Interfacing MFiX with PETSc and HYPRE Linear Solver libraries

PI: Gautham Krishnamoorthy (UND)
Lauren Clarke (Grad Student, UND)
KayLee Smith (Grad Student, UND)

Co-PI: Jeremy Thornock (U.Utah)
Surya Yamujala(Grad Student, U.Utah)
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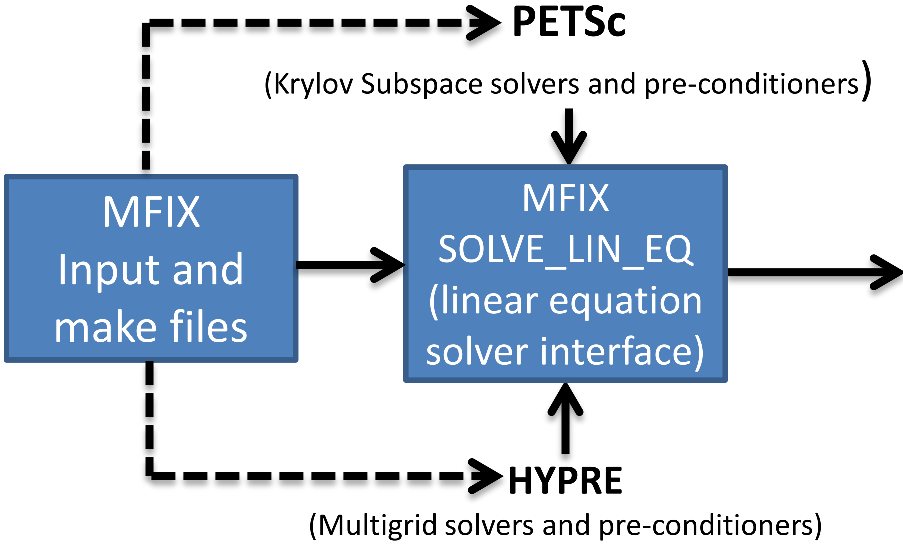
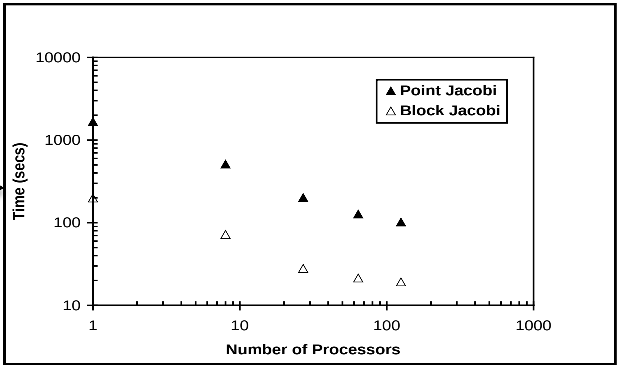
Objective/Vision

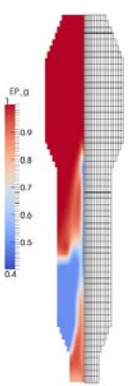
- Build a robust, well-abstracted, interface to the PETSc, HYPRE linear solver libraries from MFiX

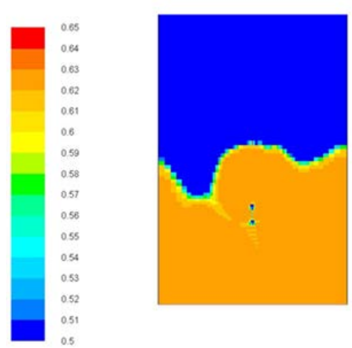


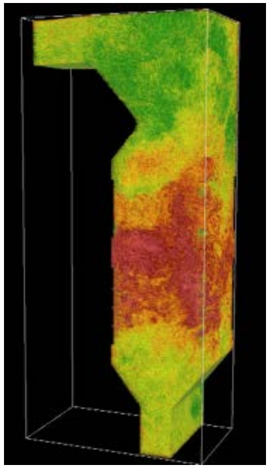


Improved speed
and scaling performance

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







Project Successes

- Lauren Elizabeth Clarke (Combined BS/MS Student, UND)
  - Mickey Leland Energy Fellow ‘17
  - 2 peer-reviewed papers (1 published, 1 under review)
  - Currently pursuing PhD at MIT

- KayLee Smith (Combined BS/MS Student, UND)
  - Mickey Leland Energy Fellow ’18
  - Placed 1st (Engineering) in UND’s Graduate Student Expo

- Surya Yamujala (MS Student, UUtah)
  - Quality and Reliability Assurance Engineer at IMFlash

- The MFiX-PETSc, MFiX-HYPRE interfaces have turned out to be faster and more robust in several problems including:
  - Domains involving local cell refinements and abrupt cell jumps
  - Complex geometries and large cell count (multi-tube BFB, multi-spout CLC reactors)
  - Large relaxation-factors
  - Large property variations (laminar sCO_2 flows)
  - Multi-fluid (different particle sizes) systems
- Increased collaboration between UND ←→ UUtah

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Our First Step

(Identification of optimum solvers and pre-conditioners)

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

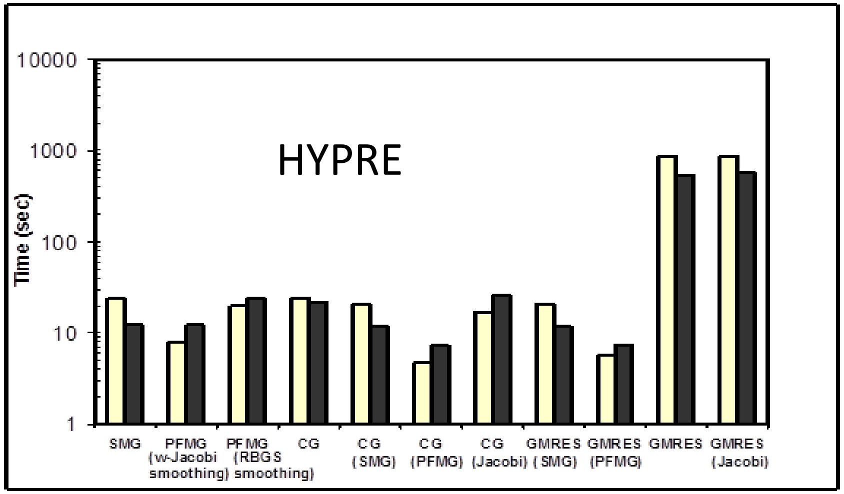
$$\nabla^2 A + k^2 A = -f$$

Stand alone solver timing studies

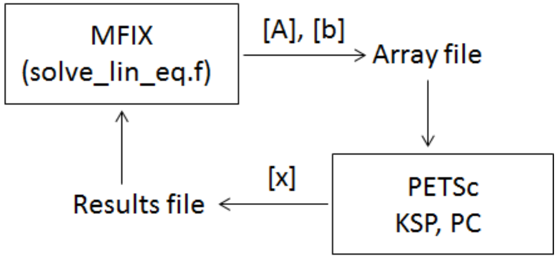
Degrees of Freedom	CG	GMRES	BiCGSTAB
150K	1.56	11.11	2.16
600K	23.45	700.00	35.56

Best stand alone solver with pre-conditioning options in brackets

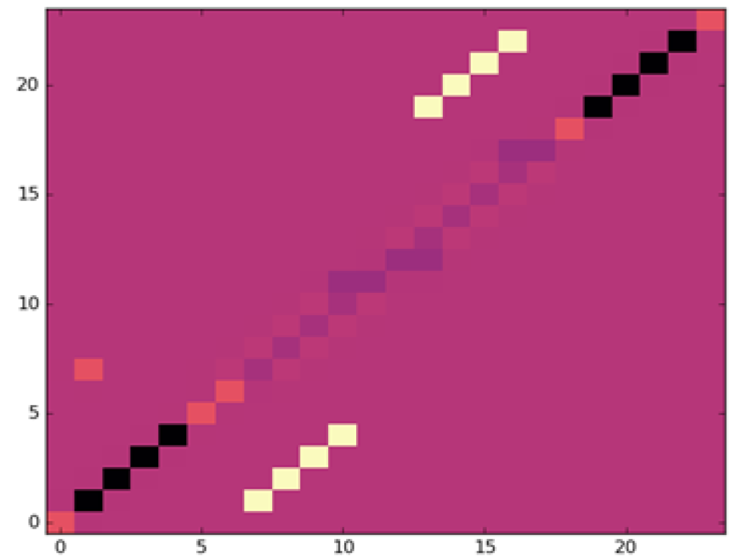
Degrees of Freedom	CG (Point Jacobi)	CG (Block Jacobi)	CG (ILU)	CG (SOR)
150K	1.29	1.06	1.06	1.00
600K	25.24	19.31	18.01	17.87
1.2M	57.64	42.94	41.76	40.00

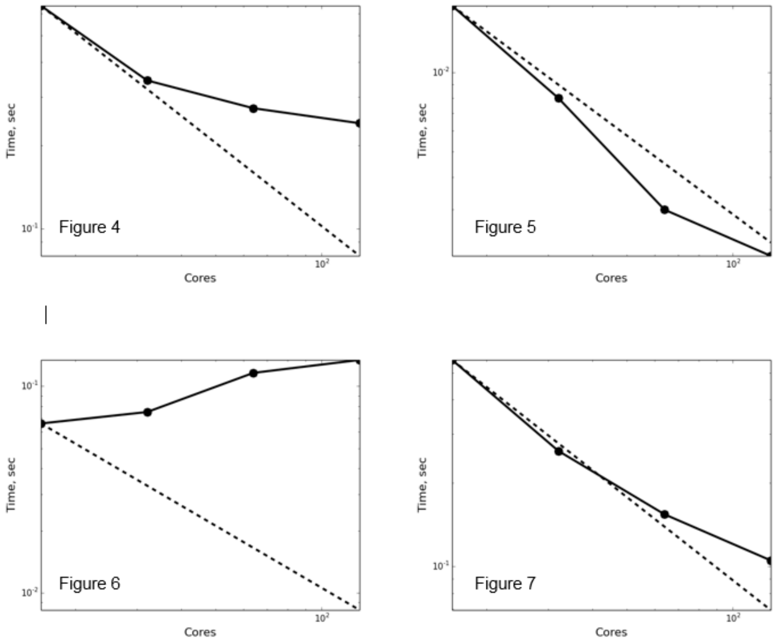


A Road Block!



