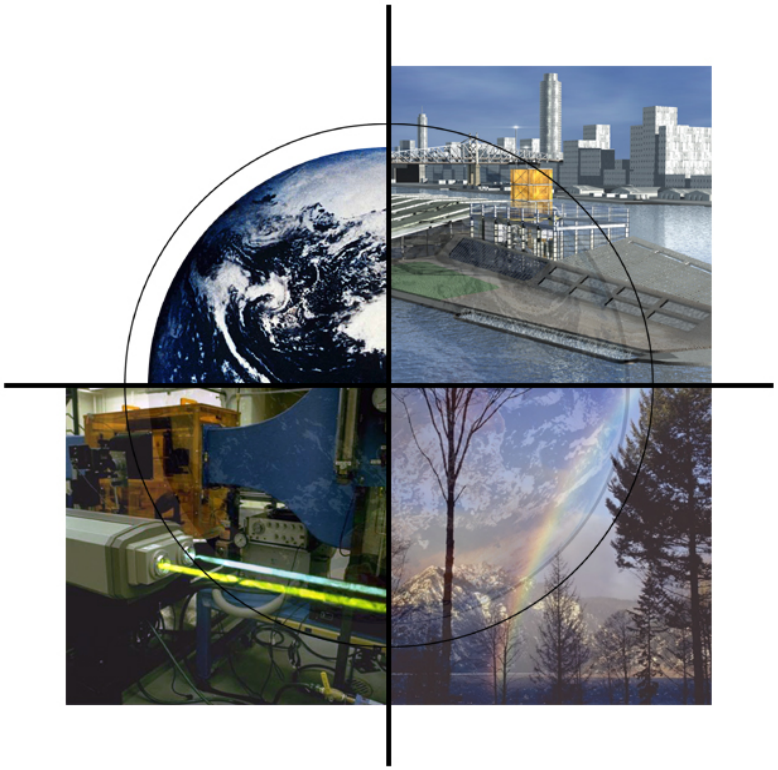
NETL-TPR-1960 DOE/NETL-IR-2008-020

Recent work in multiphase flow at NETL



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presented at

BHEL Workshop on Modeling Coal Combustion and Gasification

Tiruchy, India

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National Energy Technology Laboratory
Morgantown, WV

Outline of Presentation

- MFIX-NG
- Polydispersed Flow
- High Resolution Gasifier
- Future Outlook

MFIX-NG – Objectives

1. Improve the fidelity of multiphase flow models
   - Balance equations and constitutive relations
   - Validation studies
2. Develop fast and accurate numerical techniques
   - Accurate spatial and temporal discretization
   - Scalable parallel algorithms
   - Verification studies
3. Develop advanced post-processing capabilities
   - Data analysis
   - Visualization
   - Reduced order models

Need a software platform for these

The Path Forward

- **Continue using/developing MFIX**
  - Needs much programming
  - Cannot easily reuse modern software components
  - Cannot take advantage of available open source software written in modern programming languages
- **Use commercial software**
  - No flexibility for the concurrent development of theory, numerics, validation, and application
  - May need to abandon MFIX open source users
- **Construct software from existing software components**
  - Achieve desired features in the software
  - Reduced development cost

MFIX-NG

MFIX-NG Primary (Programmatic) Goals

- **Develop software infrastructure to model multiphase flow processes in power and process industry (e.g., coal gasifiers).**
- **Develop and validate multiphase flow theory:**
  - Transport equations,
  - Boundary conditions, and
  - Constitutive relations.
- **Develop numerical techniques for solving these multiphase flow equations efficiently and accurately.**
- **Increase the use of modeling for design and control in power and process industry.**

MFIX-NG Secondary (User-Related) Goals

- **Enable scientists to focus on model and algorithm development and validation, rather than code development and debugging.**
- **Reduce the need for scientist to understand the details of the underlying software framework, e.g., parallel computing.**
- **Reduce the development time for new applications by leveraging existing software and solver technology.**
- **Allow computational scientists to explore new algorithms through the use and modification of existing software.**

Unique Features Sought in MFIX-NG

- **Script-based front-end**: Physical models and numerical techniques are expressed in a thin layer of top-level code
  - Fast, error-free development of novel physical models and numerical techniques.
- **Components-based design**: Software system is composed of replaceable units of code with well-defined interfaces
  - Reuse advanced software components developed at other national labs and universities
- **Open-source development:** Process and infrastructure to validate and accumulate code contributions from users
  - Platform for exchanging and validating ideas
  - User contributions deepen software capabilities

Open Source Development

- Open Source (OS) Software
  - Term coined in 1998
  - Source code freely available for study, change and reuse
  - Comes with a license (GPL, LGPL, …) that requires users to follow certain rules regarding usage and redistribution
  - Success well established: **Linux** (operating system), **Apache** (Webserver)
- Advantages
  - Verification by ‘many eyes’
  - Accumulation of user contributions
  - Easier to exploit super computers
  - Information dissemination
  - **Better peer review**

Goals, Objectives and Challenges (I)

- **Building on the success of the MFIX flow solver, the next-generation solver will offer**
  - Greater geometric and modeling flexibility
    - Ability to model risers with inlets, cylinders without a centerline in grid, even entire apparatus
  - Easier extendibility and maintainability.
- **New solver will initially re-implement the MFIX solution algorithms and physical models.**
- **It will leverage externally developed libraries to easily take advantage of improvements made by other researchers.**

- **At the conclusion of the project, the new solver will**
  - Mimic the modeling capabilities now available in MFIX
  - Offer greater geometric flexibility by the use of unstructured meshes
  - Provide a platform for advanced multiphase solution algorithm development

MFIX-NG Development –1

- **Following the Unified Modeling Process adapted to the unique needs of the current project (*e.g.*, application domain, research code, legacy codes, collaboration).**
  - User Requirements Document (URD)
  - Software Requirements Document (SRD)
  - Software Design Document (SDD)
  - Software Development Plan (SDP)
  - Iterative Development process: Development goals are set every quarter based on a two-year roadmap.
  - Software Development and Testing

MFIX-NG Development –3

- Software Requirements Document (SRD)
  - Explored and qualitatively evaluated a set of alternative frameworks and PSEs based on the available documentation, examples, etc.
  - Rated each package with respect to features listed in SRD
  - Conducted user survey to determine the relative importance of various features listed in the SRD
  - Compiled the results of user survey and package ratings for determining the optimal framework

MFIX-NG Development –4

- Software Design Document (SDD)
  - Use cases (typical ways in which the software will be used)
  - class design diagram, collaboration diagrams, …External interface requirements (user, software, hardware).
  - Performance targets, quality assurance.
  - Design constraints.
  - Preliminary design - top-level architecture, main components, dataflow charts.
  - Testing strategy: unit tests, integration tests, verification tests

MFIX-NG Development –5

- Software Development Plan (SDP)
  - Tasks/features, benefits (limitations)
  - Completion criteria
  - Schedule/milestones
  - Resources
- Software Development and Testing
  - – Two-year development time to achieve full capabilities
  - – Scheduled to finish FY08-Q3
  - – Approximately 2 FTE/year development effort
- MFIX will be maintained as a well-tested legacy code

OpenFOAM Selected

Trilinos

OVERTURE

OpenFOAM

AMROC

PETSc

ROCCOM

SAMRAI

Structured Adaptive Mesh Refinement Application Infrastructure

- **Selection of the basic software libraries was the first milestone.**
- **Exhaustive evaluation of linear solvers, problem-solving environments, and CFD-specific libraries was performed.**
- **The OpenFOAM library was chosen as the most suitable.**

Framework Selection

		Feature Rating % for Objectives				
Framework	Organization	1	2	3	4	Weighted Average
OpenFOAM	OpenCFD, UK	46.1	52.0	39.6	100.0	58.8
Trilinos	CCM, Sandia	3.9	26.0	56.3	100.0	41.1
SAMRAI	CASC, Livermore	0.0	34.0	41.7	62.5	30.6
OVERTURE	CASC, Livermore	3.9	38.0	0.0	50.0	22.5
PETSc	Argonne	23.1	0.0	0.0	50.0	19.2
AMROC	CACR, CalTech	0.0	20.0	0.2	75.0	22.4
ROCCOM	U. Illinois	7.7	8.0	0.0	0.0	4.6
	WEIGHTS (Avg. of users)	0.335	0.255	0.18	0.230	

Objectives: 1 – Physics representation; 2 – Numerical scheme; 3 – SW development /maintenance; 4 – Open source

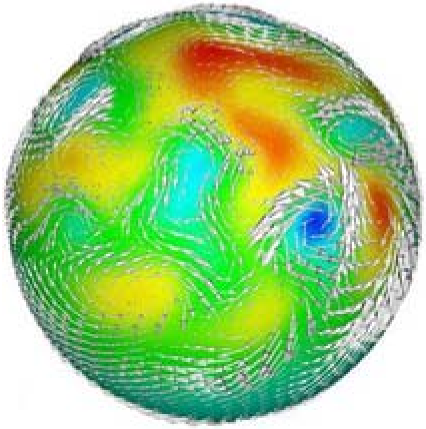
Gel et al. (2006)

OpenFOAM Strengths

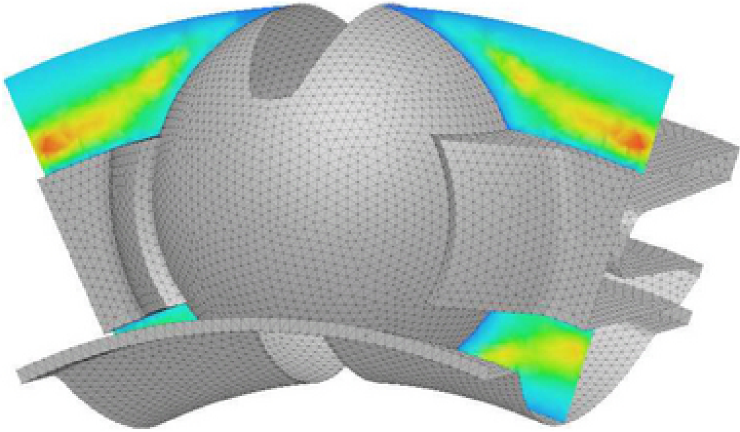
- Long development history. Marketed as a commercial product for many years.
- Code base was open sourced. A large active user group grew up quickly. Many contributors from both academia and industry. As improvements are made to the OpenFOAM core libraries, NETL's next-generation solver will be able to make use of them.
- OpenFOAM is object oriented and highly CFD specific, allowing for concise expression of CFD algorithms. Transport equations are expressed in terms of tensor calculus (i.e., div(U), grad(p)) rather than as coefficients stored in indexed matrices and vectors.
- OpenFOAM natively supports unstructured meshes, high-order discretization schemes, parallel processing without need for special coding practices.
- OpenFOAM framework exists for treating Lagrangian particles. Can be used for DEM or DPM models.
- Also supports moving meshes. Can model moving baffles, etc.

