



High Fidelity Computational Model for Fluidized Bed Experiments

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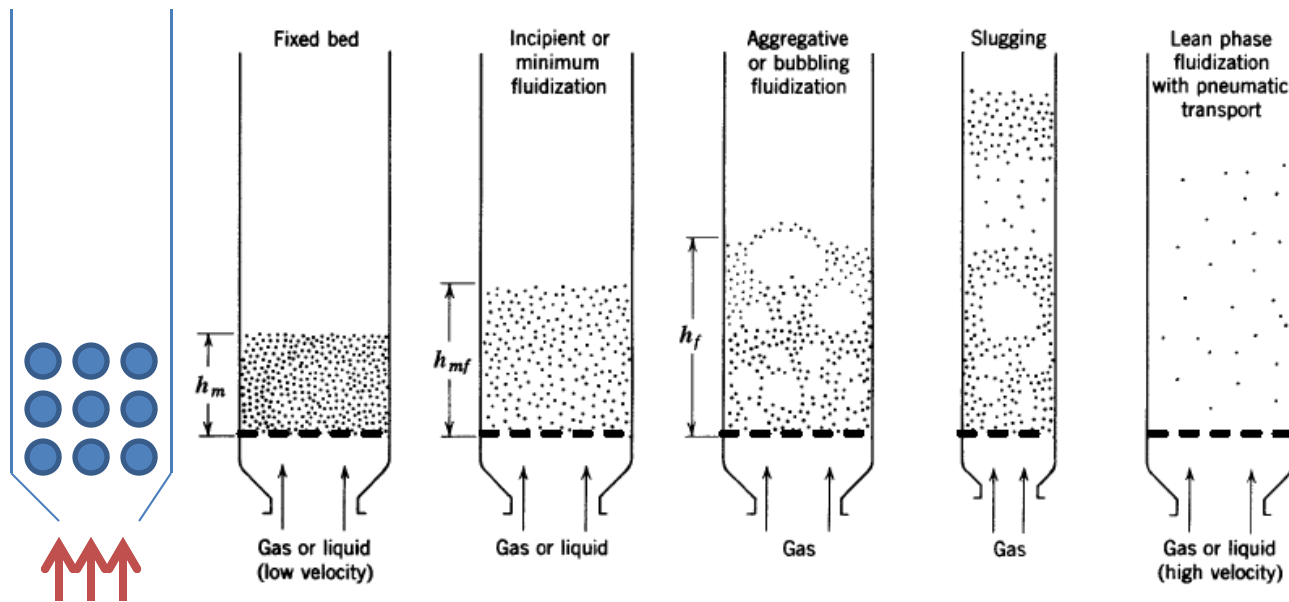
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Outline

- Background
- Goals and Objectives
- Project tasks, milestones, and schedule
- Technical approach
- Project status – results and discussions
- Accomplishments
- Concluding remarks

Fluidized Bed Reactor

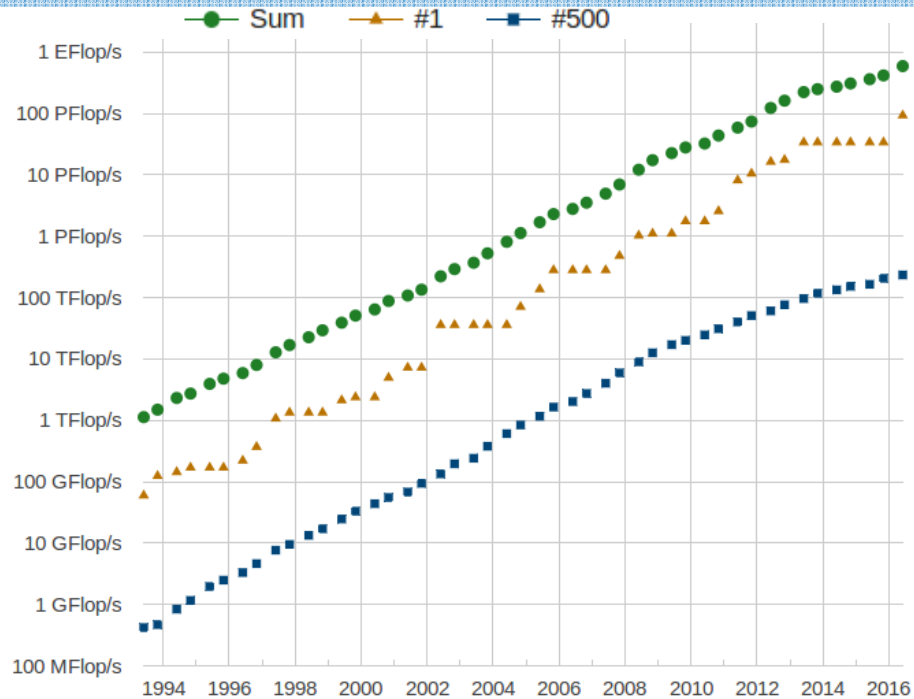


- Governing dynamics is very complicated.
- Multiple phases, interaction between particles and fluid, varying sizes of the particles makes it very difficult to predict the behavior of the bed.

The arrival time of a space probe traveling to Saturn can be predicted more accurately than the behavior of a fluidized bed chemical reactor! (Geldart, 1986)

- Greater surface area of contact for fluid and solid allowing for better mixing.
- Applications in process industry and nuclear engineering

Supercomputers



<https://www.top500.org/>

Cray X1
3 TF
2004

Cray XT3
Single-core
26 TF
2005

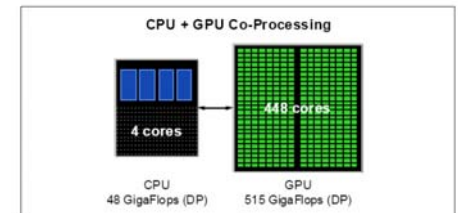
Cray XT3
Dual-core
54 TF
2006

Cray XT4
119 TF
2007

Cray XT4
Quad-core
263 TF
2008

Cray "Baker"
6-core, dual-socket SMP
~1000 TF
100TB, 2.5PB
2009

CRAY	NUDT
AMD Opteron	Intel Phi
Nvidia Tesla	54 TF
20 PF	2015



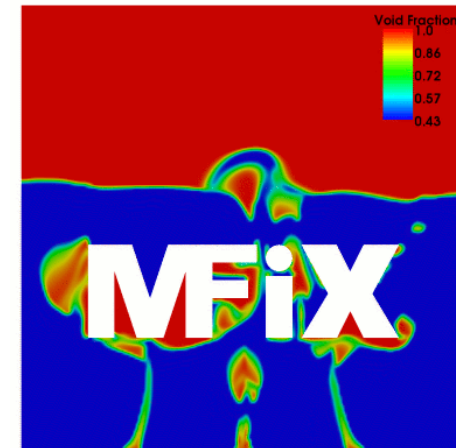
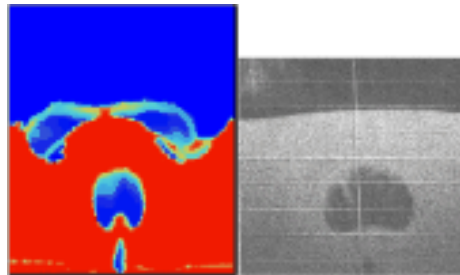
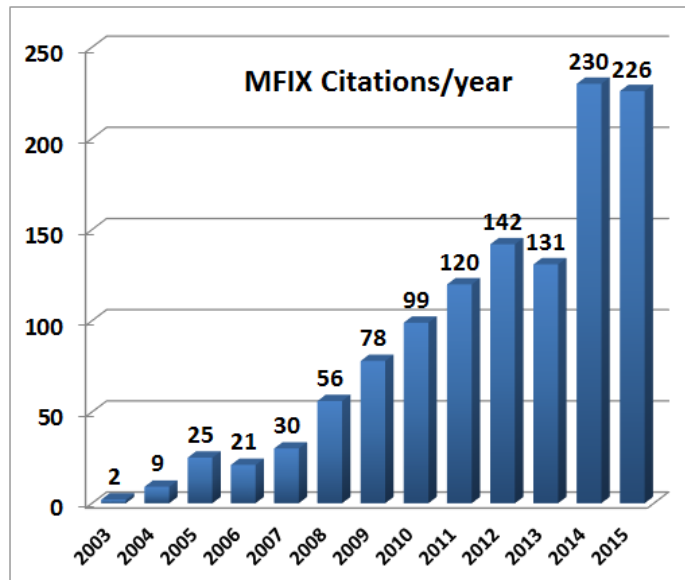
Multiphase **F**low with **I**nterphase **eX**change

The Multiphase Flow with Interphase eXchanges (MFiX) software package is

- a multiphase Computational Fluid Dynamics (CFD) software
- developed by NETL (Open-source)
- a legacy code written in Fortran

Multiphase Flow with Interphase eXchange (MFiX)

- CFD code for modeling reacting multiphase systems.
- 30 years of development history with a wide range of customers.
- Successfully modeling the complexity of fluidized bed reactor flow.



mfix.netl.doe.gov

•40% of value added by the U.S chemical industry is related to particle technology- Ennis et al. Chem Eng .Progress 1994.

•Scale up of fluidized beds is a daunting task- Knowlton et al. Powder technology, 2005.

