Enzo-P / Cello
Pursuing Petascale Astrophysics

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University of California, San Diego
San Diego Supercomputer Center

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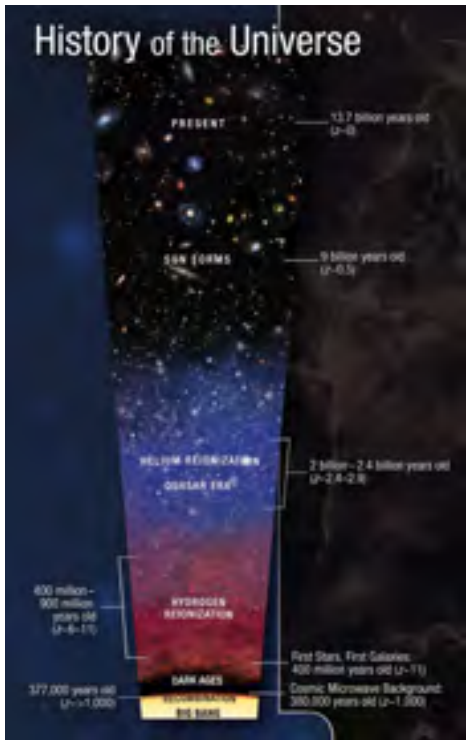
The search for missing physics

Realistic simulations of the intergalactic medium



Hubble 2010
Science Year in Review

Our project has two components:

- **cosmological simulations** (Norman)
  - investigating Helium reionization epoch
  - simulations don't match new observations
  - ran extreme simulations using *Enzo* on BW
  - more: Norman BW 2016, Pengfei Chen thesis
- **software development** (Bordner)
  - Enzo's AMR is Terascale not Petascale
  - developing next-generation *Enzo-P*
  - parallelized using Charm++
  - scalable array-of-octree AMR (*Cello*)
  - using BW for performance testing

The Enzo cosmology and astrophysics application

Enzo's strengths

Applicable to a wide range of astrophysical/cosmological problems

Physics Equations: *mathematical models*

• Hydrodynamics (Euler equations) • Gravity ($\nabla^2\Phi = 4\pi G\rho$) • Chemistry/cooling • Star formation • Magnetism • Radiation . . .

Numerical Methods: *approximate and solve*

• PPM, • ZEUS, • MUSCL • FFT • multigrid • Gadget cooling • Cloudy cooling • Grackle • Dedner MHD • MHD-CT • Implicit FLD • Moray . . .

Data Structures: *computer representation*

• Structured Adaptive Mesh Refinement (SAMR) • Eulerian fields • Lagrangian particles . . .

The Enzo cosmology and astrophysics application

Enzo's strengths

Implements a variety of sophisticated numerical methods

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Enzo's strengths

Enabled by adaptive mesh refinement with particles and fields

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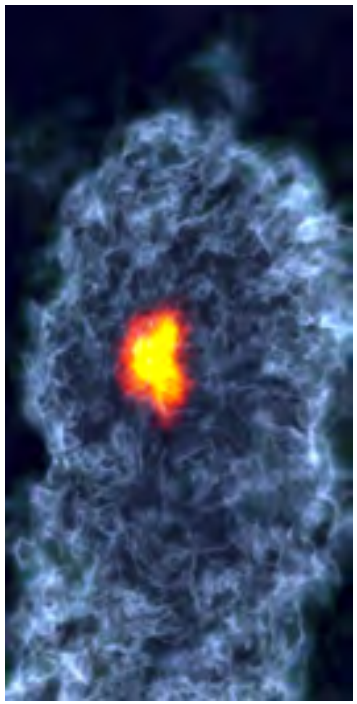
Enzo's struggles

Limitations primarily due to relentless growth of HPC platforms

- Ever-changing software requirements
  - Enzo was born in early 1990's
  - "massive parallelism" meant $P \approx 100$
  - $\times 1000$ parallelism today
- Affects different parts of Enzo differently
  - ☺ physics requirements unchanged
  - ☺ numerical methods mostly viable
  - ☹ *data structures* limit Enzo's scalability
- Motivates AMR data structure redesign
  - **Enzo-P**: "petascale" version of Enzo
  - keep Enzo's physics and many methods
  - built on **Cello** scalable AMR framework



[Sam Skillman, Matt Turk]

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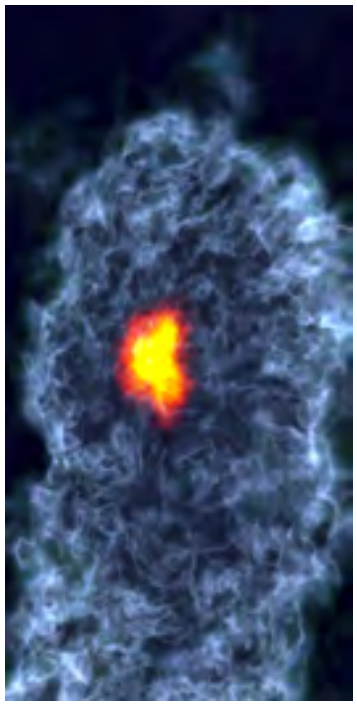