Highlights for [OpenFOAM]

- **Standalone CFD code (OOP, templated C++)**
- **Originated from Imperial College (1993)**
- **FOAM was offered as a commercial code**
- **Released as open source in December 2004**
- **3rd party software dependencies: MICO, Paraview, gcc, LAM/MPI**
- **Active community with users group lists**



Global weather prediction



Flow in a bearing

OpenFOAM Example Code

- Simple example showing the creation of a a transport equation for single-phase momentum
- The object `U` is a vector field object representing the velocity in every cell in the domain. The object `UEqn` is a vector matrix that represents the linear system defining the velocity field.
- The transient, convection, diffusion, and pressure terms are all neatly defined using the OpenFOAM notation.
- `solve(UEqn);` solves the linear system for the new velocity field.

```
fvVectorMatrix UEqn
       (
           fvm::ddt(U)
         + fvm::div(phi, U)
         - fvm::laplacian(nu, U)
        == -fvc::grad(p)
       );
solve(UEqn);
```

$$\frac{\partial U}{\partial t}$$

$$+\nabla\cdot\left(UU\right)$$

$$-\nabla\cdot\nu\nabla U$$

$$=-\nabla p$$

MFOAM – 1

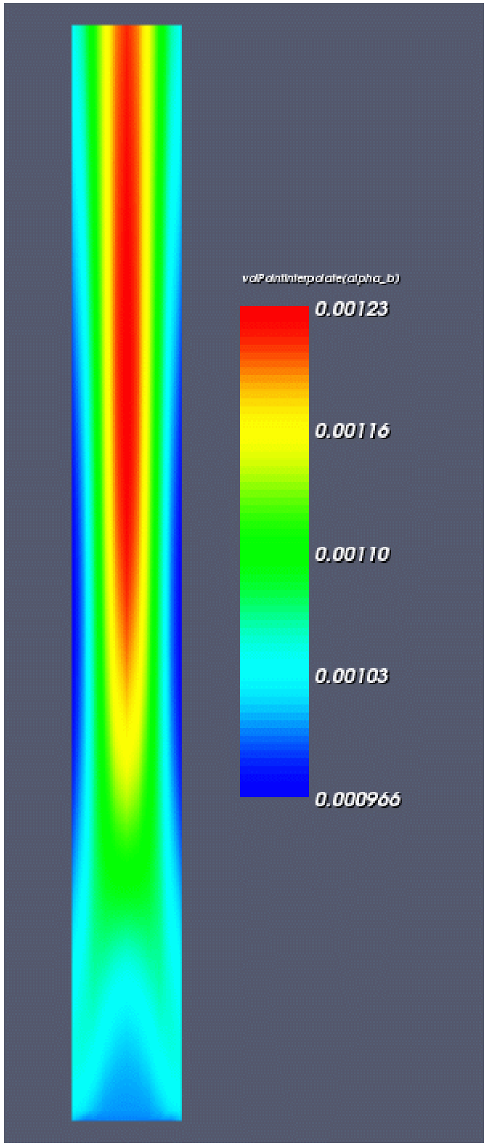
- **Initial efforts focused on learning the OpenFOAM library and building a prototype two-phase code.**
  - Followed the prototype single-phase solver codes included with the OpenFOAM source code.
  - Included isothermal gas-solids transport.
    - Included partial elimination algorithm for drag terms to promote solution stability.
    - Direct solution of the solids volume fraction equation.
    - Hard-wired solids pressure relation and constant viscosities.
  - Prototype mFoam code was successful in baseline testcases and served as the basis for the expanded solver.
  - Simple ozone decomposition chemistry and oxygen and ozone transport equations were added to replicate a well-studied MFIX case. Used as a proof-of-concept solver for reacting flows.
- **Developed a post processing program to serve as a prototype to replicate PostMFIX capabilities.**

MFOAM – 2

- **Using the mFoam prototype code, several researchers began implementation of the core MFIX model functionality.**
  - Made use of CVS to maintain consistency during development process.
- **A new storage scheme was devised to generalize the number of phases.**
  - The n-phase partial elimination algorithm was implemented for the momentum equations. mFoam could then solve flows involving a single continuous phase and one or more dispersed phases.
- **The gas transport equation was modified to include the compressibility term allowing for variable density gas flows.**
- **The energy transport equation was added to each phase.**
  - The n-phase partial elimination algorithm was used to improve inter-phase coupling due to heat transfer.

MFOAM – 3

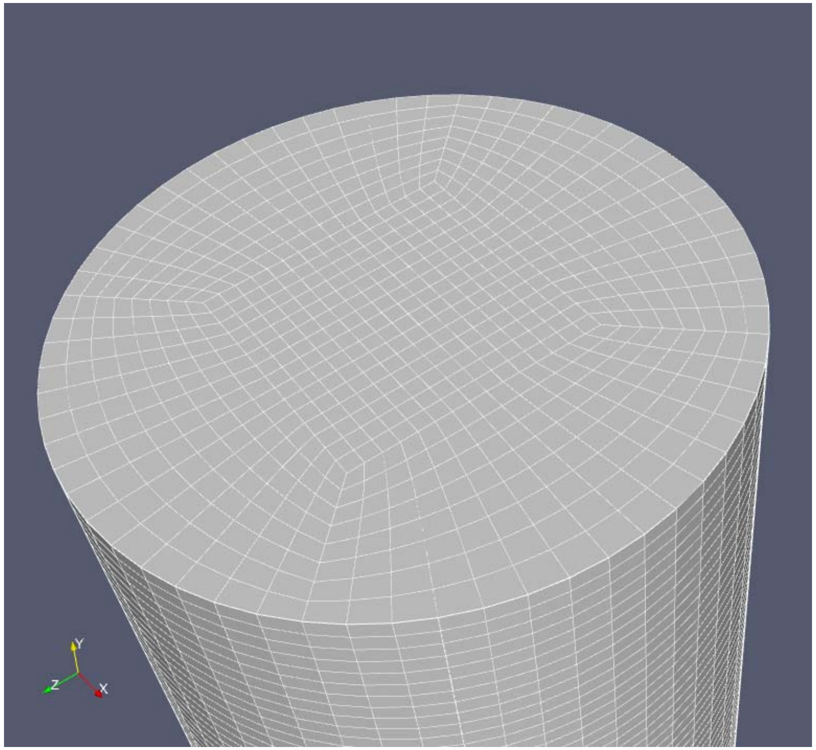
- **A general framework was assembled for handling drag models. All of the MFIX drag models were transferred to mFoam using this new framework.**
- **The MFIX algebraic and PDE kinetic theory models were implemented, including the Johnson and Jackson BCs.**
- **The Schaeffer and Princeton frictional models**
- **The Ahmadi and Simonin turbulence models**
- **The momentum equations have been modified to include an additional term that allows for the solution of periodic flows driven by a pressure gradient.**
- **A baseline automated test harness has been set up to automatically compile and test new code revisions and flag any deviation from prior results.**



MFOAM – 4

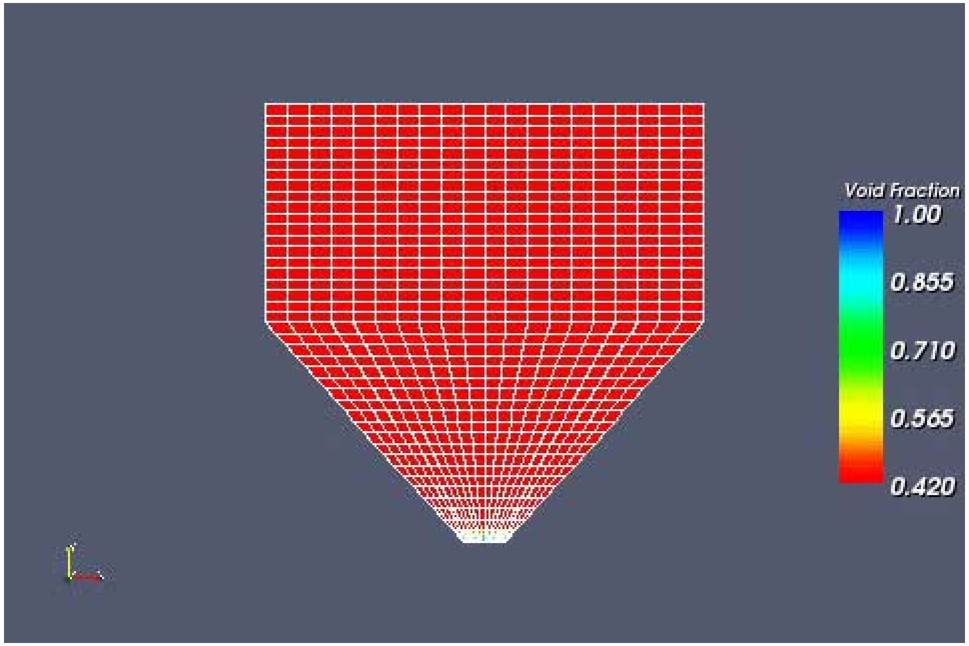
- **Adaptive time stepping algorithm used in MFIX was migrated to mFoam.**
  - This increases both the computational efficiency and stability by increasing the timestep when the solution converges smoothly and by recovering from failed time steps.
- **Modifications made to the momentum equations to remove spuriously large solids velocities when volume fraction is low.**
  - Mirroring the approach in MFIX, this modification prevents the momentum equation from becoming poorly conditioned in very dilute flow regions.

