MFIX-Exa

NATIONAL ENERGY TECHNOLOGY LABORATORY

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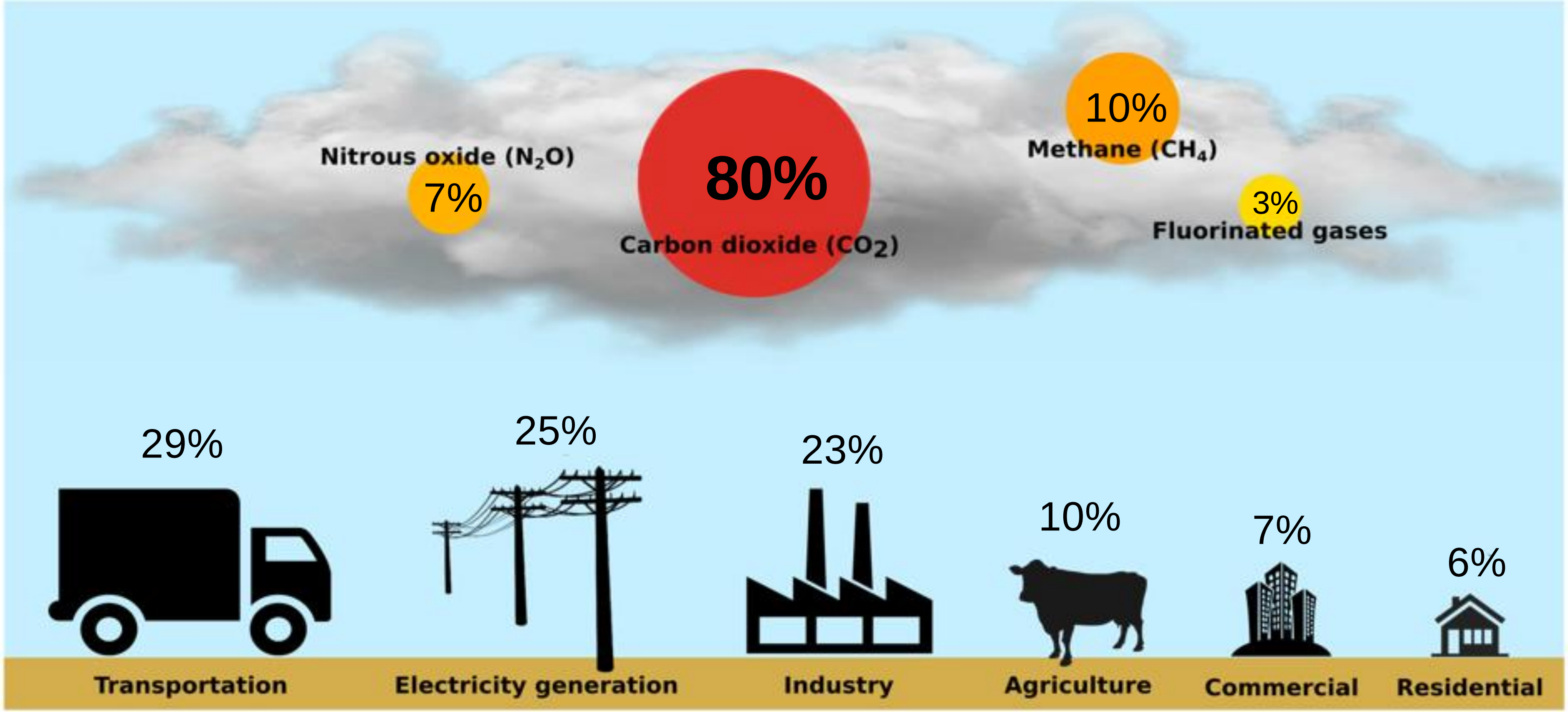
Electricity Generation is a Major Source of CO_2

Total U.S. greenhouse gas emissions by economic sector in 2019



Source:

EPA - United States Environmental Protection Agency: Greenhouse Gas Inventory Data Explorer

https://cfpub.epa.gov/ghgdata/inventoryexplorer/

Electricity is Mainly Generated from Fossil Fuels

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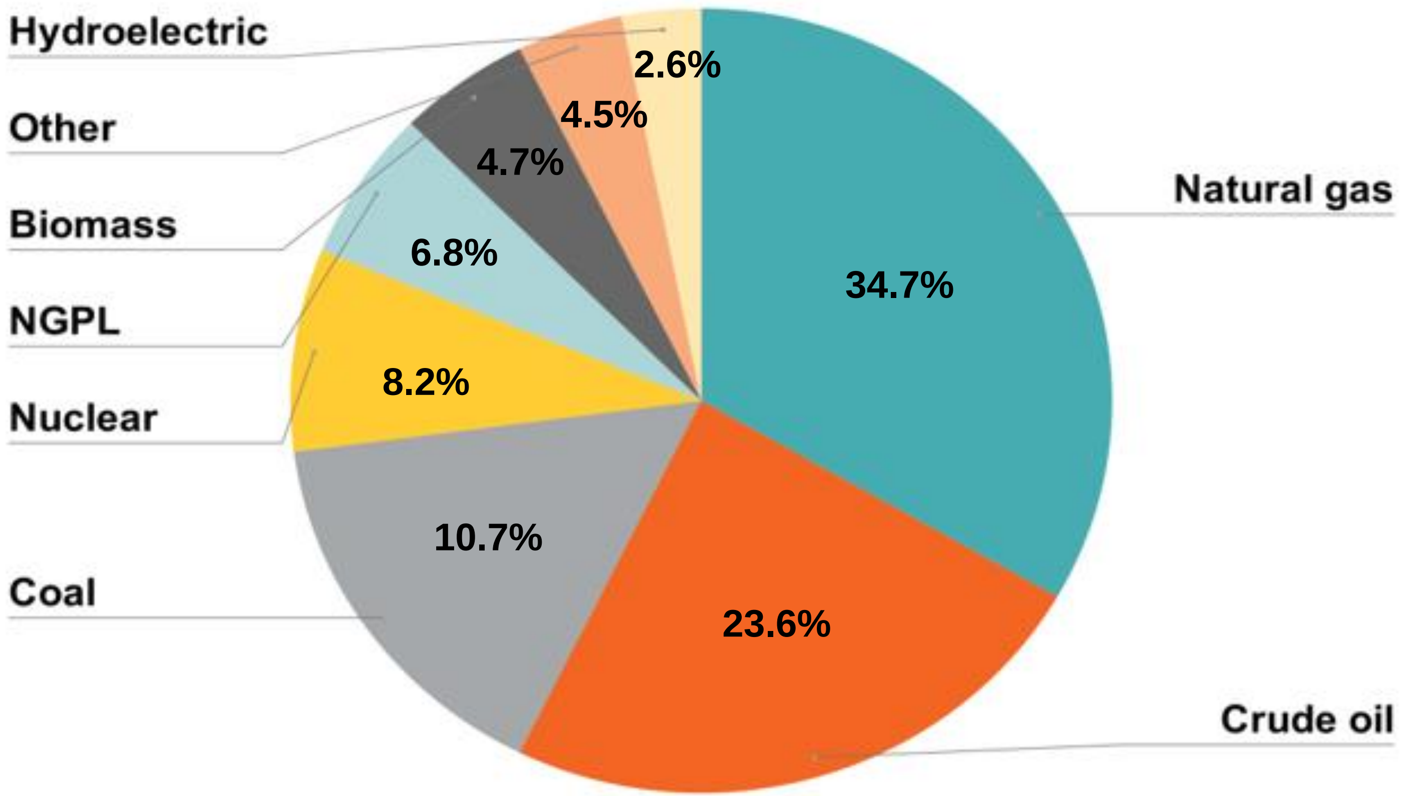
U.S. primary energy production by major sources in 2020



