MFIX-Exa development

Exascale computing for multiphase flows

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Outline

- **A brief history lesson – Where did MFIX-Exa come from?**
- MFIX-Exa overview from 3000-foot view
  - How is MFIX-Exa different from (*classic*) MFiX?
  - Built on the AMReX framework
  - Model overview
  - Utilities and tools
- A look at performance
  - Strong scaling
  - Weak scaling
- Development activities
  - Chemistry solver
  - LES viscosity models
  - Radiation

Exascale Computing Project (ECP)

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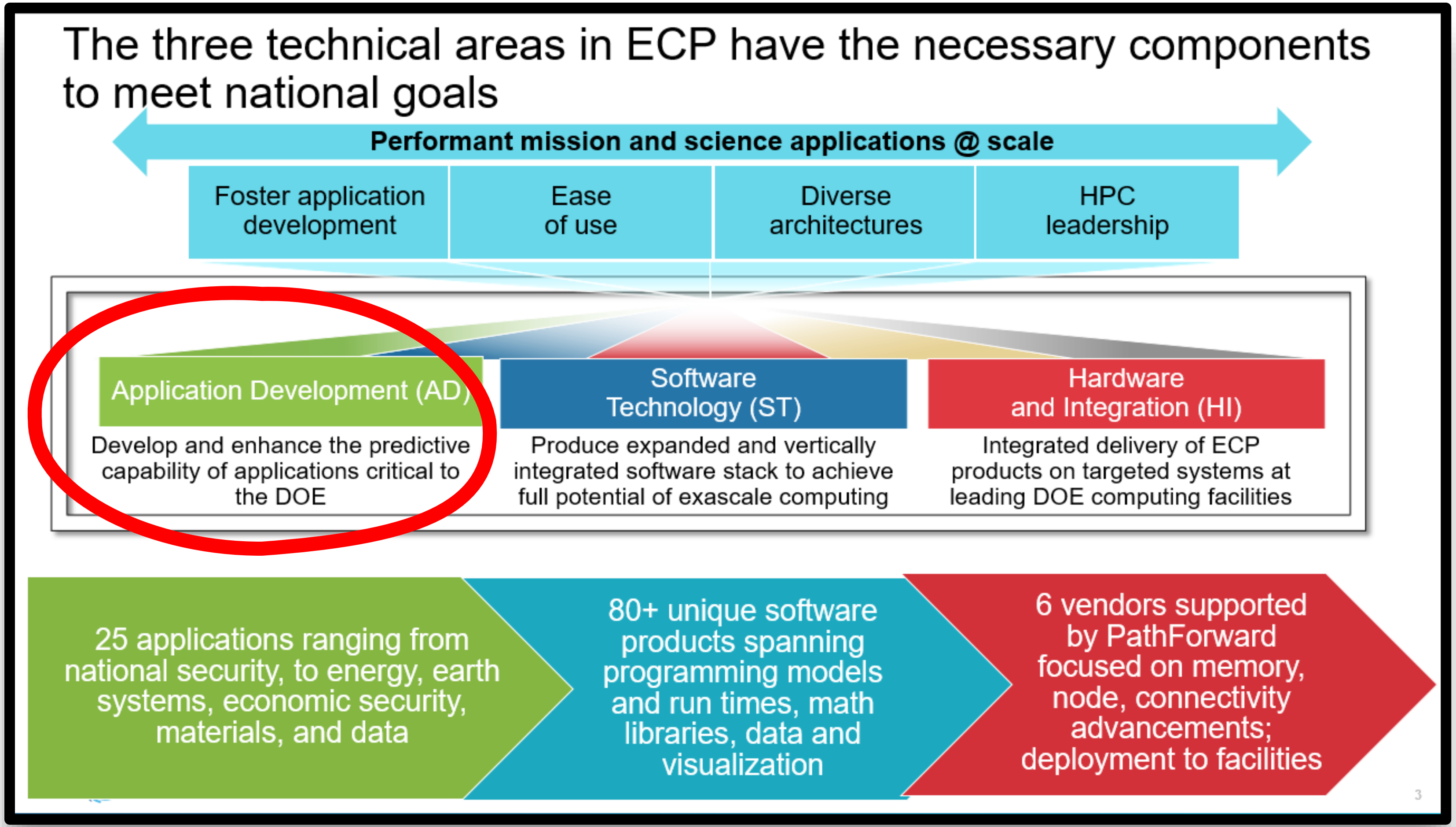
What is ECP?

