Coarse-Grid Simulation of Riser Flows

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- DOE – UCR program
- ExxonMobil Research & Engg. Co.

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Roadmap for dilute gas-particle flows

Near-term (by 2009)

• B3: Develop coarse-grained (filtered) two-fluid models

Mid-term (by 2012)

•B3: *Develop procedures to coarsen models for reactive flows*

Connection to roadmap

- Performed highly resolved simulations of a kinetic theory based two-fluid model for gas-particle flow in various test domains
- Filtered the results to learn about constitutive relations for the filtered two-fluid model
- Verified the fidelity of the filtered model. Validation remains to be done.

Characteristics of flows in turbulent fluidized beds & fast fluidized beds

- Persistent density and velocity fluctuations
  - Wide range of length and time scales
- Identifiable macroscopic inhomogeneous structures
- (Kinetic theory based) two-fluid models are able to capture the above characteristics
  - But, they require high resolution and large computational times
- Do we really want to resolve all the fine structures?
  - If we do not, then how should we modify the two-fluid model?

Solution of discretized form of the kinetic theory based two-fluid model

30 m tall

76 cm channel width

75μm particles

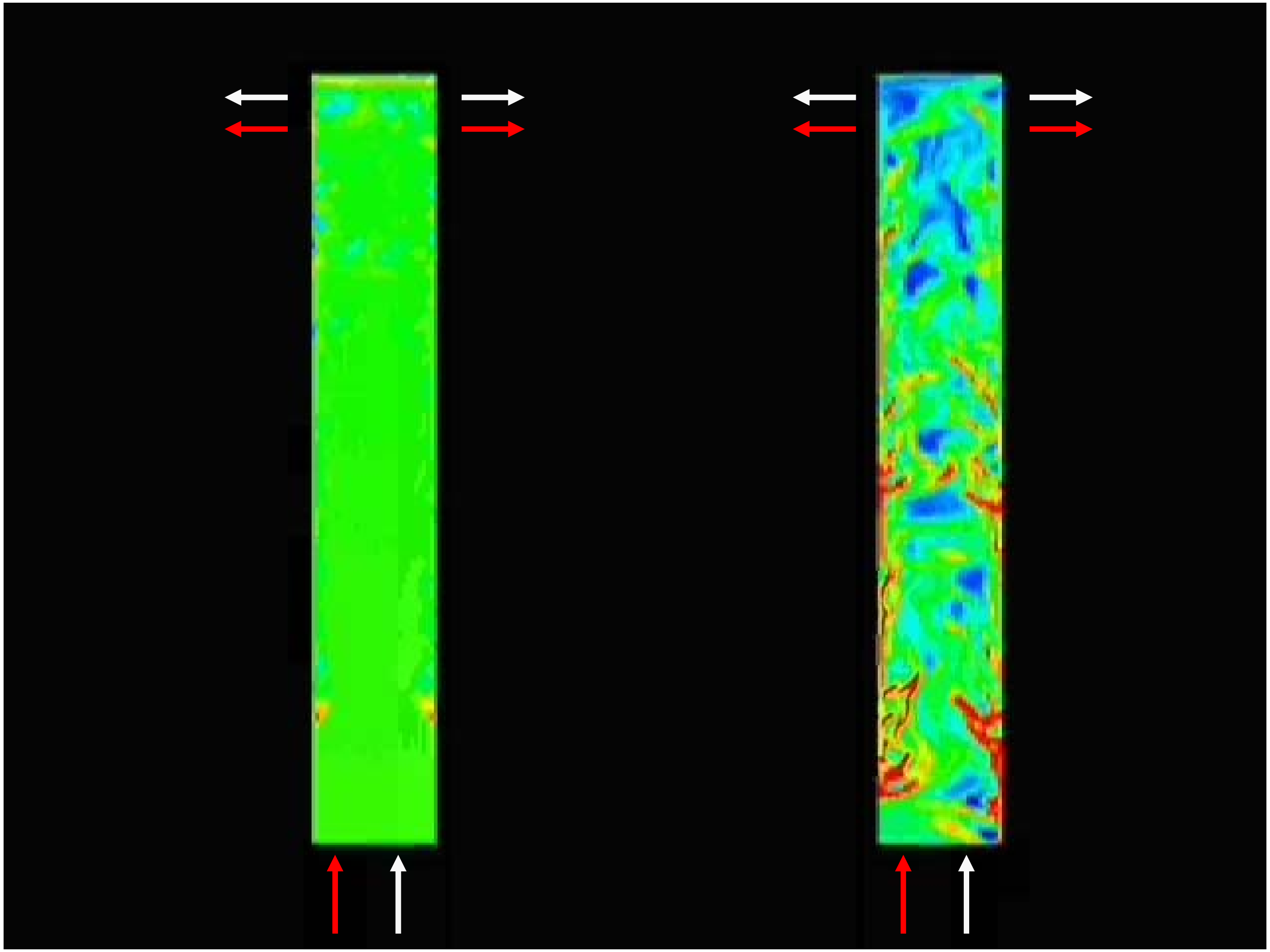
2 cm grid

2-D simulations

Solids fraction field

Red – high

Blue -low



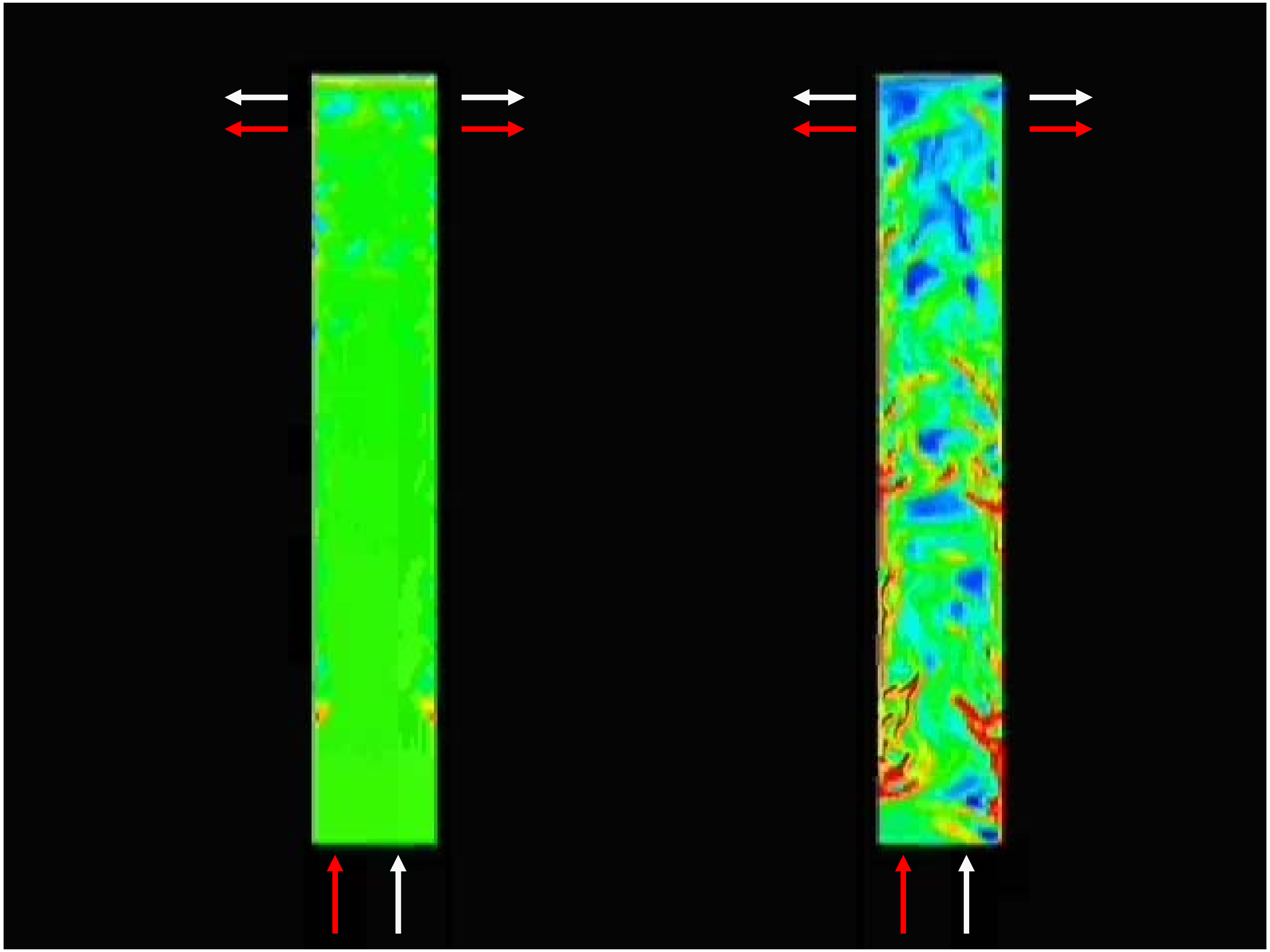
Gas vel = 6 m/s
Solids flux = 220 kg/m2.s

