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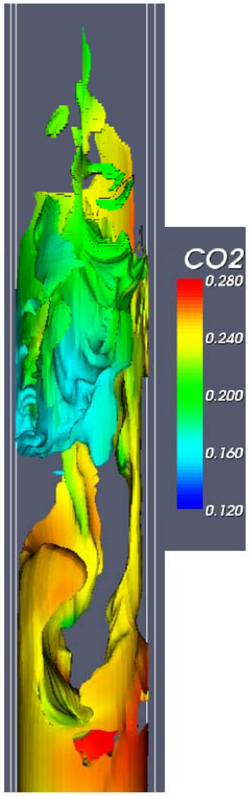
Multiphase flow simulation with MFIX



Jeff Dietiker

Workshop on Leadership-class Machines, Petascale Applications, and Performance Strategies

July 27-30, 2009, Granlibakken Resort and Conference Center, Tahoe City, CA, USA

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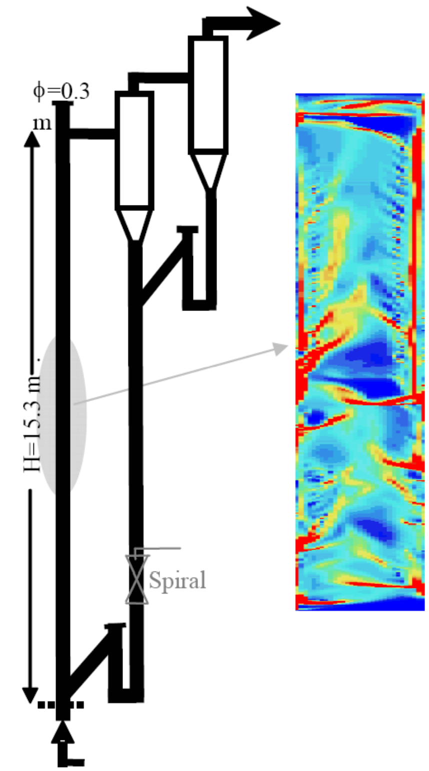
"Accelerating Clean Coal Gasifier Designs with Hybrid MPI/OpenMP High Performance Computing", 21st International Conference on Parallel Computational Fluid Dynamics – Moffett Field, CA – May 2009



Introduction

MFIX: Multiphase Flow with Interphase eXchanges

- Multiphase computational fluid dynamics software that couples multi-phase hydrodynamics, heat transfer and chemical reactions
- Eulerian-Eulerian and Eulerian-Lagrangian approach available
- 3D Finite volume with Cartesian or cylindrical structured grid with recent addition of cut-cell
- Second order accurate in space and temporal discretization
- SMP (OpenMP), DMP (MPI) and Hybrid Parallel mode of execution options that runs on many HPC platforms including Linux clusters
- Open-source code and collaborative environment (http://www.mfix.org)

Tech-Transfer Award 2006

2007 R&D100 Award

Introduction

Objectives

- Developing advanced coal technologies (as part of Clean Coal Initiative) to achieve zero emission of pollutants (e.g. CO2) while still remaining economically competitive

A coal-fired power plant in Conesville, Ohio

Source: Morgue File

An artist's rendition depicts the goal of the FutureGen initiative, which aims to build the world's first integrated sequestration and hydrogen production research power plant based on coal gasification.