[An] accelerated research and development project funded by the US DOE to ensure all necessary pieces are in place to deliver the nation's first, capable, exascale ecosystem, including mission critical applications, an integrated software stack, and advanced computer system engineering and hardware components.

ECP 101 slide deck



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MFIX-Exa: comparison with *classic* MFiX

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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: Built on the AMReX framework

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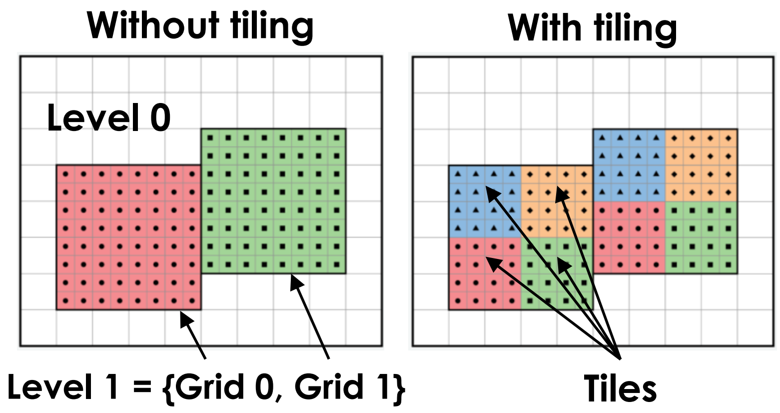
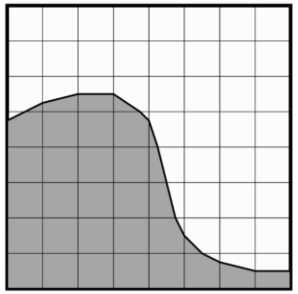
- **Iterators** (MFIter) are used to loop over **grids / tiles** owned by *this process*
- **Particle iterators** provide access to particles owned by *this process*
- Utilities are available to collect and update ghost cells and particle data
- Data structures and algorithms are provided to employ an **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…

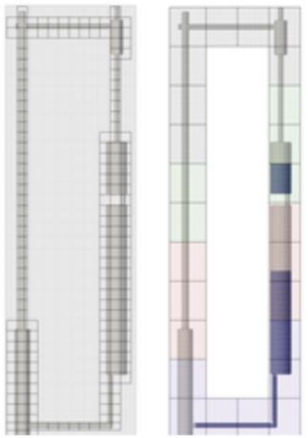
Grids and Tiling



Embedded Boundaries



Grid pruning



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) evolve 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

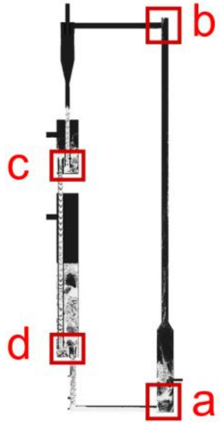
- Coupled together:
  - momentum (drag)
  - energy (convection and chemistry)
  - mass (chemistry)

