Exascale simulation for the design of industrial-scale chemical reactors

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MFIX Overview
MFiX – Open-source multiphase CFD code

4,500+ all-time MFiX registrations

Top 5 Countries:
- Germany: 162
- Brazil: 201
- India: 373
- China: 725
- USA: 1,185
Examples of MFiX GUI
Gas-solids flow in a fluidized bed reactor

Particle flow field in NETL’s Circulating Fluidized Bed (CFB) system.

MFiX offers a suite of multiphase models

- **Direct Numerical Simulation (DNS)**: Track all particles and resolve the gas flow around them.
- **Discrete Element Method (DEM)**: Track all particles; use drag laws instead of resolving gas-solids boundary.
- **Hybrid**: Some of the particles are tracked; others treated as a continuum.
- **Two-Fluid Model (TFM)**: Particles modeled as a continuum or a second fluid.
- **Particle-in-Cell (PIC)**: Track parcels or clouds of particles.
- **Reduced Order Models (ROM)**: Simplified models for specialized applications.
Gas Phase – Navier-Stokes like equations

\[
\frac{\partial}{\partial t} (\varepsilon_g \rho_g) + \frac{\partial}{\partial x_j} (\varepsilon_g \rho_g U_{gj}) = 0
\]

\[
\frac{\partial}{\partial t} (\varepsilon_g \rho_g U_{gi}) + \frac{\partial}{\partial x_j} (\varepsilon_g \rho_g U_{gj} U_{gi}) = -\varepsilon_g \frac{\partial P_g}{\partial x_i} + \frac{\partial \tau_{gij}}{\partial x_j} + f_{gi} + \varepsilon_g \rho_g g_i
\]

Particles – Newton’s law

\[
\frac{dx_{pi}}{dt} = u_{pi}
\]

\[
m_p \frac{du_{pi}}{dt} = m_p g_i + f_{pi} + m_p A_{coll}
\]

\[
I_{ij} \frac{d\omega_{pj}}{dt} = T_{pi}
\]

- Unresolved flow near particle-fluid interface → gas-particle forces drag, added mass, lift ...
- No numerical diffusion in particle phase
- Particle contacts are resolved

A_{coll} describes both enduring contacts and collisions

Two-Fluid Model

Gas and Granular Phases

\[
\frac{\partial}{\partial t} (\varepsilon_m \rho_m) + \frac{\partial}{\partial x_j} (\varepsilon_m \rho_m U_{mj}) = 0
\]

\[
\frac{\partial}{\partial t} (\varepsilon_m \rho_m U_{mi}) + \frac{\partial}{\partial x_j} (\varepsilon_m \rho_m U_{mj} U_{mi}) = -\varepsilon_m \frac{\partial p_g}{\partial x_i} + \frac{\partial \tau_{mij}}{\partial x_j} + \sum_{l=0}^{M} I_{mli} + \varepsilon_m \rho_m g_i
\]

Granular stress:

Frictional theory + Kinetic theory of granular flow

Granular energy transport equation

\[
\frac{3}{2} \varepsilon_m \rho_m \left[ \frac{\partial \theta_m}{\partial t} + U_{mj} \frac{\partial \theta_m}{\partial x_j} \right] = \frac{\partial}{\partial x_j} \left( \kappa_m \frac{\partial \theta_m}{\partial x_j} \right) + \tau_{mij} \frac{\partial U_{mi}}{\partial x_j} + \Pi_m - \varepsilon_m \rho_m J_m
\]


\begin{itemize}
\item Current workhorse in industry
\item Cannot resolve distribution in particle-scale properties: size, density, chemical conversion
\item Cannot describe regions where strain rate is zero
\item Unresolved particle contacts \rightarrow granular stress
\end{itemize}
Gas-solids flow research reactors

- High-G Reactors
- Rotating Fluidized Bed
- Rectangular Bed
- Moving Bed
- Carbon capture Unit
- Rectangular & 10 cm CFB
- Spouted Bed
- Rectangular Bed
- Vortex Bed
- Circulating Fluidized Bed

15.4 m
Reactor optimization based on CFD

Optimized Flow for Separation – Model and Experiment
Mini circulating fluidized bed
Axial pressure gradient

