SAND2006-7163C

Coupled Discrete-Time Immersed Boundary-Discrete Element Method for Multiphase Flow

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Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

Discrete Element Simulations

- An efficient, highly parallel DEM code has been developed to simulate dry granular materials
  - Mono or polydispersed particulates
  - Arbitrary material properties: hardness, coefficient of restitution, and friction coefficients
  - Particles can be poured into an arbitrary shaped container: flat or rough wall
  - Charge and adhesive, etc. interactions can be included
  - Composite particles to model non-spherical shapes
- Variety of analysis codes

Integrate Newton's equations for each particle with translational and rotational degrees of freedom

$$\mathbf{F}_n = f(\delta/d)(k_n\delta - \frac{m}{2}\gamma_n \mathbf{v}_n)$$

$$\mathbf{F}_t = f(\delta/d)(-k_t\Delta \mathbf{s}_t - \frac{m}{2}\gamma_t \mathbf{v}_t)$$

$$f(x) = \sqrt{x} \quad \text{Hertzian springs}$$

δ **Particle overlap**

Δs_t **Elastic tangential displacement**

$F_t \le \mu F_n$ **Coulomb Failure Criterion**

Multiphase Simulations

- DEM code coupled with a parallel Navier-Stokes solver for dense multiphase flow simulations is under development
  - Maintain all the capabilities of the DEM code
  - Incompressible fluids
  - Realistic solid-fluid interactions
  - Accurate effective particle/particle interactions
  - Multiple, complex, moving geometries – composite particles
  - Complex shaped system boundaries
- Number of particles ~ 10^4
- Several approaches to consider

Discrete-Time Immersed Boundary Method

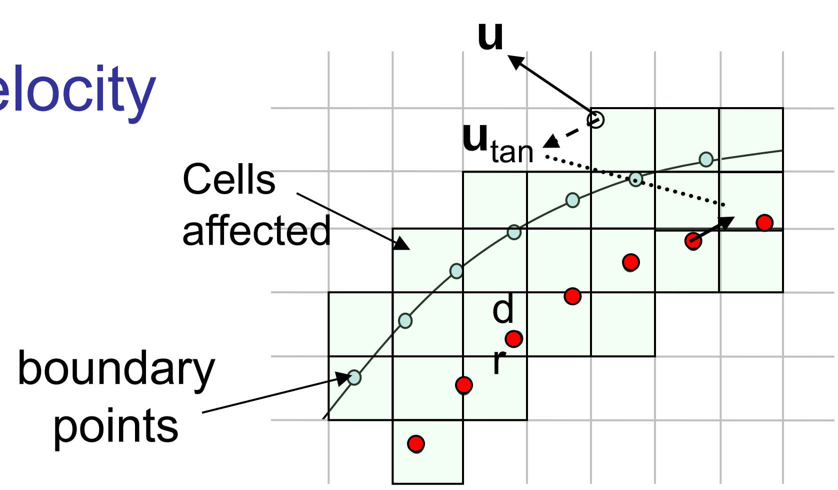
- Multiple moving boundaries (solid or flexible) without altering fluid grid
- Hybrid numerical method for solving the incompressible Navier-Stokes equations
  - Pseudo-spectral method using Fourier transforms in y- and z- directions
    - Parallel in one direction, scalar in other
    - Allows high accuracy (coarser grid?) and fast computation using FFT
    - Useful for higher Reynolds number flows
  - Space centered finite differences in x- direction
    - Parallel direction
  - Time stepping
    - No user-specified parameters from forcing – accurate and stable
  - Particle-fluid coupling
    - Solve for force at boundary that gives no-slip

Particle Fluid Coupling

- Solid/fluid coupling is achieved through a Discrete-Time Immersed Boundary Method
  - Fluid velocity, $\mathbf{u}$, must equal particle velocity, $\mathbf{v}$, on surface Ω $\mathbf{u} = \mathbf{v}(\Omega)$
  - Using the discrete-time NS equations and noting $\mathbf{u}^{n+1} = \mathbf{v}$ on Ω gives the ideal force applied to the fluid

