Self-Disturbance Corrected Two-Way Coupled Euler-Lagrange Approach for Particle-Laden Flows With Heat Transfer on Arbitrary Shaped Grids

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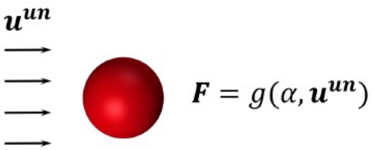
Point-Particle Model

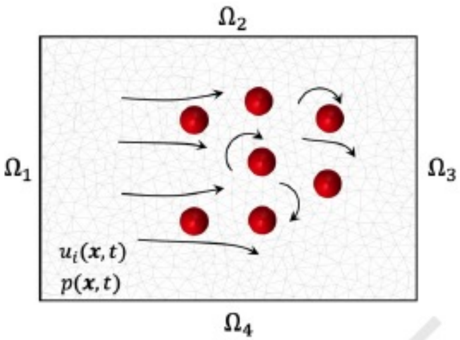
- **Several applications of particle-laden flows (fluidized beds, droplets and spray systems, coal reactors etc.) use Euler-Lagrange based point-particle model**
  - Particles assumed subgrid and much smaller than the grid resolution used in DNS/LES/RaNS
  - Particles typically assumed spherical
  - Aerodynamic forces are modeled based on typical closure models for drag(e.g. Schiller Naumann) and other forces. These typically require the fluid flow that is undisturbed by the particle
  - Originally developed for low volume loading, subgrid particles and meant to be used in the one-way coupling (particles do not affect the flow)
  - Routinely applied to higher volume loadings, particles partially resolved (of size comparable to grid resolution) with two-way, volume-filtered coupling.
  - Two-way coupling disturbs the fluid flow, and can result in significant errors in force calculations

Undisturbed Flow, Self Disturbance, and Neighbor Effects

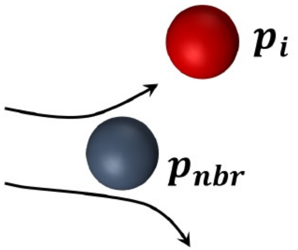
- **Standard Closures based on Undisturbed Flow**
  - Particle-flow interaction terms disturb the fluid flow (two-way coupling, volumetric coupling)
  - Undisturbed flowfield is not readily available
  - The disturbed flow interpolated to particle locations is used instead and can lead to significant errors



- **Cluster based drag models**
  - Derived for moderate-to-dense loadings based on interstitial or disturbed flow field (Subramaniam and co-workers, Tenneti et al. 2011, IJMF)
  - Undisturbed flow not needed
  - Only captures mean drag (not variations within the cluster)



- **Hydrodynamic effects due to neighbors (drafting)**
  - Deterministic Models: Pairwise Interaction Extended Point Particle (PIEP) Balachandar and co-workers-–Akiki et al. (2017, JCP), Moore et al. (2020, JCP)
  - Stochastic Models: Lattanzi et al. (2020, JFM), Esteghamatian et al. (2018, IJMF)



Theme of This Talk

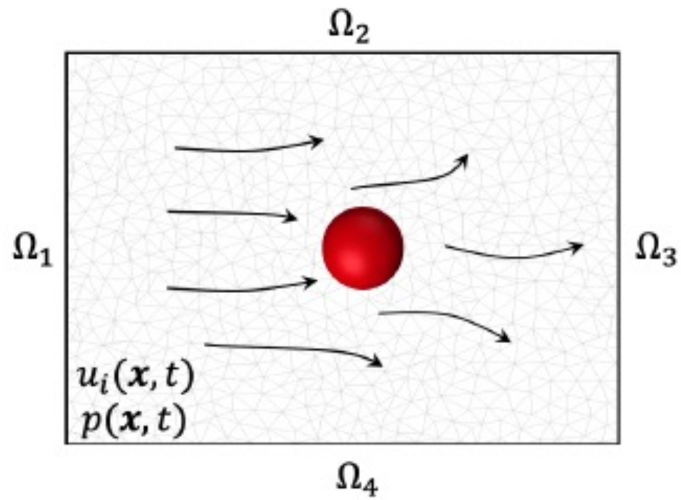
- **Develop a model to obtain the undisturbed velocity and temperature fields in two-way coupled point-particle approach based on standard closure models**
  - Derivation of an equation for self-disturbance created by a single particle
  - A simplified model for self-disturbance
  - Verification and evaluation of the model
  - Extension to multiple particle systems

(Un)Disturbed Flow

- Disturbed flow in two-way coupled formulation

$$\frac{\partial u_i}{\partial t}+u_j\frac{\partial u_i}{\partial x_j}=-\frac{1}{\rho_f}\frac{\partial p}{\partial x_i}+\nu\frac{\partial^2 u_i}{\partial x_j^2}-\frac{1}{\rho_f}f_{i,p}$$

$$\frac{\partial u_j}{\partial x_j}=0$$

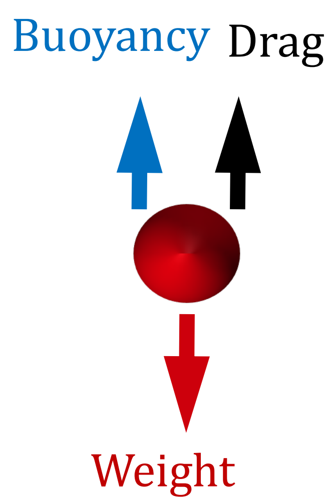


- Need the undisturbed flow that only removes the self-disturbance (not the disturbance created by neighbors)