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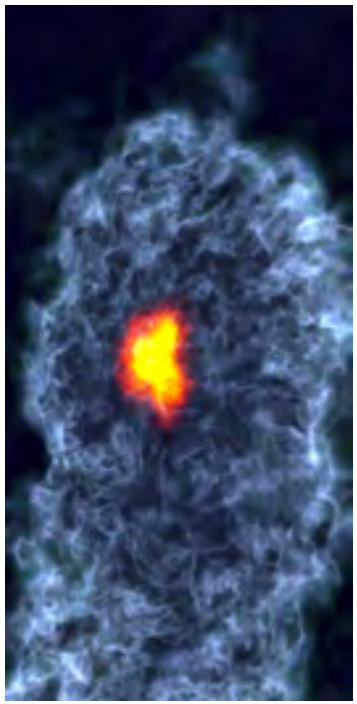
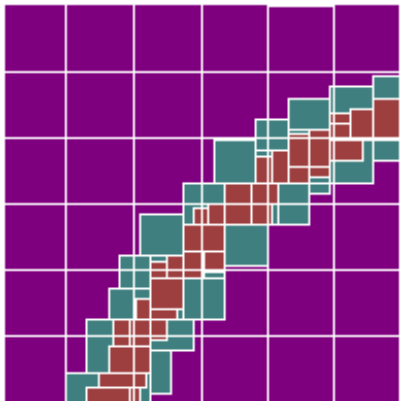


[Sam Skillman, Matt Turk]

Cello scalable adaptive mesh refinement

Differences between Enzo and Enzo-P



Enzo

structured AMR
variable shaped patches
neighbor- & parent-communication
MPI parallelization

Enzo-P/Cello

array of octrees
fixed shaped blocks
neighbor-only communication
Charm++ parallelization

Cello scalable adaptive mesh refinement

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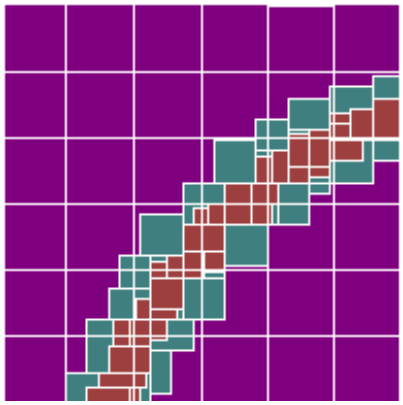

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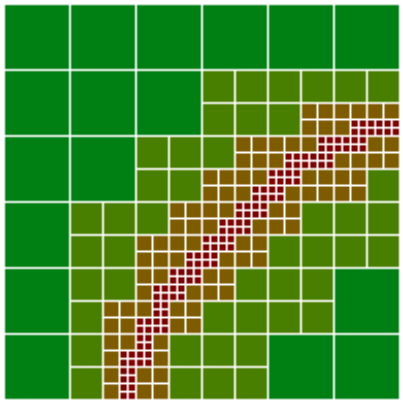

Enzo-P/Cello

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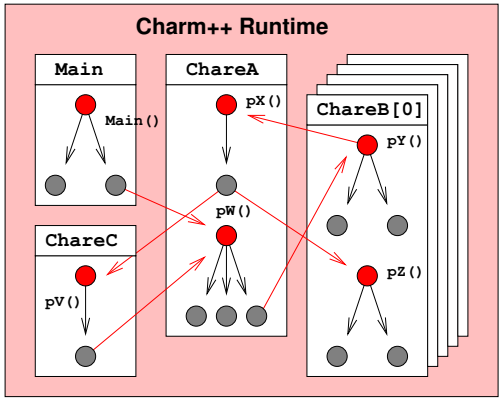
Charm++ parallelization

The Charm++ parallel programming system



A Charm++ parallel program

- Charm++ program
  - Decomposed by *objects*
  - Charm++ objects called *chares*
  - invoke *entry methods*
  - *asynchronous*
  - communicate via *messages*
- Charm++ runtime system
  - maps chares to processors
  - schedules entry methods
  - migrates chares to load balance
- Additional features
  - checkpoint/restart
  - dynamic load balancing
  - fault-tolerance

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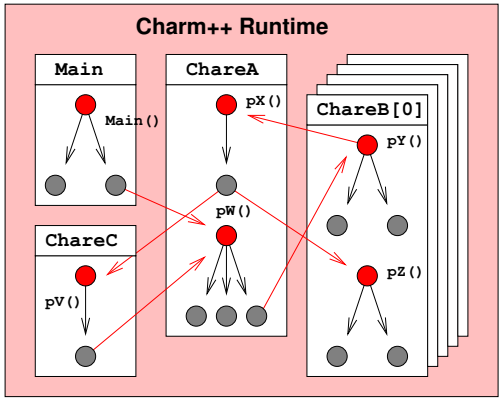