MFOAM – 5



Unstructured Mesh – no centerline.

Spouted Bed Simulation



MFOAM – 6

- **Evaluated four formats for reaction schemes and selected Cti format**
  - MFIX: easy to convert existing MFIX reaction files; non-standard format
  - Chemkin: widely-used format; OpenFOAM already has a reader; format not extensible to multiple phases; fixed-column format prone to errors.
  - OpenFOAM: similar to Chemkin format. the data is easier to input than Chemkin; format would be limited to the use with MFOAM/OpenFOAM.
  - Cti: used in Cantera; easy to write and read; utilities for converting Chemkin files into cti format; enables integration with Cantera; will need a translator

Block Solver Development

Block Solver Development

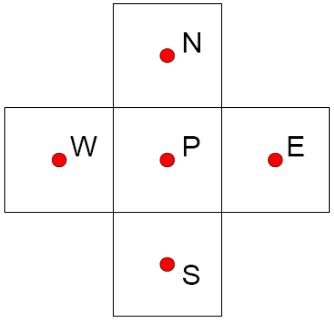
- Equation Segregation in OpenFOAM: Matrix Support.
  - Linear system and solver classes in OpenFOAM currently support scalar coefficients only.
  - As matrix coefficients are scalar, **equation segregation** is enforced: for coupled systems or vector and tensor variables, each component is solved in turn.
  - Segregated solvers do not provide sufficient level of coupling: a block matrix and solver approach is needed.
- Handling Complex Coupling
  - For coupled vector and tensor variables, basic sparseness pattern follows from mesh connectivity. For efficient solution, this fact should be used
  - Two types of coupling
    - Inter-variable coupling: vector or tensor components coupled to each other.
    - General matrix-to-matrix coupling: multiple transport equations solved together, with implicit handling of linearized coupling terms.
  - Both approaches produce the same basic effect: choice will be made based on convenience in discretization and matrix assembly.

MFOAM Future Work – 1

Sparse Matrix with Block Coefficients

- For cases of coupled vector and tensor variables, the FVM sparseness pattern is preserved: a vector component is coupled to other vector components in the same cell or to vector components in a neighboring cells.
- Example: block-coupled vector equation
  - Variable organization: (u_x, u_y, u_z).
  - Ordering of each list matches the cell ordering and sparseness pattern matches the mesh.

$$\mathbf{A}_P = \begin{bmatrix} [u_x \leftrightarrow u_x] & [u_x \leftrightarrow u_y] & [u_x \leftrightarrow u_z] \\ [u_y \leftrightarrow u_x] & [u_y \leftrightarrow u_y] & [u_y \leftrightarrow u_z] \\ [u_z \leftrightarrow u_x] & [u_z \leftrightarrow u_y] & [u_z \leftrightarrow u_z] \end{bmatrix}$$



$$\mathbf{A}_P \mathbf{u}_P + \sum_N \mathbf{A}_N \mathbf{u}_N = \mathbf{R}$$

- A_P and A_N coefficients are tensors; the rest of linear algebra generalizes naturally, including vector-matrix multiplication and linear solvers.

MFOAM Future Work – 2

General Matrix-to-Matrix Coupling

- In cases where multiple equations for multiple variables are coupled in a general manner, a block coefficient approach is not appropriate: requires re-ordering of coefficients
- Each matrix is assembled in isolation and placed into a block system. Example u1 − u2 coupling.

$$\begin{bmatrix} [\mathbf{u}_1] & [\mathbf{u}_1 \rightarrow \mathbf{u}_2] \\ [\mathbf{u}_2 \rightarrow \mathbf{u}_1] & [\mathbf{u}_2] \end{bmatrix} \begin{bmatrix} \mathbf{u}_1 \\ \mathbf{u}_2 \end{bmatrix} = \begin{bmatrix} \mathbf{R}_1 \\ \mathbf{R}_2 \end{bmatrix}$$

- [u1]: sparse matrix block containing u1 equation with implicit coupling.
- [u1 → u2]: off-diagonal block matrix containing u1 − u2 coupling terms.
- Linear solver operates on a complete block system; preconditioning is performed on diagonal blocks only.
- Implementation involves multiple blocks and arbitrary coupling: [u1 → u2] is considered a coupled interface on the [u1] block.
- Linear algebra and linear solver algorithms now operate on a block system: [u1 u2] is considered a single variable.

MFOAM Future Work – 3

- **Validation and Verification of mFoam**
  - During the current fiscal year, a testing protocol will be established.
    - Will compare mFoam results to MFIX and other CFD codes as a means of verification.
    - Will compare mFoam results to available experimental data as a means of validation.
  - These tests will be carried out in the following fiscal year.
  - Also in FY08, a careful investigation of high-order differencing schemes will be performed to mirror similar work done using MFIX by Guenther and Syamlal (2003).
- **Performance evaluation**
  - A comprehensive test will be made of the computational efficiency and scalability of mFoam. This will address single CPU performance as well as parallel performance over a tens to hundreds of CPUs.
- **Advanced algorithm development**
  - After replicating the capabilities, new solution algorithm approaches will be investigated. This will be the primary focus of research going forward.
  - These will make use of the block solver capabilities as they become available.
  - Also use of fractional step and explicit solution approaches.
  - Investigate multiphase flux limiting schemes that use the drag to compute and cap fluxes for all phases in a nonlinearly coupled manner.

Outline of Presentation

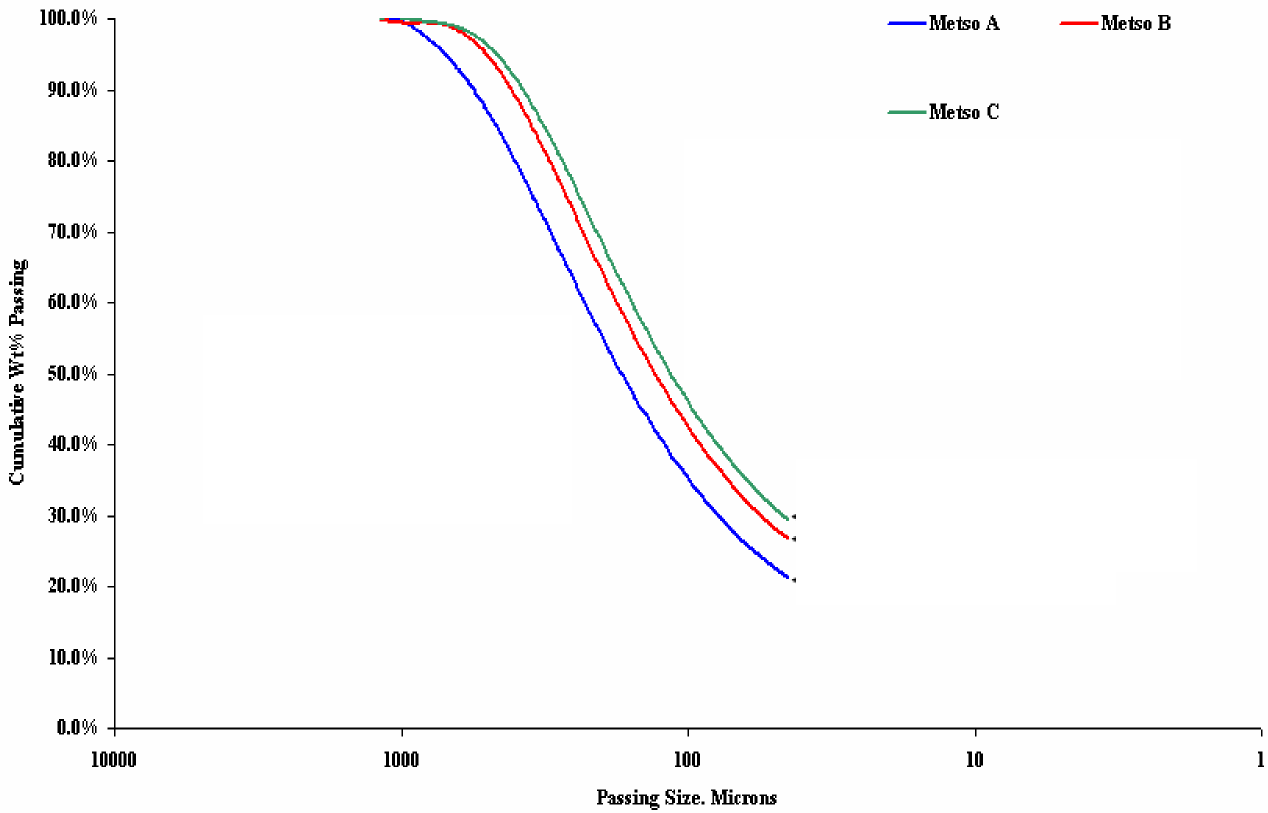
- MFIX-NG
- Polydispersed Flow
- High Resolution Gasifier
- Future Outlook

