Modeling and simulation of multiphase flows

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NATIONAL ENERGY TECHNOLOGY LABORATORY

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Outline

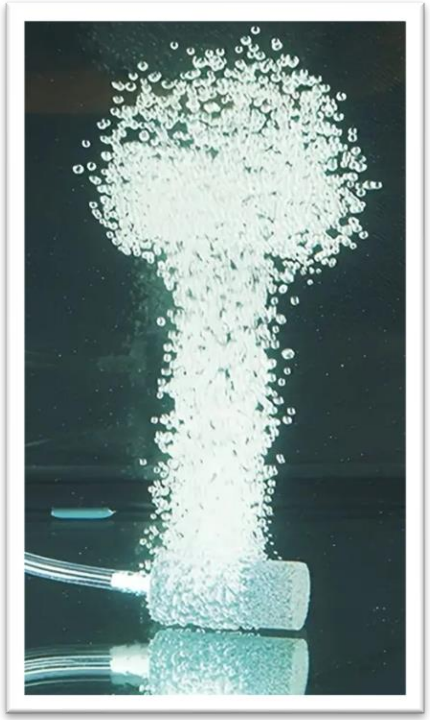
- **Background**
  - What are multiphase flows?
  - Why are they of interest?
- Multiphase flow modeling
  - Computational strategies
  - MFIX / MFIX-Exa
  - MFIX-Exa overview
  - MFIX-Exa strong & weak scaling
- Applications
  - Chemical looping
  - FCC regenerator
  - Unbounded fluidization
  - Batch slurry reactor

MFiX MFIXExa MFAL
Nodeworks Tracker

Background

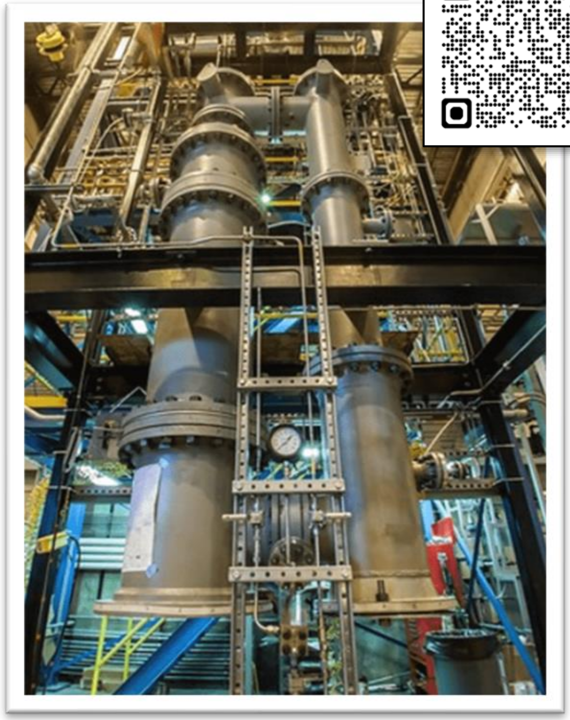
Multiphase flows: What are they?

Multiphase flows are everywhere!



Bubbles in a fish tank

Eruption of Soufriere Hills, Montserrat, November 2009
Jonathan Stone, USGS



Chemical looping reactor (CLR)
NETL

Background

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Multiphase flows: What are they?

Gas

Solid

Liquid

A multiphase flow is a flow that contains two or more phases.

Of particular interest to our work:

- Solid particles fluidized by a gas
  - gasification, combustion, carbon capture, …
- Solid particles and/or bubbles in a liquid
  - fermentation, liquefaction, …
- Liquid droplets or films in a gas
  - Sprays, solvents, …

Interface tracking / capturing is not a major focus in our development and application work.

(right) MFIX-Exa fluidized bed simulation of Geldart-A particles diameter: 148micron, density 1300 kg/m^3

Background

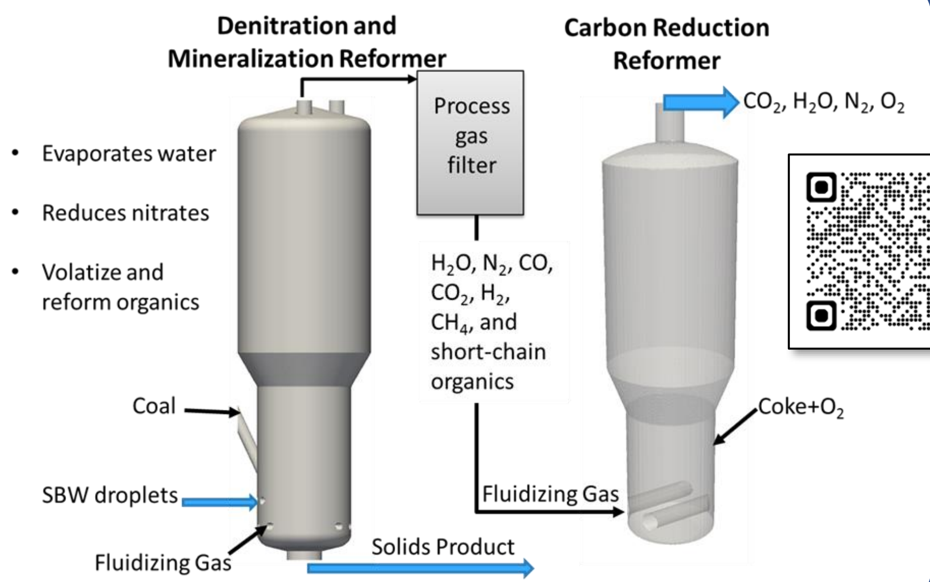
Multiphase flows: Why are they of interest?

Design and assessment of multiphase devices is ***complex*** and ***costly***.

Computational tools are used to

- *expedite deployment*
- *lower costs*
- *reduce risk*

MFIX simulations aided redesign of DOE-EM's Integrated Waste Treatment Unit



- demonstrated that the problem was inherent to the design and could not be overcome under normal operating conditions
- three alternative designs were screened in less than eight months

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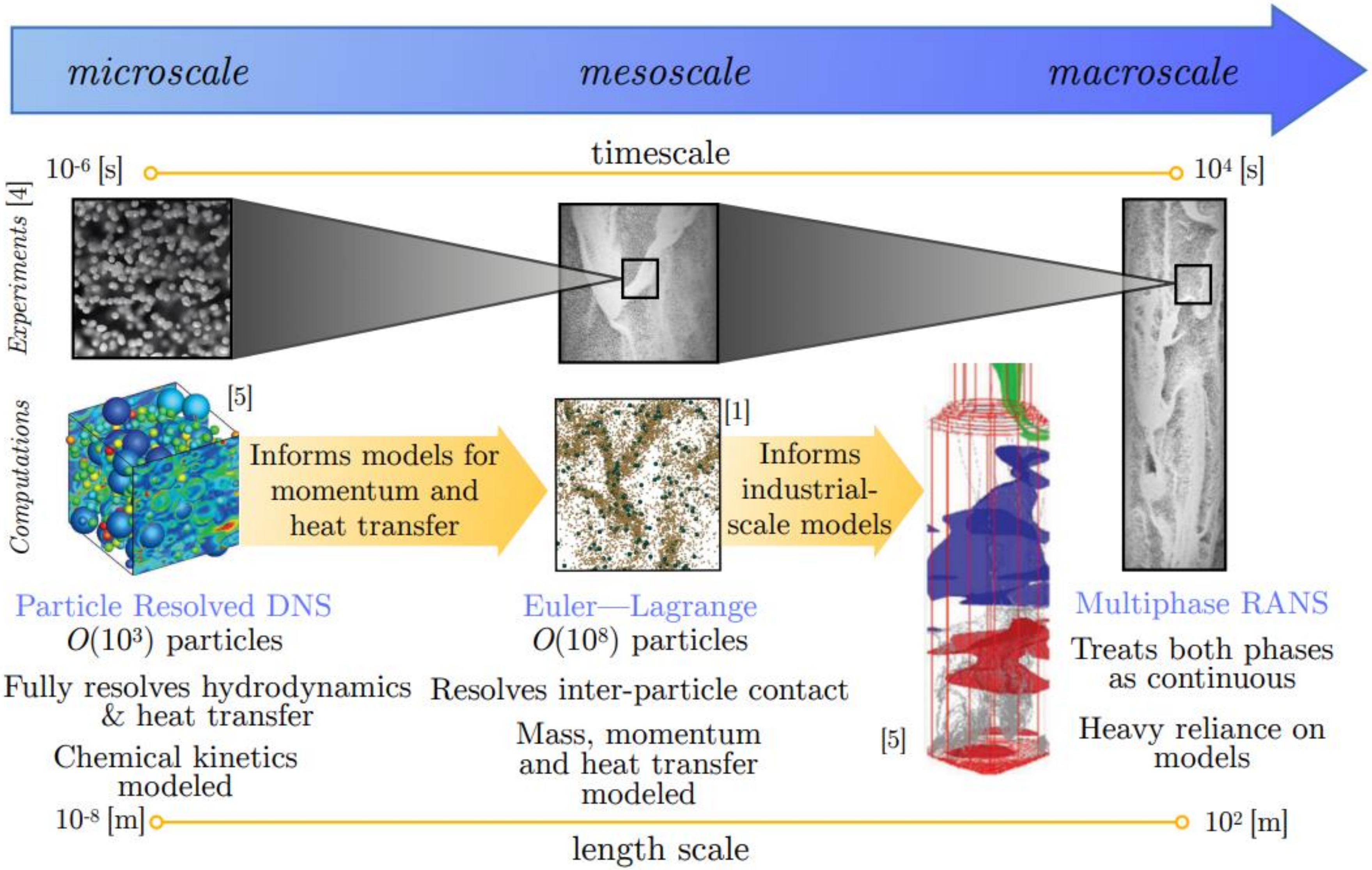
Computational strategies