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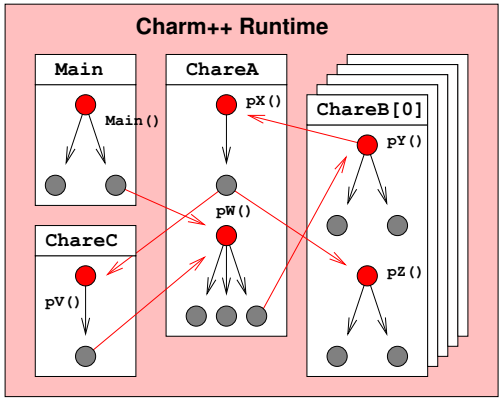

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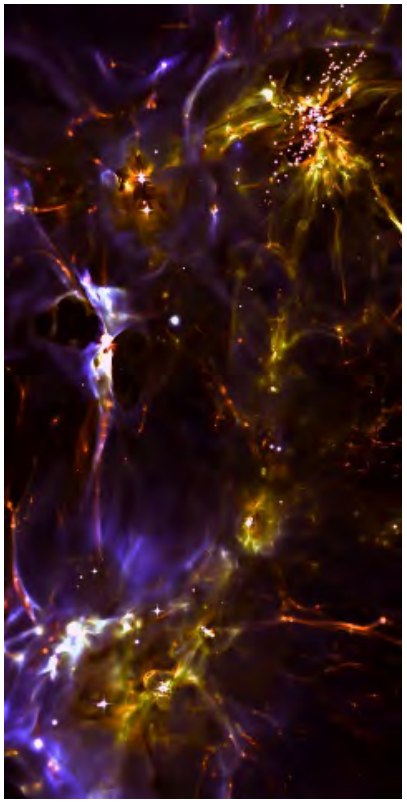
Cello scalable adaptive mesh refinement

How Enzo-P addresses Enzo's limitations

- Memory usage
  - AMR structure is fully distributed
  - uniform blocks reduce fragmentation
- Mesh quality
  - 2-to-1 refinement constraint maintained
- Parallel task definition
  - uniform field array sizes in blocks
  - sizes determined by user
- Parallel task scheduling
  - asynchronous data-driven
- Data locality
  - primarily nearest-neighbor comm.

Enzo



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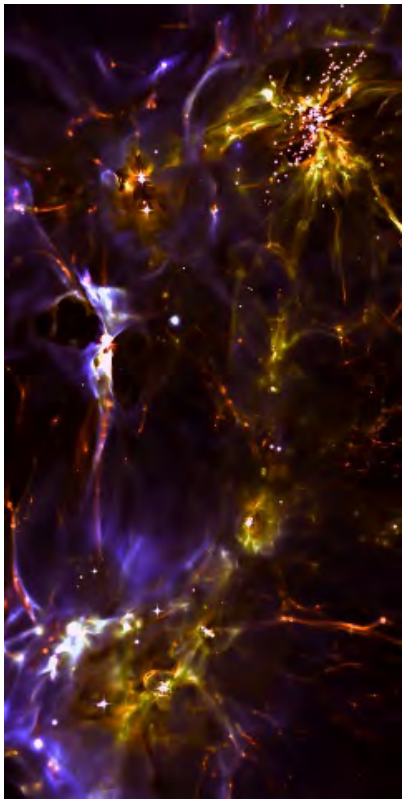

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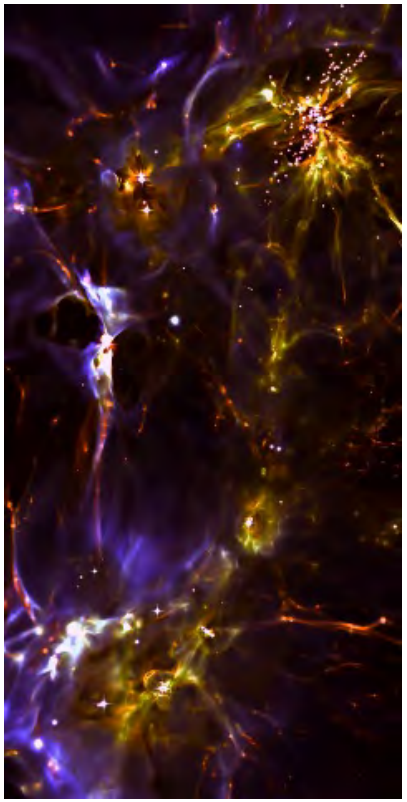

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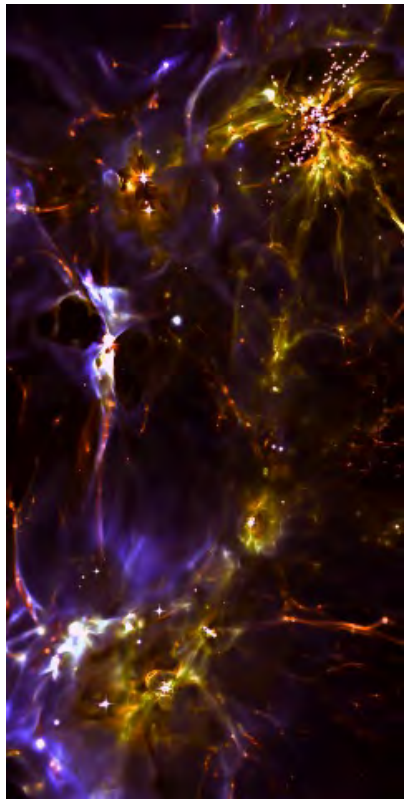

