NETL 2021 workshop

An Easily Implementable General Self-induced Perturbation Correction Model for a Finite-sized Particle in Two-way Coupled Euler-Lagrange Simulations

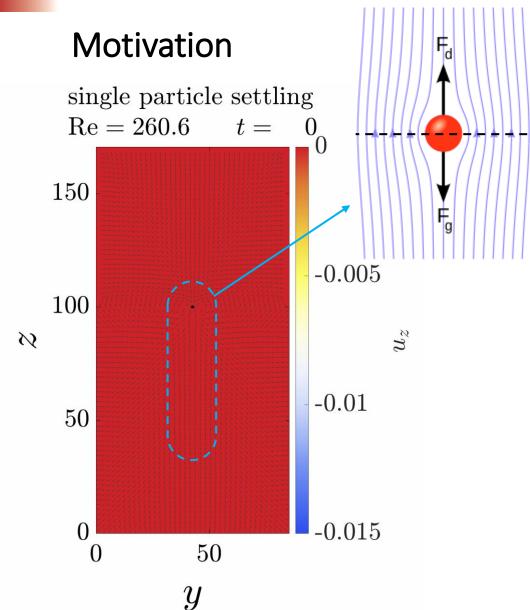
Kai Liu^{a,b}, S. Balachandar^a

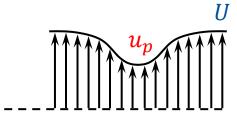
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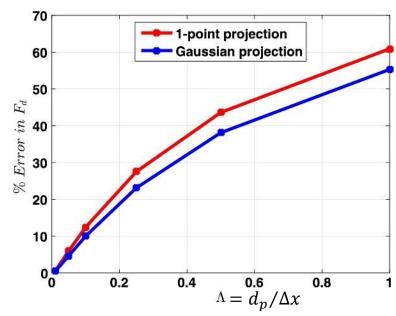






Stokes' drag:

$$F_d = \begin{cases} 3\pi\mu d_p(\mathbf{U} - \mathbf{v}_p) & \sqrt{\text{By theory}} \\ 3\pi\mu d_p(\mathbf{u}_p - \mathbf{v}_p) & \times \text{In simulation} \end{cases}$$



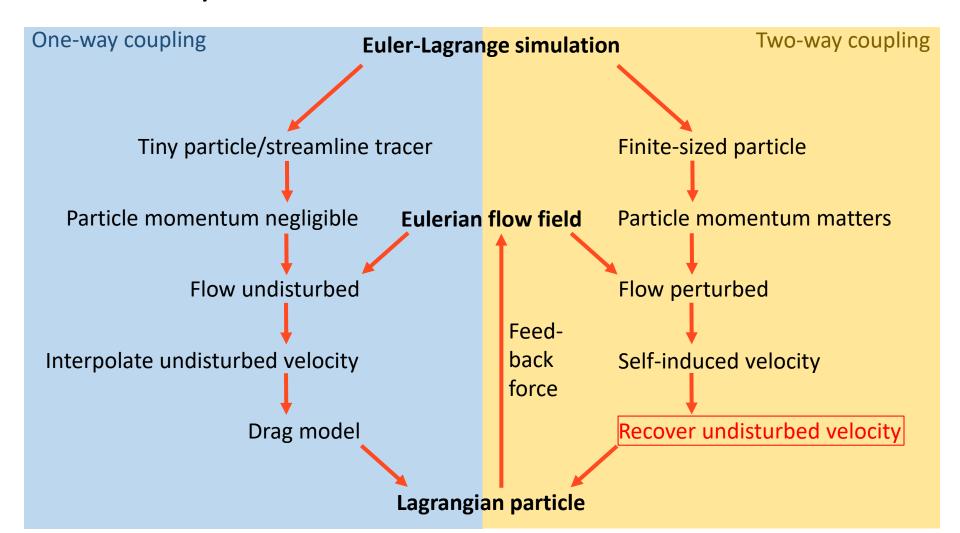
J. A. K. Horwitz and A. Mani. Journal of Computational Physics, 2016.