Multiphase Flow with Interphase eXchange (MFiX)

Gas-solids are addressed by solving

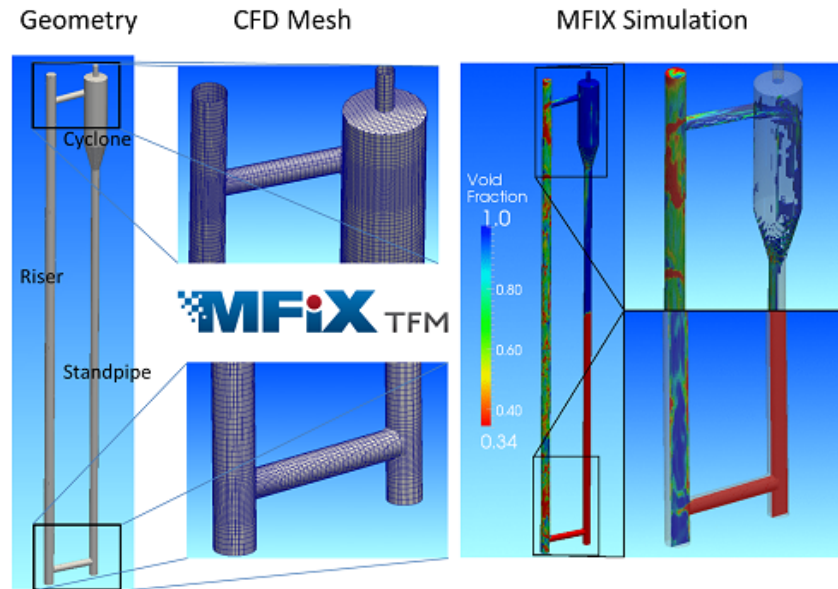
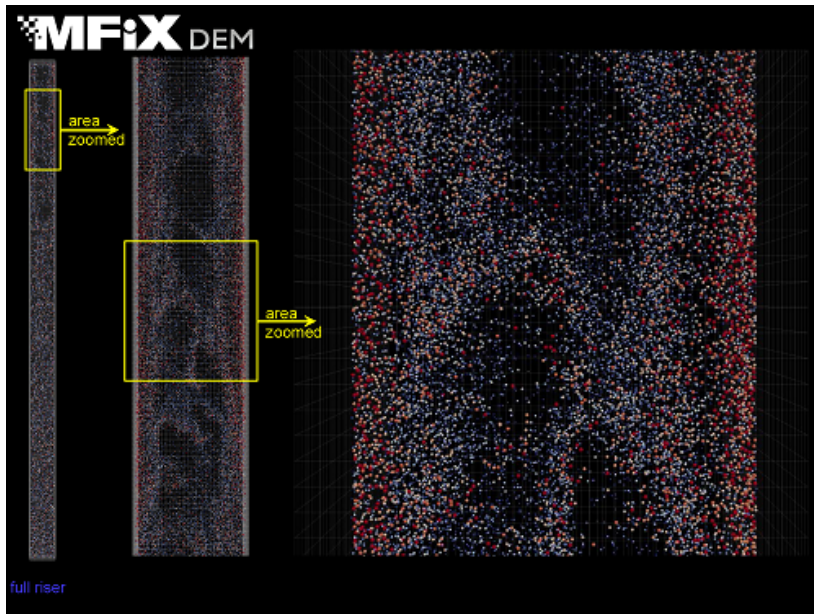
- coupled continuity
- momentum conservation
- energy equations, and
- parameterizing many effects such
 - drag force, buoyancy,
 - virtual mass effect,
 - lift force,
 - Magnus force,
 - Basset force,
 - Faxen force, etc.

Provides a suite of models that treat the carrier phase (gas phase) and disperse phase (solids phase) differently.

- MFiX-TFM (Two-Fluid Model)
- MFiX-DEM (Discrete Element Model)
- MFiX-PIC (Multiphase Particle in Cell)

In nutshell, though MFiX is widely used by the fossil fuel reactor communities to model and understand the multiphase physics in a circulating fluidized, its overall utility of the multiphase models remains **limited** due to the **computational expense** of large scale simulations. The time-to-solution however can be reduced by **leveraging** state-of-the-art **preconditions and linear solver libraries** where majority of processor-level time is spent in solving large systems of linearized equations.

Challenges with MFiX



$$\frac{\partial}{\partial t} (\varepsilon_g \rho_g) + \nabla \cdot (\varepsilon_g \rho_g \vec{v}_g) = \sum_{n=1}^{N_g} R_{gn}$$

$$\frac{\partial}{\partial t} (\varepsilon_g \rho_g \vec{v}_g) + \nabla \cdot (\varepsilon_g \rho_g \vec{v}_g \vec{v}_g) = \nabla \cdot \bar{S}_g + \varepsilon_g \rho_g \vec{g} - \sum_{m=1}^M \bar{I}_{gm} + \bar{f}_g$$

$$\frac{\partial}{\partial t} (\varepsilon_{sm} \rho_{sm}) + \nabla \cdot (\varepsilon_{sm} \rho_{sm} \vec{v}_{sm}) = \sum_{n=1}^{N_{sm}} R_{smn}$$

$$A x = B$$

- Poor Convergence, especially in complex non-linear problems.
- Increased number of Iterations as a result of poor convergence.
- Basic preconditioners.
- Not as scalable as one would like.

Technical goal

The technical goal of this project is to develop, validate and implement **advanced linear solvers** to replace the **existing linear solvers** that are used by the National Energy Technology Laboratory's (NETL) open source software package Multiphase Flow with Interphase eXchanges (**MFIX**). This goal will be achieved by integrating **Trilinos**, a publicly available open-source linear equation solver library developed by **Sandia** National Laboratory. The project will **demonstrate scalability** of the Trilinos- MFIX interface on various high-performance computing (HPC) facilities including the ones funded by the Department of Energy (DOE).

The expected results of the project will be **reduction of computational time** when solving complex gas-solid flow and reaction problems in MFIX, and reduction in time and cost of adding new algorithms and physics based models into MFIX

Objectives

- Create a framework to integrate the existing MFIX linear solver with Trilinos linear solver packages,
- Evaluate the performance of the state-of-the-art preconditions and linear solver libraries in Trilinos with MFIX, and
- Test three dimensional (3D) MFIX suites of problems on massively parallel computers with and without GPU acceleration.

Proposed Tasks and subtasks

Tasks

Task 1.0 – Project Management and Planning

Task 2.0 – Assembly of Optimum Trilinos Linear Equation Package for Integration with MFIX

Subtask 2.1: Setup a GIT/version-control repository

Subtask 2.2: Select the optimum Trilinos software package

Subtask 2.3: Develop a ForTrilinos based Fortran interface for MFIX

Task 3.0 – Performance Evaluation of Preconditions and Linear Solver Libraries

Subtask 3.1: Test and compare the linear equation solver packages in Trilinos

Subtask 3.2: Perform a scalability analysis of Trilinos-MFIX

Subtask 3.3: Improve performance of Trilinos-MFIX

Task 4.0 – Performance Evaluation of MFIX with the Trilinos Linear Solver on Massively Parallel Computers

Subtask 4.1: Secure computational time on massively parallel computers

Subtask 4.2: Compile Trilinos-MFIX on the selected massively parallel computer(s)

Subtask 4.3: Run simulations of a fluidized bed test problems with various particle sizes and shapes

Project milestones, budget and schedule

	Title	Description	Related task or subtask	Expected Completion Date	Success Criteria
Budget Year 1:					
Milestone 1.1	GIT repository setup completed	Setup GIT/version-control repository for Trilinos MFIX	Subtask 2.1	Q1	A working repository tested by at least three researchers
Milestone 1.2	Best Trilinos linear solver package decided	Choose the best Trilinos linear solver package for MFIX	Subtask 2.2	Q2	Source code for the decided package uploaded to the GIT repository
Milestone 1.3	Fortran interface for Trilinos MFIX created	Develop Fortran interface for the Trilinos linear solver to communicate with MFIX	Subtask 2.3	Q3-4	A working version of the Fortran interface uploaded
Budget Year 2:					
Milestone 2.1	>30% Linear solved speedup achieved	Test the linear solvers for its performance	Subtask 3.1	Q5	20% or better linear solver speedup achieved
Milestone 2.2	Scalability issues identified	Perform scalability analysis of Trilinos-MFIX	Subtask 3.2	Q6	Scalability testing for up to 1024 cores performed
Milestone 2.3	Bottlenecks to scalability identified and removed	Perform code profiling and identify bottlenecks	Subtask 3.3	Q7-8	Code profiling on Trilinos profiler completed and bottlenecks addressed for one HPC system
Budget Year 3:					
Milestone 3.1	Trilinos MFIX compiled on various OS/architectures	Compile Trilinos-MFIX on various cloud/HPC computers	Subtask 4.3	Q9	Trilinos MFIX compiled on 3 HPC (UTEP, DOE-Sandia, and one more)
Milestone 3.2	MFIX tests suites completed	Run simulations with various particle sizes and shapes of fluidized bed riser test problems	Subtask 4.3	Q10	All 2D runs and one 3D tests validated
Milestone 3.2	Trilinos MFIX performance analysis completed	Analyze Trilinos-MFIX performance for various computing architectures and fluidized-test problems	Subtask 4.3	Q11-12	Report submitted

Project schedule

Task Title	Budget Period: 1 st half						Budget Period: 2 nd half					
	Q1	Q2	Q3	Q4	Q5	Q6	Q7	Q8	Q9	Q10	Q11	Q12
Program Management	■											
Software preparations	■	■	■	■								
Subtask 2.1	■	■	■									
Subtask 2.2		■	■	■								
Subtask 2.3			■	■								
Trilinos MFIX Linear Solver				■	■	■	■	■				
Subtask 3.1				■	■	■						
Subtask 3.2					■	■	■	■				
Subtask 3.3							■	■				
MFIX suite tests							■	■	■	■	■	■
Subtask 4.1							■	■	■			
Subtask 4.2								■	■	■	■	■
Subtask 4.3									■	■	■	■

