Enzo-E/Cello astrophysics and cosmology

Adaptive mesh refinement astrophysics using Charm++

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University of California, San Diego
San Diego Supercomputer Center

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Charm++ and Its Applications
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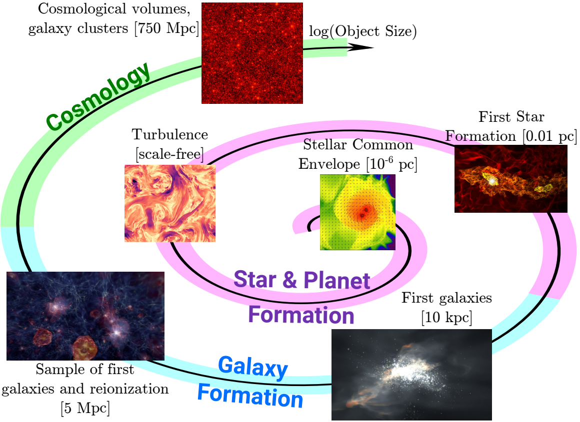
Scientific questions in astrophysics and cosmology



[John Wise]

The Enzo-E/Cello AMR Charm++ astrophysics application

Simulations require modelling multiple physics phenomena

Physics Equations: *mathematical models*

• Gravity ($\nabla^2\Phi = 4\pi G\rho$) • Hydrodynamics (Euler equations) • Chemistry/cooling • MHD • Cosmological expansion . . .

Numerical Methods *approximate and solve* **Enzo-E**

• Linear solvers (Krylov subspace, multigrid, composite) • modified PPM • Grackle chemistry/cooling • VL+CT MHD . . .

Data Structures *computer representation* **Cello**

• Adaptive mesh refinement (array-of-octrees) • Eulerian fields • Lagrangian particles

Parallel Runtime System *distribute data and computation* **Charm++**

• dynamic task scheduling • data-driven execution • asynchronous

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Numerical methods are required for solving the physics equations

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Parallel methods are enabled by distributed data structures

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Charm++ provides the support for running on large-scale HPC platforms

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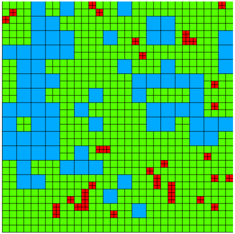
Cosmological simulations with Enzo-E/Cello

adaptive mesh



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- blocks of data
- chare array

dark matter

- particle data
- collisionless
- CIC gravity

baryonic matter

- field data
- PPM hydro
- flux-correction

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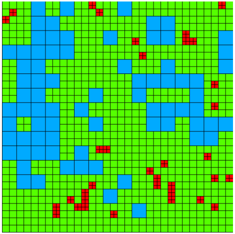

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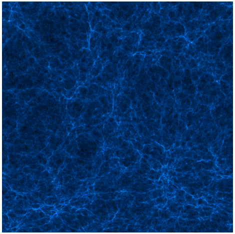

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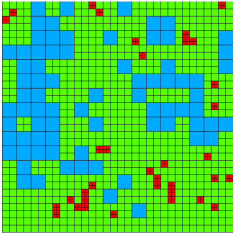

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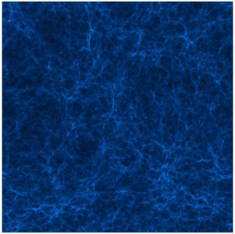

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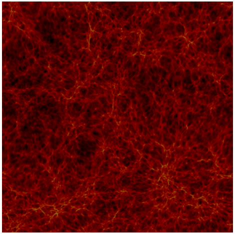

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Field and particle data communication

- **Field data exchange**
  - send `Field` face data when available
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  - scatter across 4^3 pointer array
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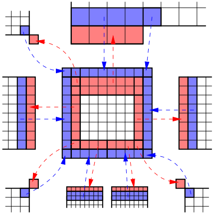

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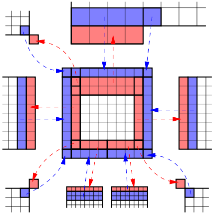

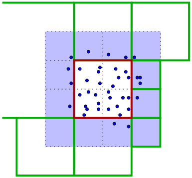

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Linear solvers in Enzo-E

Recent work has focused on scalable linear solvers

- **Krylov subspace methods**
  - CG (symmetric), BiCG-STAB (nonsymmetric)
  - easy to implement (basic linear algebra)
  - poor algorithmic scalability w/o preconditioning
  - communication intensive
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  - harder to implement (involves coarse blocks)
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The Enzo-E domain decomposition solver DD

1. `EnzoSolverMg0` for **root-level solve**
   - demonstrated good parallel scalability
   - tested to $N_0 = 2048^3$ on $P = 131$K BW fp-cores
2. `EnzoSolverBiCgStab` for **"tree-solves"**
   - use root-level solution for boundary conditions
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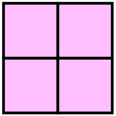

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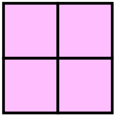