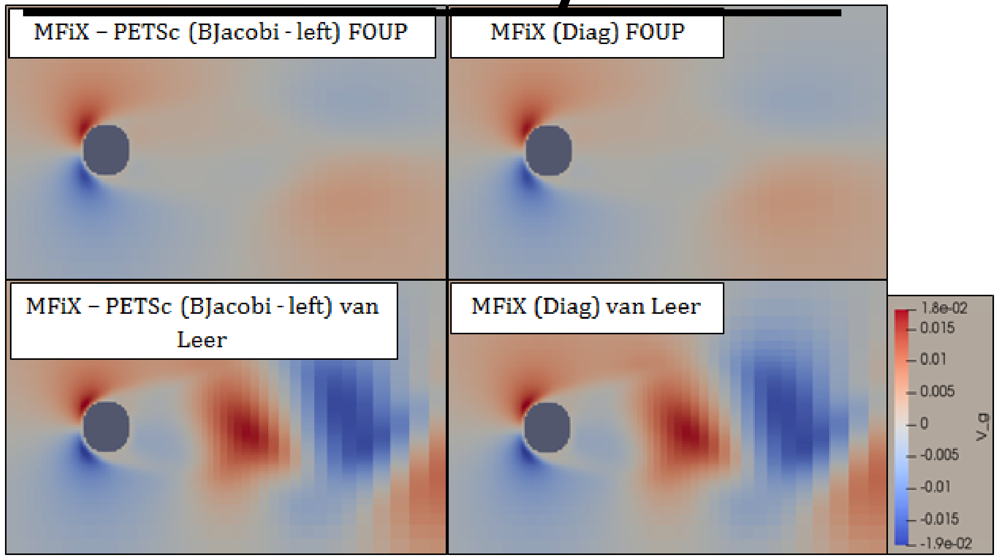
Asymmetry and the use of Conjugate Gradients

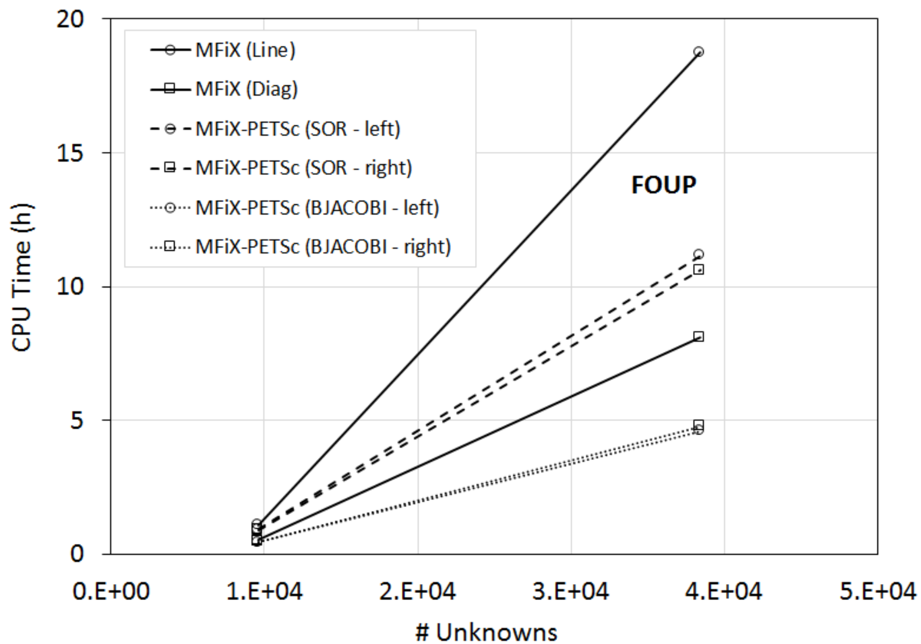


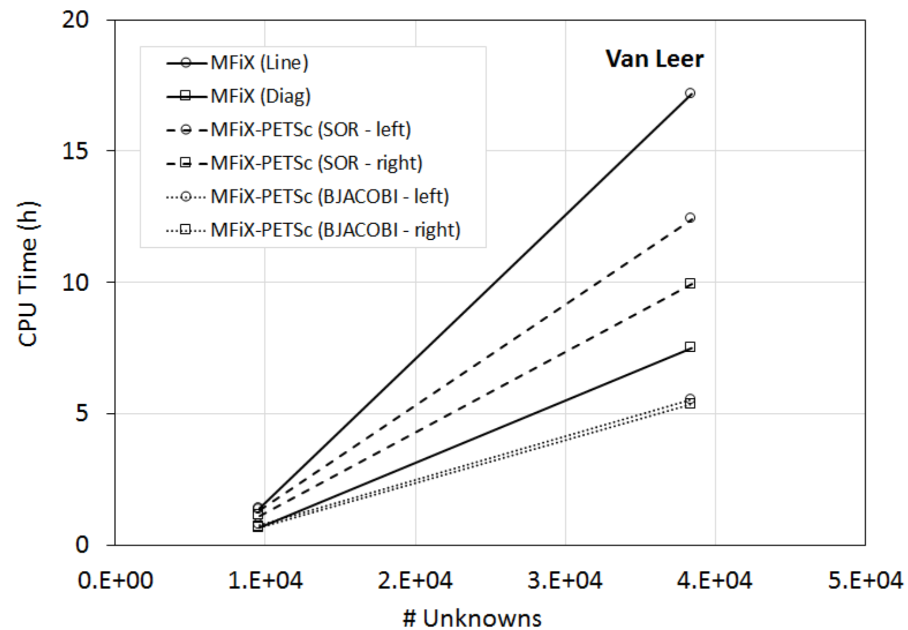


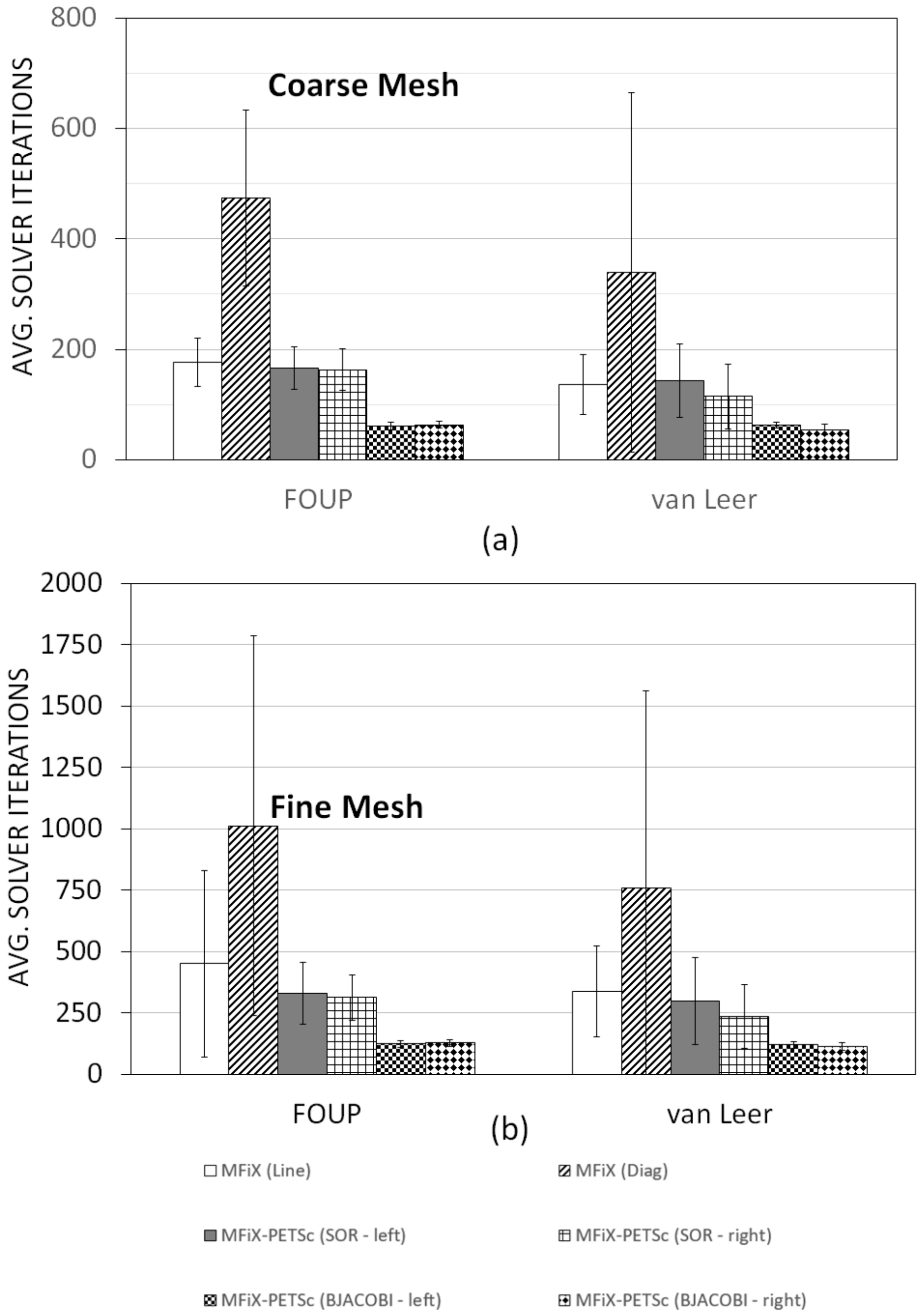
Figures 4 - 7: Plots of the (2) Total overall scaling (3) Matrix and vector object construction scaling (4) Solver object scaling and (5) BiCGStab scaling with an SMG preconditioner.