Source: DOE Office of Fossil Energy

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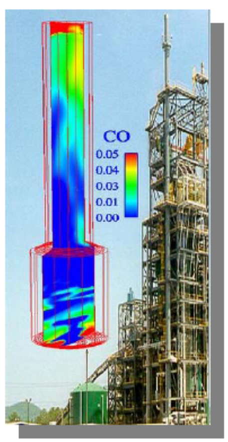
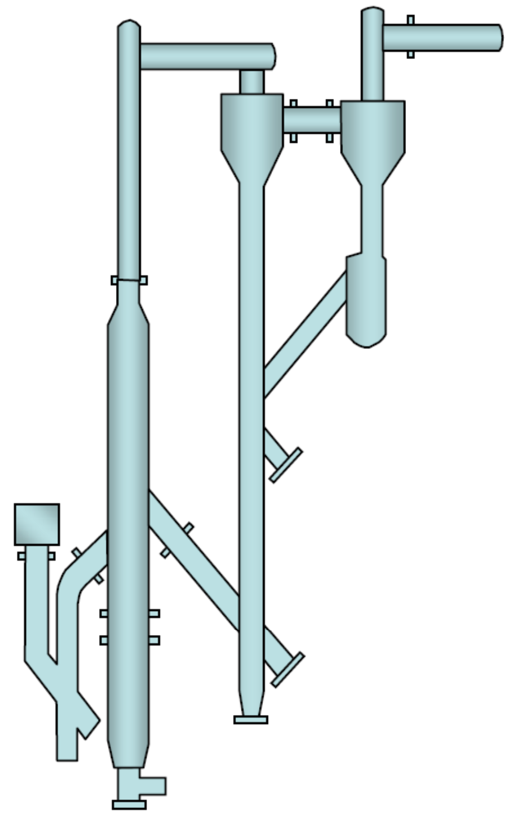
Challenge: How can we design commercial scale gasifiers for optimized operation?

Use validated computer models for answering scale up questions



MFIX simulation of pilot scale 13 MW transport gasifier at Wilsonville, AL.
Validation of the computer model with prototype system
C. Guenther et al (2003)

Parametric Study
- Length/Diameter
- Coal feed rate
- Solids circulation rate
- Recycled syngas
- Coal jet penetration



285 MW Commercial Gasifier

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Gasifier Simulations are Computationally Intensive

• ***Transient nature of gas-solid flows in industrial scale gasifier requires long computational times***

– Typical simulated time duration 10 to 15 sec

• ***Adaptive and small time-steps are required to resolve the physics, which is bounded by timescales like particle relaxation time and collision time.***

– Average timestep ranging from 10^{-5} to 10^{-4} sec

• ***Strong non-linearity stems from the complex interactions between the gas and solid phases, the chemical species reactions, and heat transfer:***

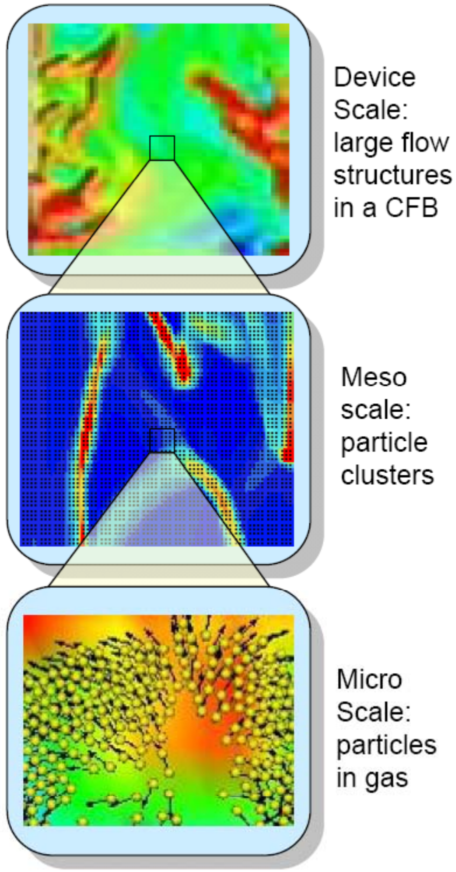
– Several non-linear iterations required per timestep

Numerical grid resolution requirement to achieve grid independent solution necessitates a grid size of few (5-10) particle diameters to fully resolve all heterogeneous flow structures, such as agglomerates of particles and small bubbles, observed during the fluidization of small particles

– For industrial scale riser of 1 m diameter & 30 m height with coal particles of 100 microns averaged:

• 24 billion cell resolution if uniformly 1 mm resolution to be reached.

• Order of billion cells if 1 mm resolution only in the regions of interest.