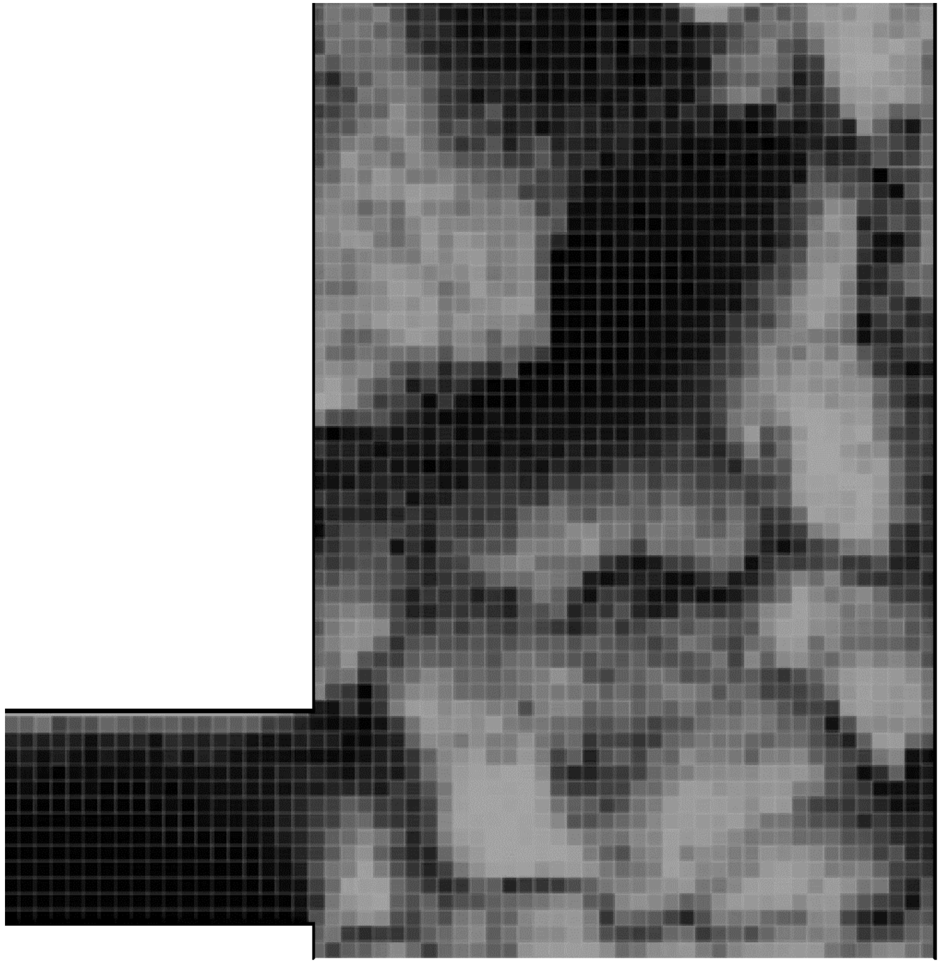
MFIX-Exa: Utilities and tools

- `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





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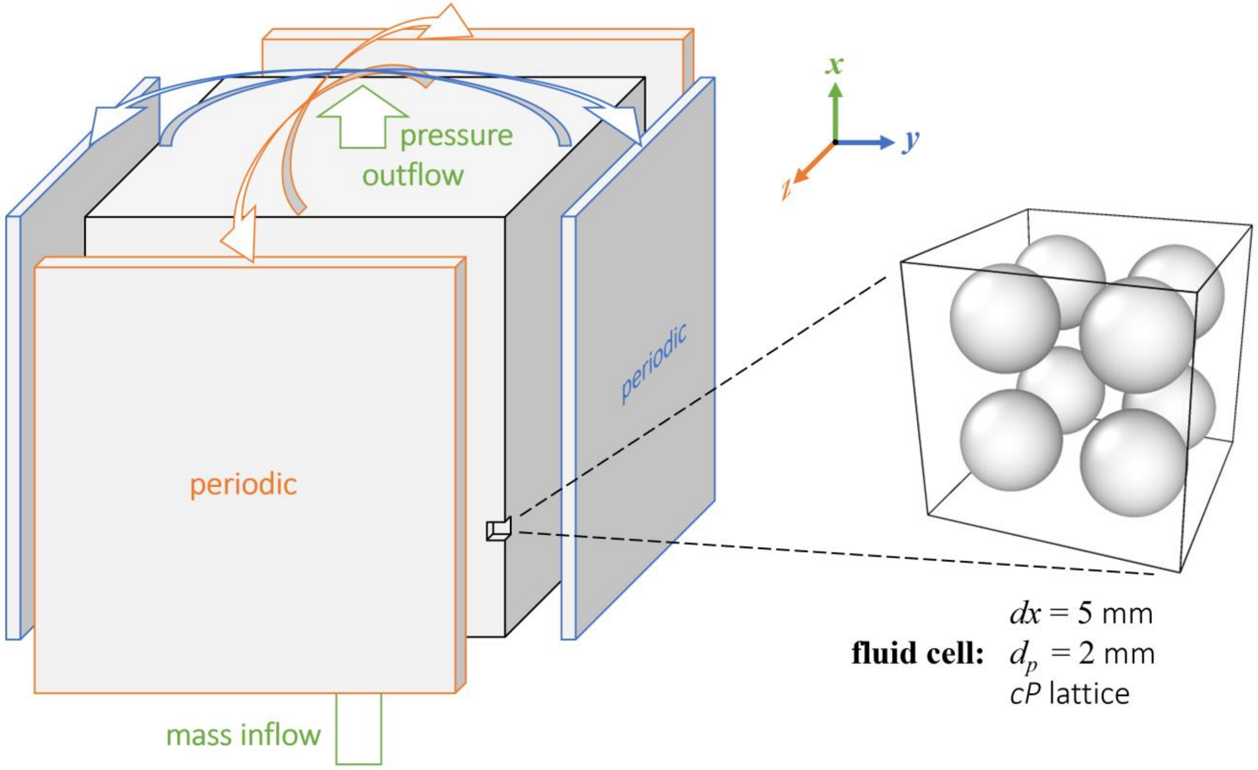
Performance: Problem Description



chemically reacting CFD-DEM using hematite reduction reactions of (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
- num. steps: 10 (3 repeats)

