LES-Style Filtering and Partly-Resolved Particles: A Process for Developing Particle Models

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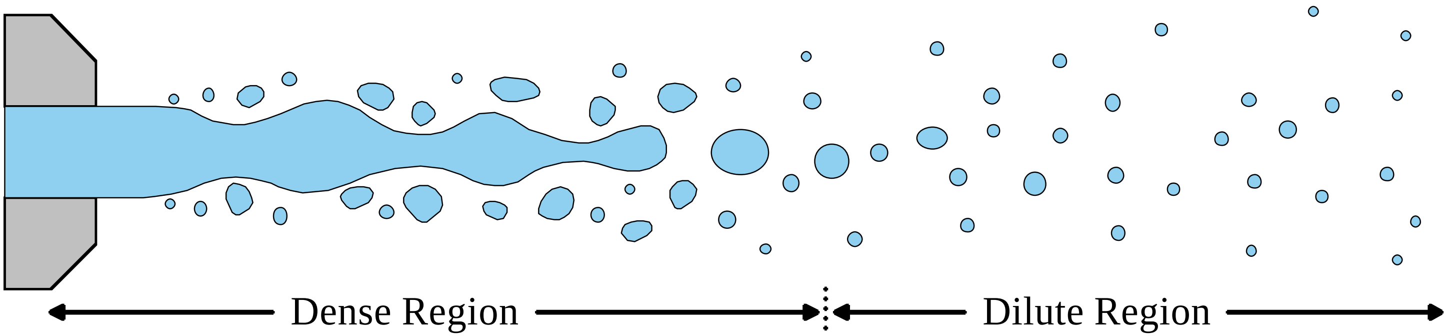
Motivation

- Mass, momentum balances in atomization processes:



- Current methods can only handle portions of the flowfield.
  - Fully-resolved methods: near-nozzle dense regime.
  - Particle methods: far-field dilute-particle regime.
- Multiphase flow models need to be consistent with LES for turbulent combustion simulations.
- Spatially filtering the multiphase flow equations provides a framework for dealing with both of these needs.
- Test problem: consider a partly-resolved particle.

Navier-Stokes on an Embedded Sub-Domain

- Mass and momentum conservation equations for an embedded subdomain corresponding to phase i:

$$\frac{\partial(\phi_i \rho_i)}{\partial t} + \nabla \cdot (\phi_i \rho_i \vec{\boldsymbol{u}}_i) = \rho_i \vec{\boldsymbol{u}}_{\text{outflow},\, i} \cdot \nabla \phi_i$$

$$\frac{\partial(\phi_i \rho_i \vec{\boldsymbol{u}}_i)}{\partial t} + \nabla \cdot (\phi_i \rho_i \vec{\boldsymbol{u}}_i \vec{\boldsymbol{u}}_i) = -\nabla(\phi_i p_i) + \nabla \cdot (\phi_i \vec{\vec{\boldsymbol{\tau}}}_i) + \vec{\vec{\boldsymbol{\sigma}}}_{\text{surface},\, i} \cdot \nabla \phi_i + \rho_i \vec{\boldsymbol{u}}_i \vec{\boldsymbol{u}}_{\text{outflow},\, i} \cdot \nabla \phi_i$$

- Phase function $\phi_i = 1$ inside the subdomain, and is zero outside it. Thus, $\nabla \phi_i$ is a delta-function distribution along the subdomain boundary.
- This formulation is valid inside and outside the fluid phase, and contains both the internal field equations and the surface conditions for the fluid.
- Thus, it can be filtered across the fluid boundary in a mathematically rigorous manner, without requiring any special treatment for the boundary.