Project risks & risk management plan

Risk Category	Description of the Risk	Probability of Occurring	Impact	Overall Level of the Risk	Risk Mitigation Strategy
Internal Data Storage Array	How will the internal data storage arrays (a setpadiagonal matrix) be reconciled with native Trilinos data structures	Med	Low	Low	<ol style="list-style-type: none"> 1) Define a class that directly copy the data 2) Compressed sparse row matrix storage 3) Discussions with experts at Sandia to determine which approach would be best
ForTrilinos	Trilinos Fortran interfaces	High	Low	Low	<ol style="list-style-type: none"> 1) Consider Python as a glue language since it provides automatic wrapper generators. 2) Leverag from collaborators' existing PyTrilinos project 3) Integrate the fortran interface fully with Stratimikos
External supercomputer access	Securing access to the external supercomputers	Low	Low	Low	<p>Added as subtask to Secure external resources. Strategies are</p> <ol style="list-style-type: none"> 1) Work with Sandia Collaborator to secure DOE's HPC for Trilinos MFIX performance testing 2) Request for more allocation on TACC HPC through UT System HPC initiatives 3) Write proposal to secure computing hours on XSEDE HPC resources 4) PI already has access to Linux and IBM clusters through UTEP's HPC facilities

Project status

- Setup ~~GIT/version control~~ repository
- Select optimum Trilinos software package
- Develop ForTrilinos based Fortran interface for MFIX
- Test and compare the linear solver packages in Trilinos
 - Run test cases of fluidized bed simulations in MFIX using the various Trilinos linear equations preconditioner. Compare the performance (computing time and accuracy) of the MFIX- Trilinos package with solutions that use MFIX and its existing linear solvers
- **Perform scalability analysis of Trilinos-MFIX**
 - Conduct scalability tests of the Trilinos-MFIX package on single node and multi-core computer clusters using distributed/shared or in hybrid environment HPC systems. Test multi-core clusters containing 4, 16, 64, 128, 512, 1024, 8192(?) cores.
- Address Trilinos-MFIX performance bottlenecks via profiling and debugging tools in Trilinos
- Run fluidized bed test problems (various particle sizes and shapes, 2D/3D, Small/Large Scale, etc.)

Technical approach

One of the main challenges for any software development is keeping the computer code up-to-date with the advancement in applied mathematics, software and hardware development in computational science and engineering. Realizing the challenge, the Computer Science Research Institute (**CSRI**) group at Sandia National Laboratories (**Sandia**) has developed and continues to develop scalable solver algorithms and software through **next-gen** (exa-scale, peta-scale, extreme-scale, etc.) computing investment. The project is called **Trilinos** project.



*Funded by various DOE entities mainly NNSA - Advanced Simulation and Computing (**ASC**)/DOE Office of Science (**SciDAC**), Advanced Scientific Computing Research (**ASCR**)*

Note: Slides in this topic mostly borrowed from M.Heroux & other trilinos members

Trilinos

*The Trilinos Project is an effort to develop and implement **robust algorithms** and **enabling technologies** using modern object-oriented software design, while still leveraging the value of established libraries such as **PETSc, Metis/ParMetis, SuperLU, Aztec, the BLAS and LAPACK**. It emphasizes **abstract interfaces** for maximum **flexibility** of component interchanging, and provides a full-featured set of concrete classes that implement all abstract interfaces. Research efforts in **advanced solution algorithms** and **parallel solver** libraries have historically had a large impact on engineering and scientific computing. Algorithmic advances increase the range of tractable problems and reduce the cost of solving existing problems. Well-designed solver libraries provide a mechanism for leveraging solver development across a broad set of applications and minimize the cost of solver integration. Emphasis is required in both new algorithms and new software (Heroux et.al., <http://trilinos.sandia.gov/>).*

What is Trilinos?

- Object-oriented software framework for...
- Solving big complex science & engineering problems
- More like LEGO™ bricks than Matlab™



Trilinos provides the state-of-the-art preconditions and **linear solver** libraries

- demonstrate **scalability** on **current HPC systems**
- illustrate plans for **continued maintenance**
- include **support for new hardware technologies**

Target Platforms

Desktop: Development and more...

Capability machines:

Redstorm (XT3), Clusters

Roadrunner (Cell-based).

Multicore nodes.

Parallel software environments:

MPI

UPC, CAF, threads, vectors,...

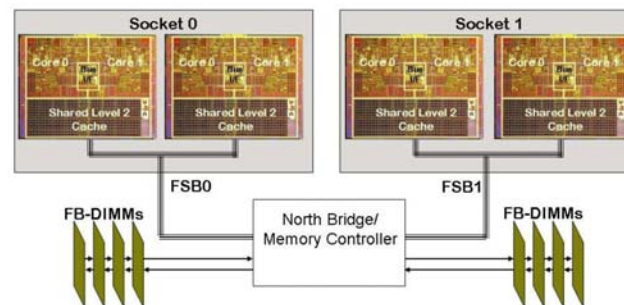
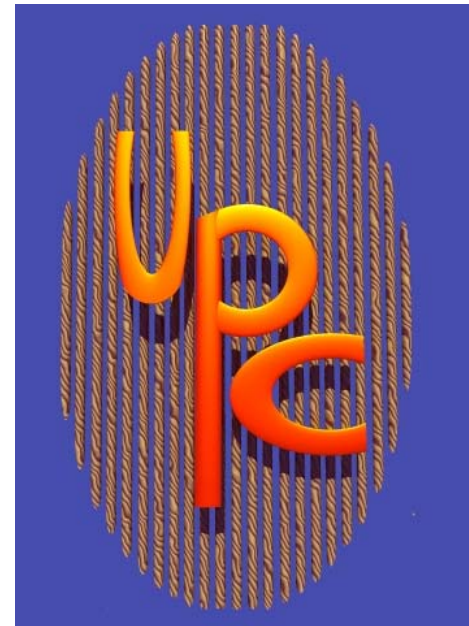
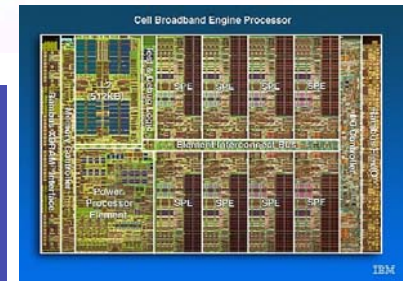
Combinations of the above.

User "skins":

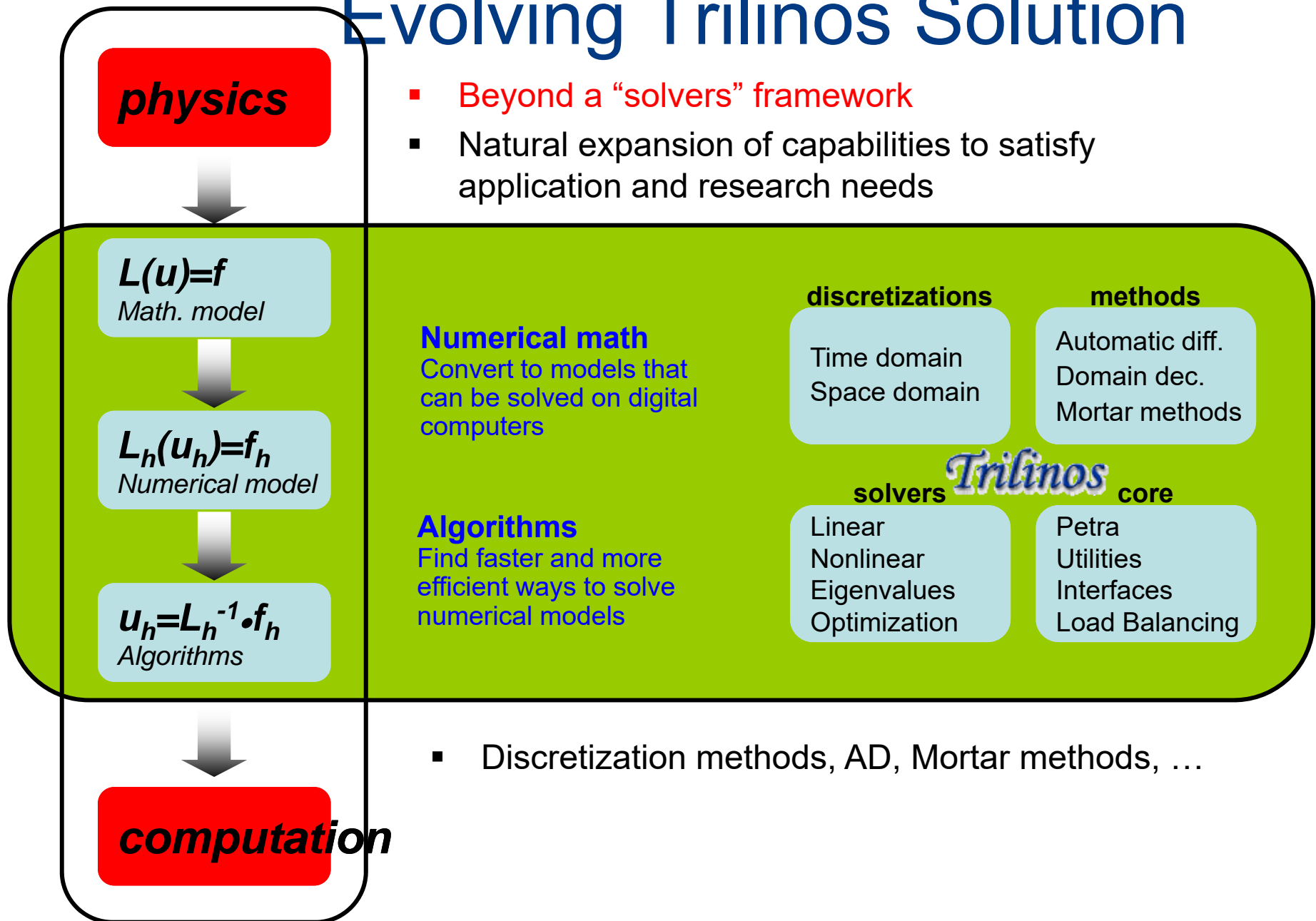
C++/C, Python

Fortran.