Slide reproduced with permission:

Beetham (2024) On the Clustering and Settling Behavior of Polydisperse, Gas-solid Flows.

Experimental images

Shaffer and Gopalan (2013) The Science and Beauty of Fluidization

Simulation images

Tenneti and Subramaniam (2014) Particle-Resolved Direct Numerical Simulation for Gas-Solid Flow Model Development.

MFIX Technology Development Timeline

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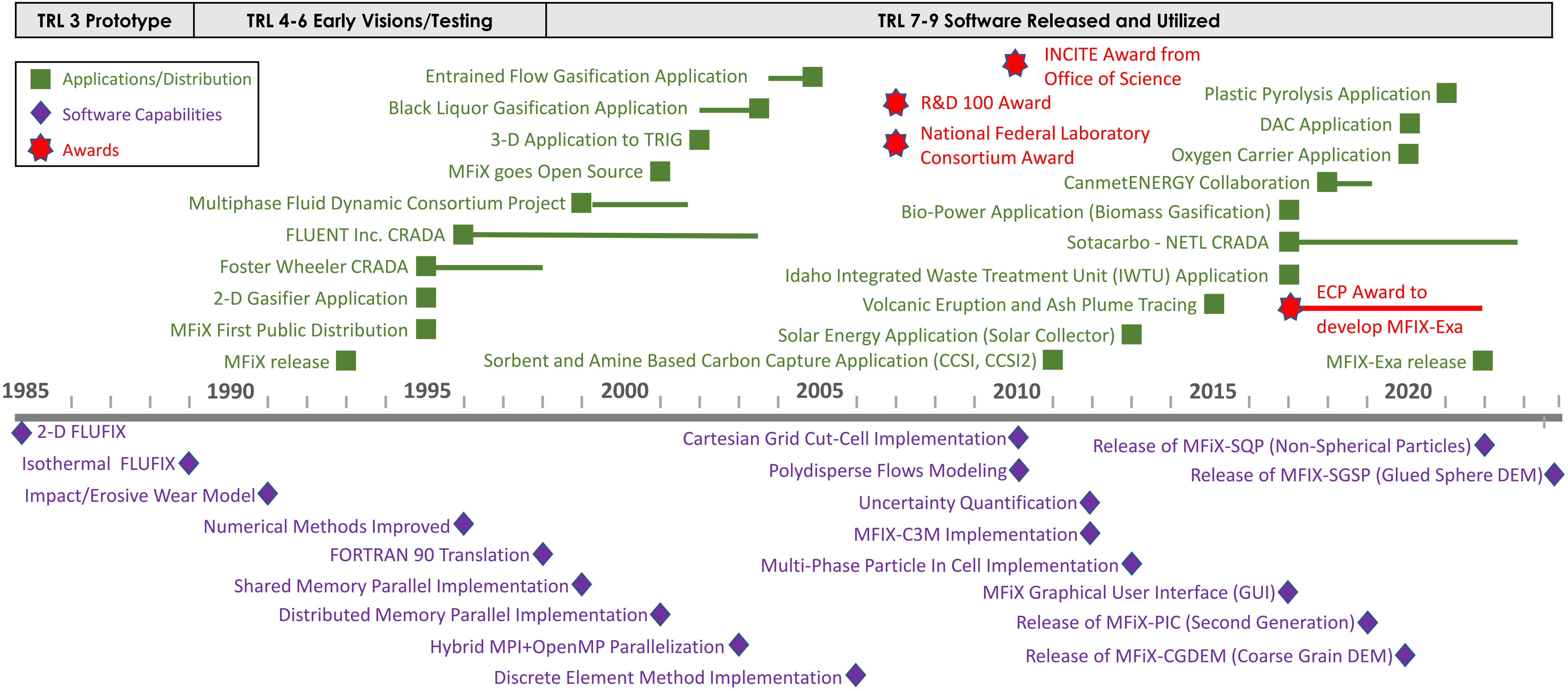
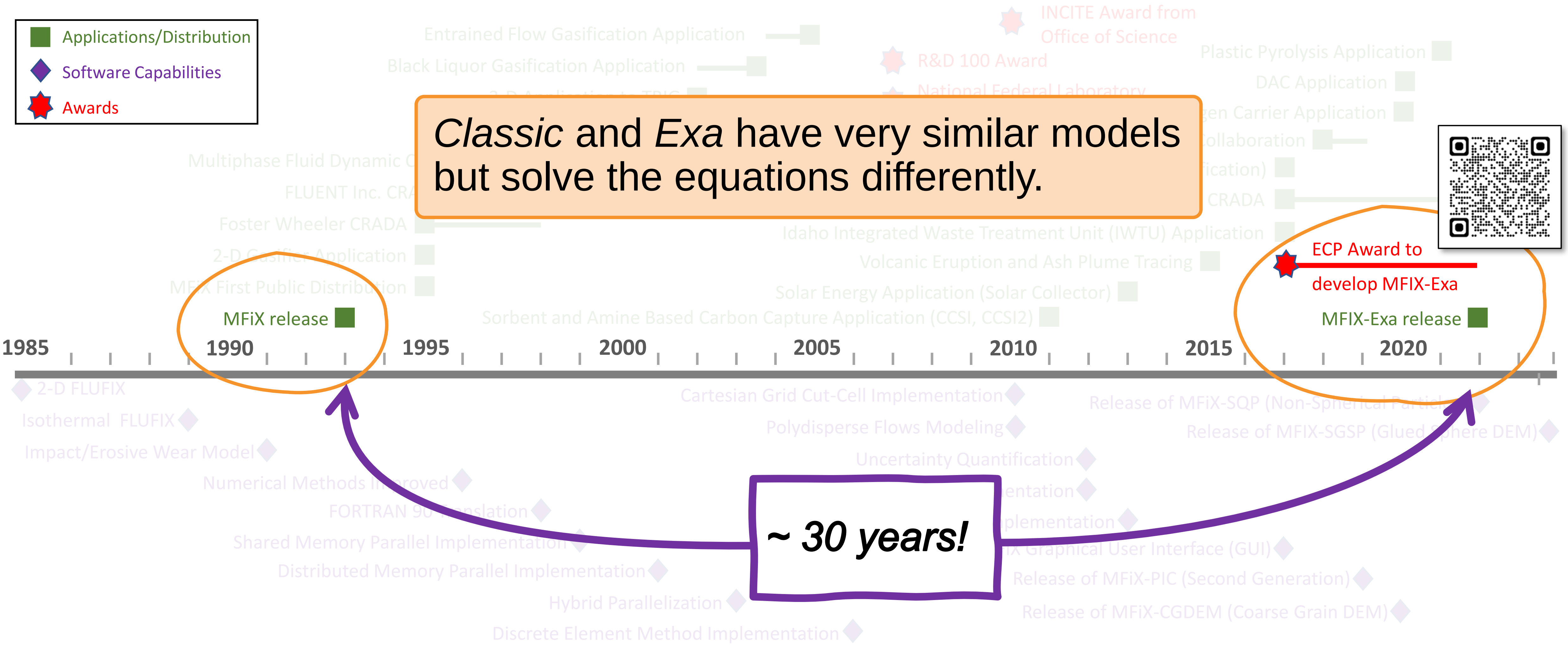