Polydispersity – Goals

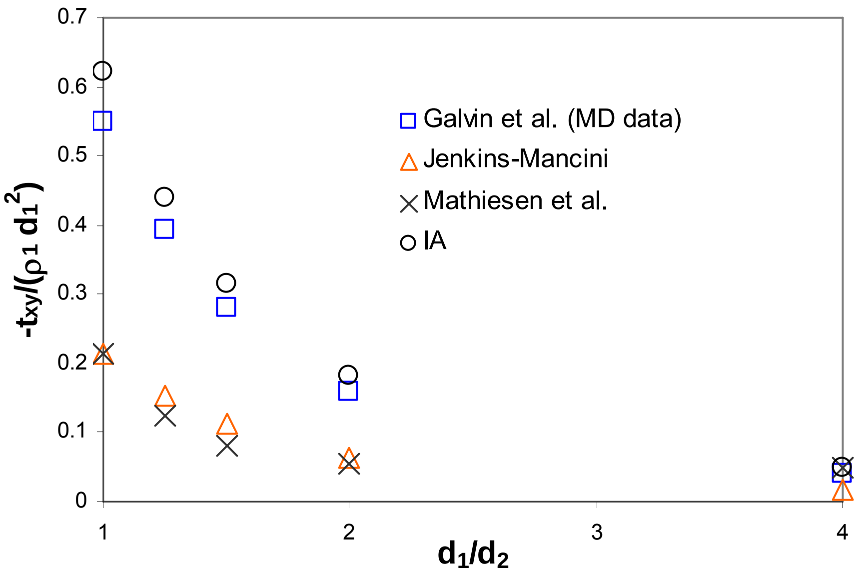
- **Implementation of I-A theory in MFIX (*www.mfix.org*)**
- **Verification and validation of theory with:**
  - Experimental data produced at NETL, U. of Colorado and PSRI as well as data from the literature.
  - Numerical-experiments using discrete particle techniques.
- **Application of theory to large-scale coal gasifier**

Motivations and Justification

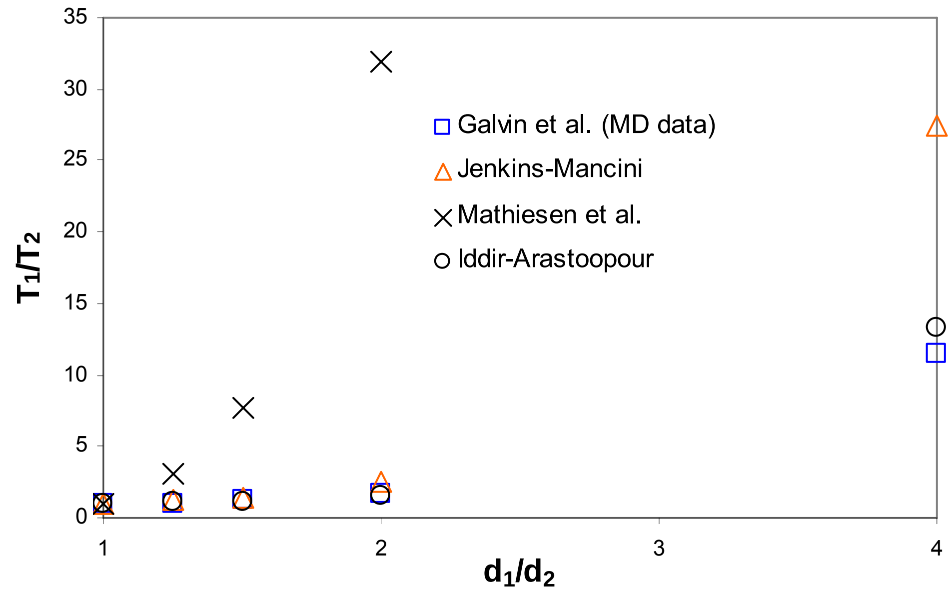
- **Powders found in nature and those used in industry usually have wide size distribution. E.g. coal used in transport gasifiers**



Motivation: results of simple shear flow



$$\frac{\rho_1}{\rho_2} = 1,\ \varepsilon_s = 0.3,\ \frac{\varepsilon_{s1}}{\varepsilon_{s2}} = 0.5,\ e = 0.95$$



$$\frac{\rho_1}{\rho_2} = 1,\ \varepsilon_s = 0.3,\ \frac{\varepsilon_{s1}}{\varepsilon_{s2}} = 0.5,\ e = 0.8$$

Energy dissipation in IA theory: $N_{ip} = N_{s,ip}\left(T_p - T_i\right) + N_{sT,ip} + N_{svp,ip}\nabla\cdot\mathbf{v}_p + N_{svi,ip}\nabla\cdot\mathbf{v}_i$

[1] Galvin et al. (2005), [2] Jenkins and Mancini (1987), [3] Mathiesen et al. (1999)
[4] Iddir and Arastoopour, (2005)

Brief description of I-A theory

$$\frac{\partial}{\partial t}(\varepsilon_i \rho_i \mathbf{v}_i) + \nabla\cdot(\varepsilon_i \rho_i \mathbf{v}_i \mathbf{v}_i) = -\nabla\cdot(\mathbf{P}_{ki} + \mathbf{P}_{ci}) + \frac{\varepsilon_i \rho_i}{m_i}\mathbf{F}_{iext} + \sum_{p=1,\, p\neq i}^{N} \mathbf{F}_{Dip}$$

$$\mathbf{P}_{ki} + \mathbf{P}_{ci} = P_{s,i}\mathbf{I} - 2\mu_i^{\,1}\mathbf{S}_i - \xi_i^{\,1} tr(\mathbf{D}_i)\mathbf{I} - 2\sum_{p=1}^{N}\left(\mu_{ip}^{\,2}\mathbf{S}_p\right) - \sum_{p=1}^{N}\left(\xi_{ip}^{\,2} tr(\mathbf{D}_p)\mathbf{I}\right)$$

$$\mathbf{F}_{Dip} = F_{s,ip}(\mathbf{v}_p - \mathbf{v}_i) + F_{snu,ip}(n_p \nabla n_i - n_i \nabla n_p) + F_{sTi,ip}\nabla T_i + F_{sTp,ip}\nabla T_p$$

$$\frac{3}{2}\frac{\varepsilon_i \rho_i}{m_i}\frac{D\Theta_i}{Dt} + \nabla\cdot(\mathbf{q}_{ki} + \mathbf{q}_c) + (\mathbf{P}_{ki} + \mathbf{P}_{ci}):\nabla \mathbf{v}_i = \sum_{p=1}^{N}\left(N_{ip} - \mathbf{v}_i \mathbf{F}_{\mathrm{Dip}}\right)$$

$$\mathbf{q}_{ki} + \mathbf{q}_{ci} = -K_{sTi,i}\nabla\Theta_i + \sum_{p=1,\, p\neq i}^{N} K_{sTp,ip}\nabla\Theta_p$$

$$+\sum_{p=1}^{N} K_{sv,ip}(\mathbf{v}_i - \mathbf{v}_p) + \sum_{p=1}^{N} K_{snu,ip}(n_i \nabla n_p - n_p \nabla n_i)$$

$$N_{ip} = N_{s,ip}(\Theta_p - \Theta_i) + N_{sT,ip} + N_{svp,ip}\nabla\cdot\mathbf{v}_p + N_{svi,ip}\nabla\cdot\mathbf{v}_i$$

Accomplishments

- **I-A theory was implemented in MFIX open-source CFD code.**

- **I-A model modifications include:**
  – Removed drag term contribution to granular energy equation.
  – Granular stresses and fluxes are now additive.
  – Correct dilute limit for granular viscosity and conductivity.
  – Modified Johnson-Jackson and Jenkins wall BC's.

- **Other code enhancements for polydisperse systems:**
  – Added 3 radial distribution functions.
  – Added gas/solids drag law based on LBM.

- **Code verified for simple granular shear flow.**

- **Code validation with experimental data:**
  – Currently under way using Joseph et al. (2007) data.
  – Qualitative validation in dilute riser flow.

Assessment of Kinetic Theory in Dense Fluidized Beds

- **Assess the validity of the binary kinetic theory of Iddir & Arastaoopour theory (IA) (2005)**
  - Compare with axial segregation results of Joseph et al. (2007): experiments of a bidisperse fluidized bed at low gas velocities

- **Assess the impact of a kinetic theory model in bidisperse fluidized beds and identify dominate terms:**
  - Compare predictions from:
    - rigorous binary kinetic theory model of IA
    - formally monodisperse kinetic theory model of Lun et al. (1984)
    - without any kinetic theory model

Joseph et al. (2007)

Assessment of Kinetic Theory in dilute riser

- **Assess the validity of the binary kinetic theory of Iddir & Arastaoopour theory (IA) (2005)**
  – Compare with radial segregation results of Mathiesen et al. (1999): experiments of a bidisperse dilute riser flow

- **Assess the impact of a kinetic theory model in bidisperse riser flow and identify dominate terms that cause lateral segregation**

Mathiesen et al. (1999)

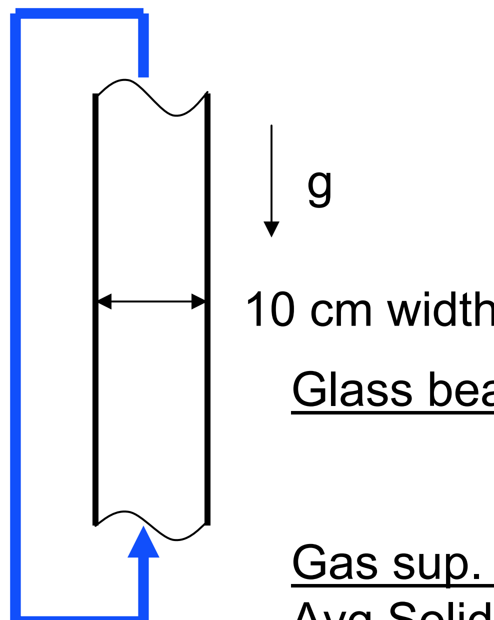
Fully-developed upward *dense* gas/solids flow in a channel

1-D channel has 1 computational cell in flow-wise direction.

2-D channel has cell aspect ratio equal to one.

Johnson-Jackson wall BC with ϕ = 1e-04 and e_w = 0.7.