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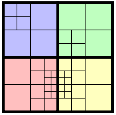

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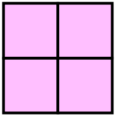

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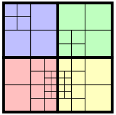

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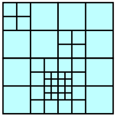

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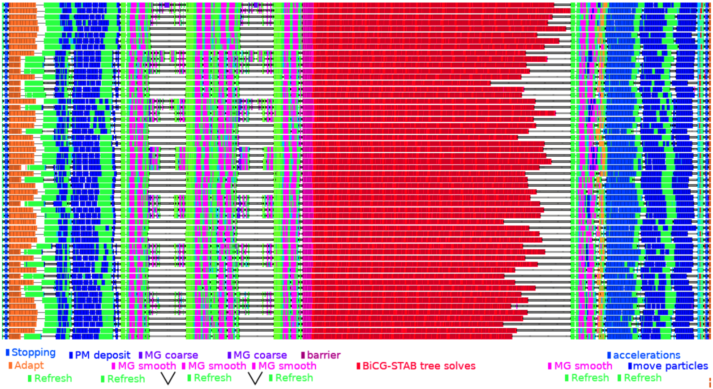
One cycle of a DM-only cosmology simulation using DD



Issue #2: robust refresh

Implementing DD Solver uncovered communication issues

Previous Refresh

- send face data when available
- copy data to ghosts when received
- race condition: may not be ready!
- extra synchronization added for correctness

Current Refresh

- sends face data when available
- 1. receives but not ready ⇒ copy data to buffer
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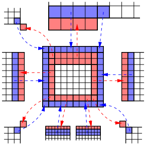

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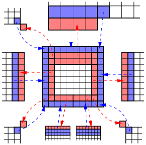

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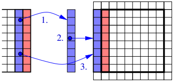

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AMR cosmology simulations with DM + gas

- Enzo-E can run DM-only AMR simulations
- and DM + gas non-AMR simulations
- but DM + gas with AMR leads to non-physical behavior

- clue: always at refinement-level boundaries

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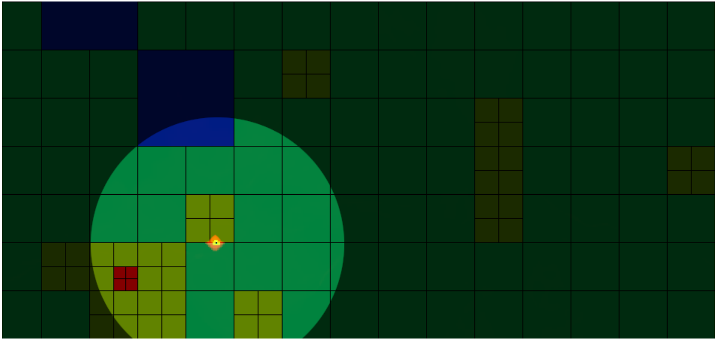

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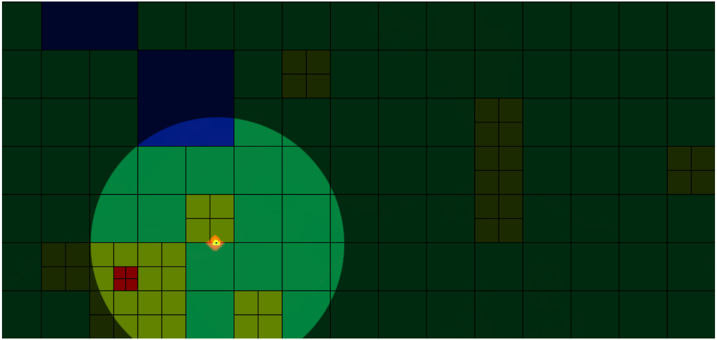

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Issue #3: flux-correction

Conserved quantities were not conserved at refinement jumps

- consider two fine blocks adjacent to a coarse block
- hydro computations depend on ghost values
- ghost values available from previous refresh

- fluxes at both fine and coarse faces
- conservation requires consistent fluxes
- not consistent in general

- apply a "flux-correction" step
- update coarse values along face so fluxes match
- requires coarse-to-fine block communication

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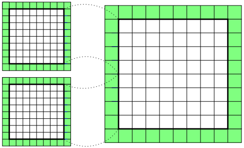

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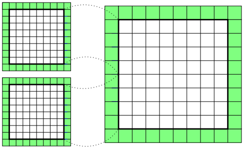

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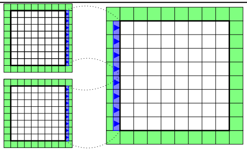

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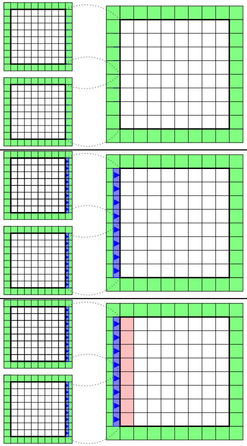

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Issue #4: improved interpolation