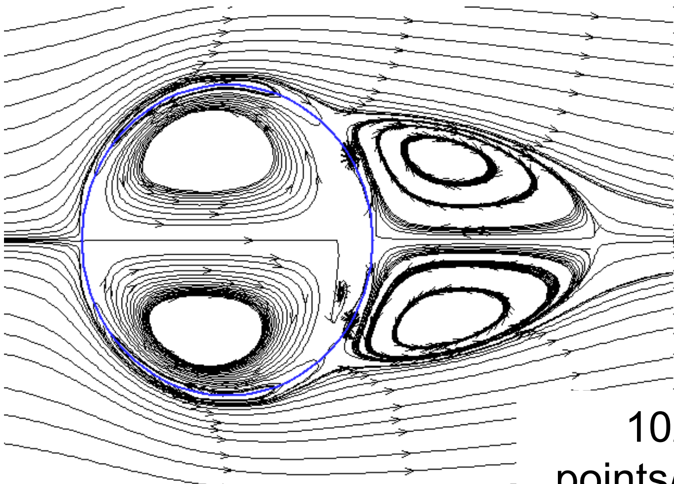
$$\mathbf{g}(\Omega) = \mathbf{S} + \nabla P - \nu \nabla^2 \mathbf{u} + \frac{1}{\Delta t}(\mathbf{v} - \mathbf{u}^n)$$

  - Smooth local tangential velocity for no-slip

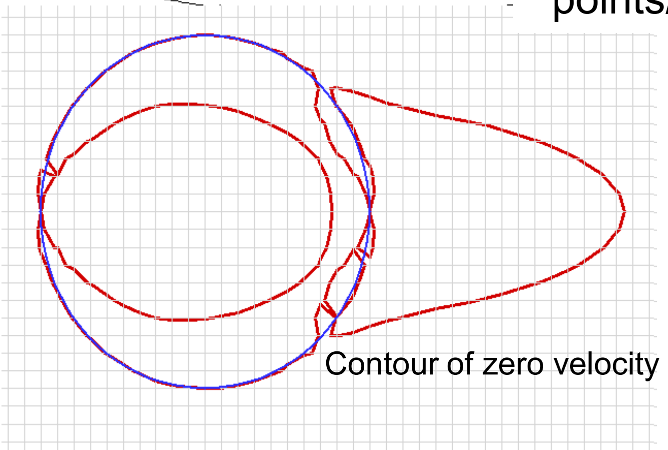


Example: Particle Resolution

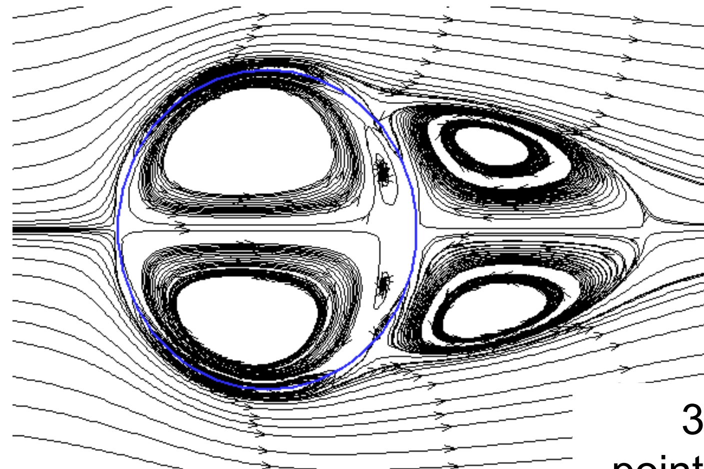
$Re_p = 50$



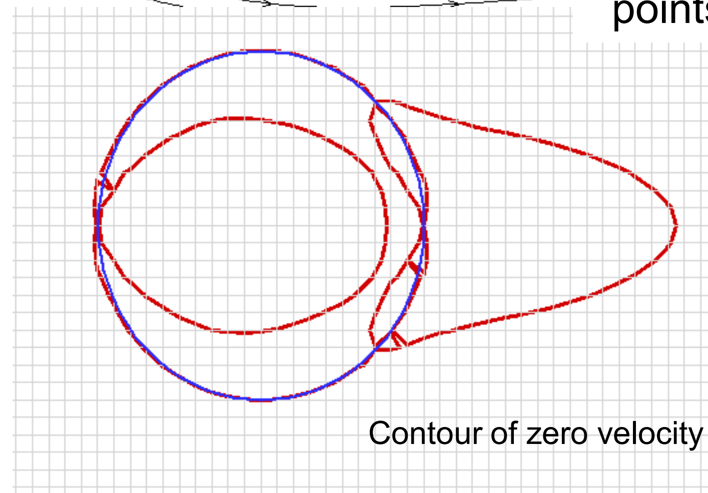
102 points/area



Contour of zero velocity (red)