Upward flow with periodic boundaries



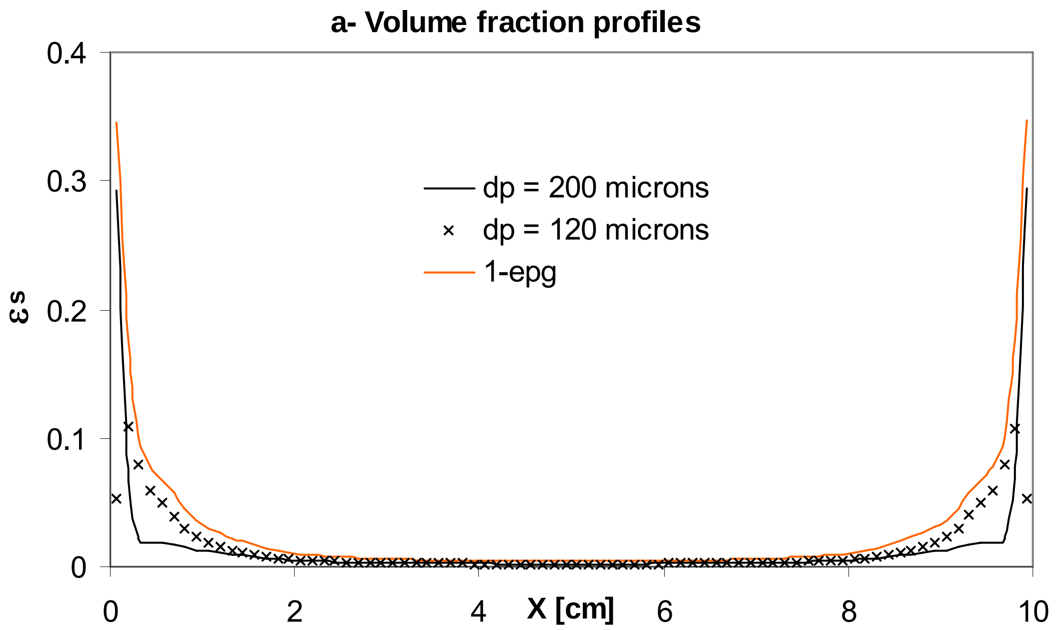
<u>Glass beads</u> : 2.4 g/cm3 density
200 &120 micron diameter
0.95 restitution coef.

<u>Gas sup. Velocity fixed at</u>: 5.5 m/s

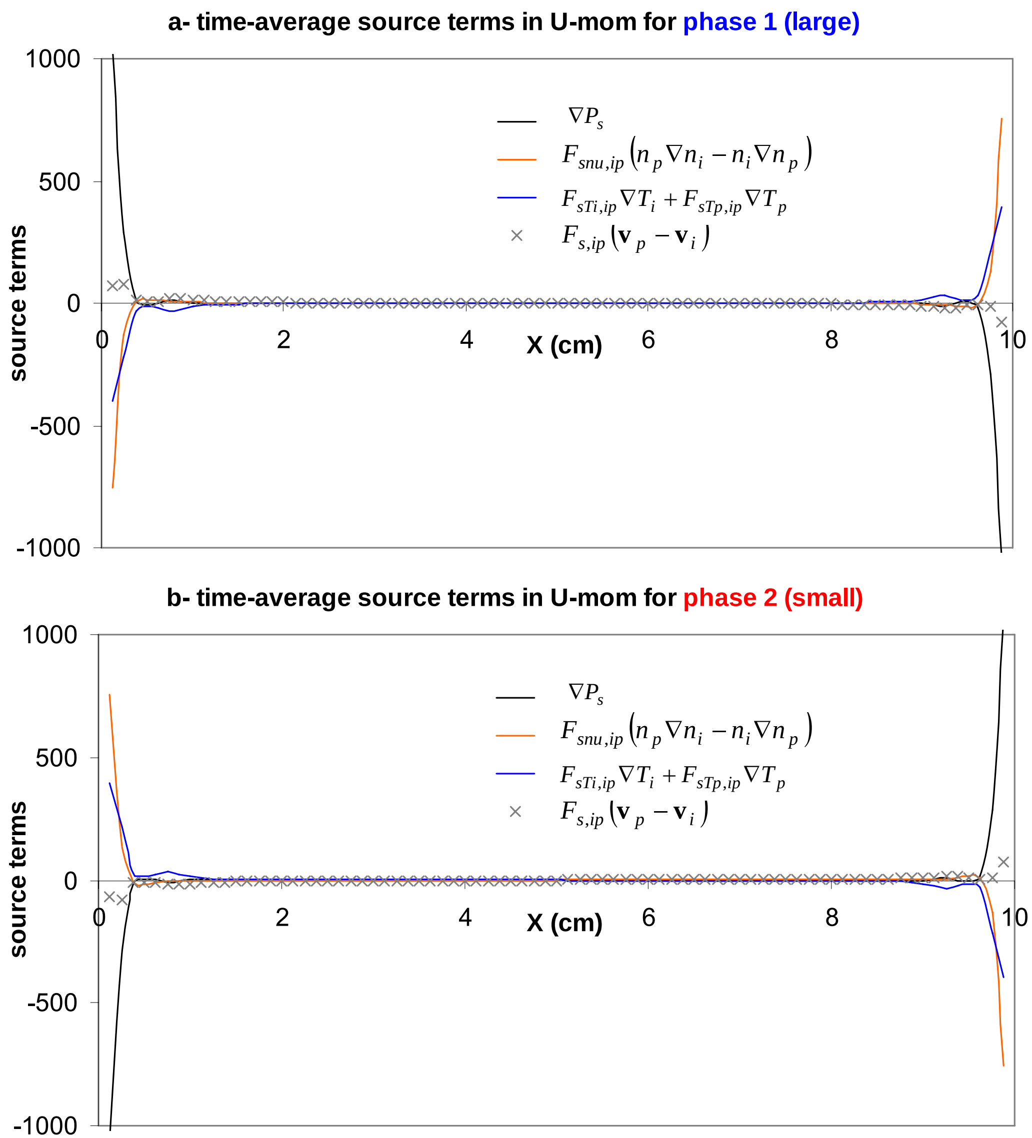
<u>Avg Solids volume fraction fixed at</u>: 3%

Three concentration of initial powder mixtures was used (10, 50 and 90%).

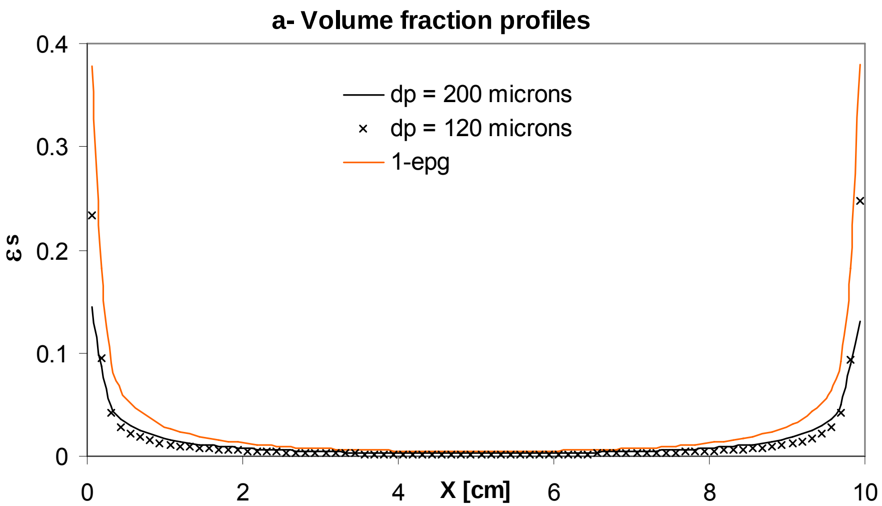
Time-averaged solids volume fraction profiles

