Structured Mesh Activities

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FASTMath structured mesh frameworks support SciDAC and other applications with a wide range of capabilities and a focus on synergistic interoperability.

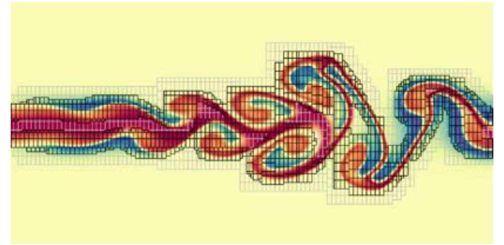
Overview

FASTMath supports structured mesh frameworks with a wide range of capabilities. Features include support for:

- Adaptive Mesh Refinement (AMR)
- Higher-order interior spatial discretizations
- Higher-order time-stepping
- Higher-order tools for interface dynamics
- Particle dynamics and particle-mesh operations
- Mapped multi-block methods
- Dynamic load balancing

Improved interoperability includes:

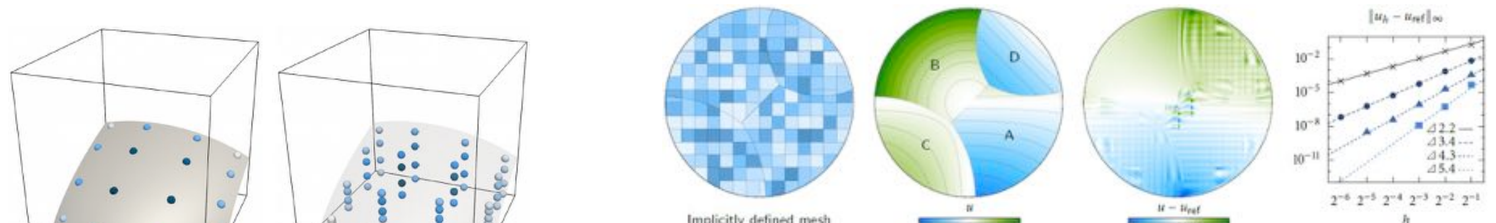
- New connections to SUNDIALS – serving as testbed for new time integrators
- New support for SDC (spectral deferred corrections) time-stepping
- New connection between AMR frameworks and higher-order interface dynamics tools
- Interoperability with new hypre semi-structured solver
- Improvements to non-linear solvers



High-Order Accurate Interface Dynamics

Algorithms and numerical software for high-order accurate interface dynamics, centered around the theme of implicitly defined geometry.

- Open-source high-order accurate quadrature algorithms for implicitly defined domains.
- Numerical tools for high-order accurate interface dynamics, including finite difference implementations of the Voronoi implicit interface method for multi-phase interface dynamics, accurate closest point algorithms for implicitly defined surfaces, high-order level set reinitialization, and k-d trees optimized for codimension-one point sets.
- Integration of some of the ideas and techniques underlying *implicit mesh discontinuous Galerkin* methods into AMReX with a view to adding new capabilities for high-order accurate multi-physics interface dynamics.



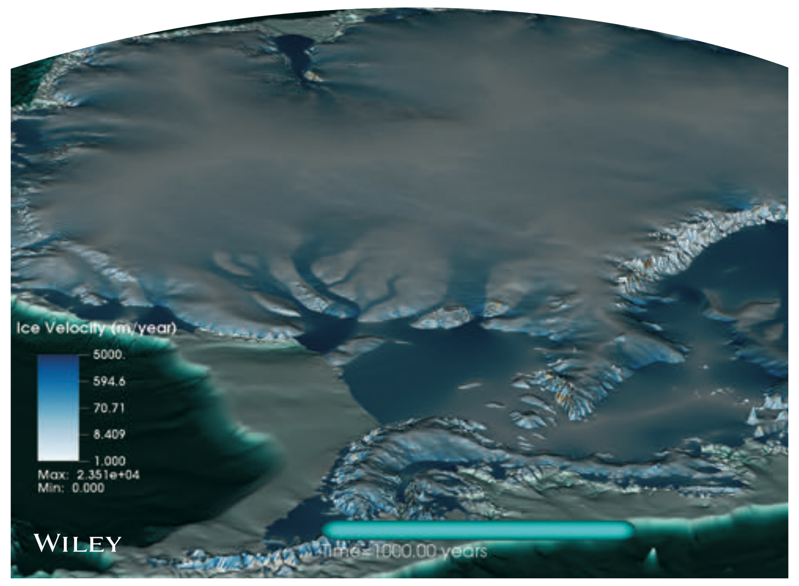
High-order accurate convergence in the maximum norm for an elliptic interface problem in a curved four-phase domain with interconnected interfaces.