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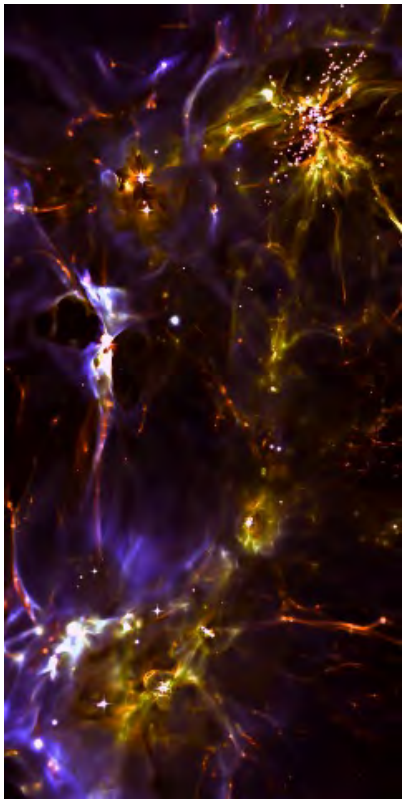

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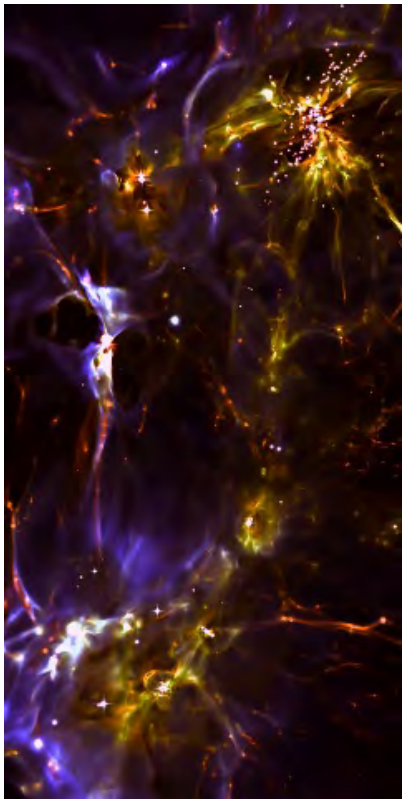
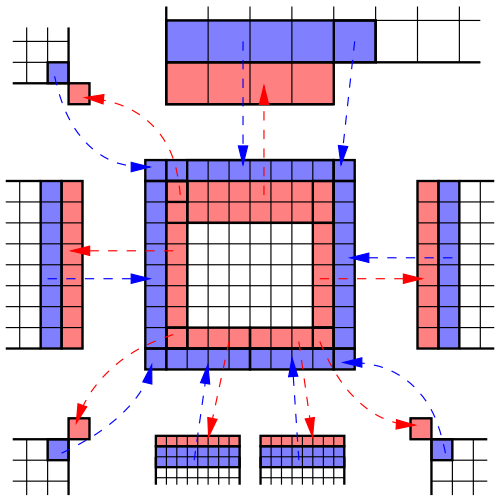


[John Wise]

Cello distributed adaptive mesh refinement

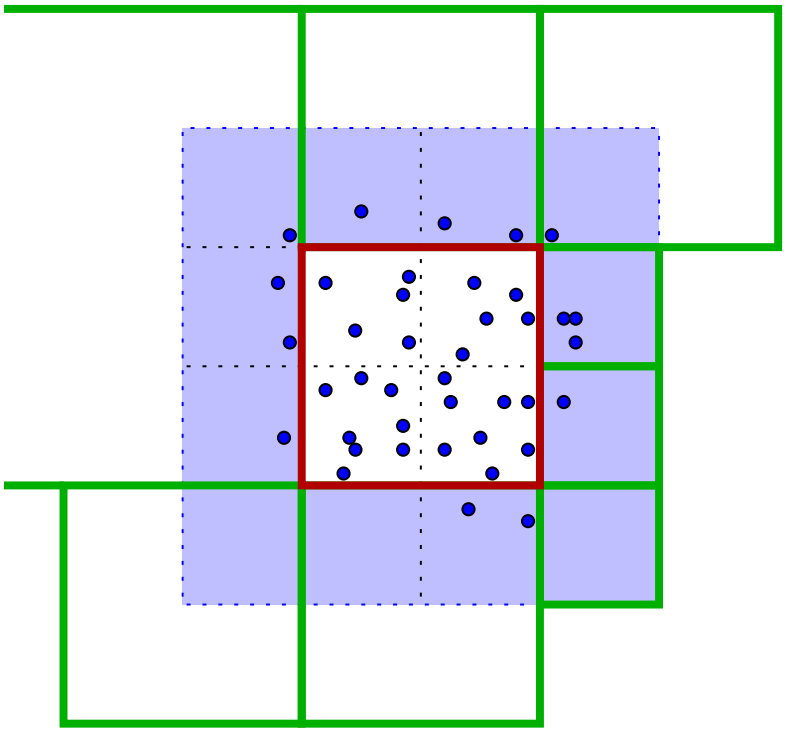
Cello implements a *fully-distributed* array-of-octree mesh hierarchy using a Charm++ *chare array* of `Blocks`. `Block` chare elements are indexed using a bit-coding of the array and octree indices.