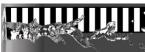




Hierarchy







Our plan

- Simple model
- Drag not in same direction of flow
- Near wall
- Compatible for common projection filters
- Compatible for common difference schemes

Oseen's equation:

$$\nabla \cdot (\phi_{c1} \mathbf{u}'_{1c}) = 0$$

$$\rho \mathbf{U} \cdot (\phi_{c1} \mathbf{u}'_{1c}) = -\nabla (\phi_{c1} p'_{1c}) + \mu \nabla^2 (\phi_{c1} \mathbf{u}'_{1c}) - \mathbf{F}G$$

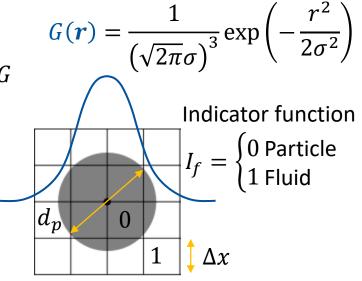
Solution:

$$\boldsymbol{U}(\boldsymbol{x},t) = \phi_{c1}\boldsymbol{u}_{c}(\boldsymbol{x},t) - \phi_{c1}\boldsymbol{u}_{1c}'(\boldsymbol{x},t)$$

Undisturbed velocity

EL particle

Self-induced Center velocity perturbation velocity



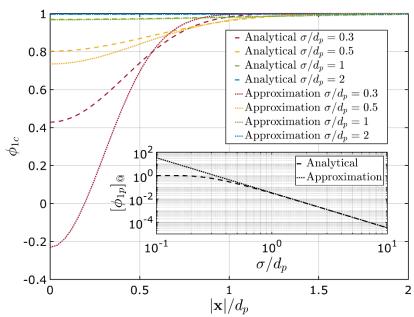








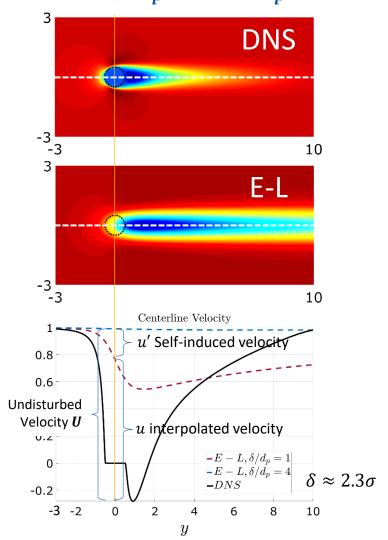
Filter effect



$$\phi_{1c} = \begin{cases} 1 - \operatorname{erf}\left(\frac{d_p}{2\sqrt{2}\sigma}\right) + \frac{d_p}{\sqrt{2\pi}\sigma} \exp\left(-\frac{d_p^2}{8\sigma^2}\right) \text{Analytical} \\ 1 - \frac{\pi d_p^3}{6} \frac{1}{\left(\sqrt{2\pi}\sigma\right)^3} \exp\left(-\frac{0^2}{2\sigma^2}\right) \text{Approximation} \end{cases}$$

- Recommend using the analytical form
- σ/d_p \longrightarrow fluid volume fraction \mathcal{J}
- σ/d_p \longrightarrow self-induced velocity \mathcal{J}