Flow Over Cylinder

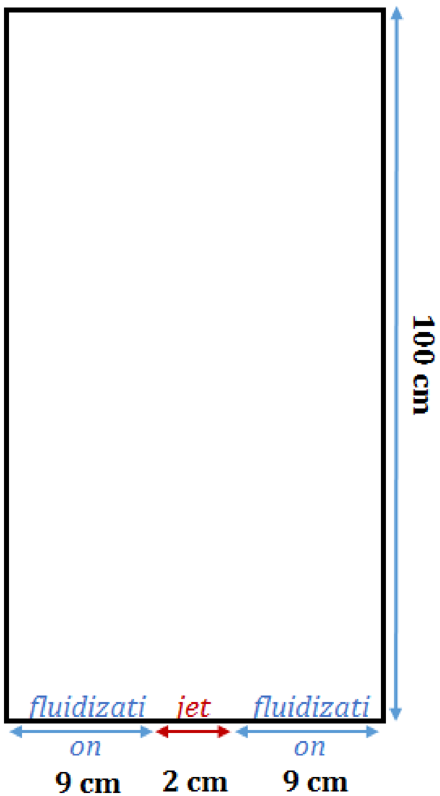




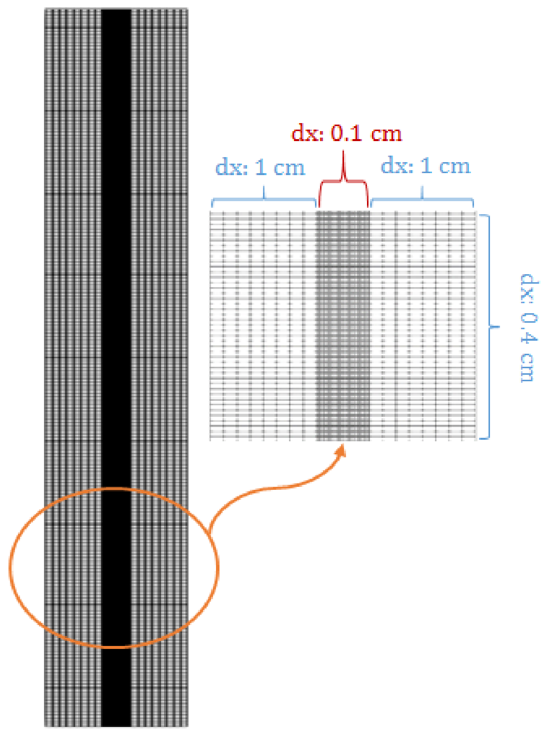




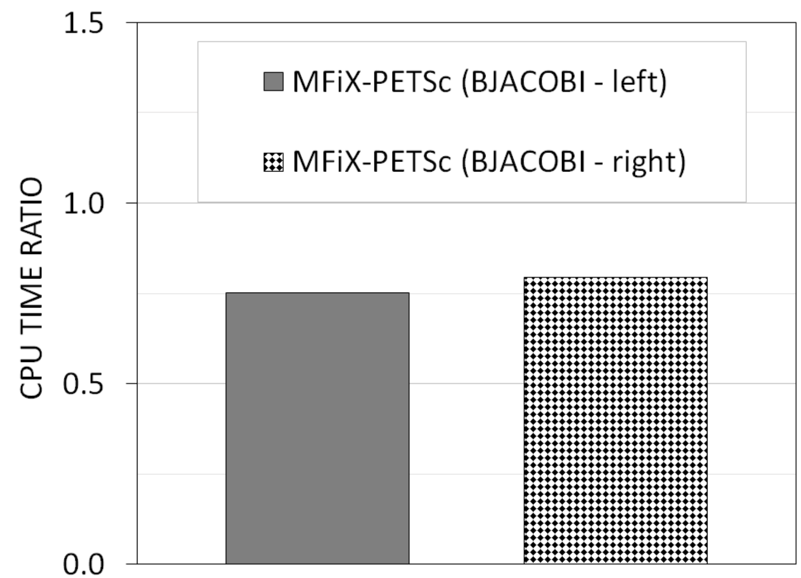
800
600
400
200
0
AVG. SOLVER ITERATIONS
Coarse Mesh
FOUP
van Leer
(a)
2000
1750
1500
1250
1000
750
500
250
0
AVG. SOLVER ITERATIONS
Fine Mesh
FOUP
van Leer
(b)
MFiX (Line)
MFiX (Diag)
MFiX-PETSc (SOR - left)
MFiX-PETSc (SOR - right)
MFiX-PETSc (BJACOBI - left)
MFiX-PETSc (BJACOBI - right)

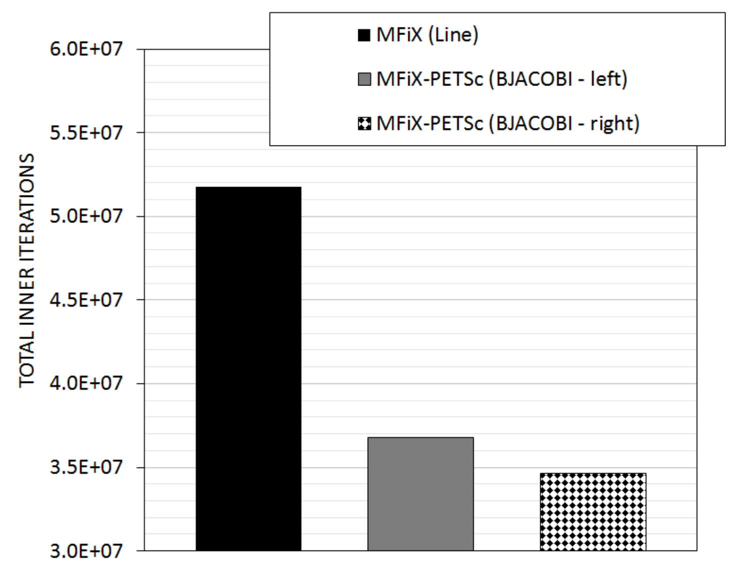

100 cm
fluidizati
on
9 cm
jet
2 cm
fluidizati
on
9 cm

(a)


dx: 0.1 cm
dx: 1 cm
dx: 1 cm
dx: 0.4 cm

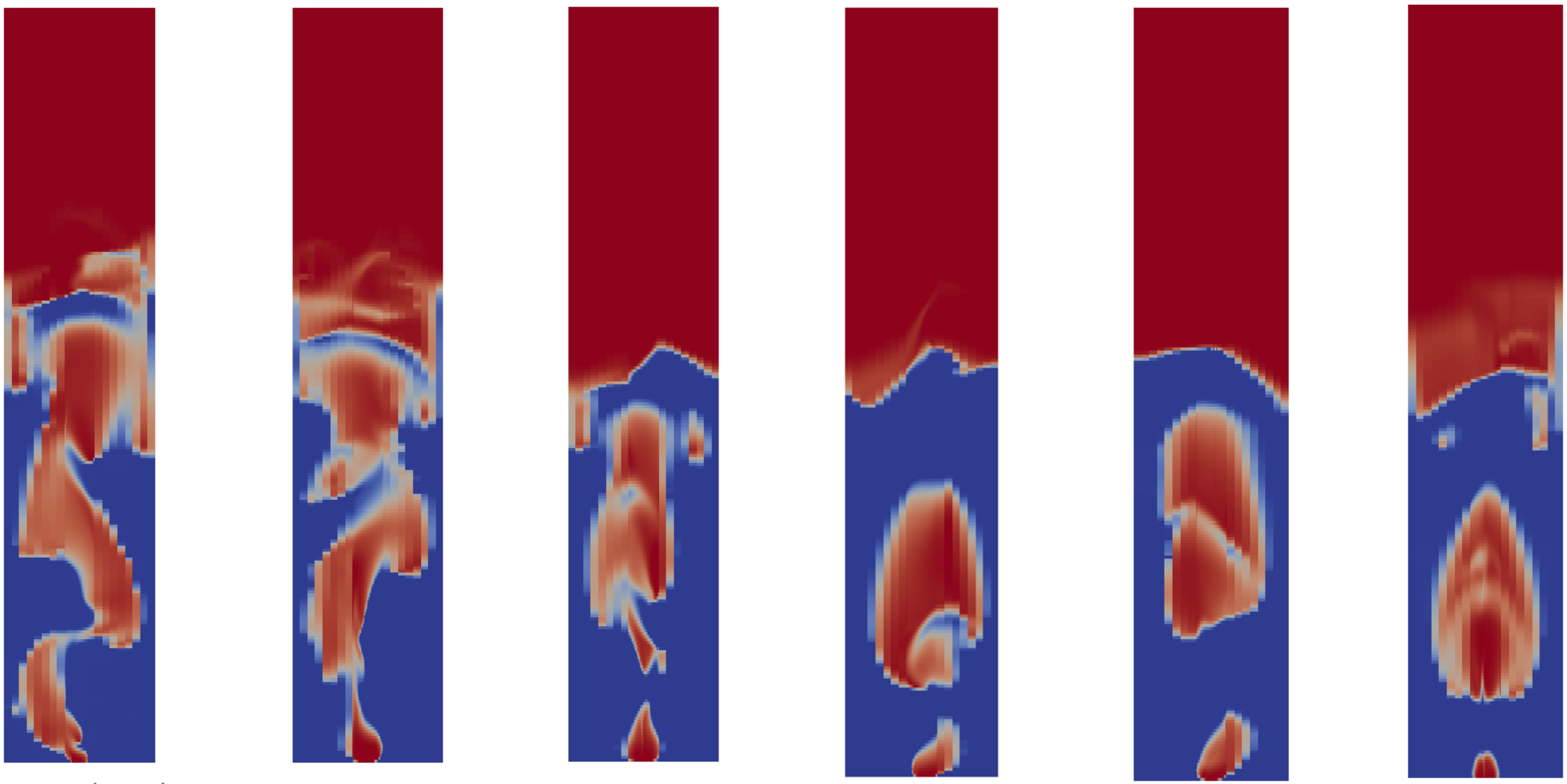
(b)


CPU TIME RATIO
1.5
1.0
0.5
0.0
MFiX-PETSc (BJACOBI - left)
MFiX-PETSc (BJACOBI - right)