MFIX Technology Development Timeline

TRL 3 Prototype	TRL 4-6 Early Visions/Testing	TRL 7-9 Software Released and Utilized



Comparison between MFIX and MFIX-Exa

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	MFiX	MFIX-Exa
Codebase:	• Fortran	• C++
Fluid layout:	• Face centered velocities • Cell centered scalar fields	• Cell centered velocities and scalar fields • Nodal pressure
Solids:	• Two-Fluid Model (TFM) • Discrete Element Model (DEM) • Multiphase Particle-in-Cell (PIC)	• Discrete Element Model (DEM) • Multiphase Particle-in-Cell (PIC)
Fluid algorithm:	**S**emi **I**mplicit **M**ethod for **P**ressure **L**inked **E**quations (SIMPLE)	Explicit update with approximate projection to enforce incompressibility constraint
Geometry:	Cartesian grid cut-cell	Cartesian grid cut-cell
Linear solver:	Native BiCG-STAB	AMReX multilevel geometric multigrid solver with option to call hypre for bottom solve
Distribution map:	• Each MPI task manages one grid • Fluid/particles co-exist on single grid	• MPI tasks can manage multiple grids • Fluid/particles can co-exist on single grid or use separate (dual) grids for load balancing • Option to “prune” fully covered grids
Parallelism:	MPI+MPI, MPI+OpenMP	MPI+MPI, MPI+OpenMP, MPI+Cuda, MPI+HIP, MPI+DPC++

MFIX-Exa: Model overview

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- **Fluid conservation equations solved on a mesh**
  - supports density, species, and enthalpy advection
  - multicomponent ideal mixture with three incompressibility constraints
    - incompressible fluid
    - ideal gas (open system) :: thermodynamic pressure (scalar) is constant
    - ideal gas (closed system) :: thermodynamic pressure (scalar) evolves in time

- **Particle models:**
  - DEM: tracks individual particles
    - computes collisions
    - advances using time step smaller than fluid
  - PIC: tracks particle clouds
    - approximates particle interactions
    - advances at the fluid time step

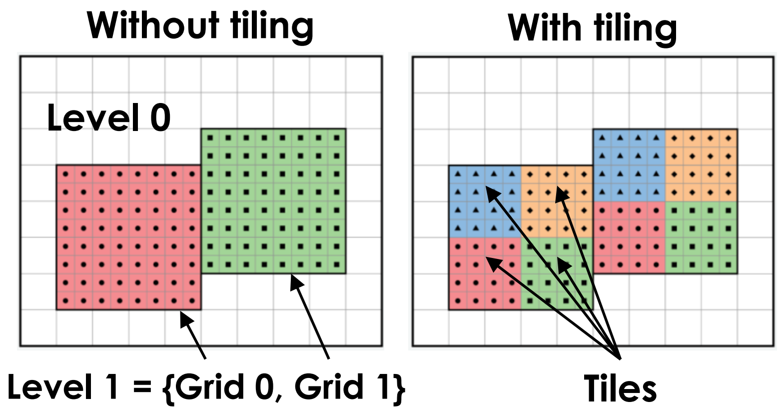
Fluid-particles models are coupled

- volume fraction
- momentum (drag)
- energy (convection and chemistry)
- mass (chemistry)

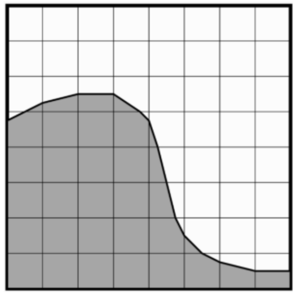
MFIX-Exa: Built on the AMReX framework

- **Iterators** (MFIter) are used to loop over **grids / tiles** owned by *this process*
- **Particle iterators** provide access to particles owned by *this process*
- Utilities are available to collect and update ghost cells and particle data
- Data structures and algorithms are provided to employ an **embedded boundary** (EB) approach
- **`amrex::ParallelFor`** construct for portability
  - Normal "for loop" when running on CPUs
  - GPU kernel launch when running with CUDA / HIP / SYCL
- This doesn't even touch the AMR capabilities…

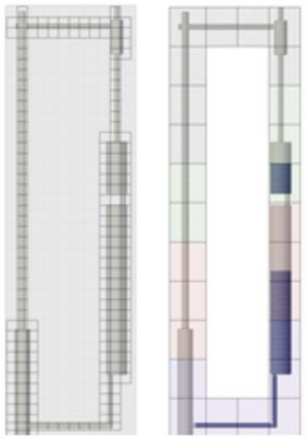
Grids and Tiling



Embedded Boundaries



Grid pruning



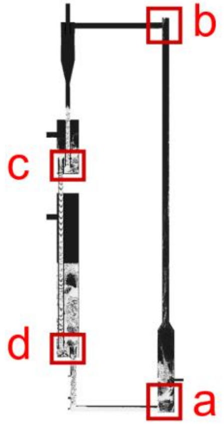
Images source: AMReX online documentation