$U = 1, d_p = 1, Re_p = 170$









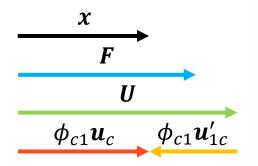


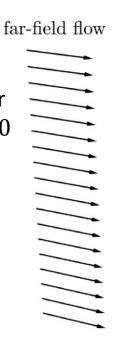


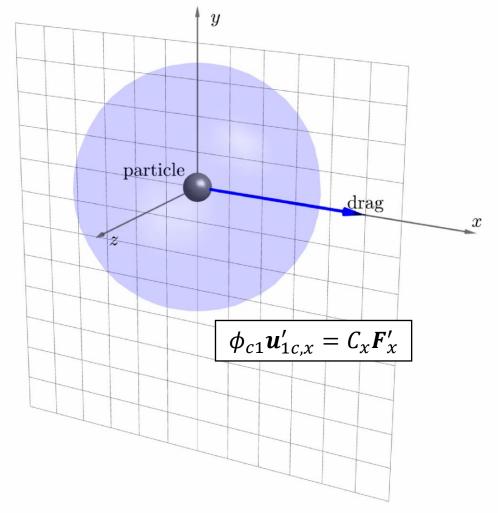


Scenario 1: x-dir scalar

- Drag is parallel to flow
- self-induced velocity in x-dir
- No y,z perturbation @ x = 0









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Scenario 2: 3D vectorial

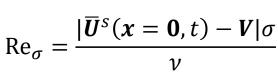
- Drag is not parallel to flow

• Drag is not parallel to flow
• Due to not only
$$\mathbf{F}'_{qs}$$

• Diagonal relation
$$\begin{bmatrix} \phi_{c1}\mathbf{u}'_{1c,x} \\ \phi_{c1}\mathbf{u}'_{1c,y} \\ \phi_{c1}\mathbf{u}'_{1c,z} \end{bmatrix} = \begin{bmatrix} M_x & 0 & 0 \\ 0 & M_y & 0 \\ 0 & 0 & M_z \end{bmatrix} \begin{bmatrix} \mathbf{F}'_x \\ \mathbf{F}'_y \\ \mathbf{F}'_z \end{bmatrix}$$



far-field flow



$$M_{\chi}(\mathrm{Re}_{\sigma}) = -\frac{1}{2\pi^{2}\mathrm{Re}_{\sigma}^{2}} \left[\pi - \sqrt{2\pi}\mathrm{Re}_{\sigma} + \frac{\pi}{2}\mathrm{Re}_{\sigma}^{2} - \pi\mathrm{exp}\left(\frac{\mathrm{Re}_{\sigma}^{2}}{2}\right) \mathrm{erfc}\left(\frac{\mathrm{Re}_{\sigma}}{\sqrt{2}}\right) \right]$$













y

particle

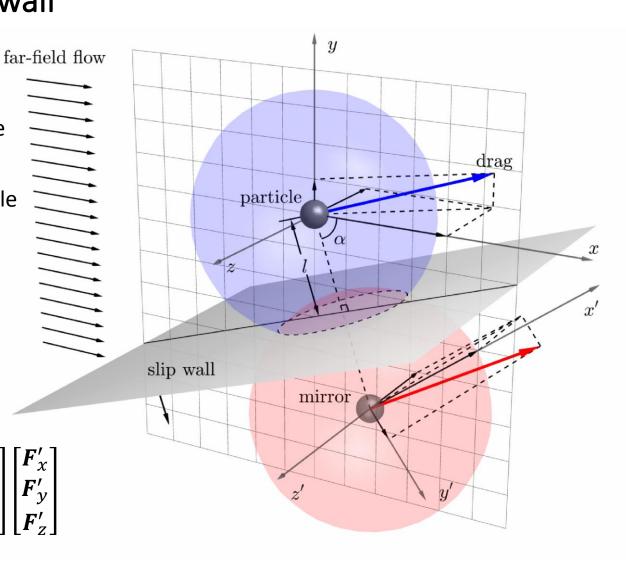


drag

Scenario 3: near-wall

- Free-slip wall nearby
- Projection point in x-y plane
- Modelled by a mirror particle
- Symmetric by the wall
- Drag symmetric by the wall
- Not only diagonal relation

$$\begin{bmatrix} \boldsymbol{\phi}_{c1} \boldsymbol{u}'_{1c,x} \\ \boldsymbol{\phi}_{c1} \boldsymbol{u}'_{1c,y} \\ \boldsymbol{\phi}_{c1} \boldsymbol{u}'_{1c,z} \end{bmatrix} = \begin{bmatrix} \boldsymbol{M}_{xx} & \boldsymbol{M}_{xy} & 0 \\ \boldsymbol{M}_{yx} & \boldsymbol{M}_{yy} & 0 \\ 0 & 0 & \boldsymbol{M}_{zz} \end{bmatrix} \begin{bmatrix} \boldsymbol{F}'_{x} \\ \boldsymbol{F}'_{y} \\ \boldsymbol{F}'_{z} \end{bmatrix}$$







