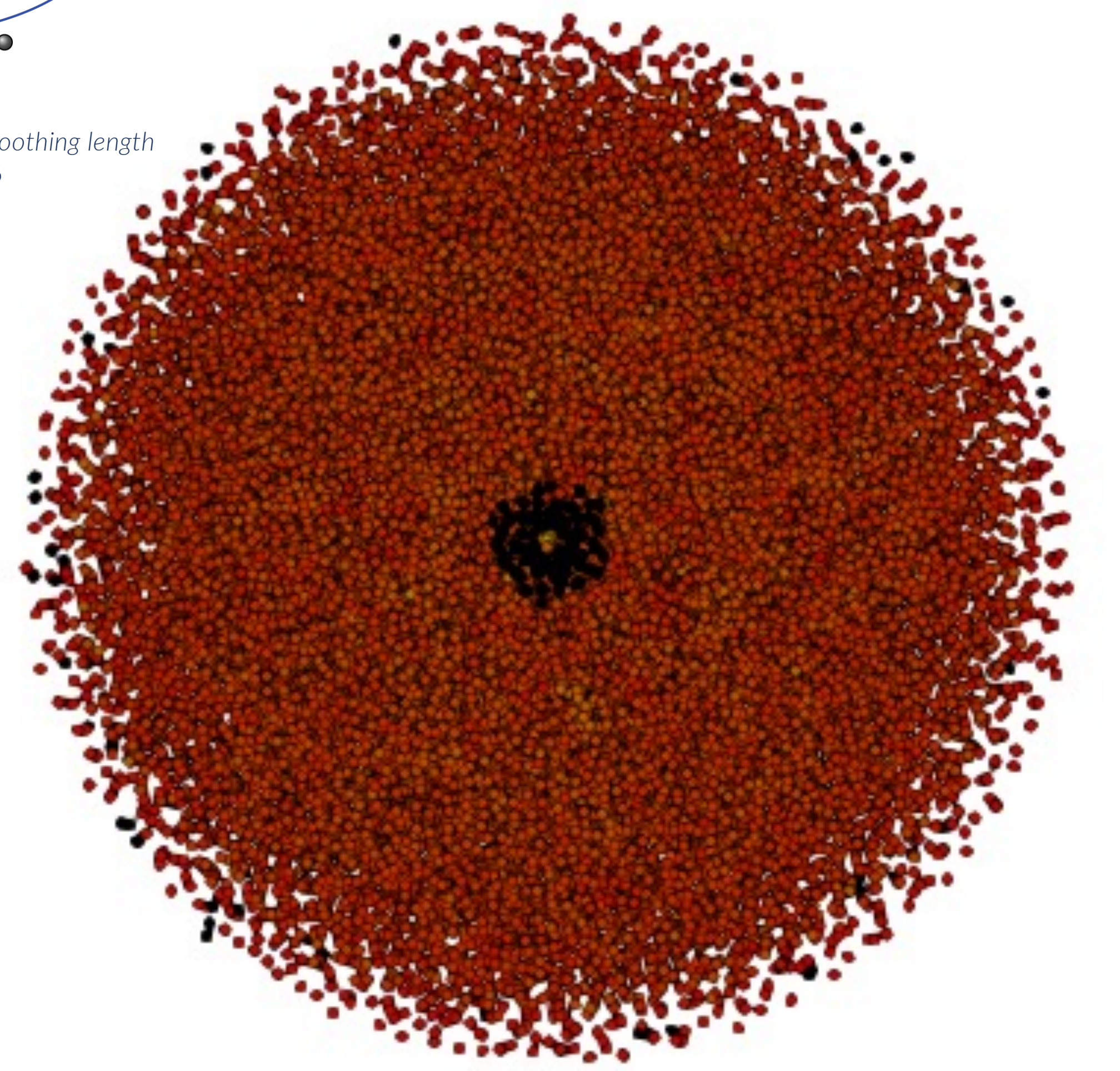
Integrated and unit tested tabular EOS