Source:

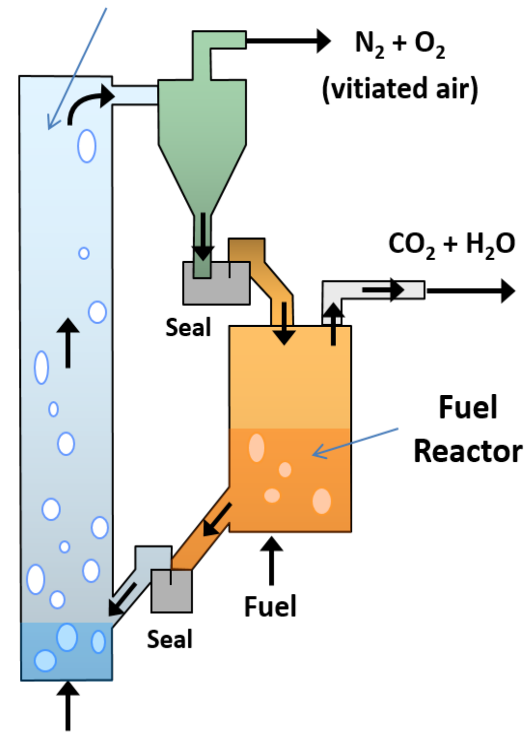
EIA - United States Energy Information Administration

https://www.eia.gov/energyexplained/us-energy-facts/

Numerical Simulations are Necessary for Industrial-Scale CLR Design

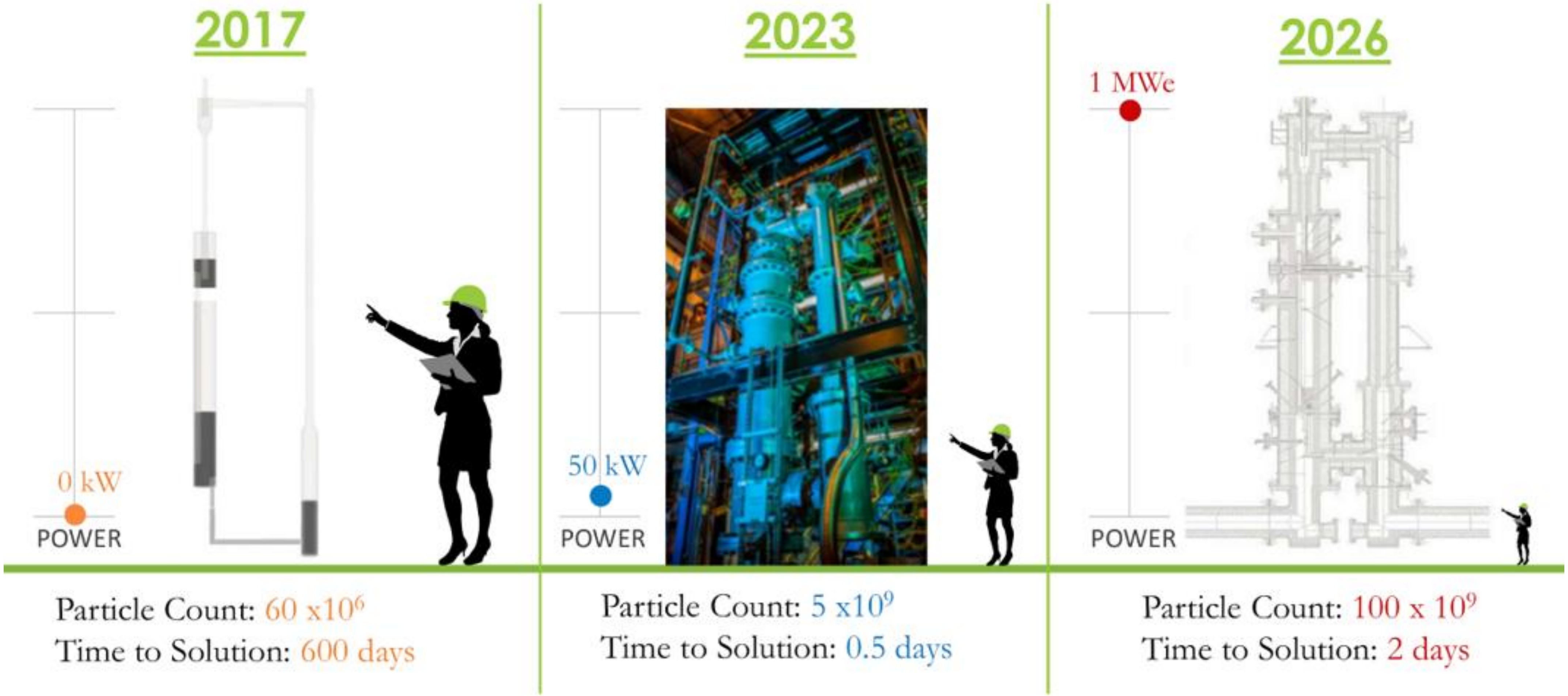
NETL's 50 kW hot flow chemical looping reactor (CLR)

Chemical looping combustion



Objective: CLRs to be Operative by 2026

The 2023 and 2026 values are rough estimates.



MFIX-Exa: CFD-DEM Multiphase Flows

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Fluid phase

- *Particle-unresolved multi-component low-Mach number* formulation
- *Embedded boundaries*
- *Finite volumes* in space, *Godunov scheme* for time integration
- Conservation of *mass*
- *Navier-Stokes momentum equation* in convective form
- Conservation of *species mass*
- Conservation of *energy*
- *Incompressibility* or *ideal gas equation of state*

