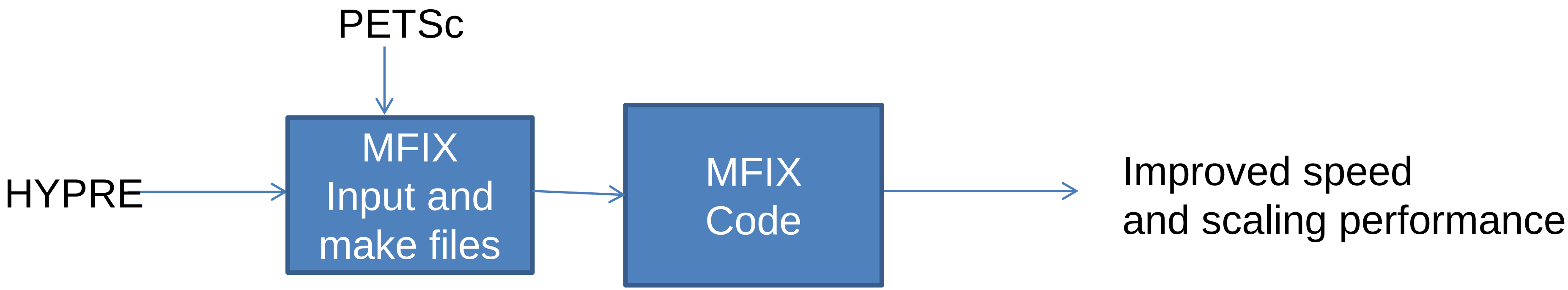
Interfacing MFIX with PETSc and HYPRE Linear Solver libraries

Award #: DE-FE0026191

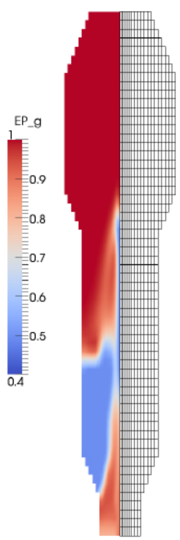
PI: Gautham Krishnamoorthy (UND)
Co-PI: Jeremy Thornock (U.Utah)
October 28th , 2015
Presentation at:
DOE-NETL

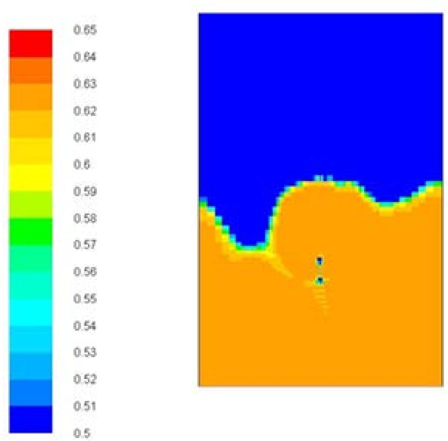
Objective/Vision

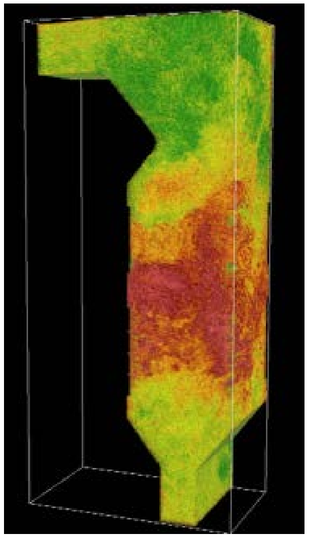
- Build a robust, well-abstracted, interface to the PETSc, HYPRE linear solver libraries from MFIX



- Code verification against established MFIX solutions and code to code comparisons