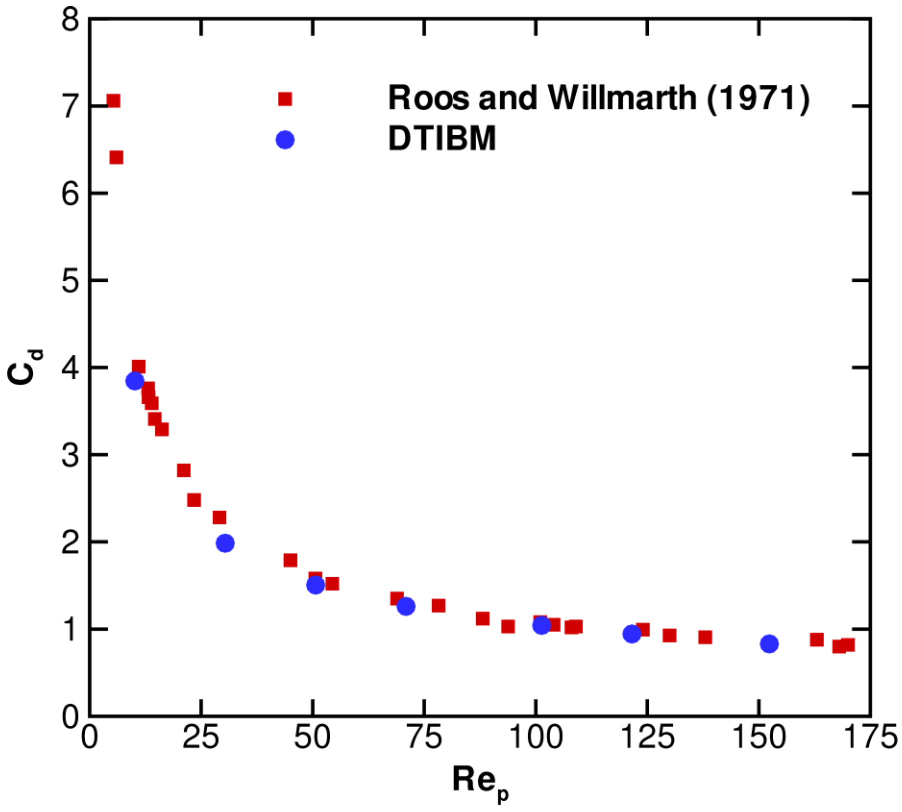


321 points/area



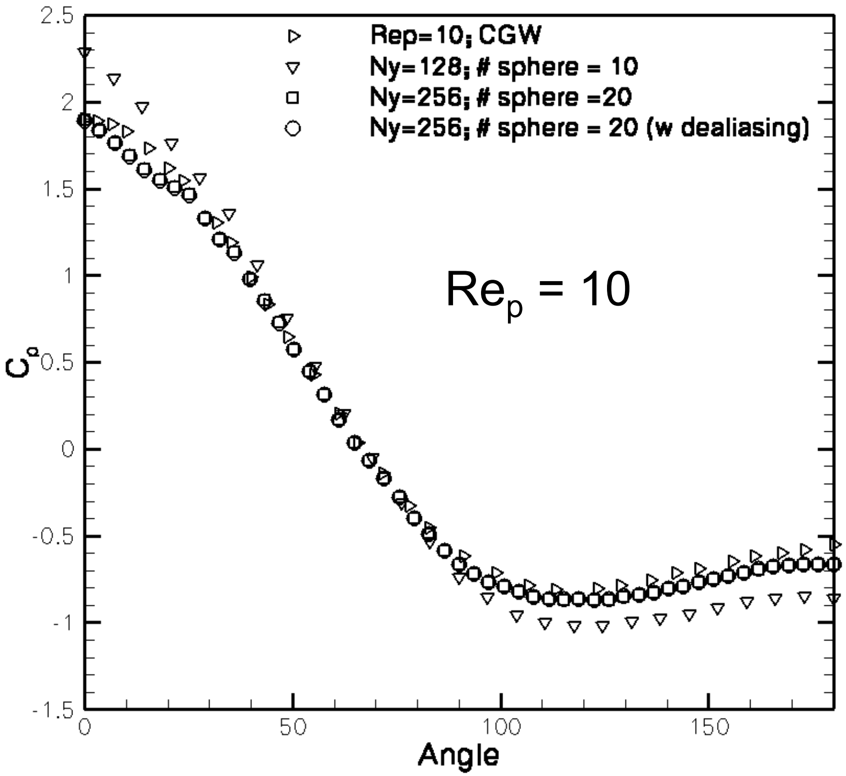
Contour of zero velocity (red)