Performance: Strong Scaling on Perlmutter

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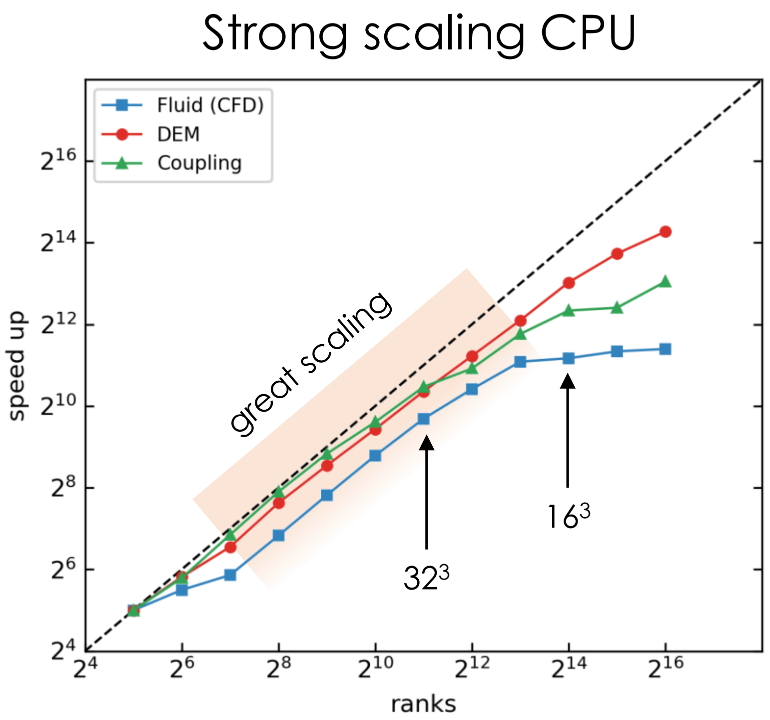
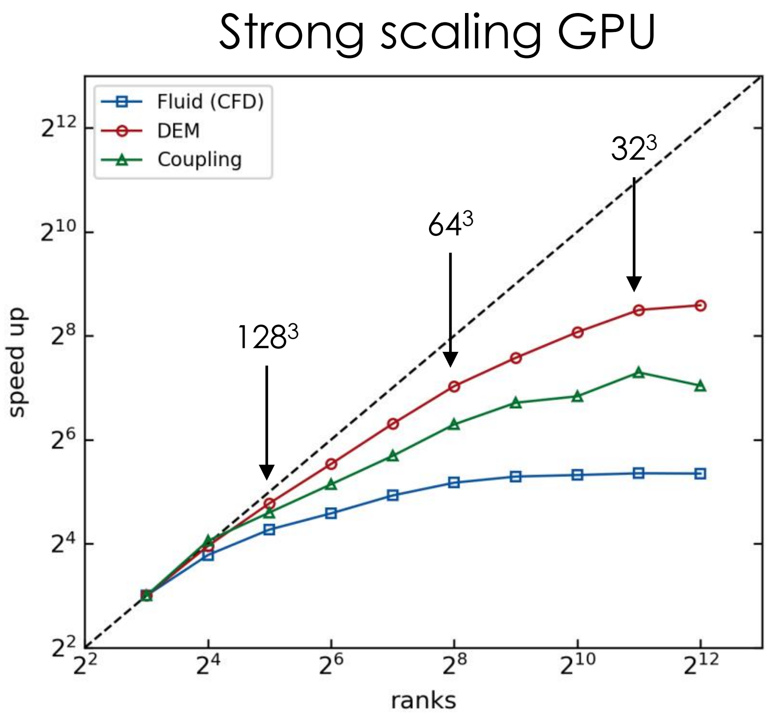
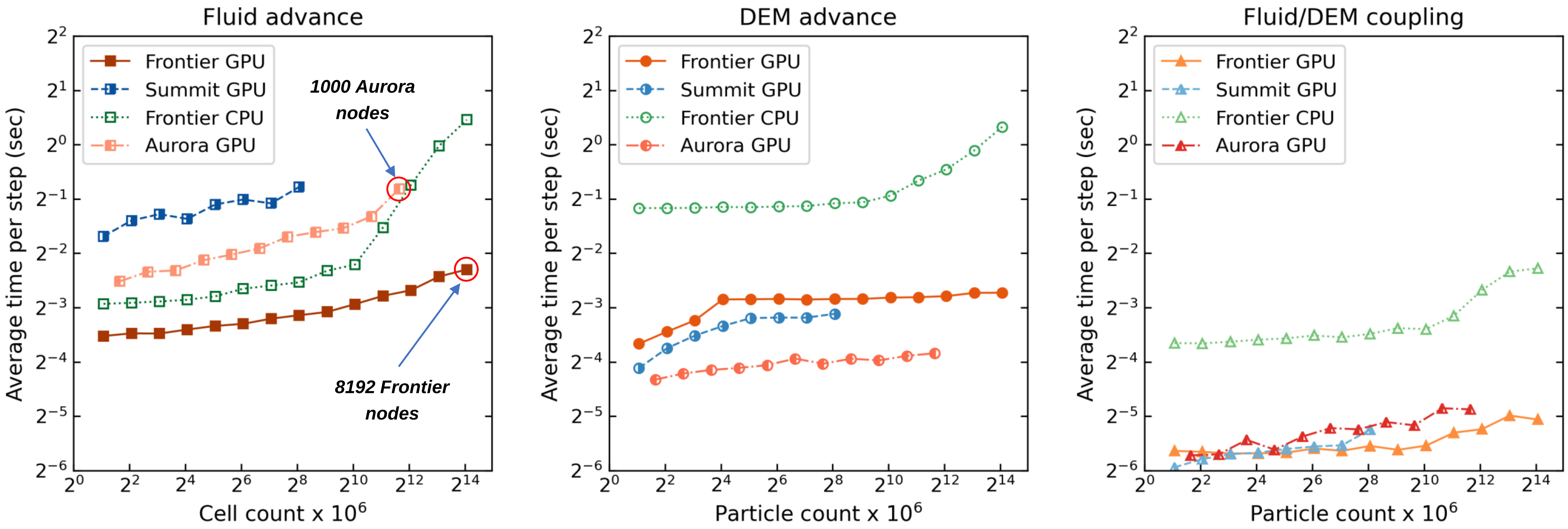