Levels of averaging: discrete particles to continuum to filtered-continuum models

Implementation of Cut-cell technique

MFIX: Multiphase Flow with Interphase eXchanges

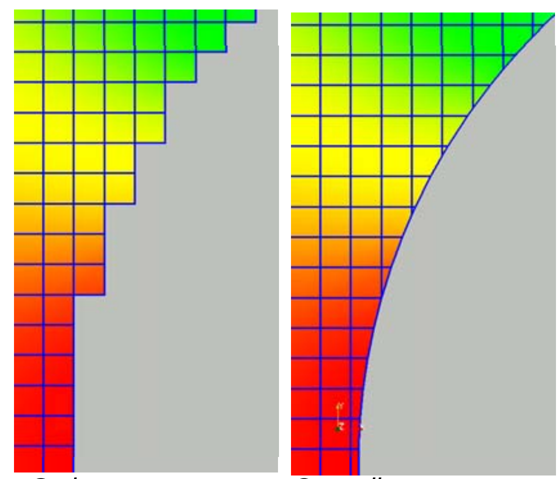
- Finite volume , 3D Cartesian or cylindrical coordinate system
- Continuum model (Interpenetrating fluid and solids phases)
- Boundary conditions typically specified along planes, aligned with grid

Cartesian Grid (Cut-cell) technique:

- Based on: M.P. Kirkpatrick, S.W. Armfield, J.H. Kent, "A representation of curved boundaries for the solution of the Navier–Stokes equations on a staggered three-dimensional Cartesian grid," *Journal of Computational Physics*, 184 (2003) 1–36.

Representation of curved boundaries: Computational cells are truncated to conform to the shape of the boundaries

- **Preprocessing:**
  - Representation of curved or sloping boundary
  - Identify boundary cells (cut cells)
  - Identify "Problematic" cells
  - Computation of cells volumes and face areas
- **Solution**
  - Flux computation through cut cell faces
  - Pressure forces
  - Wall shear stress
- **Postprocessing**: VTK files (geometry must be saved in every file)

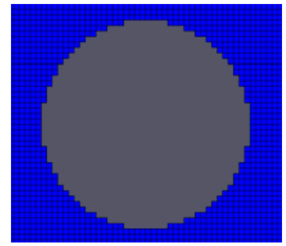


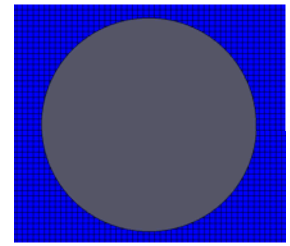
Staircase steps *Cut cells*

Implementation of Cut-cell technique

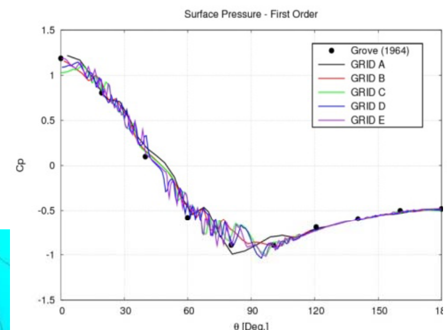
2D flow over a cylinder, Re = 40 (Steady)

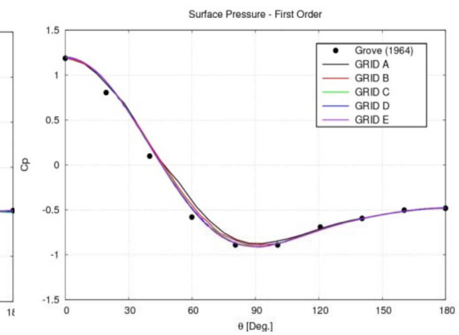
- *Surface Pressure*
  - *Staircase: General trend captured, even with coarse grid, with pressure oscillations*
  - *Cut-cell: Accurate and smooth surface distribution*
- *Surface Vorticity*
  - *Staircase: Vorticity under-predicted with coarse grid, Large oscillations even with fine grid*
  - *Cut-cell : Smooth distribution, Accuracy improves as grid is refined*