Comparison of MFIx-TFM and MFIx-DEM (Coarse-grained) results with experimental data

1. T. Li, MFIx simulations of gas-solid flow in large scale fluidized bed reactors, the 39th IFPRI Annual General Meeting, Jun. 17-21, 2017, Philadelphia.
Micro-Encapsulated Carbon Sorbent (MECS)

MECS\(^1\) capsules
*(Image: John Vericella, LLNL)*

- Elastic, deformable shell
- Capsule size/density changes
- Precipitation of solids inside capsule
- Water loss/uptake during \(CO_2\) capture
- Complex liquid equilibrium reactions

\(^1\)Vericella et al., *Nature Comms.*, v. 6, 2015

MECS Capsule model

MECS fluidized bed simulation
Integrated Waste Treatment Unit, Idaho

Guide performance improvement of nuclear waste clean up reactor

Low Flow
0.6 gpm

High Flow
1.25 gpm

Evaporates water
Reduces nitrates
Volatile and reform organics

Carbon Reduction Reformer

CO₂, H₂O, N₂, O₂

H₂O, N₂, CO₂, CO, CH₄, and short-chain organics

Denitrification and Mineralization Reformer

Process gas filter

SBW droplets
Fluidizing Gas
Coal
Solids Product

Fluidizing Gas
Biofuels reactor

Upgrading reactor models to help pilot-scale testing

- Riser: Height: 7.05 m, diameter: 0.092 m
- Outlet diameter: 0.038 m
- Solids inlet diameter: 0.049 m
- Pyrolysis vapor inlet diameter: 0.047 m
- Distributor: 16 holes with diameter of 0.00625 m
Using Solids as Heat Transfer “Fluid” for CSP Receivers

**Challenge:** Molten salts unstable > 600°C

**Idea:** Use inert solids (e.g., sand) as heat transfer “fluid”
- can operate at higher T and thus increased efficiency
- good thermal storage for on/off diurnal cycle
- Sand is inexpensive
Using Solids as Heat Transfer “Fluid” for CSP Receivers

MFIX DEM simulations (~10⁷ particles on Titan)

Informed design

Drove development of continuum theory

Morris et al., AIChE J. (2016)
Morris et al., Solar Energy (2016)
Morris et al., Int. J. Heat Mass Transfer (2015)
Volcanic hazards from explosive eruptions

Soufrière Hills volcano   MFiX-TFM simulation


George Bergantz/University of Washington
Path of ‘magma mush’ inside a volcano

Crystal mixing by granular vorticies

Crystals entrained into mixing bowl


George Bergantz/University of Washington
MFIX-Exa Project
Acknowledgments

This research was supported by the Exascale Computing Project (http://www.exascaleproject.org), a joint project of the U.S. Department of Energy’s Office of Science and National Nuclear Security Administration, responsible for delivering a capable exascale ecosystem, including software, applications, and hardware technology, to support the nation’s exascale computing imperative.

Project Number: 1.2.1.21
The Exascale Computing Project (ECP)

Collaboration
2 US Department of Energy organizations
- Office of Science
- National Nuclear Security Administration

Execution
800 researchers (22 laboratory and agency partners; 39 universities) engaged in:
- 66 software projects
- 25 science application projects
- 5 co-design centers

Goal
Drive pre-exascale science, application development, hardware and software R&D to ensure that the US has a capable exascale ecosystem in 2021
What is a **capable** exascale computing system?

- Delivers 50× the performance of today’s 20 PF systems, supporting applications that deliver high-fidelity solutions in less time and address problems of greater complexity
- Operates in a power envelope of 20–30 MW
- Is sufficiently resilient (perceived fault rate: ≤1/week)
- Includes a software stack that supports a broad spectrum of applications and workloads

This ecosystem will be developed using a co-design approach to deliver new software, applications, platforms, and computational science capabilities at heretofore unseen scale
From Giga to Exa, via Tera & Peta*

Performance from parallelism

*S. Borkar, Intel
Exascale simulation for the design of industrial-scale chemical reactors

Goal: Develop an efficient high-fidelity multiphase flow modeling capability to aid in the design of industrial-scale chemical reactors

Simulation with high-fidelity, physics-based models is essential to scaling up from lab → pilot → commercial scale reactors
• Reduction in cost
• Reduction in time to deployment
• Risk mitigation at large scales

