Domain Partitioning and Problem Space Representations for Compact Binary Mergers

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Introduction

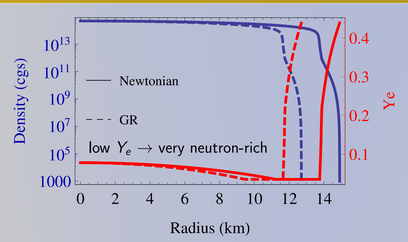
- **Our project** is a collaboration between computer and domain scientists to simulate binary neutron star mergers
- **Our starting point** is the highly scalable 2HOT code
- **Our algorithms of choice** are smoothed particle hydrodynamics and the hashed octree data structure

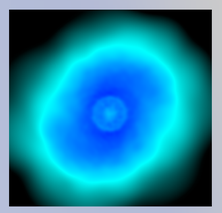
Physics Accomplishments
- Add Equation of State in 2HOT
- Generate realistic initial data for SPH code
- Add gravitational radiation-reaction
- Merge binary neutron stars
- Analyse the ejecta

Computer Science Accomplishments
- Improve the Equation of State lookup
- Improve the data distribution and the structure generation
- Use and benchmark efficient runtimes with a proxy application

Astrophysical Motivation

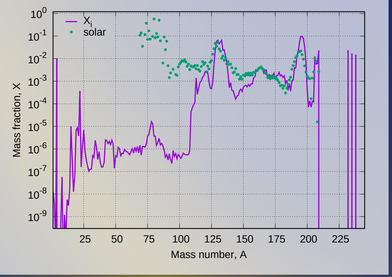
- **Neutron stars (NS)**
  - Remnants of stellar core-collapse
  - Compact objects supported against gravity by the strong nuclear force and neutron degeneracy pressure
  - Density and electron fraction plotted to the right





- **Binary NS mergers:** observational signatures
  - Gravitational waves ($\sim 10^{57}$ erg/s in ~ 1 ms)
  - Short gamma-ray bursts ($\sim 10^{50}$ erg/s in ~ 0.2 s)
  - Produced in ejecta, or unbound flow (plotted on the left):
    - Infrared "macronova/kilonova" transients ($\sim 10^{40}$ erg/s for ~ 7 d)
    - Radio transients ($\sim 10^{50}$ erg over $5-100$ years)

- **r-process nucleosynthesis**
  - Ejecta conducive to rapid neutron capture by heavy-seed nuclei
  - r-process may help explain abundance of heavy elements in universe (residuals plotted to the right).
  - "Kilonova" afterglow (faint supernova-like transient) powered by radioactive decay of freshly synthesized heavy elements



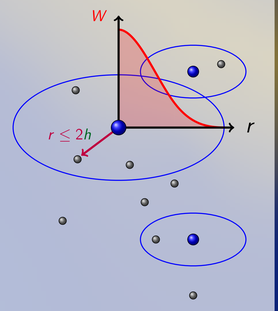
Smoothed Particle Hydrodynamics (SPH)

- **Why?** can handle deformations (mergers), low densities (ejecta) and vacuum
- **What?** explicit numerical *mesh-free* method → solve hydrodynamic PDE: Lagrangian, discretized in set of fluid elements called "particles"
- **How?** their smooth field variables (density, velocity, internal energy, pressure) and derivatives interpolated via smoothing kernel W

$$\langle A \rangle (\vec{r}) \approx \sum_b \frac{m_b}{\rho_b} A(\vec{r}_b) W(|\vec{r} - \vec{r}_b|, h)$$

h smoothing length (hydro interaction range) evolved for each particle (adaptive resolution)

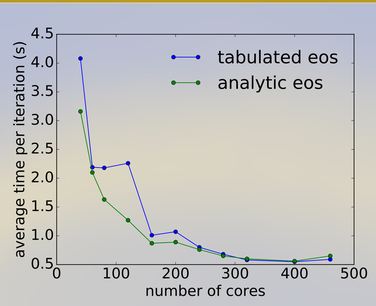
- Equation of state (matter behavior) to close system