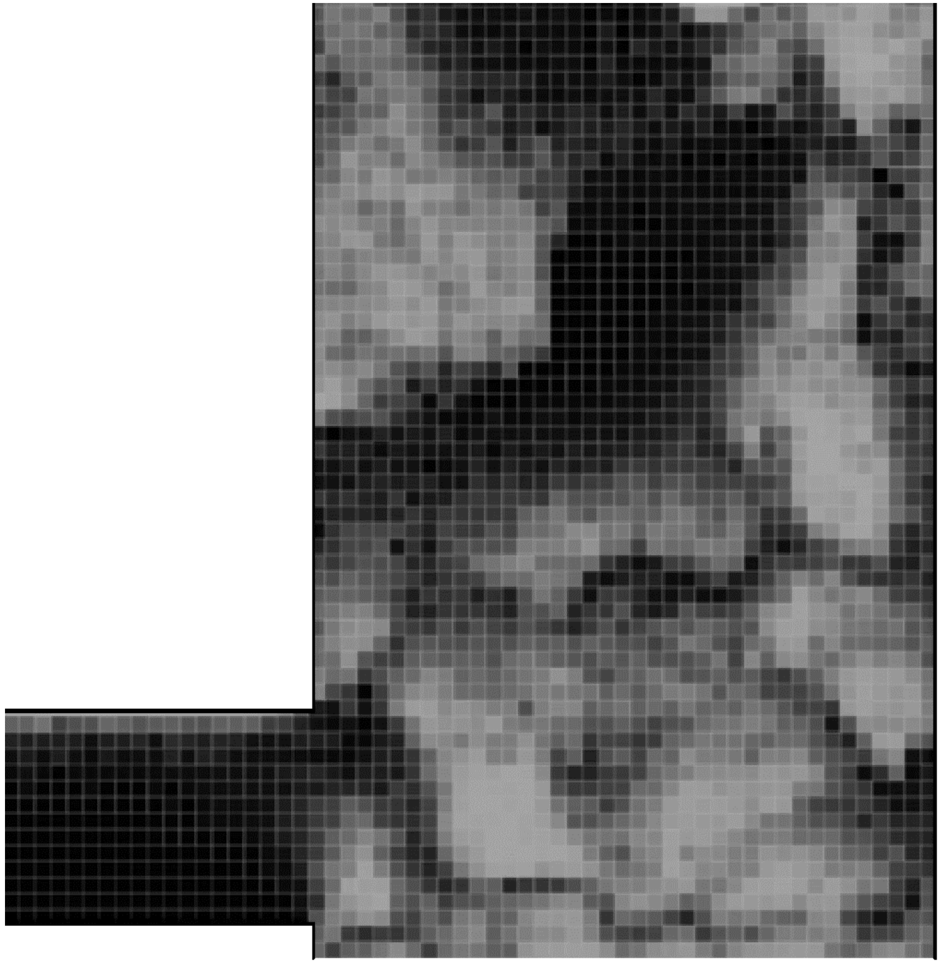
MFIX-Exa: Utilities and tools

- **`pic2dem`** an application to bootstrap CFD-DEM simulation initial conditions from PIC simulations
- **`FilterML`** and **`post`** are applications designed to extract and process simulation data primarily targeting the development of ML models
- in situ visualization with **Ascent** and **ParaView Catalyst** and native monitors for data extraction

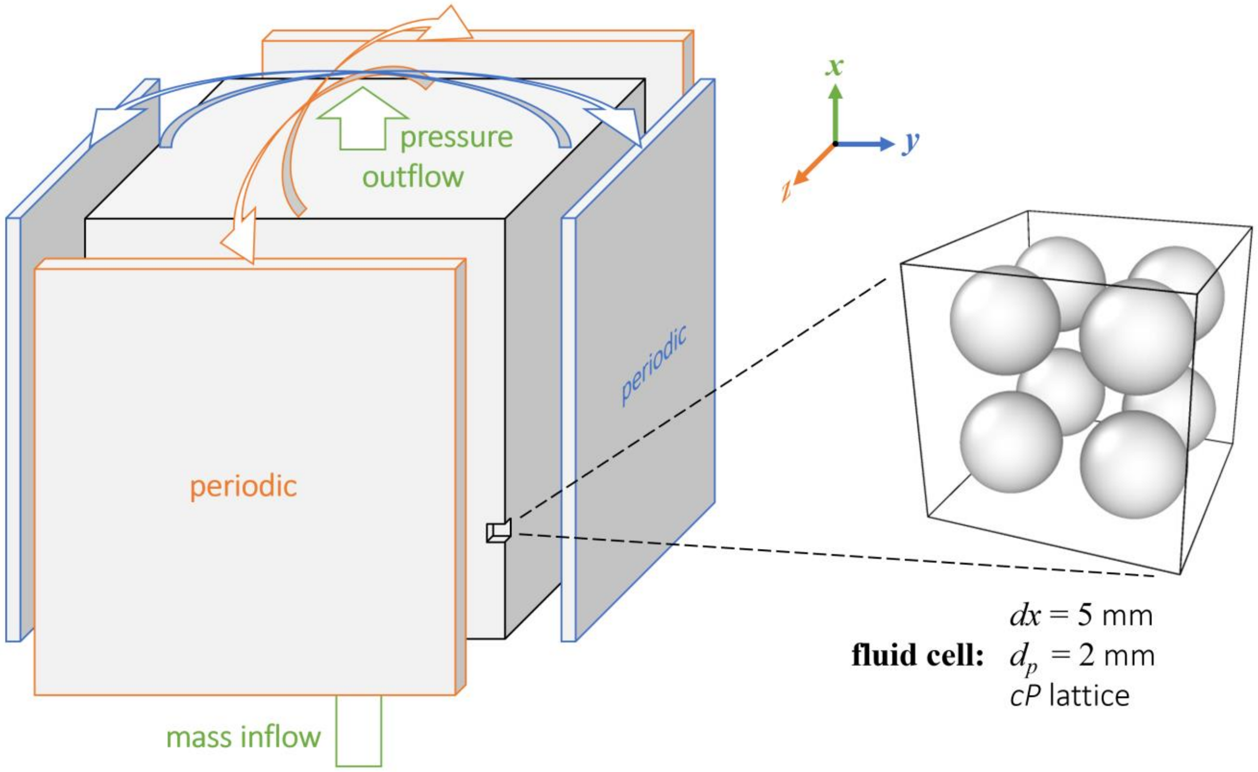
Animation shows up-close view of CFD-DEM simulation bootstrapped from PIC simulation.

a) bottom of air reactor
b) blind-T at top of riser
c) bottom of loop-seal
d) bottom of fuel-reactor





MFIX-Exa: Performance - *problem description*



chemically reacting CFD-DEM using hematite reduction reactions (Abad et al. 2011)

- 1-grid is a 3D block of fluid cells ($N_x \times N_y \times N_z$ – often cubic N^3)
- grids are the basic work elements and include all particles within the grid
- *typically,* we assign one grid to one resource (CPU or GPU)
- domain size is equal to the number of grids × the grid size × fluid mesh
- timestep: 4.0e-5 s
- number of steps: 10 (3 repeats)

MFIX-Exa: Performance - *strong scaling*

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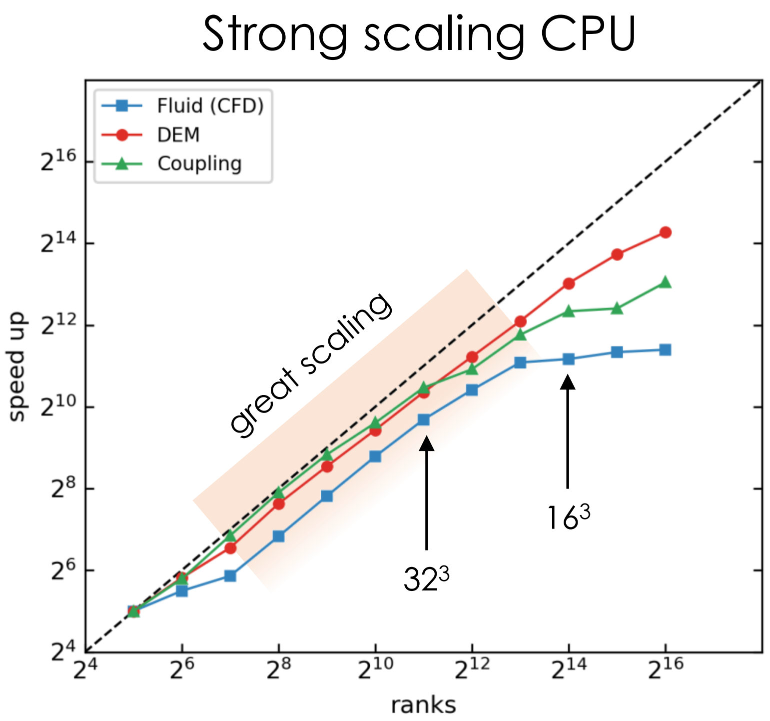

