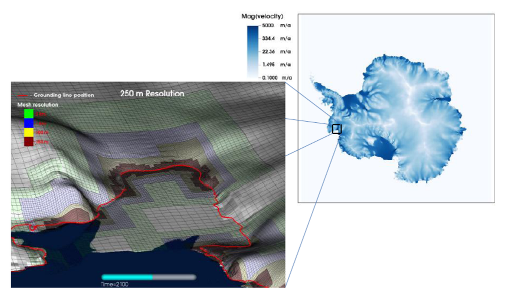
Impact of FASTMath Structured Mesh Technologies

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.

BISICLES: Ice Sheet Modeling

Mark Adams, Stephen Cornford, Daniel Martin

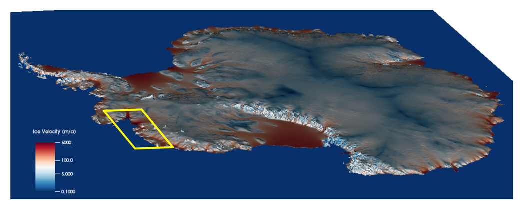
The dynamics of ice sheets span a wide range of scales. Very fine (sub-kilometer) resolution is needed to correctly resolve the dynamics in key regions like grounding lines and ice streams. Resolving all of Antarctica at such fine resolutions is computationally prohibitive. Adaptive Mesh Refinement (AMR) enables us to focus fine resolution only where needed.



BISICLES-computed Antarctic ice velocity. Inset: AMR meshing for Pine Island Glacier. Grounding line shown in red.

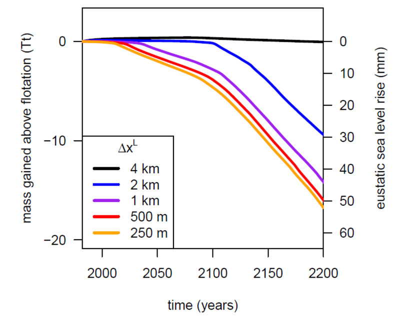
BISICLES (part of the PISCEES SciDAC application partnership) is a finite-volume block-structured AMR ice-sheet model built on FASTMath-supported Chombo.

Parallel, scalable, block-structured mesh refinement resolves the *grounding line* (Ice/Land/Ocean interface)



Above: location of Amundsen Sea

An Amundsen Sea example demonstrates the importance of adequate mesh resolution. Modeling the effects of warm-water incursion into the Amundsen Sea, the plot at right shows contribution to sea level rise vs. time and mesh resolution.

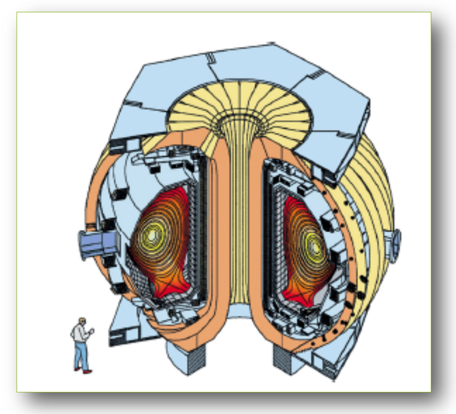


Finer than 1 km resolution is required – made possible through Chombo-supported AMR.

COGENT: Edge Plasma Simulation

Milo Dorr, Jeffrey Hittinger, Peter McCorquodale, Phil Colella

Simulation of tokamak edge plasmas requires the solution of PDEs in a geometry defined by magnetic flux surfaces. To better accommodate anisotropy, there is strong motivation for the use of mapped multiblock coordinates aligned with the flux surfaces.

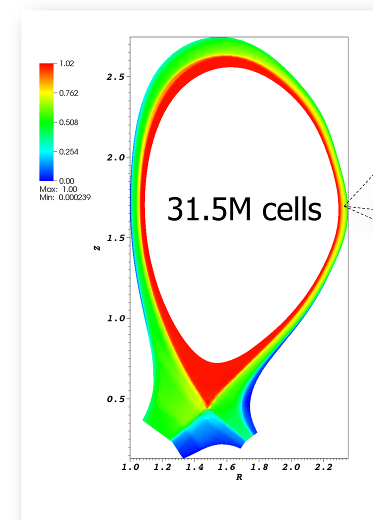


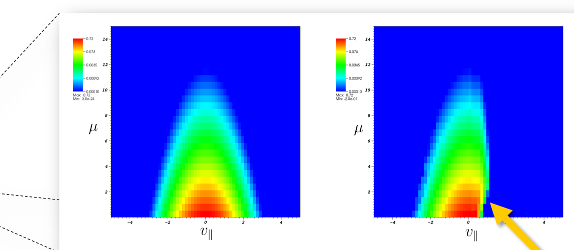
A new interface couples Chombo mapped multiblock objects and the *hypre* Sstruct (semi-structured) interface.