Spatially-Filtered Multiphase Flow Equations

- Filtering these equations (with $(\phi_i \rho_i)$, $(\phi_i \rho_i \vec{\boldsymbol{u}}_i)$, and $(\phi_i p_i)$ chosen as the primary variables) produces:

$$\frac{\partial \overline{(\phi_i \rho_i)}}{\partial t} + \nabla \cdot \overline{(\phi_i \rho_i \vec{\boldsymbol{u}}_i)} = \overline{\rho_i \vec{\boldsymbol{u}}_{\text{outflow},\, i} \cdot \nabla \phi_i}$$

$$\frac{\partial \overline{(\phi_i \rho_i \vec{\boldsymbol{u}}_i)}}{\partial t} + \nabla \cdot \overbrace{(\phi_i \rho_i \vec{\boldsymbol{u}}_i \vec{\boldsymbol{u}}_i)}^{\text{resolved part}}$$

$$= -\nabla \overline{(\phi_i p_i)} + \nabla \cdot \overbrace{(\phi_i \vec{\vec{\boldsymbol{\tau}}}_i)}^{\text{resolved part}} - \vec{\boldsymbol{T}}_{\text{SFS}} + \vec{\boldsymbol{T}}_{\text{SFS-viscous}}$$

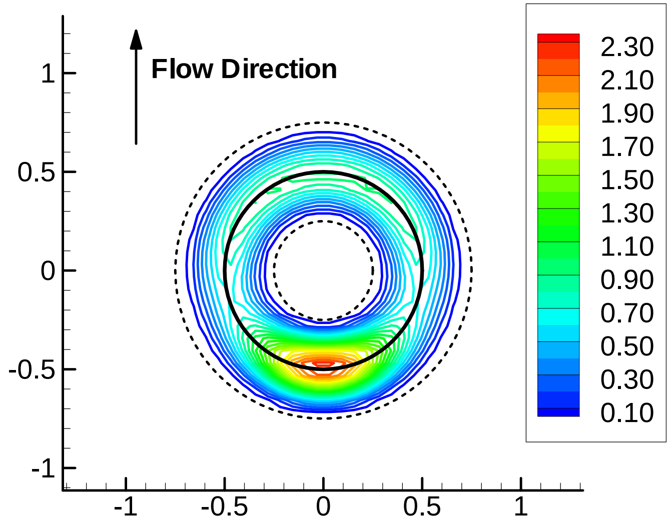
$$+ \overline{\vec{\vec{\boldsymbol{\sigma}}}_{\text{surface},\, i} \cdot \nabla \phi} + \overline{\rho_i \vec{\boldsymbol{u}}_i \vec{\boldsymbol{u}}_{\text{outflow},\, i} \cdot \nabla \phi_i}$$

- These contain unclosed terms, which are provided by various models (wall models, particle models, turbulence models, phase-interaction models, etc.):
  - (blue) Mass and momentum fluxes across the surface.
  - (purple) Subfilter-scale convection term (as in LES).
  - (green) Subfilter-scale viscous term.

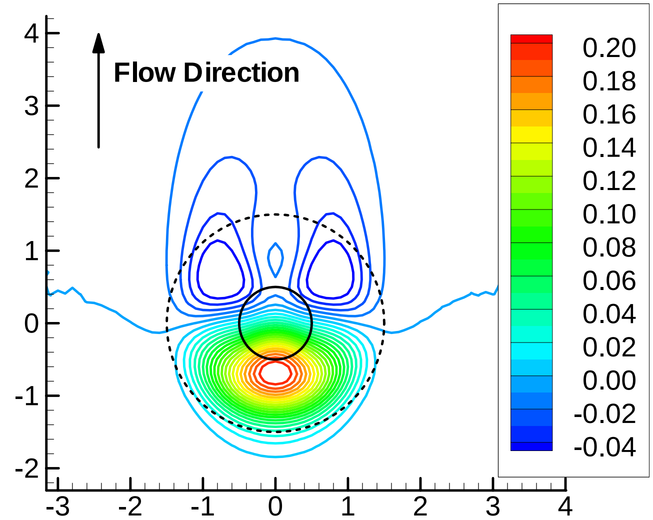
Particle Model Development Process

- In general, models for the unclosed terms can be developed by the following process:
  - Start with well-resolved calculations of representative flowfields.
  - Filter the resolved flowfields to the desired resolution.
  - Calculate exact forms of the subfilter-scale terms using fluxes from the filtered and well-resolved flowfields.
  - Approximate the exact subfilter-scale terms with a parameterized model. (As with turbulence, this is not always easy!)
- These models can be combined with existing phase tracking methods (level-set, VOF, particle-tracking, etc.) to produce a complete simulation method.
- As a demonstration of this, consider the case of a single partly-resolved cylinder (a "2D particle") in a steady uniform flow at Re=26.