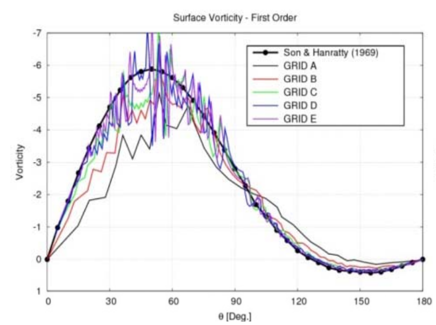


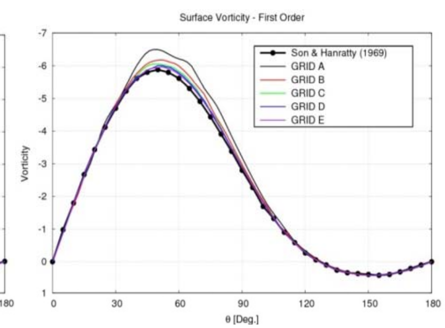


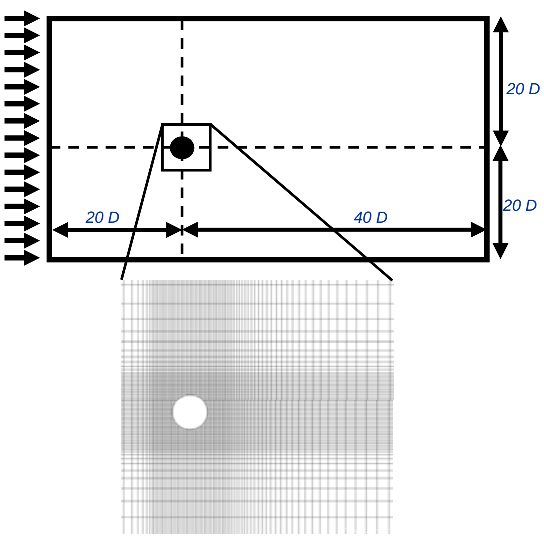
Staircase ***Cut-cell***

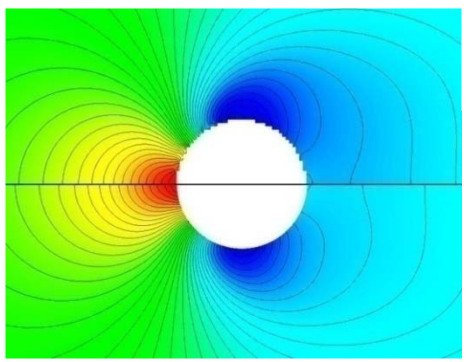












GRID	IMAX x JMAX	cells/diameter
A	120x80	20
B	200x140	40
C	320x240	80
D	420x320	120
E	520x420	160

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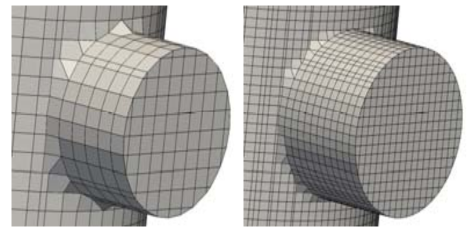
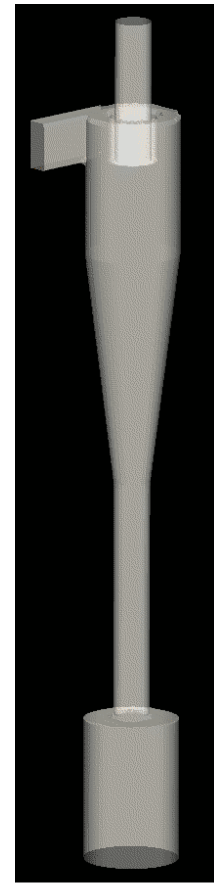
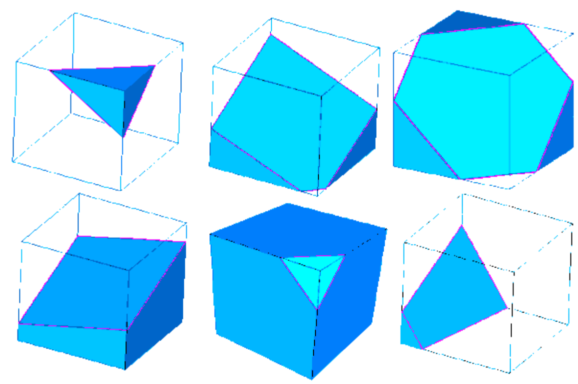
Implementation of Cut-cell technique



Coarse grid   Fine grid



- Cut cell technique useful to represent geometry with fairly coarse grid, but still limited to background Cartesian grid
- Future Improvements:
    - *Remove the dead cells and perhaps use a space-filling curve to index the cells*
    - *Ability to accept mesh information from an external Mesh generator such as Gambit*
    - *Hanging-nodes*
    - *Adaptive mesh refinement*
    - *Moving boundaries and immersed objects*