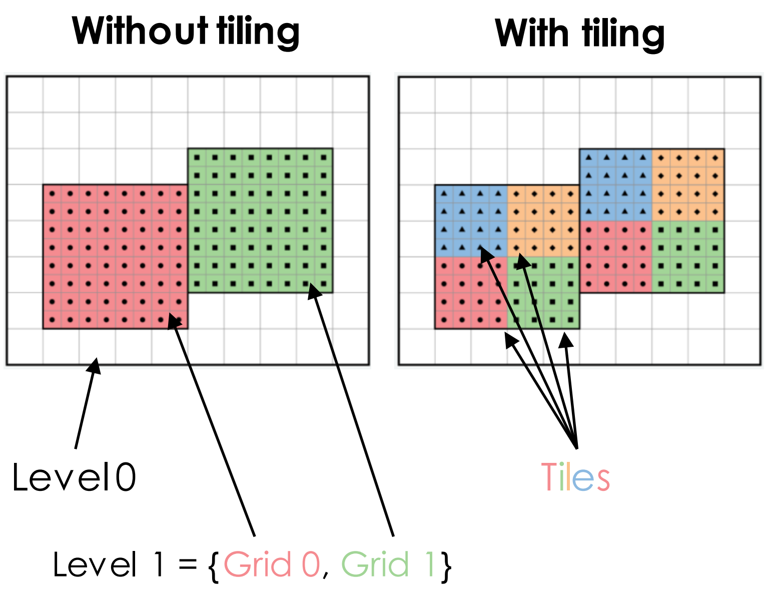
Solid phase: particles

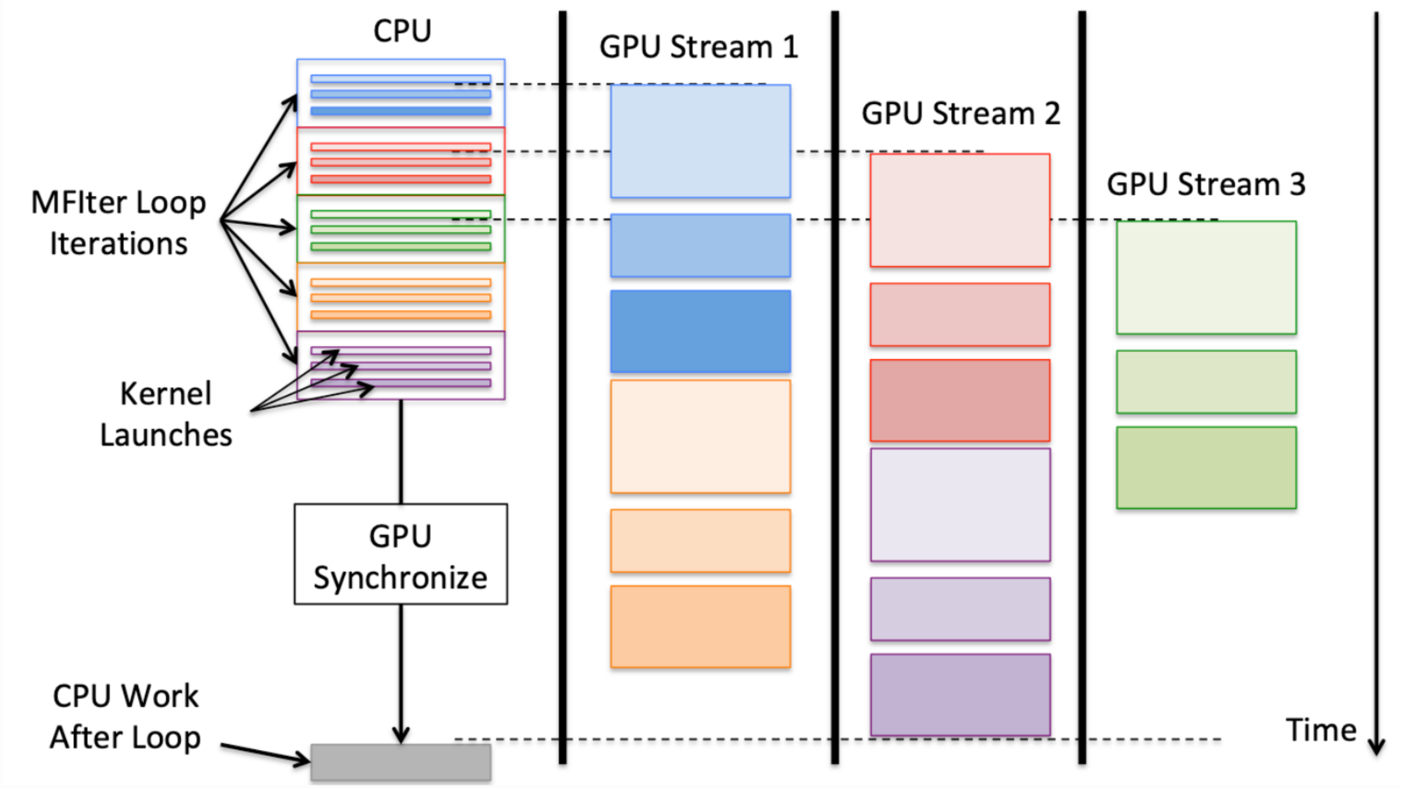
- *Soft-sphere spring-dashpot* model
- *Forward Euler* time integration with *subcycling*
- Conservation of *mass*
- Conservation of *linear momentum*
- Conservation of *angular momentum*
- Conservation of *species mass*
- Conservation of *energy*

Hybrid Parallelism

AMReX inside

Levels, Grids and Tiling



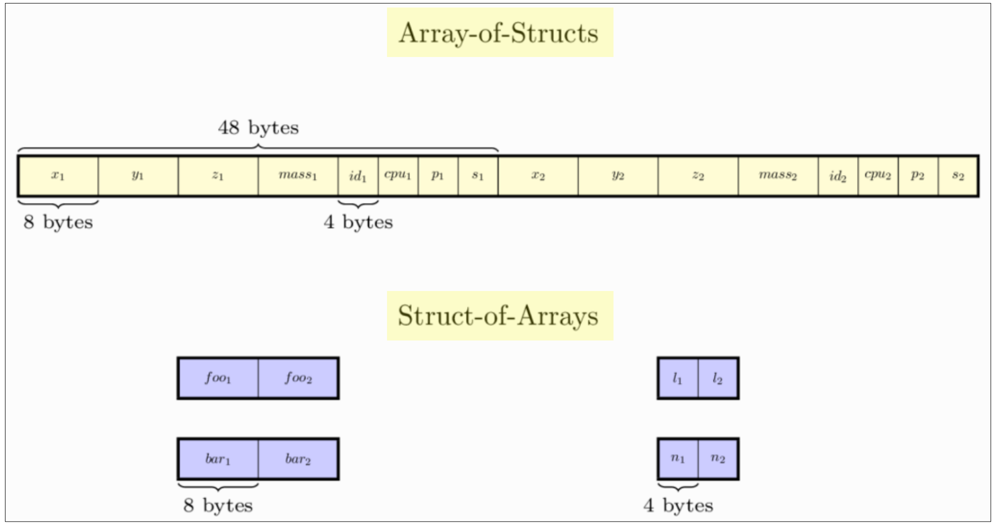


Images source: AMReX online documentation

Improve Coalescence + Reduce Communication

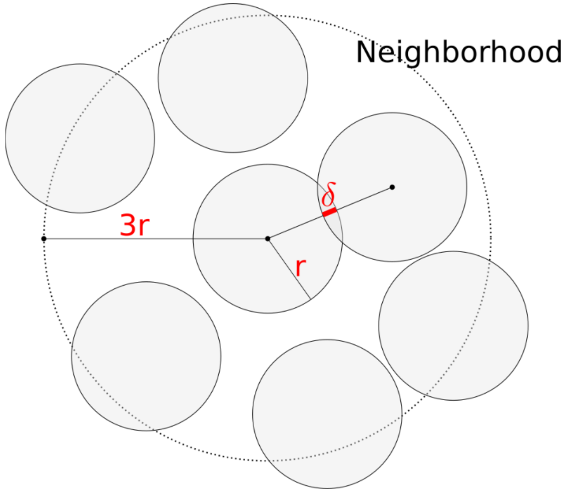
AoS → SoA

ParticleContainer<NStructReal, NStructInt, NArrayReal, NArrayInt>



Images source: AMReX online documentation

"Halving" the neighborlist



Take advantage of particle-particle mutual interaction:

if particle "i" ***is*** *in particle "j" neighborhood,*

then particle "j" ***is not*** *in particle "i" neighborhood*

Improve Coalescence + Reduce Communication

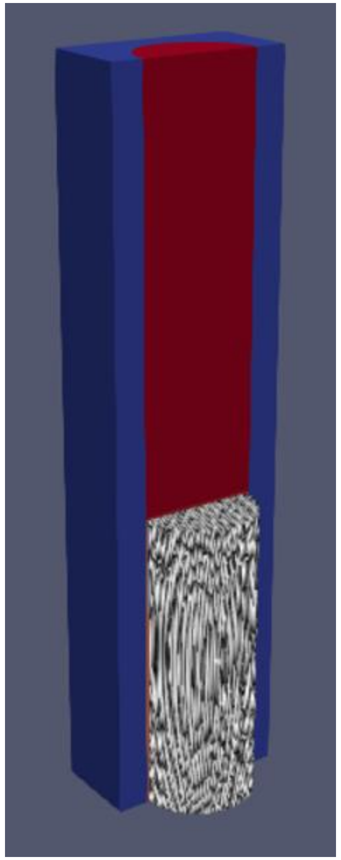
Real domain extents
lower bound (*m*): (0, 0, 0)
upper bound (*m*): (0.64, 0.16, 0.16)

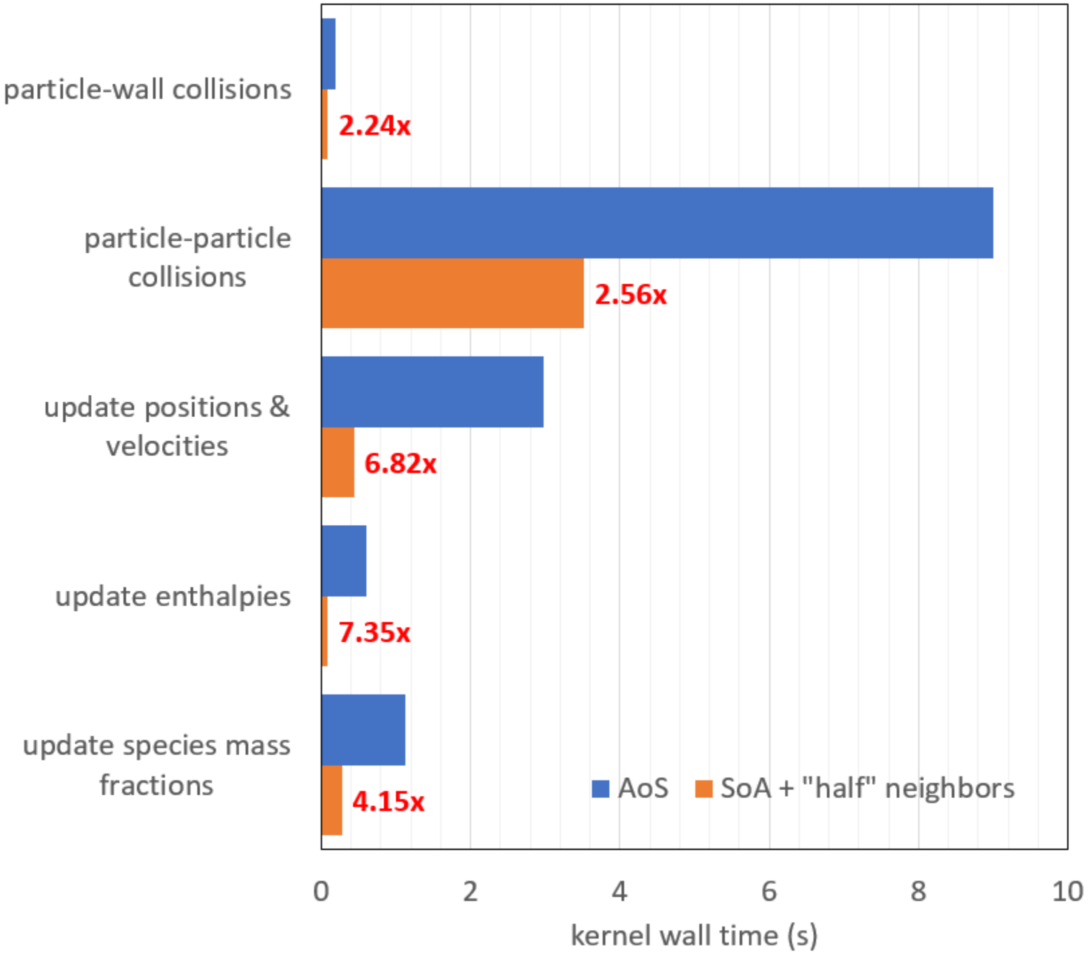
Computational domain
number of cells: (256, 64, 64)

Embedded boundaries
geometry: cylinder
cylinder radius (*m*): 0.1016
cylinder center (*m*): (0.64, 0.16, 0.16)

Solid particles
initial volume fraction = 60%

Chemical reactions
$4Fe_2O_3 + CH_4 \rightarrow 8FeO + CO_2 + 2H_2O$
$Fe_2O_3 + H_2 \rightarrow 2FeO + H_2O$
$Fe_2O_3 + CO \rightarrow 2FeO + CO_2$
$4FeO + O_2 \rightarrow 2Fe_2O_3$