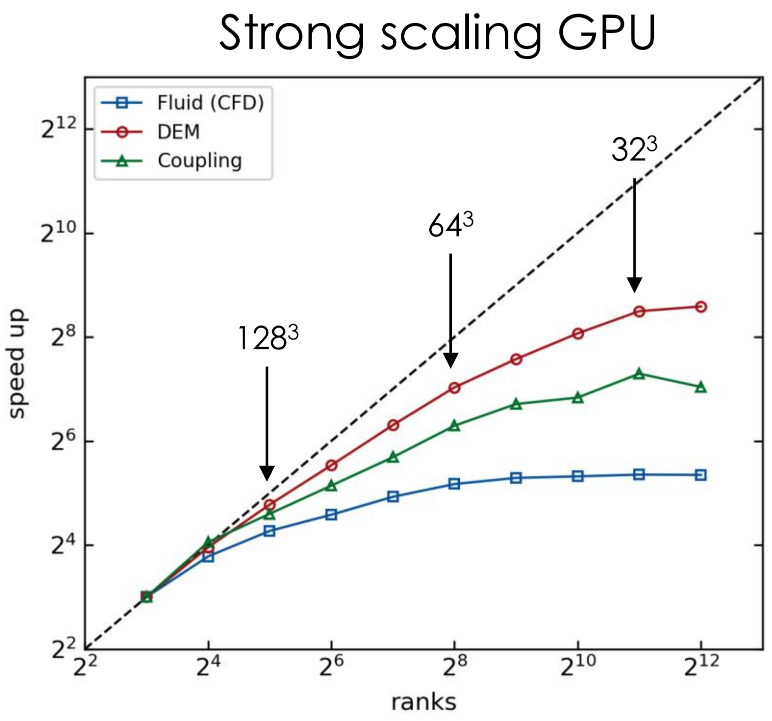

- CPUs have region of near-perfect scalability
- Fluid work flatlines at 8192 CPUs, corresponding to a grid of 32 x 16 x 16
- GPUs don't show any significant region of
- Fluid work saturates on a 64^3 grid size

Reported data collected on NERSC's Perlmutter

This research used resources of the National Energy Research Scientific Computing Center (NERSC), a Department of Energy Office of Science User Facility using NERSC awards ALCC-ERCAP0025948 ASCR-ERCAP0027134.

MFIX-Exa: Performance - *weak scaling*

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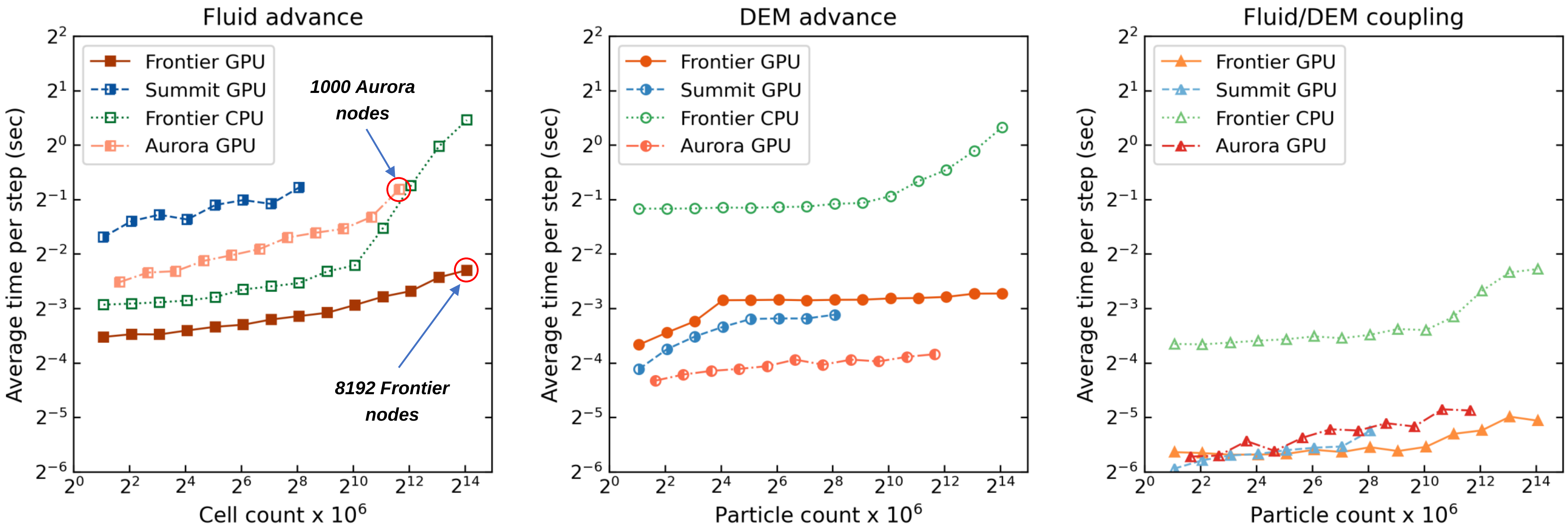

- Problem is setup to be trivially scalable so the **work per MPI task is constant**
- Work is reported by total particle count to adjust for different hardware configurations:
  - Summit: 6-NVIDIA V100 GPUs per node (6 accelerators per node).
  - Frontier: 4-AMD MI250X, each with 2 Graphics Compute Dies (8 accelerators per node).
  - Aurora: 6-Intel Data Center Max 1550 Series, each with 2 Stacks (12 accelerators per node).

This research was supported by the Exascale Computing Project (17-SC-20-SC), a collaborative effort of the U.S. Department of Energy Office of Science and the National Nuclear Security Administration.P0027134.

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This figure contains results from work done on a pre-production super-computer with early versions of the Aurora software development kit.

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MFiX MFIXExa MFAL

Nodeworks Tracker

Applications: Chemical Looping

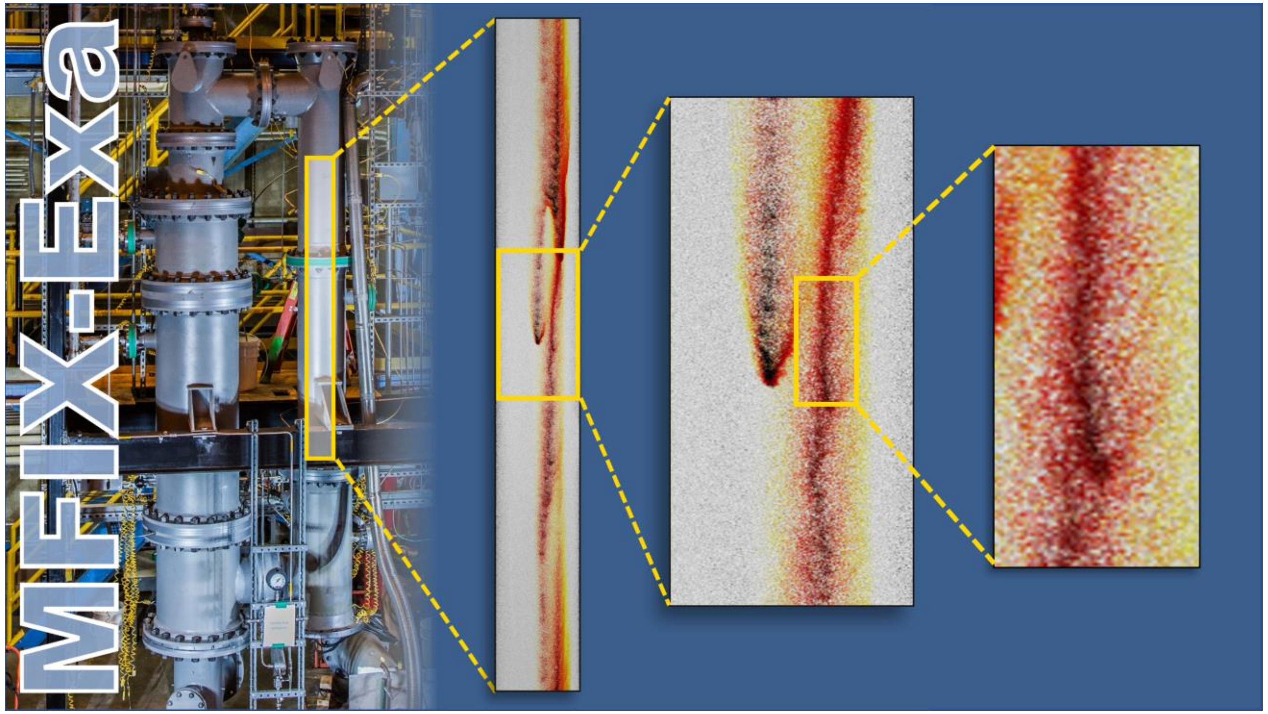
MFIX-Exa simulation of NETL's Chemical Looping Reactor

MFIX-Exa CFD-PIC simulation of CLR startup.