Milestone calculation: Fourth-order (spatial and temporal) solution of the 4D gyrokinetic model in DIII-D edge geometry: Loss cone test problem

Physical explanation:

- Advection in phase space
- Open field lines carry particles into diverter plates
- Density depletes in SOL (scrape-off layer)



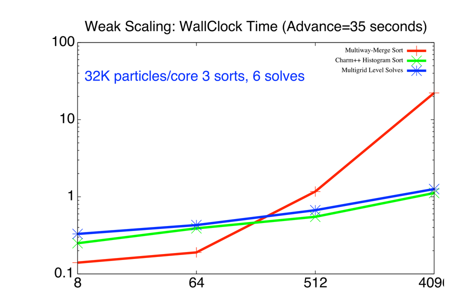


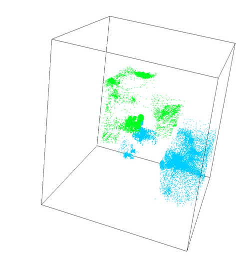
Magnetic well traps particles ("banana" orbits), so loss boundary is curved

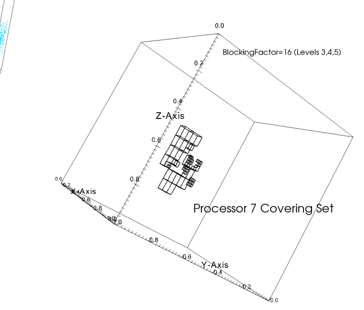
ComPASS: Comp. Accelerator Physics Tools

Mark Adams, Phil Colella, Christos Kavouklis, Brian Van Straalen

- Using the same domain decomposition for the field solve grids and for the particle deposition results in load imbalance.
- For simulations in which there are a large number of particles per grid cell, we perform field solves and field-particle transfers with different grids.
- Particles handled with sorted space-filling curve, transfers to local "covering set" grids (distributed sorting can be hard!)
- The transfer between the two sets of grids is done efficiently, since the amount of field data is small relative to the particle data.







Basic algorithm development work done through FY13:

- MLC: initial implementation of the algorithm will be complete, with demonstration of convergence and dependence on numerical parameters (ARRA and ASCR Base Math programs).
- PIC: Completion of scalable fast sorting algorithm, and initial release of two-grid PIC infrastructure in Chombo (FASTMath).

During FY14, we will use a combination of SciDAC funding and ComPASS funding to develop and release a high-performance version of the MLC Poisson solver.

Nyx: Cosmological N-body/Hydrodynamics

Peter Nugent, Zarija Lukić, Martin White, Casey W. Stark, Ann Almgren

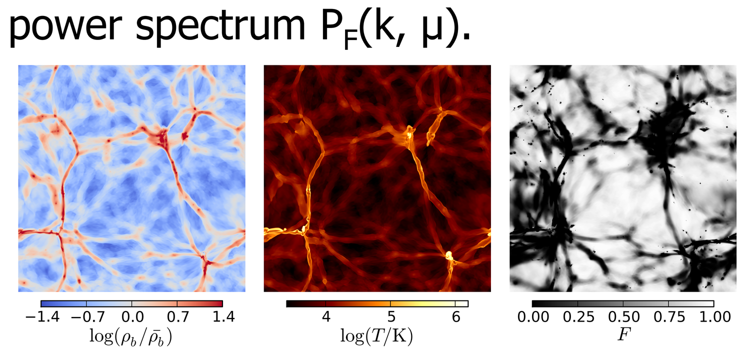
We have recently developed a new cosmological N-body/hydrodynamics code, Nyx, which is built on the BoxLib framework. Nyx is designed to perform simulations of the intergalactic medium (IGM) and model the Lyman-α forest (LyAF).

The scalability of Nyx allows us to simulate dynamic ranges that capture enough linear modes while resolving the Jeans scale in the IGM for redshifts relevant to LyAF observations (z=2-3).

As part of the SCIDAC-3 project, "Computation-Driven Discovery for the Dark Universe", Nyx simulations will be used to provide robust predictions of the various LyAF statistics including the mean flux, the flux PDF, and the 1D power spectrum.