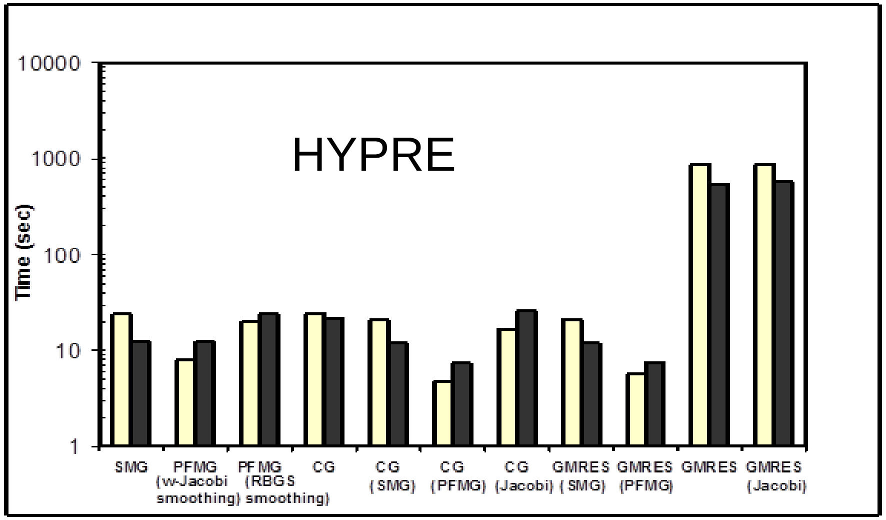


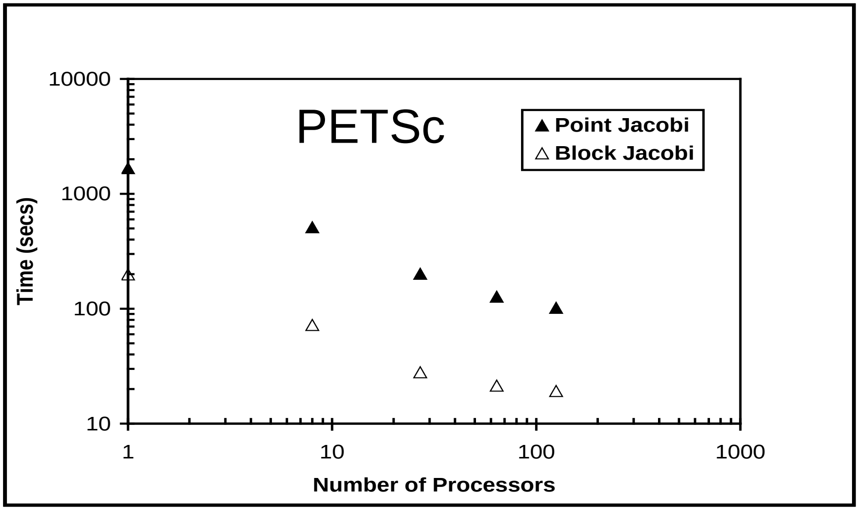




Objective/Vision (continued)

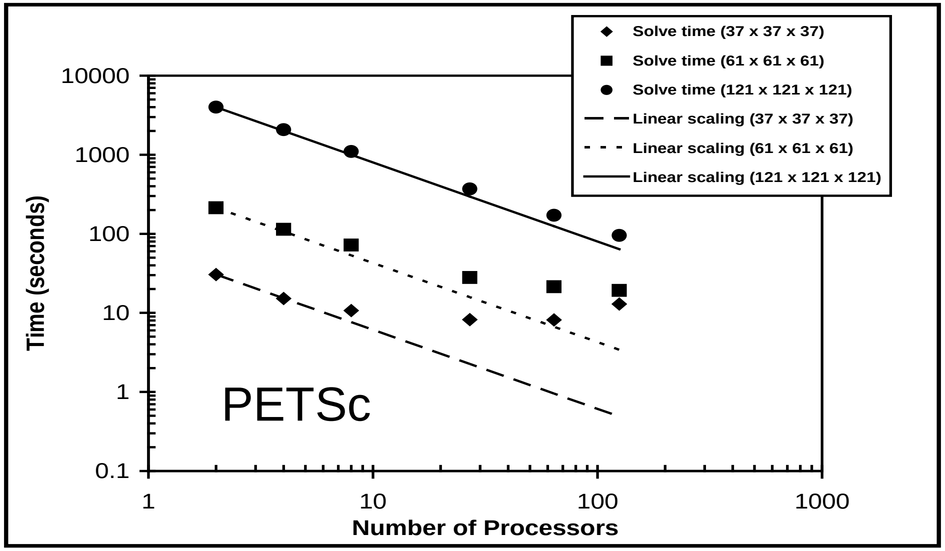
- Identification of <u>optimum</u> solvers and pre-conditioners

