FASTMath Structured Mesh and Particle Technologies

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Scientific phenomena happen over a wide range of length and time scales. FASTMath is developing and deploying state-of-the-art structured mesh technologies that allow scientific application codes to capture these scales efficiently and enable scientific discoveries at scale. Chombo and BoxLib provide evolving algorithms and computational frameworks for these applications.

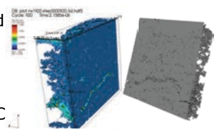
Applications-Aware Algorithms and Software

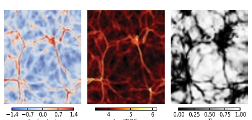
Algorithms and Software

- Hybrid and hierarchical parallelism for structured grid AMR.
- Particle methods: two-grid and single-grid methods (cosmology, plasmas).
- New grid generation for embedded boundaries (subsurface flow).
- Grid generation for mapped grids (edge plasmas).
- PETSc Interface (subsurface flow)
- High-order accurate finite-volume methods (climate, edge plasmas)

Applications Impact

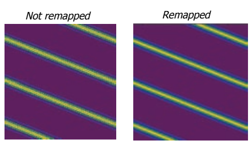
- Embedded boundary simulation of of fully resolved flow in fractured shale
- 0.18 porosity including fracture,100 micron block sample
- 48 nm resolution.60,000 processor cores at NERSC



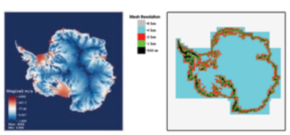


Left: A slice (one cell thick) through a L=10 Mpc/h simulation at z=2.5. The flux line-of-sight is into the page.

- The cosmological N-body/hydrodynamics code, Nyx, is built on the BoxLib framework.
- Nyx is designed to perform simulations of the intergalactic medium (IGM) and to model the Lyman-α forest (LyAF).

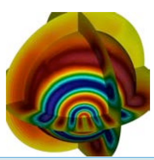


- Robust PIC support to enable research to eliminate spurious clumping
- Two-grid scheme allows high particle count simulations that weren't possible before



Ice sheet initial condition: Initial basal velocity field (left), and initial AMR meshes (right)

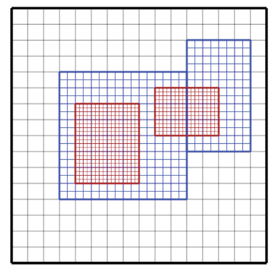
- AMR model of land ice dynamics (BISICLES)
- High-resolution coupled land ice (BISICLES) and ocean (POP2X) simulation of the full Antarctic continent and surrounding Southern Ocean.



- AMR for 3D non-hydrostatic models of the atmosphere for climate modeling
- Dynamic, anisotropic mesh refinement on the mapped multiblock cubed-sphere grid"
- Semi-implicit treatment of vertical acoustic wave propagation using ARK methods.

Overview

- Refined regions are organized into rectangular patches.
- Refinement in time and space, including region-based refinement in time.
- Higher-order temporal and spatial discretization methods.
- Implemented as layered C++ / Fortran software libraries.
- High-performance implementations using hybrid parallelism.



Collaborations

- Interoperability with PETSc solvers, collaboration within FastMath.
- Fast parallel sorting methods for particles (UIUC Charm++)
- Roofline toolkit (SUPER).
- Prototype implementation of resilience to resource loss (GVR).

Future Plans

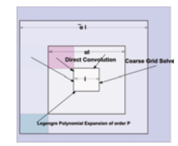
- Continued periodic releases of Chombo and BoxLib.
- Continued support of climate, accelerator modeling, and cosmology applications.
- Continue exploration of abstractions interplay in the context of AMR
- Systematically study the impact of turning off more demanding and logically complex AMR features on different class of applications
  - Fix the box-size (more cells, less book-keeping and meta-data)
  - Subcycling (may not be needed for all applications)
- Release of higher-order finite-volume infrastructure

Architecture-aware Algorithms and Techniques

Hybrid and hierarchical parallelism in both Chombo and BoxLib using tiling (*see Almgren et al. poster*).

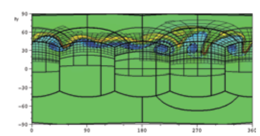
Method of Local Corrections for Poisson's equation

- Potential-theoretic domain-decomposition leads to low-communication algorithm.
- Mathematically systematic convergence theory.
- Production version as part of Chombo distribution currently being implemented.



Embedded Boundary Optimization

- Node execution time reduced by a factor of more than 2, geometry generation time reduced by a factor of 400 and peak memory use reduced by a factor of 3.
- Examination of memory footprint – closely related to the geometry configuration
  - Introspective load balancing does not help, different operators have conflicting demands. The right solution is to parameterize load balancing and tailor it for overall execution time.



Barotropic instability test (cubed sphere)

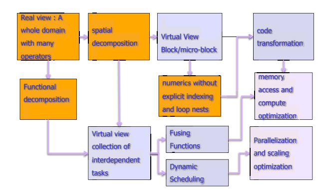
- Higher order methods for mapped multiblock grids, embedded boundaries, particles for emerging architectures.
  - Higher arithmetic intensity
  - Smaller memory footprint for a given level of accuracy.

Exploration of dynamic runtime management

- Interface with Charm++ for embedded boundary applications
- More heterogeneity in work distribution and memory use, potential for better performance with tasking

Design of software architecture for heterogeneity

- Differentiate between logical (virtual) and physical view
- Explore abstraction interplay
- Maintain separation of concerns



More Information: http://www.fastmath-scidac.org or contact Lori Diachin, LLNL, diachin2@llnl.gov, 925-422-7130

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