- **Pros:**
  - Discretized form exactly conserves mass, energy, linear & angular momentum $\forall$ resolutions
  - Exactly advects fluid properties
  - Easily combines with tree methods for solving Newtonian gravity via N-body
- **Cons:**
  - Special care must be taken when handling high gradients (shocks, NS surface)
  - Restricted to low-order convergence
  - Can struggle to resolve turbulence dominated flows
  - Requires careful setup of initial distribution of particles

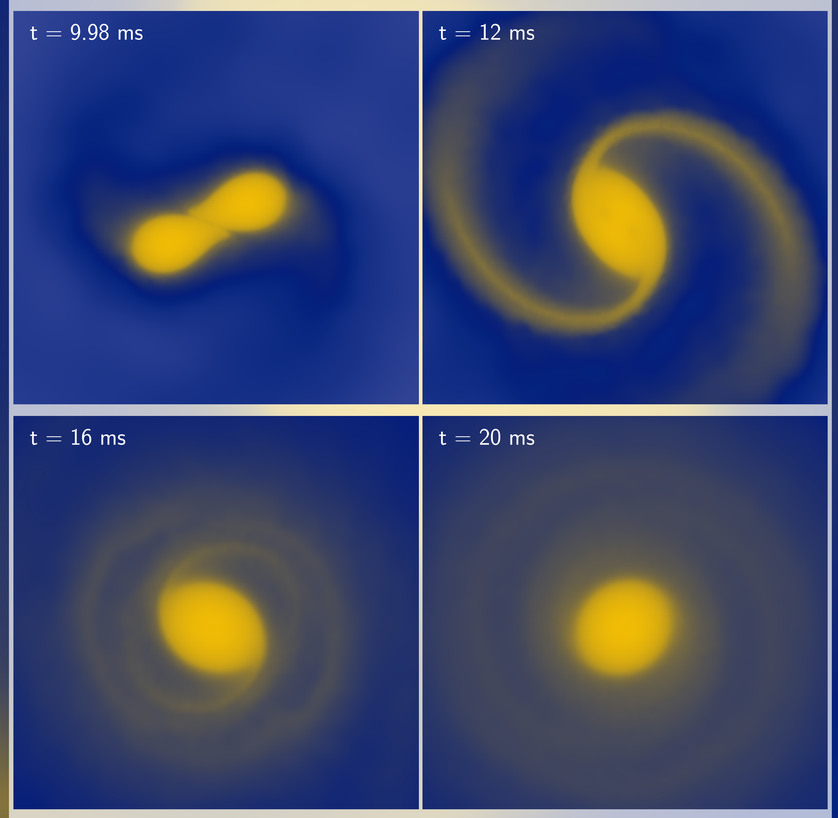
2HOT: A Provenly Scalable Astrophysics Code

- **2**HOT
  - A highly-scalable N-body code
  - Written by Mike Warren (originally HOT)
  - Based on:
    - Multipole acceptance criterion
    - Hashed octree data structure
  - Later extended by Chris Fryer and others to handle SPH (SNSPH)
  - Computational time scales as $\mathcal{O}(n \ln n)$.
- **O**ur Additions
  - Several realistic equations of state, many of which are tabulated
  - Gravitational wave radiation-reaction
  - Realistic neutron star initial data



A strong scaling test for a single neutron star with 2 million particles.