What we get

What we expect based on experimental data

Solution of discretized form of the kinetic theory based two-fluid model

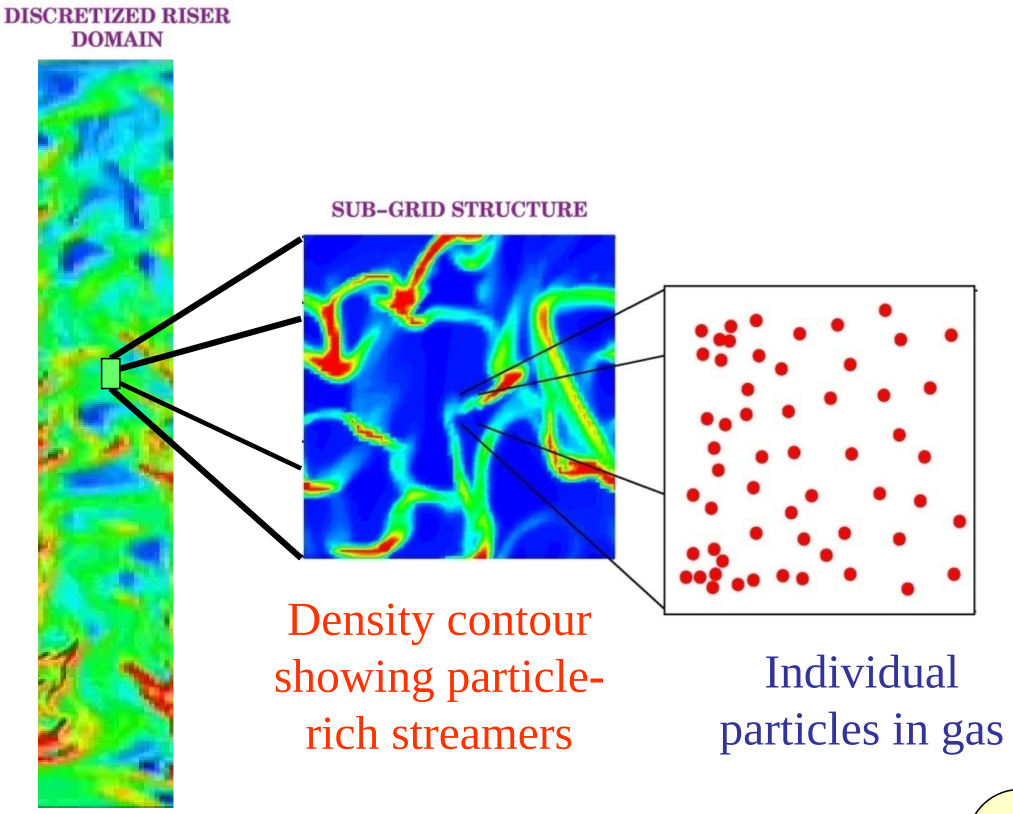
But in smaller channels and with finer grid resolution, kinetic theory based model does produce the right kind of spatial and temporal variations



What we get in wide channels and coarse grids

What we get in narrow channels with fine grids

Overview of the coarse-graining (filtering)



All the constitutive models for the two-fluid models are for nearly homogeneous mixtures

Multiphase flow computations via two-fluid models

Reaction engineering need: Tools to probe macro-scale reactive flow features directly

Modeling challenge for gas-particle flows

Develop models that allow us to focus on large-scale flow structures, without ignoring the possible consequence of the smaller scale structures.

Original two-fluid model and constitutive relations

Significant advances in the past three decades

→

Filtered two-fluid model

Modified constitutive relations for

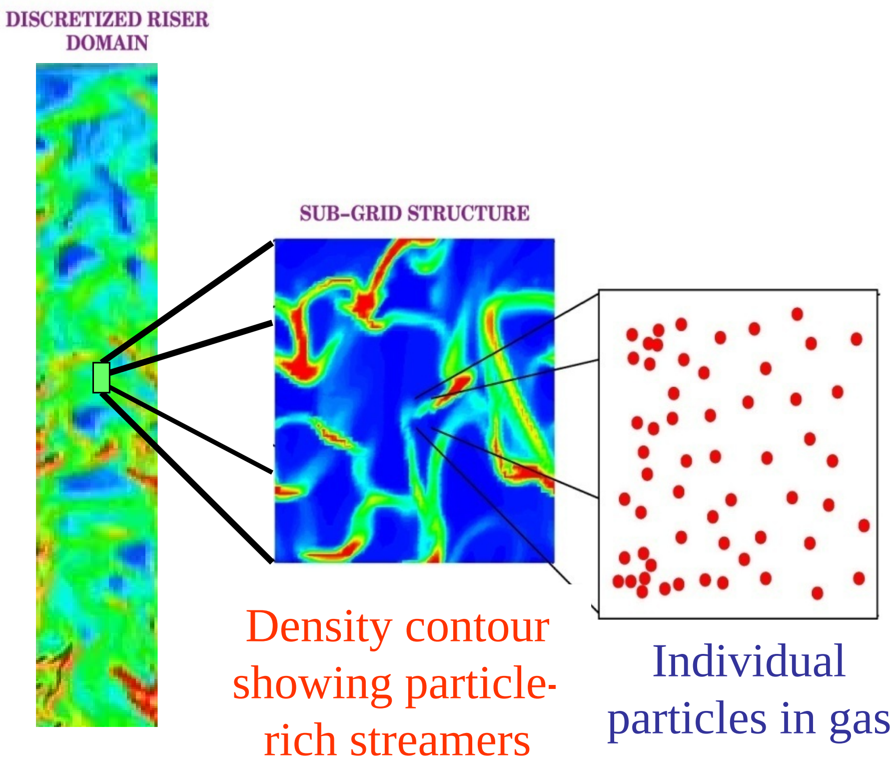
hydrodynamic terms

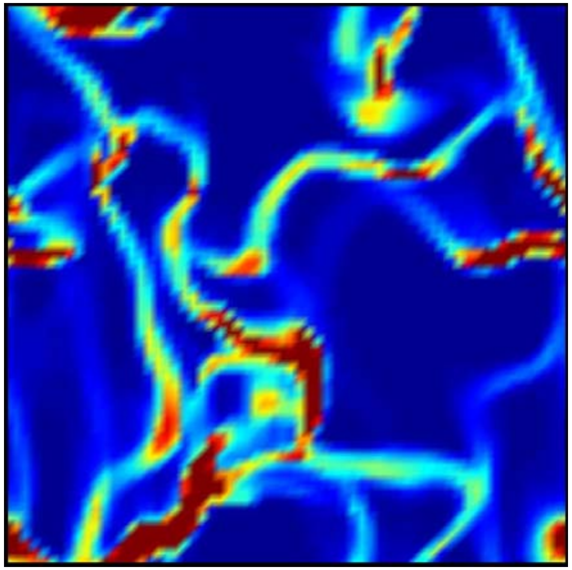
species and energy dispersion

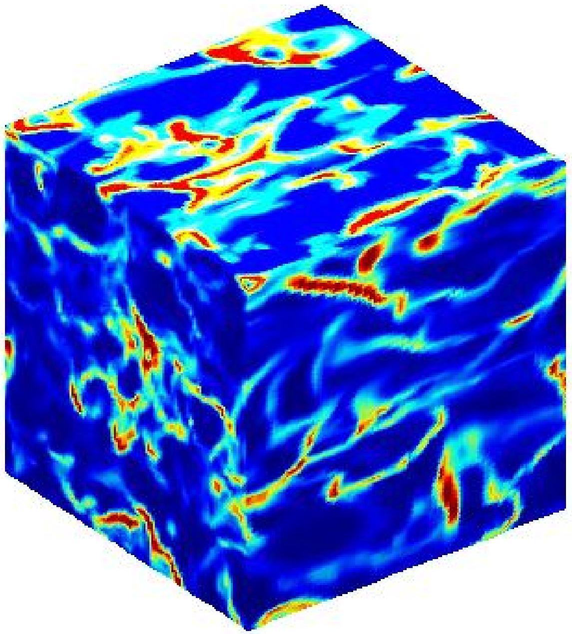
interphase heat and mass transfer rates

even modified reaction rate expressions!