Visualization of Particle Model Terms



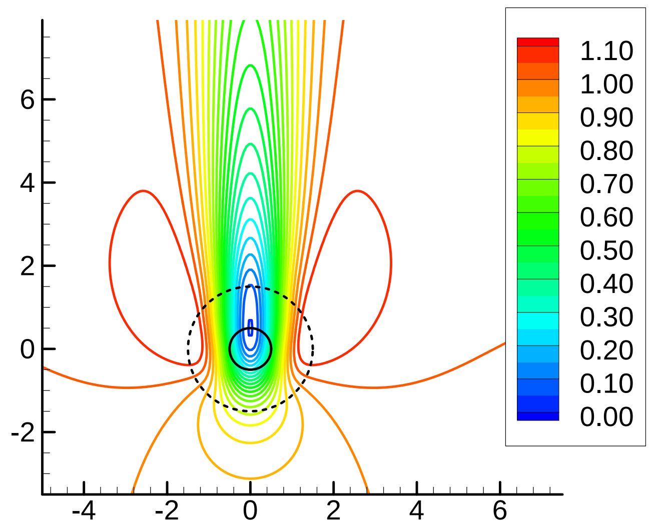
Filtered streamwise surface force density, $r_{\text{filter}} = 0.25 D_{\text{particle}}$



Streamwise subfilter convection, $r_{\text{filter}} = 1.0 D_{\text{particle}}$

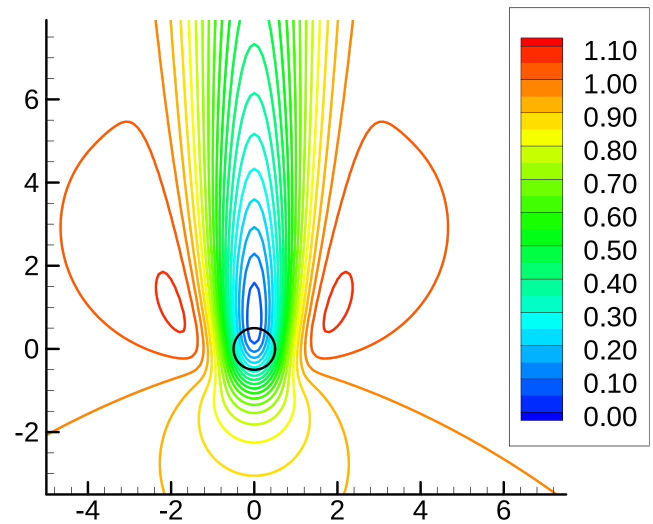
- We will model the unclosed terms are as follows:
  - Surface force density is represented by a multiple-filtered-point interpolation over the particle surface.
  - Subfilter-scale convection is represented by three filtered point forces.

