An Orthogonal Recursive Bisection (ORB) Based Time Advancement Algorithm for CFD-DEM Solvers

Hari Sitaraman, Ray Grout

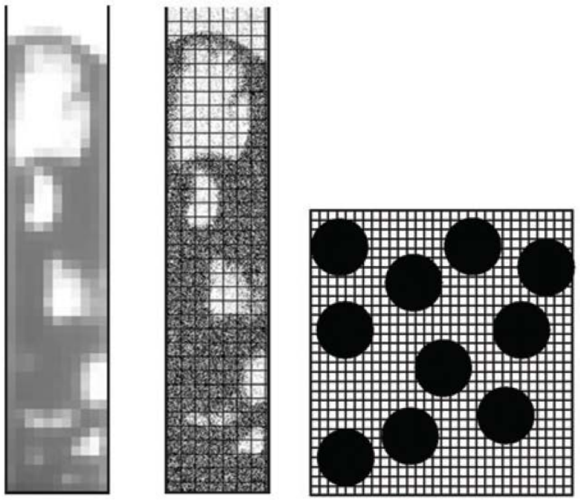
Venue: AIChE Annual Meeting 2018, Pittsburgh, PA, USA

Date: 29th October 2018

NREL/PR-2C00-72822

This work was authored by the National Renewable Energy Laboratory, operated by Alliance for Sustainable Energy, LLC, for the U.S. Department of Energy (DOE) under Contract No. DE-AC36-08GO28308. Funding provided by the U.S. Department of Energy Office of Fossil Energy. The views expressed in the article do not necessarily represent the views of the DOE or the U.S. Government. The U.S. Government retains and the publisher, by accepting the article for publication, acknowledges that the U.S. Government retains a nonexclusive, paid-up, irrevocable, worldwide license to publish or reproduce the published form of this work, or allow others to do so, for U.S. Government purposes.

