FASTMath Structured Mesh Technologies

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.

Structured Adaptive Mesh Refinement

Region-Based Adaptive Mesh Refinement (RAMR) and Optimal Subcycling

We have developed a new paradigm for adaptive mesh refinement (AMR) in **BoxLib**.

In the newly-named region-based AMR (RAMR), different regions at the same level of spatial refinement may have different temporal refinement.

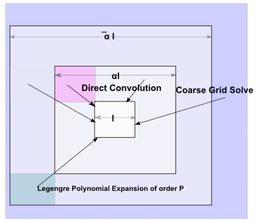
When combined with optimal subcycling, which selects a timestep for each region based on maximizing the efficiency of the overall algorithm, the use of RAMR can result in significant computational savings over traditional AMR approaches.

Method of Local Corrections

Potential-theoretic domain-decomposition Poisson solver compatible with AMR grids

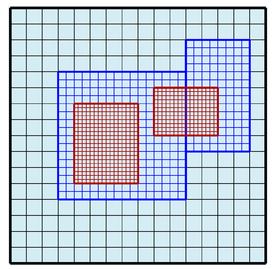
One V-cycle solve

- Downsweep: build RHS for coarser grids using discrete convolutions and Legendre polynomial expansions. Exploits higher-order FD property of localization.
- Convolutions performed with small FFTs and Hockney (1970)
- Coarse solve: Either MLC again, or FFT



No iteration, accurate, no self-force problems, large number of flops per unit of communication (messages and DRAM).

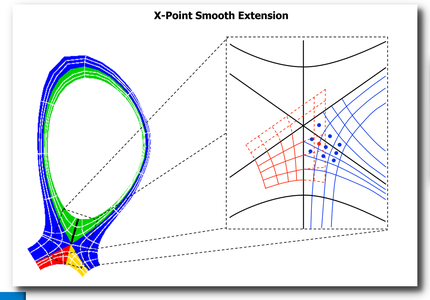
- Upsweep Solve for Φ_h on boundary of patch
- Interpolation and summations
- Local Discrete Sine Transform solve



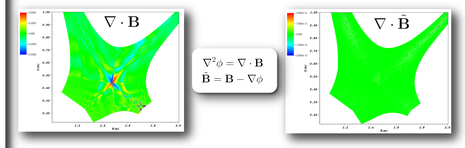
Mapped Multiblock Methods

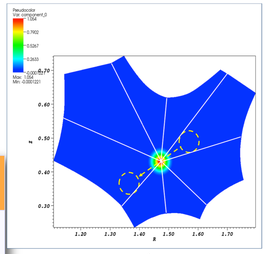
We have addressed a variety of issues related to high-order spatial discretization in edge plasma geometries:

- Modifications for free-stream preservation in axisymmetric geometries
- Smooth extension of block mappings through the X-point
- Fourth-order phase space boundary conditions

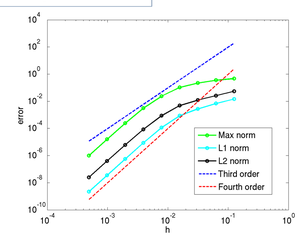


Magnetic field "divergence cleaning"

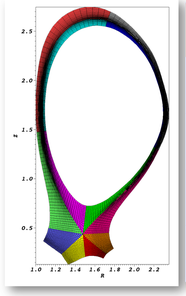




Left/Below: 4th-order accurate schemes across complex discontinuous mapping intersections



- Single-null geometry decomposition:

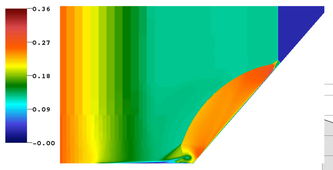


Block	Resolution
Left/Right Core	16 x 128 x 64 x 64
Central SOL	24 x 128 x 64 x 64
Left/Right SOL	12 x 32 x 64 x 64
Left/Right Private Flux	24 x 32 x 64 x 64

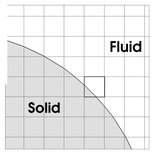
Interoperability

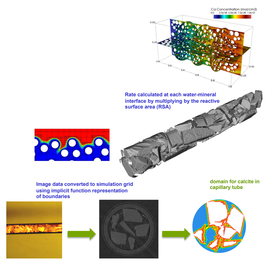
- Level matrix operator classes added to Chombo to create linearization of Chombo operators: Petsc matrices
- Solver classes build on Matrix Op classes
  - Interface to linear solvers (KSP)
  - Linear variable coefficient Poisson solver in EBAMRINS
- Interface to nonlinear solver (SNES)
  - Callback functions for apply and form Jacobian.
- Non-linear viscous tensor solver in BISICLES: Recently stood up full AMR matrix construction. Viscous tensor operator and solver deployed to BISICLES.
- Boxlib has native mutigrid solvers for cell- and node-centered data and also provides interfaces to PETSc, hypre and SuperLU solvers.

Embedded Boundary Methods

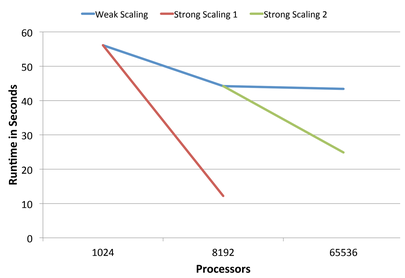


Comparison of viscous vs. inviscid high Mach number flow reflection from inclined surface. Resolved boundary layer-shock interaction



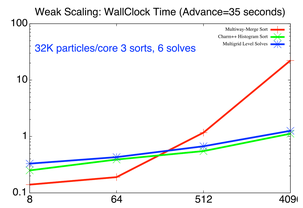


- CFD + multi-component geochemical reactive transport in very complex pore (micro) scale geometries
- Adaptive, finite-volume methods for advection-diffusion in Chombo
- Accurate reactive surface area using embedded boundaries
- Dynamic local refinement (AMR)
- Direct simulation of image data



Weak and strong scaling on the NERSC Cray XE6 (Hopper)

Particle-Mesh Methods

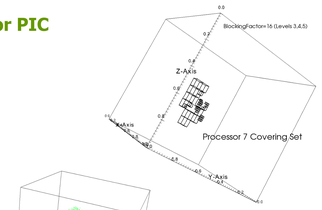


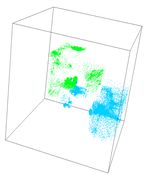
Distributed space-filling curve sort algorithms for 2-grid particle schemes compared to field solve time. Parallel distributed sort schemes are not a commodity programming element

Two-Grid Schemes for PIC

Using the same domain decomposition for the field solve grids and for the particle deposition results in load imbalance.

For simulations for which the are a large number of particles per grid cell, we perform field solves and field-particle transfers with *different* grids.





Particles handled with parallel distributed sorted space-filling curve, transfers to local "covering set".

The transfer between the two sets of grids is done efficiently. Only accumulated data is transferred using grid-grid native methods.

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