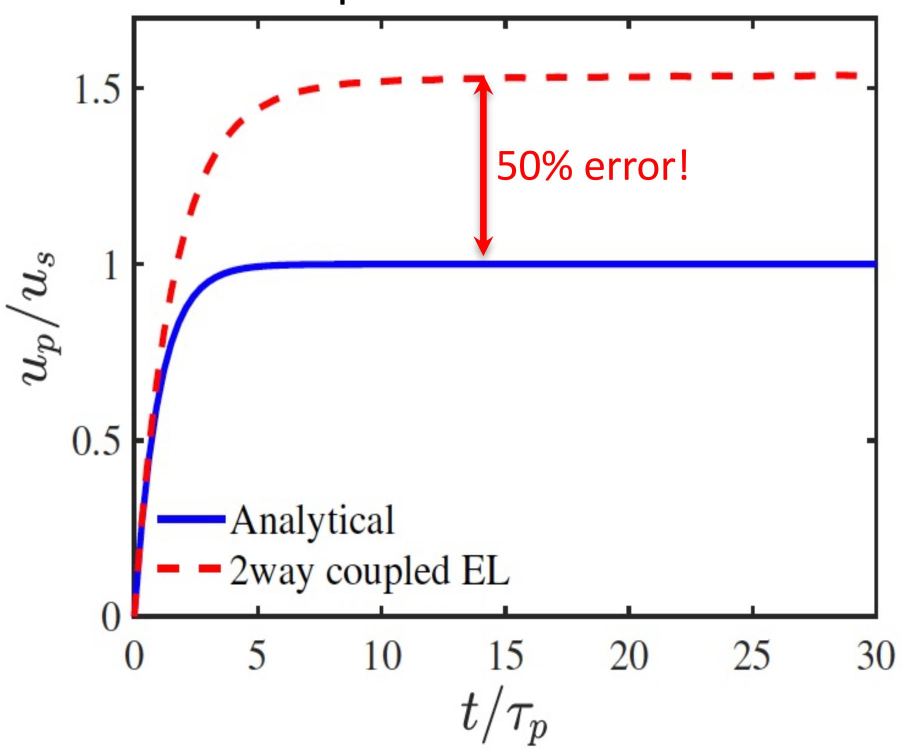
- How much does it matter?

(Un)Disturbed Flow

- Particle settling in a quiescent flow



Re_p = 0.1; St=10;



- Large error if the disturbed flow is used in drag calculation
- Error increases with particle size to grid ratio, but decreases with Reynolds number

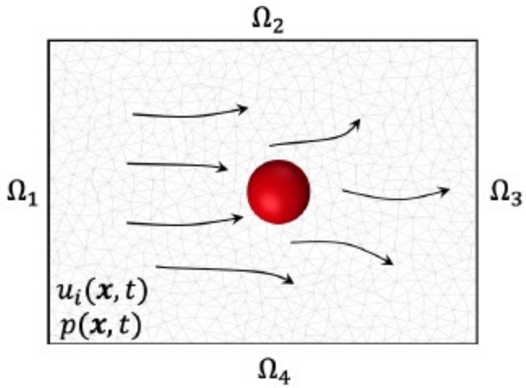
Self-Disturbance Flowfield

- Mass, momentum, and energy equations in the zero Mach number limit
- Focus on a single particle
- For simplicity, temperature induced density variations within the fluid due to inter-phase heat transfer assumed small
  - Energy equation becomes decoupled
- Analysis can be extended to variable density, multiple species reacting flows, as well as multiple particles or particle clusters

(Un)Disturbed Flowfield

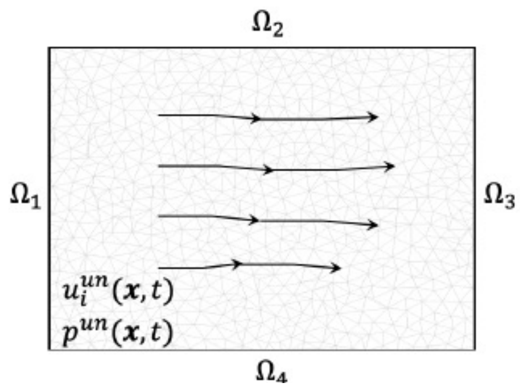
- Disturbed flow from two-way coupling

$$\begin{aligned}
\frac{\partial u_j}{\partial x_j} &= 0, \\
\frac{\partial \rho_g u_i}{\partial t} + \frac{\partial \rho_g u_i u_j}{\partial x_j} &= -\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j}\left(2\mu S_{ij}\right) + \dot{S}_i, \\
\frac{\partial \rho_g h}{\partial t} + \frac{\partial \rho_g h u_j}{\partial x_j} &= \frac{\partial}{\partial x_j}\left(\rho_g \alpha_h \frac{\partial h}{\partial x_j}\right) + \dot{S}_h,
\end{aligned}$$