Web, CCA.



Evolving Trilinos Solution



Trilinos Strategic Goals

Scalable Computations: As problem size and processor counts increase, the cost of the computation will remain nearly fixed.

Hardened Computations: Never fail unless problem essentially intractable, in which case we diagnose and inform the user why the problem fails and provide a reliable measure of error.

Full Vertical Coverage: Provide leading edge enabling technologies through the entire technical application software stack: from problem construction, solution, analysis to optimization.

Algorithmic
Goals

Grand Universal Interoperability: All Trilinos packages will be interoperable, so that any combination of packages that makes sense algorithmically will be possible within Trilinos and with compatible external software.

Universal Accessibility: All Trilinos capabilities will be available to users of major computing environments: C++, Fortran, Python and the Web, and from the desktop to the latest scalable systems.

Universal Capabilities RAS: Trilinos will be:

The leading edge hardened, efficient, scalable solution for each of these applications (**Reliability**).

Integrated into every major application at Sandia (**Availability**).

Easy to maintain and upgrade within the application environment (**Serviceability**).

Software
Goals

C++ Objected
Oriented
Framework

Parallel/Distribut
ed Templated
classes for matrix
generations



Flexibility in
terms of
generic
programming
with Tpetra

State-of-The -
Art Linear and
Non-Linear
Solvers

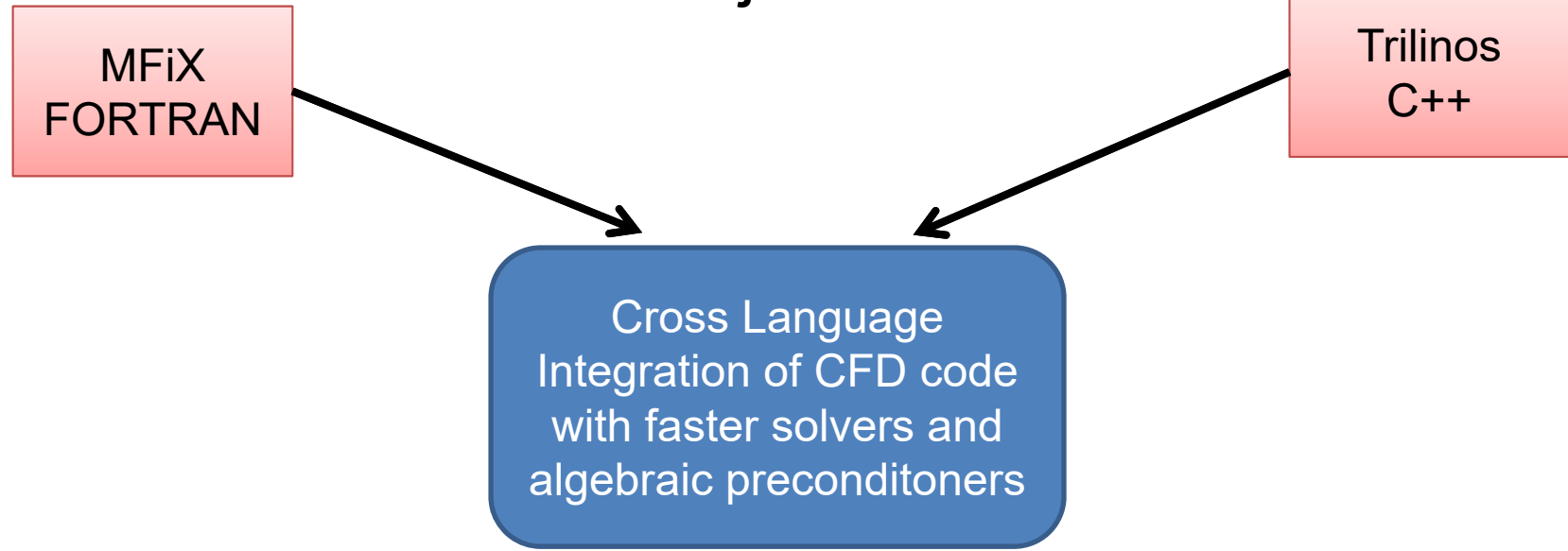
Run time load
balancing
between CPU
and GPU via
Kokkos

Parallel Data
Decomposition
data structures
Map

Native support for
exascale(>2
billion unknowns)
computing

Hardware
Exploitation for
large scale
number
crunching

Objective



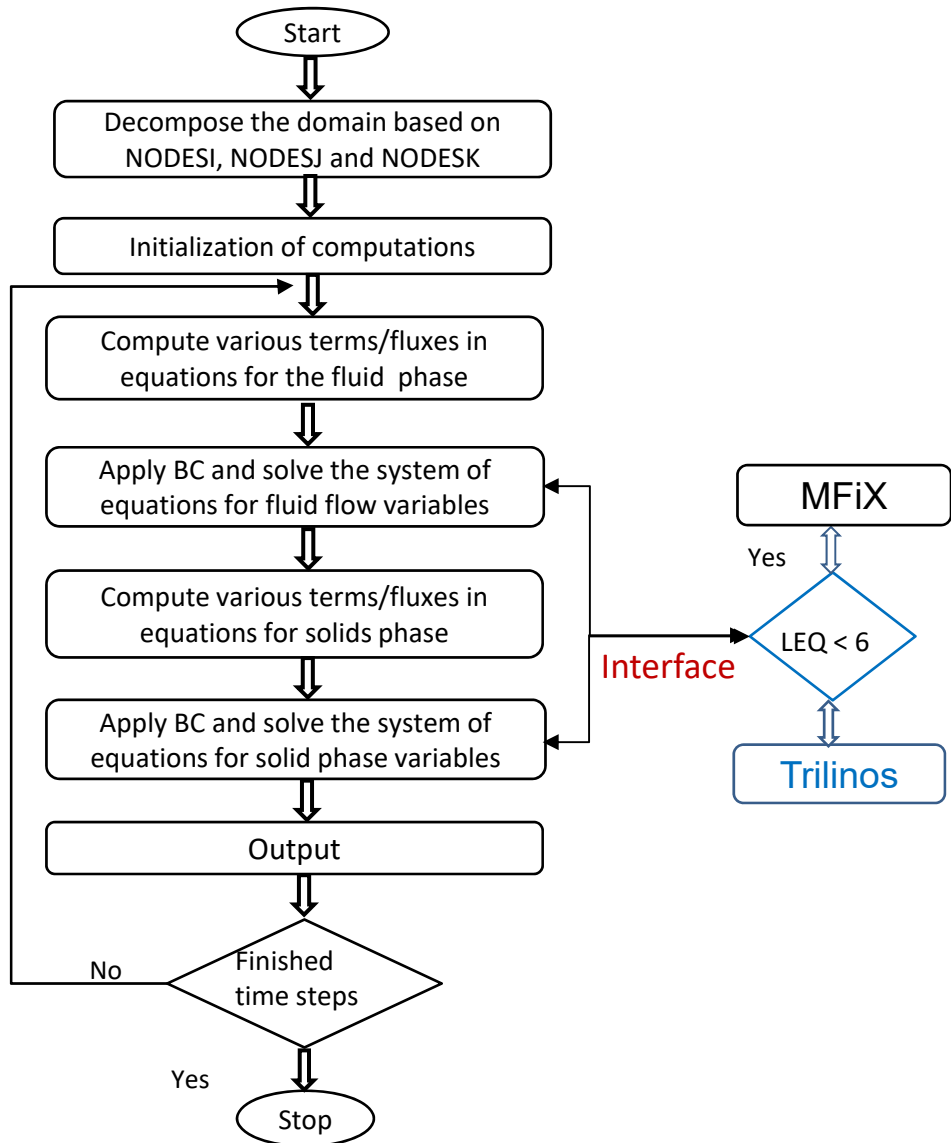
Advantages

- Exploit legacy codes' expertise in setting up large scale problems
- Use Trilinos as a faster and modern solver platform integrated with legacy codes.