First Step in development of Filtered Model







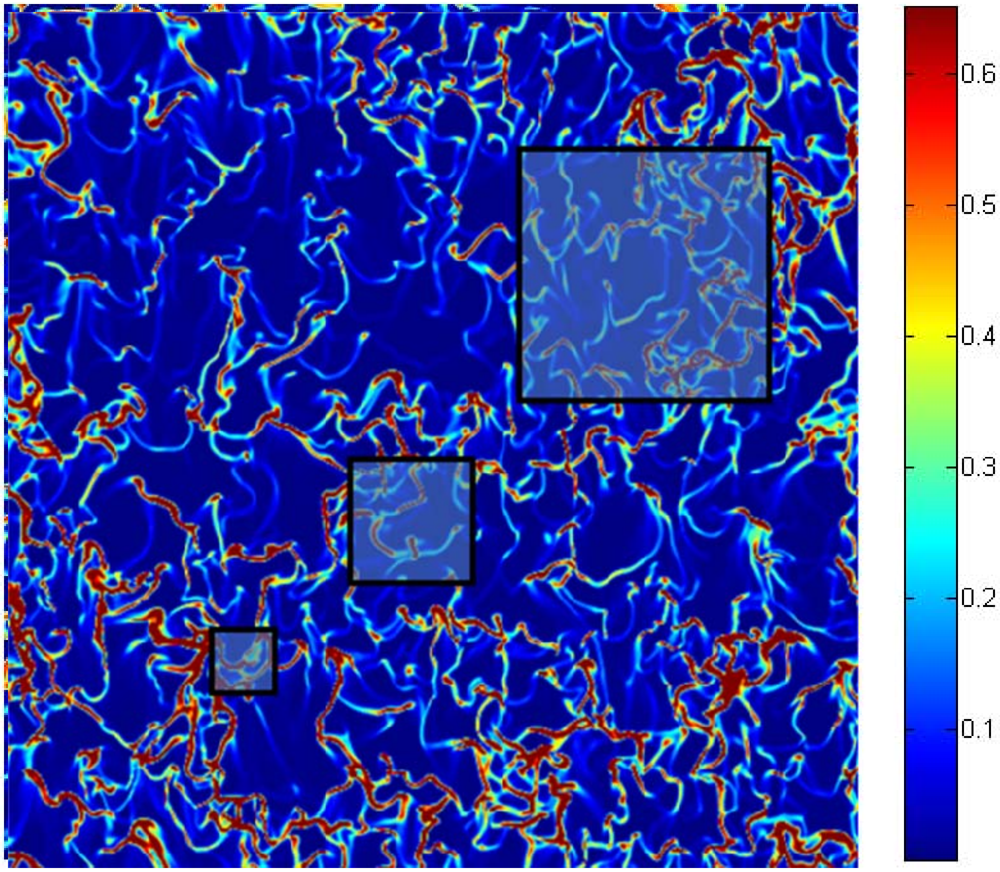
Approach: Probe details of mesoscale structures and develop effective coarse-grained equations

Igci, et al., AIChE J., 54, 1431 (2008)

Filter "data" generated through highly resolved simulations of two-fluid models

Snapshot of particle volume fraction fields obtained in highly resolved simulations of gas-particle flows. Squares illustrate regions (i.e. filters) of over which averaging over the cells is performed.

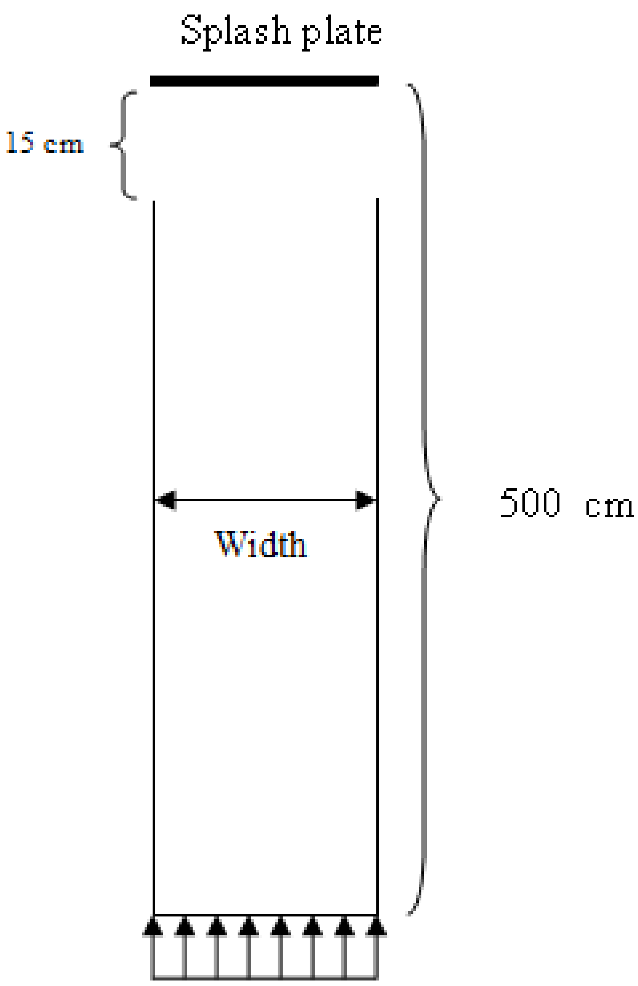
The filtered drag coefficient, particle phase pressure and viscosity are now functions of particle volume fraction and filter size.



Igci, et al., AIChE J., 54, 1431 (2008)

Wall correction to the filtered closures

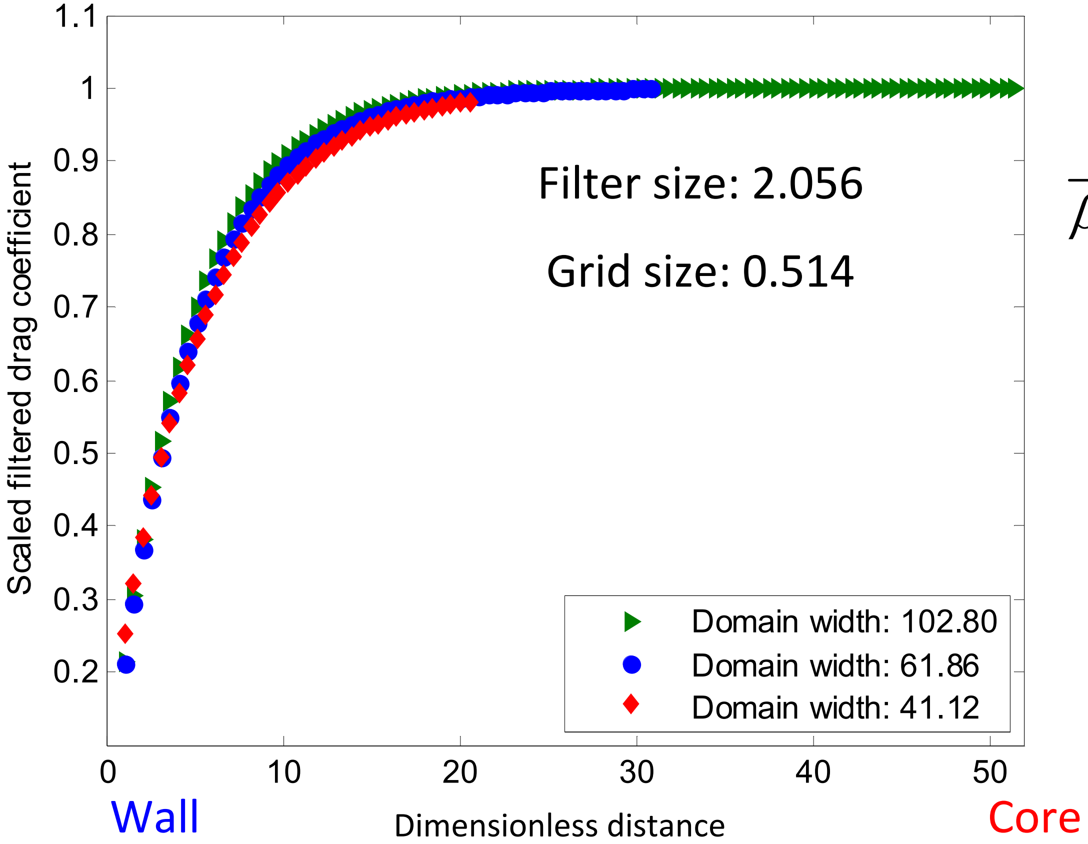
75 μm particles in air



- 2-D Kinetic theory based simulations
- Height: 500 cm
- Width: 20 cm, 30 cm, 50 cm
- The inlet gas superficial velocity: 93 cm/s.
- The inlet particle phase superficial velocity is 2.38 cm/s.
- The inlet particle phase volume fraction is 0.07.
- Partial-slip BC for particle phase and free-slip BC for gas phase

Grid size: 0.25 cm (0.514 dimensionless units)

The filtered drag coefficient is noticeably different in the core and the wall regions



$$\overline{\beta_{filtered,\ \mathrm{scaled}}} = \frac{\overline{\beta_{filtered,\ \mathrm{with\ wall\ correction}}}(\phi_s, \mathrm{r})}{\overline{\beta_{filtered}}^{*}(\phi_s)}$$

$$\overline{\beta_{filtered}}^{*}(\phi_s) = \overline{\beta_{filtered,\,periodic}}(\phi_s, Fr_{\Delta_{\mathrm{filter\ size}}})$$

Dimensionless filter size:

$$\frac{g\Delta_{\mathrm{filter\ size}}}{V_t^2} = \frac{1}{Fr_{\Delta_{\mathrm{filter\ size}}}}$$