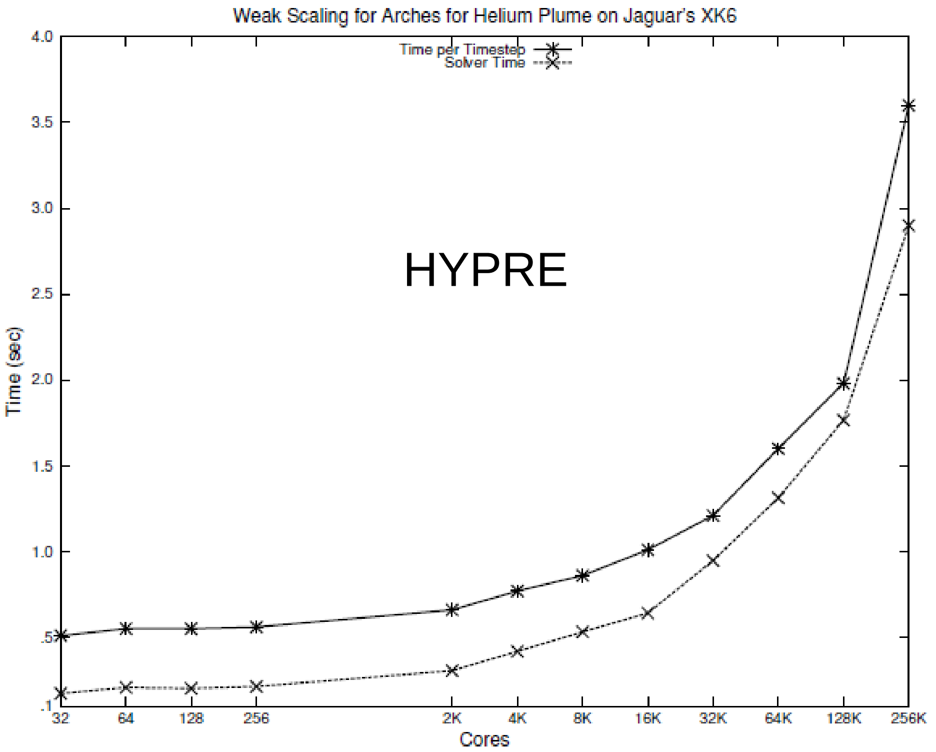




Objective/Vision (continued)

Examining the scaling of MFIX when invoking PETSc and HYPRE





Background
Software Abstraction

The problem:

- MFIX already has linear solver options
- Interfacing with the linear solver packages is not universal (different stencil setup operations)
- Fortran (MFIX is written in F90) isn't an object-oriented programming language

Our approach:

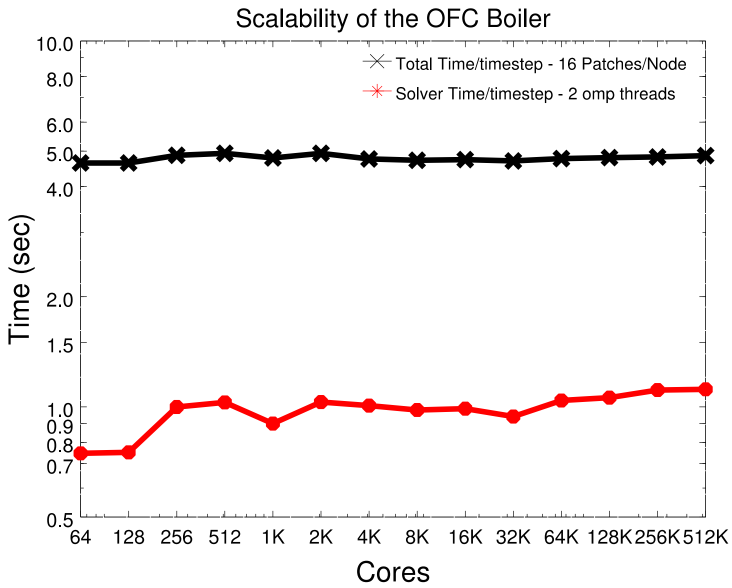
- To enable programmers and users, a well abstracted 'linear solver interface' is required
- Operations to setup a general linear solve (Ax=b), is easily abstracted
    - ➢ Compute matrix and vector elements (local to global mapping in PETSc and HYPRE)
- Object orientation can be simulated in F90 with some clever use of existing F90 features
- Define a common interface (a.k.a base class) and derive specific solver interface for existing MFIX solvers, HYPRE, and PETSC, etc.