Proposed increase in fidelity will aid in the development of CO$_2$ capture technology (supported by DOE-FE) as well as unlock the ability to simulate a host of relevant problems in energy, chemical processing and pharmaceutical industries

Lab-scale testing of a novel CO$_2$ capture method at NETL

Petra Nova, world’s largest post-combustion CO$_2$ capture plant, began operation in January 2017
MFIX-Exa challenge problem
Simulate 1 MWe chemical looping reactor with CFD-DEM

<table>
<thead>
<tr>
<th>Year</th>
<th>Particle Count</th>
<th>Time to Solution</th>
</tr>
</thead>
<tbody>
<tr>
<td>2017</td>
<td>$60 \times 10^6$</td>
<td>600 days</td>
</tr>
<tr>
<td>2023</td>
<td>$5 \times 10^9$</td>
<td>0.5 days</td>
</tr>
<tr>
<td>2026</td>
<td>$100 \times 10^9$</td>
<td>2 days</td>
</tr>
</tbody>
</table>

Time-to-solution is estimated for 5 minutes of real time in all cases; the 2023/2026 values are guestimates.
Achieving the desired performance in MFIX-Exa
The 10 Year Challenge Problem

Risk mitigation strategies
- Hybrid method
- Coarse grained DEM

Improved solver
- Modern low-Ma projection method
- Adaptive mesh refinement

Increased computational power

Parallel Performance
- Balanced fluid & particle work load
- Optimized particle-particle interaction tracking: increased on-node performance and reduced off-node communication
- Scalable linear equation solver

Baseline: MFIX-2016-1
MFIX-Exa brings together three teams and two codes

- 60+ years of experience in multiphase modeling and MFIX (NETL and CU)
- 60+ years of experience in large-scale, multiscale multiphysics applications (LBNL)
- 90+ years of experience in high performance computing

- 30+ years of development
- 12 developers at NETL
- 4,000+ registered users
- 175+ downloads per month
- 200+ citations per year
- Applied for reactor design and troubleshooting in fossil, bio, nuclear, and solar energy; chemicals industry; and nuclear waste treatment

- Block-structured AMR software framework supported by ECP Co-Design Center
- Supports multiple DOE codes: accelerator modeling, astrophysics, combustion, cosmology, and subsurface
- Long development history
Open source software

- Support for solution of PDE's on hierarchical adaptive mesh with particles and embedded boundary representation of complex geometry
  - Core functionality in C++ with frequent use of Fortran90 kernels
- Support for multiple modes of time integration
- Provides support for explicit and implicit single-level and multilevel mesh operations, multilevel synchronization, particle, particle-mesh and particle-particle operations
- Hierarchical parallelism -- hybrid MPI + OpenMP with logical tiling to work efficiently on new multicore architectures
- Native multilevel geometric multigrid solvers for cell-centered and nodal data
- Highly efficient parallel I/O for checkpoint/restart and for visualization – native format supported by Visit, Paraview, yt

https://www.github.com/AMReX-Codes/amrex

Applications: accelerator modeling, astrophysics, combustion, cosmology, multiphase flow…
First version of MFIX-Exa developed and verified

Many verification cases

Four benchmark cases that mimic sections of a CLR

Freely falling particle with wall collision

Couette flow in a channel

Two stacked compressed particles

Fluidized Bed

Settling Bed

Riser Flow

Homogeneous Cooling System
Preliminary performance analysis conducted

Scaling of MFIX-Exa and MFIX-2016-1 Release on Cori-KNL (run for 50ms)
MFIX-Exa released with hybrid parallelism and dynamic load balancing

- Take full advantage of many-core architectures through Hybrid parallelism (MPI + OpenMP)
- Minimize run time through Dynamic load balancing

Two load balancing strategies

Based on number of grid cells

Based on number of particles
Migrated MFIX-DEM hydrodynamics to the AMReX framework.

MFIX-Exa Status and Development Plans

- EB Particles
  - Replace SIMPLE
  - Performance! Performance! Performance!

- EB Fluid
  - Performance!

- CLR Demonstration

Timeline:
- 2017
- 2018
- 2019
Thank You!

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