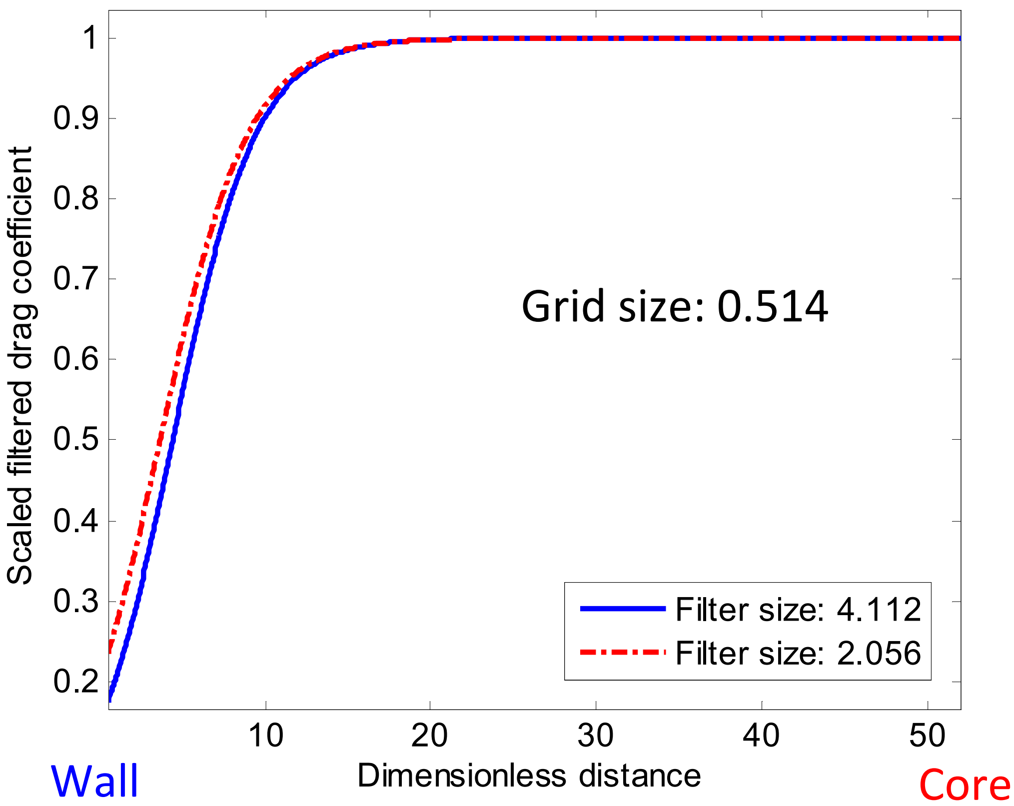
Dimensionless distance:

$$\frac{g\Delta_{\mathrm{distance}}}{V_t^2} = \frac{1}{Fr_{\Delta_{\mathrm{distance}}}}$$

The wall correction for the filtered drag coefficient is independent of channel width.

The same conclusion applies for filtered particle phase pressure and viscosity.

The filtered drag coefficient is noticeably different in the core and the wall regions



$$\overline{\beta_{filtered,\ \text{scaled}}} = \frac{\overline{\beta_{filtered,\ \text{with wall correction}}}(\phi_s, \text{r})}{\overline{\beta_{filtered}}^{*}(\phi_s)}$$

$$\overline{\beta_{filtered}}^{*}(\phi_s) = \overline{\beta_{filtered,\, periodic}}(\phi_s, Fr_{\Delta_{\text{filter size}}})$$

<u>Dimensionless filter size:</u>

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<u>Dimensionless distance:</u>

$$\frac{g\Delta_{\text{distance}}}{V_t^2} = \frac{1}{Fr_{\Delta_{\text{distance}}}}$$

The wall correction for the filtered drag coefficient is nearly independent of filter size.

The same conclusion applies for filtered particle phase pressure and viscosity.

Verification of the filtered model

Original two-fluid model → Filtered two-fluid model

1-D Linear Stability Analysis of filtered two-fluid model equations

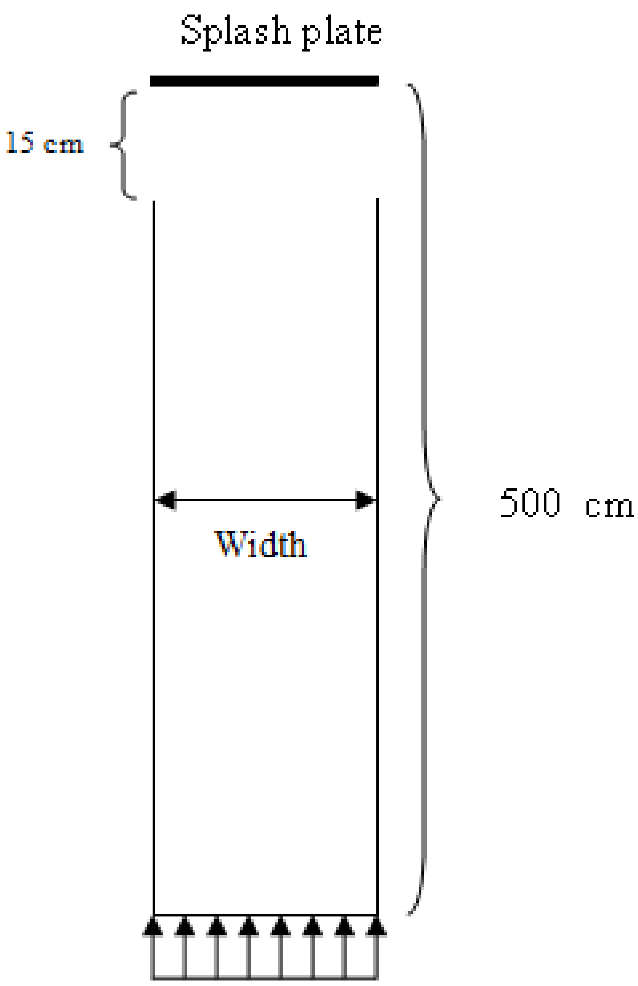
Solve a test problem using the original two-fluid model equations