Implementing flux-correction didn't fix the problem :-(

Ran experiments to narrow down the problem

mesh ie ac

- problem only occurs when including gas dynamics
- internal energies blow up at level interfaces

- *linear interpolation* was main suspect
- got further with injection but grid effects

- suspected mismatched *time-centering*
- using $\alpha = 0.0$ instead of $\alpha = 0.5$ didn't help

- reducing *order of accuracy* only delayed problem
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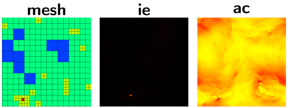

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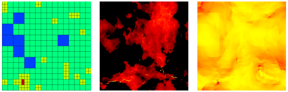

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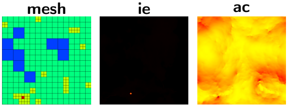

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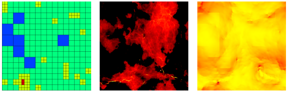

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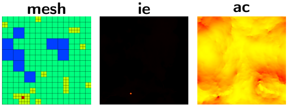

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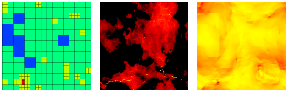

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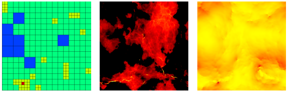

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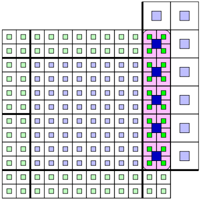

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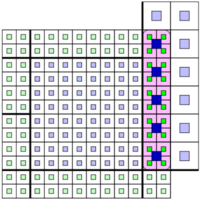
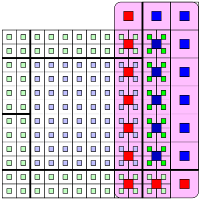


- ideally **accurate**, **monotonic**, **conservative**
- linear interpolation: coarse block values only
- some ghost cells must be extrapolated
- non-monotonic: negative densities, etc.



- ENZO's `SecondOrderA` method
- uses an extra layer of coarse zones
- overlaps some other adjacent blocks
- additional communication required

Issue #4: improved interpolation

New interpolation scheme involves additional blocks

- consider interpolating ghost cells $B_i \rightarrow B_j$
- coarse array overlaps additional blocks B_k
- B_k needs to know it participates in $B_i \rightarrow B_j$
- can take advantage of symmetry
- assume fully-balanced octree
- B_k must be same level as B_i or B_j
- if same level as B_i, then $B_k \rightarrow B_j$
- if same level as B_j, then $B_i \rightarrow B_k$

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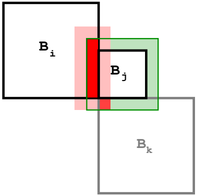

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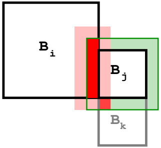

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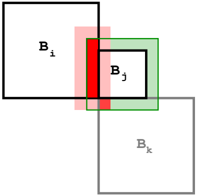

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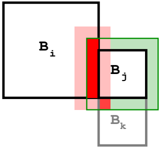

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Issue #4: improved interpolation

Indexing gets complicated and error-prone: introduced `Box` class

- **define blocks**
  - size (nx, ny)
  - ghosts (gx, gy)
- **define neighbor**
  - level L
  - face (fx, fy)
  - child (cx, cy)
- variable ghost depths to refresh
- optional ghost depths on send (e.g. mass deposit to total density)
- extra coarse-zone padding (px, py) for ENZO interpolation
- easily test block B_k intersection with defined region

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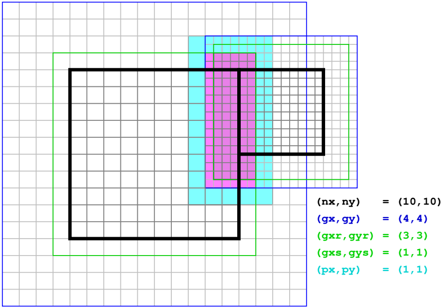

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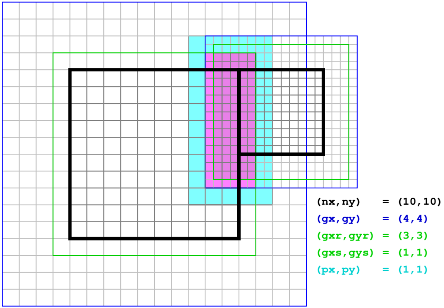

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Conclusions

- Finishing up last steps before production runs
  - 1. scalable gravity
  - 2. buffered refresh
  - 3. flux-correction
  - 4. improved interpolation
- Just a couple remaining loose ends
  - scalable I/O
  - ~~scalable checkpoint/restart~~ (thanks Ronak!)
- Performance optimization required
  - Enzo-E much slower than ENZO
  - over-refinement relative to ENZO
  - refresh across edges/corners
  - less communication in ENZO's gravity solver
  - ENZO uses adaptive time-stepping

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Acknowledgements

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