FASTMath + ProSPect

The Antarctic Ice Sheet (particularly in West Antarctica) is believed to be vulnerable to collapse driven by warm-water incursion under ice shelves, which causes a loss of buttressing, subsequent grounding-line retreat, and large (up to 4m) contributions to sea level rise. Very fine (finer than 1km) spatial resolution needed to resolve ice dynamics around grounding lines (the point at which grounded ice begins to float).

FASTMath-supported BISICLES ice sheet model is part of ProSPect (Probabilistic Sea Level Projections from Ice Sheet and Earth System Models). BISICLES uses adaptive mesh refinement (AMR) to enable sufficiently-resolved modeling of full-continent ice sheet response to climate forcing.

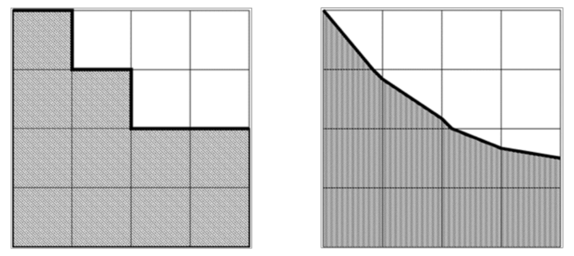
In SciDAC4, FASTMath continues to work with SOLVER LBNL team to improve numerical performance of PETSc solvers for BISICLES non-linear velocity solve. We are also contributing toward better accuracy of grounding lines using multifluid discretizations.



Surface velocities in Antarctica, highlighted on cover of *Geophysical Research Letters* (see Antarctic Vulnerability below)

Multifluid discretization

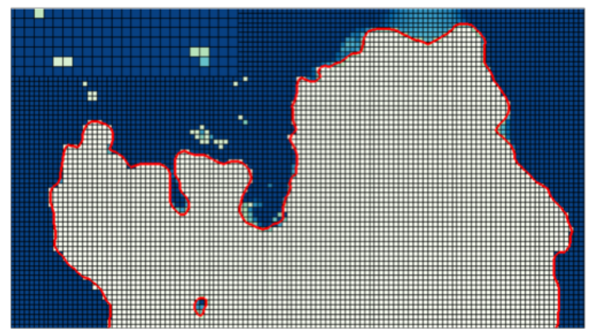
Recent results have demonstrated that very fine spatial resolution (< 1 km, maybe ~250m) is needed to resolve ice-dynamic features near grounding lines.



Representing a grounding line using stair-step (left) and embedded-boundary (right) discretizations. BISICLES currently uses an interpolated stair step grounding line (below, red contours).

Grounding lines can move arbitrarily fast depending on bathymetry and ice thickness → contact point problem.

Chombo's Embedded-boundary (EB) discretization could improve representation of grounding lines, grounded areas, and ice margins using a cut-cell approach.

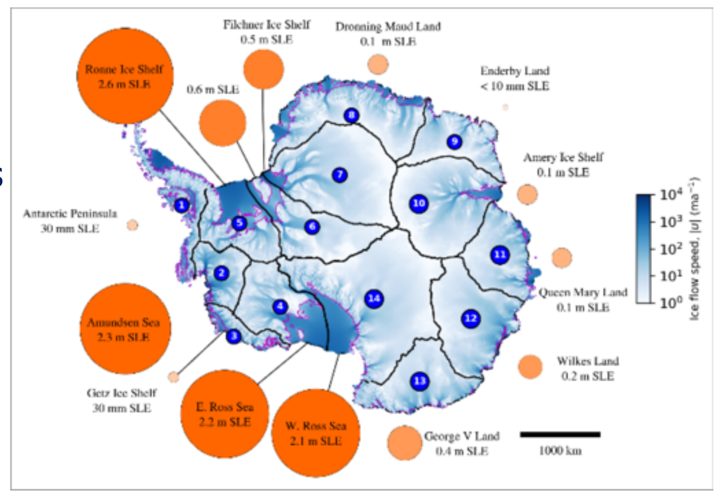


Antarctic Vulnerability

Used BISICLES to study Antarctic vulnerability to regional ice shelf collapse.