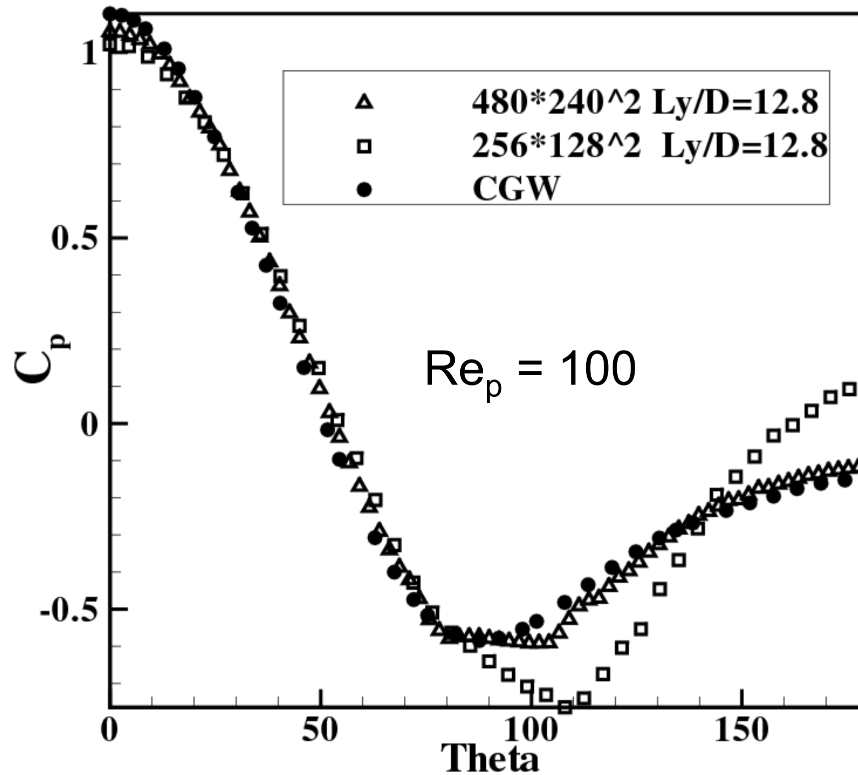
Drag Coefficient on Single Particle



- Drag force on sphere agrees very well with published results

Pressure Part of Drag

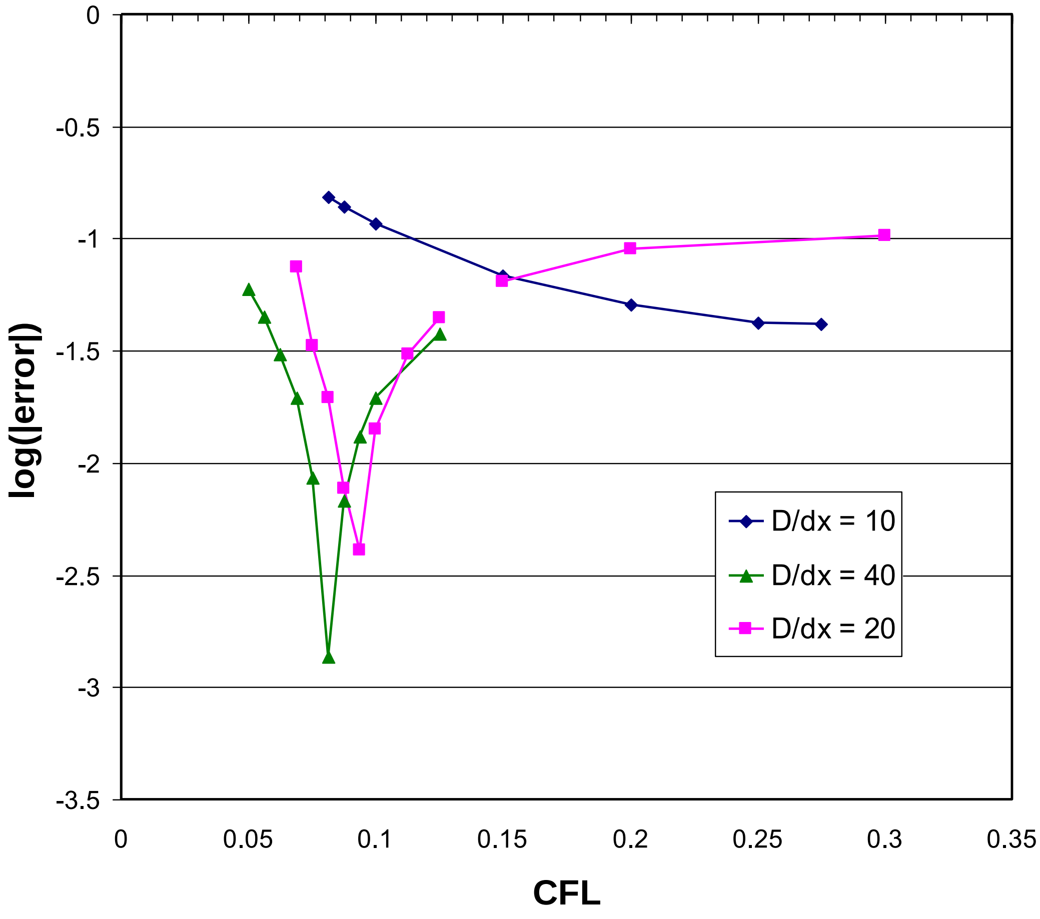




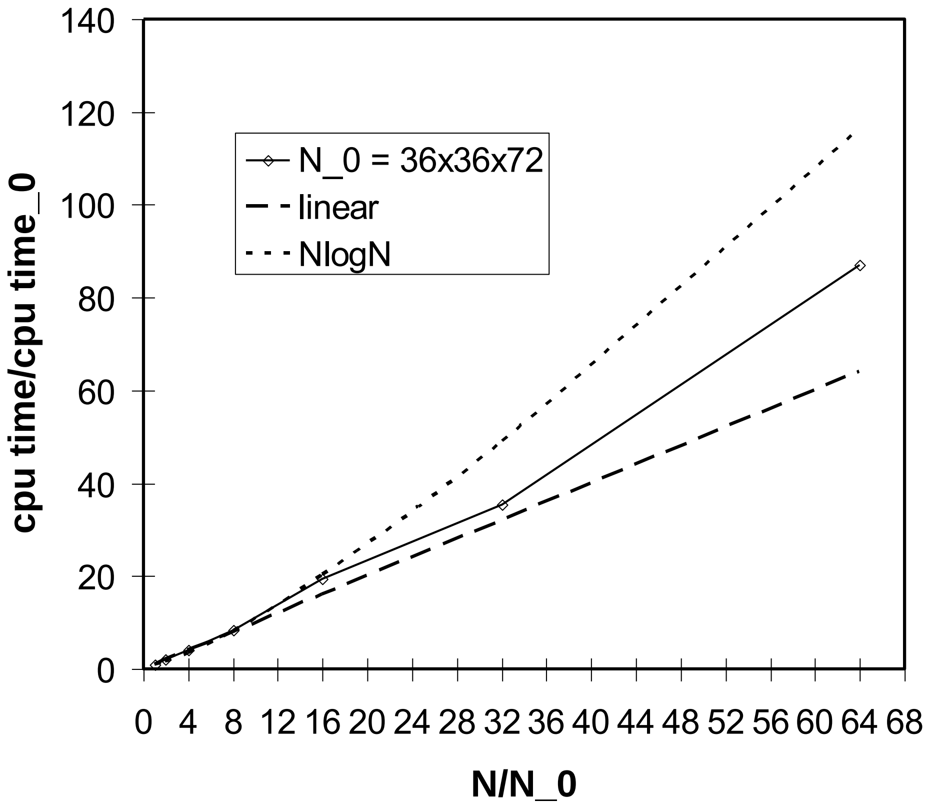
- Pressure distribution deviates from expected behind the particle at low D/dx
- At low Re_p a coarser mesh can be used
  - further Re_p-mesh studies being carried out