- 4mm fluid mesh (coarse)
- One parcel represents 512 'real' particles

Experience and knowledge gained from modeling the CLR is being leveraged to support NETL's Advanced Scale Up Reactor Experiment (ASURE) facility.

The ASURE facility will be used to test decarbonization technologies at scales needed to attract commercial investment for deployment.



Fullmer, Musser, Weber, Porcu, Rangarajan (2023) MFIX-Exa PIC simulation of NETL 50kW CLR. *This research was supported by the Exascale Computing Project (17-SC-20-SC).*

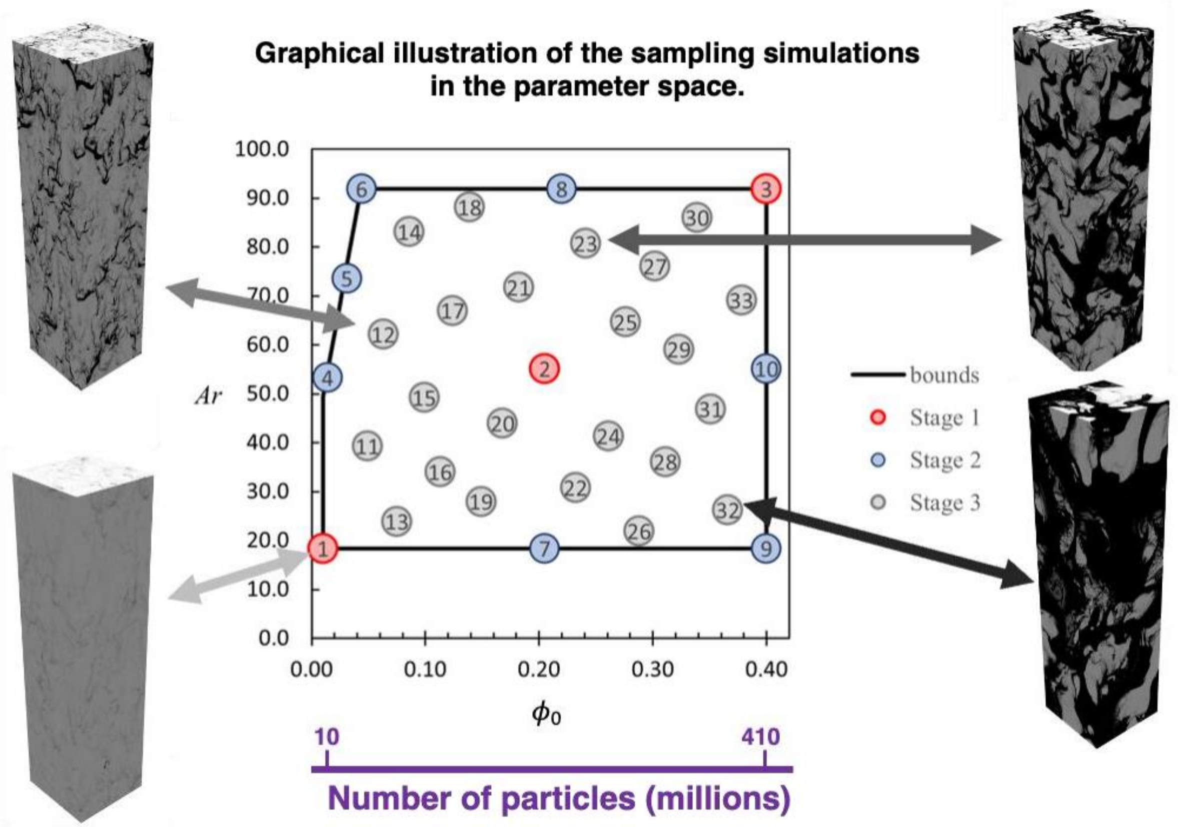
Applications: Unbounded fluidization

MFIX-Exa simulation campaign to generate ML training datasets

Project goals:

- model unbounded fluidization sweeping a range of Archimedes numbers and solids concentrations
- save ‘snapshots’ of fluid and particle fields for ML training
  - 33 total runs
  - 100 ‘snapshots’ per run

  } **Total of 46.8 TB**
- demonstrated in-situ ML training with SmartSim



Gel, Shao, Musser and Fullmer. (2024) Pioneering Real-Time (In-Situ) Machine Learning Integration for Multiphase Flow Analysis: A First-of-Its-Kind Workflow Demonstration with MFIX-Exa.

This research used resources of the National Energy Research Scientific Computing Center (NERSC), a Department of Energy Office of Science User Facility using NERSC award ALCC-ERCAP0025948.

Fullmer, Musser, Gel and Beetham. (2024) Machine Learning-Enhanced Multiphase CFD for Carbon Capture Modeling Run Data. web. https://doi.org/10.18141/2344941

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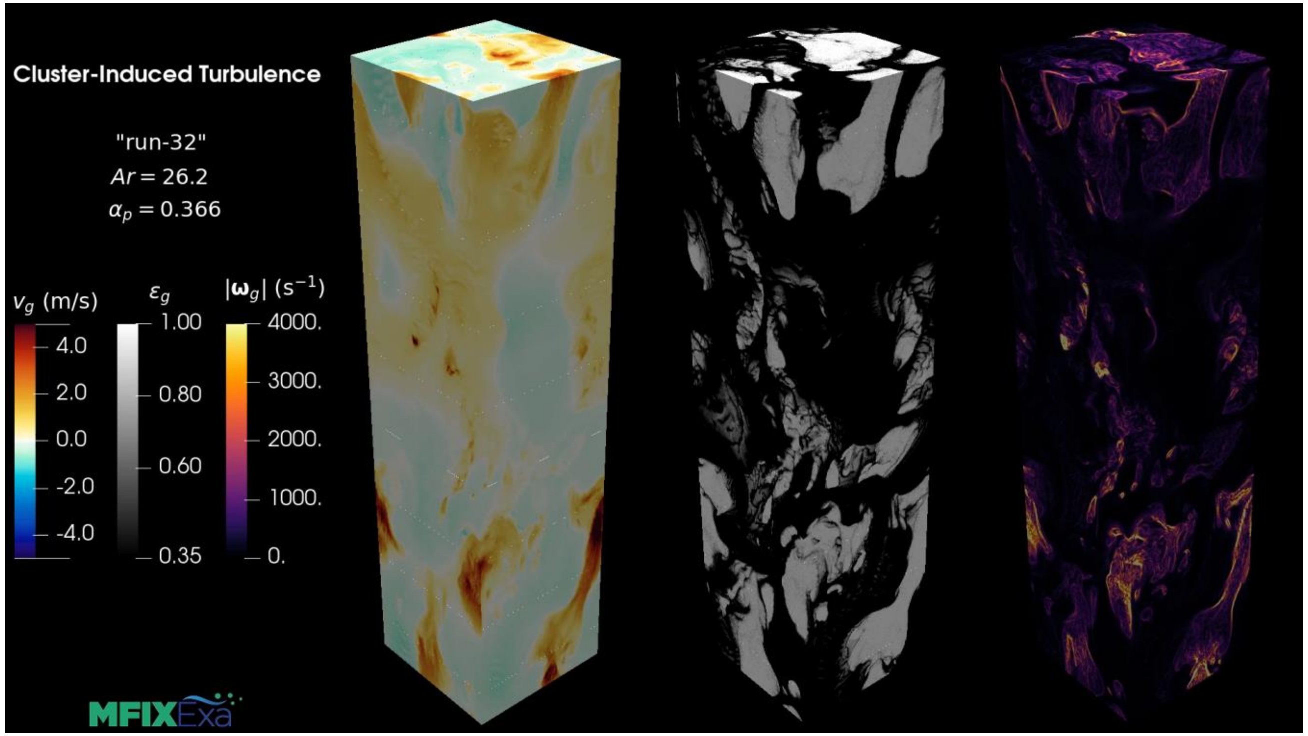