- CPUs have region of near-perfect scalability
- Fluid work flatlines at 8192 CPUs, corresponding to a grid of 32 x 16 x 16
- GPUs don't show any significant region of
- Fluid work saturates on a 64^3 grid size

TL;DR? GPUs need sufficient work to offset kernel launches.

Performance: weak scaling



- 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 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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Development: Chemistry solver

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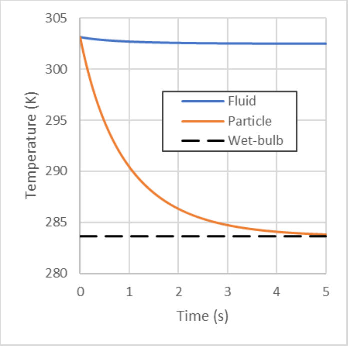
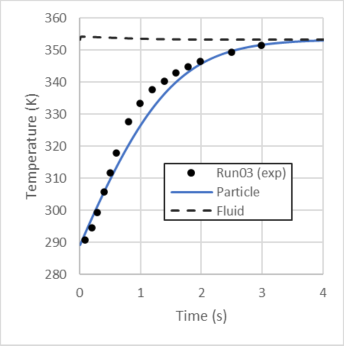
- **Goal:** Improve the accuracy and time-to-solution for simulations using chemical reactions.
- **Approach:** Incorporate a chemistry management interface that supports a collection of GPU-enabled integrators
  - Construct a memory handler to bridge between field variable data (MultiFabs) and local memory allocation for integrators
  - Leverage the work of AMReX-Astro / Microphysics [1] to create custom GPU-enabled integrators.
  - Resize integrators dynamically based on number of chemical species, reactions, and particles in a computational cell
  - Construct a suite unit tests using the method of manufactured solution (MMS) to ensure code correctness