Error Traces for Total Drag Force on Sphere

- Decreasing CFL gives near collapse of data
- For moderate to high grid resolution: optimal dt ~ 0.0875



Single Processor Scaling

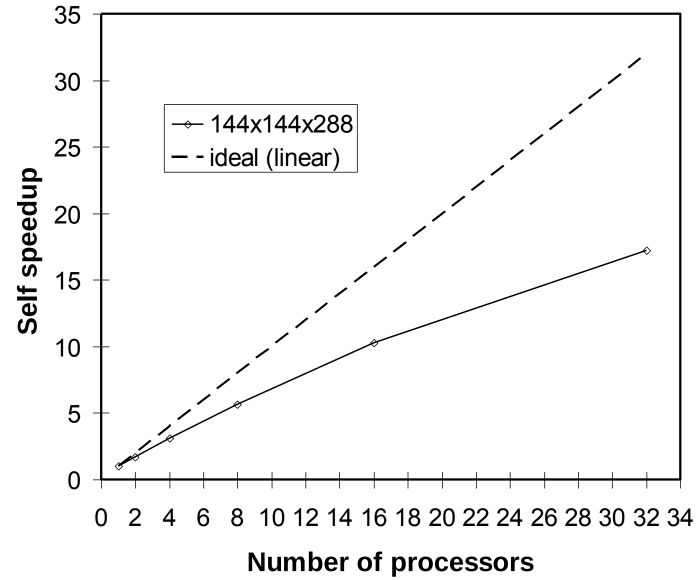


- Test performed with single particle centered in domain, Re = 100, D/dx = 16, time for 100 Δt_{NS}
  - Optimal number of NS nodes,N per processor ~ $O(10^6)$