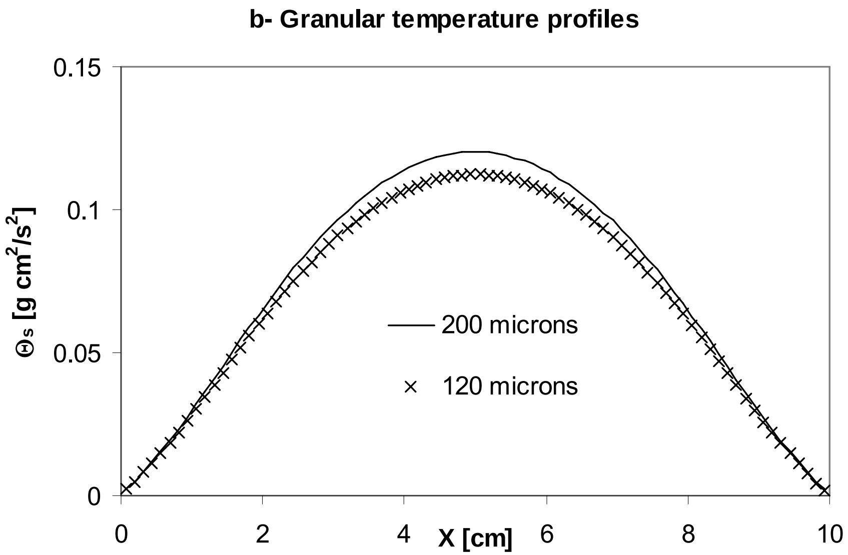


Time-averaged lateral momentum of major source terms

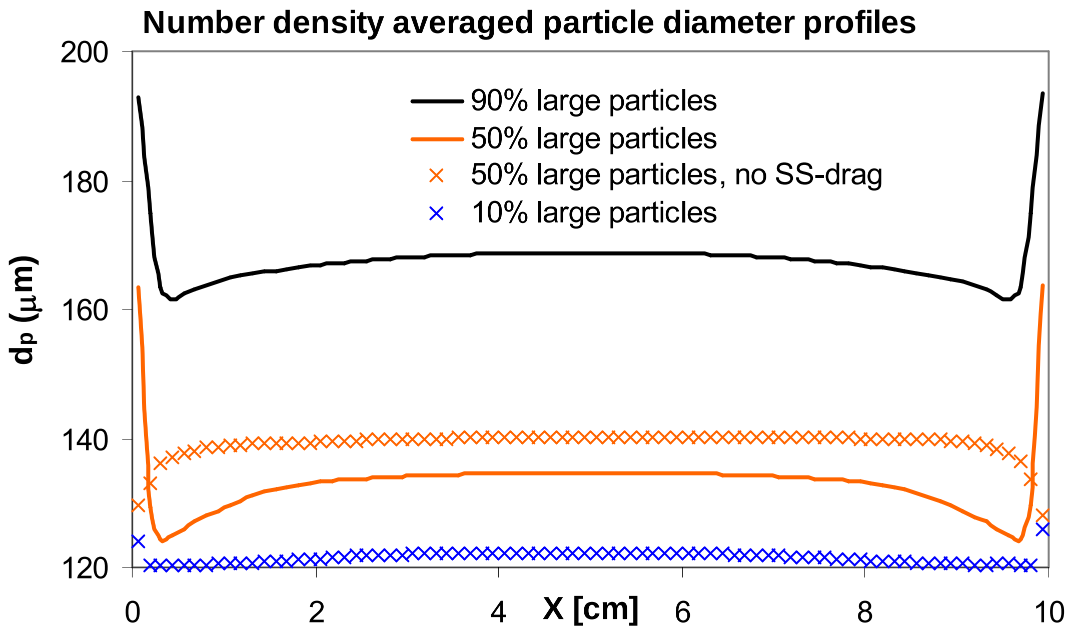


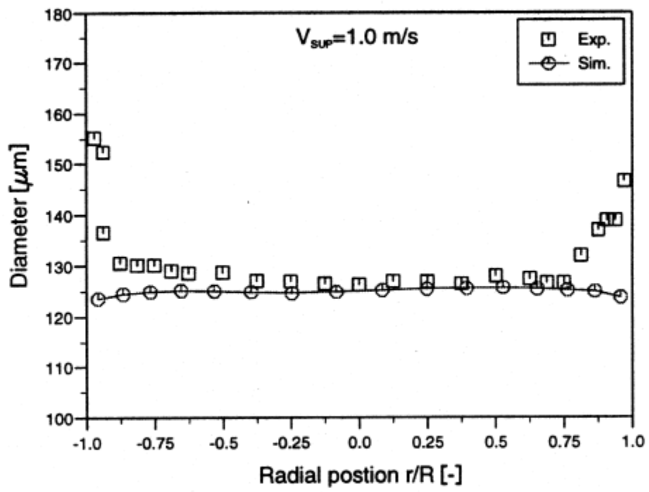
Time-averaged solids volume fraction profiles without S-S drag terms





Time-averaged particle diameter (number averaged) profiles using the full I-A theory





From experimental data of Mathiesen et al. *(Inter. J. of multiphase flow, 26 (2000) 387-419)* using 120 and 185 microns glass beads.

Polydispersity Summary

- **I-A theory was implemented in MFIX and verified using a simple granular shear flow.**

- **I-A theory comparison with experiments:**
  - predicts the right segregation trends in dilute riser flow.
  - Disagreements observed in dense systems are currently under investigation[1].

1. Gera et al. (2004)

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High Res Gasifier Objectives

- **Programmatic goal: High resolution (~1 mm grid-size) gasifier simulations to help with the design of commercial-scale gasifiers**
- **Project goal: Capability to sufficiently resolve the CCPI gasifier**
  - Conduct a 10 M grid production simulation of CCPI gasifier with roughly one week turn-around time
  - Develop the capability for conducting such MFIX simulations

Challenges

- **Simply running the gasifier simulation on a large number of processors (cores) will not help**
  - Parallel efficiency reduces below 50,000 cells per processor in typical CFD codes → at most 200 cores, ~ ten weeks run time
- **Need to use 2000 cores to reduce the turn around time**
  - Current gasifier simulations use 10's of cores and achieve 20 GFlop/s
  - Increase the number of cores by 100x and the speed to 1 TFlop/s
- **Current mode of I/O handling introduces a bottleneck when the number of cores is increased**
  - e.g., In a 2M-cell case the I/O time increased from1.4 % on 16 cores to 5.9 % on 64 cores
- **Two things must be done to enable high resolution simulations**
  1. Increase the parallel scaling efficiency of MFIX
  2. Develop the ability to do distributed I/O from 100 to 1000's of cores

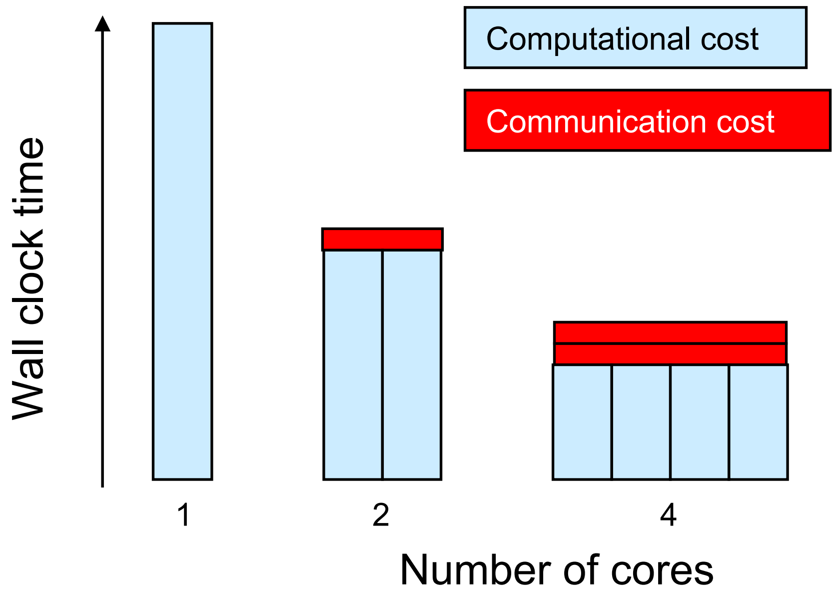
Benchmarking

- **Setup standardized test cases of increasing complexity (A. hydrodynamics only, B. simple chemistry, C. char combustion, D. coal gasification and combustion)**
- **Benchmarking for coarse (262 K cells) and fine grid (2 million cells) performed for Cases A & B.**
  - Cray XT3 (PSC), AMD Opteron cluster (NERSC), and Cray XT4 (NCCS)
- **Extensive TAU-based profiling of MFIX showed the need for reducing global collective operations**

Improve Existing Algorithm

- **Reduced the number of global collective operations (dot products) in BiCGStab linear equation solver from 6 to ~3**
  - Reduced the communication cost by 50%
- **The net speed increase was found to be 10%**

Global collectives become expensive on a large number of cores because of high latency



- Communication time = Latency + (message size)/(band width)
- Latency is the time needed to initiate a message transfer and bandwidth is the rate of message transfer
- The size of messages passed during collective operations on a large number of cores is small
- Then latency accounts for most of the communication cost

Standard BiCGStab iteration needs 6 vector-vector dot products (Original Algorithm)

Compute $r^{(0)} = b - Ax^{(0)}$ for some initial guess $x^{(0)}$
Choose $\tilde{r}$ (for example, $\tilde{r} = r^{(0)}$)
for $i = 1, 2, \ldots$

I $\quad \rho_{i-1} = \tilde{r}^T r^{(i-1)}$

if $\rho_{i-1} = 0$ **method fails**
if $i = 1$
$\quad p^{(i)} = r^{(i-1)}$
else
$\quad \beta_{i-1} = (\rho_{i-1}/\rho_{i-2})(\alpha_{i-1}/\omega_{i-1})$
$\quad p^{(i)} = r^{(i-1)} + \beta_{i-1}(p^{(i-1)} - \omega_{i-1} v^{(i-1)})$
endif
solve $M\hat{p} = p^{(i)}$
$v^{(i)} = A\hat{p}$

II $\quad \alpha_i = \rho_{i-1}/\tilde{r}^T v^{(i)}$

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

III $\quad$ check norm of s; if small enough: set $x^{(i)} = x^{(i-1)} + \alpha_i \hat{p}$ and stop

solve $M\hat{s} = s$
$t = A\hat{s}$

IV, V $\quad \omega_i = t^T s / t^T t$

$x^{(i)} = x^{(i-1)} + \alpha_i \hat{p} + \omega_i \hat{s}$
$r^{(i)} = s - \omega_i t$

VI $\quad$ check convergence; continue if necessary

for continuation it is necessary that $\omega_i \neq 0$
end

6 collectives

Eliminated 2 dot products and combined two into one operation (New Algorithm)

Compute $r^{(0)} = b - Ax^{(0)}$ for some initial guess $x^{(0)}$
Choose $\tilde{r}$ (for example, $\tilde{r} = r^{(0)}$)
for $i = 1, 2, \ldots$
I
$\rho_{i-1} = \tilde{r}^T r^{(i-1)}$
if $\rho_{i-1} = 0$ **method fails**
if $i = 1$
$p^{(i)} = r^{(i-1)}$
else
$\beta_{i-1} = (\rho_{i-1}/\rho_{i-2})(\alpha_{i-1}/\omega_{i-1})$
$p^{(i)} = r^{(i-1)} + \beta_{i-1}(p^{(i-1)} - \omega_{i-1} v^{(i-1)})$
endif
solve $M\hat{p} = p^{(i)}$
II
$v^{(i)} = A\hat{p}$
$\alpha_i = \rho_{i-1}/\tilde{r}^T v^{(i)}$
III
$s = r^{(i-1)} - \alpha_i v^{(i)}$
check norm of s; if small enough: set $x^{(i)} = x^{(i-1)} + \alpha_i \hat{p}$ and stop
solve $M\hat{s} = s$
$t = A\hat{s}$
IV, V
$\omega_i = t^T s / t^T t$
$x^{(i)} = x^{(i-1)} + \alpha_i \hat{p} + \omega_i \hat{s}$
VI
$r^{(i)} = s - \omega_i t$
check convergence; continue if necessary
for continuation it is necessary that $\omega_i \neq 0$
end