- **Data-driven execution**
  - `Field` face data sent when available
  - last update triggers computation
- **Dynamic task scheduling**
  - multiple `Blocks` per process
  - overlaped communication/computation
- Charm++ **also provides**
  - cutting-edge load-balancing schemes
  - double in-memory checkpoint/restart



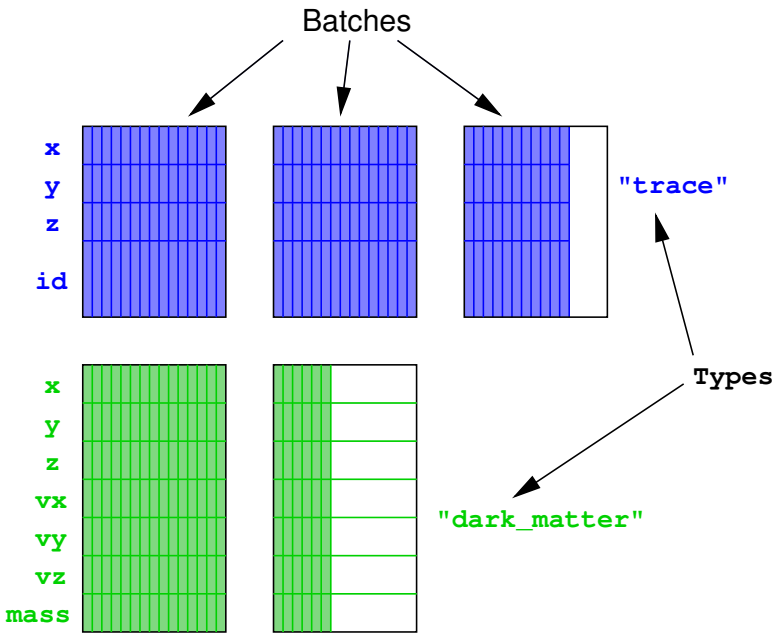
How particle data is communicated between Blocks

- communication is required when particles move outside a Block
- this is done using a 4x4x4 array
  - array contains pointers to ParticleData (PD) objects
  - one PD object per neighbor Block



- migrating particles are
  - `scatter()`-ed to PD array objects
  - sent to associated neighbors
  - `gather()`-ed by neighbors
- one sweep through particles
- one communication step per neighbor

How `Particle` objects store particle data



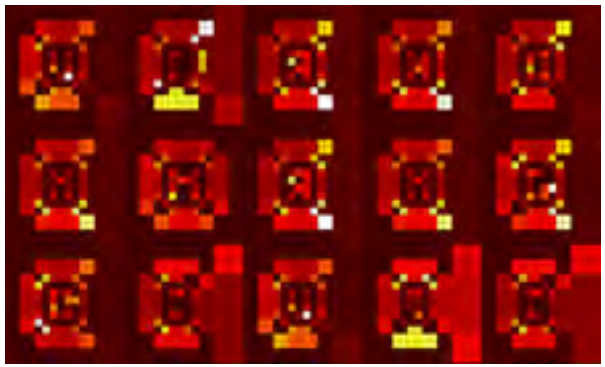
- multiple particle *types*
- particles allocated in *batches*
  - fixed size arrays
  - fewer new/delete operations
  - efficient insert/delete operations
  - potentially useful for GPU's
- batches store particle *attributes*
  - (position, velocity, mass, etc.)
  - 8,16,32,64-bit integers
  - 32,64,128-bit floats

- particle positions may be floating-point or integers
  - floating-point for storing global positions
  - integers for `Block`-local coordinates
    - solves reduced precision issue for deep hierarchies
    - less memory required for given accuracy

Enzo-P/Cello Blue Waters scaling test

Hydro and particles: "Alphabet Soup" problem

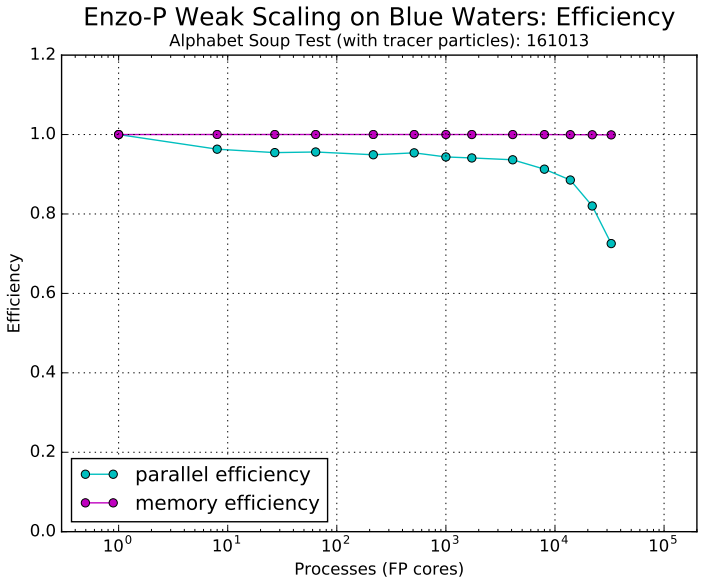
We tested basic Enzo-P hydrodynamics and particles scalability