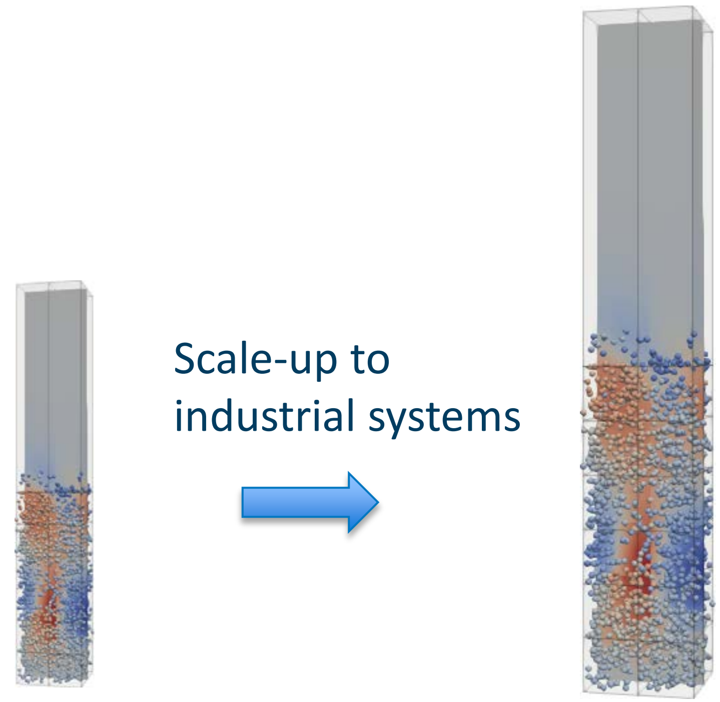
Motivation



TFM CFD-DEM DNS

Less closure models

Computational cost



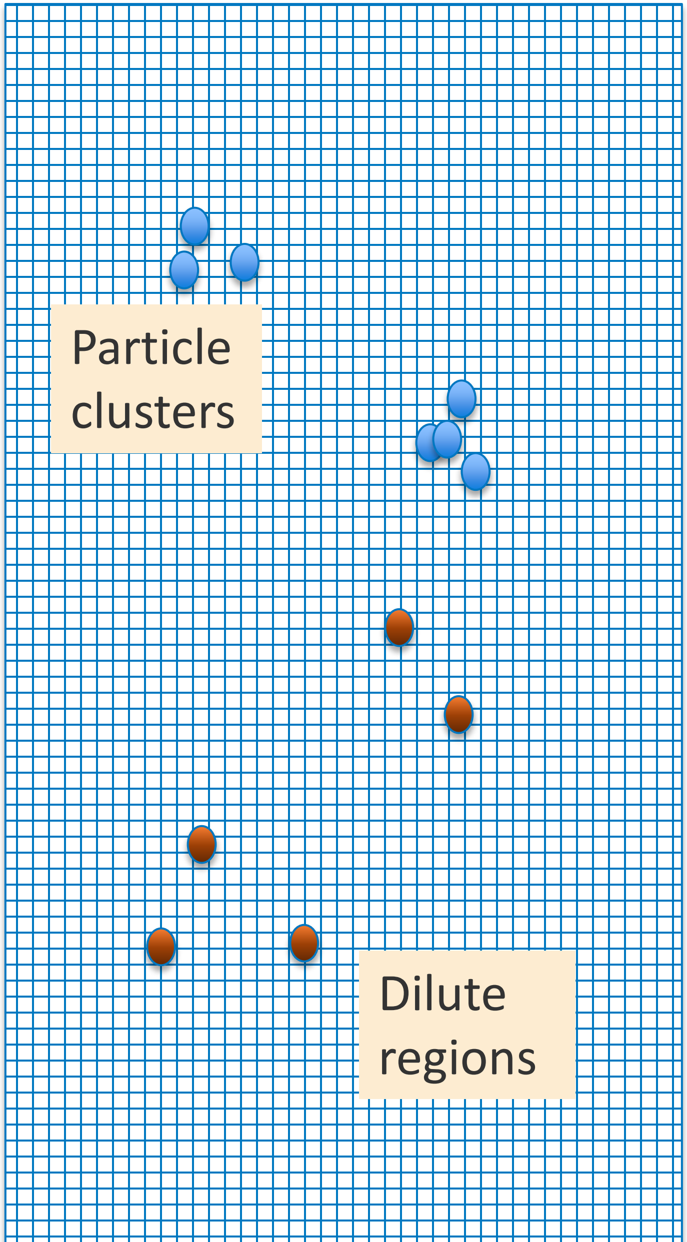
N_p ~ 10^4-10^7 N_p ~ 10^9-10^{12}

- CFD-DEM – balance between computational cost and modeling closures
- Goal: Achieve simulations of industry relevant granular flows
- Specifically, increase performance of well-established CFD-DEM solver, MFIX
- MFIX – Multiphase Flow with Interface Exchanges
  - Developed at National Energy Technology Laboratory
  - MFiX-Exa – being developed as part of DOE Exascale Computing Project

Current approaches for particle advance

- 2^{nd} order explicit-Verlet scheme
  - $\vec{v}_i^{n+1/2} = \vec{v}_i^{n-1/2} + \Delta t \frac{\vec{F}_i^n}{m_i}$
  - $\vec{x}_i^{n+1} = \vec{x}_i^n + \Delta t \, \vec{v}_i^{n+1/2}$
- Constant time step size for all particles
  - Collisional time scale determined by solid phase properties
- Challenge with constant time step
  - Fluid residence time scales with system dimensions
  - Particle time scale is intrinsic to phase properties
- For large-scale systems computational cost increases
  - More number of particles
  - More number of time steps

Adaptive time stepping - idea



- Particle clustering is common in industrial systems
- Reduce overall computational cost with localized time stepping method
- Adaptive time stepping approach
  - Identify particle clusters
  - Advance particle subsets with local timescale
    - Lower costs for dilute regions
  - Identify dilute/clustered regions?
  - synchronization in a global fluid time step?
  - Collision misses?

Mathematical model and numerical methods

Computational model

Continuous phase equations solved by SIMPLE/projection schemes

$$\frac{\partial(\epsilon_g \rho_g)}{\partial t} + \nabla \cdot (\epsilon_g \rho_g \mathbf{v}_g) = 0$$

$$\frac{\partial(\epsilon_g \rho_g \mathbf{v}_g)}{\partial t} + \nabla \cdot (\epsilon_g \rho_g \mathbf{v}_g \mathbf{v}_g) = \nabla \cdot \bar{\bar{S}} + \epsilon_g \rho_g \mathbf{g} + I_{gs}$$

Interaction term

Discrete phase equations solved using 2nd order velocity-verlet scheme

$$\frac{d\mathbf{X}_i}{dt} = \mathbf{V}_i$$

$$m_i \frac{d\mathbf{V}_i}{dt} = \mathbf{F}_T = m_i \mathbf{g} + \mathbf{F}_d + \mathbf{F}_c$$

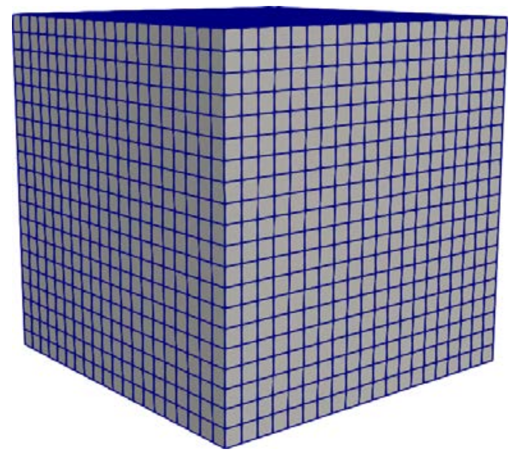
Collisional term

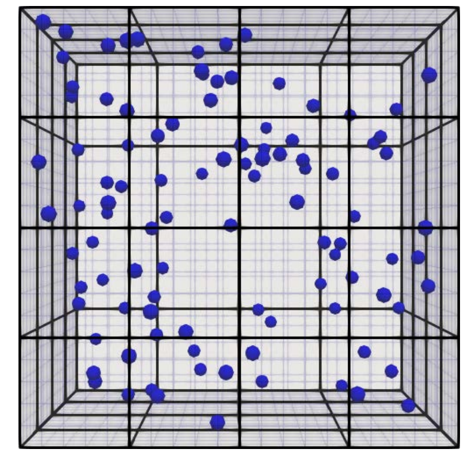
Viscous and pressure drag

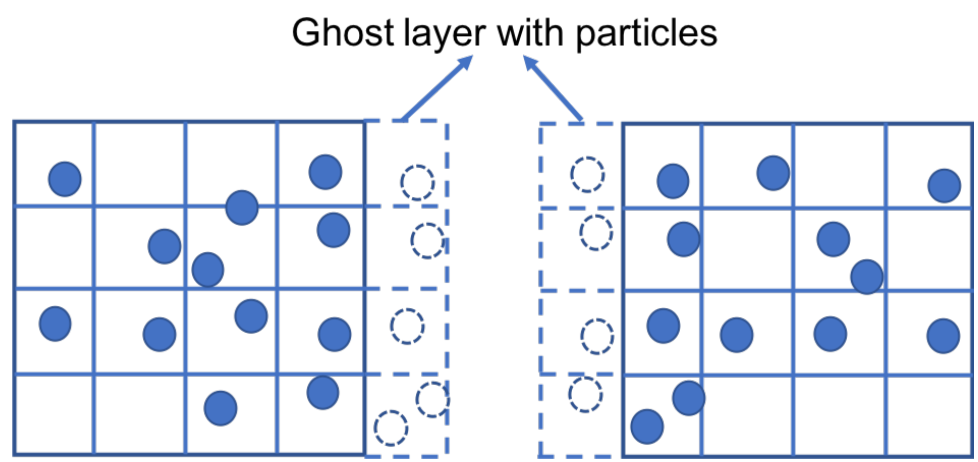
- Continuous to discrete coupling through void fraction and momentum interaction term
- Discrete to continuous coupling through viscous and pressure drag