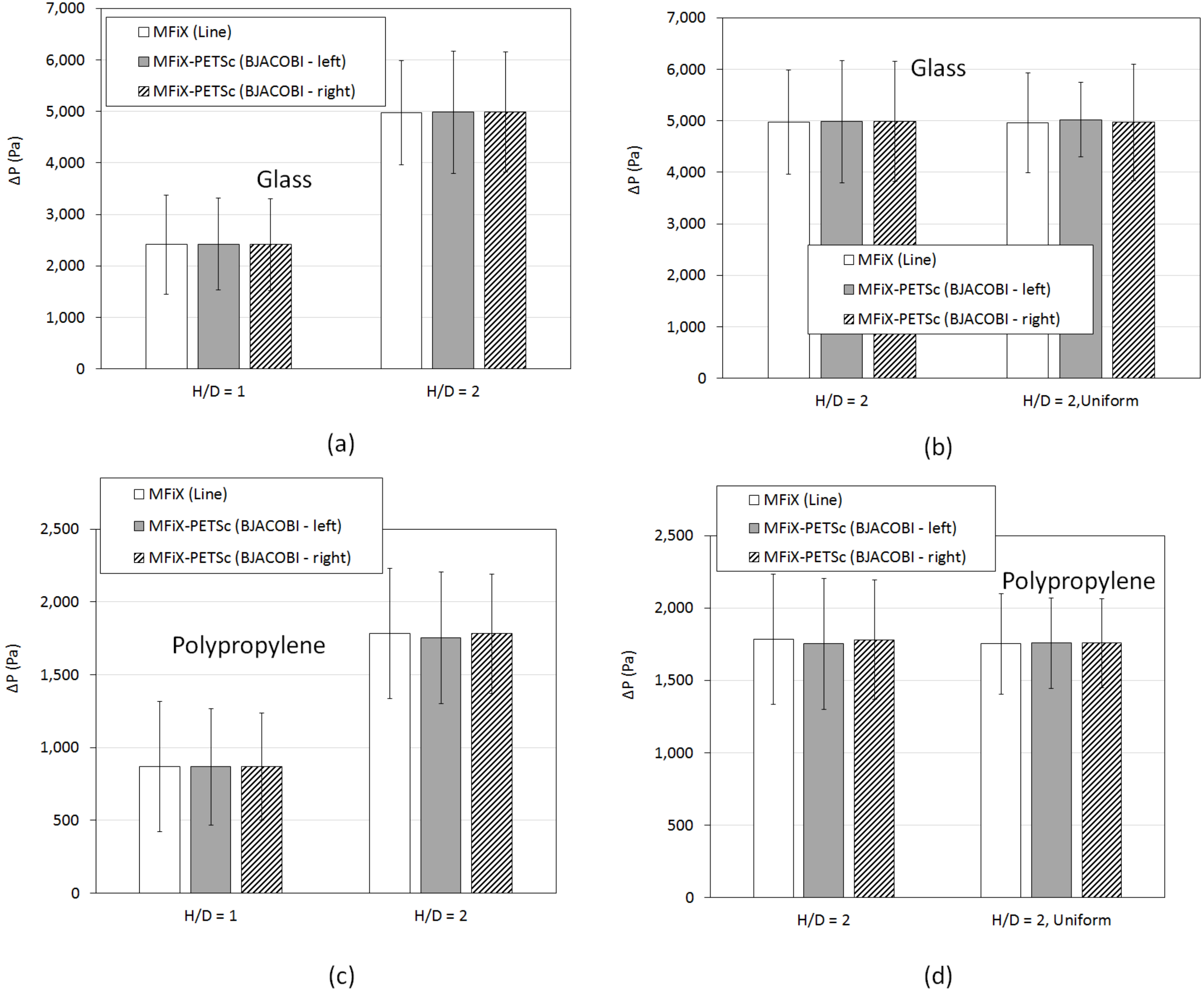

TOTAL INNER ITERATIONS
6.0E+07
5.5E+07
5.0E+07
4.5E+07
4.0E+07
3.5E+07
3.0E+07
MFiX (Line)
MFiX-PETSc (BJACOBI - left)
MFiX-PETSc (BJACOBI - right)

Polypropylene (Non-Uniform Grid, 2D, H/D = 2)

Glass (Non-Uniform Grid, 2D, H/D = 2)



MFiX (Line) | MFiX-PETSc (BJACOBI - Left) | MFiX-PETSc (BJACOBI - Right) | MFiX (Line) | MFiX-PETSc (BJACOBI - Left) | MFiX-PETSc (BJACOBI - Right)



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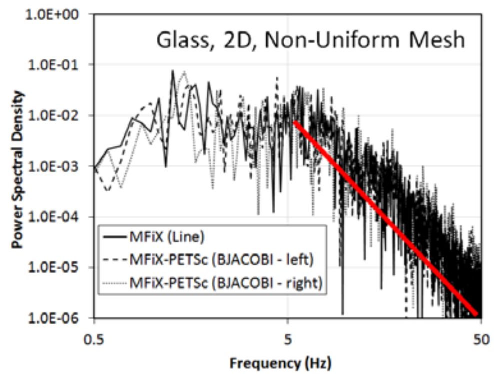
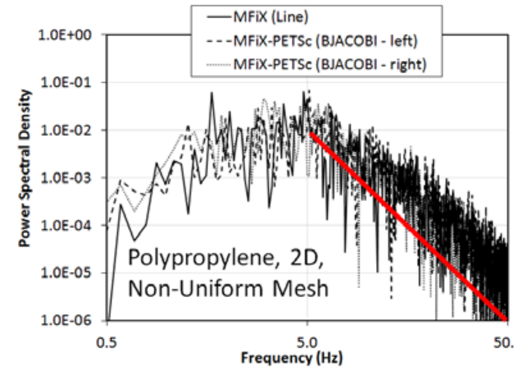
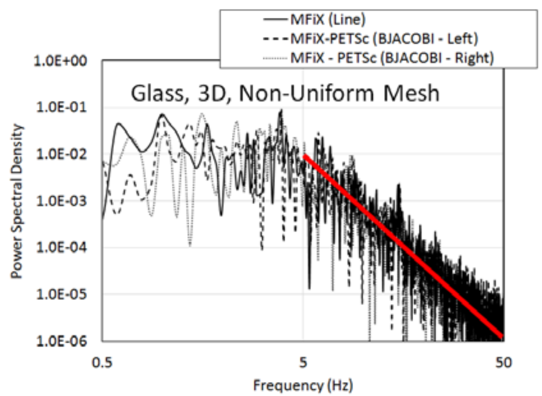


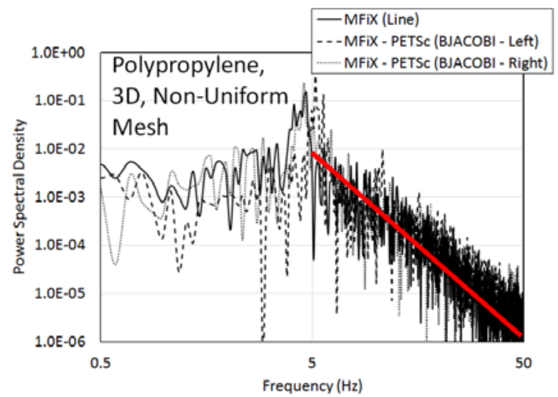
(a)



(b)

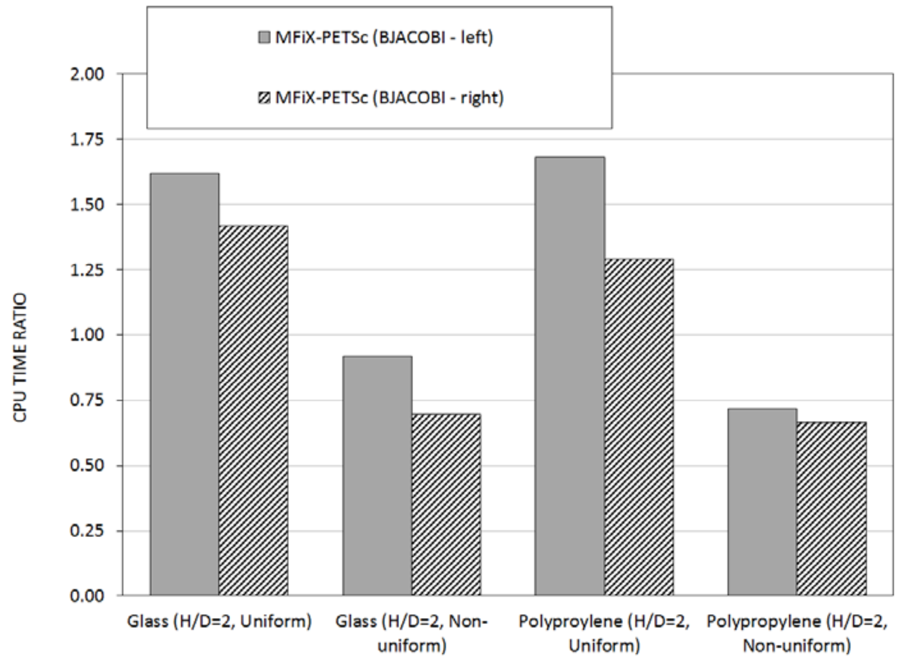


(c)



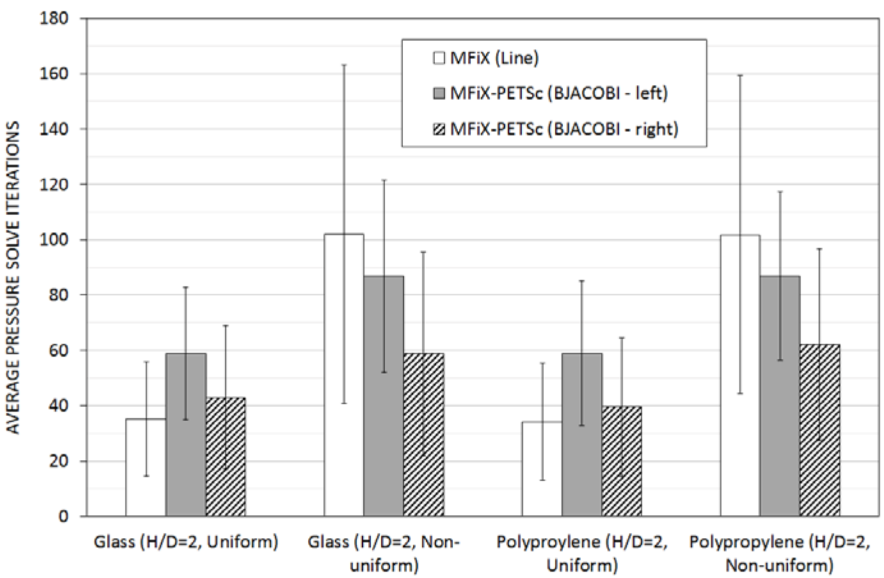
(d)

	Glass (H/D = 2)		PP (H/D = 2)	
Preconditioner	**2D, Non-Uniform**	**3D, Non-Uniform**	**2D, Non-Uniform**	**3D, Non-Uniform**
MFiX – line relaxation	1.3	3.8	4.8	4.7
MFiX-PETSc – BJACOBI (left)	1.3	3.9	5.0	5.2
MFiX PETSc – BJACOBI (right)	1.5	1.6	3.0	4.6



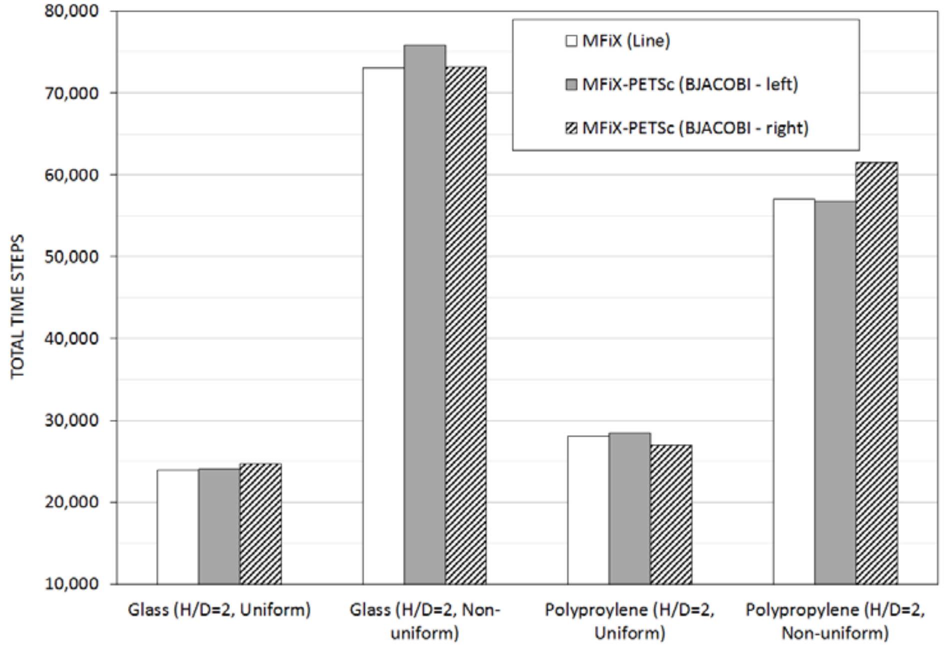
MFiX-PETSc (BJACOBI - left)
MFiX-PETSc (BJACOBI - right)
2.00
1.75
1.50
1.25
1.00
0.75
0.50
0.25
0.00
CPU TIME RATIO
Glass (H/D=2, Uniform)
Glass (H/D=2, Non-uniform)
Polyprolyene (H/D=2, Uniform)
Polypropylene (H/D=2, Non-uniform)