- Undisturbed flow (without the self-disturbance)

$$\begin{aligned}
\frac{\partial u_j^{un}}{\partial x_j} &= 0, \\
\frac{\partial \rho_g u_i^{un}}{\partial t} + \frac{\partial \rho_g u_i^{un} u_j^{un}}{\partial x_j} &= -\frac{\partial p^{un}}{\partial x_i} + \frac{\partial}{\partial x_j}\left(2\mu S_{ij}^{un}\right), \\
\frac{\partial \rho_g h^{un}}{\partial t} + \frac{\partial \rho_g h^{un} u_j^{un}}{\partial x_j} &= \frac{\partial}{\partial x_j}\left(\rho_g \alpha_h \frac{\partial h^{un}}{\partial x_j}\right),
\end{aligned}$$



Self-Disturbance Flowfield

- Self-disturbance $u_i^{un} = u_i + u_i^d; \ \ p^{un} = p + p^d; \ \ h^{un} = h + h^d$

Disturbed flow

$$\frac{\partial u_j^d}{\partial x_j} = 0,$$

$$\rho_g \frac{\partial u_i^d}{\partial t} + \rho_g u_j \frac{\partial u_i^d}{\partial x_j} + \rho_g u_j^d \frac{\partial u_i^{un}}{\partial x_j} = -\frac{\partial p^d}{\partial x_i} + \frac{\partial}{\partial x_j}\left(2\mu S_{ij}^d\right) - \dot{S}_i,$$

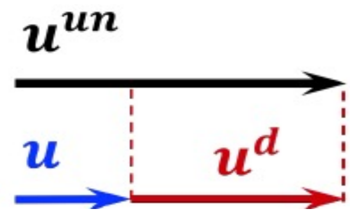
$$\rho_g \frac{\partial h^d}{\partial t} + \rho_g u_j \frac{\partial h^d}{\partial x_j} + \rho_g u_j^d \frac{\partial h^{un}}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\rho_g \alpha_h \frac{\partial h^d}{\partial x_j}\right) - \dot{S}_h.$$

- Gradients in undisturbed flow much smaller than disturbed flow
  - Flows without strong mean shear
  - Can be corrected with presumed mean gradient in undisturbed flow

$$\frac{\partial u_i^{un}}{\partial x_j} << \frac{\partial u_i^d}{\partial x_j} \qquad \frac{\partial h^{un}}{\partial x_j} << \frac{\partial h^d}{\partial x_j}$$

Self-Disturbance: Direct Method

$$u^d = u^{un} - u$$



- **Direct Solution-**-Requires solution of three additional equations for disturbance velocity field, a disturbance pressure Poisson equation, and disturbance enthalpy for each particle
- Can use same solvers and framework as for the main flow
- Expensive

$$\frac{\partial u_j^d}{\partial x_j} = 0,$$

$$\rho g \frac{\partial u_i^d}{\partial t} + \rho g u_j \frac{\partial u_i^d}{\partial x_j} = -\frac{\partial p^d}{\partial x_i} + \frac{\partial}{\partial x_j}\left(2\mu S_{ij}^d\right) - \dot{S}_i,$$

$$\rho g \frac{\partial h^d}{\partial t} + \rho g u_j \frac{\partial h^d}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\rho g \alpha_h \frac{\partial h^d}{\partial x_j}\right) - \dot{S}_h.$$

Approximate Method

disturbance of point-particle **disturbance of actual particle**

- Stokes flow

$$F_{\text{drag}}^{\text{Stokes}} = \underbrace{\pi \mu d_p u_p^{rel}}_{\text{Pressure force}} + \underbrace{2\pi \mu d_p u_p^{rel}}_{\text{Viscous force}}$$

Same form for pressure and viscous drag

- Rewrite as

$$F_{\text{drag}}^{\text{Stokes}} = 2\pi \mu_{eff} d_p u_p^{rel}; \quad \mu_{eff} = K_\mu \mu; \quad K_\mu = 1.5$$

- Model pressure force per unit volume as half of an effective viscous force per unit volume ➔ Advection-Diffusion-Reaction

$$\rho_g \frac{\partial u_i^d}{\partial t} + \rho_g u_j \frac{\partial u_i^d}{\partial x_j} = \frac{\partial}{\partial x_j}\left(2K_\mu \mu S_{ij}^d\right) - \dot{S}_i,$$

$$\rho_g \frac{\partial h^d}{\partial t} + \rho_g u_j \frac{\partial h^d}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\rho_g \alpha_h \frac{\partial h^d}{\partial x_j}\right) - \dot{S}_h$$