Parallel Performance

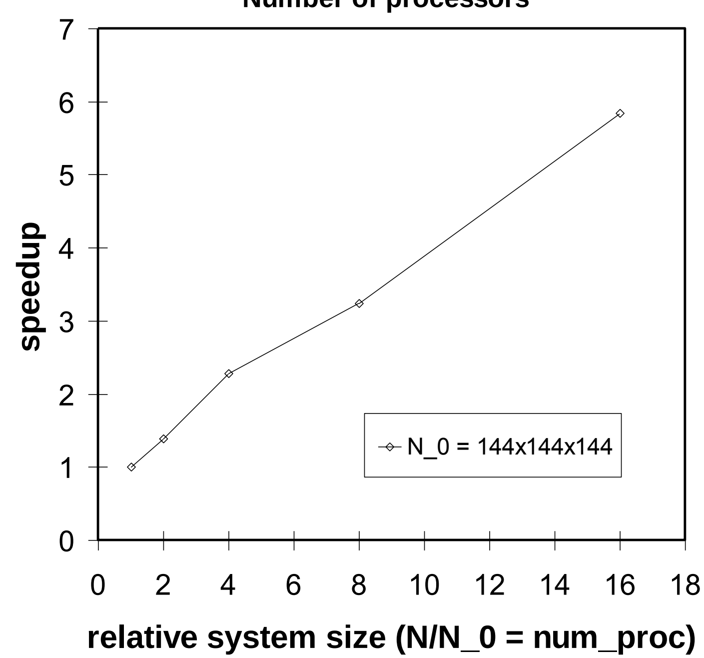
- Fix the system size and increase number of processors

$$S_p^{self} = \frac{\text{execution time on 1 proc}}{\text{excution time on p proc}}$$



- Fix number of NS nodes per processor and increase system size
  – assume linear scaling with N_{NS} for single processor

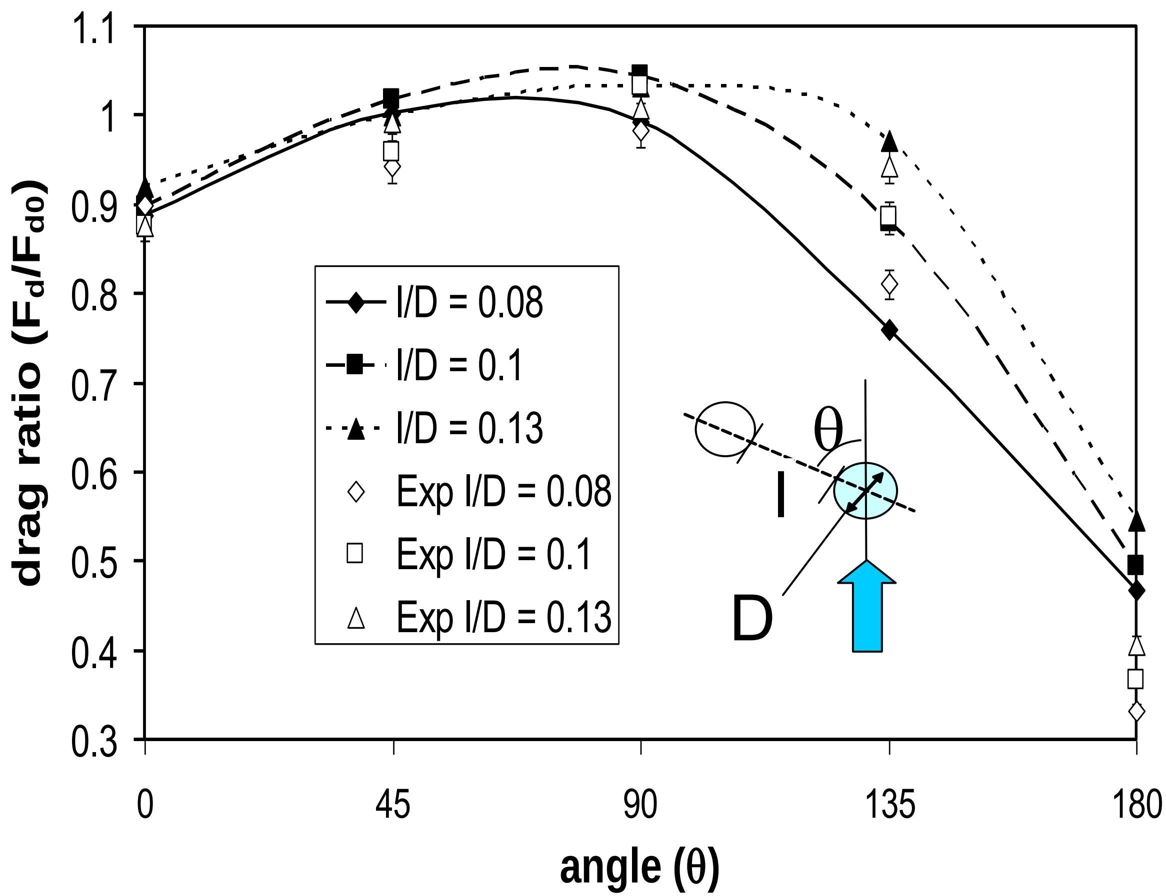
$$S_p = \frac{\text{number of proc} * \text{execution time on 1 proc}}{\text{execution time on p proc}}$$