Challenges

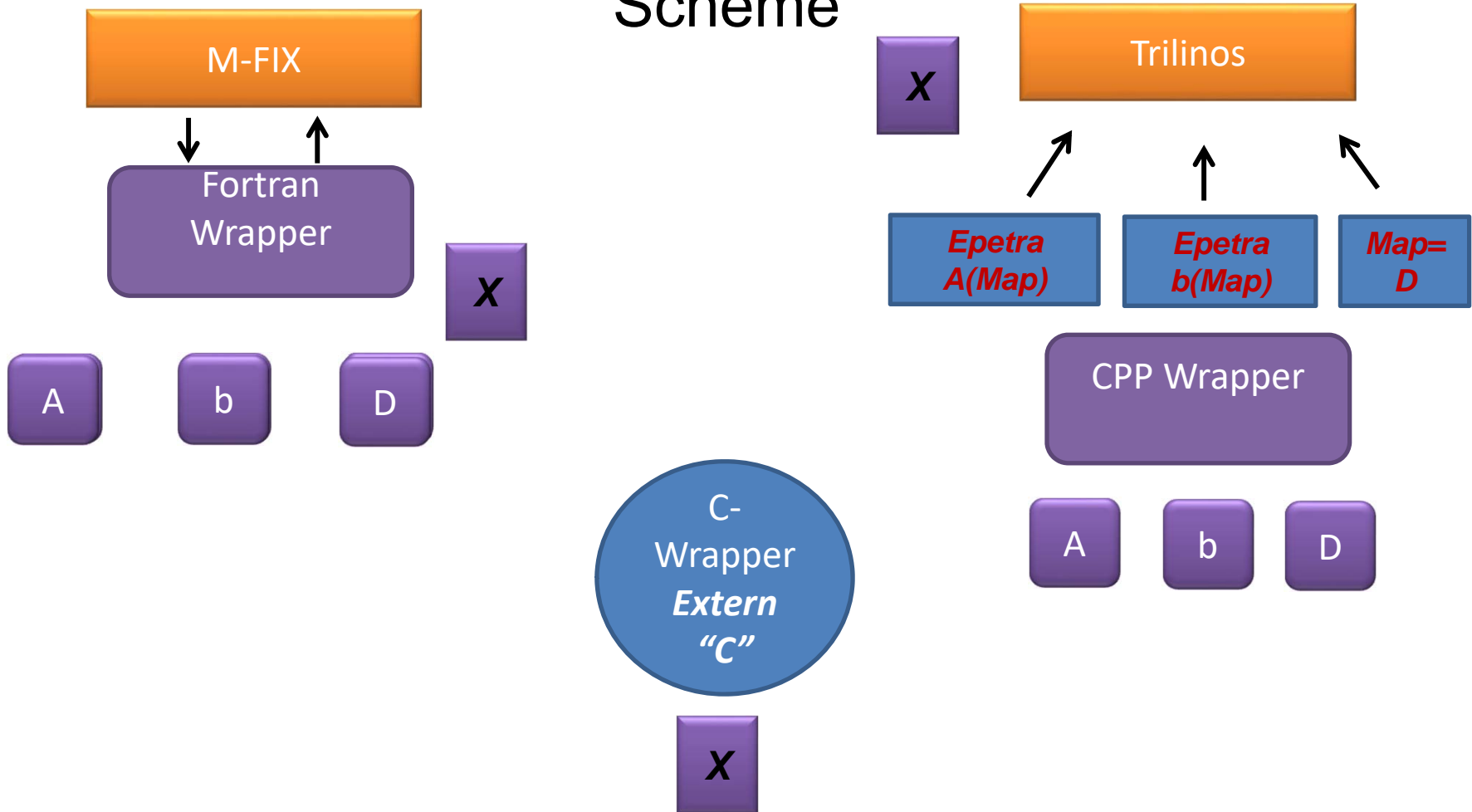
- FORTRAN has no objected oriented framework.
- Trilinos has been developed in C++(objected oriented) framework.
- No semantic support for C++ in FORTRAN.

Flow chart

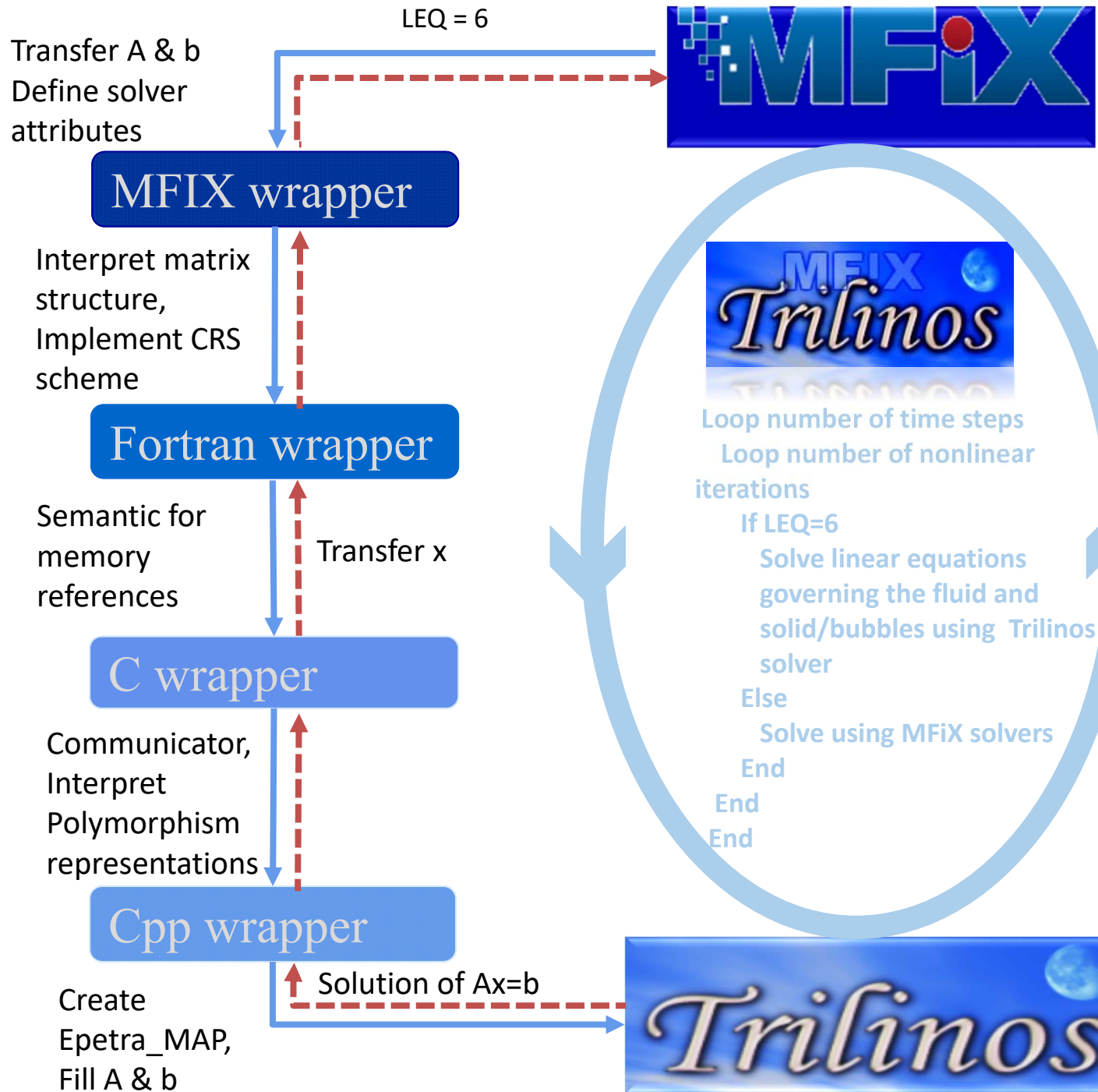


LEQ	Method	Description
1	SOR	Point Successive Over Relaxation
2	BiCGSTAB	Bi-Conjugate Gradient STABILized method
3	GMRES	Generalized Minimal RESidual algorithm
4	BICGSTAB + GMRES	
5	CG	Conjugate Gradient
6	BiCGSTAB/GMRES/CG/Direct/....	Trilinos

Cross Language Integration Scheme



A language independent interface
to integrate legacy codes



MFIX Wrapper

```
nstart = istart;      nend   = iend

ie = 0
do k = kstart,kend
  do i = nstart,nend
    do j = jstart, jend
      IJK = funijk(i,j,k)
      IJK_GL = funijk_gl(i,j,k)
      ie = ie + 1
      Anew(ie,1) = A_M(IJK,-3)
      Anew(ie,2) = A_M(IJK,-1)
      Anew(ie,3) = A_M(IJK,-2)
      Anew(ie,4) = A_M(IJK,0)
      Anew(ie,5) = A_M(IJK,2)
      Anew(ie,6) = A_M(IJK,1)
      Anew(ie,7) = A_M(IJK,3)
      Bn(ie)     = B_M(IJK)
      locgl(ie)  = IJK_GL
      pos(ie,1)  = KM_OF(IJK) - IJK
      pos(ie,2)  = IM_OF(IJK) - IJK
      pos(ie,3)  = JM_OF(IJK) - IJK
      pos(ie,4)  = JP_OF(IJK) - IJK
      pos(ie,5)  = IP_OF(IJK) - IJK
      pos(ie,6)  = KP_OF(IJK) - IJK
    enddo
  enddo
enddo
```