THE UNIVERSITY OF UTAH

Background
Hypre

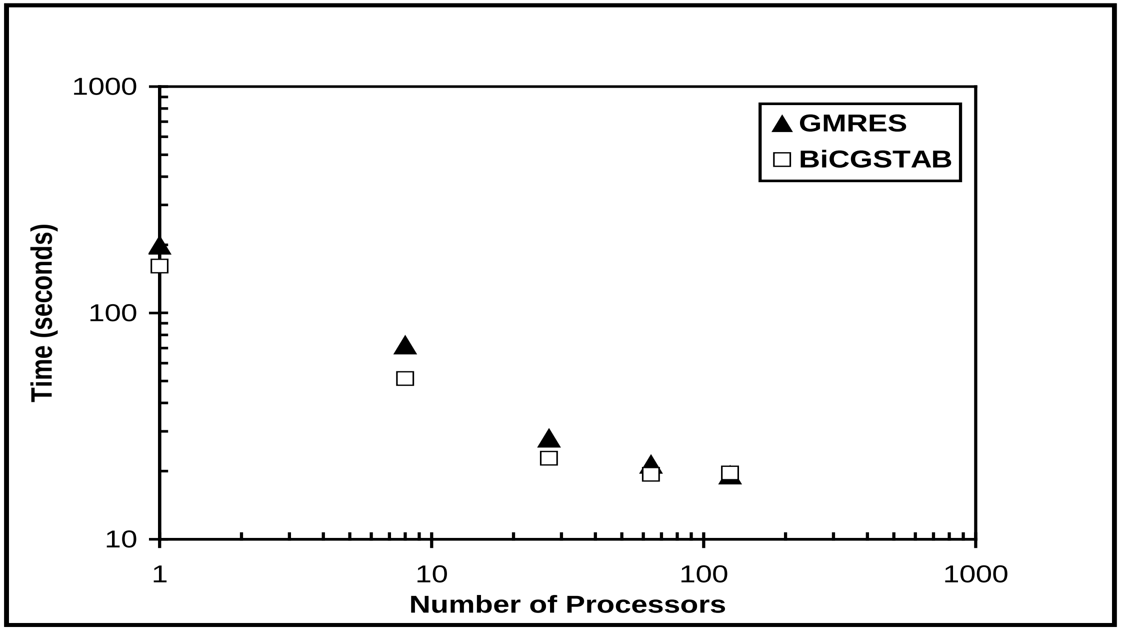
- Hypre (LLNL) is a linear solver package for the solution of preconditioned, sparse linear systems (including multigrid)
- Hypre includes native support for Fortran codes (MFIX)
- U.Utah and UND have extensive experience using Hypre for septa-diagonal matrix systems (Pressure-Poisson and P-1 radiation model)
- Hypre is current production linear solver for the U. of Utah's combustion (including PC) Arches code (Thornock; current software architect)

Arches/Hypre weak scaling up to 512K cores for a PC combustion simulation (simulations performed on Mira)