Solve the same test problem using the filtered two-fluid model equations

Compare macroscopic features

Verification of the filtered model

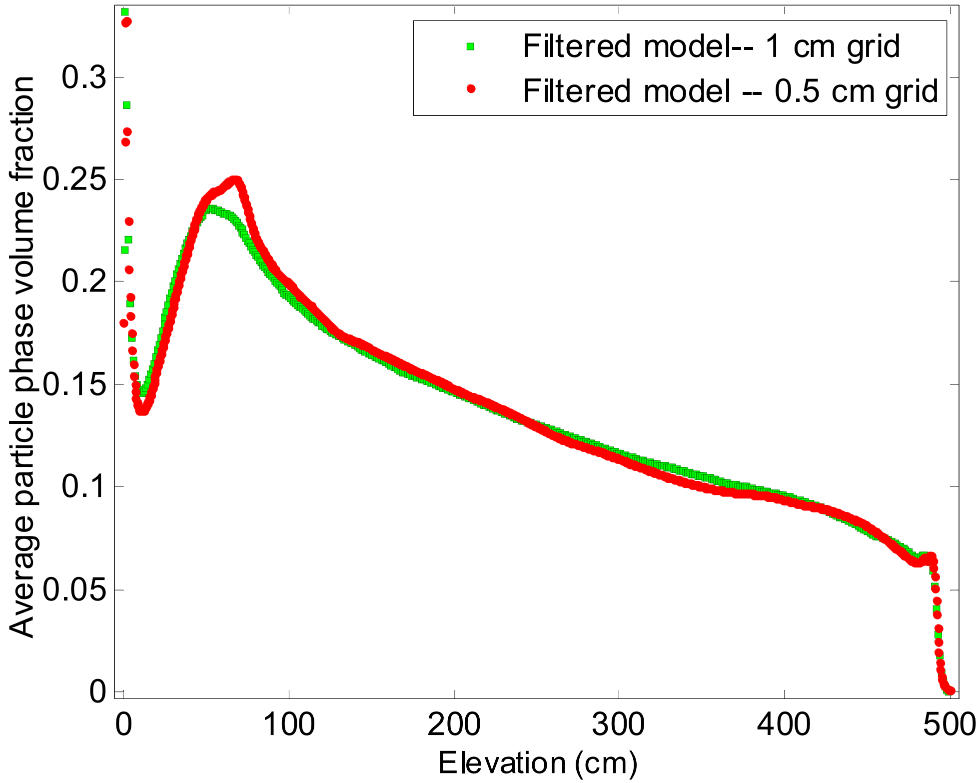
75 μm particles in air

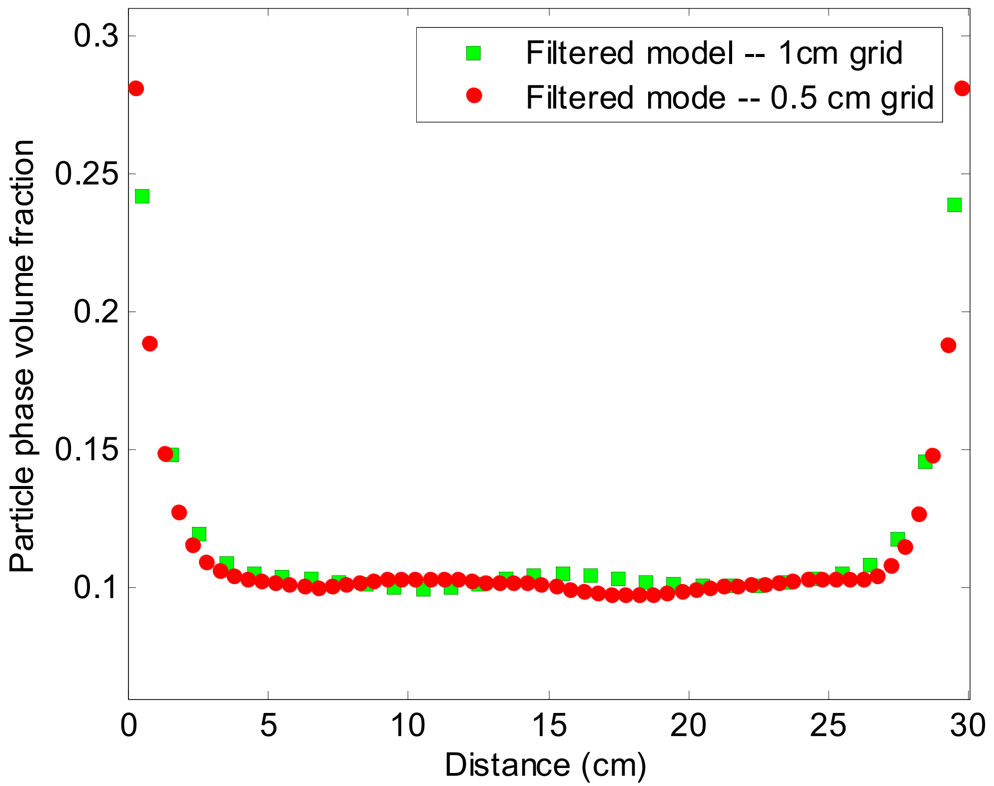


- **Compare predictions of kinetic theory and filtered models**
- Height: 500 cm
- Width: 30 cm
- The inlet gas superficial velocity: 93 cm/s.
- The inlet particle phase superficial velocity is 2.38 cm/s.
- The inlet particle phase volume fraction is 0.07.
- Free-slip boundary conditions

- Kinetic theory model: Grid size: 0.25 cm (0.514 dimensionless units)
- *Filtered model with closures corresponding to a filter size of 2 cm*

Solution of discretized form of the filtered two-fluid model

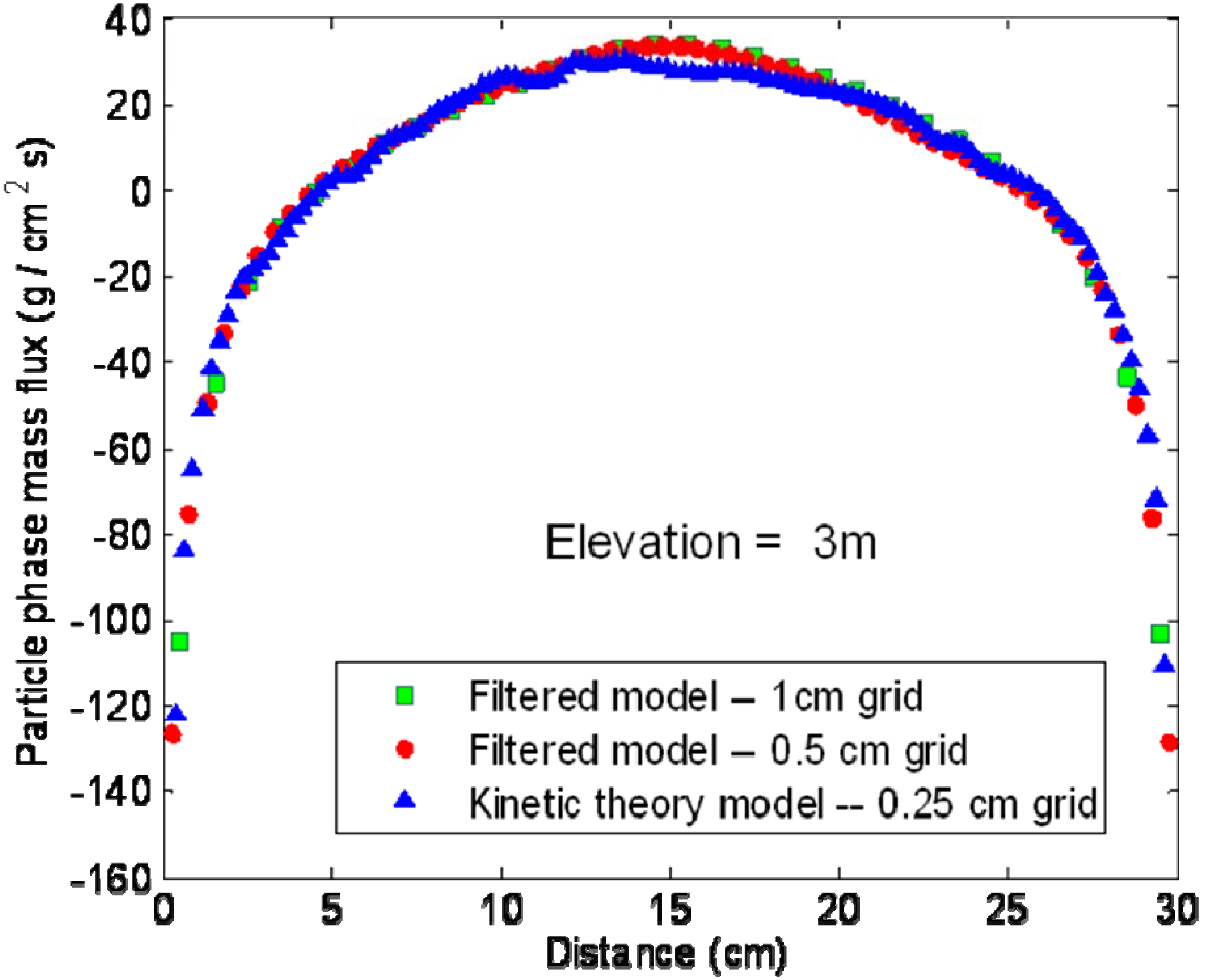




Filtered model with closures corresponding to a filter size of 2 cm

Nearly grid-size independent time-averaged profiles when grid size is less than or equal to one-half of the filter size.

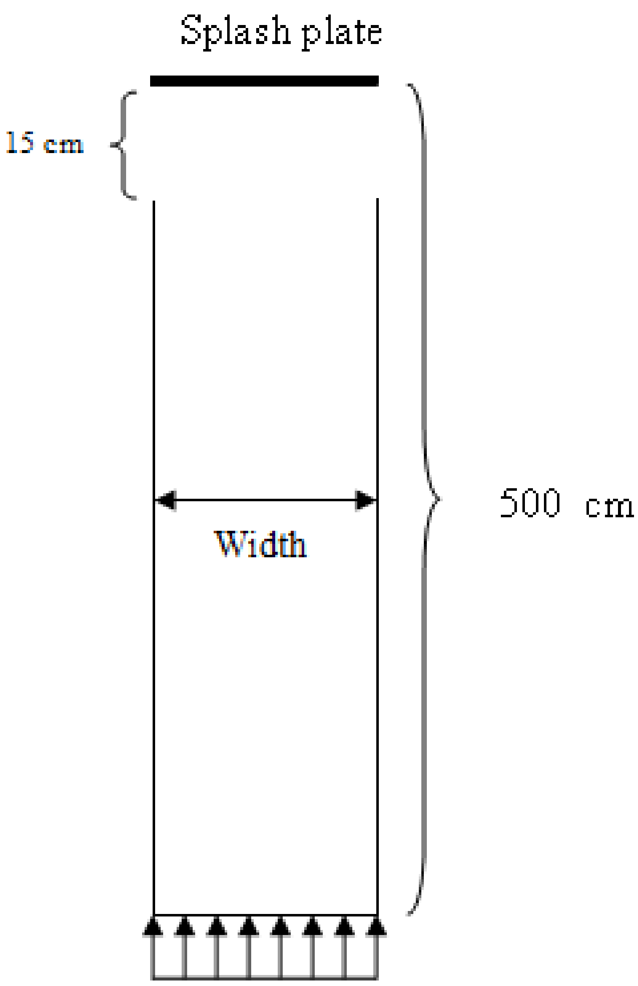
Solution of discretized form of the filtered two-fluid model



- Kinetic theory model: Grid size: 0.25 cm (0.514 dimensionless units)
- *Filtered model with closures corresponding to a filter size of 2 cm*