Code base – MFIX-Exa

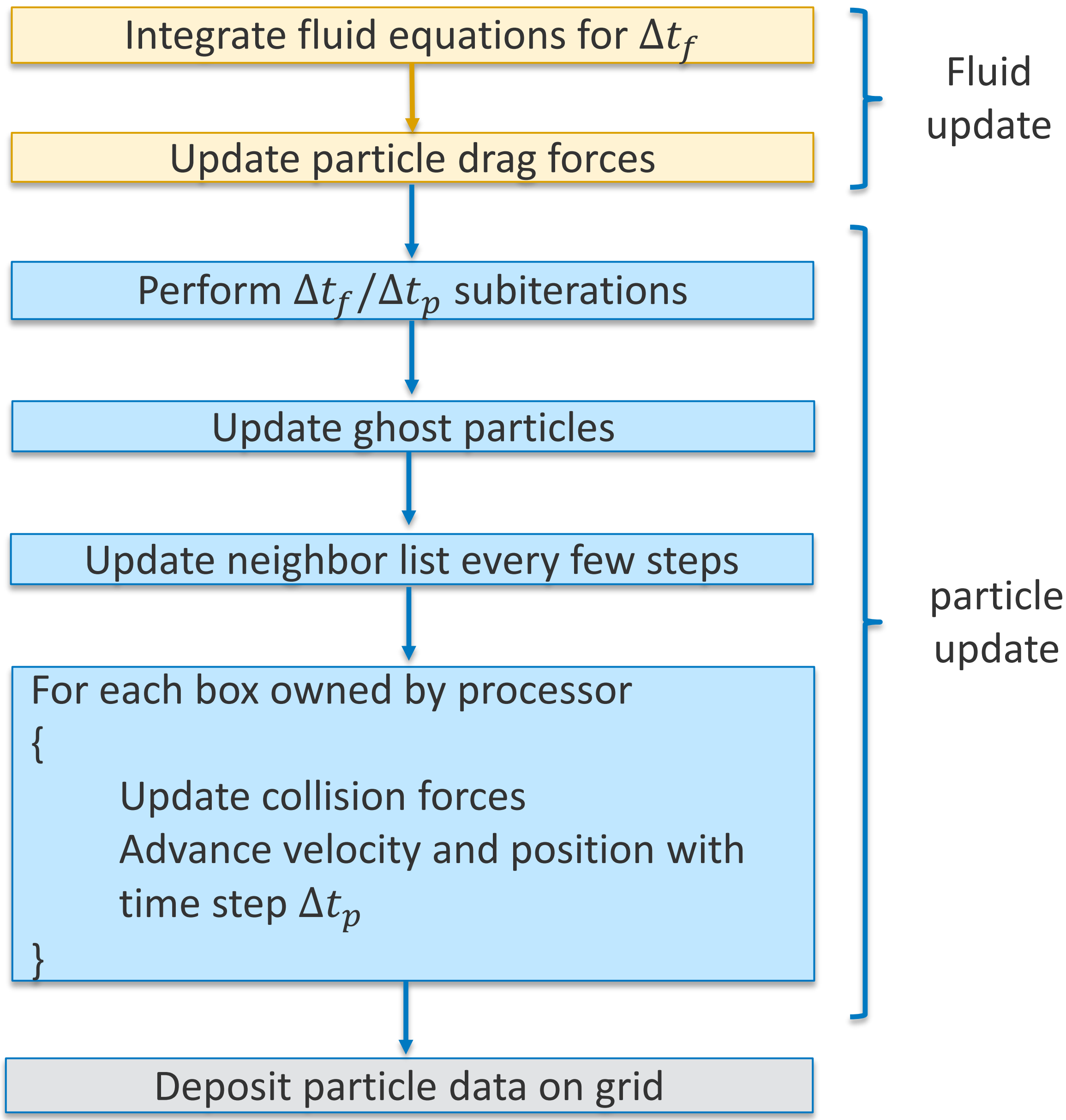
- Slimmed down version of multiphase code – MFIX
  - developed at LBNL, NETL, NREL and CU, Boulder
  - Test bed for performance optimizations
  - uses adaptive-mesh refinement library, AMReX
  - Decomposition of domain into boxes
    - Boxes distributed among processors
    - load balancing
      - Space filling curve
      - knapsack