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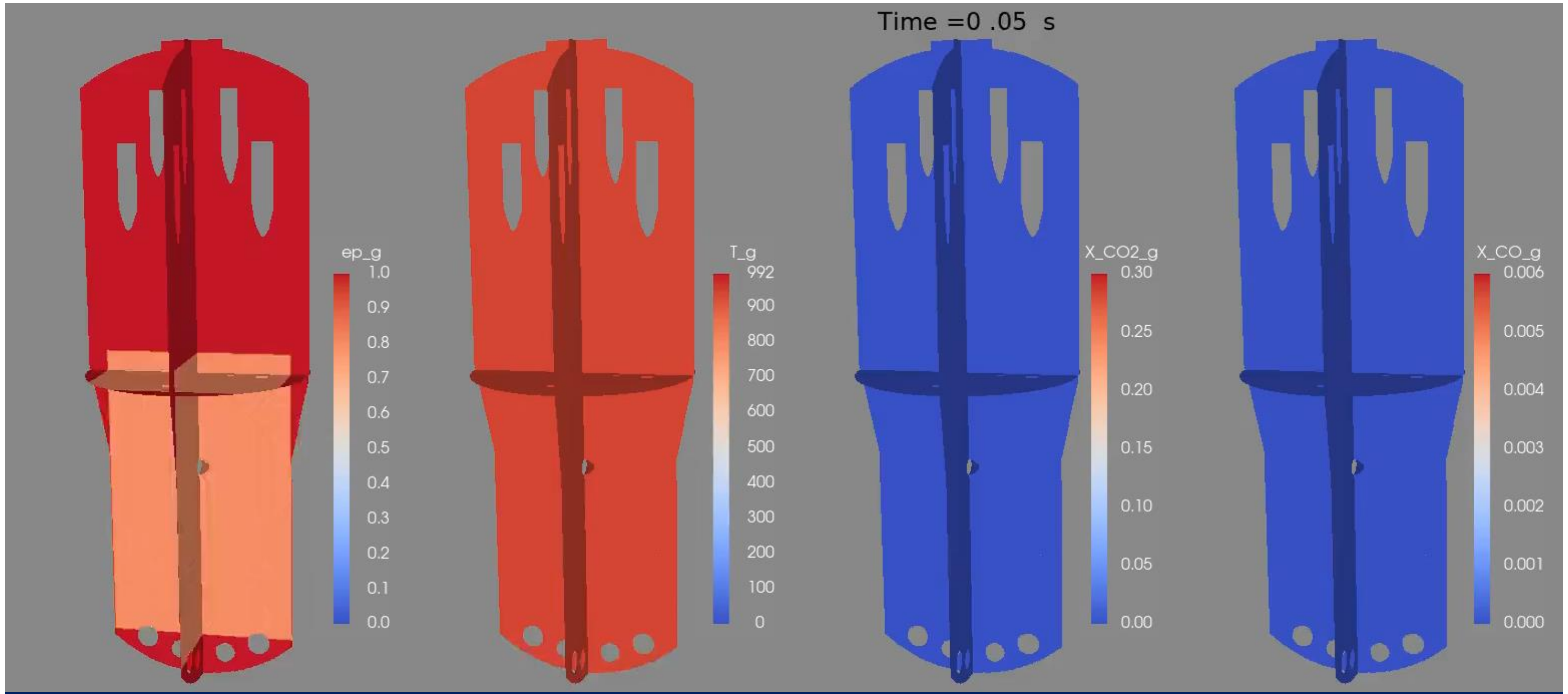
Applications: Fluid Catalytic Cracker (FCC)

MFIX-Exa simulation of a 2,500 mTPD Biogenic FCC Regenerator

Project goals:

- develop a biogenic coke oxidation kinetic model
- validate against experimental results
- assess performance of a demonstration-scale FCC regenerator
- investigate key parameters regarding the reactor performance



Solids concentration | Fluid temperature (K) | CO_2 mass fraction | CO mass fraction

ChemCatBio
Chemical Catalysis for Bioenergy

Xu, Adkins, Musser and Shahnam. (2024) Numerical Simulation of a Biogenic Fluid Catalytic Cracking (BFCC) Regenerator with MFIX-Exa. web. doi:10.2172/2429409.

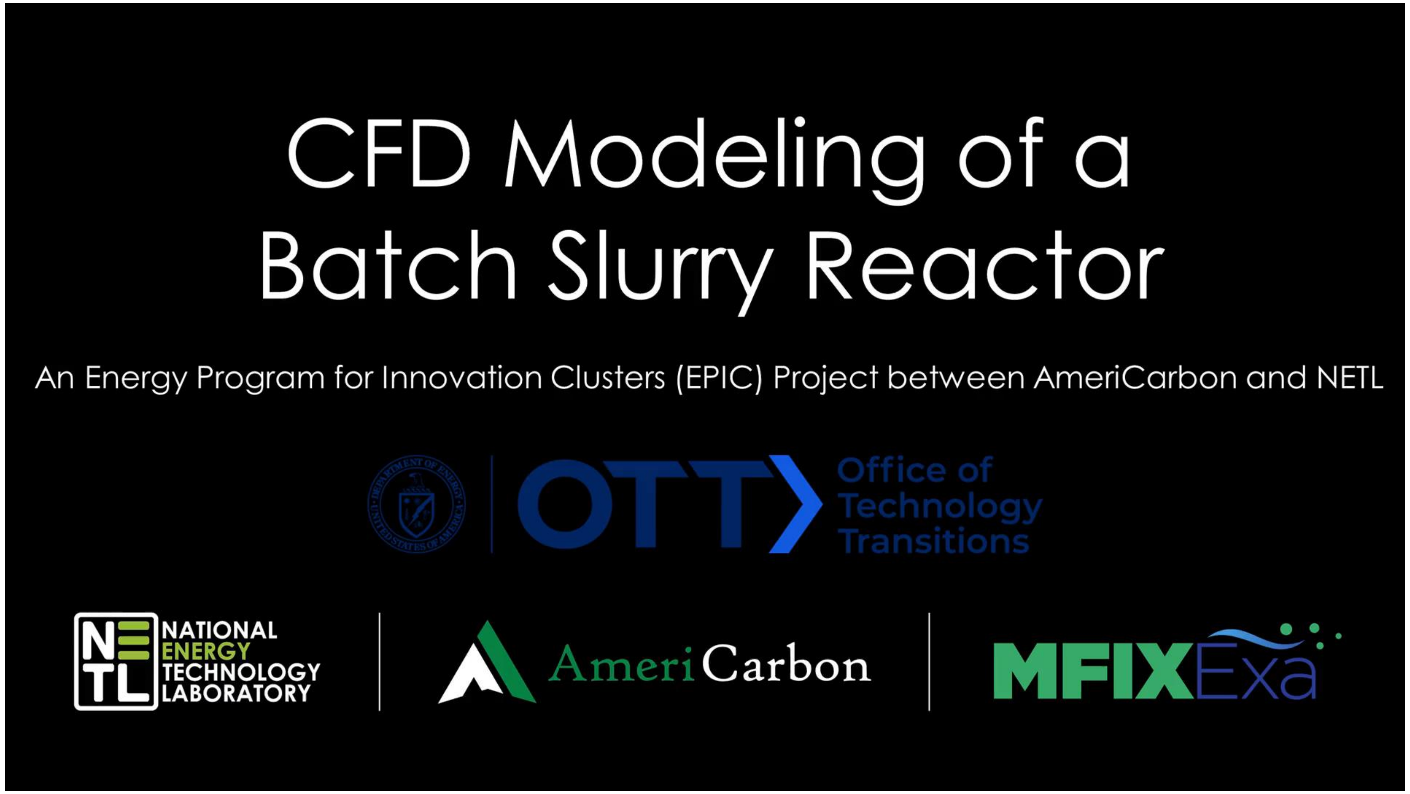
Project funding provided under FOA DE-LC-0000015

Applications: Batch slurry reactor

MFIX-Exa simulation of a batch slurry reactor

Project goals:

- develop a homogeneous mixture model with LES of batch slurry reactor
- assess effect of changes to reactor geometry
- provide insight into flow characteristics