Cpp Wrapper

```
Tpetra_Map map(numGlobalElements, numMyElements, indexBase, comm)

Tpetra_crsMatrix A(map,7);

Tpetra_multivector x (map,1);
Tpetra_multivector b (map,1);

for (LO i = 0; i < static_cast<LO> (numMyElements); ++i) {
    Values = Anew[][];
    Indices = pos[][];
    A->insertGlobalValues (gblRow, NumEntries, Values, Indices);
}
A->fillComplete (map,map);

for (LO i= 0; i < static_cast<LO> (numMyElements); ++i) {
    const GO gblRow = map->getGlobalElement (i);
    b->sumIntoGlobalValue(gblRow, 0, Bn[i]);
}

Tpetra_LinearProblem problem(&A, &x, &b);

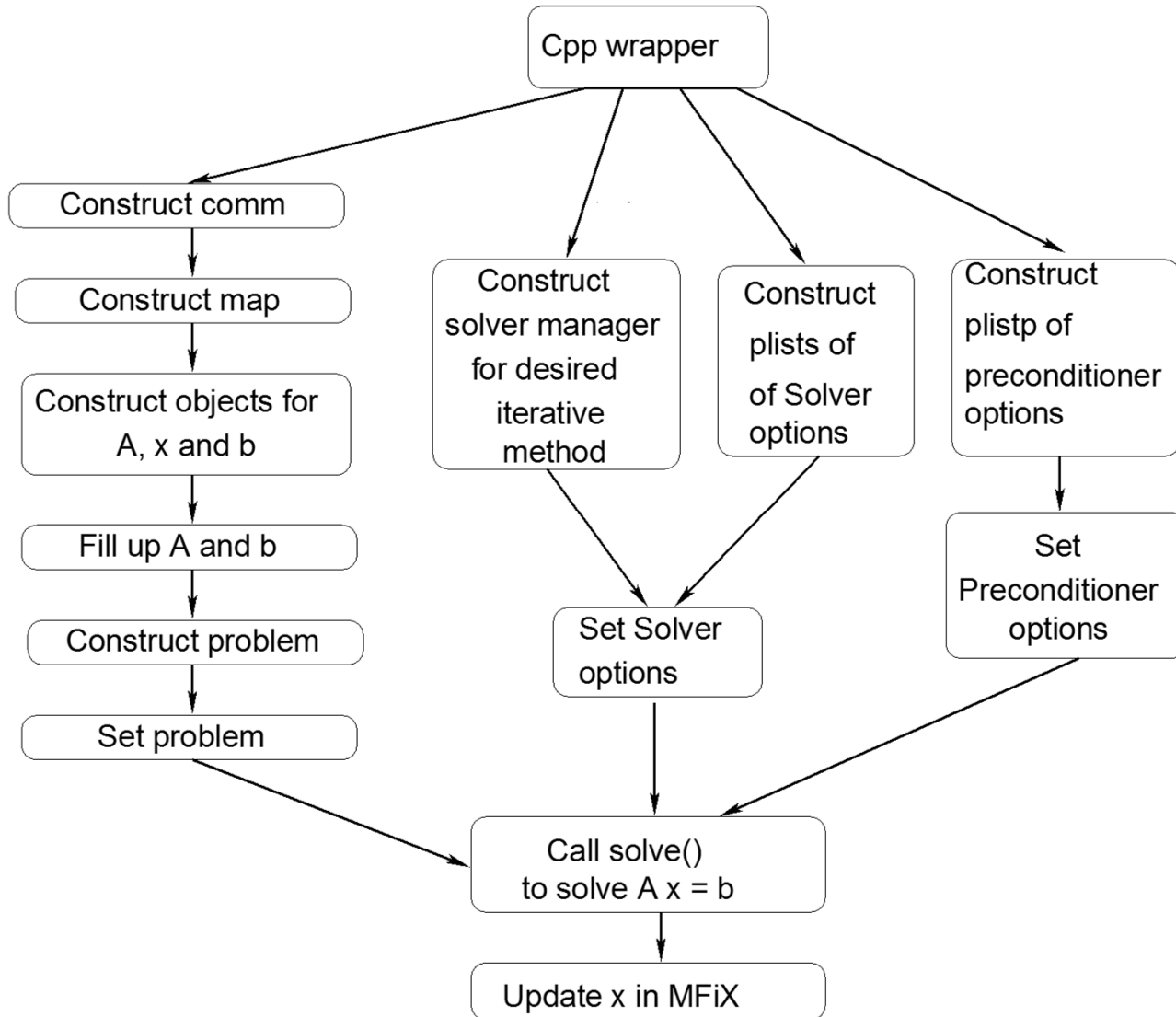
Problem->setRightPrec (plistp);

belos_bicgstab_manager_type solver(Problem, plists));

solver->solve();
```

Flow chart of Cpp wrapper

for preconditioned iterative solver in Belos



Abstract Numerical Algorithms

An **abstract numerical algorithm** (ANA) is a numerical algorithm that can be expressed solely in terms of vectors, vector spaces, and linear operators

Example Linear ANA (LANA) : Linear Conjugate Gradients

Given:

$A \in \mathcal{X} \rightarrow \mathcal{X} : \text{s.p.d. linear operator}$

$b \in \mathcal{X} : \text{right hand side vector}$

Find vector $x \in \mathcal{X}$ that solves $Ax = b$

- ANAs can be very mathematically sophisticated!
- ANAs can be extremely reusable!

Linear Conjugate Gradient Algorithm

Types of operations

Types of objects

Compute $r^{(0)} = b - Ax^{(0)}$ for the initial guess $x^{(0)}$.

for $i = 1, 2, \dots$

$$\rho_{i-1} = \langle r^{(i-1)}, r^{(i-1)} \rangle$$

$$\beta_{i-1} = \rho_{i-1} / \rho_{i-2} \quad (\beta_0 = 0)$$

$$p^{(i)} = r^{(i-1)} + \beta_{i-1} p^{(i-1)} \quad (p^{(1)} = r^{(1)})$$

$$q^{(i)} = Ap^{(i)}$$

$$\gamma_i = \langle p^{(i)}, q^{(i)} \rangle$$

$$\alpha_i = \rho_{i-1} / \gamma_i$$

$$x^{(i)} = x^{(i-1)} + \alpha_i p^{(i)}$$

$$r^{(i)} = r^{(i-1)} - \alpha_i q^{(i)}$$

check convergence; continue if necessary

end

linear operator applications

vector-vector operations

scalar operations

scalar product $\langle x, y \rangle$ defined by vector space

Linear Operators

- A

Vectors

- r, x, p, q

Scalars

- $\rho, \beta, \gamma, \alpha$

Vector spaces?

- \mathcal{X}

Gas-solid flow in a 2D bubbling fluidized bed

Cartesian vessel: 10cm length and 100cm height

Sand particle diameter	= 0.04cm
Sand particle density	= 2.0 g/cm ³
Restitution co-efficient	= 0.80
Angle of internal friction	= 30
The minimum void fraction	= 0.42
Fluid viscosity	= 0.00018 g/cm s
Fluid density	= 0.0012 g/cm ³

Boundary conditions

Inlet: constant mass inflow

124.6 cm/s for $4.3 < x < 5.7$; 25.9cm/s for $0 < x < 4.3$, $5.7 < x < 10$

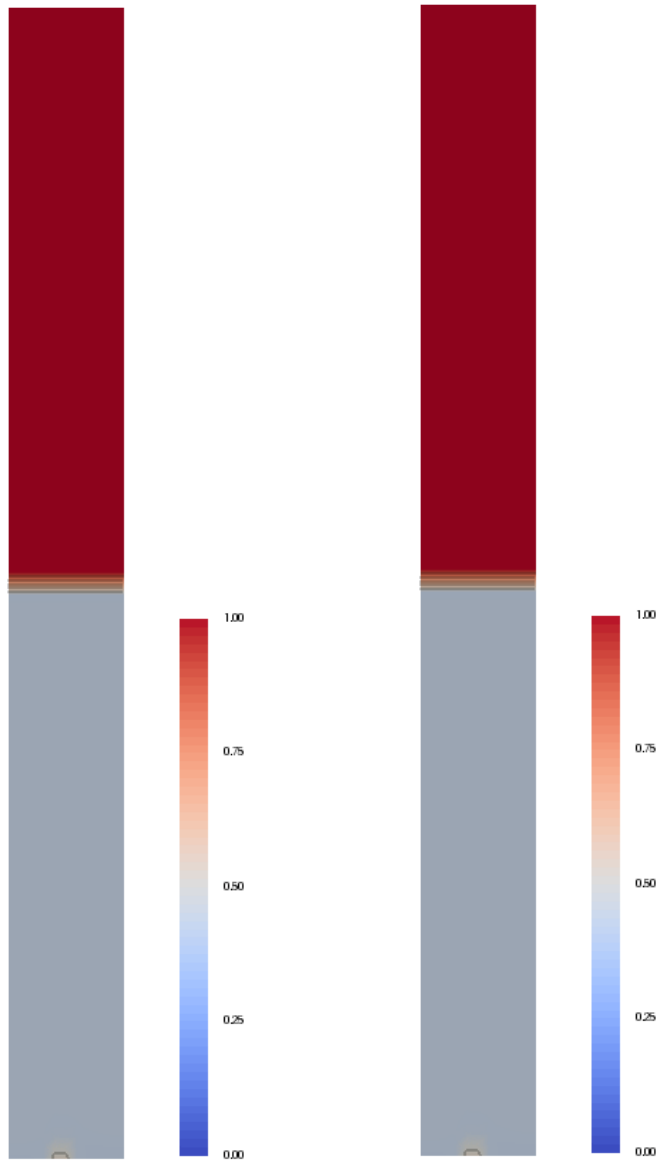
Sidewalls: slip condition

Outlet : pressure outflow condition ($p = 0$)

Mesh

Structured: IMAX = 10, JMAX= 100

Flow (void fraction) in a fluidized bed



MFiX

MFiX-Trilinos

Gas-solid flow in a 3D bubbling fluidized bed

Cartesian vessel: 10cm length, 10cm width and 100cm height.

