Use of a DNS Method to Reduce Uncertainties in Two-Fluid Models

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Principal Approaches for the Study of Particulate Flows

• Continuum model (two-fluid model)
  – Both the fluid phase and solid phase are treated as continuous media
    \[
    \partial_t (\rho_s \vec{u}_s) + \vec{\nabla} \cdot (\rho_s \vec{u}_s \vec{u}_s) = -\epsilon_s \vec{\nabla} p - \vec{\nabla} \cdot (\epsilon_s \vec{r}_s) + \beta (\vec{u}_g - \vec{u}_s) + \rho_s \vec{g}
    \]
    \[
    \partial_t (\rho_g \vec{u}_g) + \vec{\nabla} \cdot (\rho_g \vec{u}_g \vec{u}_g) = -\epsilon \vec{\nabla} p - \vec{\nabla} \cdot (\epsilon \vec{r}_g) - \beta (\vec{u}_g - \vec{u}_s) + \rho_g \vec{g}
    \]
  – Need empirical inputs: \( \epsilon_s, \beta \) some of which cannot be measured directly;
  – Not very accurate at present, accuracy depends greatly on empirical inputs.

• Discrete particle model (one-way coupling)
  – The solid particles are treated as point particles; hydrodynamic drag force is given by closure equations.
  – The fluid phase is treated as continuous phase; the effect of solid particles to the fluid phase is modeled.

• Direct Numerical Simulation (DNS)
  – The Navier-Stokes equation for the fluid phase and the equations of motion for the solid particles are solved simultaneously.
  – Two-way coupling.
  – Exact method.
DNS Methods for Particulate Flow

- **Stokesian Dynamics** (Brady & Bossis, 1980s)
  - Valid for Stokes flow (Re<<1), spherical particles
- **Finite Element Method** (Dan Joseph’s group, 1990s)
  - High Reynolds number, high accuracy, need mesh-adaptive, very expensive, two dimensional simulations.
- **Fictitious Domain Method** (Glowinski et al, 1998)
  - Low to medium Reynolds number, complicated to implement, computationally intensive.
- **Lattice Boltzmann Method** (Ladd, 1994 and after)
  - Low Reynolds number, high efficiency and fast, suitable for parallel computing
- **Proteus Method** (Feng and Michaelides, 2005)
  - Low to medium Reynolds number, easy to implement, improved accuracy compared to LBM.
Inclusion of Heat Transfer - Objectives

• Extend the DNS method to take into account the energy transfer to/from particles.
• Apply the Immersed Boundary Method (IBM) and the Direct Forcing (DF) scheme to momentum as well as the energy transfer problems.
• This is accomplished by substituting the surface of the particle with a series of forces and heat sources/sinks.
Conceptual Model and Governing Equations

Continuity, Momentum and Energy Equations

\[ \nabla \cdot \vec{u} = 0 \]

\[ \Gamma \rho_f \frac{\partial \vec{u}}{\partial t} + \rho_f \vec{u} \cdot \nabla \vec{u} = -\nabla p + \mu_f \nabla^2 \vec{u} + \beta_f (T - T_{fo}) \vec{g} \]

\[ \rho_f c_f \frac{\partial T}{\partial t} + \rho_f c_f \vec{u} \cdot \nabla T = k_f \nabla^2 T + q \]

Modified Momentum and Energy Equations

\[ \rho_{f0} \frac{\partial \vec{u}}{\partial t} + \rho_{f0} \vec{u} \cdot \nabla \vec{u} = -\nabla p + \mu_f \nabla^2 \vec{u} + \beta_f (T - T_{fo}) \vec{g} + \vec{f} \]

\[ \rho_f c_f \frac{\partial T}{\partial t} + \rho_f c_f \vec{u} \cdot \nabla T = k_f \nabla^2 T + q + \lambda \]
Immersed Boundary Method

\[ \rho \left( \frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right) = \mu \nabla^2 \mathbf{u} - \nabla p + \mathbf{f} \]

\[ \nabla \cdot \mathbf{u} = 0 \]

\[ f(x, t) = \int_{\Gamma} F(s, t) \delta(x - X(s, t)) ds \]

\[ \frac{\partial \mathbf{X}}{\partial t} = \int_{\Omega} \mathbf{u}(x, t) \delta(x - X(s, t)) dx \]
Assumptions