Dual Grids Load Balancing

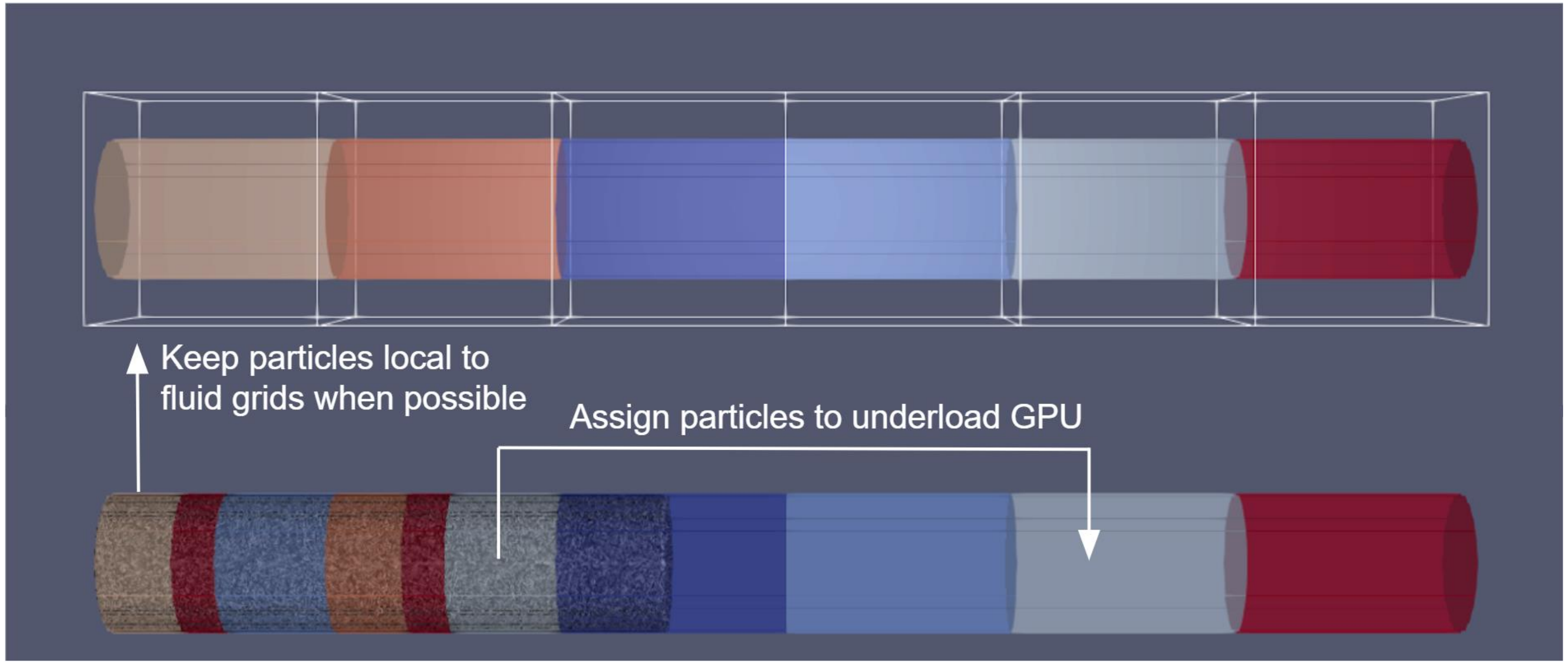
Fluid Grids: one grid per GPU

Particle Grids:

- balance particle counts among GPUs.
- minimize the communication between particle and fluid grids.

Fluid grids

Particles grids

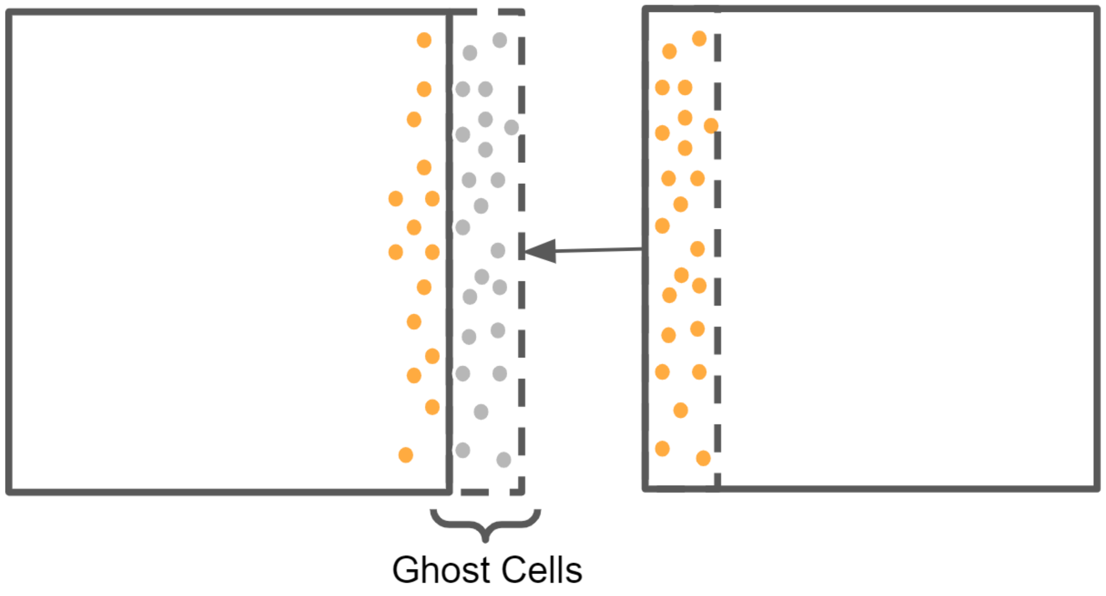


Load Balance Example. Each color represents a GPU.

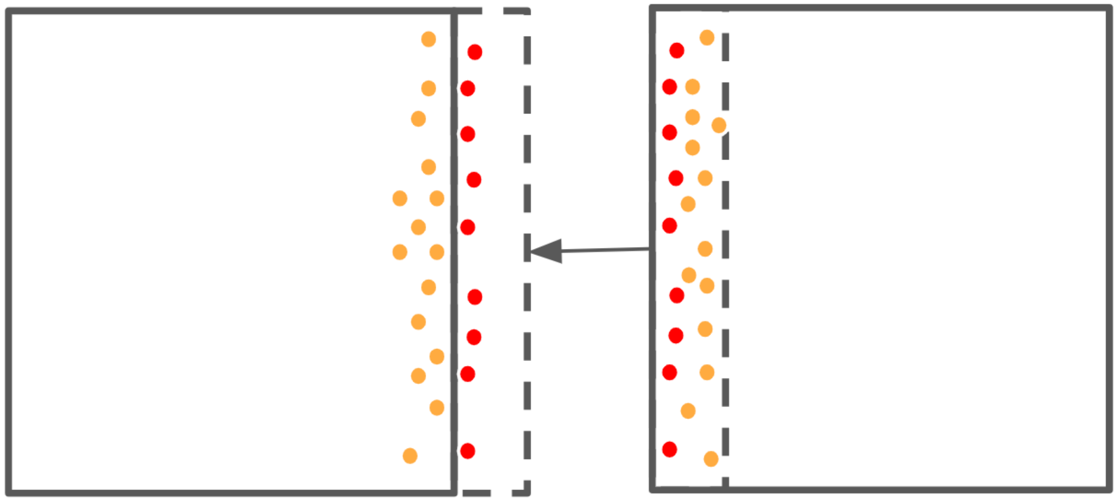
Courtesy of Hengjie Wang

Reduce Particle Communication

- We need to communicate particles in the ghost regions.
- Only the neighbor particles are used in the computation in the destination grid.
- Reduce particle variables used in communication.