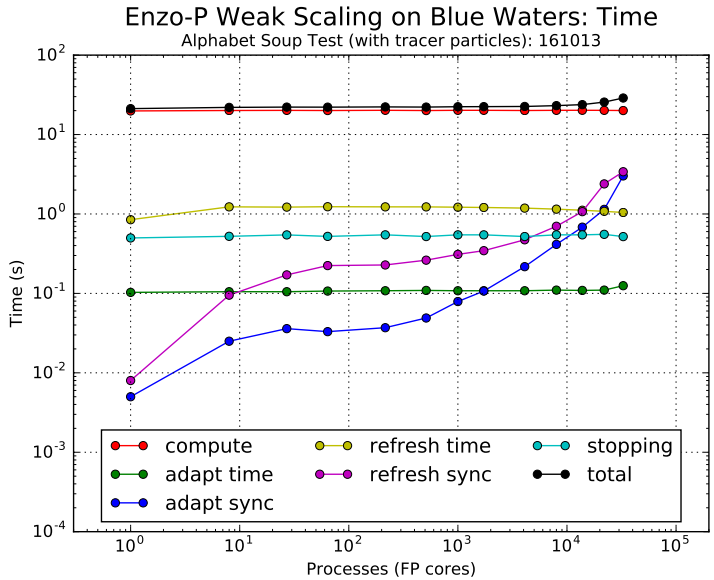


- variation of "array of Sedov Blast" test
- letters instead of spheres
  - inhibits lockstep coarsen/refine
- one letter per BW fp-core
- tested with/without tracer particles
- 32^3 or 24^3 cells per block
- among largest AMR runs ever done
  - $256K$ fp-cores
  - $1.7T$ cells; $0.7T$ (cells + particles)
  - $50M$ Blocks
- Enzo would require $72GB$ / process

Enzo-P/Cello Blue Waters hydro/particle scaling

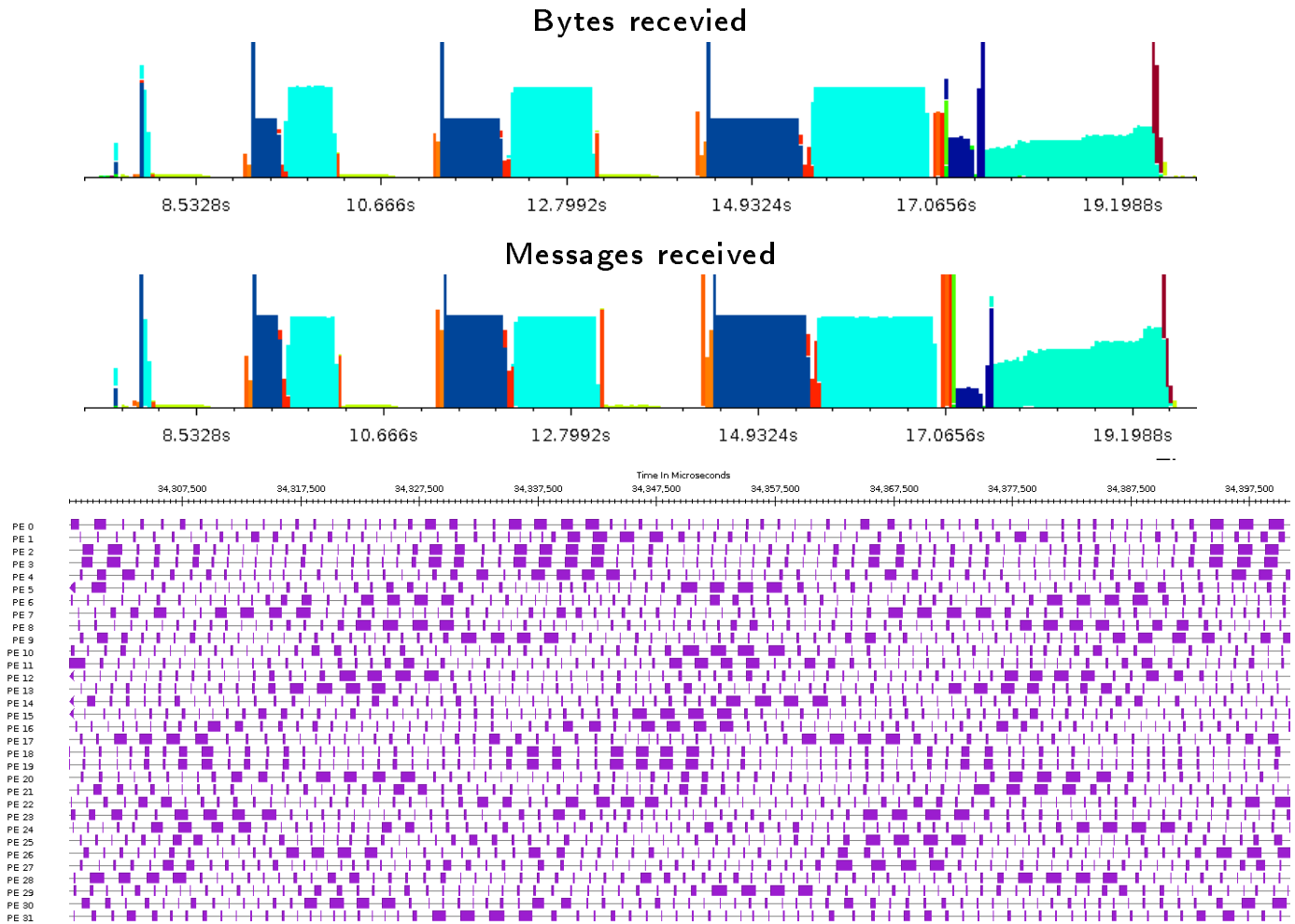
Initial tests: efficiency dropoff before $32K$ fp-cores