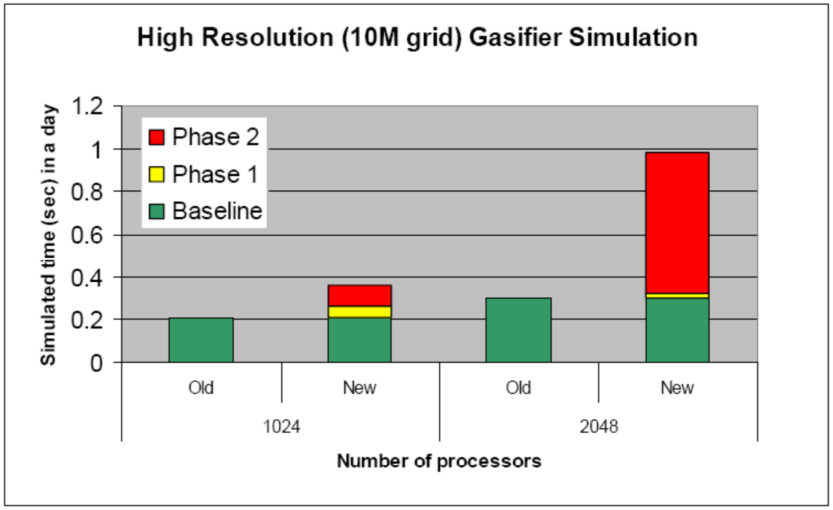
•Data visualization: *In 3D, cut face can have between 3 and 6 vertices → vtk file*

Cost of Cut-cell Method:

Geometry	Grid size	Number of cells	Standard cells	Cut cells	Blocked cells	Overhead	Overhead/ cut cell
2D	40x80	3200	71.50%	7.25%	21.25%	5.52%	0.75
3D	60x100x30	180000	9.55%	3.70%	86.75%	2.49%	0.67

Performance Improvements (MFIX baseline)

- *Extensive profiling of MFIX on various HPC platforms to understand bottlenecks was performed.*
- *Multiple improvement phases were incorporated & are under progress:*
    - ***Phase I: Choice of compiler flags and MPI tuning parameters***
    - ***Phase II: Reduction of MPI collective calls in linear equation** solver and compile with PathScale instead of PGI.*
    - ***Phase III: Hybrid mode operation of MFIX to take** advantage of multi-core platforms with MPI and OpenMP.*
    - *Phase IV: Integration of a standard high level I/O library to address I/O bottlenecks (netCDF/pnetCDF) [under progress].*
    - *Phase V: Integration with highly scalable and tuned solver library such as Trilinos [under progress].*



Phase 1, tuning the settings in PBS batch queuing software and in the MPI library; Phase 2, reduction of global dot-products in linear solver and residual calculations, and switching from PGI to Pathscale compiler. The time-simulated increased from 0.3 s/day to 1 s/day and surpassed the initial target of 0.5 s/day.

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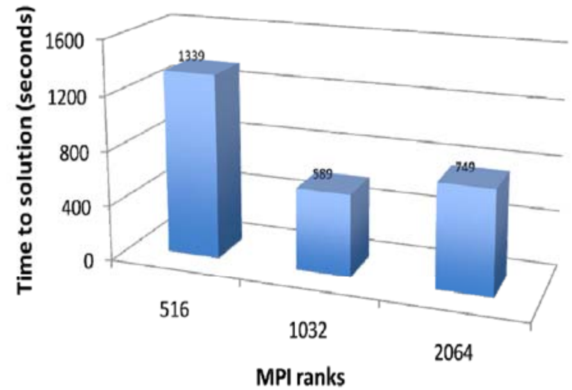
Preliminary Benchmarking Results on XT5