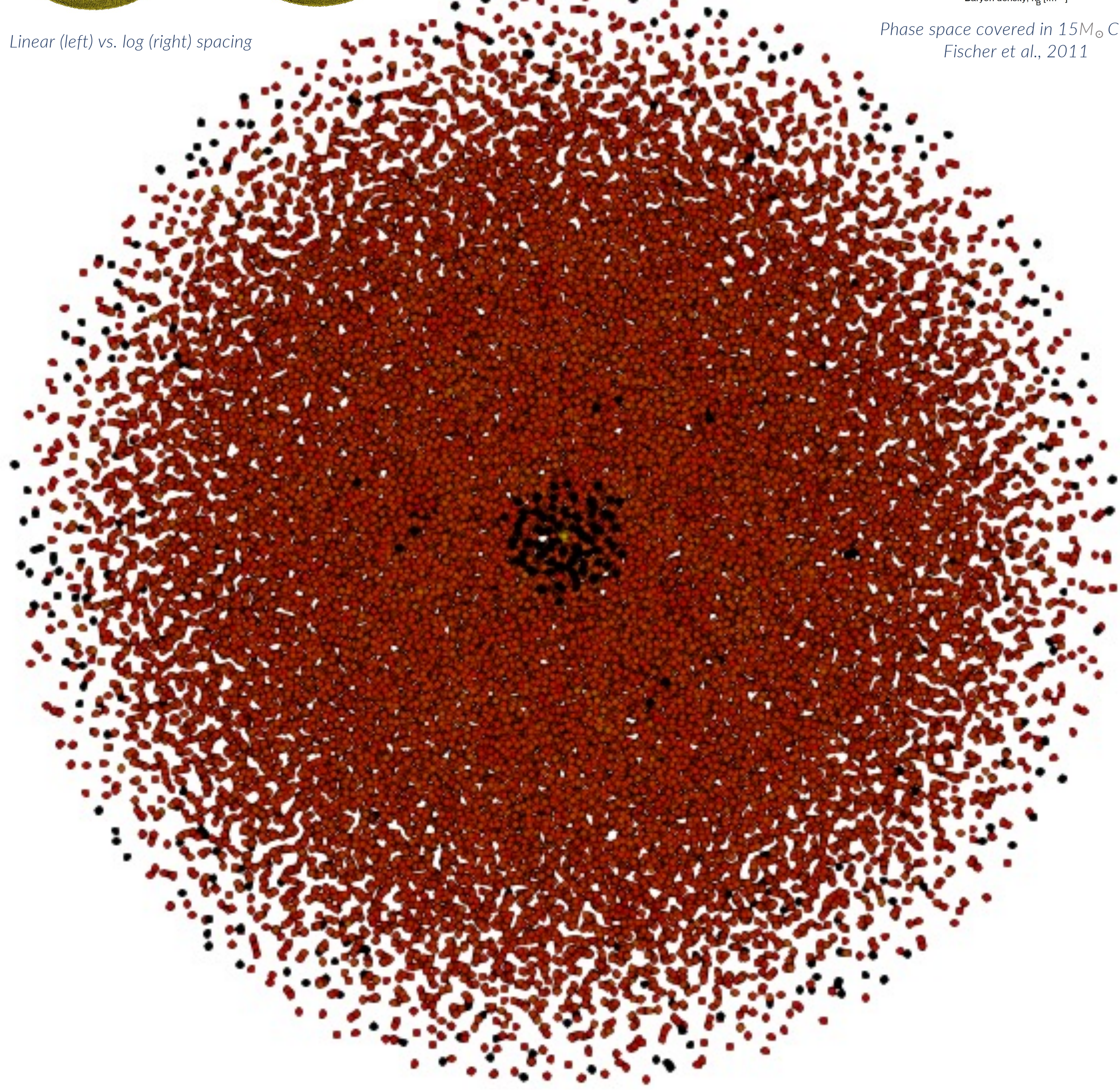
Implemented tracking and evolution of particle electron fraction (Y_e)