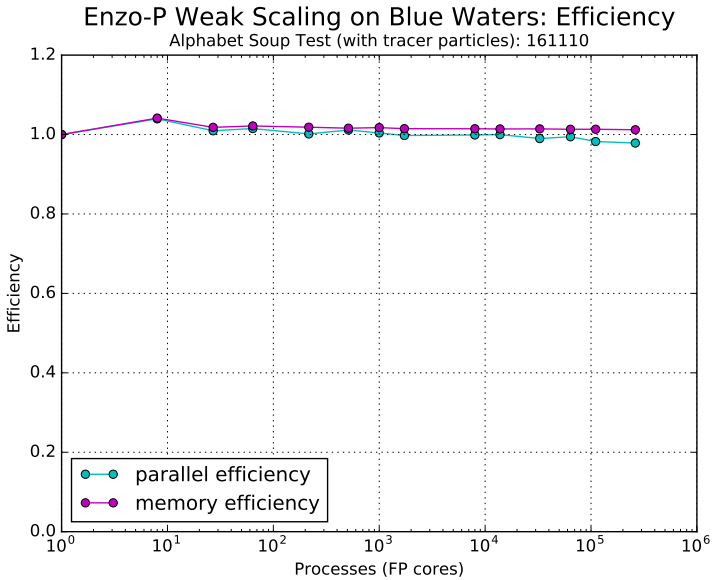
Enzo-P/Cello Blue Waters hydro/particle scaling

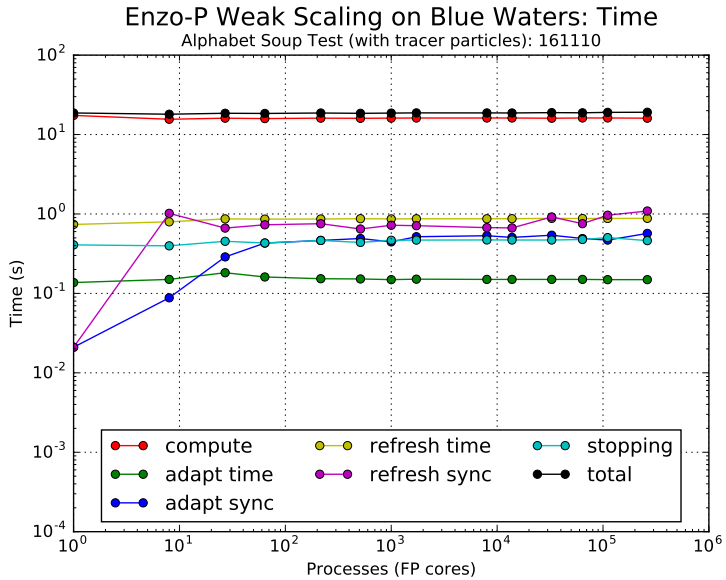
`Projections` analysis: hidden $O(N)$ or $O(P)$



Enzo-P/Cello Blue Waters hydro/particle scaling

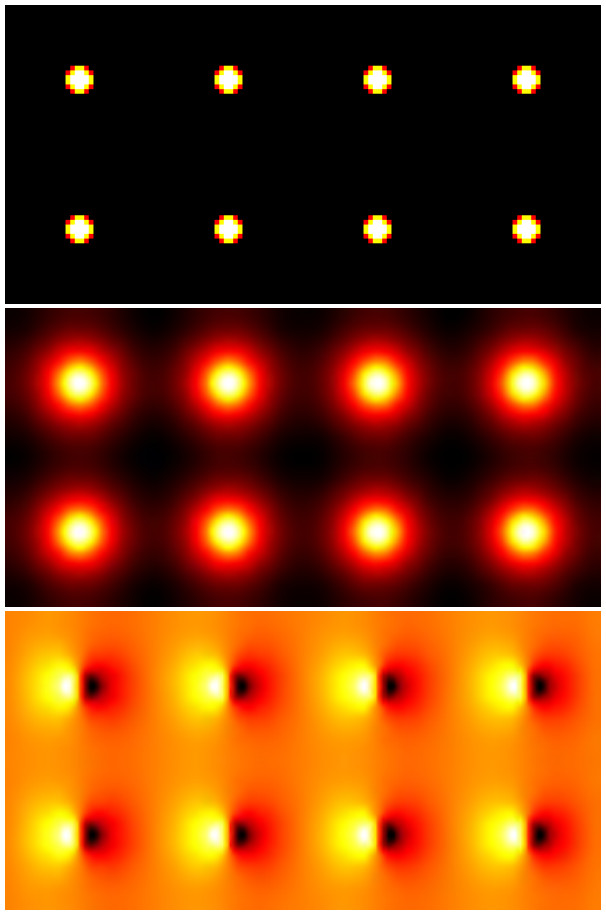
Charm++ SMP mode: excellent efficiency through 256K fp-cores