Execution Mode: MPI only and on 8 cores/node

Benchmarking problem with 10M cell grid resolution

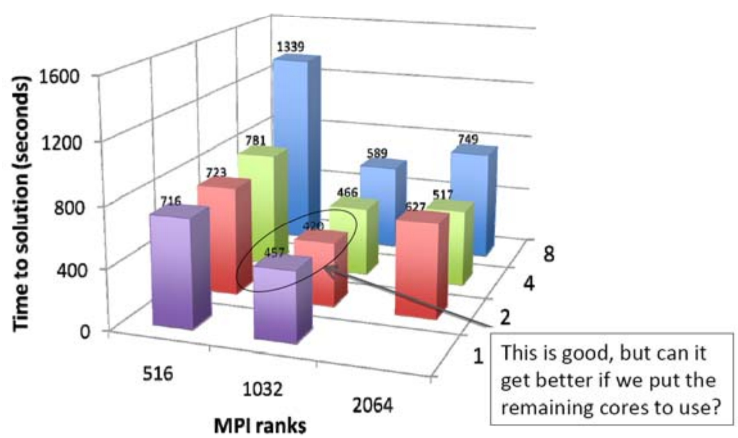
- *Platform: Cray XT5@NCCS*
- *MPI only and using all 8 cores on a node*
- *Time to solution measured for integrating over 100 steps of 2.5e-4 sec*
  - *Initialization and I/O times are ignored and no replication of timings*
- *Above 1032, more MPI ranks makes it slower for the current problem size*



Execution Mode: MPI only & using fewer cores/node

As wall-clock time is valuable, used more nodes although not all cores were utilized.

- *Having fewer MPI ranks per node gives solution faster*
  - *Memory bandwidth limited portions of the code which are accelerated*



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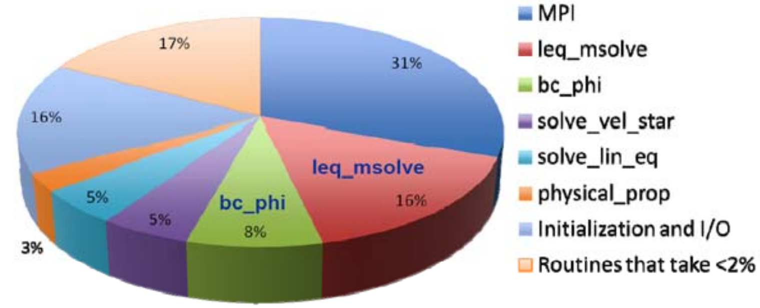
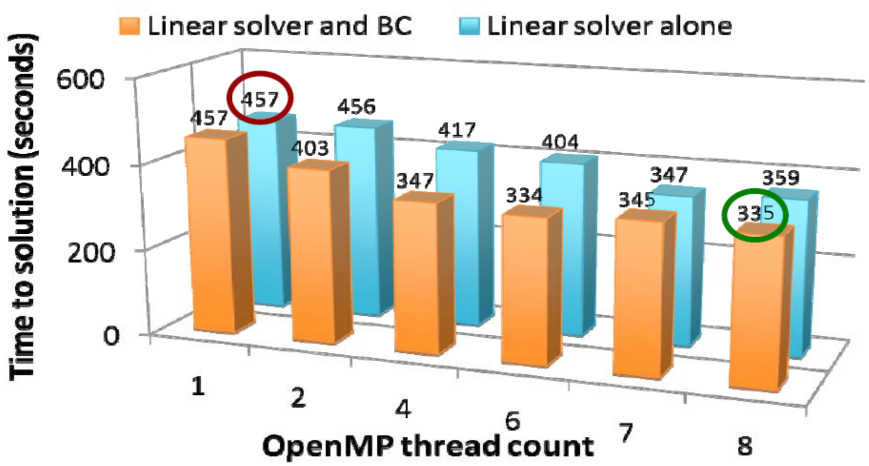
Preliminary Benchmarking Results on XT5

Hybrid MPI + OpenMP Execution Mode



Multiple OpenMP threads can exist within a single MPI rank
Distribute compute intensive loops/sections among several cores within the node
Performance profiling of the 1032-rank MPI only job gave the 25 % of time spent in two routines: leq_msolve and bc_phi have the most potential for improvement through OpenMP threading

First OpenMP enabled in the linear solver routines alone (leq_msolve) and then also in the BC routine
OpenMP brought the time down by 25%
but OpenMP in BC did not seem to help as much as the linear solver



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Conclusions

•Parametric study using simulation based engineering is critical in understanding design factors and operational efficiencies for various configurations

•Time-to-solution is key in the success of design and optimization of commercial scale gasifiers

•Implementation of cut-cell technique will help define complex geometries with coarser grids, and it will need to be optimized for parallel execution

•Efforts to improve performances of MFIX are under way . Using hybrid MPI+OpenMP enabled a better performance to be achieved – better than attainable with MPI alone