Initial Model Results



Computed streamwise velocity,

$r_{\text{filter}} = 1.0 D_{\text{particle}}$

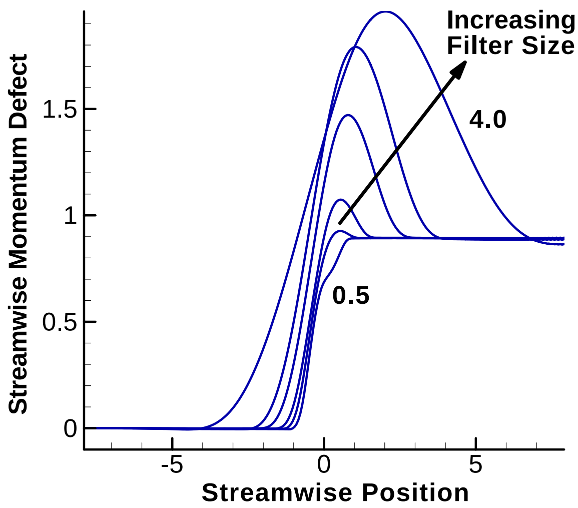


Filtered "exact" velocity,

$r_{\text{filter}} = 1.0 D_{\text{particle}}$

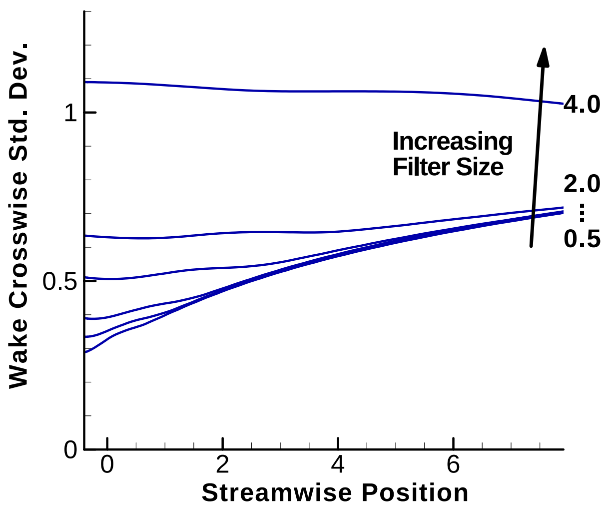
- Computational parameters:
  - $16 D_{\text{particle}} \times 16 D_{\text{particle}}$ flow domain.
  - $\Delta x_{\text{grid}} = 1/16\, r_{\text{filter}}$, for grid-converged results.
- The resulting simulation is a close match for the exact filtered flow, both qualitatively and quantitatively.

Results for Various Filter Sizes



Wake momentum defects

(in units of ρU_0^2).



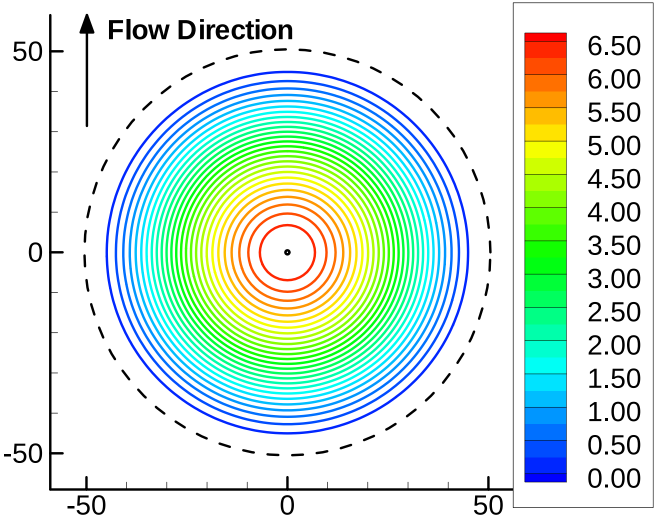
Wake width

(in units of D_{particle}).

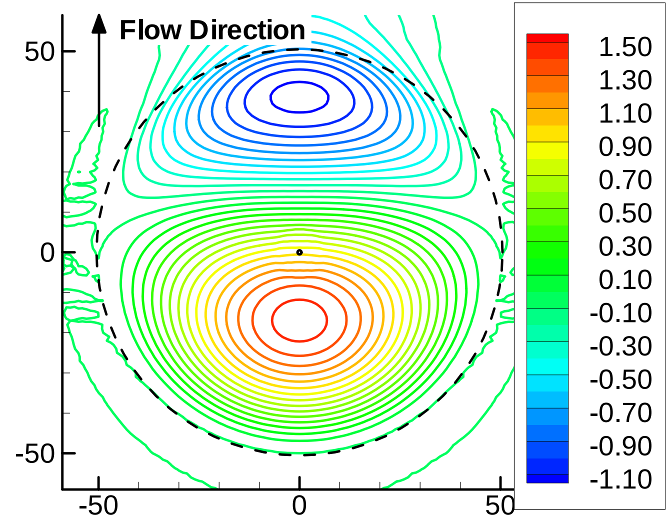
- The amount of momentum flux hidden in the subfilter scales increases with increasing filter size.
- Net wake defect across the particle is constant, and is equal to the particle drag force.
- Wake widths converge to the same size when the wake becomes resolved downstream.

