Solver – Mesh Interactions

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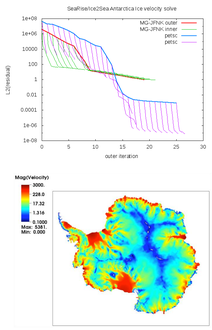
Structured and unstructured mesh interaction with equation solver libraries: BoxLib, Chombo & MeshAdapt with hypre, PETSc & Trilinos

Overview

One of the goals of FASTMath is the interoperability of existing FASTMath software. Recent FASTMath efforts have defined interfaces that allow the structured mesh frameworks to use external linear and nonlinear solver libraries for improved performance and robustness, and allowed the integration of unstructured mesh adaptation with PDE solution procedures. Below are four examples of structured mesh frameworks calling the hypre and PETSc solvers. On the right is an example of coupling between a general mesh adaptation procedure and existing unstructured mesh solvers.

Chombo/PETSc – BISICLES ice sheet modeling



BISICLES ice sheet modeling code

- Viscous tensor non-linear eqs.
- Large jumps in material coefs
- Use AMG solvers (hypre,GAMG,ML)

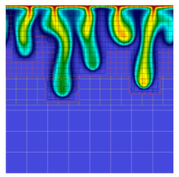
PETSc non-linear JFNK level solver

- Map AMR sparse index space to global equation for sparse solver.
  - PETSc solver is more robust than Chombo geometric MG solver.

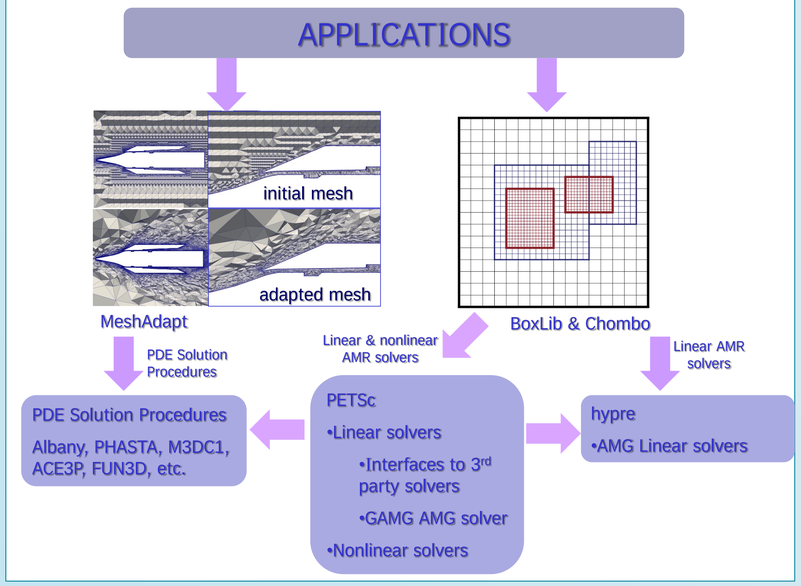
BoxLib/PETSc – Amanzi structured solver

Amanzi porous media code

- Simulation of time-dependent multiphase reacting flow in porous media requires nonlinear solve on multilevel AMR hierarchy
- Semi-structured interface to PETSc Mat, Vec and SNES objects for trust-region, damped Newton methods, Krylov and ILU-based solvers
- 4-level steady AMR flow solver coupled to solute transport/reaction integration
- BoxLib/PETSc example in Tutorials soon



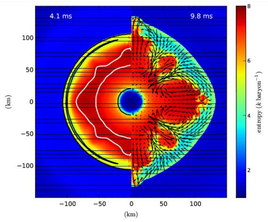
Component interactions



BoxLib/hypre – CASTRO radiation solver

CASTRO hydro/radiation code

- Multi-group radiation solve on multilevel AMR hierarchy
- Structured or semi-structured grid interface to hypre
- GMRES with PMG as preconditioner
- Scaling to 32K cores with 3 AMR levels
- BoxLib/hypre examples in Tutorials



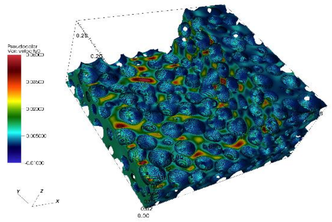
Chombo/PETSc – EBAMRINS porous media

Embedded boundary AMR method

- Complex geometry (BCs)
- Geometric MG coarse grids can not capture BCs accurately

Use AMG solvers (hypre,GAMG,ML)

- Able to solve problems where GMG failed.



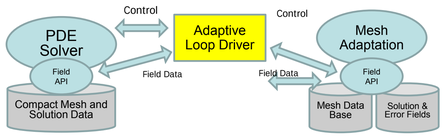
In-Memory Unstructured Adaptive Simulations

Couple existing unstructured mesh solvers with FASTMath's general mesh adaptation procedure with focus on high performance and low development costs. Possible approaches:

- Passing data through existing file structures – major bottleneck
- Integrating mesh adaptation data structures in solver – requires massive code rewrite
- "In-memory" approach, replace file I/O with functional interfaces – extra copy of data during transfer

In-Memory Coupling

- Adaptive driver that is based on high-level APIs to control flow of execution and data




```
//execute adaptive loop
while(solveReturn == asysComp::Adapt) {
  transferToAdapt(adaptComp, asysComp);
  adaptComp->adapt();
  adaptComp->preProcess();
  transferToSolver(adaptComp, asysComp);
  solveReturn = asysComp->Solve();
}
```

- Refactor I/O procedures to use functional interfaces for data
- Provide memory management procedures to resize structures

Current efforts on in-memory integration with MeshAdapt

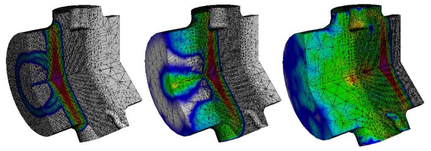
- MeshAdapt interacts through FMDB/iMeshP
- Albany, a demonstration application using the Trilinos framework
- PHASTA CFD

Status of Development

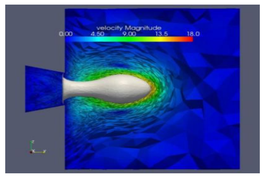
- Integration with Albany taking advantage of Trilinos and MeshAdapt interfaces (PISCEES ice sheet modeling, laser welding)
- In-memory version working with Phasta (multiphase reactor flow) On 2048 proc. file-based took 91 sec while in-memory took 1 sec.
- Other applications being developed
  - Fusion Edge Physics (XGCI)
  - Fusion Plasmas (M3DC1)
  - Accelerator Modeling (ACE3P)
  - High-speed viscous flows (FUN3D)

PHASTA CFD in-memory transfer vs. file based transfer on NERSC Hopper

Number of processes	File-based elapsed time (sec)	In-memory elapsed time (sec)
512	49	2
2048	91	1



Adaptive curved moving mesh short-range wakefield (ACE3P)



Adaptive two-phase flow with PHASTA CFD

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