No need to solve Pressure Poisson equation

Model for Self-Disturbance

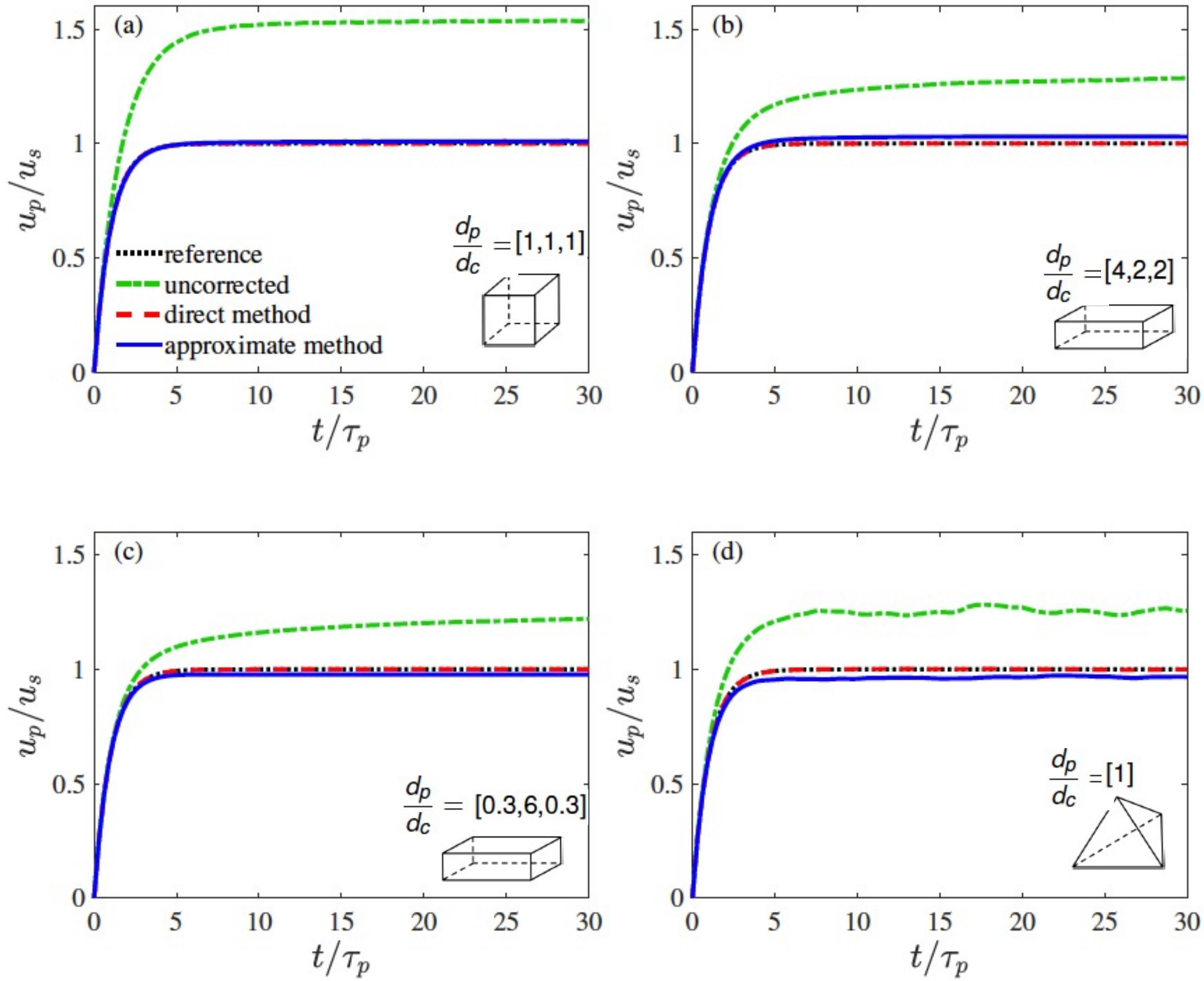
$$\rho_g \frac{\partial u_i^d}{\partial t} + \rho_g u_j \frac{\partial u_i^d}{\partial x_j} = \frac{\partial}{\partial x_j}\left(2K_\mu \mu S_{ij}^d\right) - \dot{S}_i, \qquad K_\mu = 1.5$$

$$\rho_g \frac{\partial h^d}{\partial t} + \rho_g u_j \frac{\partial h^d}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\rho_g \alpha_h \frac{\partial h^d}{\partial x_j}\right) - \dot{S}_h$$

- Eliminates expensive pressure solve
- Continuity constraint for disturbance field only approximately satisfied.
- Coefficient K_μ can be made function of Re
- ADR equation can be solved in a region of influence around droplet
- Fast computation and easy implementation in any solver
- Valid for any type of grid (structured/unstructured) as well as wall-bounded flows, and particle sizes on the order of grid resolution
- Can use PDE solver used in main fluid flow analysis