Verification of the filtered models

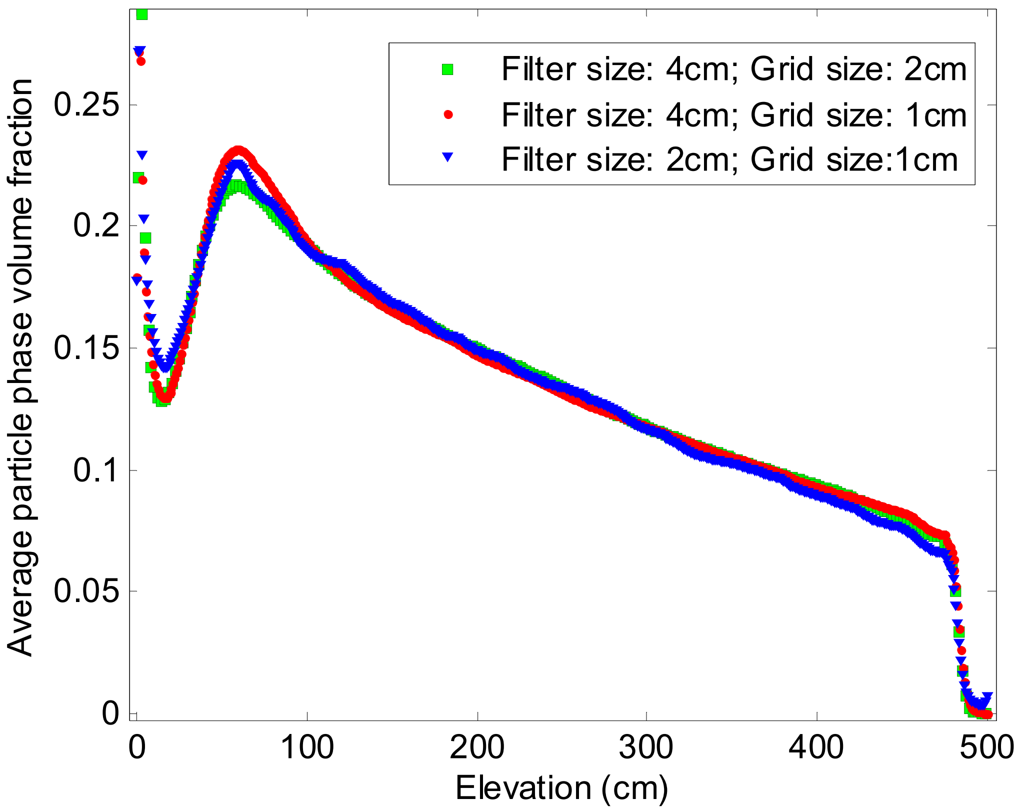
75 µm particles in air

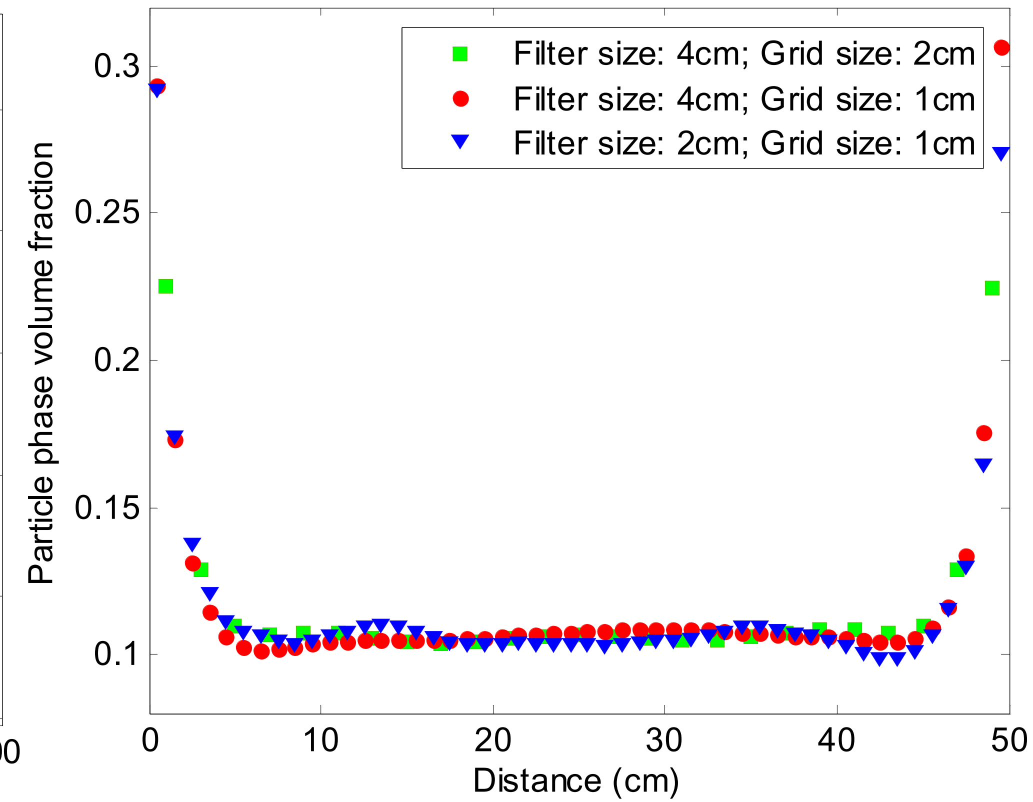


- **Compare predictions of filtered models with different filter sizes**
- Height: 500 cm
- Width: 50 cm
- The inlet gas superficial velocity: 93 cm/s.
- The inlet particle phase superficial velocity is 2.38 cm/s.
- The inlet particle phase volume fraction is 0.07.
- Free-slip boundary conditions

- Kinetic theory model: Grid size: 0.25 cm (0.514 dimensionless units)
- *Filtered model with closures corresponding to a filter sizes of 2 and 4 cm*

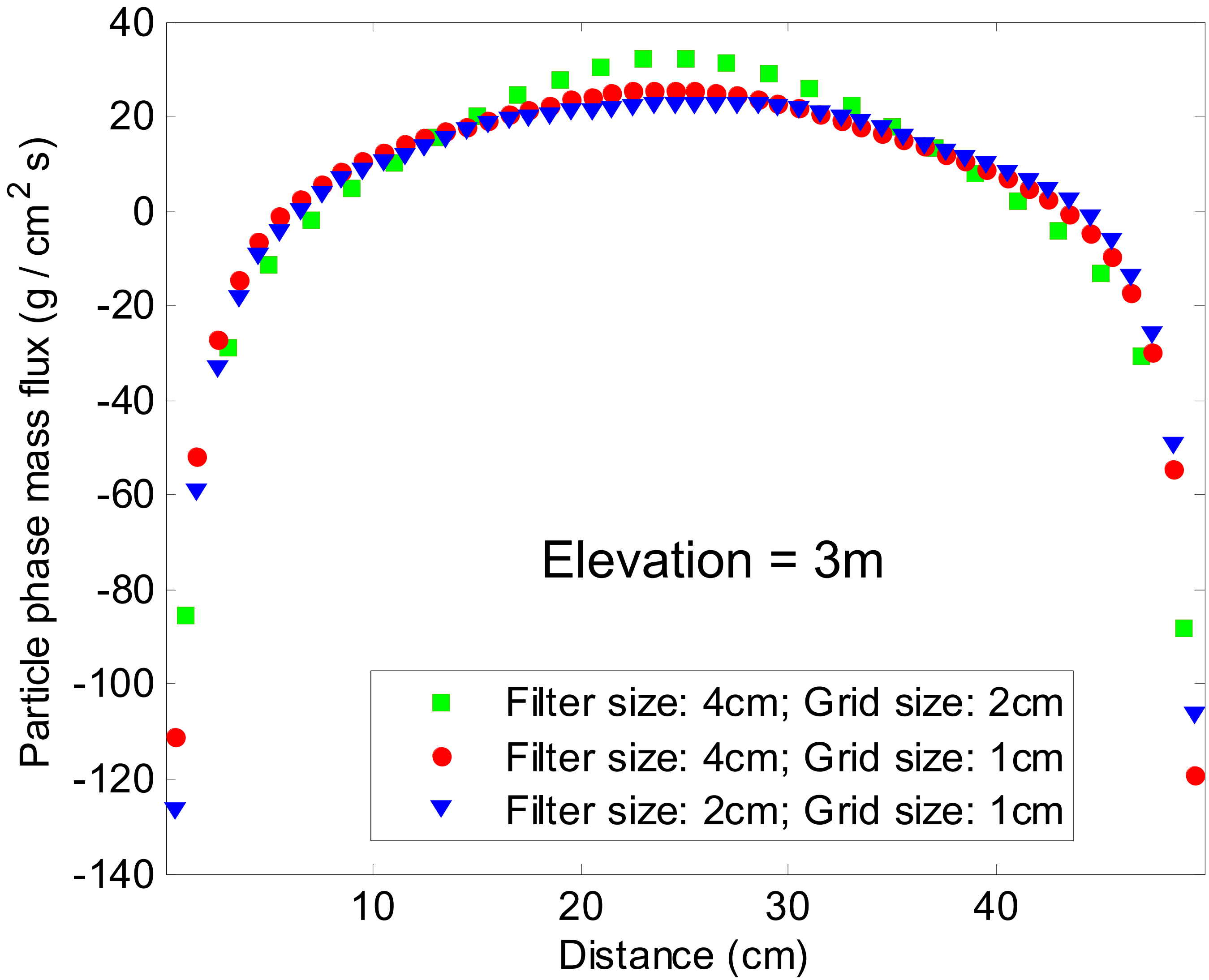
Solution of discretized form of the filtered two-fluid models





Filtered model with closures corresponding to filter sizes of 2 and 4 cm yield nearly the same time-averaged results as long as grid size is less than equal to 0.5 (filter size)

Solution of discretized form of the filtered two-fluid models



Filtered model with closures corresponding to filter sizes of 2 and 4 cm

Computational times

- Assumption: Irrespective of the process device size, accurate integration of the kinetic theory based model will require grids as small as 0.25 cm (or smaller) for 75 μm particles.