Transfer all the particles in the ghost region



Just transfer the neighbor particles (red)

Courtesy of Hengjie Wang

Performance Evaluation of a Riser with 18 GPUs

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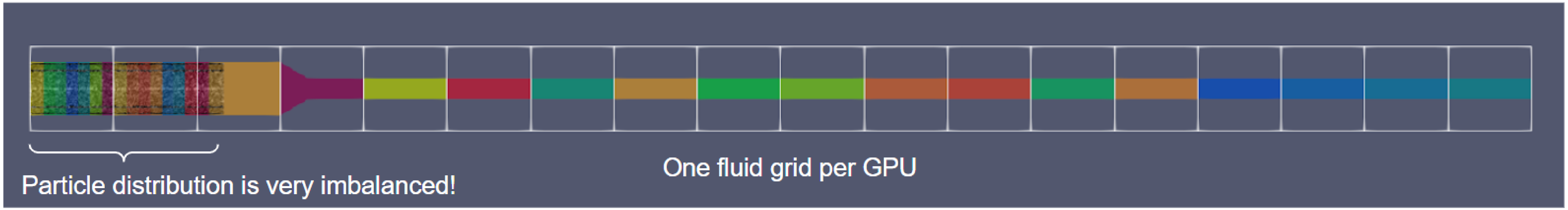
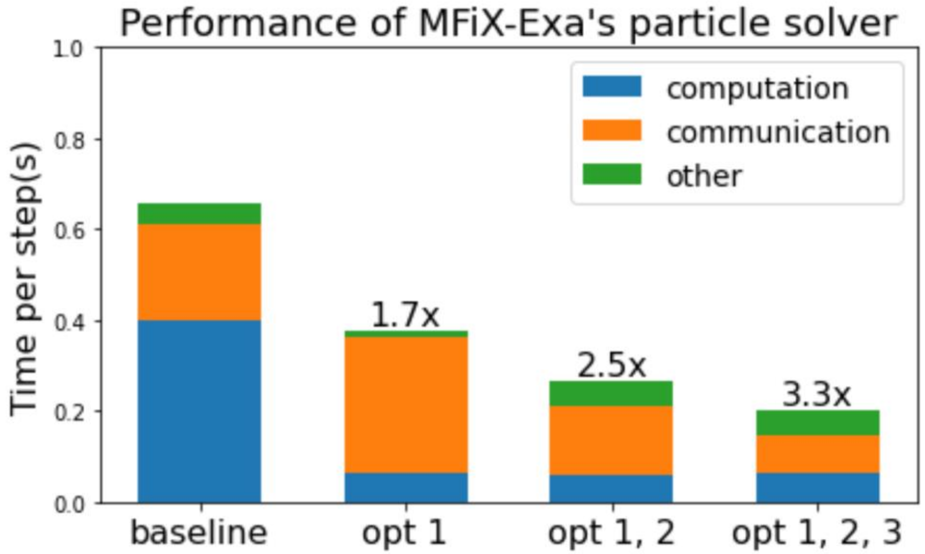
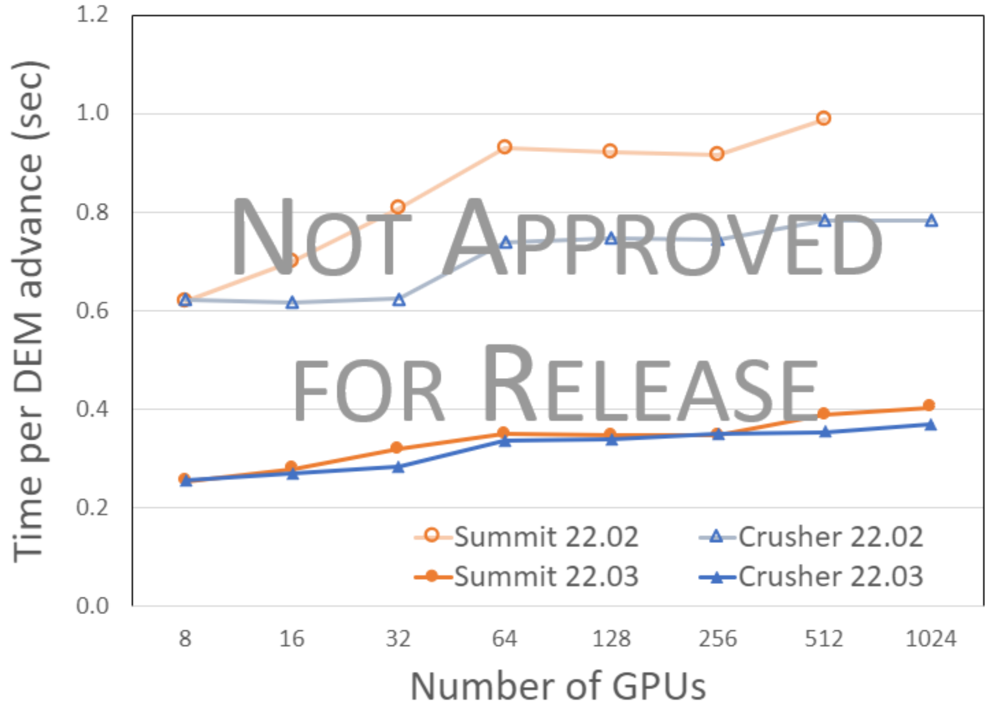


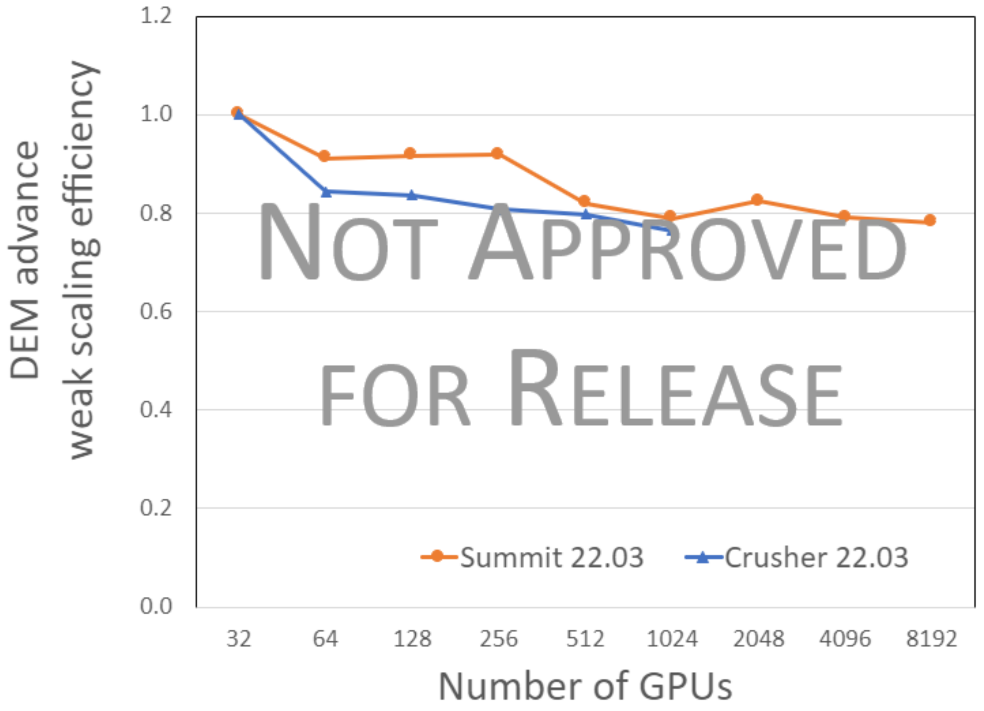


Baseline	Use the same grids for fluid and particles
Optimization 1	Use dual grids with load balance
Optimization 2	Only communicate neighbor particles
Optimization 3	Reduce particle variables