Phase space covered in 15M$_\odot$ CCSN Fischer et al., 2011







White Dwarf test case: Toy model supernova

Specific internal energy in white dwarf explosion.
Left to right: Simulation at 0, 1.3, and 3.5 s

Post-processing nucleosynthesis

NuGrid⁺ used to analyze thermal conditions

Isotopic yields consistent with those of supernovae

Large yield of Ni56 as typically observed

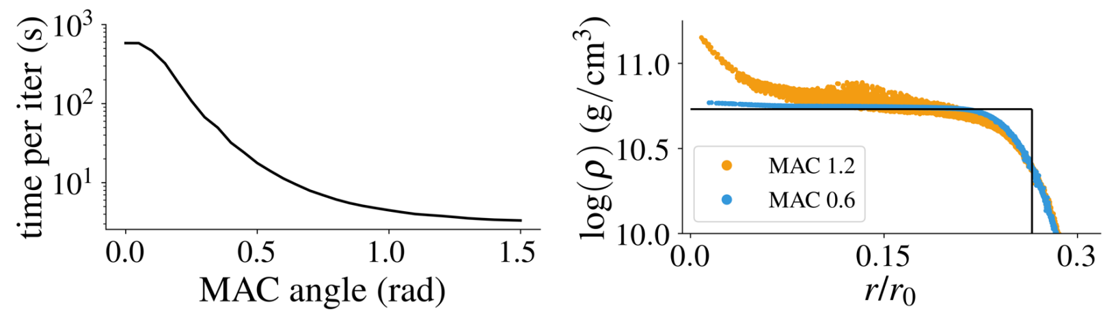
⁺NuGrid collaboration (http://www.nugridstars.org)

Improvements of FleCSPH to facilitate large-scale simulations of CCSNe

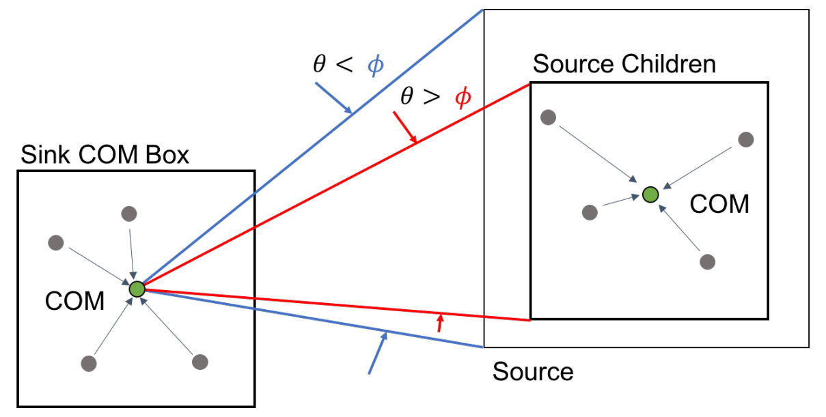
Gravitational interaction ①

Fast multipole method (FMM) approximation reduces *O(N^2)* to *O(N log N)*

Multipole Acceptance Criterion (MAC) angle determines runtime speed and accuracy



MAC angle vs. run time (left), and radial density profile comparison for different MAC angles (right)