Correction model

standard drag

$$F'_{qs} = 3\pi\mu d_p [\overline{\phi_{c1}u_c}^s - V] \Phi - \mathcal{V}$$
 Interpolated relative flow velocity $\overline{\phi_{c1}u_c}^s - V$

Renew $\overline{U}^{S} - V$ and

Iterate

Coordinates rotation
$$[\mathbf{M}][\overline{\phi_{c1}}\overline{u_c}^s - V]$$

Compute $\operatorname{Re}_{\sigma}$, Re_{p} , Φ , $[\mathbf{B}]$, $[\mathbf{C}]$ using $[\mathbf{M}][\overline{\mathbf{U}}^{s} - \mathbf{V}]$

Start

$$\overline{\boldsymbol{U}}^{S} - \boldsymbol{V} = [\mathbf{M}]^{T} \left\{ [\boldsymbol{I}] - \frac{d_{p}}{\sigma} \frac{\Phi}{\sqrt{2\pi}} [\mathbf{B}] ([\boldsymbol{I}] + [\mathbf{C}]) \right\}^{-1} [\mathbf{M}] (\overline{\phi_{c1} \boldsymbol{u}_{c}}^{S} - \boldsymbol{V})$$

True drag $F'_{as} = 3\pi\mu d_p [\overline{U}^s - V]\Phi$

$$[\mathbf{B}] = \begin{bmatrix} \Psi_{xx-os} & \Psi_{xy-os} & 0 \\ \Psi_{yx-os} & \Psi_{yy-os} & 0 \\ 0 & 0 & \Psi \end{bmatrix} - \frac{d_p^2}{24\sigma^2} \begin{bmatrix} \Psi_{xx-Lap} & \Psi_{xy-Lap} & 0 \\ \Psi_{yx-Lap} & \Psi_{yy-Lap} & 0 \\ 0 & 0 & \Psi_{xy-Lap} \end{bmatrix} [\mathbf{C}] = [\mathbf{M}] \begin{bmatrix} \overline{\mathbf{F}}'_{ot} \\ \overline{\mathbf{F}}'_{qs} \end{bmatrix} \begin{bmatrix} \overline{\boldsymbol{\phi}_{c1} \boldsymbol{u}_c}^s - \mathbf{V} \\ \overline{\boldsymbol{v}}^s - \mathbf{V} \end{bmatrix} [\mathbf{M}]^T$$

$$[\mathbf{C}] = [\mathbf{M}] \left[\frac{\mathbf{F}'_{ot}}{\mathbf{F}'_{qs}} \right] \left[\frac{\overline{\phi_{c1}} \mathbf{u}_c}{\overline{\mathbf{U}}^s - \mathbf{V}} \right] [\mathbf{M}]$$