Courtesy of Hengjie Wang

Scaling on Crusher

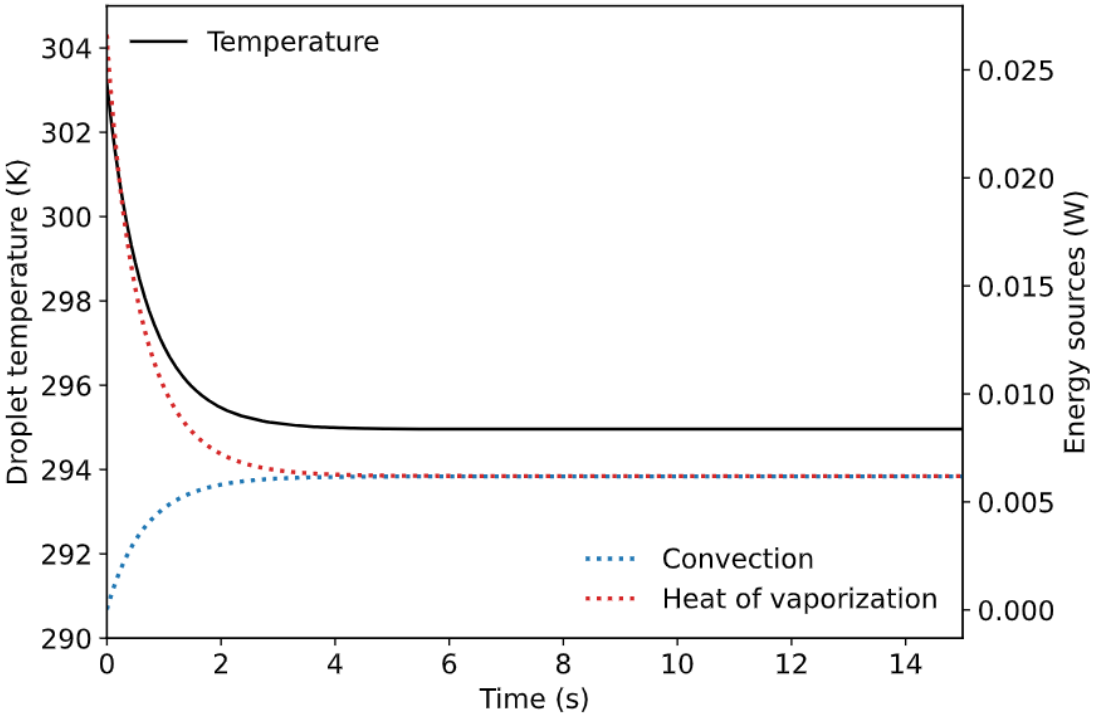




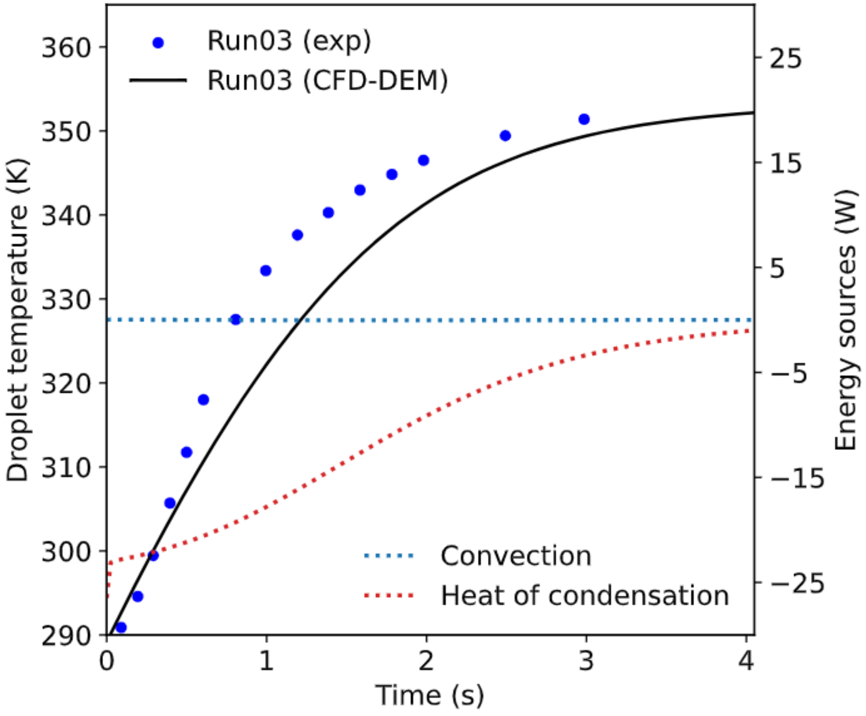
Numerical Results

Wet-bulb: water droplet in a humidified air stream

Droplet evaporation



Water vapor condensation



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Numerical Results

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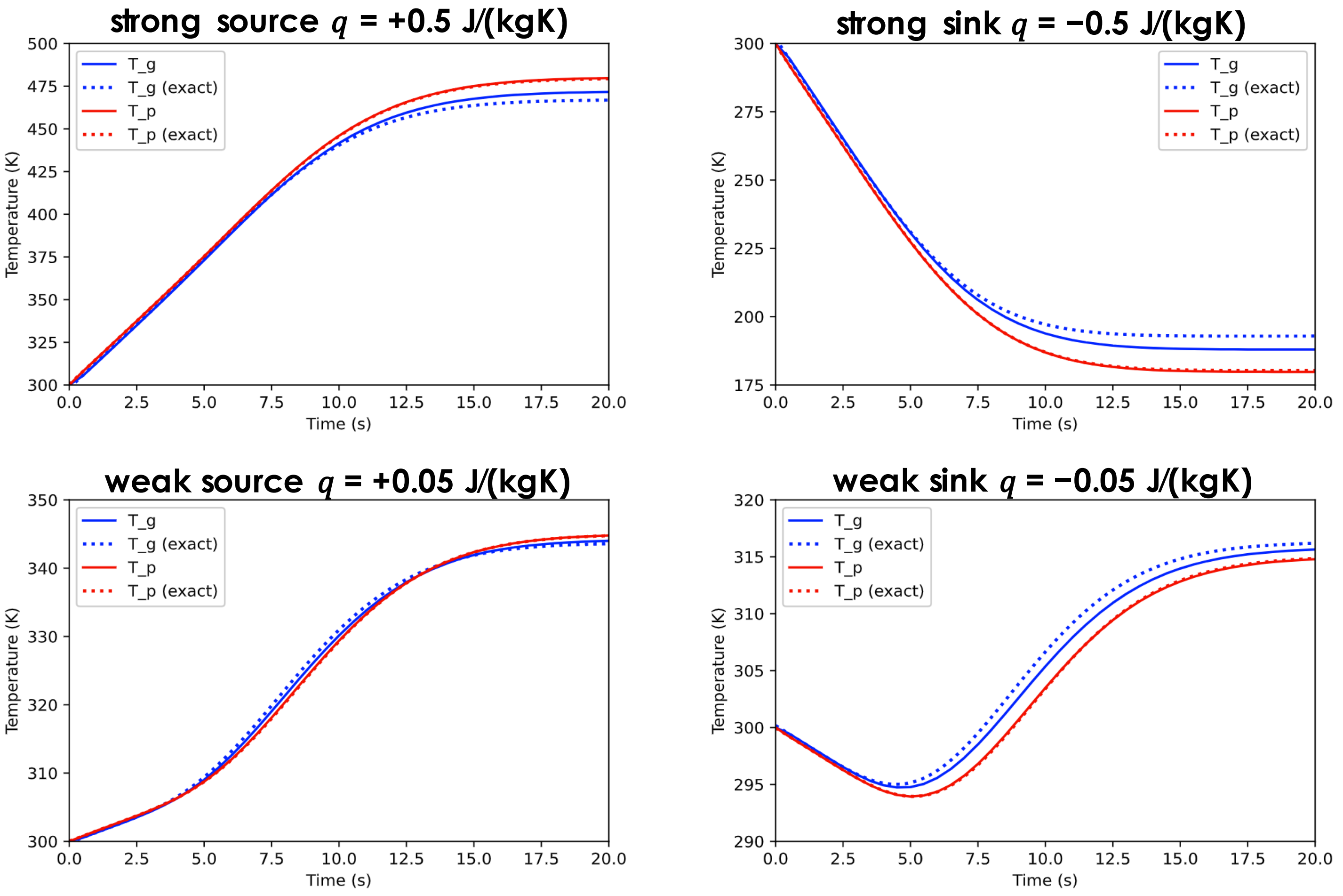
Transient heat conduction in packed beds