(a)



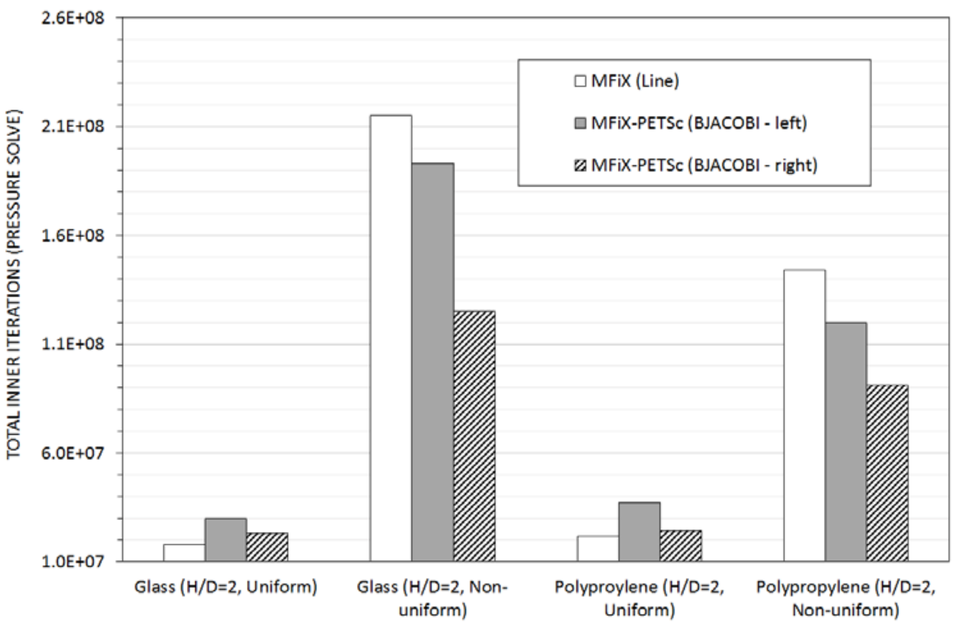
180
160
140
120
100
80
60
40
20
0
AVERAGE PRESSURE SOLVE ITERATIONS
MFiX (Line)
MFiX-PETSc (BJACOBI - left)
MFiX-PETSc (BJACOBI - right)
Glass (H/D=2, Uniform)
Glass (H/D=2, Non-uniform)
Polyprolyene (H/D=2, Uniform)
Polypropylene (H/D=2, Non-uniform)

(b)



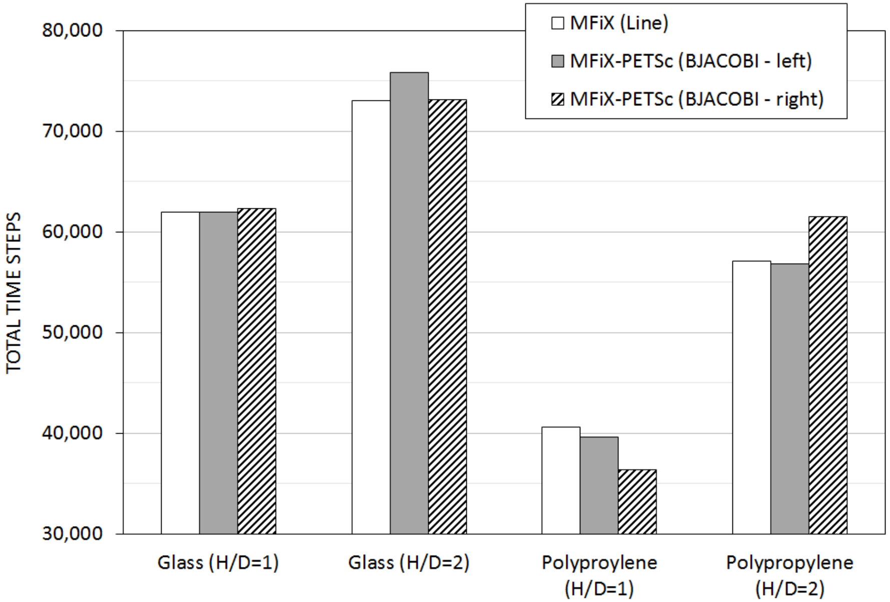
80,000
70,000
60,000
50,000
40,000
30,000
20,000
10,000
TOTAL TIME STEPS
MFiX (Line)
MFiX-PETSc (BJACOBI - left)
MFiX-PETSc (BJACOBI - right)
Glass (H/D=2, Uniform)
Glass (H/D=2, Non-uniform)
Polyproylene (H/D=2, Uniform)
Polypropylene (H/D=2, Non-uniform)

(a)



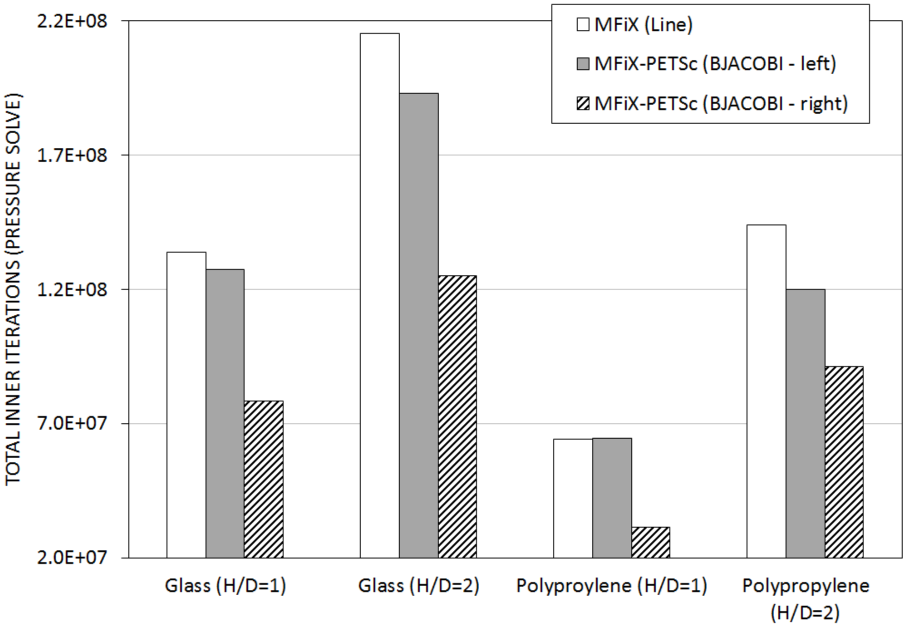
2.6E+08
2.1E+08
1.6E+08
1.1E+08
6.0E+07
1.0E+07
TOTAL INNER ITERATIONS (PRESSURE SOLVE)
MFiX (Line)
MFiX-PETSc (BJACOBI - left)
MFiX-PETSc (BJACOBI - right)
Glass (H/D=2, Uniform)
Glass (H/D=2, Non-uniform)
Polyproylene (H/D=2, Uniform)
Polypropylene (H/D=2, Non-uniform)

(b)



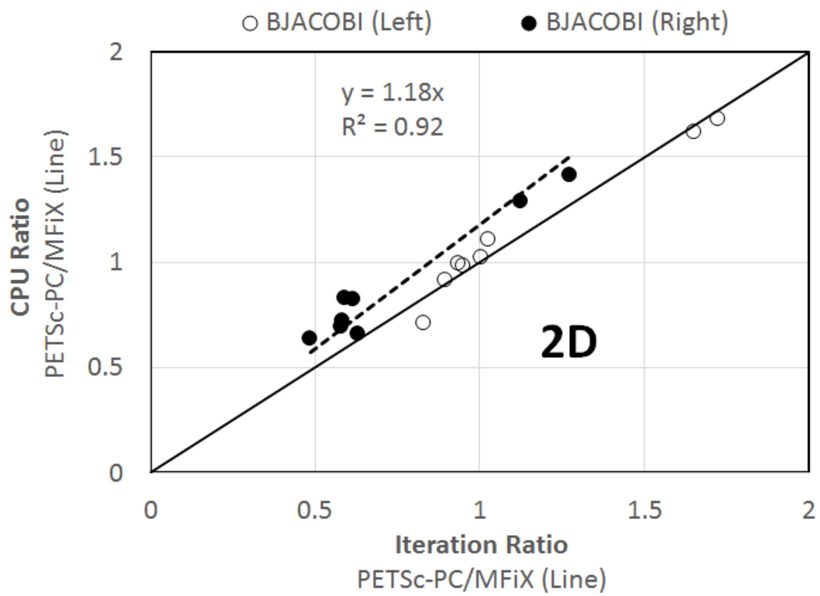
MFiX (Line)
MFiX-PETSc (BJACOBI - left)
MFiX-PETSc (BJACOBI - right)
TOTAL TIME STEPS
80,000
70,000
60,000
50,000
40,000
30,000
Glass (H/D=1)
Glass (H/D=2)
Polyproylene (H/D=1)
Polypropylene (H/D=2)

(a)