Multipole Method Loiseau et al., 2017

"Grad-h" terms ②

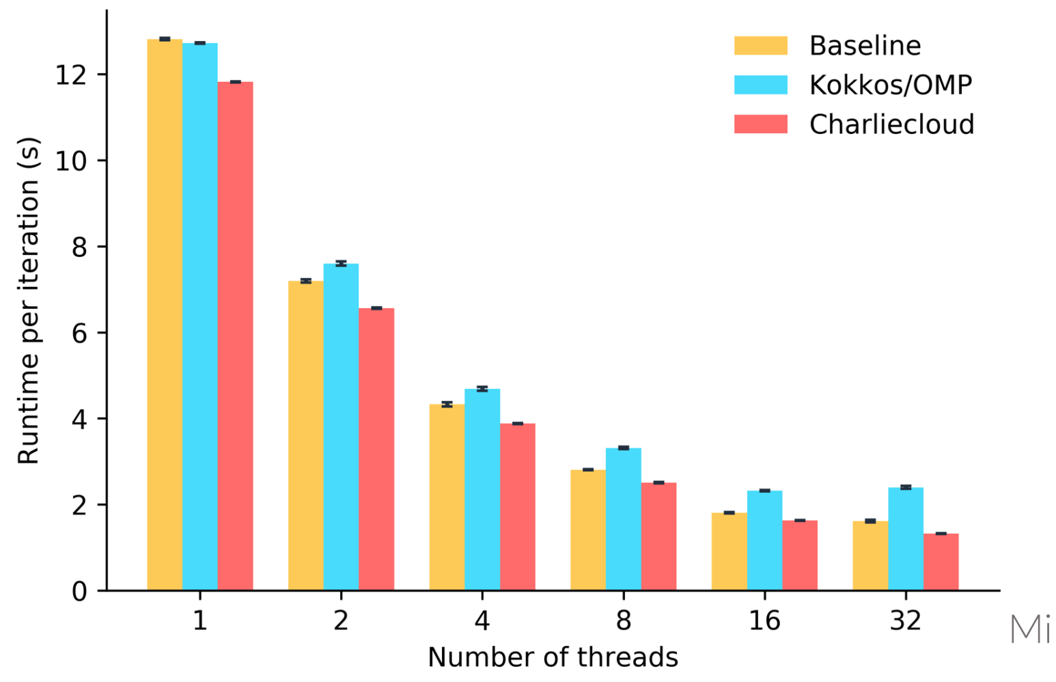
Variable smoothing length introduces extra terms

Important for cases with large shocks, relativistic environments

$$\rho_a = \Sigma_b m_b W(r_{ab}, h_a)$$

$$\frac{d\rho_a}{dt} = \frac{1}{\Omega_a} \sum_b m_b \vec{v_b} \cdot \nabla_a W_{ab}(h_a),$$

$$\text{with} \quad \Omega_a \equiv \left(1 - \frac{\partial h_a}{\partial \rho_a} \sum_b m_b \frac{\partial W_{ab}(h_a)}{\partial h_a}\right)$$