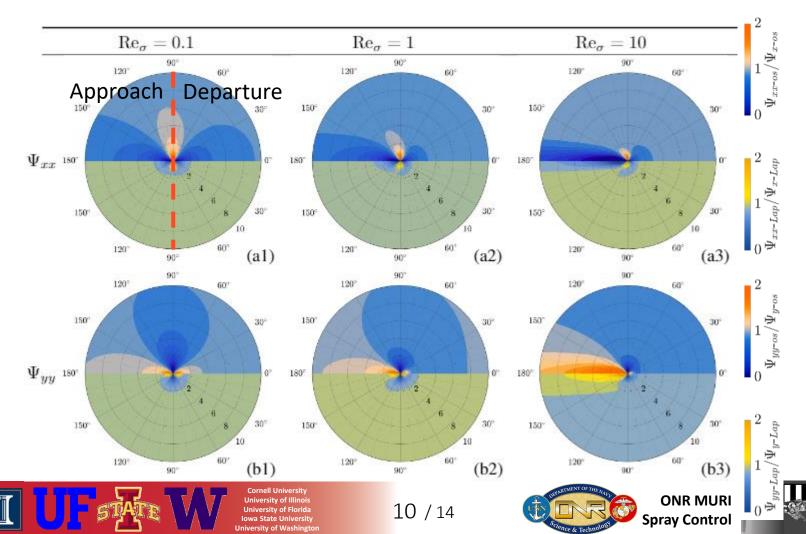




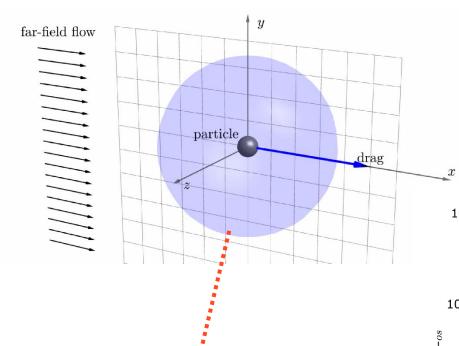


Ψ components

Obtained totally 10 components of $\Psi\left(\operatorname{Re}_{\sigma},\frac{l}{\sigma},\alpha\right)$ with explicit asymptotic functions for low $\operatorname{Re}_{\sigma}$



Different filters

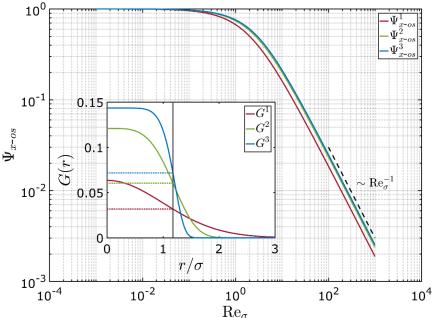


Scalar case for example, different choice of filter does not change general solution

$$\overline{\phi_{c1}u_c'}^s = C \operatorname{Re}_{\sigma} F_x' \Psi_{x-os}$$
 but slightly changes the specific values of

 $C, \Psi_{x-\alpha s}$

 $G^{2}(r) = \frac{1}{\pi \Gamma(\frac{3}{4})(\ln 16)^{3/4} \sigma^{3}} \exp\left[-\frac{r^{4}}{(\ln 16)\sigma^{4}}\right]$ $G^{3}(r) = \frac{2^{5/8}}{\pi \Gamma(\frac{3}{2})(\ln 4)^{9/8} \sigma^{3}} \exp\left[-\frac{r^{8}}{2(\ln 4)^{3} \sigma^{8}}\right]$









 $G^{1}(r) = \frac{1}{(2\pi)^{3/2}\sigma^{3}} \exp\left(-\frac{r^{2}}{2\sigma^{2}}\right)$







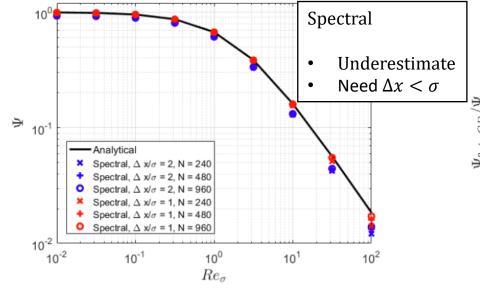
 $\begin{array}{l} \text{Differentiation schemes} \\ \text{Self-induced velocity derived by Fourier Transform } \widehat{\phi_{c1} \boldsymbol{u}_c'} = -\frac{F_x' \text{Re}_{\sigma} \left(1 - \iota \frac{\text{Re}_{\sigma} k_x}{\left|\tilde{k}\right|^2}\right)}{\left|\tilde{k}\right|^2 \left(1 + \frac{\text{Re}_{\sigma}^2 \tilde{k}^2}{\left|\tilde{k}\right|^4}\right)} \left(1 - \frac{\tilde{k}_x^2}{\tilde{k}^2}\right) \widehat{G} \end{array}$