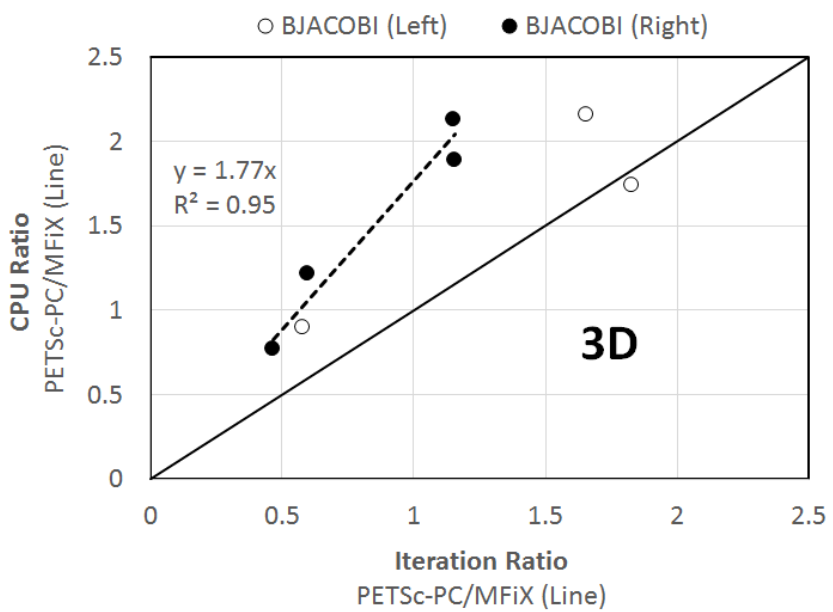
MFiX (Line)
MFiX-PETSc (BJACOBI - left)
MFiX-PETSc (BJACOBI - right)
TOTAL INNER ITERATIONS (PRESSURE SOLVE)
2.2E+08
1.7E+08
1.2E+08
7.0E+07
2.0E+07
Glass (H/D=1)
Glass (H/D=2)
Polyproylene (H/D=1)
Polypropylene (H/D=2)

(b)



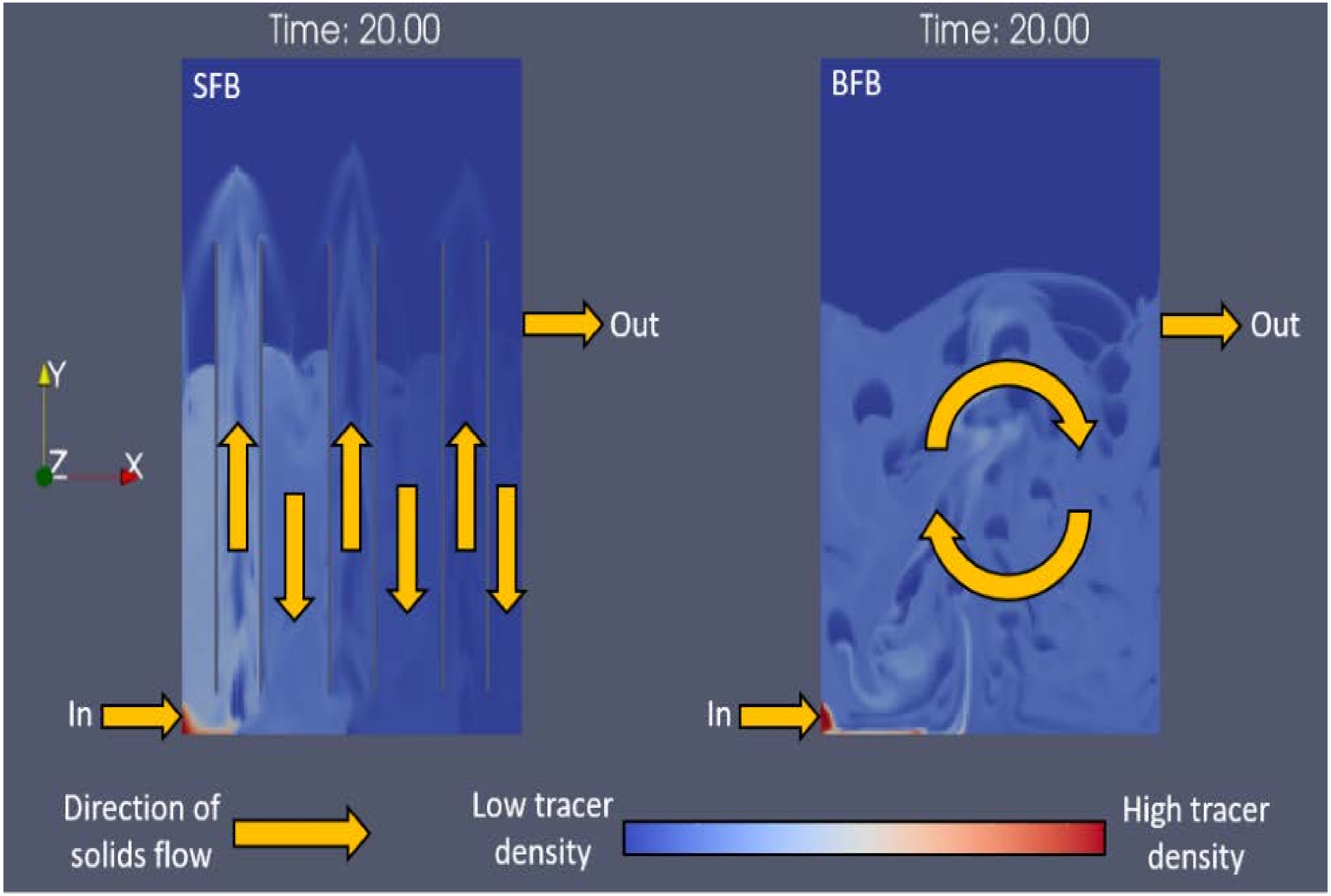
○ BJACOBI (Left)
● BJACOBI (Right)
y = 1.18x
R² = 0.92
2D
CPU Ratio
PETSc-PC/MFiX (Line)
Iteration Ratio
PETSc-PC/MFiX (Line)
0
0.5
1
1.5
2

(a)



○ BJACOBI (Left)
● BJACOBI (Right)
y = 1.77x
R² = 0.95
3D
CPU Ratio
PETSc-PC/MFiX (Line)
Iteration Ratio
PETSc-PC/MFiX (Line)
0
0.5
1
1.5
2
2.5

(b)



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Scalability

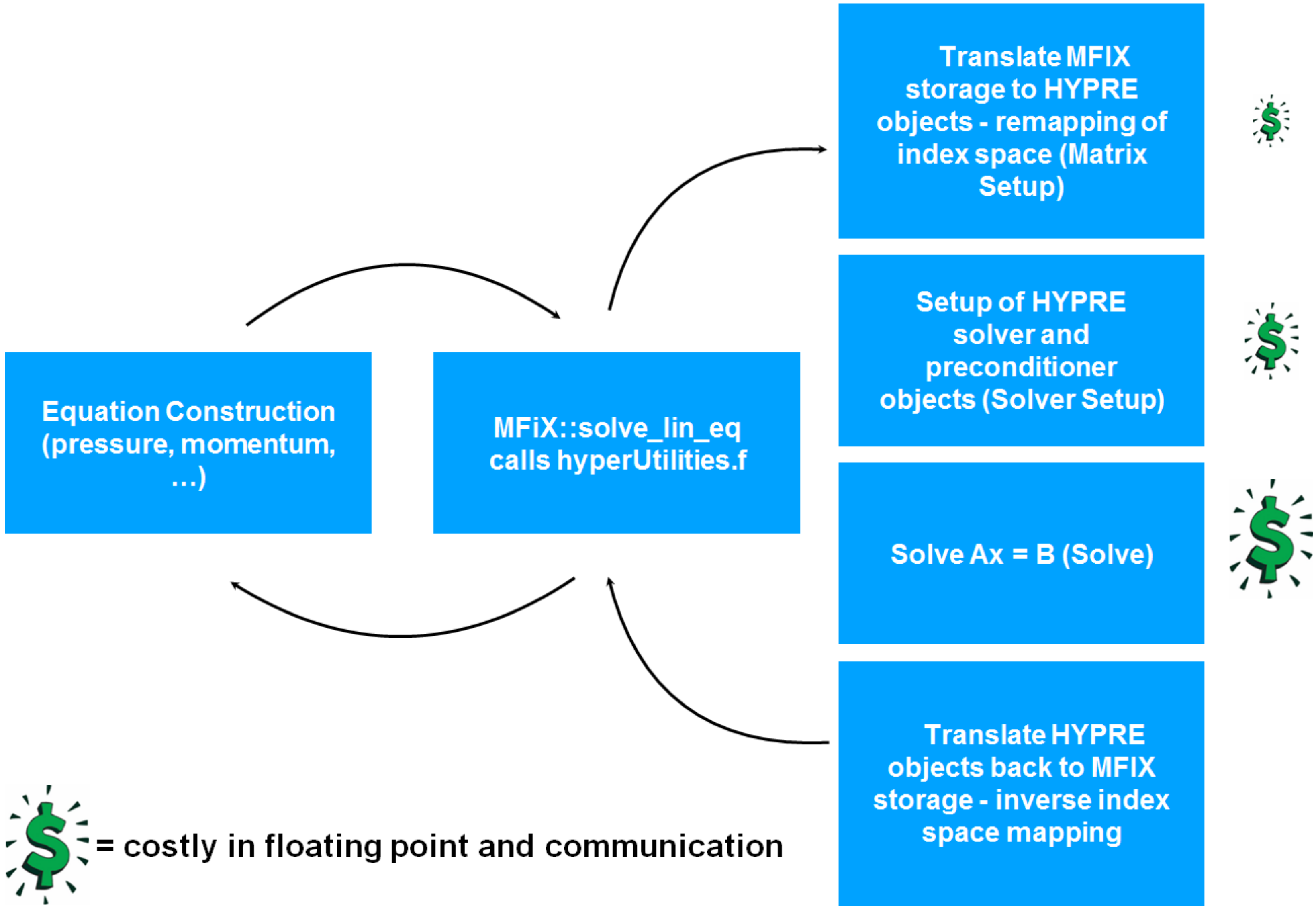
- Machine latency is a fixed cost - when computational work gets close or runs below this cost, parallel scalability (strong) breaks down
- Algorithmic decisions/design/methods contribute to scalability - some methods/algorithms (weak) scale better than others
- Multigrid solvers scales like O(n) whereas CG scales like $O(n^{1.5})$-$O(n^2)$
- Multigrid scalability has shown problem dependency

Method	Storage	Flops
GE(banded)	n^5	n^7
Gauss-Seidel	n^3	$n^5 \log n$
Optimal SOR	n^3	$n^4 \log n$
CG	n^3	$n^{3.5} \log n$
Full MG	n^3	n^3

To solve the Poisson problem in 3D ($N = n^3$)