- 2D simulations in the 30 cm x 500 cm channel:
  - 2 cm filtered model with 1 cm grid size ~ 40 times faster than the kinetic theory model
- Had it been done in 3D, the ratio would be ~ 100

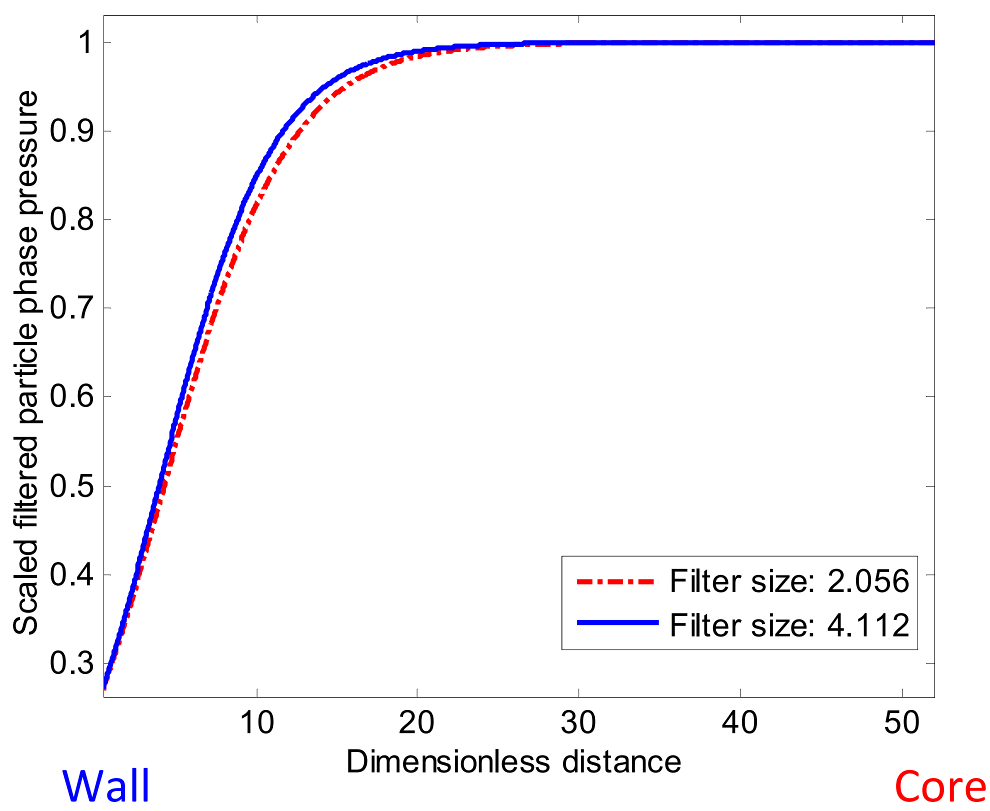
- With a 2 cm filter size, the filter volume (3D) ~ 8 cm^3 ; the grid volume (3D) ~ 1 cm^3
- Large scale devices: grid volume (3D) ~ 100 - 1000 cm^3
  - The filtered model is expected to be ~ 10^5 – 10^6 times faster than the original model!
- Thus, the filtered model converts a virtually impossible problem to a manageable problem!

Summary

- Performed highly resolved simulations of a kinetic theory based two-fluid model for gas-particle flow in various test domains
- Filtered the results to learn about constitutive relations for the filtered two-fluid model
- Verified the fidelity of the filtered model
- Validation remains to be completed – in progress.
- Filtered species and energy balance equations (and rate of chemical reactions) remain to be developed: future research project.

Extra slides

The filtered particle phase pressure is noticeably different in the core and the wall regions.



$$\overline{P_{s,\,filtered,\text{ scaled}}} = \frac{\overline{P_{s,\,filtered,\text{ with wall correction}}}(\phi_s, \text{r})}{\overline{P_s}^*(\phi_s)}$$

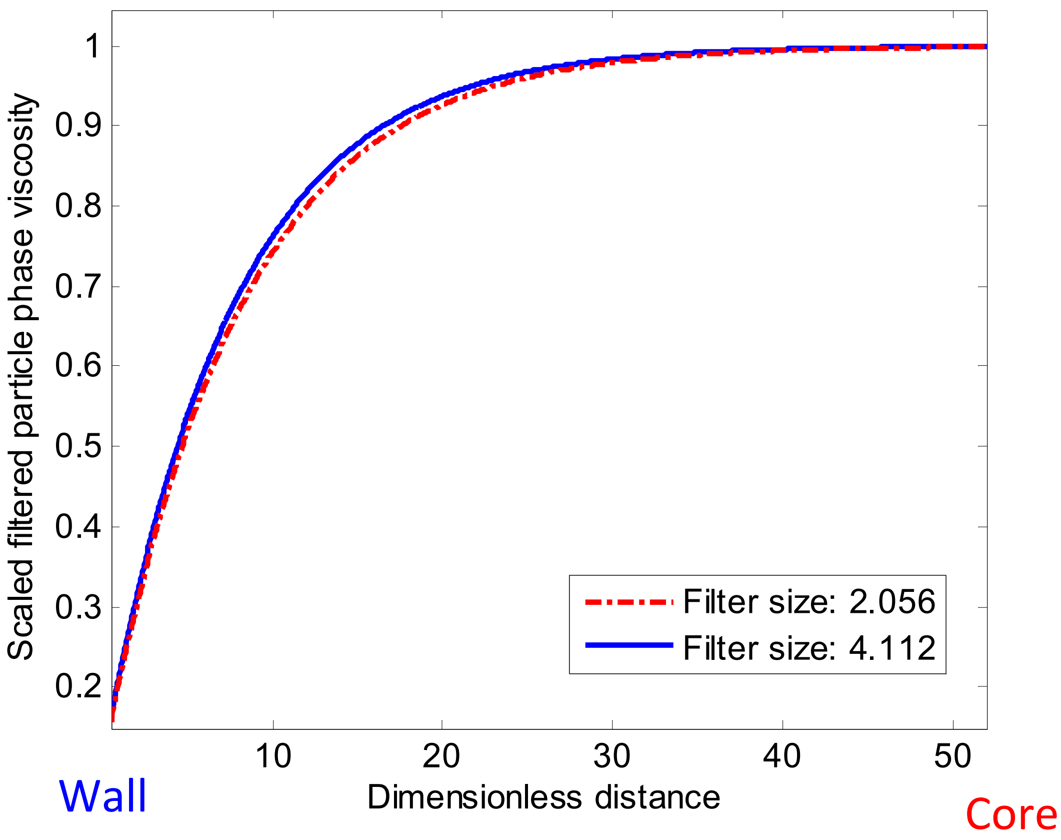
$$\overline{P_s}^*(\phi_s) = \overline{P_{s,\,filtered,\,periodic}}(\phi_s, Fr_{\Delta_{\text{Filter size}}})$$

$$\frac{g\Delta_{\text{filter size}}}{V_t^2} = \frac{1}{Fr_{\Delta_{\text{filter size}}}}$$

$$\frac{g\Delta_{\text{distance}}}{V_t^2} = \frac{1}{Fr_{\Delta_{\text{distance}}}}$$

The wall correction for the filtered particle phase pressure is nearly *independent of filter size*.

The filtered particle phase viscosity is noticeably different in the core and the wall regions.



$$\overline{\mu_{s,\,filtered,\ \text{scaled}}} = \frac{\overline{\mu_{s,\,filtered,\ \text{with wall correction}}}(\phi_s, \text{r})}{\overline{\mu_s}^*(\phi_s)}$$

$$\overline{\mu_s}^*(\phi_s) = 1.15 \times \overline{\mu_{s,\,filtered,\,periodic}}(\phi_s, Fr_{\Delta_{\text{Filter size}}})$$

$$\frac{g\Delta_{\text{filter size}}}{V_t^2} = \frac{1}{Fr_{\Delta_{\text{filter size}}}}$$

$$\frac{g\Delta_{\text{distance}}}{V_t^2} = \frac{1}{Fr_{\Delta_{\text{distance}}}}$$

The wall correction for the filtered particle phase viscosity is nearly *independent of filter size*.