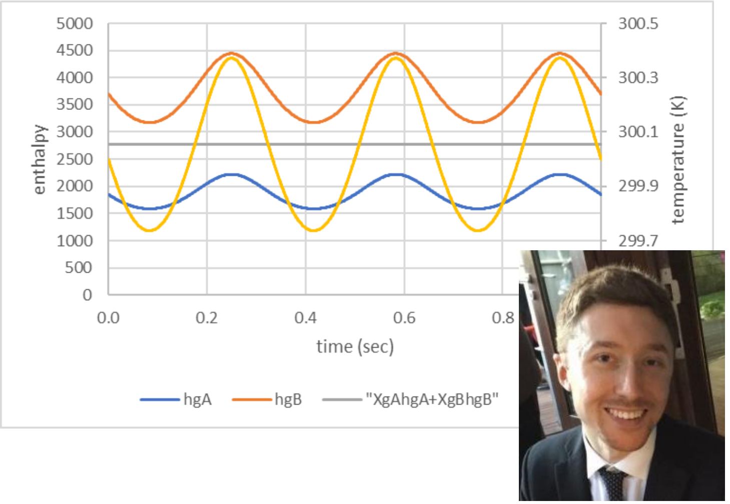
Evaporation



Condensation



MMS: Multicomponent species enthalpy

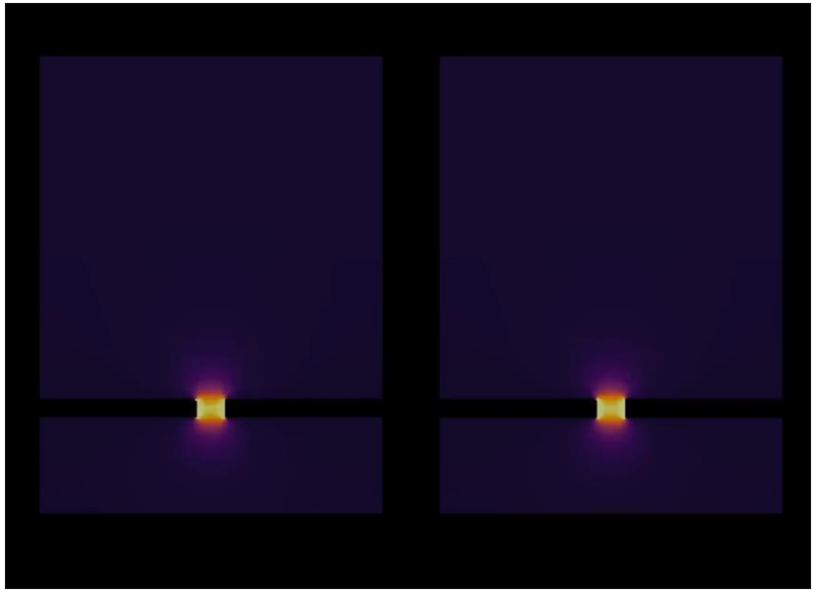


Roberto Porcu

1. *AMReX-Astro Microphysics Development Team (2024) “AMReX-Astro/Microphysics: Release 24.03”. Zenodo. doi: 10.5281/zenodo.10732065.*

Development: LES viscosity models

- **Goal:** Expand modeling capabilities to support new applications, particularly in liquid systems
- **Approach:** Incorporate multiple viscosity models to capture sub-grid effects
  - *Molecular viscosity: Sutherland; mixture*
  - *Eddy viscosity*: Smagorinsky-Lilly; WALES
  - *Suspension viscosity*: Einstein; Brinkman-Gibilaro; Sato;
- **Synergistic efforts**: Incorporate virtual (added) mass and Saffman lift forces to particle models



Single phase liquid jet injection at two different mesh sizes

Will Fullmer

Deepak Rangarajan

1. *"Gas-phase velocity fluctuations in statistically homogeneous fixed particle beds and freely evolving suspensions using particle-resolved direct numerical simulation", Mehrabadi et. al 2012*
2. *"Momentum And Energy Equations For Disperse Two-phase Flows And Their Closure For Dilute Suspensions", Zhangt And Prosperetti, 1996 (Eq. 5.9)*
3. *"Momentum And Heat Transfer In Two-phase Bubble Flow - I", Sato et al., 1980 (Eq. 10)*
4. *"On the apparent viscosity of a fluidized bed", Gibilaro et al., 2006 (Eq. 19)*
5. *Ducros, Nicoud, & Poinsot (1998). Wall-adapting local eddy-viscositymodels for simulations in complex geometries. Numerical Methods for Fluid Dynamics VI, 293-299.*