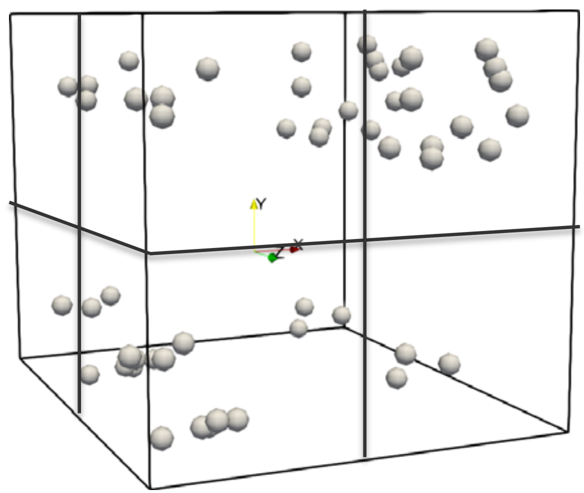




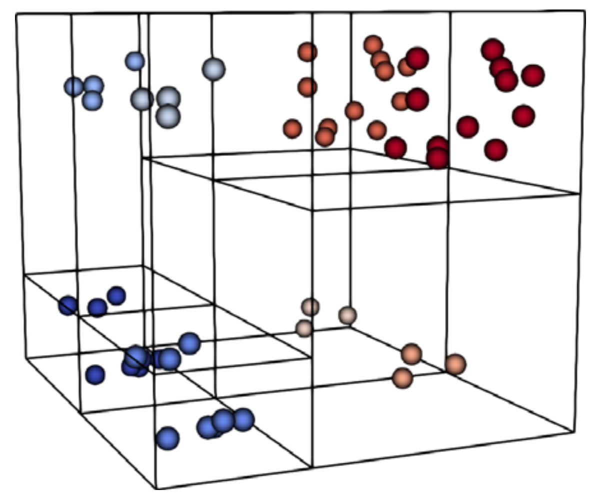
Tasks in a coupled time step



Orthogonal Recursive Bisection (ORB) method



Classic explicit scheme

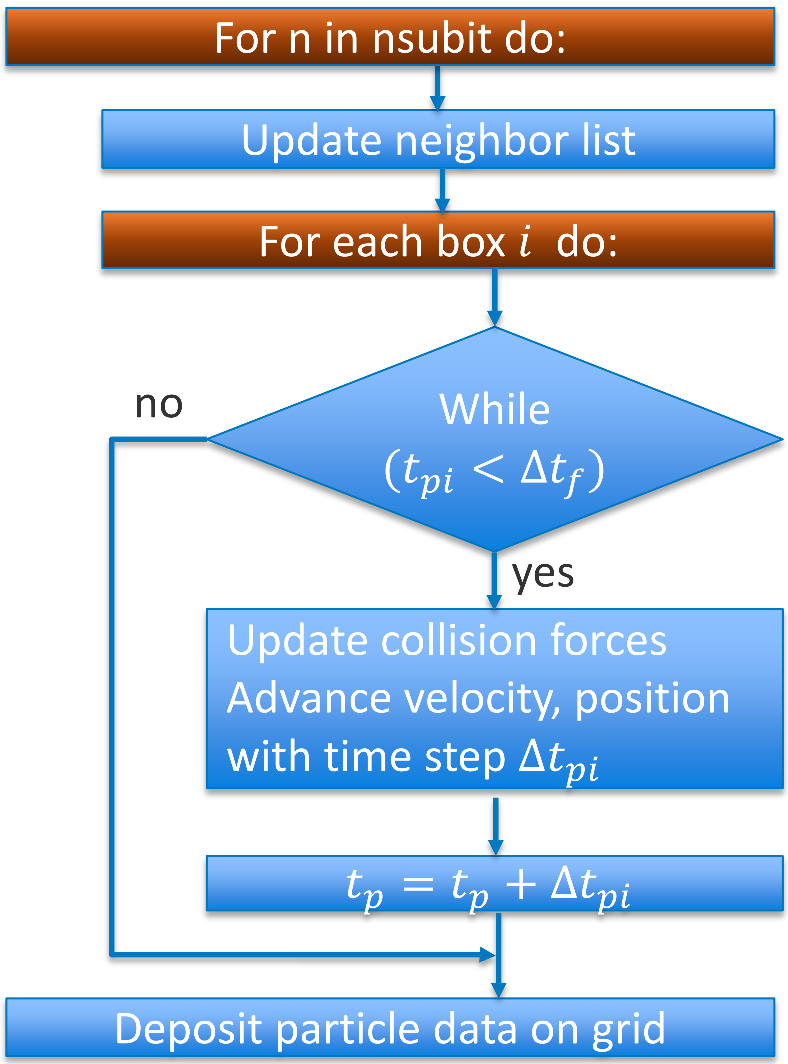


Explicit ORB scheme

- Find global minimum time step, dt_{min}
- N_subit = dt/dt_{min}
- Update neighbor data
- Perform N_subit sub iterations
    - Loop over each box
        - Compute forces
        - Advance using explicit scheme

- Build the ORB tree
- Update neighbor data
- Loop over each box
    - Find minimum time step, dt_{min}
    - N_subit=dt/dt_{min} (can be 1!!)
    - Perform N_subit sub iterations
        - Compute forces
        - Advance using explicit scheme

Reduce neighbor exchange errors – strategy 1



- Advance in smaller timestep chunks
  - Particle update to fluid time level happens in a few iterations of smaller time steps
  - This will increase number of neighbor updates
  - More number of updates will increase accuracy
  - Algorithm tends to constant global timestep method for large number of sub-iterations

Reduce neighbor exchange errors – strategy 2

Δt_{ps} = user defined sub time step

While ($t_{pi} < \Delta t_f$)

First pass

- Redistribute, Update neighbor list
- Do adaptive time stepping for time Δt_{ps}
- Store particle position and velocity

second pass

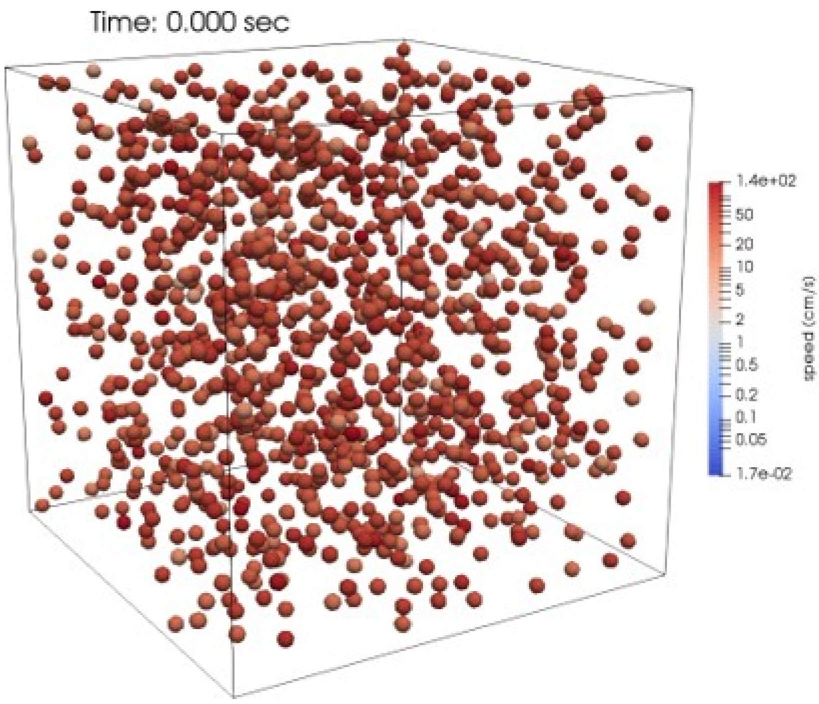
- Repeat 2 times
  - Redistribute, Update neighbor list
  - Do adaptive time stepping for time $\Delta t_{ps}/2$