- Boussinesq approximation on the effect of temperature on fluid properties.
- Particles have uniform temperature (Bi=0) that is, particles are very small or their conductivity is much higher than that of the fluid.
- No-slip at the particle surface.
- Equal temperatures ($T_f=T_s$) at the particle surface.
Momentum-side equations for the domain of particles

Translational motion

\[ (\rho_p - \rho_f) V_p \frac{d\bar{U}_p}{dt} = \rho_f \int_S f d\nu + (\rho_p - \rho_f) V_p \bar{g} \]

Rotational motion

\[ I_p \left(1 - \frac{\rho_p}{\rho_f}\right) \frac{d\bar{\omega}_p}{dt} = -\rho_f \int_{V_p} (\bar{x} - \bar{x}_p) \times \bar{f} d\nu \]

Force density

\[ \bar{f} = \rho_f \frac{\partial \bar{u}}{\partial t} + \rho_f \bar{u} \cdot \nabla \bar{u} + \nabla p - \mu_f \nabla^2 \bar{u} \]

Particle interior motion

(rigid body rotation)

\[ \bar{u} = \bar{U}_p + \bar{\omega}_p \times (\bar{x} - \bar{x}_p) \]
Heat transfer-side equations for the
domain of particles

In analogy with the momentum forcing:

\[ \rho_p c_p \frac{dT}{dt} + \rho_f c_f \bar{u} \cdot \nabla T = k_f \nabla^2 T + q + \lambda \]

Or, in the solid region:

\[ \lambda = \rho_f c_f \frac{dT}{dt} + \rho_f c_f \bar{u} \cdot \nabla T - k_f \nabla^2 T + q \]

Particle temperature change:

\[ \rho_p V_p c_p \frac{dT_p}{dt} = \int_{S} k_f \nabla T_f \cdot \bar{n} \, ds + \int_{S} q_s \, dv \]
Model validation/verification

Comparison with falling particle data by ten Cate et al. (2002)
The Drafting-Kissing-Tumbling motion of two light particles – A

Physical parameters:

• Domain size: $\Omega = [-1,1] \times [0,6]$;
• particle radius: $r = 0.125$;
• initial position of the two particles: $x_{p1} = [0, 5.2]$, and $x_{p2} = [0.001, 4.8]$;
• Particle/fluid density ratio: $\rho_r = 1.01$.
• Fluid viscosity: $\nu = 0.001$.
• The grid is 200x600, and the dimensionless time step $\delta t = 0.005$. 

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The Drafting-Kissing-Tumbling motion of two light particles – B

Case A: $\Theta_p = \Theta_f = 0; \ Gr = 0$;
Case B: ambient fluid $\Theta_f = 0$; $\Theta_p = -1; \ Gr = 1000$;
Case C: ambient fluid $\Theta_f = 0$; $\Theta_p = 1; \ Gr = 1000$.
The Drafting-Kissing-Tumbling motion of two light particles – C

T=112

T=185

T=210

T=315
Sedimentation of 56 “hot” particles – A
Sedimentation of 56 “hot” particles – B
Use of the DNS model to determine the behavior of the particulate phase(s) near walls

• Use a physically meaningful wall-particle interaction model.

• Observe the behavior of a statistically large number of particles in the wall region.

• Determine the average behavior of the particles.