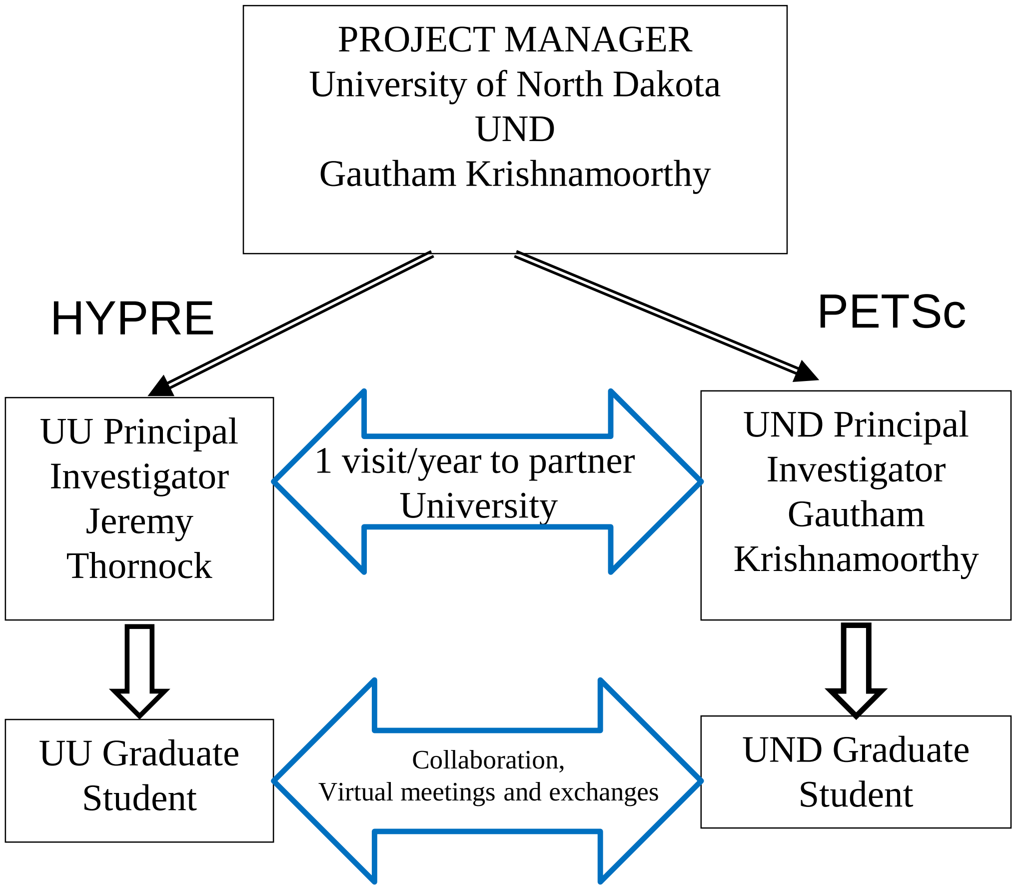


Background
PETSc

- PETSc (ANL) is a linear solver package for the solution of preconditioned, sparse linear systems (KSP)
- PETSc includes native support for Fortran codes (MFIX)
- U. Utah and UND have extensive experience using PETSc (non-symmetric matrices resulting from the discrete ordinates radiation model)



Team Description



Task 1 (Description): Project Management

- UND and U.Utah have discussed and concurred on a plan to move forward on this project
- MFIX, PETSc and HYPRE have been downloaded, compiled and tutorials have been run at both centers
- A graduate student has been recruited at UND, recruitment efforts ongoing at Utah

UND

THE UNIVERSITY OF UTAH

Task 2 (Description): Interfacing MFIX with PETSc and HYPRE

- Problem Setup*: Solver parameters (solver tolerances, maximum number of iterations, solver types, pre-conditioners etc...)
- Solver Setup*: Solver object creation (allocation of A, x, and b) and initialization methods.
- Communication Linear System: Handshake (or "mapping") function for passing the linear system coefficients (A) and right-hand-side values (b) in the current native MFIX data-structure to the solver-specific types.
- Solve System: Compute the solution (x) to the linear system
- Return/Copy Solution: Conversion of the solver type solution (x) to the current, native MFIX type
- Cleanup: De-allocation and destruction of solver objects

*one-time costs during simulation start-up during a transient calculation

Task 3 (Description): Code verification

- Established solutions from MFIX tutorials on serial and parallel machines
- Code-to-code comparisons (ANSYS FLUENT, ARCHES)

Task 4 (Description): Solver optimization

- PETSc (GMRES, BiCGSTAB)
- HYPRE (Pre-conditioned multigrid)