Performance comparison of FleCSPH builds

Performance portability ③

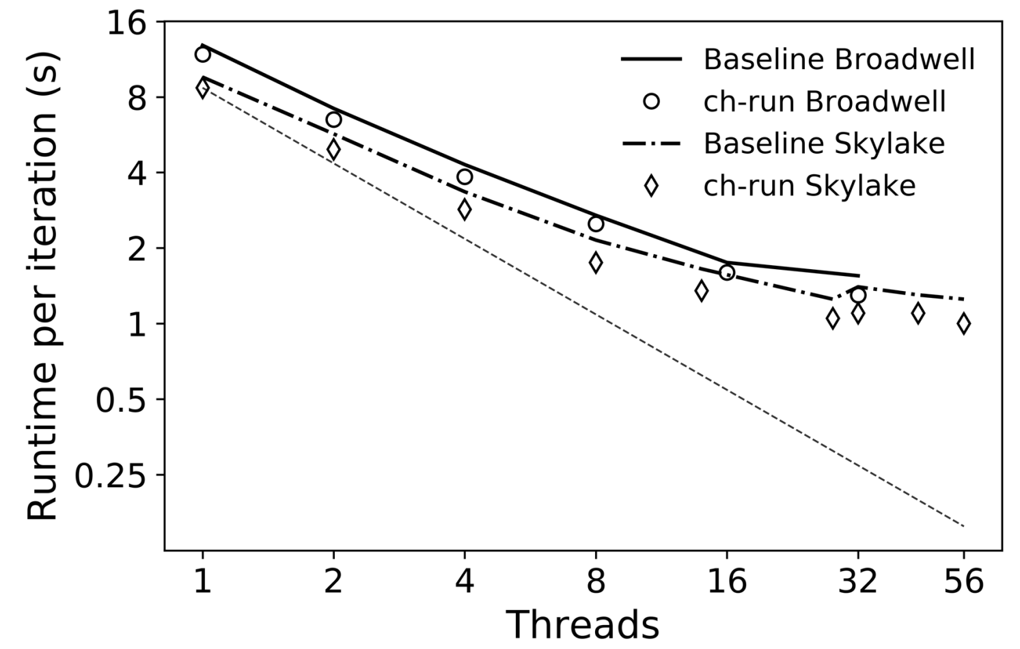
Integrated **Kokkos C++** library

Supports multiple backends, OpenMP, Pthreads, CUDA

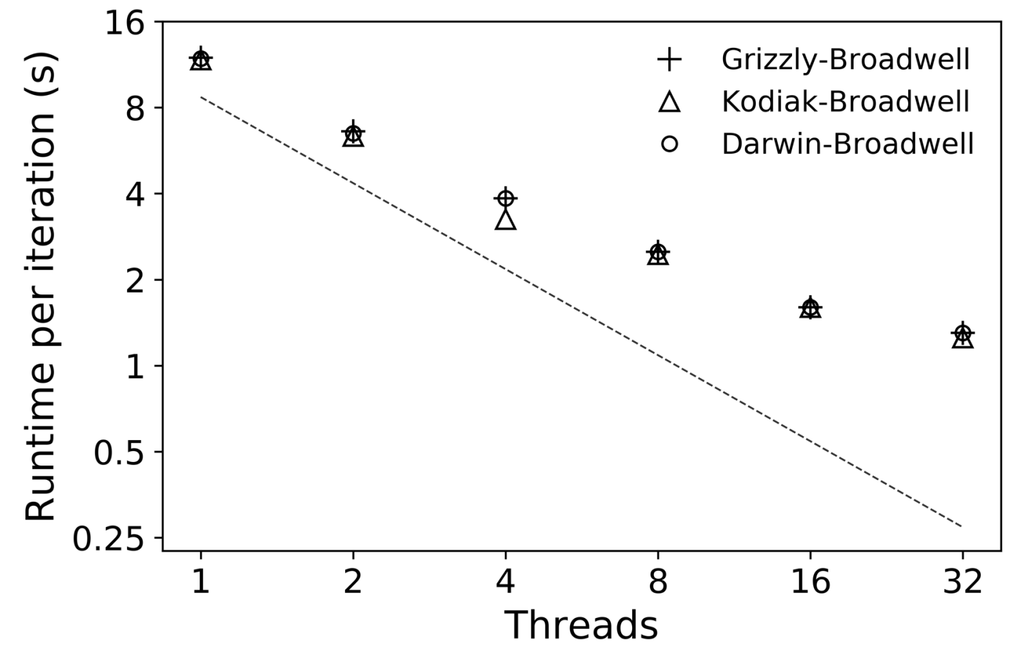
Port STL data structures to **Kokkos Views**

Kokkos parallel dispatch for loops

Minimal performance penalty with Kokkos



Intra-node scaling (strong) of FleCSPH with baseline (bare metal) and Charliecloud container on Darwin test bed cluster