Sand particle diameter	= 0.04cm
Sand particle density	= 2.0 g/cm ³
Restitution co-efficient	= 0.80
Angle of internal friction	= 30
The minimum void fraction	= 0.42
Fluid (gas) viscosity	= 0.00018 g/cm s
Fluid density	= 0.0012 g/cm ³

Boundary conditions

Inlet: constant mass inflow (124.6 cm/s for $4.3 < x < 5.7$, $4.3 < z < 5.7$)

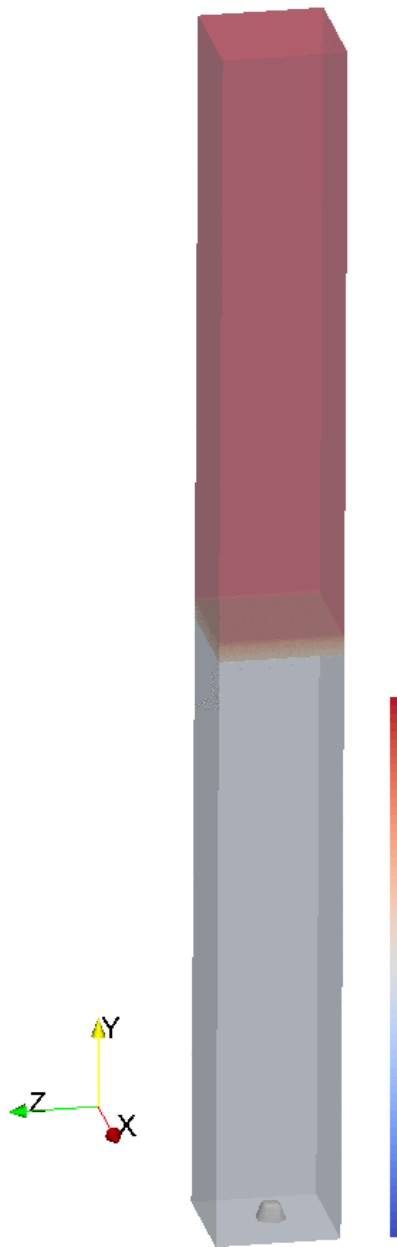
Sidewalls: slip condition

Outlet : pressure outflow condition ($p = 0$)

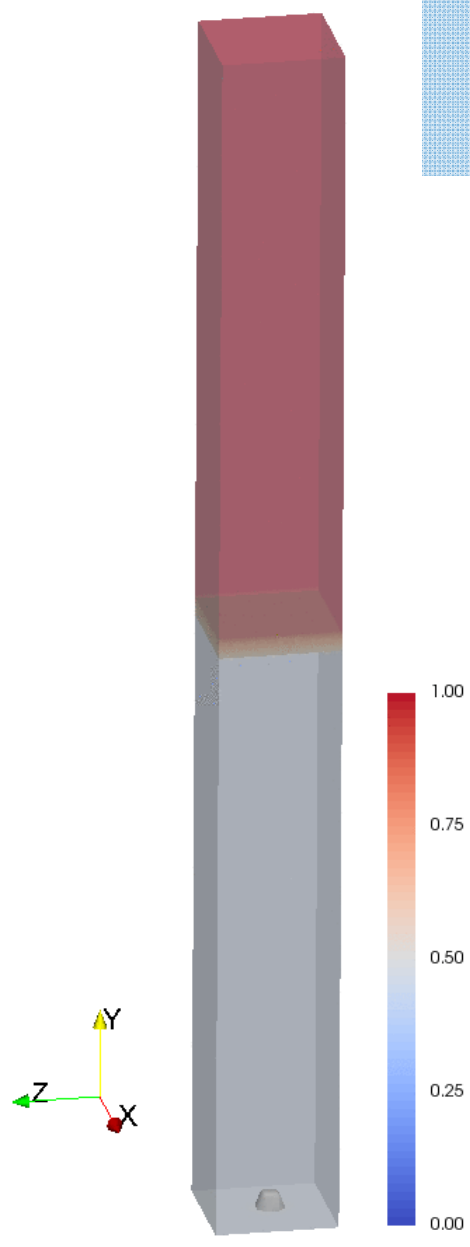
Mesh

Structured: IMAX = 10, JMAX = 100, KMAX = 10

Flow (void fraction) in a fluidized bed



MFiX



MFiX-Trilinos

Gas-solid flow in a circulating fluidized bed

Cylindrical vessel: 10cm diameter 100cm height.

Sand particle diameter	= 0.04cm
Sand particle density	= 2.0 g/cm ³
Restitution co-efficient	= 0.80
Angle of internal friction	= 0
The minimum void fraction	= 0.42
Fluid (gas) viscosity	= 0.00018 g/cm s
Fluid density	= 0.0012 g/cm ³

Boundary conditions

Inlet: constant mass inflow (124.6 cm/s for $0 < r < 0.7$)

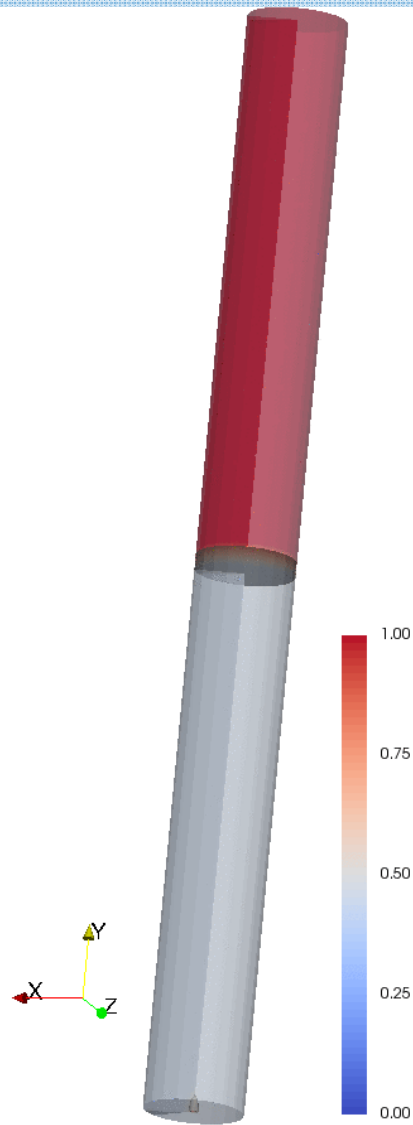
Sidewalls: slip condition

Outlet: pressure outflow condition ($p = 0$)