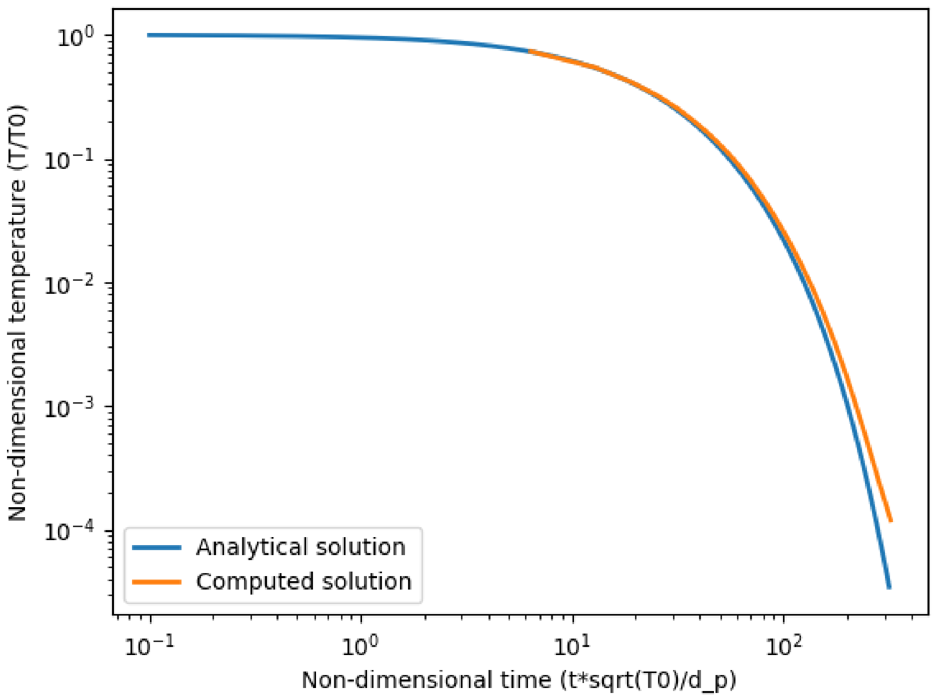
- Compute error between first and second pass
- $t_{pi} = t_{pi} + \Delta t_{ps}$
- If error is large $\Delta t_{ps} = \Delta t_{ps}/2$

- Two-pass error correction method
  - Adaptively change particle update time step based on an error metric
- Advantages
  - Detect time stepping failure
  - Reduces neighbor update MPI communication events
  - Temporal locality in Cache
    - Repeated usage of memory
- Disadvantage
  - More floating point operations

Results

Test case 1 – Homogenous cooling system (HCS)