3 + 1/(frequency) collectives

Intermediate residual check is eliminated

Combined two independent dot products into one global operation

Final residual checked infrequently

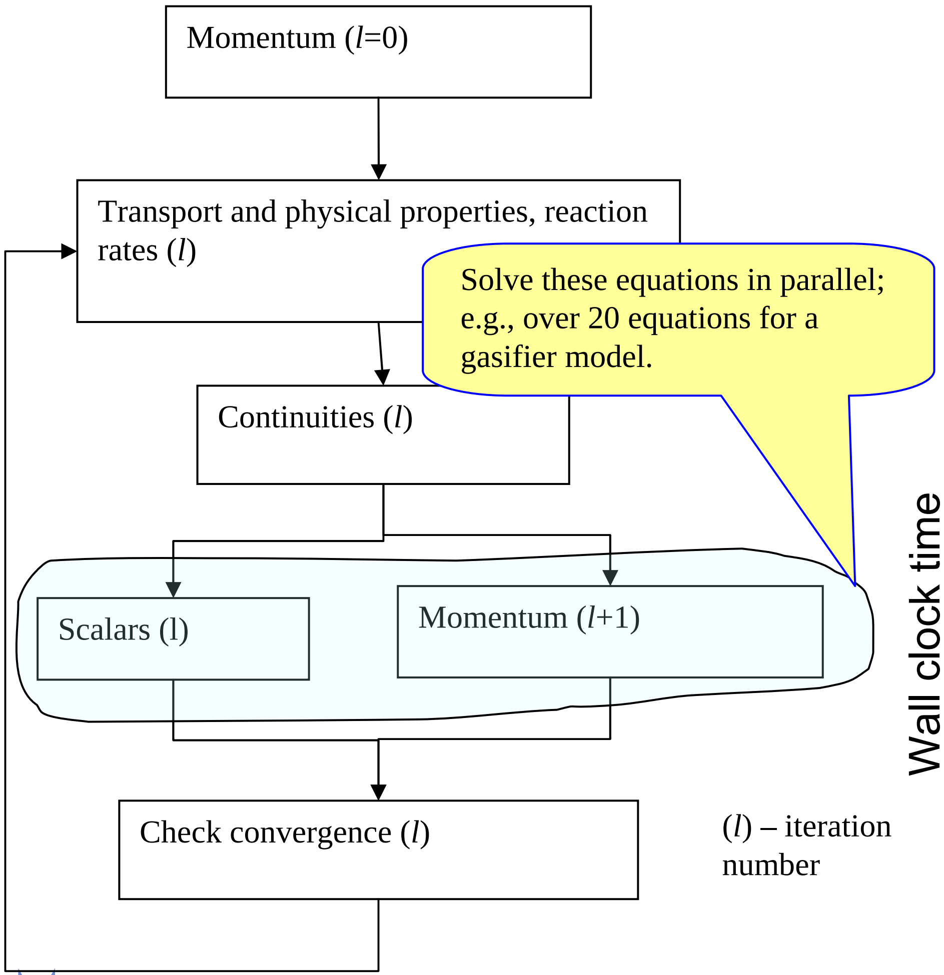
Improve Existing Algorithm

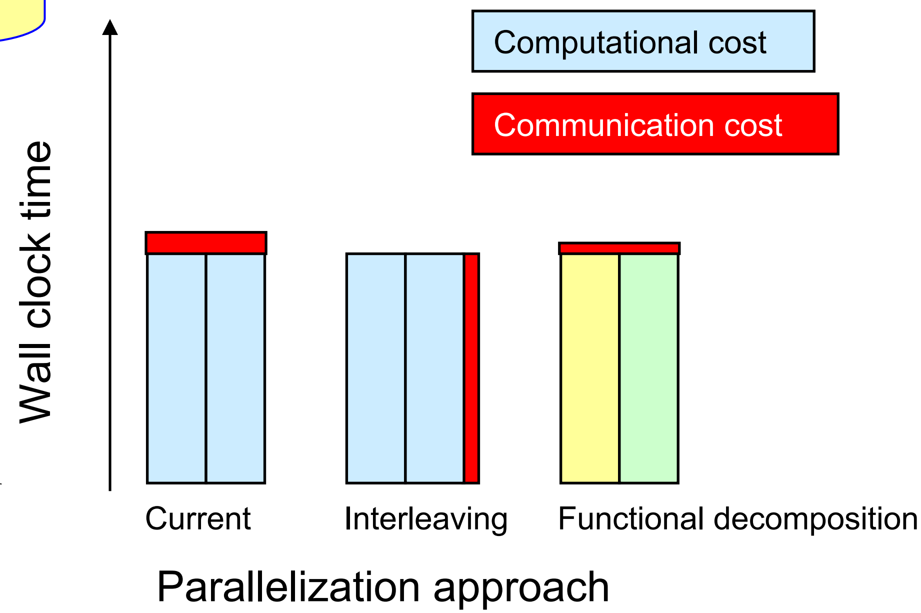
- **Use successive over relaxation (SOR) for all variables except for gas pressure and solids volume fraction**
  - SOR parallelizes better because it does not include any global collectives
  - SOR routine was updated to work with the latest version of the code
  - The gasifier test cases have been tested with this option and seem to run stably
  - Further improvements (e.g., red-black algorithm) to make SOR performance independent of processor decomposition are being considered

Develop New algorithm

- **Evaluated two approaches for solving multiple equations in parallel**
  - Functional decomposition
  - interleaving communications and computations (in linear equation solver)
- **Determined interleaving as the better method**
- **Evaluated a NBC library**

Parallel Solving of Multiple Equations (New Algorithm)





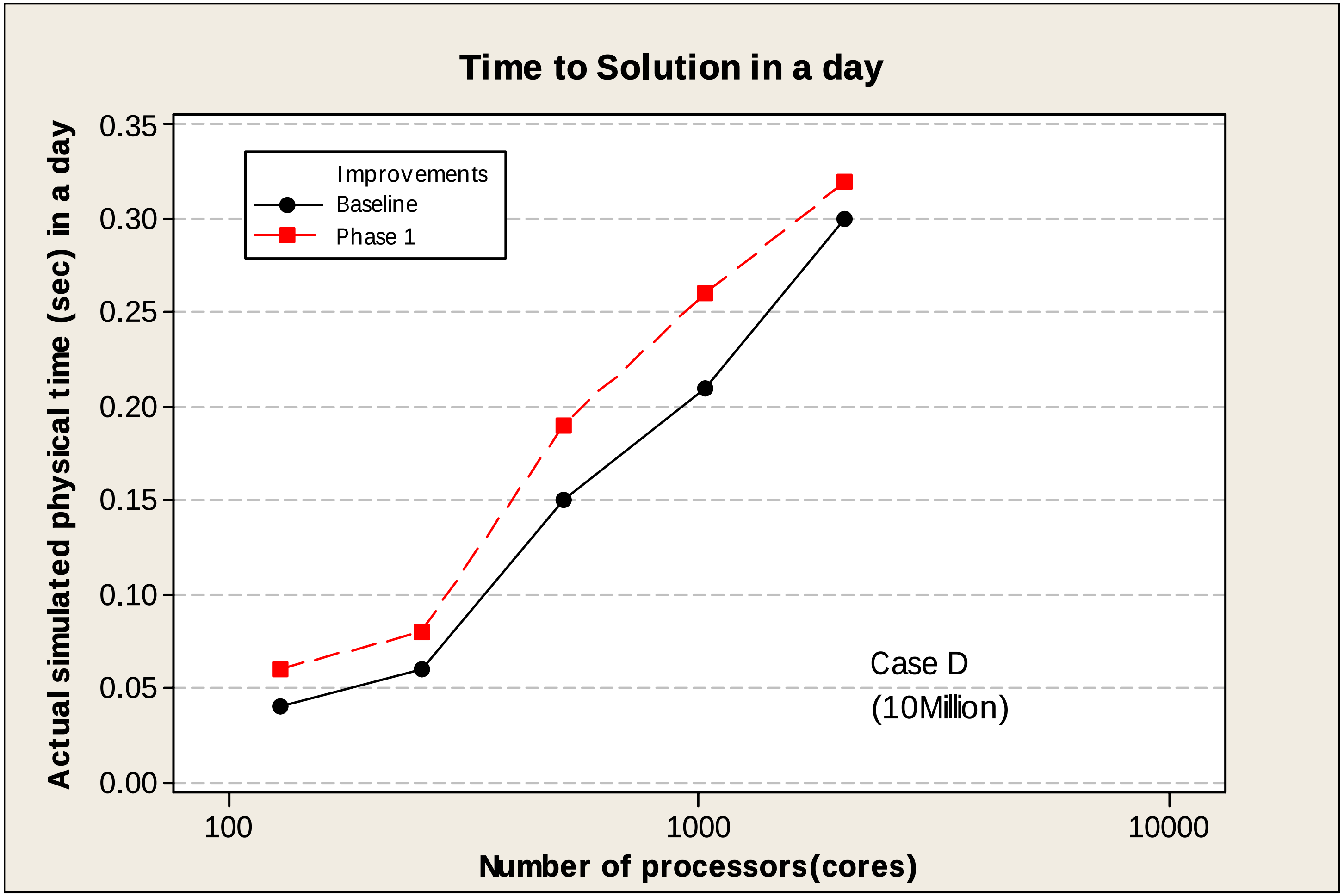
Improving I/O for Massively Parallel Environment

- **Problem: Single files that accumulate all time records become unwieldy to handle and slow to read when the grid size is large**
  - stopping the run and doing a restart_2 requires user intervention and does not retain data from before the restart
- **Solution: Create multiple files with a user defined time interval**
  - Post-processing codes were modified to read this format