Gravitational Settling w/o Heat Transfer

Re_p=0.1



Gravitational Settling w/o Heat Transfer

Normalized fluid velocity

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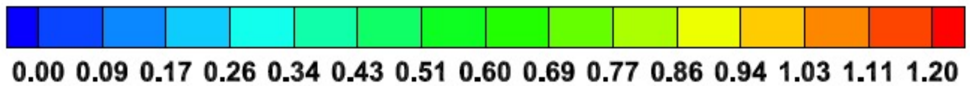
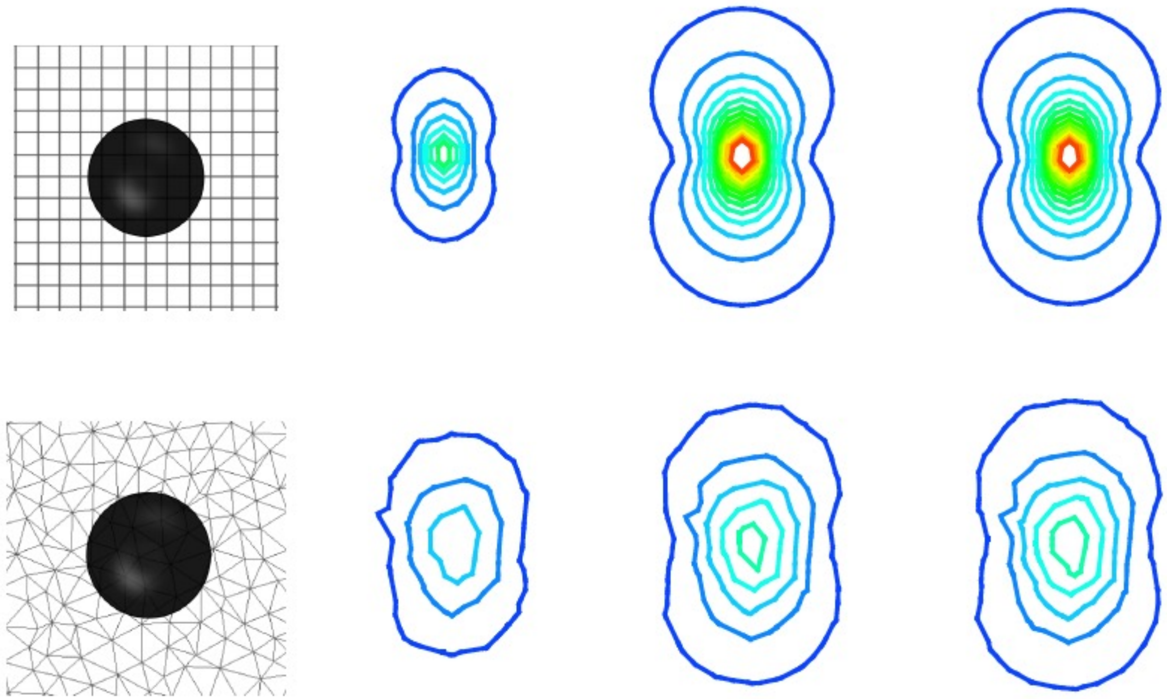
U_g/U_s