Software stack portability of FleCSPH container

Stack portability ④

Charliecloud offers rootless image build and modification capabilities

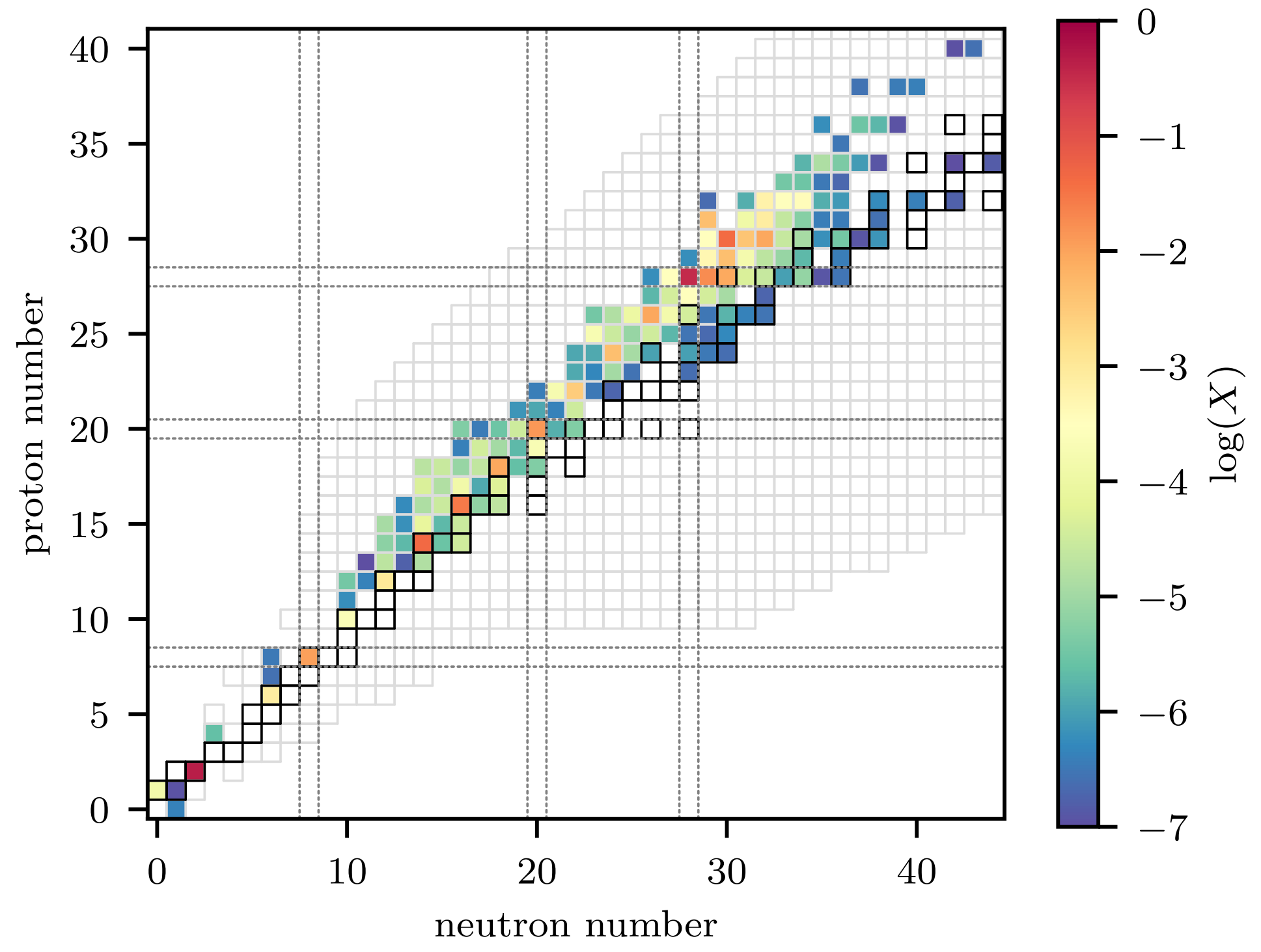
Dependencies for FleCSPH **GCC - C++ 17, MPI, HDF5 parallel, GSL, CMake, FleCSI**

Better performance of the application image in the container

Stack portability demonstrated on different HPC platforms

LANL HPC Systems **Grizzly, Kodiak** on Intel Broadwell

ASC and ASCR funded test bed cluster **Darwin** on Intel Broadwell & Skylake



Nucleosynthetic yield mass fractions (X) from white dwarf test

CONCLUSIONS

1. Enabled higher density resolution with new logarithmic spacing in particle generator
2. Emulated the effect of shock revival via energy injection at the shock radius
3. Implemented tabulated EOS and Y_e
4. Validated approximations in SPH
5. Utilized Kokkos for performance portability
6. Containerized FleCSPH for stack portability
7. Successfully reproduced basic supernova features: unbound outer envelope, overall energy released, and nucleosynthetic yields
8. Demonstrated core capabilities of FleCSPH for numerical simulations of CCSNe

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