High Fidelity Computational Model for Fluidized Bed

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BACKGROUND

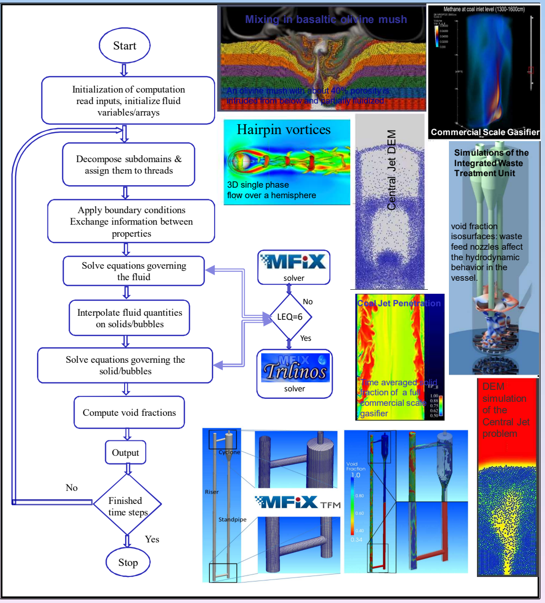
A requirement of many engineering and scientific applications is the need to solve linear and non-linear systems of equations. Research efforts in advanced solution algorithms and parallel solver libraries have a large impact on engineering and scientific computing. Algorithmic advances increase the 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. Sandia has developed a scalable solver algorithms and software (Trilinos) to provide a good robust solver and minimize the cost of solver integration.

OBJECTIVES

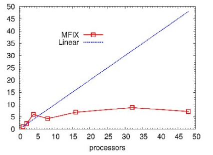
- Create a framework to integrate the existing MFIX (Multiphase Flow with Interphase eXchanges) linear solver with Trilinos linear solver packages,
- Evaluate the performance of the state-of-the-art preconditions and linear solver libraries in Trilinos with MFIX.

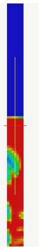
The project will reduce the computational cost as well as convergence instabilities when solving gas-solid flow in large scale flow problems using MFIX.

MFIX


Start
Initialization of computation read inputs, initialize fluid variables/arrays
Decompose subdomains & assign them to threads
Apply boundary conditions Exchange information between properties
Solve equations governing the fluid
Interpolate fluid quantities on solids/bubbles
Solve equations governing the solid/bubbles
Compute void fractions
Output
Finished time steps
No
Yes
Stop
MFIX solver
LEQ=6
No
Yes
Trilinos solver
Mixing in basaltic olivine mush
An olivine mush with about 40% porosity is intruded from below and partially fluidized
Methane at coal inlet level (1300-1600cm)
Commercial Scale Gasifier
Hairpin vortices
3D single phase flow over a hemisphere
Central Jet DEM
Simulations of the Integrated Waste Treatment Unit
void fraction isosurfaces: waste feed nozzles affect the hydrodynamic behavior in the vessel.
Coal Jet Penetration
Time averaged solid fraction of a full commercial scale gasifier
DEM simulation of the Central Jet problem
Cyclone
Riser
Standpipe
MFIX TFM
Void Fraction
1.0
0.80
0.60
0.40
0.34

S. No.	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	Trilinos	Trilinos





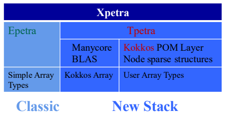
Intel Xeon E5649, 2.53GHz
4GB/core, 6 cores/processor
IBM 300GB 10K RPM 6Gbps