AmeriCarbon

Office of Technology Transitions

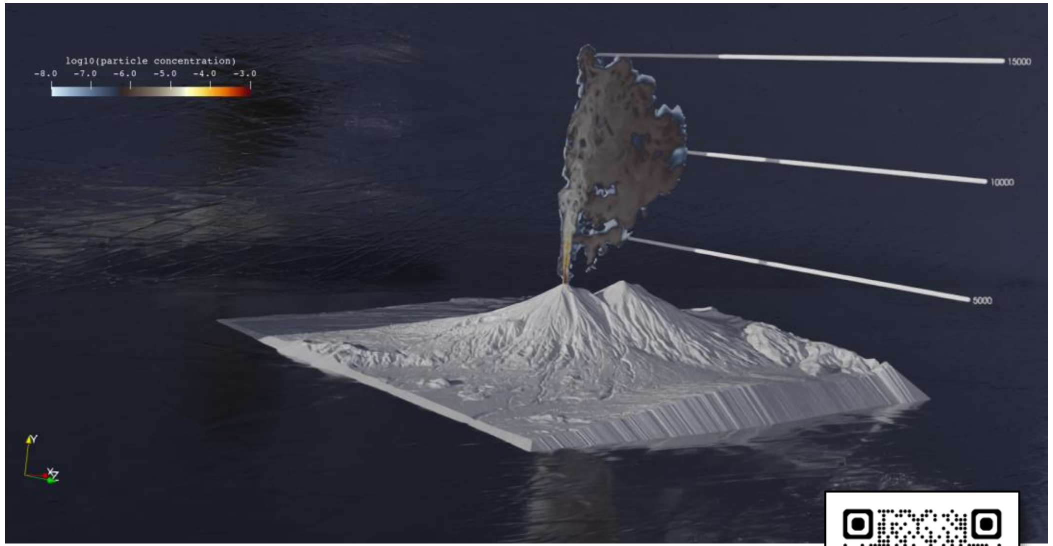
Fullmer, Tambe, Berry, Musser and Shahnam. (2024) CFD modeling of a batch slurry reactor. web. doi:10.2172/2429409. Project funding provided by the Office of Technology Transitions (OTT) Energy Program for Innovation Clusters (EPIC) under agreement 1024033.

Applications: Volcanic eruptions

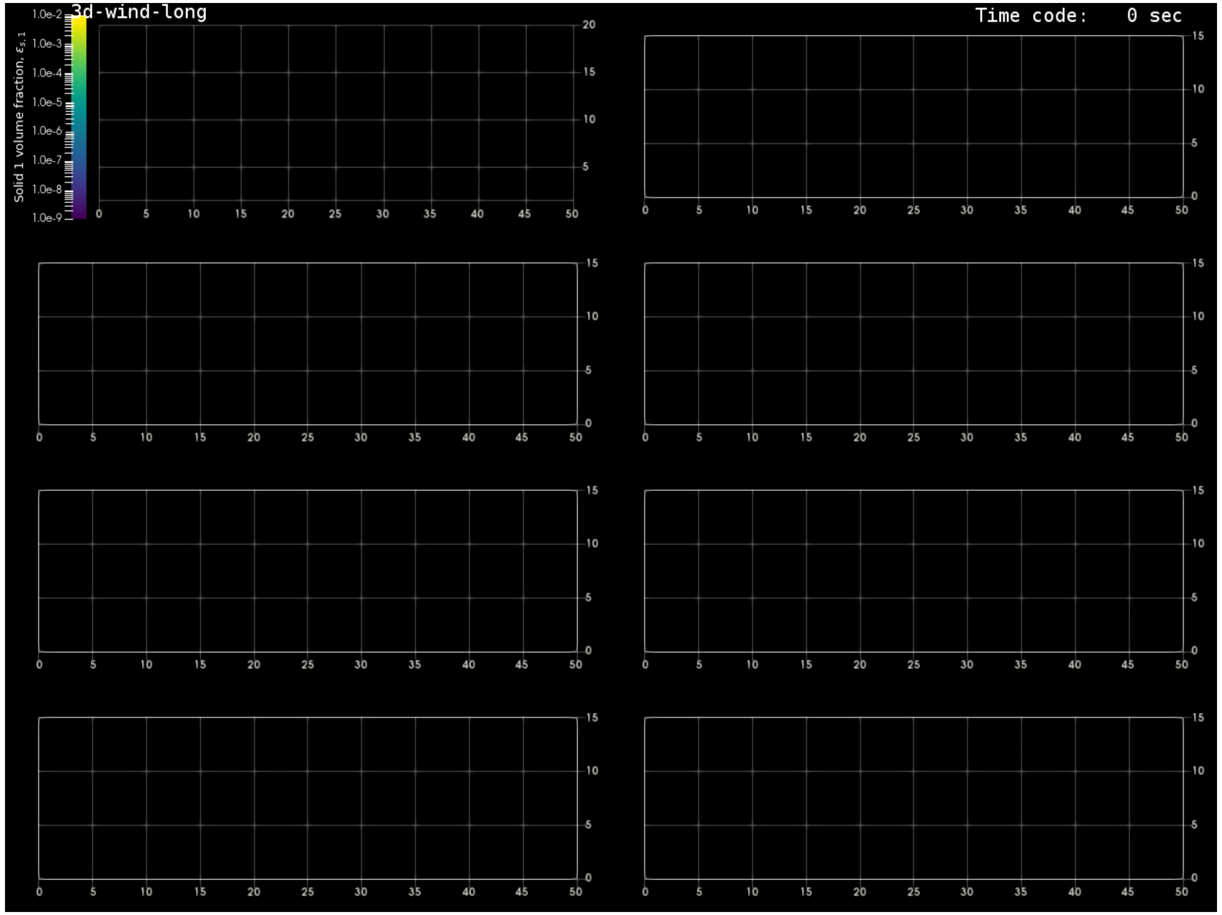
MFIX simulation weak plume volcanic eruption

Investigations include:

- weak and strong volcanic plumes
- pyroclastic flows



Eric Breard, NERC Independent Research Fellow
University of Edinburgh (UK)



Additional interesting examples using MFIX to volume volcanic flows, see Dufek, Breard and Musser (2023) Granular and Fluid Instabilities in Explosive Volcanic Eruptions.

Computational CFD Tools

IN-HOUSE CODE

MFiX

MFIXExa

COMMERCIAL CODE

ANSYS FLUENT

BARRACUDA

COMSOL MULTIPHYSICS

cpfd

OTHER OPEN-SOURCE

OpenFOAM®

Computational Resources

IN-HOUSE COMPUTING

JOULE NETL SUPERCOMPUTER

WATT The Power of Ai

COMPUTE AWARDS

U.S. DEPARTMENT OF ENERGY INCITE LEADERSHIP COMPUTING

Computational Support Tools

IN-HOUSE CODE

Nodeworks

Tracker

C3M

OTHER OPEN-SOURCE

blender

User (NETL) Outreach

Support Forum

EDX Energy Data eXchange

Experimental Resources

MFAL

Researcher Skill Sets

- Apply CFD tools to investigate multiphase reactors from bench to device scale.
- Develop fundamental physics-based models from first principles.
- Translate mathematical models from literature to code (C++, fortran, python).
- Apply machine learning to improve accuracy of fast running, lower fidelity models.
- Apply verification and validation methods to assess code quality.
- Create surrogate models from CFD simulations to inform process scale models.

Proven Demonstrations/ Applications

- Detailed chemical kinetics (CRECK) for gasification.
- IWTU
- O2 Production from perovskite fixed beds.
- CO2 capture using MECS, MOFS and PIMS.
- 100k GPU node hours to generate high fidelity datasets for ML.
- Microwave heating of plastics/bio for gasification.
- Alaska-Fairbanks moving bed gasifier.
- Bioreactor optimization (HPC4EI).
- EERE-BETO Regeneration of bio-FCC catalyst particles.
- EERE-FCIC Fast pyrolysis of biomass for sustainable aviation fuel.

NETL RESOURCES

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