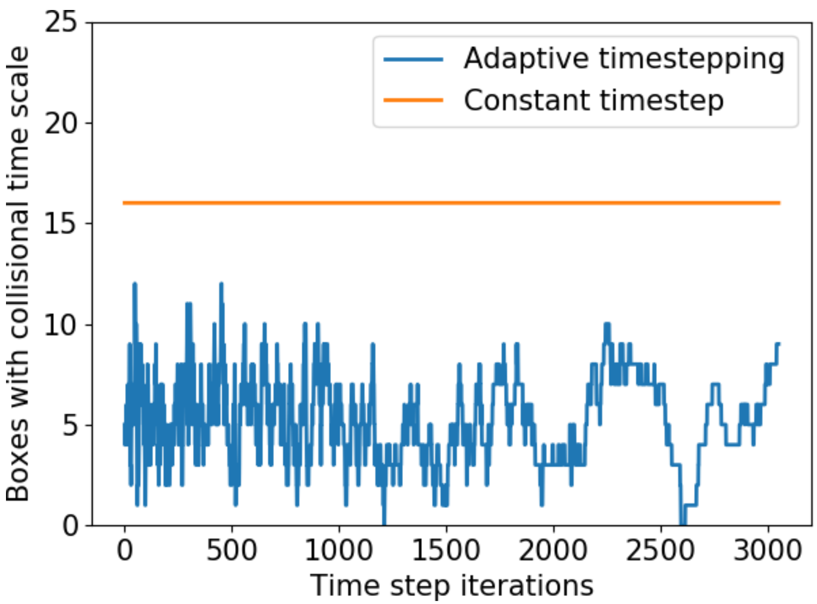


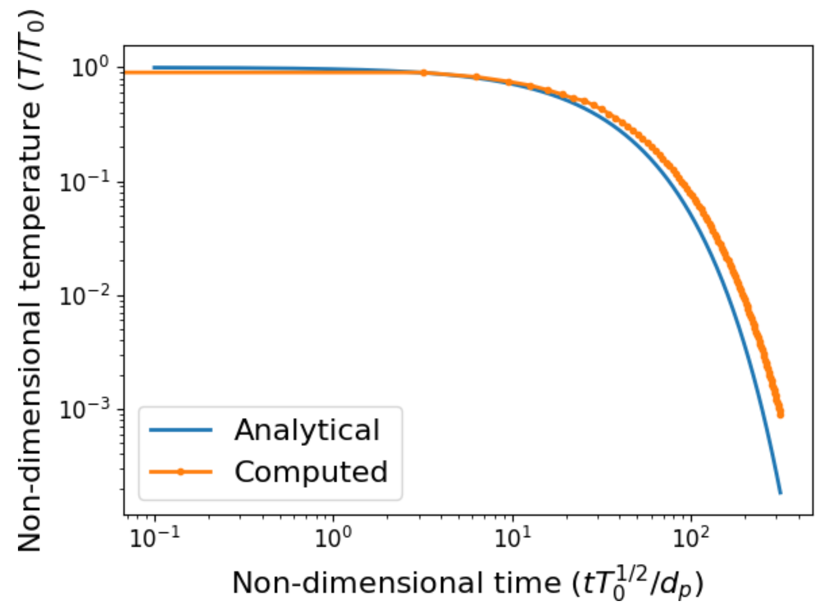
- Decay of total particle energy with time
  - Viscous and collisional losses
- Initial conditions – random velocity and position distribution

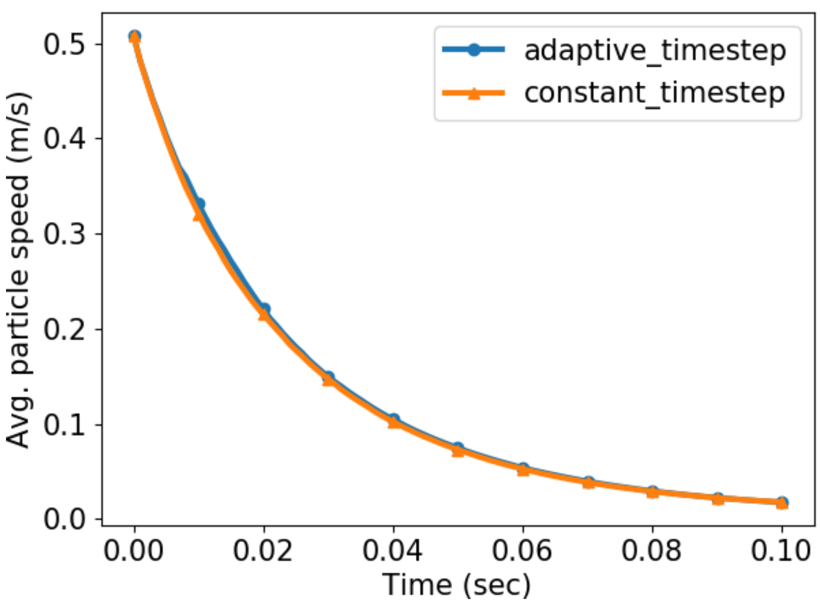
- Analytic solution – Haff's law[1] predicts decay of non-dimensional temperature

[1] Haff, P., "Grain flow as a fluid-mechanical phenomenon," Journal of Fluid Mechanics, Vol. 134, 1983, pp. 401–430.

Test case 1 – Homogenous cooling system (HCS)