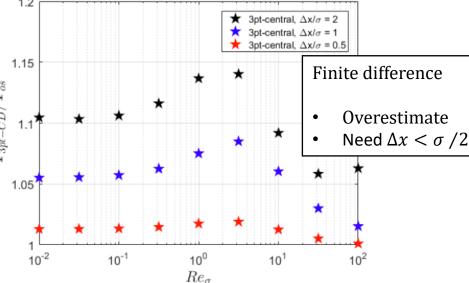
Wave number in spectral method

$$\tilde{k}=k$$
 and $\tilde{k}^2=k^2$ for $k=0,\pm k_{min},\pm 2k_{min},\cdots,\pm \frac{N}{2}k_{min}$

Wave number in second-order finite difference scheme

$$\tilde{k} = \frac{1}{\Delta x} \sin(k\Delta x) \text{ and } \tilde{k}^2 = \frac{1}{\Delta x^2} [1 - \cos(k\Delta x)] \text{ for } k = 0, \pm k_{min}, \pm 2k_{min}, \cdots, \pm \frac{N}{2} k_{min}$$

















Conclusion

Subject: provide the self-induced perturbation velocity correction model

Aim: recover the true drag force in Two-way coupled Euler-Lagrange simulation

Needs: $\Delta x < \sigma$ for spectral method, $\Delta x < \sigma / 2$ for finite difference scheme

Inputs: $\sigma, d_p, \nu, X_w, (\overline{\phi_{c1}u_c}^s - V), [\frac{F'_{ot}}{F'_{qs}}]$

Outputs: corrected drag

Capability:

- Arbitrary velocity vectors of flow, particle, and force
- Free-slip wall

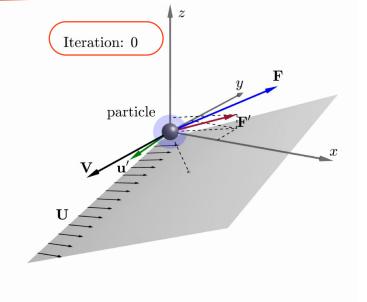
Feature:

- Analytically derived
- Explicit form without table interpolation
- Easy to extend to different filters, DS, finite Re_σ , fast-varying, heat/mass transfer







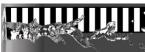


Thank you for watching!

You can send me questions by email: kailiu@ufl.edu

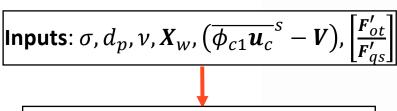
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Supplementary pages

Test



Model: a black box of functions Matlab < 100 lines, < 0.01s/iteration

Outputs: correct drag force

$$F' \rightarrow F$$

Example inputs:

$$\sigma = 2$$

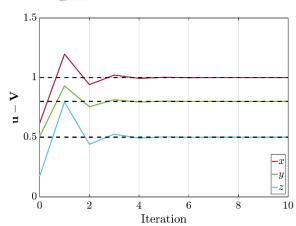
$$d_p = 2$$

$$\nu = 2$$

$$X_w = [2,1,-5]'$$

$$\frac{\mathbf{X}_{w} = [2,1,-5]'}{\phi_{c1}\mathbf{u}_{c}^{S} - \mathbf{V} = [1,0.8,0.5]'}$$

$$\begin{bmatrix} \underline{F'_{ot}} \\ \overline{F'_{qs}} \end{bmatrix} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix}$$



Iteration: 0

particle



 10^{-5}

Relative error of 10^{-3} 10^{-4}





Supplementary pages

Extension

- 1. Finite Reynolds number $\text{Re}_{\sigma}\gg 1$ correction
 - Moderate derivation
 - Small self-induced velocity, less important to correct
- 2. Fast transient correction
 - Derive time history term
 - Commonly not used
- 3. Self-induced temperature/concentration corrections
 - Scalar form
 - Adiabatic/inpermeable wall