On large scales, we aim to accurately determine the bias b and the redshift-space distortion parameter β.

On small scales, our ultimate goal is to emulate the anisotropic power spectrum $P_F(k, \mu)$.

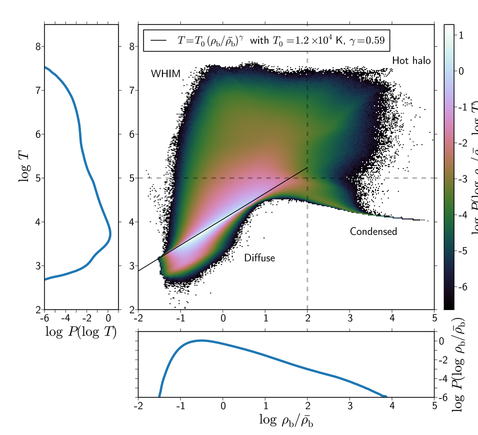


Left: A slice (one cell thick) through a L=10 Mpc/h simulation at z=2.5. The flux line-of-sight is into the page.

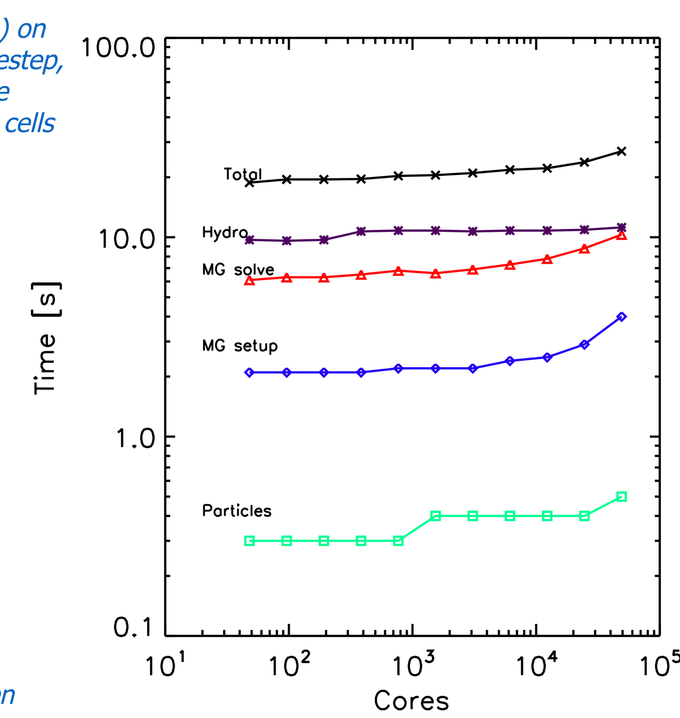
The scalability of Nyx allows us to run large problems with very quick turnaround. We are able to run 2048^3 simulations down to z=2 on 32,000 cores on Hopper at NERSC in a matter of hours rather than days.

Preliminary tests on the Edison Phase I machine indicate that Nyx runs about 3 times faster than on Hopper.

Right: Weak scaling of Nyx (up to 50,000 cores) on Hopper, based on the average walltime per timestep, broken down by task. We used the problem size such that each NUMA node (6 cores) held 128^3 cells and particles.



Above: Two-dimensional PDF of baryon density (in units of mean density) and temperature (in K), taken from a L=100 Mpc/h, 2048^3 simulation at z=2.5.



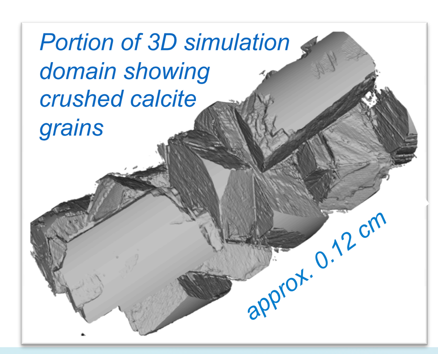
Chombo-Crunch: Subsurface Pore Scale Modeling

D. Trebotich, S. Molins, T.J. Ligocki, M.F. Adams, C. Shen, B.V. Straalen, L. Yang, J.B. Ajo-Franklin, C.I. Steefel

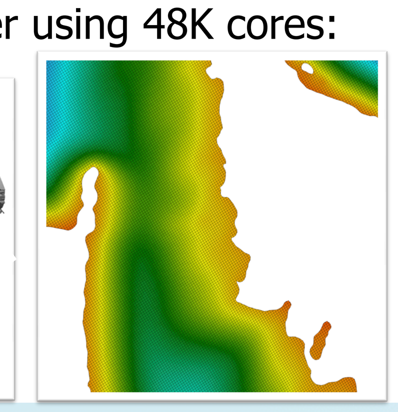
EFRC-NCGC is developing investigative tools (experimental, imaging and modeling) to build a new understanding of molecular-to-pore-scale processes in fluid-rock systems, and to demonstrate the ability to control critical aspects of flow and transport in porous rock media, in particular, as applied to geologic sequestration of CO_2.