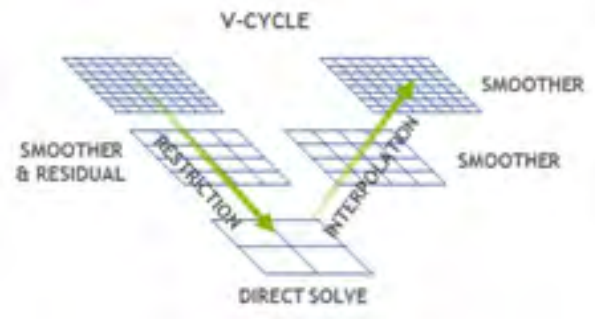




Enzo-P/Cello Blue Waters gravity test

We tested scalability of a recently implemented gravity solver





- "array of collapsing spheres" problem
- varied both block size and problem size
- multigrid V-cycle solve (uniform-mesh)
- debugging scalable AMR gravity
  - Reynolds "HG" algorithm
  - BiCG-STAB Krylov solver
  - multigrid-based preconditioner

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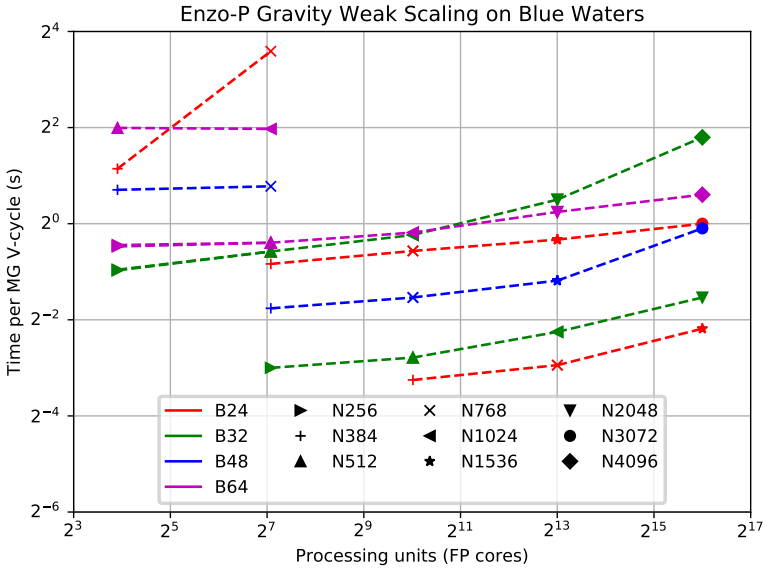

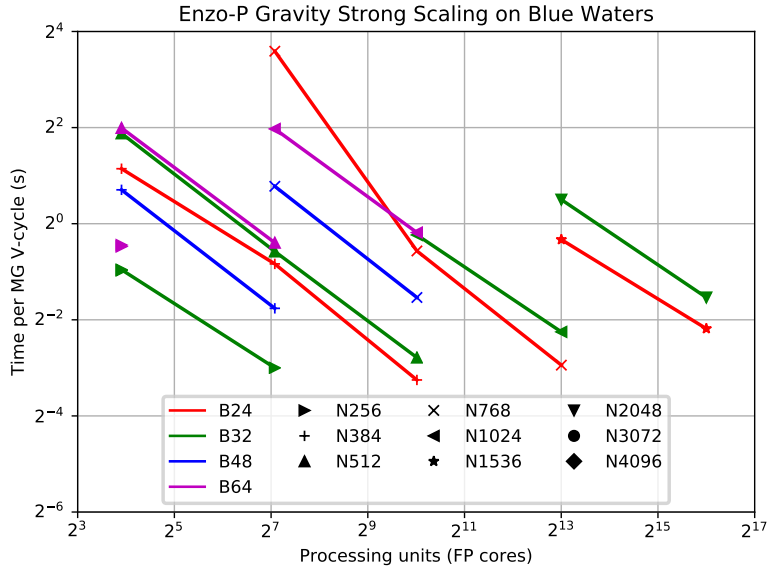

Conclusions and next steps

We are developing Enzo-P/Cello, the next-generation of the Enzo parallel AMR cosmology and astrophysics application

- Scalability of AMR hydro is excellent through $256K$ cores
- Scalability of uniform grid gravity is very good through $64K$ cores
- Scalable AMR gravity capability is around the corner

Next steps include the following

- Analyse and optimize uniform grid gravity
- Test and optimize AMR gravity
- More rigorous and realistic scaling problems
- Exercise Charm++ load balancing algorithms

`http://cello-project.org/`

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