• Deduce the appropriate “boundary condition.”
Collision Model with the Wall – reflection method (Glowinski et al. (2001))

When the gap between a particle and the wall is less than a given threshold, \( \zeta \), a repulsive force is applied to the particle, which is added to a total force the particle experiences.

\[
F_{ij}^{\text{rep}} = \begin{cases} 
0, & \|x_i - x_{ij}\| > 2R_i + \zeta \\
\frac{c_{ij}}{\varepsilon_w} \left( \frac{\|x_i - x_{ij}\| - 2R_i - \zeta}{\zeta} \right)^2 \left( \frac{x_i - x_j}{\|x_i - x_j\|} \right), & \|x_i - x_{ij}\| \leq 2R_i + \zeta 
\end{cases}
\]

where \( c_{ij} \) is the force scale factor, \( \varepsilon_w \) is the stiffness parameter of the collision, \( R_i \) is the radius of the particle, \( \zeta \) is the threshold or the “safe zone, and \( x_{ij} \) is the position of the fictitious particle \( P_{i,j} \), which is located symmetrically on the other side of the wall.
Near-wall particle trajectories – 264 particles of d=0.6 cm
Vertical Velocities at the Wall

$V_a, \text{cm/sec}$

$1,000,000$  $3,000,000$  $5,000,000$  $10,000,000$  $14,000,000$
The effect of the parameter $c_{ij}$

$V_a$, dimensionless

$c_{ij}$

$1,000,000$
$3,000,000$
$5,000,000$
$8,000,000$
$10,000,000$
$14,000,000$
The effect of the parameter $c_{ij}$ – all averaged results for $d=0.4$ and 0.6 cm

$y = -5.2967E-10x - 3.8253E-01$

$y = 1.34727E-09x - 4.09610E-01$
Single-sphere collision with walls – the soft sphere collision scheme

Spring-dashpot model with normal and tangential forces

\[ f_{ij}^n = -k_n \delta^n_{ij} - \eta_n v^n_{ij} \]

\[ f_{ij}^t = -k_t \delta^t_{ij} - \eta_t v^t_{ij} \]

The relative tangential velocity component at the contact point may be computed as follows

\[ \vec{v}_{ij}^t = \vec{v}_{ij} - (\vec{v}_{ij} \cdot \hat{n}_{ij})\hat{n}_{ij} + \left[ \vec{\omega}_i \times r_i \hat{n}_{ij} - \vec{\omega}_j \times r_j (\hat{n}_{ij}) \right] \]

With friction at contact, the tangential contact force becomes:

\[ f_{ij}^t = \begin{cases} 
-\kappa \delta^t_{ij} - \eta v^t_{ij}, & \text{if } |f_{ij}^t| \leq \mu_s |f_{ij}^t| \\
\mu_k |f_{ij}^t| \frac{\delta^t_{ij}}{|\delta^t_{ij}|}, & \text{if } |f_{ij}^t| > \mu_s |f_{ij}^t|
\end{cases} \]
Results of the soft-sphere collision scheme – A

\[ \theta = 45^\circ, \eta = 50 \text{ dyn.s/cm} \]

\[ r \approx 0.65 \]
Results of the soft-sphere collision scheme – B

\[ \theta = 45^\circ, \ k = 1,000,000 \ \text{dyn/cm} \]

\[ 0.54 < r < 0.76 \]
Summary – Conclusions

• A DNS with a forcing scheme, used to ensure rigid body motion, has been developed for the motion of the particles. In analogy with the momentum forcing scheme, a heat transfer forcing scheme was developed for the determination of the temperature field in the fluid.

• The collision parameters affect significantly the behavior of particles close to the wall. Having an accurate collision model is paramount for accuracy.

• Particle interactions close to the wall influence the trajectories, the wall collisions and, hence, the boundary conditions at the wall.

• There is significant evidence that particles “slip” near a vertical wall with a velocity close to 0.4 of their terminal velocity.

• The single-particle collision model with viscous fluids may be used more extensively to analyze better single-particle collisions with a wall.
Publications and Acknowledgements

On the DNS model:

On the particle-wall interactions:

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