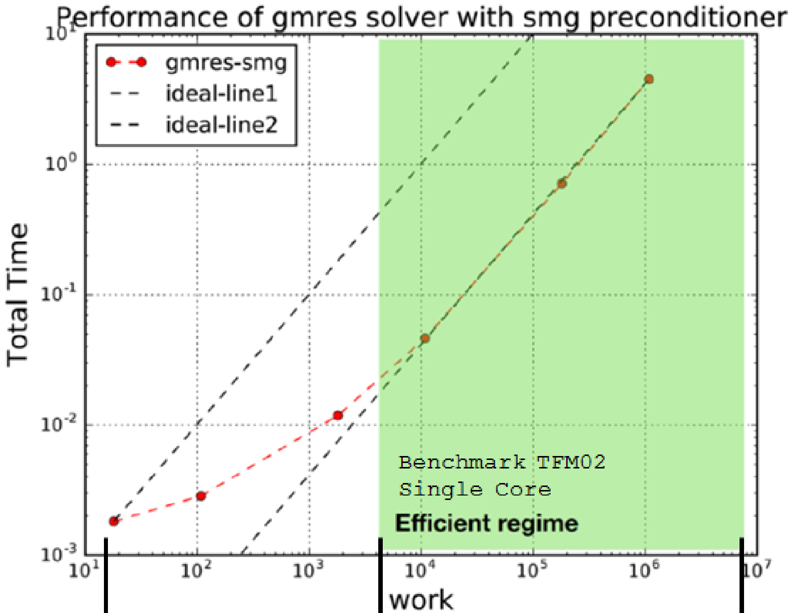
Source: Kab Seok Kang, GIST HPC Summer school 2015

Modified “inner solve” - MFIX coupled with HYPRE



HYPRE Scaling in MFiX

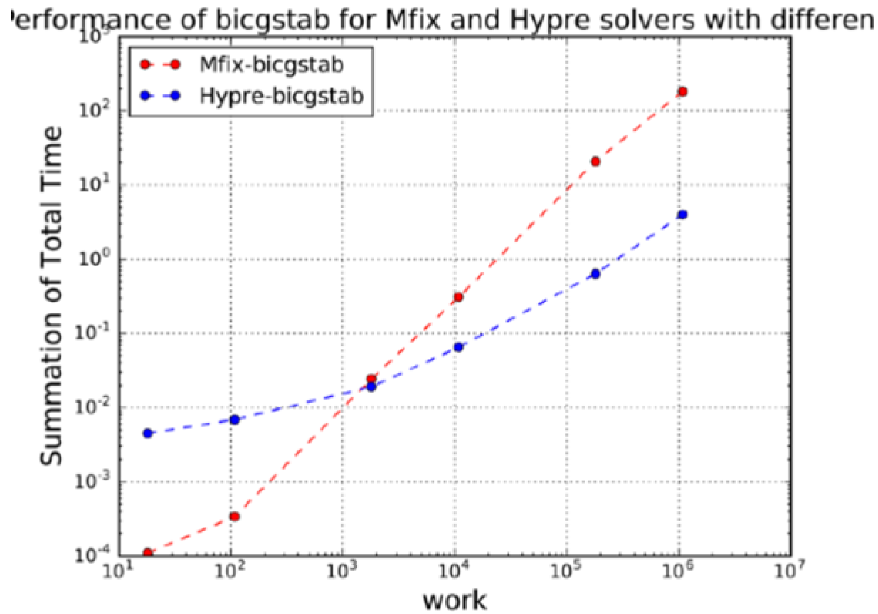
HYPRE Solver and Matrix setup costs must be overcome with enough work



*for this problem

setup cost dominates

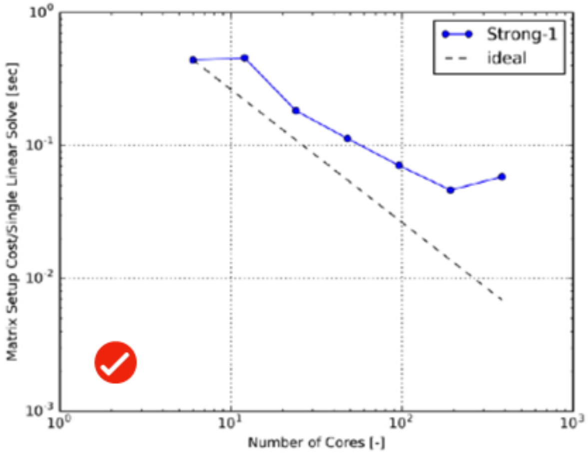
scaling like O(n)



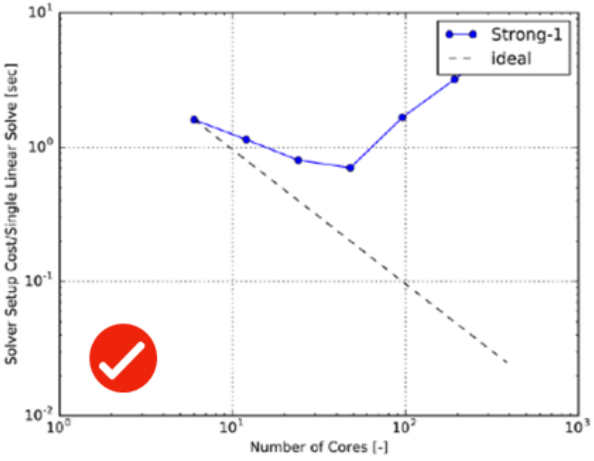
Comparison with MFiX on a single core

Where is the HYPRE overhead?

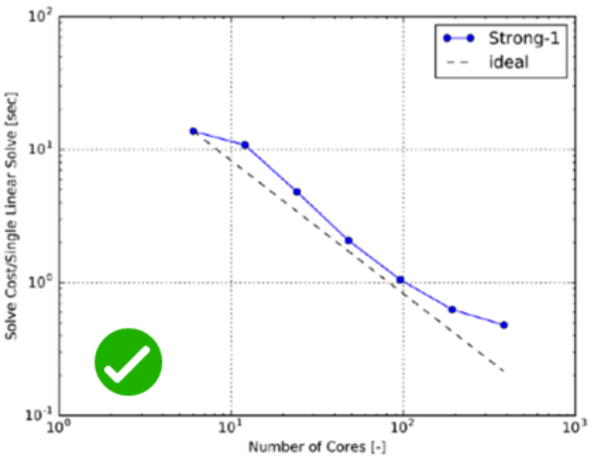
Matrix Setup



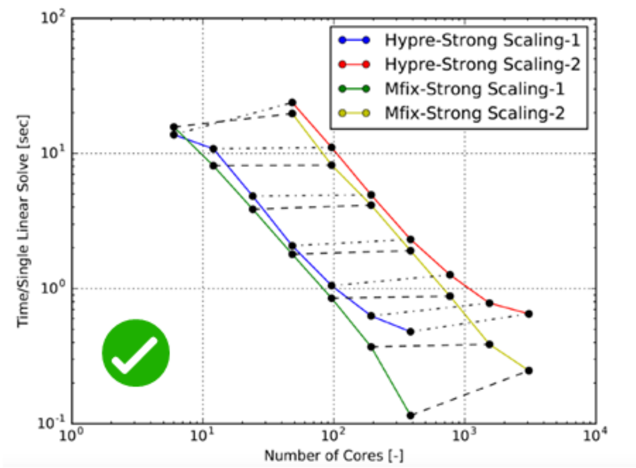
Solver Setup



Actual Solve



Actual Solve - strong and weak scaling



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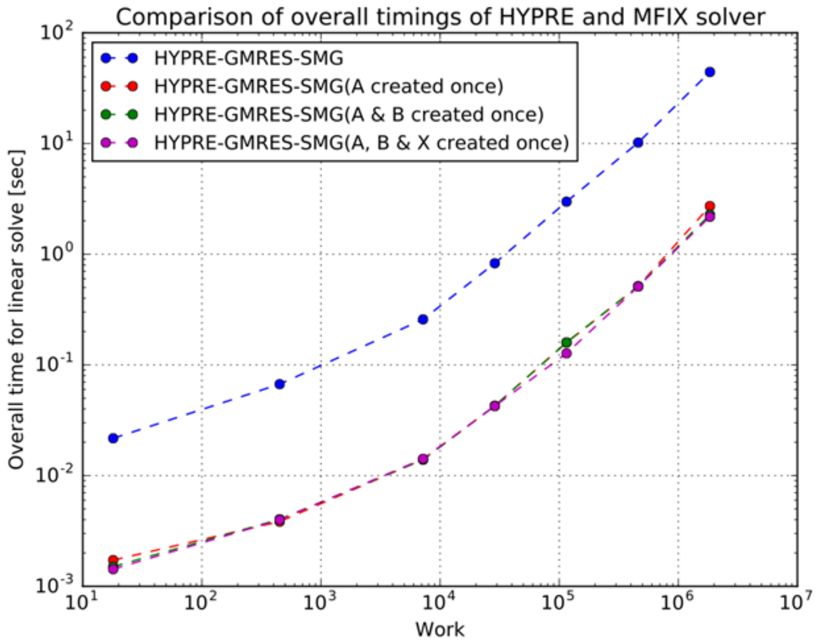
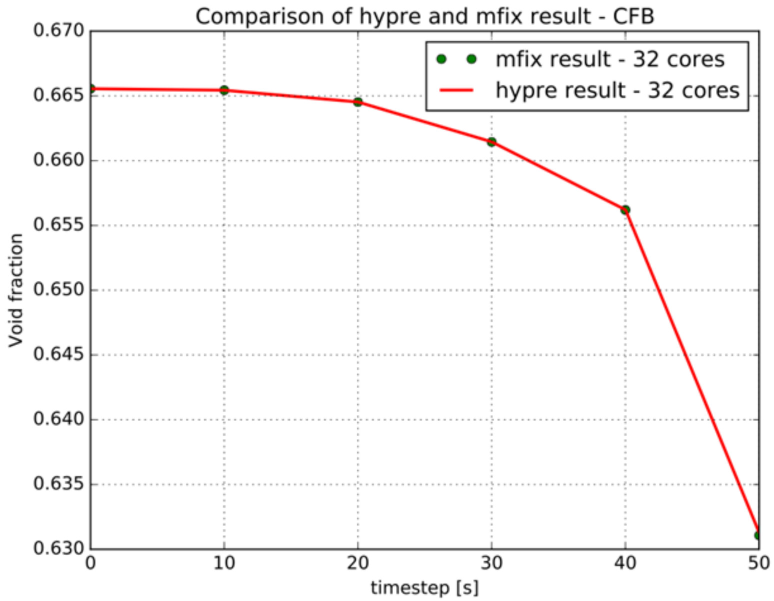
Setup Cost Mitigation

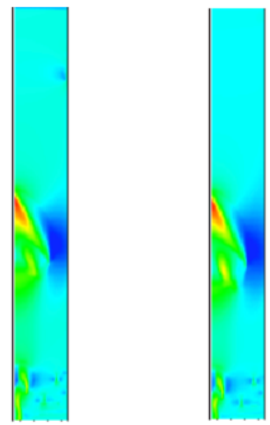
- Can setup costs be mitigated by:
  - reusing the solver/matrix objects every iteration?
  - over the lifetime of the simulation?