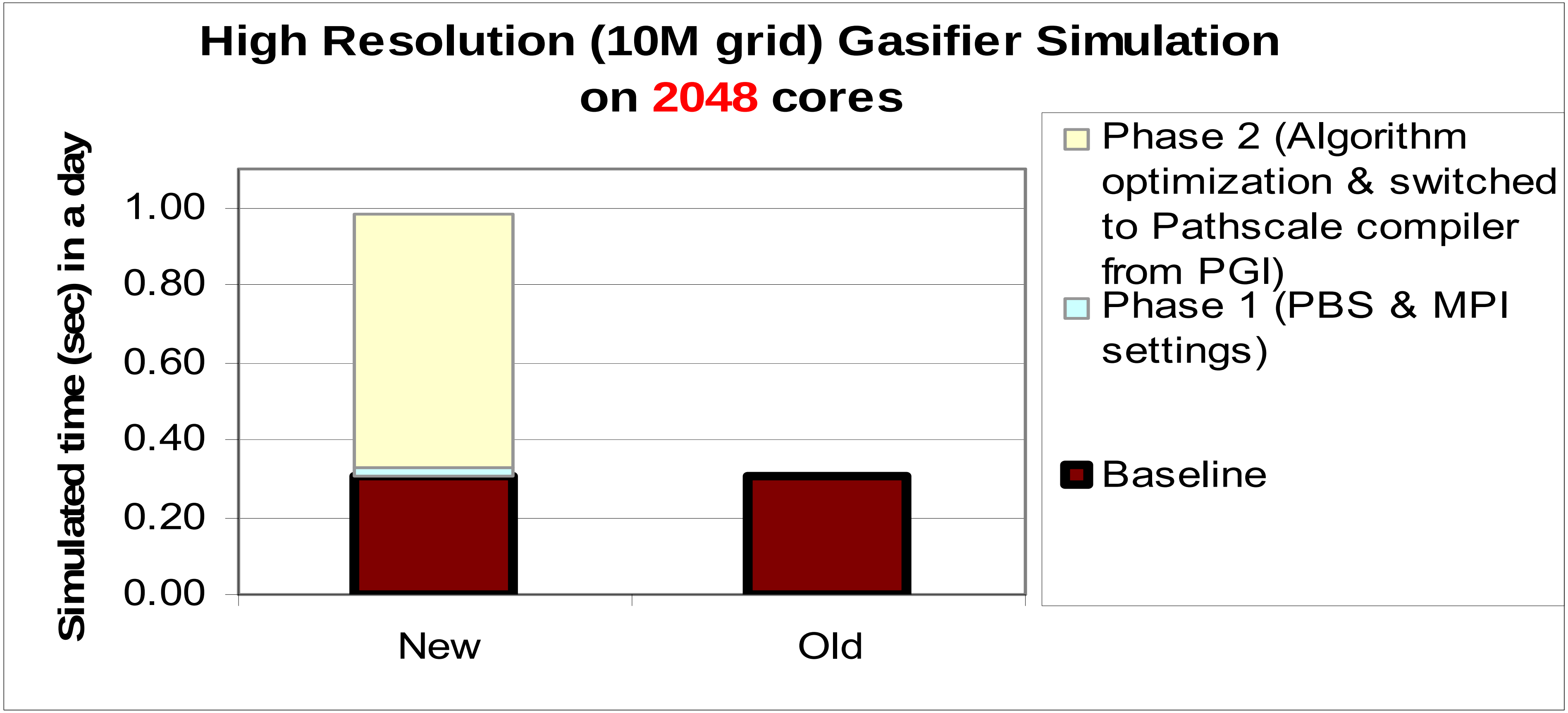
Improving I/O for Massively Parallel Environment

- **Problem: Reading large files containing species mass fraction data was slow**
- **Solution:**
  - Post-processing codes were modified to read data only for the requested species instead of all the species
  - Time required to post-process the results of a case on a 20 x 1176 x 40 grid, 16 species, and 100 time steps
    - Original code: 715 seconds
    - Modified code: 50 seconds

Actual simulated physical time per day for Case D with 10 million cells



Performance improvements achieved



Outline of Presentation

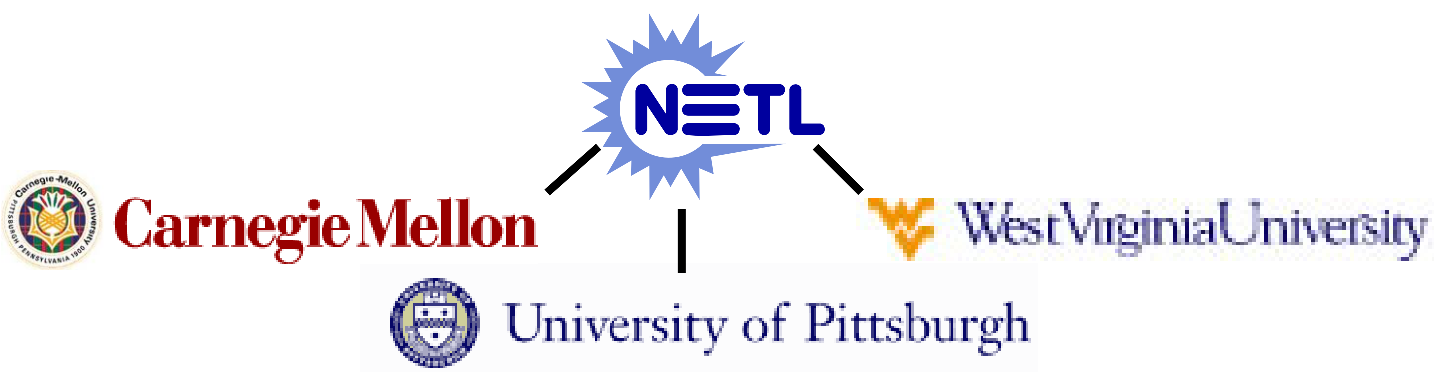
- MFIX-NG
- Polydispersed Flow
- High Resolution Gasifier
- Future Outlook

Goal

- **Ensure that by 2015 multiphase science based computer simulations play a significant role in the design, operation, and troubleshooting of multiphase flow devices in fossil fuel processing plants.**
- **Benefits**
  - Reduce the time and cost to develop efficient fossil fuel plants
  - Troubleshoot and mitigate problems
  - Enable the invention of novel reactor designs for next generation power plants and coal refineries

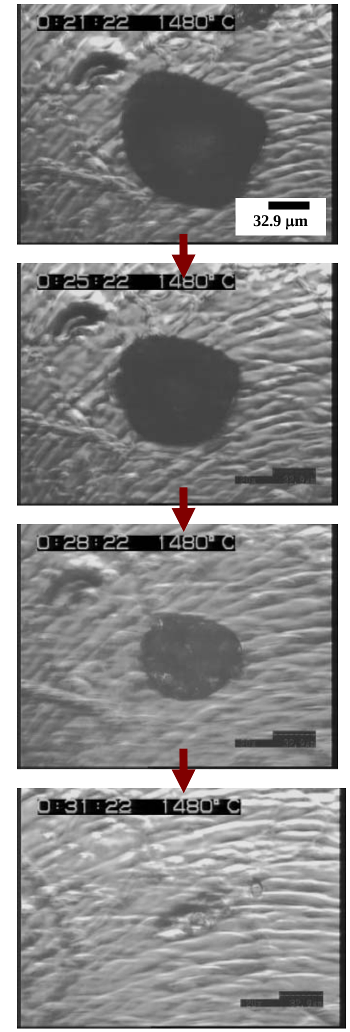
Collaboratory for Multiphase Flow Research (CMFR)

- Develop multiphase flow models and numerical techniques
- Validate the models with well calibrated experiments
- Promote the use of computational tools in industrial practice
- Provide a focal point for collaboration with academic and national labs
- Disseminate information and attract young researchers to the subject



Current Projects – CMFR

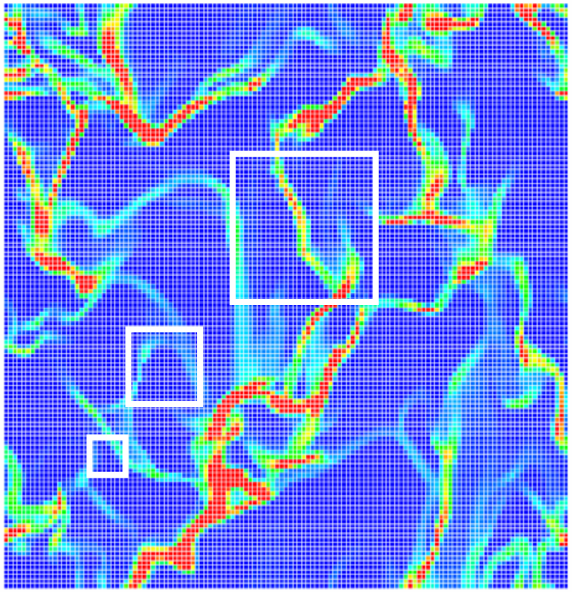
- Task 1: High Resolution Discretization Schemes for Multiphase Flow – TBD (WVU)
- Task 2: OpenFOAM Block Solver Development – Jasak (Wikki/WVU)
- Task 3: Evaluation and Benchmarking of Arches Code – Clarke (WVU)
- Task 4: Dispersion in CFB Riser: Effect of Riser Inlet Configuration – Johnson and Kang (WVU), Monazam (REM)
- Task 5: Discrete Particle Dynamics Simulations – McCarthy (Pitt), Higgs (CMU)
- Task 6: Coal Partitioning/Gasifier Fouling Project – Shadle (NETL), Kuhlman (WVU), Fruehan (CMU), Seetharaman (CMU), REM, NEA, PSU, LTI, SRI
- Task 7: Next generation multiphase flow solver – Prinkey (Aeolus/WVU)
- Task 8: Image Analysis of Circulating Fluid Bed Hydrodynamics – Ross (WVU)



Mineral particle dissolution in high temperature slag.

Extramural Projects

- **Dispersion Coefficient**
  - D. Gidaspow, IIT
- **Filtered two-fluid equations**
  - S. Sundaresan, Princeton U.
- **Kinetic theory of polydispersed systems**
  - C. Hrenya, U. Colorado
  - R. Fox, Iowa State U.
  - S. Subramaniam, Iowa State U.
  - S. Sundaresan, Princeton U.
  - R. Cocco, PSRI
- **Frictional flow Regime**
  - S. Sundaresan, Princeton U.
  - S. Subramaniam, Iowa State U.
  - G. Tardos, CCNY



Filtered “data” generated through highly resolved MFIX simulations. Andrews and Sundaresan (Princeton University), 2005.

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- Dr. Hrv Jasak – Wikki Ltd.

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