Development: Radiation modeling

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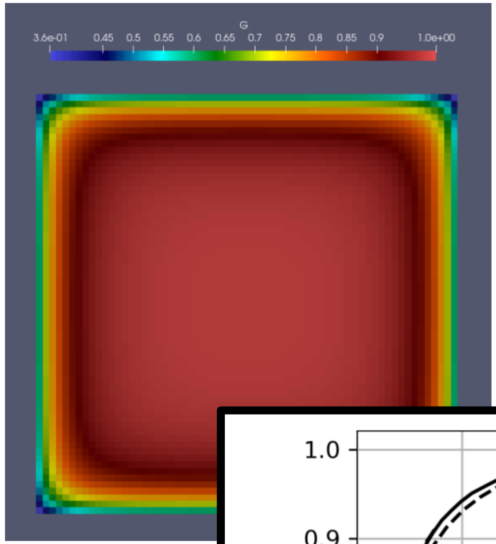
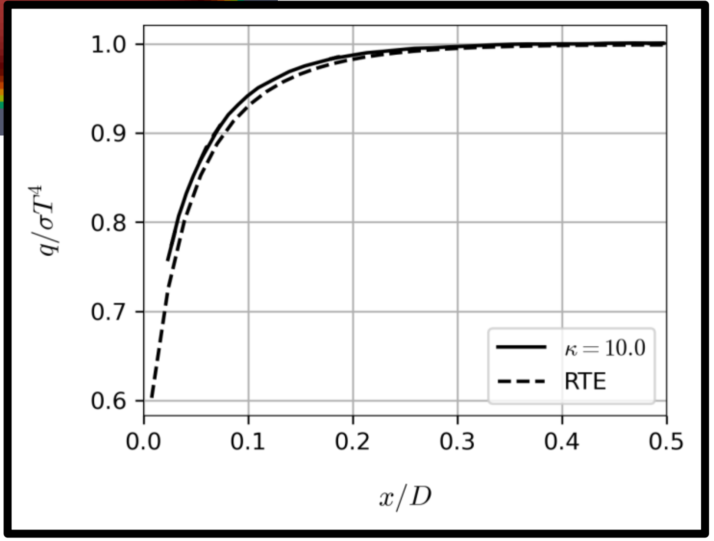
- **Goal:** Advance development and understanding of novel energy reactors that incorporate microwave heating.
- **Approach:** Implement an EB aware finite volume method for solving the radiation transport equation

$$\frac{\partial I_\eta}{\partial s} = \kappa_\eta I_{b\eta} - \kappa_\eta I_\eta - \sigma_{s\eta} I_\eta + \frac{\sigma_{s\eta}}{4\pi}\int_{4\pi} I_\eta(\hat{s}_i)\Phi_\eta(\hat{s}_i, \hat{s})d\Omega_i$$

  - Follows work of Chai, Lee and Patankar [1,2]
  - Leverage hypre for linear solves
  - Procedural development approach as standalone ‘app’
    - 2D box geometry followed by 2D with EB
    - 3D box geometry followed by 3D with EB



Aashish Goyal



1. *Chai, Lee, and Patankar (1994) Finite volume method for radiation heat transfer. Journal of Thermophysics and Heat Transfer. 1994.8:419-425.*
2. *Chai, Lee, and Patankar (1994) Treatment of irregular geometries using a cartesian coordinates finite-volume radiation heat transfer procedure. Numerical Heat Transfer, Part B: Fundamentals. 26(2):225–235.*
3. *Raithby and Chui (1990) A finite-volume method for predicting a radiant heat transfer in enclosures with participating media. Journal of Heat and Mass Transfer. 112(2):415-423.*

Thanks for your attention

Primary references:

J. Musser, A.S. Almgren, W.D. Fullmer, et al., (2022). MFIX-Exa: A Path Towards Exascale CFD-DEM Simulations. The International Journal of High Performance Computing Applications. 36(1): 40-58. doi:10.1177/10943420211009293

R. Porcu, J. Musser, Jordan; A.S. Almgren, et al., (2023) MFIX-Exa: CFD-DEM simulations of thermodynamics and chemical reactions in multiphase flows. Chemical Engineering Science. 273(5): 118614. doi:10.1016/j.ces.2023.118614

MFIX-Exa online documentation:
https://mfix.netl.doe.gov/doc/mfix-exa/guide/latest/

Feature articles:

Feature extraction and visualization algorithm improves functional memory and research outcomes in multiphase flow simulation analysis, Fader, April 2023.

Supercomputer code can help capture carbon, reduce global warming. Bernard, July 2022.

MFIX-Exa - Exascale supercomputing to model chemical looping reactors for industrial carbon capture. Farber, June 2020.

Optimizing a new technology to reduce power plant carbon dioxide emissions. January 2019.