Speedup study with MFIX for two-fluid fluidized bed problem

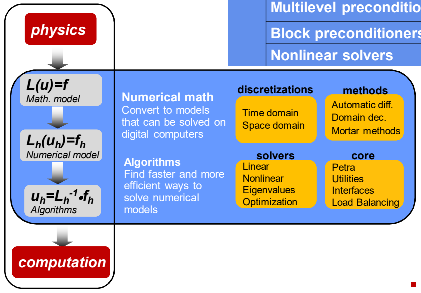
Trilinos

	Objective	Package(s)
Services	Linear algebra objects	Epetra, Tpetra, Xpetra
	Interfaces	Xpetra, Thyra, Stratimikos, Piro
	Load Balancing	Zoltan, Isorropia, Zoltan2
	Utilities, I/O, thread API	Teuchos, EpetraExt, Kokkos, Phalanx
Solvers	Iterative linear solver	AztecOO, Belos, Komplex
	Direct sparse linear solver	Amesos, Amesos2, ShyLU
	Direct dense linear solver	Epetra, Teuchos, Pliris
	Iterative eigenvalue solver	Anasazi
	Incomplete factorizations	AztecOO, Ifpack, Ifpack2
	Multilevel preconditioners	ML, CLAPS, MueLu
	Block preconditioners	Meros, Teko
	Nonlinear solvers	NOX, LOCA

Data Classes Stacks



Xpetra
Epetra
Tpetra
Manycore BLAS
Kokkos POM Layer Node sparse structures
Simple Array Types
Kokkos Array
User Array Types
Classic
New Stack



- A challenge for any software development is keeping the computer code up-to-date with the advancement in applied mathematics, software and hardware development.

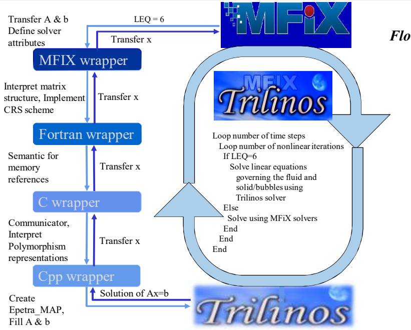
- Sandia group has developed and continues to develop **Trilinos, a scalable** solver algorithms and software through next-gen (exa-scale, peta-scale, exteme-scale, etc.) computing investment. The project is called project.
- It is an effort to develop and implement **robust algorithms** and **enabling technologies** using modern object-oriented software design, while still leveraging the value of established libraries.

AztecOO provides access to preconditioners and solvers such as CG, GMRES, BiCGSTAB by implementing an interface using Epetra. It uses Epetra objects for defining matrix and vectors. It provides a mechanism for using Ifpack, ML and AztecOO itself as preconditioners. It was Sandia's workhorse solver.

Kokkos

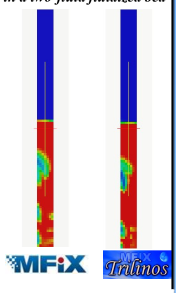
- Performance-portable abstraction over many different thread-parallel programming models: OpenMP, CUDA, Pthreads, …
- Abstract away physical data layout & target it to the hardware Solve "array of structs" vs. "struct of arrays" problem
- Memory hierarchies getting more complex; expose & exploit
- Data structures & idioms for thread-scalable parallel code Automatic memory management, atomic updates, vectorization, …
- Stand-alone; does not require other Trilinos packages

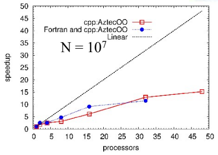
MFIX Trilinos



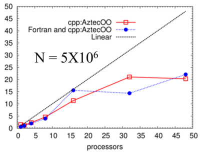
```
Loop number of time steps
  Loop number of nonlinear iterations
    If LEQ=6
      Solve linear equations
        governing the fluid and
        solid/bubbles using
        Trilinos solver
    Else
      Solve using MFiX solvers
    End
  End
End
```

Flow in a two-fluid fluidized bed





Speedup study with Trilinos and the interface for 1D heat conduction problem



CONCLUSIONS

•A framework is developed to call Trilinos from a Fortran program.

•The framework can be extended to integrate softwares written in Fortran and C/C++.

•The performance of integrated solver is better compared to the actual solver.

•The two open source softwares written in different programming languages are integrated and performance will be studied on large scale multiphase flow problem.

•GPU capabilities(via Kokkos) through a functional language interface(thread safe codes) will be exploited.

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