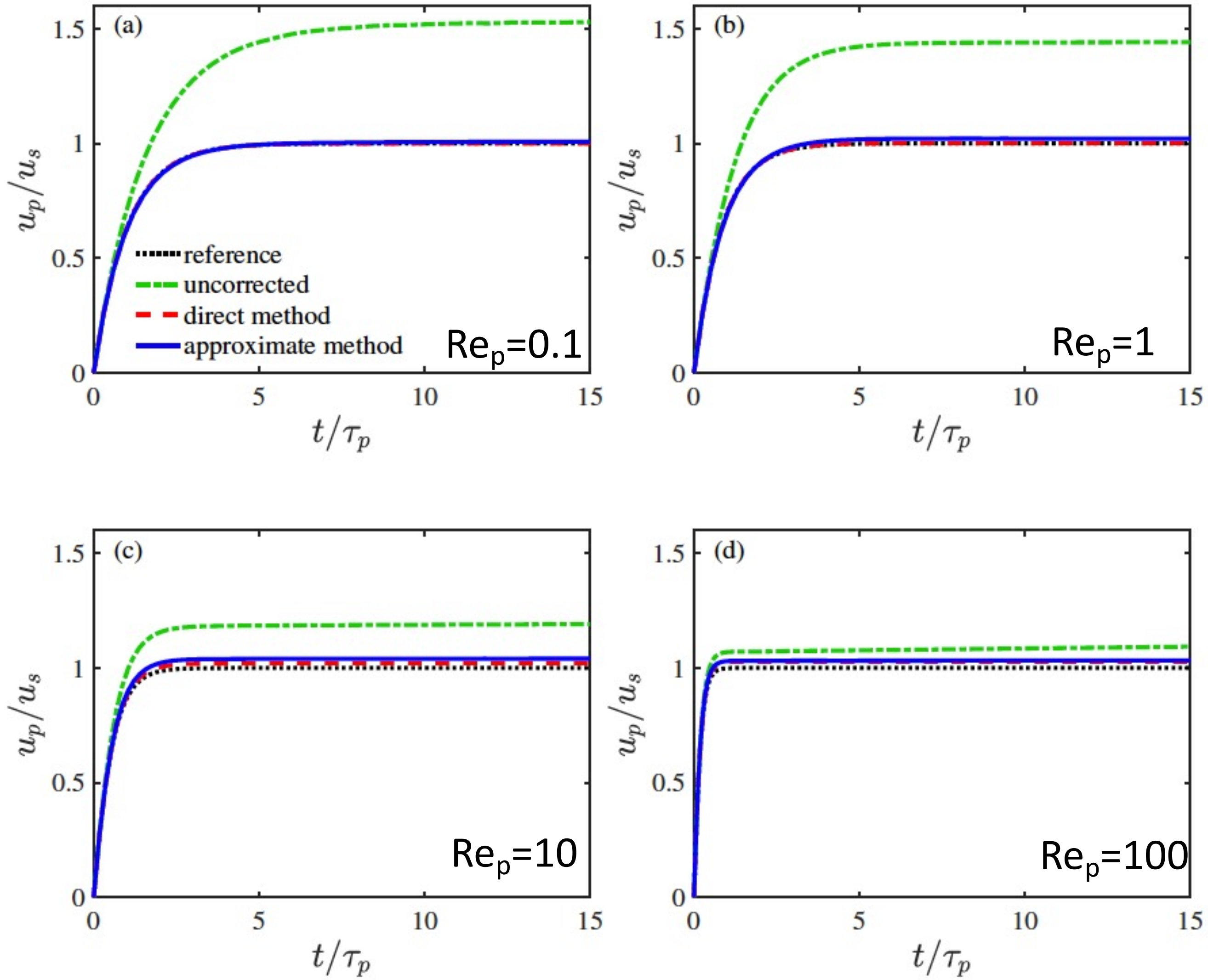


Re_p=0.1



Grid Uncorrected Direct Approximate

Gravitational Settling w/o Heat Transfer



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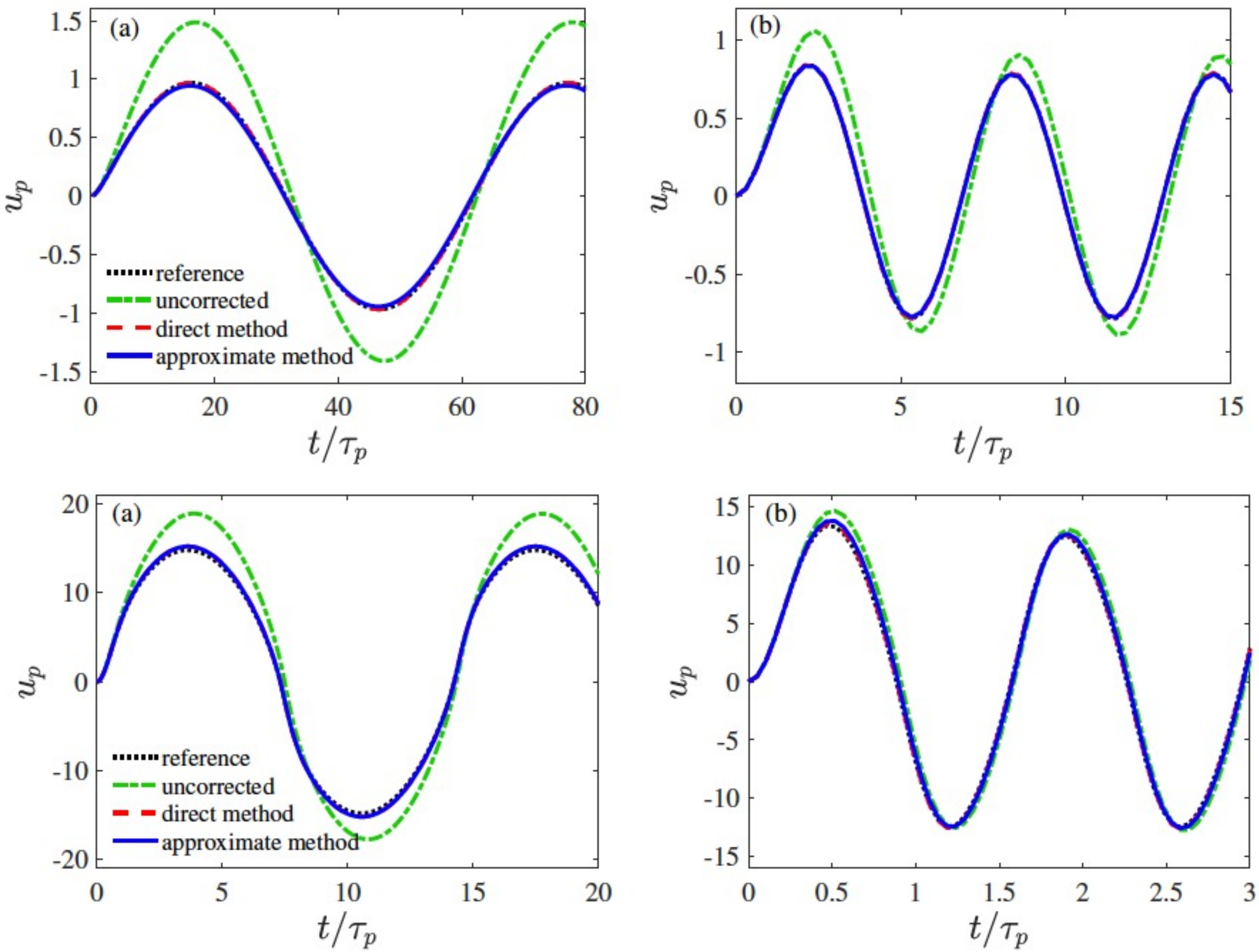
Particle in Oscillatory Motion