A flow-through capillary tube experiment is being used to validate a new state-of-the-art simulation capability known as Chombo-Crunch. In the image-to-simulation process, the computational domain is constructed from experimentally-derived μCT images using implicit functions to represent the mineral surface locally on a grid.

Below is an example of a highly resolved simulation (1.16 μm resolution, 1.6 billion grid points) performed on NERSC XE6 Hopper using 48K cores:



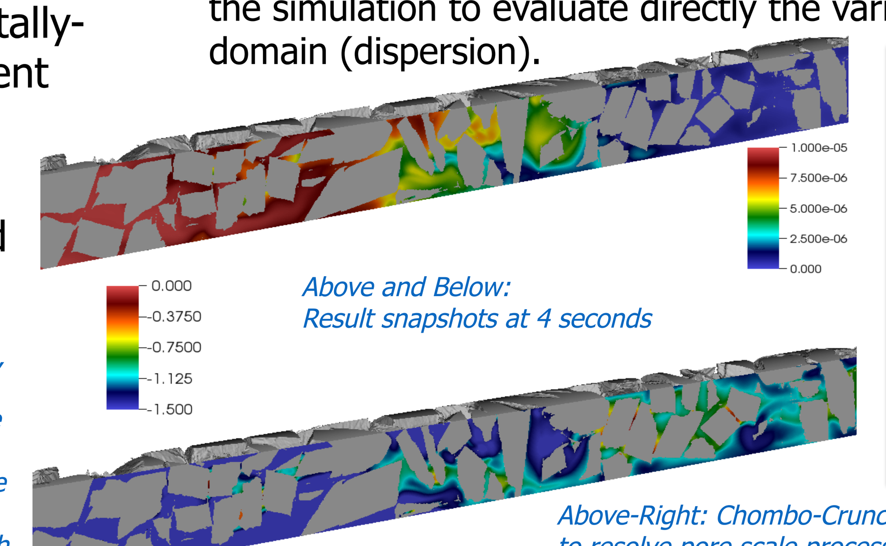
Portion of 3D simulation domain showing crushed calcite grains



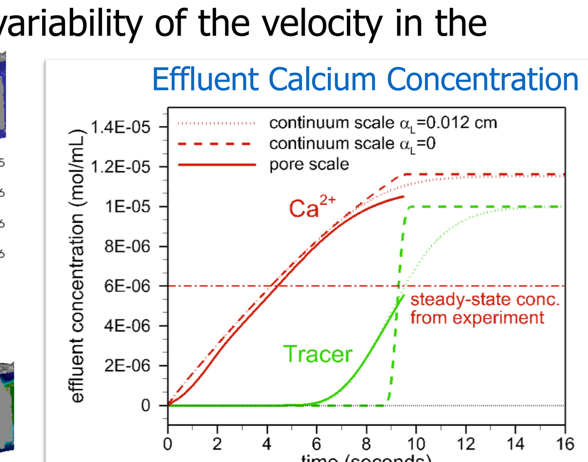
Left: 2D section, zooming in to a single pore. The dissolution rate, calculated at the mineral surface, depends on both the transport of reactants to the surface and the intrinsic rate of attachment and detachment of ions.

A **first-of-its-kind production run** has been performed for validation of the pore scale reactive transport simulation capability by an experiment:

- Current simulation time: More than 9 secs at 2 μm resolution using 2 weeks of runtime.
- Reaction rate parameters obtained by fitting the experiments for high pCO_2. In initial test run with Chou et al. (1989) rate law overshot measured effluent concentration. Pokrovsky et al. (2005) model improves the validation.
- In addition to reactants and products, a non-reactive tracer is added to the simulation to evaluate directly the variability of the velocity in the domain (dispersion).



Above and Below: Result snapshots at 4 seconds



Above-Right: Chombo-Crunch validation. 2 micron resolution was found to resolve pore scale processes, saving much time and resources compared to 1 micron runs. Pore scale simulation shows dispersion in the scalar transport breakthrough curve which can be upscaled to improve the continuum model.

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

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