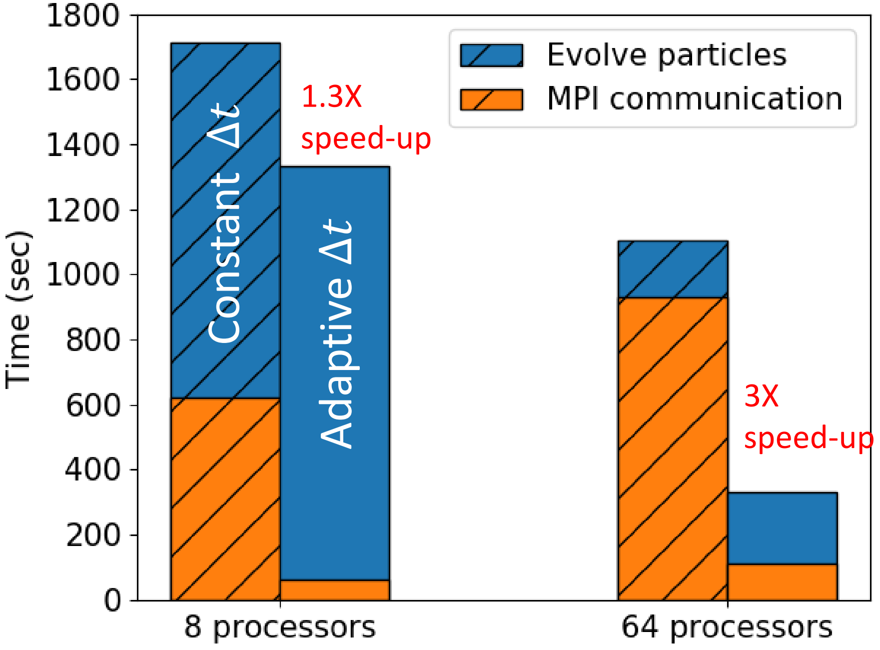


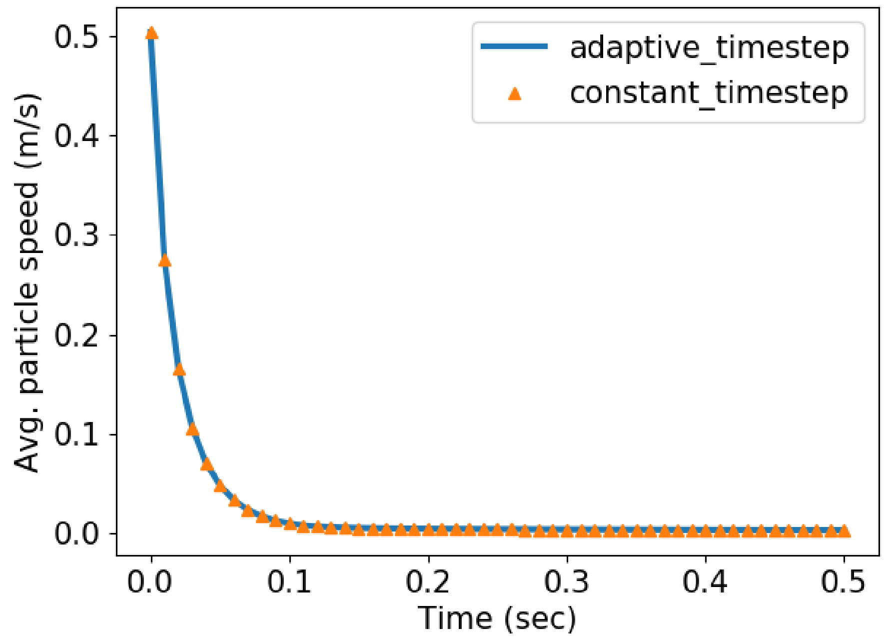
- 300 particles,16 ORB leaves, 8000 cells
- Single processor run

- Initial guess for adaptive timestep = 10 μs
- Collisional time step = 0.3 μs

- Speed-up of 1.6x obtained with adaptive time stepping

Test case 1 – Homogenous cooling system (HCS)



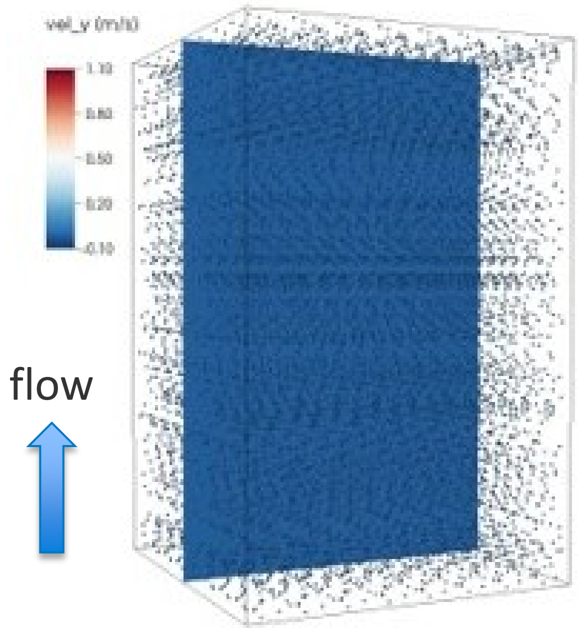


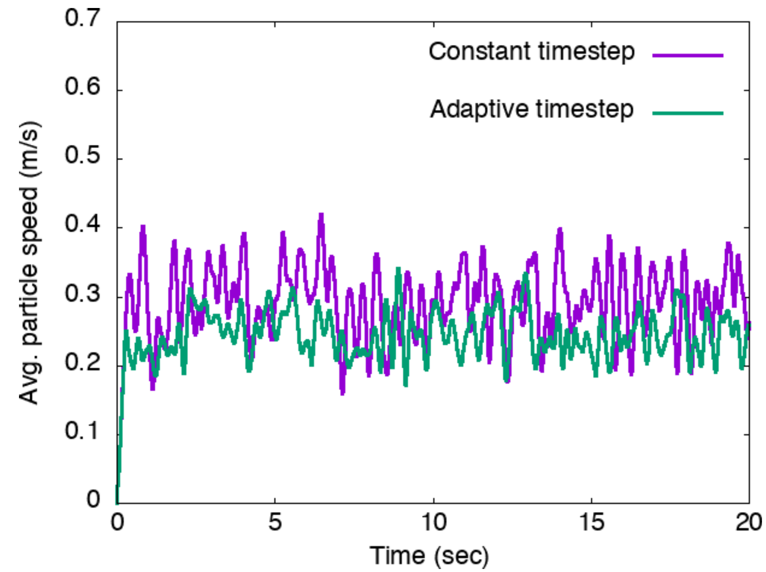
- Multi-processor HCS run with 40,000 particles with 128 ORB leaves

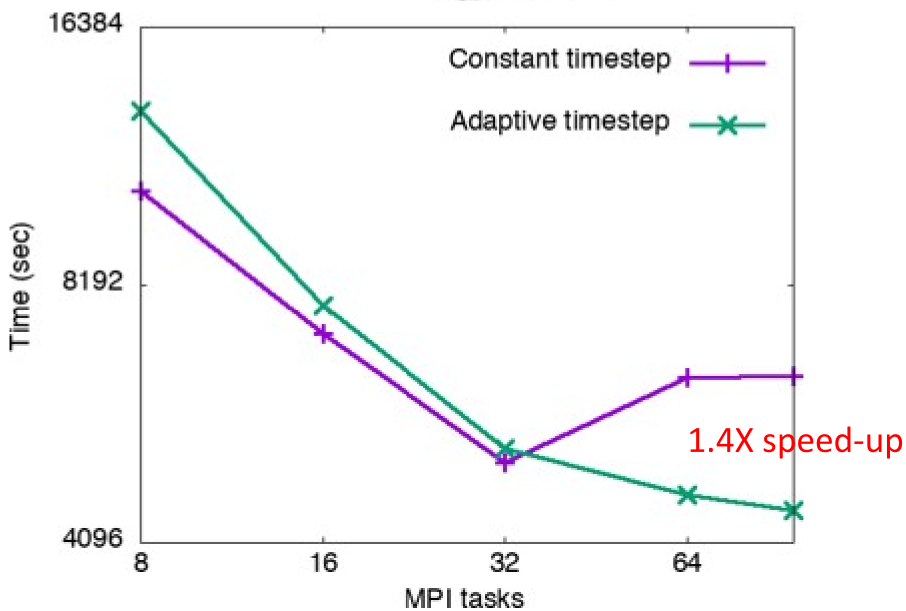
- Improvements are more pronounced at larger processor counts
    - Less MPI communications with respect to neighbor communication
    - ~ 3X improvement seen with 64 processors

