Interfacing MFIX with PETSc and HYPRE Linear Solver Libraries

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Abstract

High computational cost associated with the solution of large, sparse, poorly conditioned matrices is currently a serious impediment towards increasing the utility of computational fluid dynamic models for resolving multiphase flows.

This project will interface NETL's Multiphase with Interphase Exchanges (MFIX) code with Portable Extensible Toolkit for Scientific Computation (PETSc) and High Performance Preconditioners (HYPRE) linear solver libraries with the goal of reducing the time to solution for the large, sparse, and often ill-conditioned matrix equations resulting during the solution process.

The lack of robust convergence associated with the current iterative methods in MFIX can be alleviated through appropriate preconditioning techniques to Krylov Subspace solvers and Multigrid methods accessible from these third-party solver libraries.

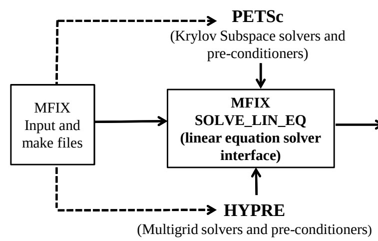
The overall objectives of this project are to:

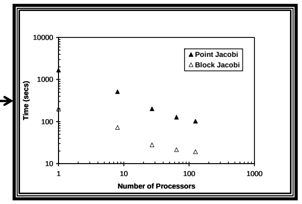
- Establish a robust well-abstracted solver interface that will present an extensible back-end that would allow MFIX to successfully interface with various solver libraries.
- Demonstrate this extensibility by interfacing MFIX with PETSc and HYPRE linear solver libraries with the goal of reducing the time to solution for large, sparse, linearized matrix equations resulting from the discretization of multiphase transport equations.

It is anticipated that this project could cut down the time to solution when compared to current linear solver options in MFIX, by at least 50 percent. It also could show that near linear scaling in parallel performance can be achieved to at least 1000 processors.

Objective/Vision

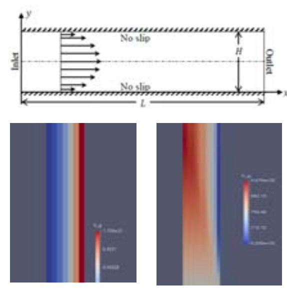
Build a robust/well-abstracted interface to PETSc and HYPRE linear solver libraries from MFIX





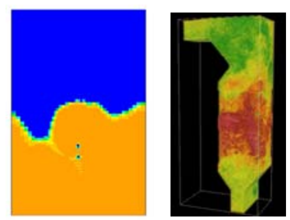
Improved speed and scaling performance

Code verification against established solutions



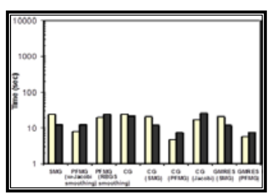
laminar turbulent

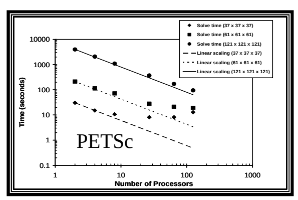
Plane Poiseuille Flow
(Comparisons against analytical solutions)

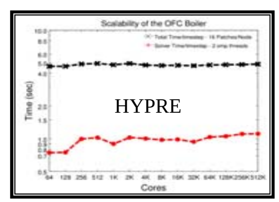


Code to code comparisons

Identification of optimum solvers and pre-conditioners, scaling studies







Results

PETSc relative solve times for solution to the inhomogeneous Helmholtz Equation (3D) (Septadiagonal matrix, uniprocessor)

$$\nabla^2 A + k^2 A = -f$$

Stand alone solver timing studies

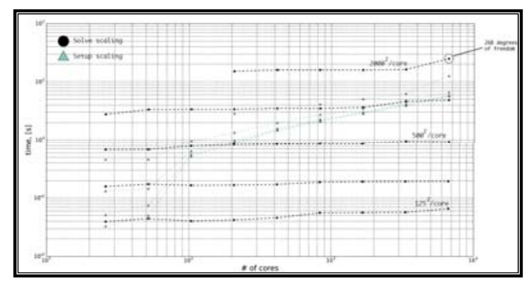
Degrees of Freedom	CG	GMRES	BiCGSTAB
150K	1.56	11.11	2.16
600K	23.45	700.00	35.56

Best stand alone solver with pre-conditioning options in brackets

Degrees of Freedom	CG (Point Jacobi)	CG (Block Jacobi)	CG (ILU)	CG (SOR)
150K	1.29	1.06	1.06	1.00
600K	25.24	19.31	18.01	17.87
1.2M	57.64	42.94	41.76	40.00

HYPRE scaling study
2D Poisson Equation
Solver: CG; Pre-conditioner: PFMG

$$\nabla^2 A = -f$$



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