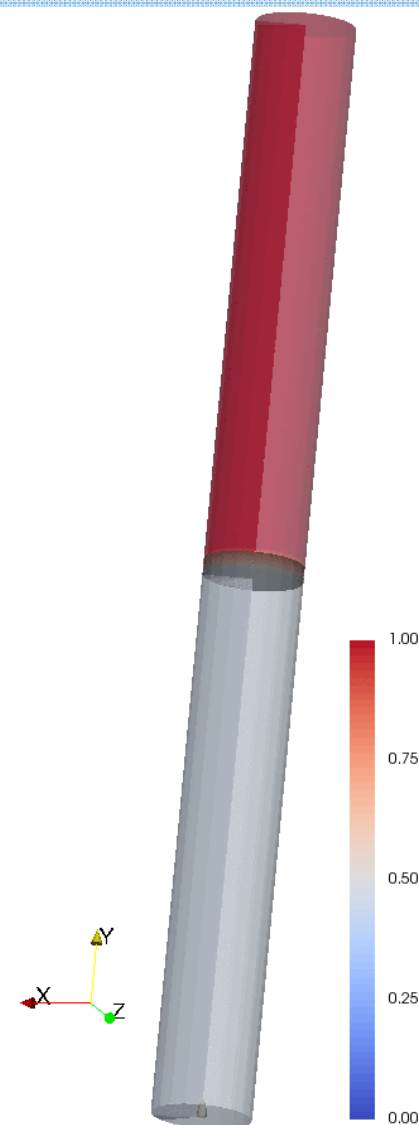
Mesh

Structured: IMAX = 10, JMAX = 100, KMAX = 10

Flow (void fraction) in a fluidized bed



MFiX



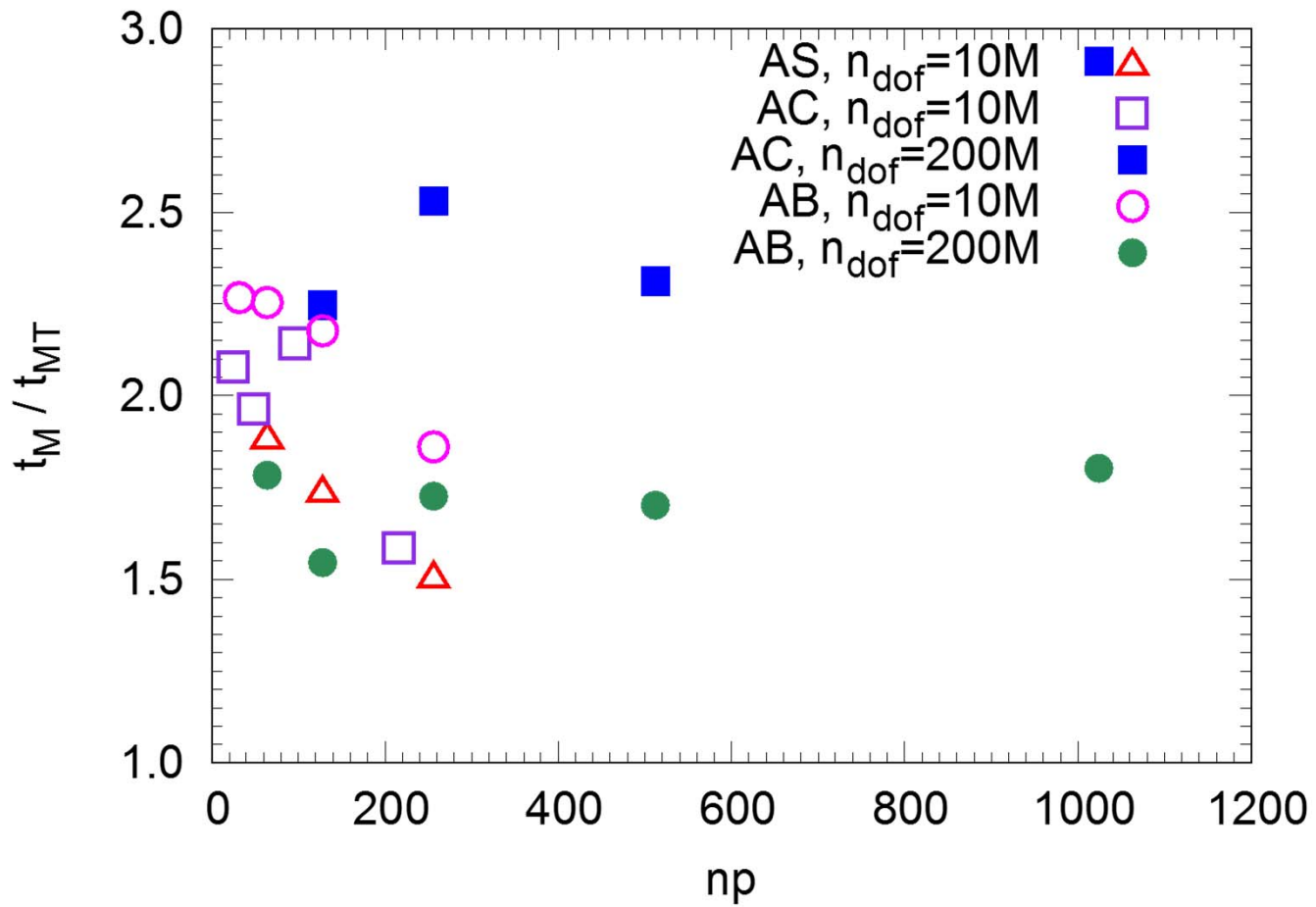
MFiX-Trilinos

Various computer architectures

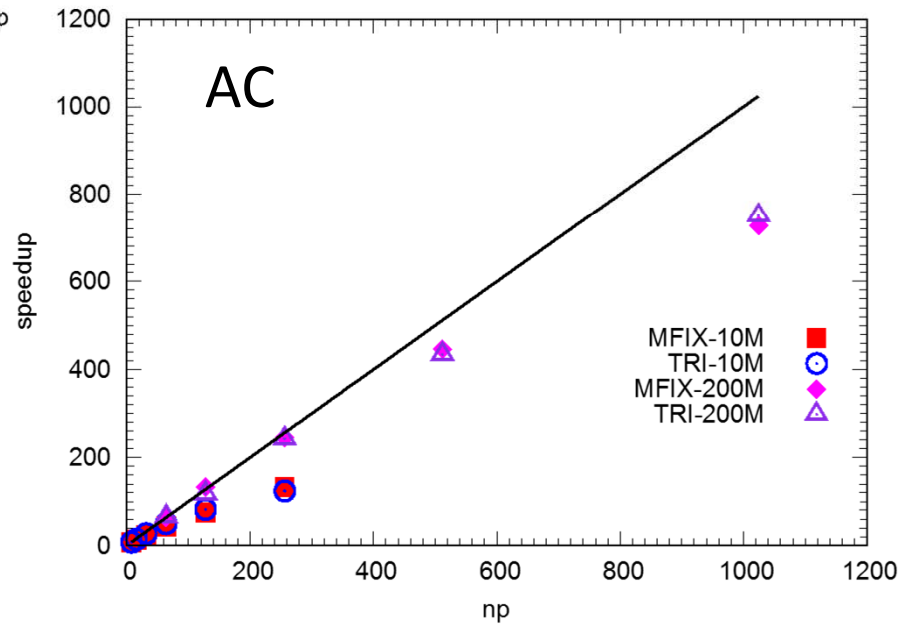
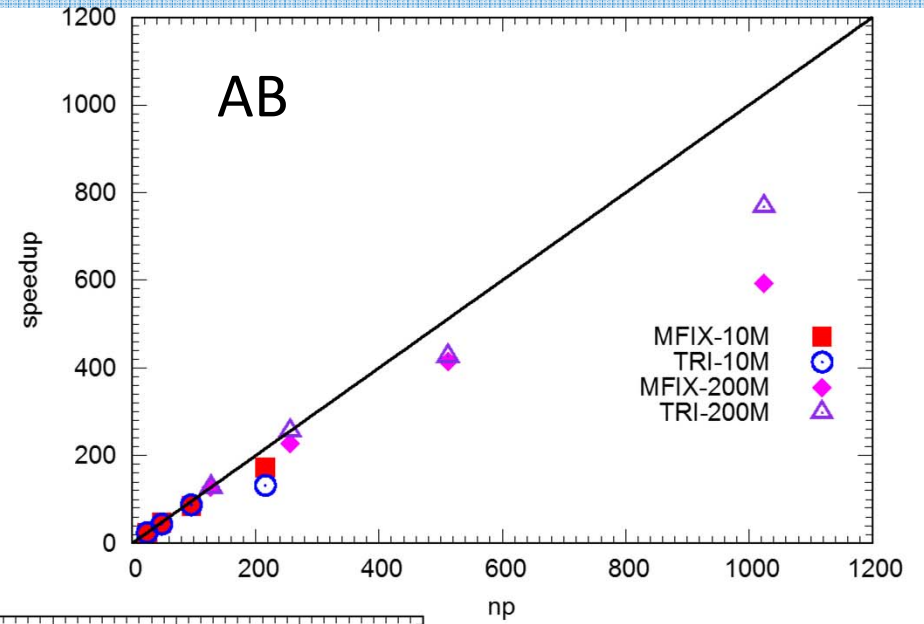
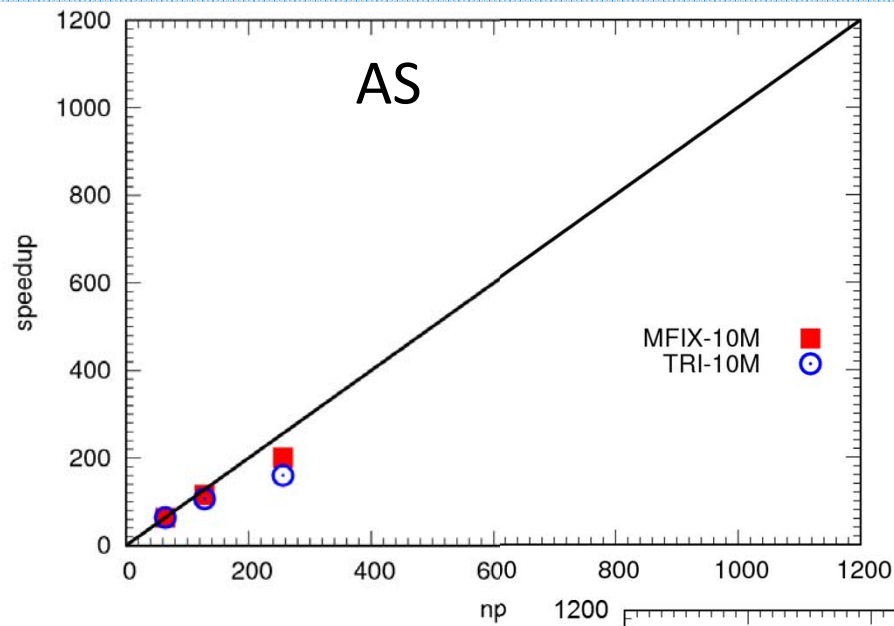
used for the performance analysis study

	Stampede (AS)	Comet (AC)	Bridges (AB)
Model (Intel Xeon)	E5-2680 2.7GHz	E5-2695 2.5GHz	E5-2695 2.30 GHz
Cores per socket	8	12	14
Sockets	2	2	2
L1 cache (KB)	32	32	32
L2 cache (KB)	256	256	256
L3 cache (KB)	20480	30720	35840
RAM (GB)	32	128	130

Performance of MFiX-Trilinos



Speedup study



Remarks:

- Trilinos linear solver was integrated with MFiX
- Scalability and speed-up tests for 2D & 3D bubbling flow problems were performed for upto 1024 processors
- >50% speed is observed but further investigation is required to examine any biases of the solver parameters

Scholarly dissemination

- V. Kotteda, A. Chattopadhyay*, V. Kumar, W. Spatz, “Next generation exascale capable multiphase solver with Trilinos”, ASME Journal of Fluid Engineering, under review
- V. Kotteda, A. Chattopadhyay*, V. Kumar, W. Spatz, “Next-generation multiphase flow solver for fluidized bed applications”, ASME FEDSM2017-69555
- A. Chattopadhyay*, V. Kumar, V. Kotteda, W. Spatz, “Next generation exascale capable multiphase solver with Trilinos”, ASME IMECE2016-67962 (2016)
- A. Chattopadhyay*, V. Kumar, V. Kotteda, W. Spatz, Leveraging Trilinos’s Next Generation Computing Framework for an Exa-Scale Poro-Elastic Network Simulator Implementation, 2016 IEEE High Performance Extreme Computing (HPEC) (2016)
- V. Kotteda, A. Chattopadhyay*, V. Kumar, W. Spatz, A Framework to Integrate MFiX with Trilinos for High Fidelity Fluidized Bed Computations, 2016 IEEE High Performance Extreme Computing (HPEC) (2016)

Q & A ?

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