Our Binary NS Mergers



COOL is for Optimized Object Lookup

Nearest-neighbor search **proxy application:**
- Key generation
- Distributed particle sort
- Tree construction
- k-nearest neighbor search

- Uses the same data structures and algorithms as 2HOT
- Supports multiple domain decomposition schemes to improve **data locality**
- Makes additional development simpler
- Implemented in three runtimes:

MPI
- Very well known runtime
- Hard to get performance
- Useful as a baseline comparison tool

STAPL
- Task-graph driven library
- STL-like containers and algorithms
- Easy to read and write

Charm++
- Object-focused asynchronous parallelism
- Efficient
- Mature

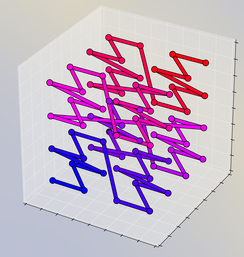
Domain Decomposition

- Distributed nearest-neighbor search is communication-bound
- The choice of domain decomposition affects the amount of communication required
- Domain decompositions from space-filling curves provide good locality and fast tree construction
- 2HOT only supports Morton-order decomposition
- COOL supports both Morton- and Hilbert-order domain decomposition

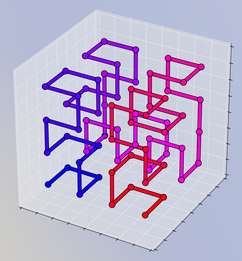
Morton-order Decomposition
- Simple algorithm for n dimensions
- Creates spatial discontinuities
- Can result in unnecessary communication

Hilbert-order Decomposition
- More complex to implement
- Algorithm varies by number of dimensions
- Preserves spatial locality within nodes

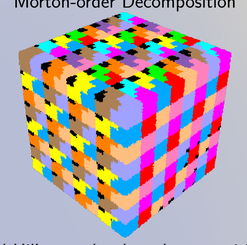
Morton Curve



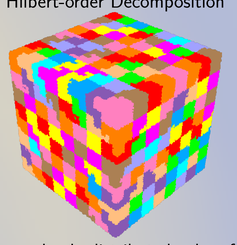
Hilbert Curve



Morton-order Decomposition

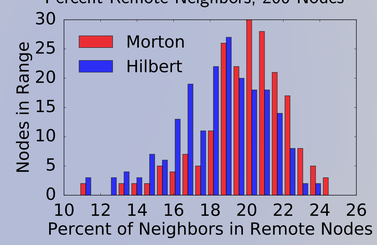


Hilbert-order Decomposition

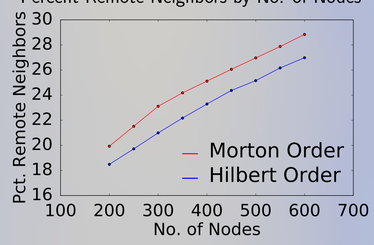


Morton- and Hilbert-order data decompositions for a uniformly randomly distributed cube of particles. Particles are distributed among 512 nodes, which are colored with a rotating set of twelve colors. Spatial discontinuities are colored black.

Percent Remote Neighbors, 200 Nodes

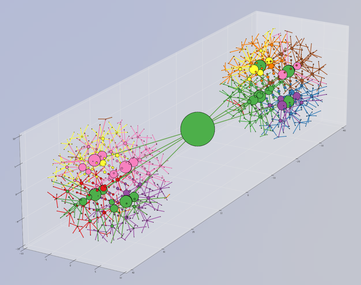


Percent Remote Neighbors by No. of Nodes

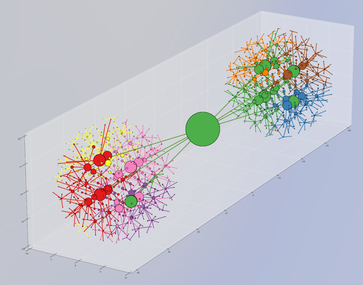


Data locality for Morton- and Hilbert-order nearest-neighbor search for a uniformly randomly distributed cube of one million particles. Hilbert-order decomposition results in a smaller average percentage of remote neighbors, resulting in less communication during tree construction and nearest-neighbor search.

Morton-order Octree



Hilbert-order Octree



Morton- and Hilbert-order octrees generated from a binary neutron star system, distributed over eight nodes. Tree vertices and edges are colored by the node that owns them. The Morton octree has a high degree of spatial discontinuity, with all nodes owning particles from each star.

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