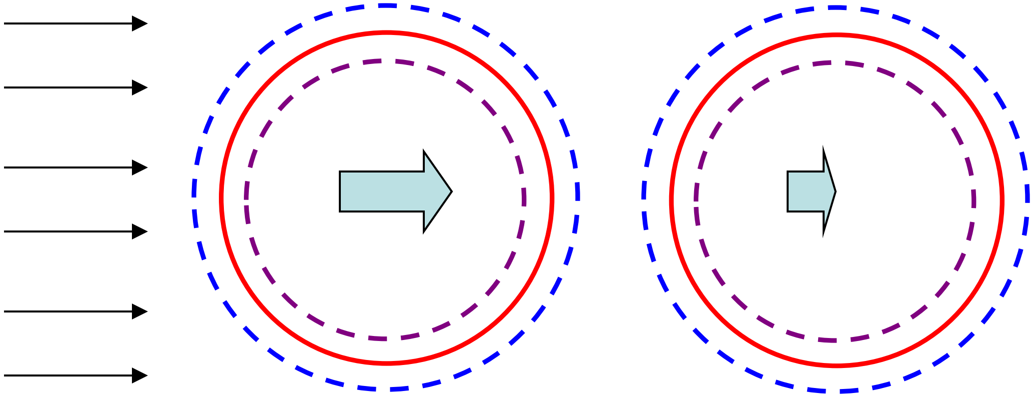
Multi-particle Hydrodynamic Interactions: Trailing Particle Drag

- Ratio of drag force on test particle to that of isolated particle
- Compares well with experimental results

(Zhang et al. 1993)

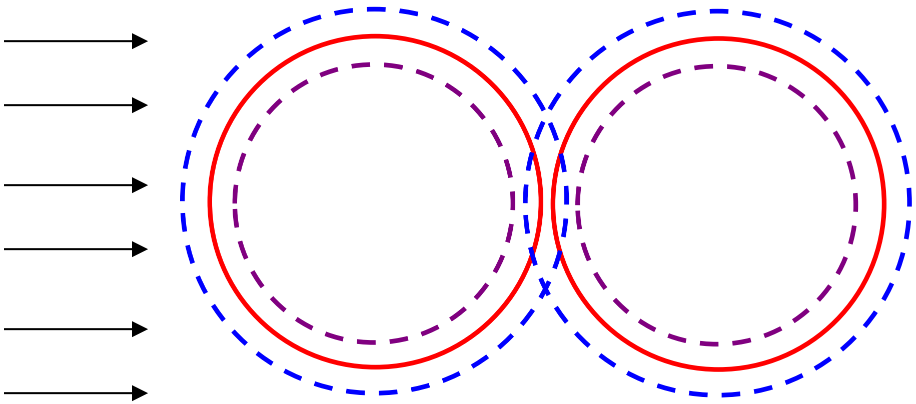


Particle Contact (subgrid physics)

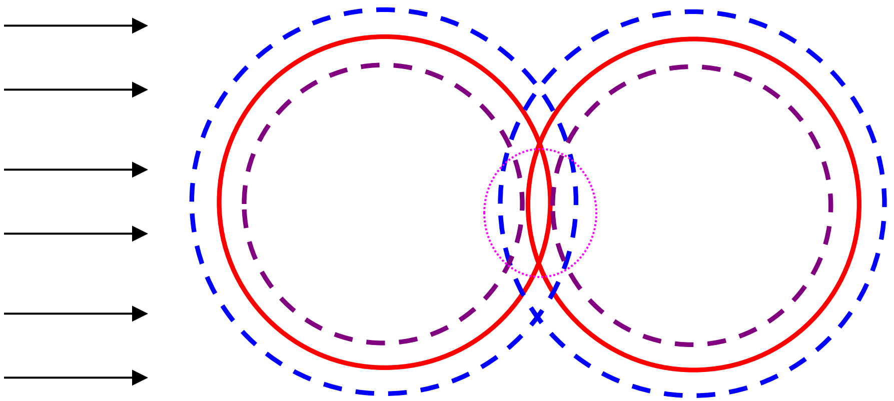


- Separated particles: proceed normally with NS solver to get liquid forces on particles.