Str=0.1 **Str=1**

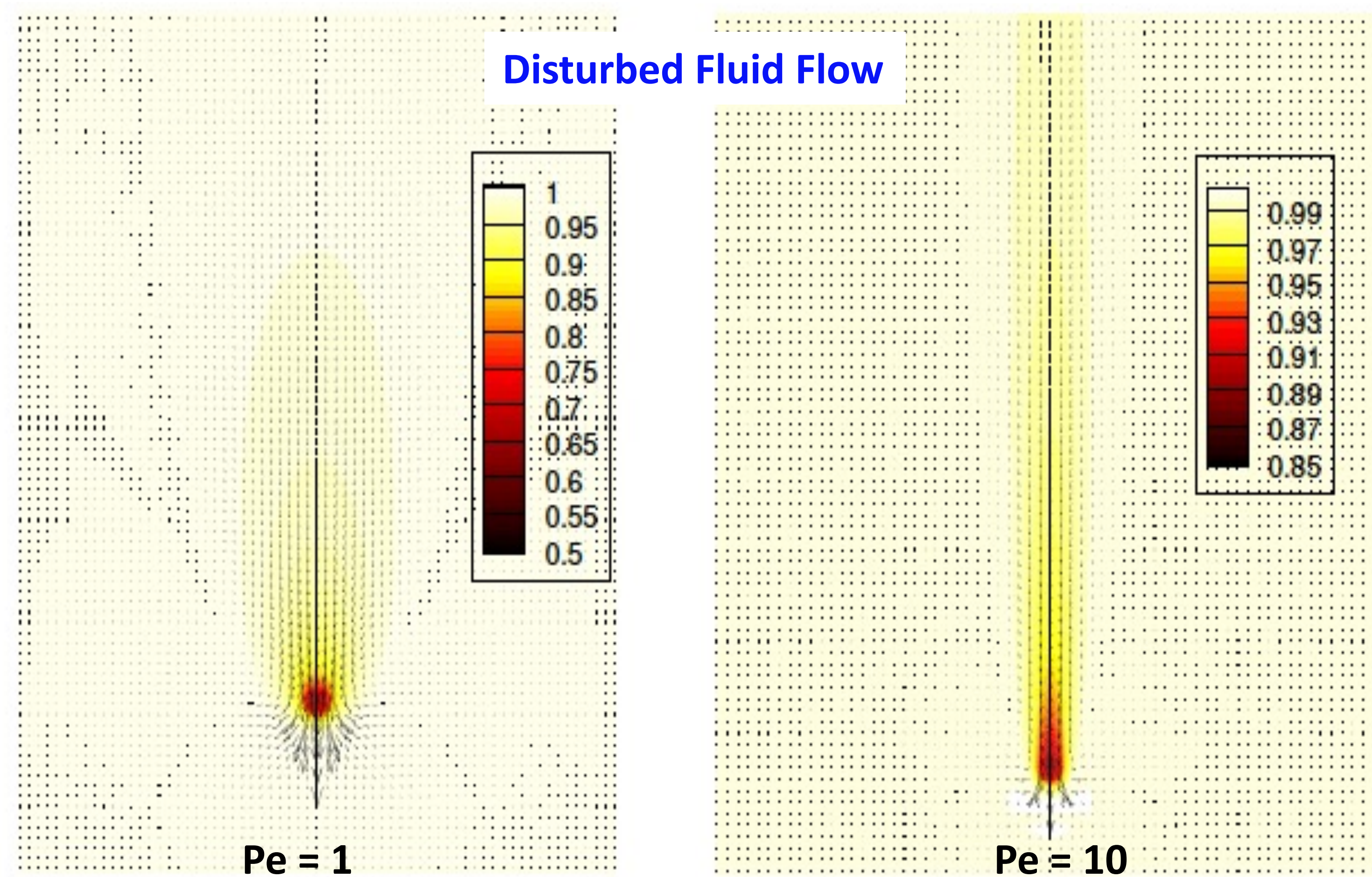
$Re_{p,max}$=0.1

$Re_{p,max}$=100

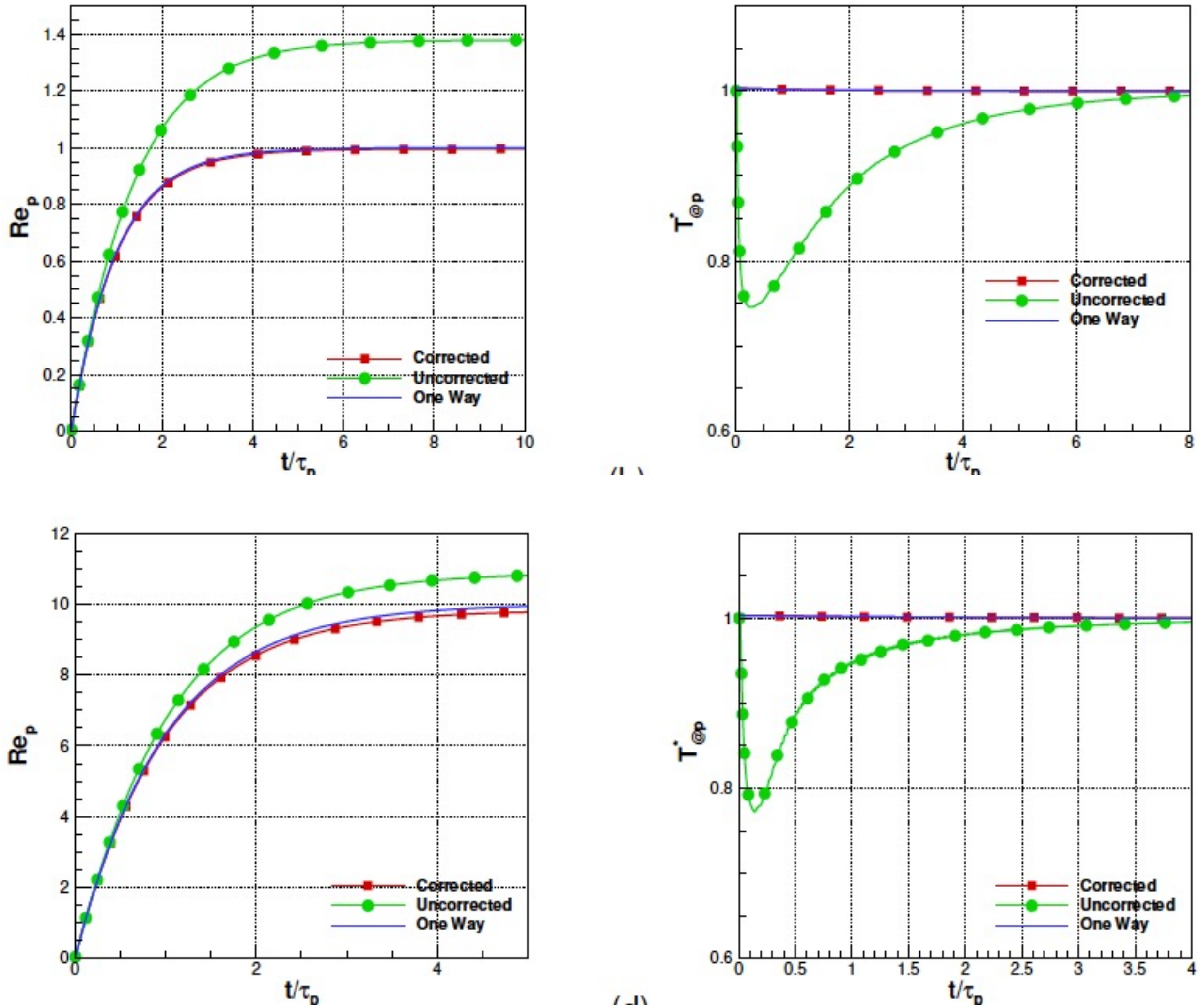


Gravitational Settling with Heat Transfer

Uniformly hot quiescent fluid flow $Pr=1$ $C_{p,\ell}/C_{p,g} = 1.0$



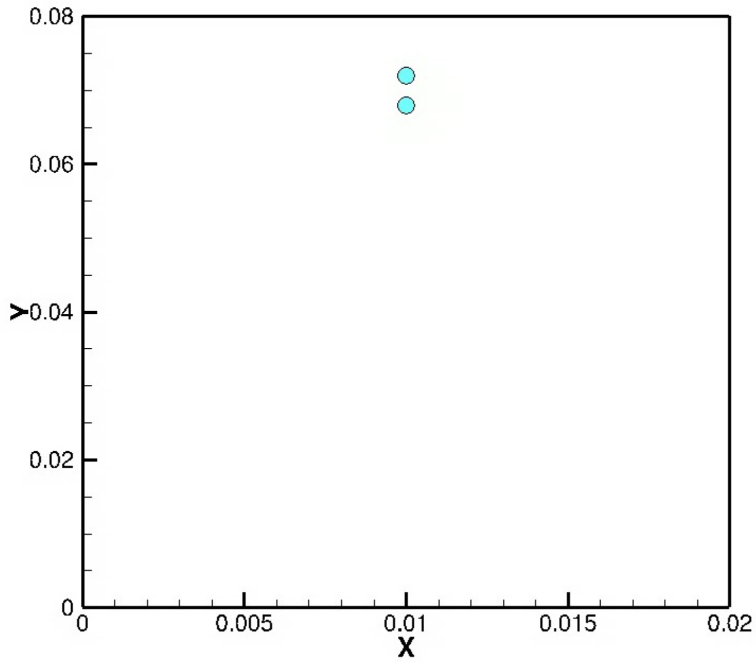
Gravitational Settling with Heat Transfer



Pe = 1

Pe = 10

Multi-Particle Systems: Neighboring Particle Effects



Drafting captured with corrected point-particle model

Summary

- Developed a simple model to obtain the undisturbed fluid flow (velocity and temperature) required for accurate modeling of particle dynamics in point-particle model.
- The disturbance model is shown to be accurate for a range of Reynolds and Peclet numbers, arbitrary shaped grids, and particles comparable or larger than grid resolution.
- The model can be easily implemented into any solver using the same solver routines for momentum and scalar transport.
- The model can be easily extended to multiple particle systems by solving the self-disturbance field for each particle in a small region of influence around the particle.
- This can be easily parallelized and is suitable for GPU-type algorithms as the disturbance field for each droplet is independent of each other.