- Reuse of matrix objects shows same scaling behavior with a reduction in time
- Reuse of solver objects was met with memory leaks and other issues - still needs investigation
- Solver object problems could be due to underlying communication requirements in HYPRE for Struct interface
- For the Hypre-Struct interface, no solver reinitialize option was available (as opposed to other interfaces, e.g. IJ-Interface)

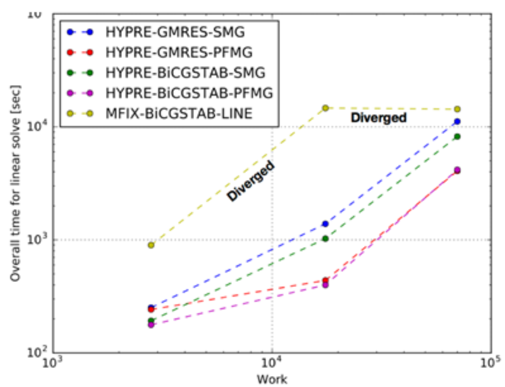
Fluidized Bed Problem





HYPRE **MFIX**

Solid volume fraction after some time



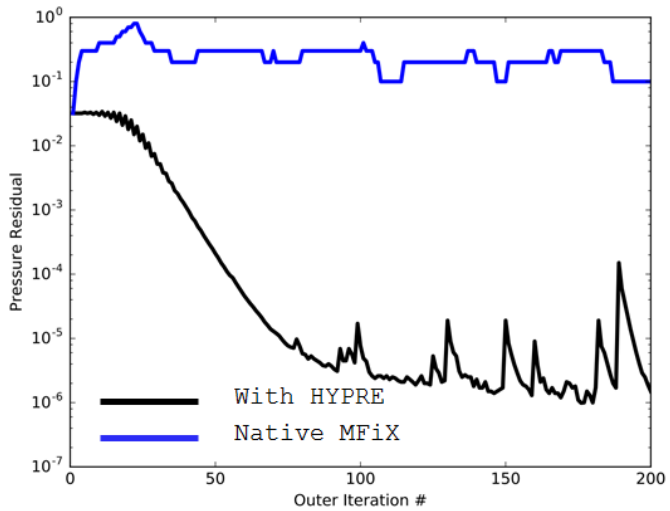
- Initial apple-to-apples comparison (same solver tolerance, max iterations)
- MFiX native solver diverged while HYPRE converged
- PFMG preconditioner consistently offers better performance (well known)

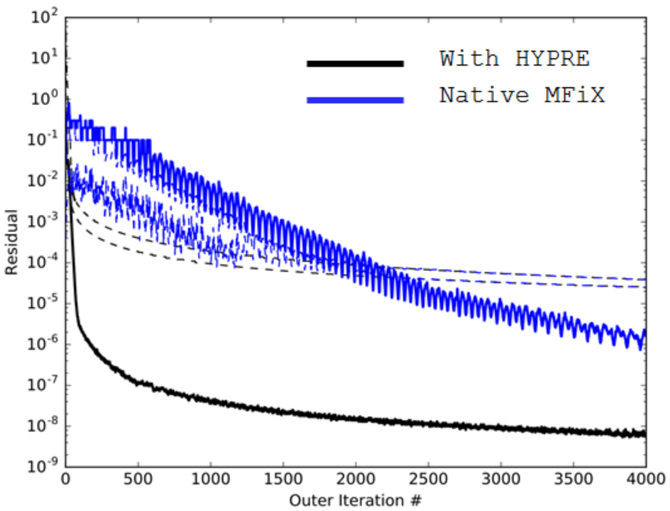
Outer Solve Parameters Impact on Efficiency

Can HYPRE inner solver robustness be exploited?

`Benchmark TFM03 Multiple Cores`

`Pressure Convergence with high outer relaxation factors`





- HYPRE appears to support higher relaxation factors (it converges) for the outer solve
- Stalling or slow/noisy convergence seen with MFiX native solver with higher relaxation factors

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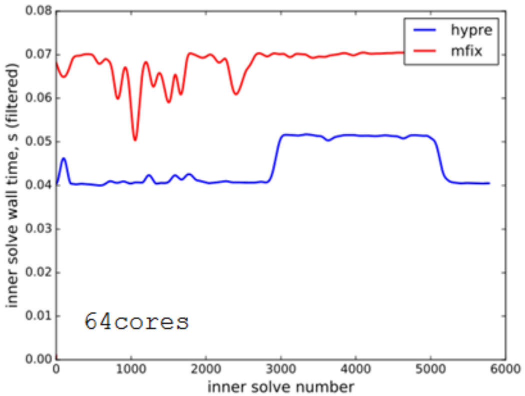
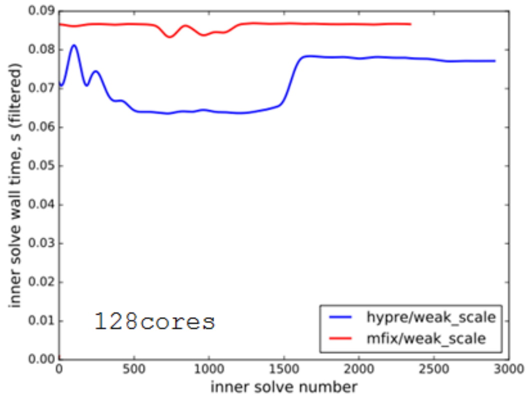
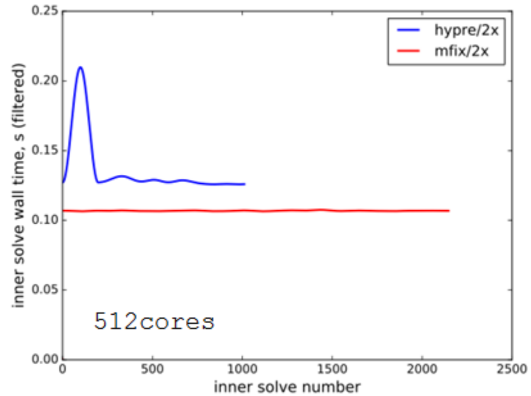
Challenge Problem: Flow over a tube bank

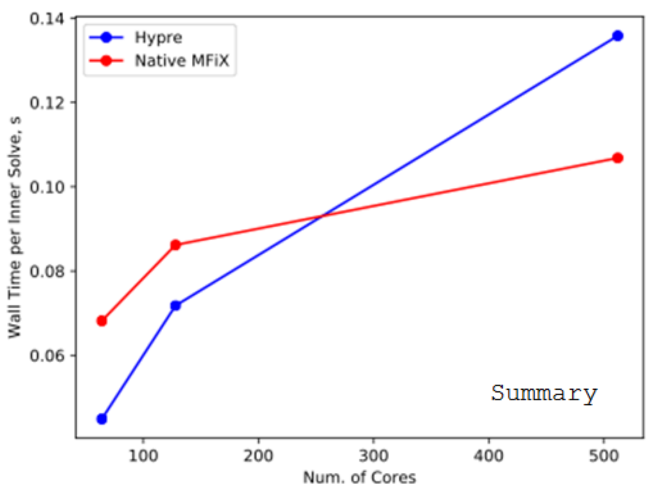
Same Workload per Core







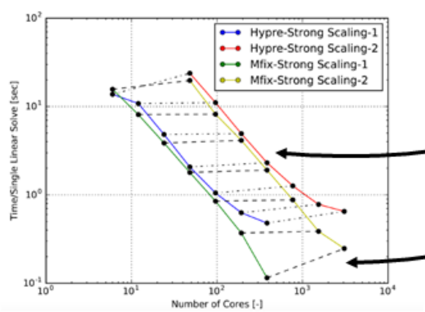
Increasing problem size -> -> ->



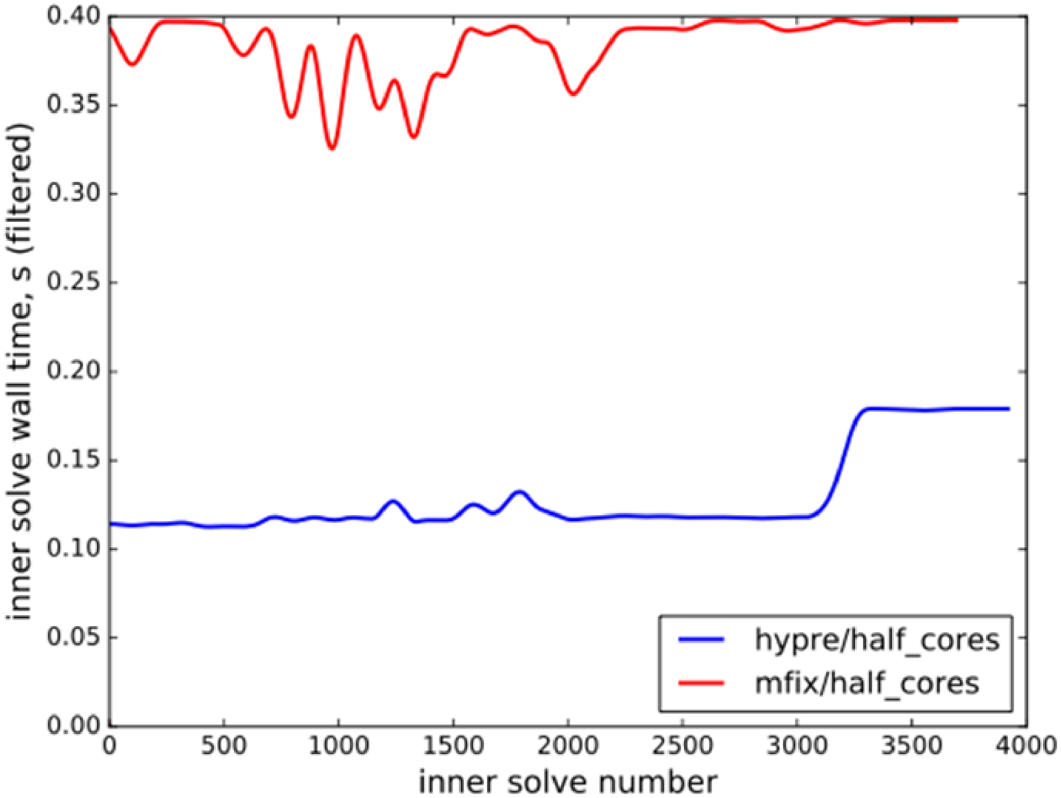
- Workload/Core O(10^4)
- Promising at lower core counts
- Should repeat with more workload/core

should be here

was here



Challenge Problem: Flow over a tube bank



- 5X more work/core
- ~3.5-2.5X speedup
- Needs more work, further study