Filtering and the Point Particle Model

- Consider the model terms for a small particle typically treated as a “point particle”:



Filtered streamwise surface force density, $r_{\text{filter}} = 50 D_{\text{particle}}$



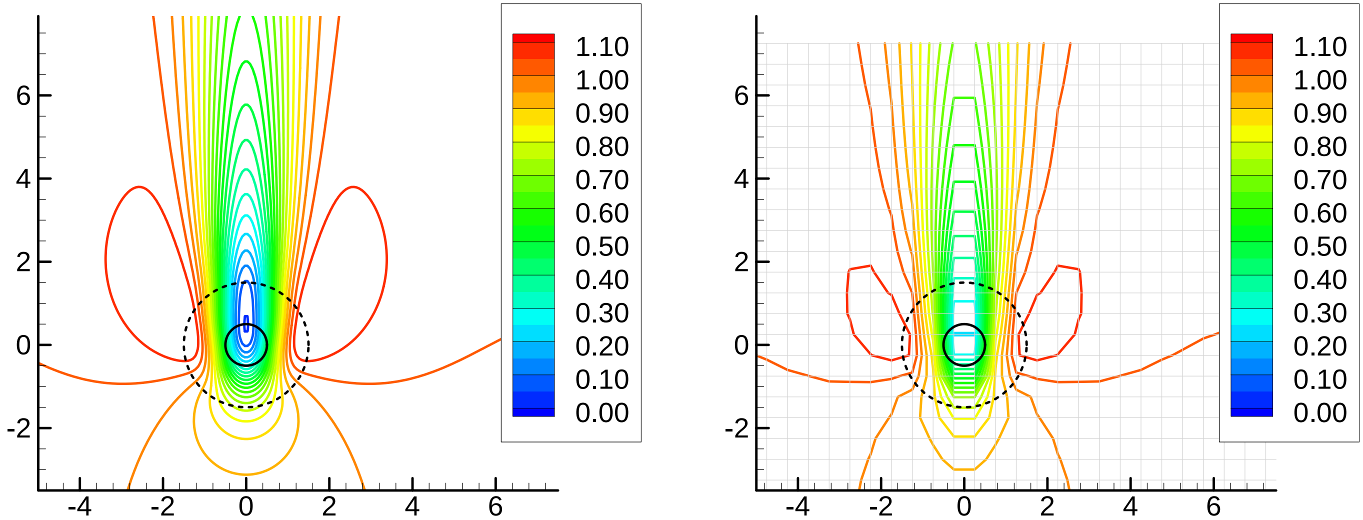
Streamwise subfilter convection, $r_{\text{filter}} = 50 D_{\text{particle}}$

- Even for a case where the filter is $100\times$ larger than the particle, the subfilter-scale convection term is a sizable fraction (around 25%, at peak) of the filtered surface force, and may be computationally significant.

Summary and Conclusions

- We have derived general LES-compatible equations for multiscale, multiphase flow by spatially filtering the conservation equations for an embedded subdomain.
- These equations can be used to develop models for typical partly-resolved particles, and these models produce accurate results over a range of filter scales.
- The grid resolution requirements for the particle models are comparable to requirements for turbulence LES.
- The subfilter-scale term is important over a wide range of scales – well into the "resolved" and "point-particle" regimes.
- Work to extend the 2D cylinder models to 3D spheres is currently in progress.

Results for Grid Resolution Study



Filtered-computation results, $\Delta x_{\text{grid}} = 1/16\, r_{\text{filter}}$

Filtered-computation results, $\Delta x_{\text{grid}} = 1/2\, r_{\text{filter}}$

- For a grid spacing of half the filter radius:
  - The results are still qualitatively very good.
  - There are some primary grid-coarsening effects (e.g., the centerline velocity deficit is washed out due to finite-width grid cells).