- Retrieves identical solution with respect to constant timestep case

Test case 2 – Riser flow

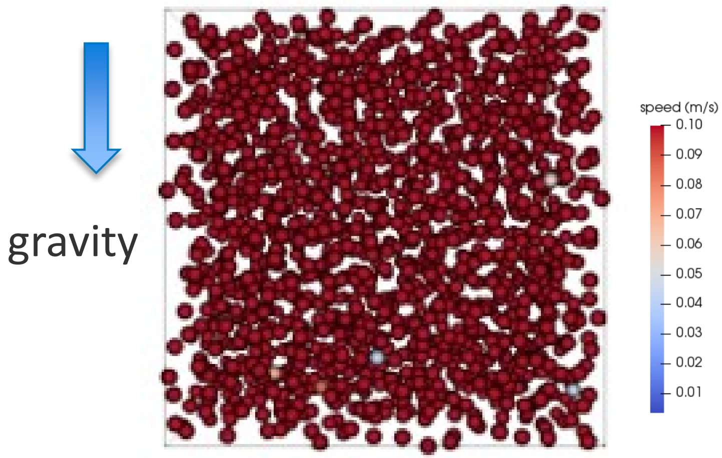


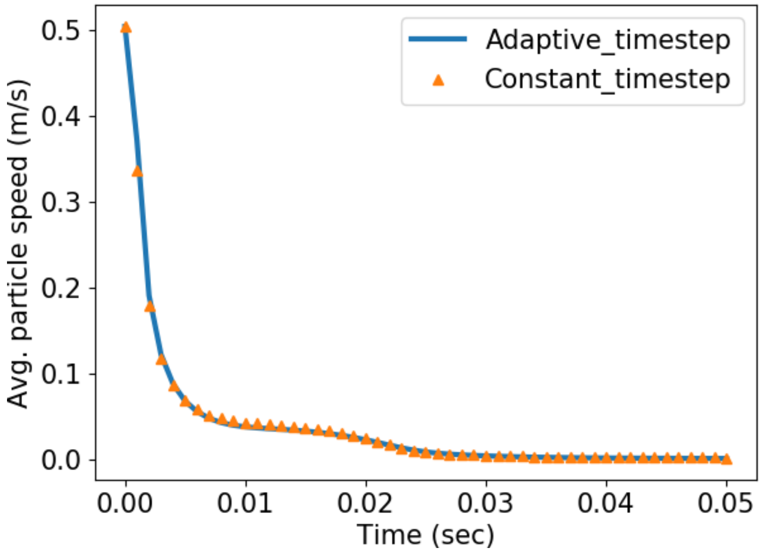


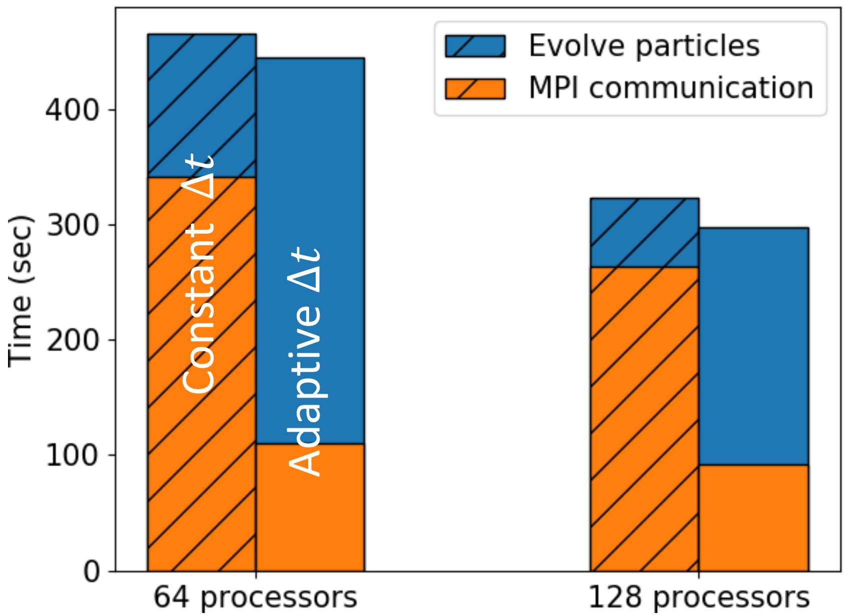


- Case set up
  - Lateral wall boundaries
  - Constant y pressure gradient
  - 51200 cells, 14000 particles
- Better strong scaling observed with adaptive timestep
  - Less MPI communications
- Average speed solutions are very similar

Test case 3 – Settling due to gravity







- Case set up
  - Top/bottom walls
  - Gravity along -y direction
  - 64000 cells, 100,000 particles
- Lower MPI overhead for adaptive timestepping
- Less performance improvement due to execution overhead
- Average particle speed solutions match

Conclusions and future work

- Conclusions
  - Developed an adaptive time stepping algorithm
    - Using Orthogonal recursive bisection
    - Local time steps for subsets of particles at the ORB leaves
    - Two-pass error correction method to reduce collision misses
  - Performance improvement
    - Significant performance improvement for parallel cases
      - Reduces MPI communication overheads
- Future work
  - Other decomposition methods
    - K-means clustering
  - Currently studied 3 canonical DEM cases
    - Application to realistic systems
  - What is the correct error tolerance for different DEM systems?

Acknowledgements

- Funding from DOE, Office of Fossil Energy
- Ann Almgren from LBNL and Jordan Musser from NETL for MFIX-Exa code, funded by ASCR Exascale Computing Project (ECP)
- Researchers at CU Boulder:
  - Prof. Christine Hrenya, Dr. Peiyuan Liu, Steven Dahl
  - Prof. Thomas Hauser, Aaron Holt, Shandong Lao, Mike Page
- Deepthi Vaidhynathan, Ray Grout at NREL