Findings include high vulnerability of WAIS to loss of any of its ice shelves, with limited vulnerability elsewhere.

D. F. Martin, S. L. Cornford, A. J. Payne "Millennial-scale Vulnerability of the Antarctic Ice Sheet to Regional Ice Shelf Collapse" Geophysical Research Letters, January 9, 2019, DOI:10.1029/2018gl081229



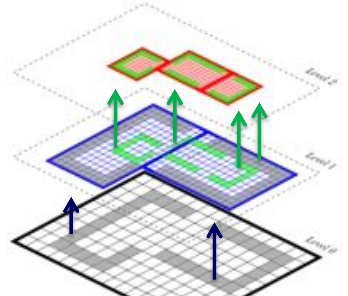
Antarctic vulnerability (in mm Sea Level Equivalent (SLE) to regional ice shelf collapse for each of 14 sectors.

FASTMath + ComPASS

QuickPIC is a highly efficient, fully parallelized, fully relativistic, three-dimensional particle-in-cell code for simulating particle or laser beam driven wakefield acceleration.
(https://plasmasim.physics.ucla.edu/codes/quickpic)

As part of the HEP ComPASS project, mesh refinement – both static and adaptive – will be added to QuickPIC to enable faster, more efficient simulation

FASTMath support provides source code and expertise to enable quick prototyping of multilevel algorithm and eventual optimization on new HPC architectures of the multilevel algorithm in the context of QuickPIC



Mapped Multiblock

Support for high-order mapped-multiblock:

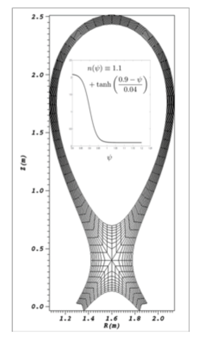
- Grid -> discretization infrastructure for 4th-order finite-volume methods on mapped grids.
- High-order interpolation of ghost-cell values between block boundaries.
- Managing flux-matching conditions at block boundaries.
- For kinetics problems (dimension > 3), specialized versions that take advantage of block-tensor-product structure of phase space mapping.
- Ongoing work under FASTMath 4: extension to multiblock mappings that are nonconforming in one of the coordinate directions.

Bolded blue quadrilaterals are examples of ghost cells for grid 2 that must be interpolated; adjacent shaded regions indicate cells in the interpolation stencils.

FASTMath + COGENT

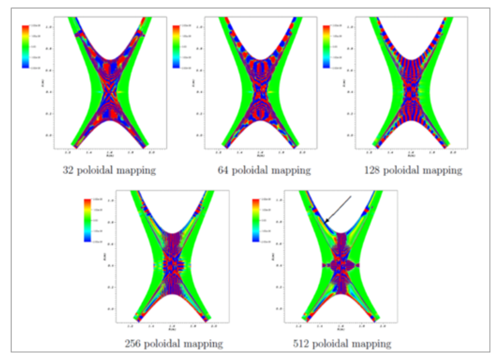
First-ever 4D continuum gyrokinetic simulation capability for problems in the edge plasma region of tokamak reactors that spans both sides of the magnetic separatrix.

- Uses FASTMath-supported mapped-multiblock software to discretize PDE in a nearly field-aligned coordinate system (4TH ORDER CODE??)
- Enables the simulation of kinetic effects on transport across the separatrix.
- Is the starting point for a 5D edge plasma turbulence capability.



(left): Representative COGENT edge plasma meshes and domain. Inset shows example of prescribed magnetic flux

(right): Study of local flux dealignment of grids enabled by the ability to plot truncation error.



Reference: M. R. Dorr, P. Colella, M. A. Dorf, D. Ghosh, J. A.F. Hittinger, P. O. Schwartz, "High-order discretization of a gyrokinetic Vlasov model in edge plasma geometry" 2018, J. Comp. Physics, vol. 373, (605-630), DOI:10.1016/j.jcp.2018.07.008

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