Boundary points – Red
Reversal points – Blue and Purple

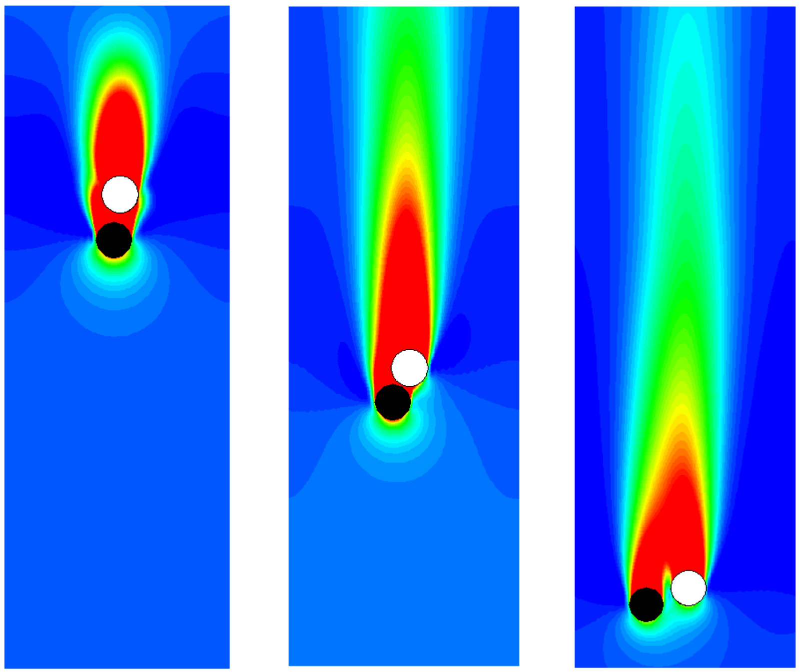


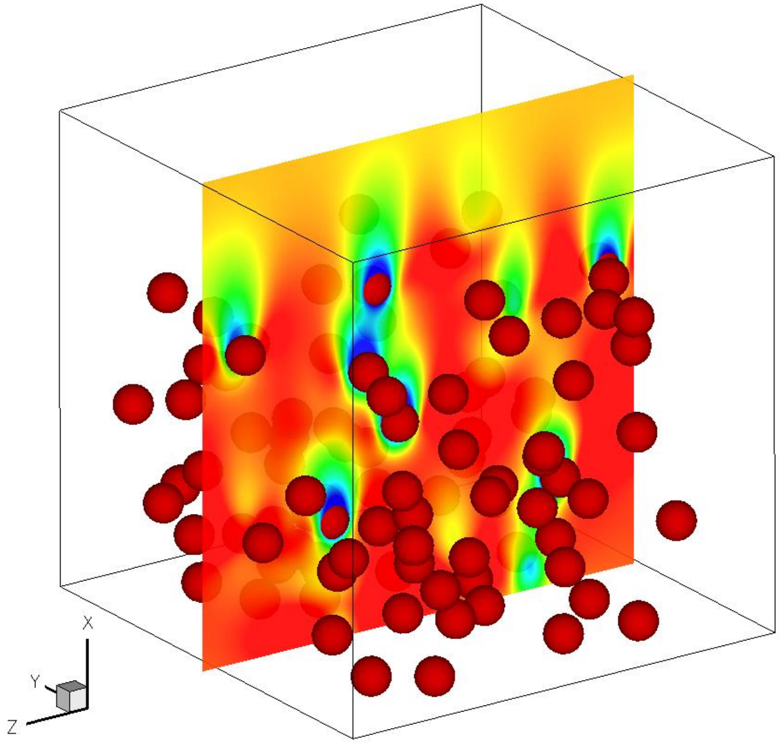
- Reversal points start to overlap: continue NS unchanged, but include, e.g., lubrication forces.



- As particles overlap, the boundary and reversal points at the intersection are turned off, contact forces calculated

Examples: Simple Particle Interaction Tests





Open Issues

- Finite grid size
  - Mesh refinement: accuracy vs. number of particles
  - Subgrid physics
    - Lubrication
    - Effective potentials
- Scaling with and maximum number of particles
  - Parallelize other PS- direction
- Relationship to other methods
  - Efficiency and accuracy: spatial and temporal
  - Regime of applicability: dense suspensions? low Re?
- Generalize particle shape
  - High surface curvature could lead to complications
- Generalize system boundary conditions
  - Pseudo-spectral methods in other coordinate systems

Summary

- A 3D, parallel, hybrid Pseudo-spectral/Finite Difference NS solver has been coupled with our existing 3D, parallel DEM code via the DTIBM
  - Preliminary scaling can be improved!
- Particle contact, longer range interaction potentials, and “subgrid physics” can be incorporated naturally through DEM
- Can handle polydispersed systems and can be generalized to complex shapes
- In the works
  - Detailed validation of the parallel NS/DTIBM-DEM code
  - System size range (scaling with number of particles)