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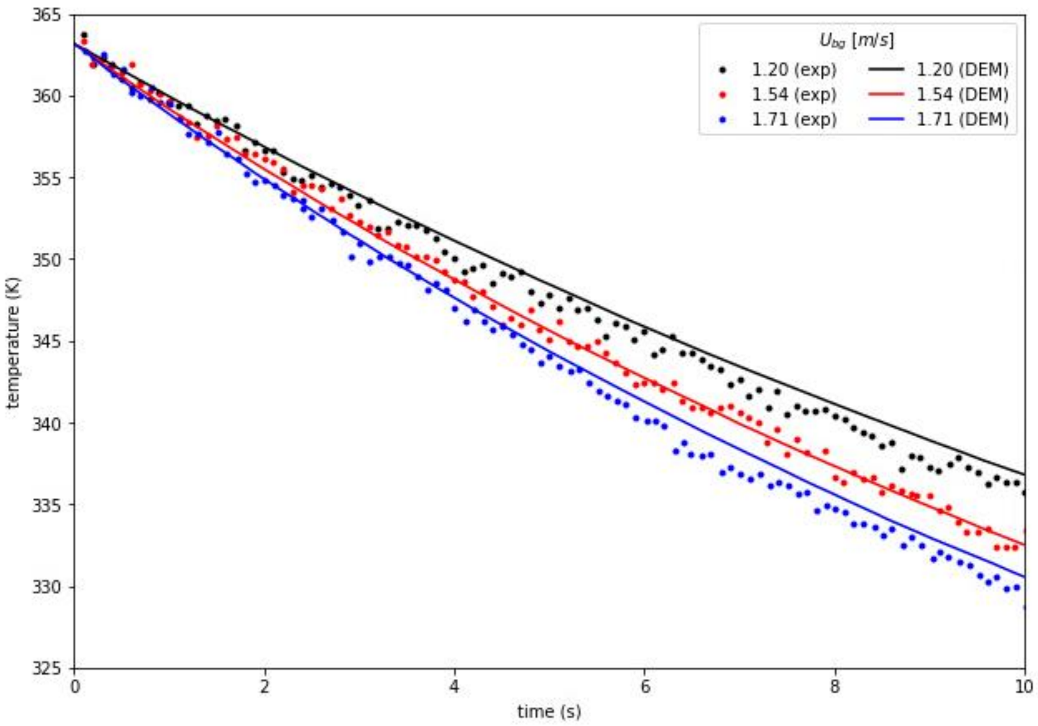
Salehi, M.S., Askarishahi, M., Radl, S. (2017). **Analytical solution for thermal transport in packed beds with volumetric heat source**. *Chemical Engineering Journal*

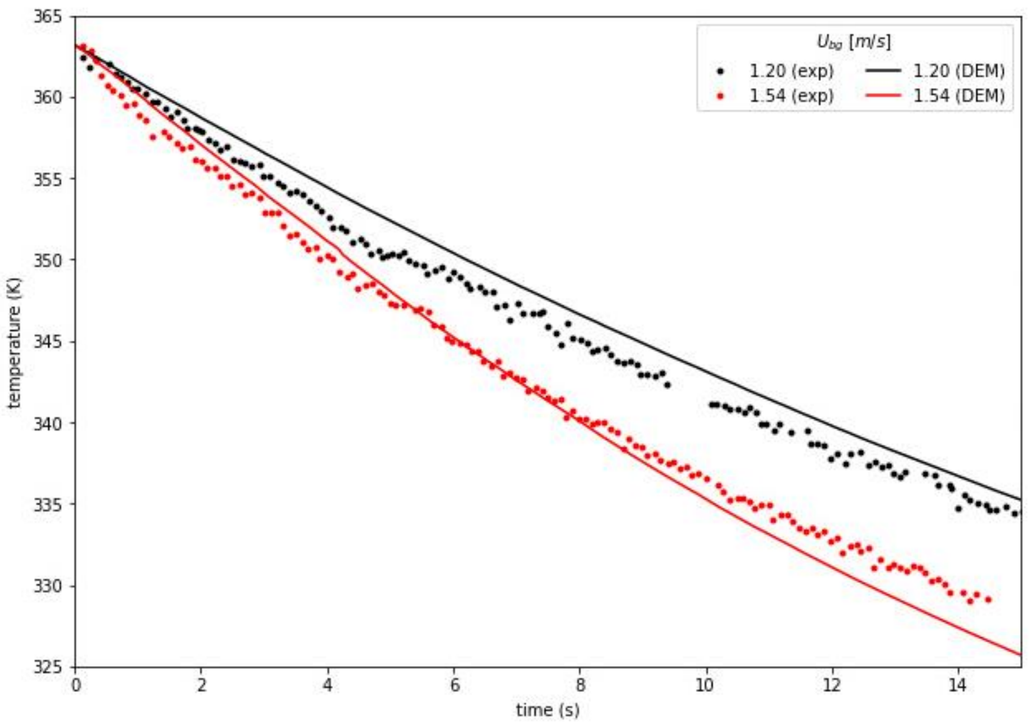
Numerical Results

Bench-scale fluidized bed

Light



Heavy



Patil, A.V., Peters, E.A.J.F., Sutkar, V.S., Deen, N.G., Kuipers, J.A.M. (2015). **A study of heat transfer in fluidized beds using an integrated dia/piv/ir technique**. *Chemical Engineering Journal*

THANKS!!

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