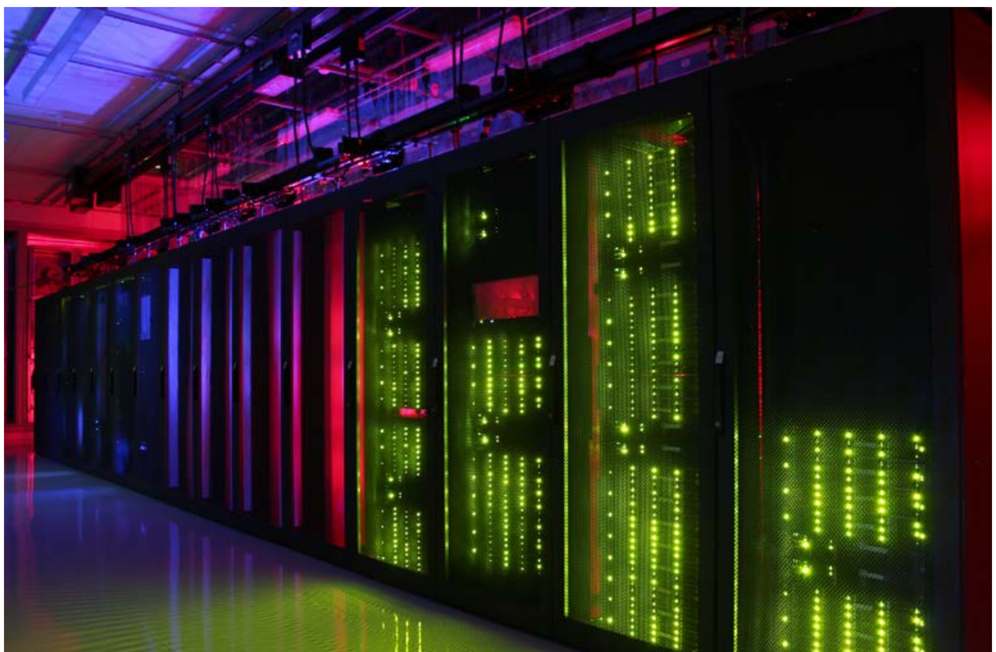
THE UNIVERSITY OF UTAH

Task 5 (Description): Scaling studies

U. Of Utah's Ash cluster will be used for scaling tests

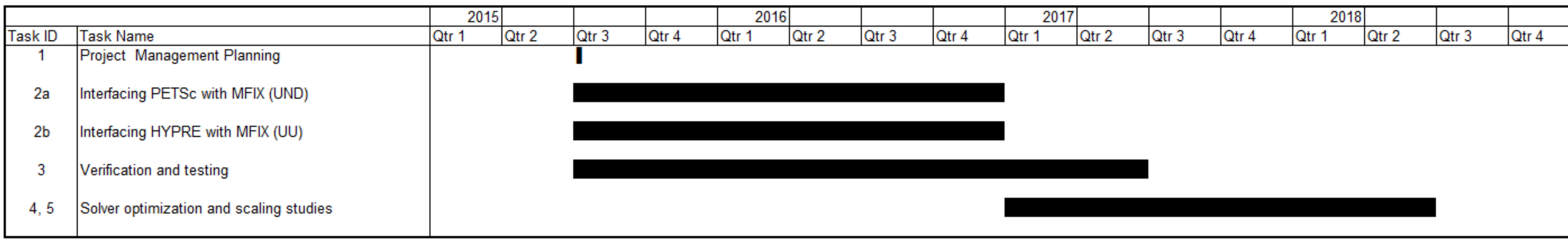
Ash Cluster Hardware Overview

- 253 12 Core Nodes and 164 20 Core Nodes (6316 total cores)
- 2.8 GHz Intel Xeon (Westmere X5660) processors
- 24 Gbytes memory per node on the 12 core nodes
- 64 Gbytes memory per node on the 20 core nodes
- Mellanox FDR Infiniband interconnect
- Gigabit Ethernet interconnect for management



(photo credit: Sam T. Liston)

GANTT chart



2015
2016
2017
2018
Task ID
Task Name
Qtr 1
Qtr 2
Qtr 3
Qtr 4
Qtr 1
Qtr 2
Qtr 3
Qtr 4
Qtr 1
Qtr 2
Qtr 3
Qtr 4
Qtr 1
Qtr 2
Qtr 3
Qtr 4
1
Project Management Planning
2a
Interfacing PETSc with MFIX (UND)
2b
Interfacing HYPRE with MFIX (UU)
3
Verification and testing
4, 5
Solver optimization and scaling studies

Milestones

Year 1 (9/1/2015 – 8/31/2016)

- Successful mapping of "A" and "b" elements from native MFIX data structure to PETSc and HYPRE solver objects
- MFIX runs with PETSc and HYPRE linear solver options on serial machines. Solutions verified against existing MFIX tutorials
- Solver options are specified within the source code

Year 2 (9/1/2016 – 8/31/2017)

- Refinement of the solver interface
- Extension of MFIX-PETSc-HYPRE coupling to parallel machines and solution verification

Year 3 (9/1/2017 – 8/31/2018)

- Identification of optimum solvers (explore dependency on flow regimes)
- Scaling performance
- Rigorously assess improvement in time to solution compared to native MFIX linear solvers

THE UNIVERSITY OF UTAH