Two-fluid model equations

Solids $$\frac{\partial(\rho_s\phi_s)}{\partial t}+\nabla\cdot(\rho_s\phi_s\boldsymbol{u}_s)=0$$

Fluid $$\frac{\partial(\rho_f\phi_f)}{\partial t}+\nabla\cdot(\rho_f\phi_f\boldsymbol{u}_f)=0$$

$$\phi_s+\phi_f=1$$

Solids $$\frac{\partial}{\partial t}(\rho_s\phi_s\boldsymbol{u}_s)+\nabla\cdot(\rho_s\phi_s\boldsymbol{u}_s\boldsymbol{u}_s)=-\nabla\cdot\boldsymbol{\sigma}_s \quad -\phi_s\nabla\cdot\boldsymbol{\sigma}_f \quad +\boldsymbol{f} \quad +\rho_s\phi_s\boldsymbol{g}$$

inertia | solid phase stress | effective buoyancy | interphase interaction | gravity

Fluid $$\frac{\partial}{\partial t}(\rho_f\phi_f\boldsymbol{u}_f)+\nabla\cdot(\rho_f\phi_f\boldsymbol{u}_f\boldsymbol{u}_f)= \quad -\phi_f\nabla\cdot\boldsymbol{\sigma}_f \quad -\boldsymbol{f} \quad +\rho_f\phi_f\boldsymbol{g}$$

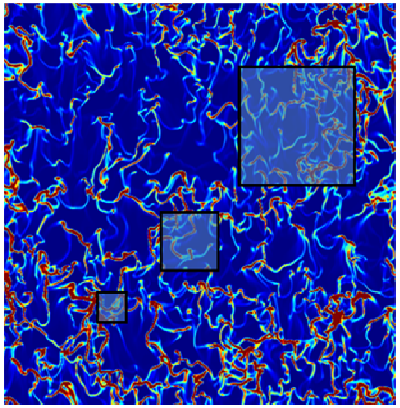
Filtered continuity equations

$$\frac{\partial\left(\rho_s\phi_s\right)}{\partial t}+\nabla\cdot\left(\rho_s\phi_s\boldsymbol{u}_s\right)=0 \qquad \frac{\partial\left(\rho_f\phi_f\right)}{\partial t}+\nabla\cdot\left(\rho_f\phi_f\boldsymbol{u}_f\right)=0$$

$$\phi_s=\overline{\phi_s}+\phi_s' \qquad \phi_f=\overline{\phi_f}+\phi_f' \qquad \overline{\phi_s'}=0$$

$$\boldsymbol{u}_s=\overline{\boldsymbol{u}_s}+\boldsymbol{u}_s' \qquad \overline{\phi_s}\,\overline{\boldsymbol{u}_s}=\overline{\phi_s\boldsymbol{u}_s} \qquad \overline{\phi_s\boldsymbol{u}_s'}=0$$

$$\boldsymbol{u}_f=\overline{\boldsymbol{u}_f}+\boldsymbol{u}_f' \qquad \overline{\phi_f}\,\overline{\boldsymbol{u}_f}=\overline{\phi_f\boldsymbol{u}_f} \qquad \overline{\phi_f\boldsymbol{u}_f'}=0$$



$$\frac{\partial\left(\rho_s\overline{\phi_s}\right)}{\partial t}+\nabla\cdot\left(\rho_s\overline{\phi_s}\,\overline{\boldsymbol{u}_s}\right)=0$$

$$\frac{\partial\left(\rho_f\overline{\phi_f}\right)}{\partial t}+\nabla\cdot\left(\rho_f\overline{\phi_f}\,\overline{\boldsymbol{u}_f}\right)=0$$

All filtered quantities are functions of space and time

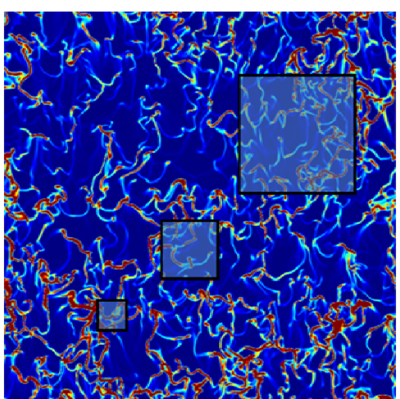
Filtered particle phase momentum balance

$$\frac{\partial}{\partial t}\left(\rho_s\phi_s\boldsymbol{u}_s\right)+\nabla\cdot\left(\rho_s\phi_s\boldsymbol{u}_s\boldsymbol{u}_s\right)=-\nabla\cdot\boldsymbol{\sigma}_s\quad-\phi_s\nabla p_f\quad+\boldsymbol{f}_{drag}\quad+\rho_s\phi_s\boldsymbol{g}$$

Upon filtering,

$$\frac{\partial}{\partial t}\left(\rho_s\overline{\phi_s}\,\overline{\boldsymbol{u}_s}\right)+\nabla\cdot\left(\rho_s\overline{\phi_s}\,\overline{\boldsymbol{u}_s}\,\overline{\boldsymbol{u}_s}\right)=-\nabla\cdot\left(\overline{\boldsymbol{\sigma}_s}+\underbrace{\rho_s\overline{\phi_s\boldsymbol{u}'_s\boldsymbol{u}'_s}}_{\text{stress due to sub-filter scale fluctuations}}\right)-\overline{\phi_s}\nabla\overline{p_f}$$

$$\underbrace{-\overline{\phi'_s\nabla p'_f}+\overline{\boldsymbol{f}}_{drag}}_{\text{effective sub-filter scale fluid-particle interaction force}}\quad+\rho_s\overline{\phi_s}\boldsymbol{g}$$



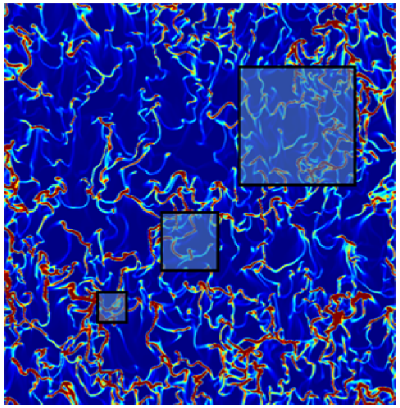
Filtered fluid phase momentum balance

$$\frac{\partial}{\partial t}\left(\rho_f \phi_f \boldsymbol{u}_f\right) + \nabla\cdot\left(\rho_f \phi_f \boldsymbol{u}_f \boldsymbol{u}_f\right) = -\phi_f \nabla p_f - \boldsymbol{f}_{drag} + \rho_f \phi_f \boldsymbol{g}$$

Upon filtering,

$$\frac{\partial}{\partial t}\left(\rho_f \overline{\phi_f}\,\overline{\boldsymbol{u}_f}\right) + \nabla\cdot\left(\rho_f \overline{\phi_f}\,\overline{\boldsymbol{u}_f}\,\overline{\boldsymbol{u}_f}\right) = -\nabla\cdot\left(\underbrace{\rho_f \overline{\phi_f \boldsymbol{u}'_f \boldsymbol{u}'_f}}_{\text{stress due to sub-filter scale fluctuations}}\right) - \overline{\phi_f}\,\nabla\overline{p_f}$$

$$\underbrace{-\overline{\phi'_f \nabla p'_f} - \overline{\boldsymbol{f}}_{drag}}_{\text{effective sub-filter scale fluid-particle interaction force}} + \rho_f \overline{\phi_f}\,\boldsymbol{g}$$



Sub-filter scale correlations

$$\underbrace{\rho_s \overline{\phi_s \boldsymbol{u}'_s \boldsymbol{u}'_s}}_{\text{stress due to sub-filter scale fluctuations}}$$

$$\underbrace{\rho_f \overline{\phi_f \boldsymbol{u}'_f \boldsymbol{u}'_f}}_{\text{stress due to sub-filter scale fluctuations}}$$

$$\underbrace{-\overline{\phi'_f \nabla p'_f} - \overline{\boldsymbol{f}}_{drag}}_{\text{effective sub-filter scale fluid-particle interaction force appearing in the fluid phase equation}} = -\left(\underbrace{-\overline{\phi'_s \nabla p'_f} + \overline{\boldsymbol{f}}_{drag}}_{\text{effective sub-filter scale fluid-particle interaction force appearing in the particle phase equation}} \right)$$

$$\boldsymbol{u}'_s \sim \boldsymbol{u}'_f ,$$

If $\quad \rho_s \phi_s >> \rho_f \phi_f ,\quad$ then

$$\rho_s \overline{\phi_s \boldsymbol{u}'_s \boldsymbol{u}'_s} \quad >> \quad \rho_f \overline{\phi_f \boldsymbol{u}'_f \boldsymbol{u}'_f}$$

So, only two terms to focus on

Sub-filter scale correlations

$$\rho_s \overline{\phi_s \boldsymbol{u}_s' \boldsymbol{u}_s'} + \underbrace{\overline{\boldsymbol{\sigma}_s}}_{\text{from kinetic theory}} = p_{s,eff} \mathbf{I} + 2\mu_{s,eff} \boldsymbol{S}$$

$$-\overline{\phi_s' \nabla p_f'} + \overline{\boldsymbol{f}}_{drag} = \beta_{eff} \left(\overline{\boldsymbol{u}_f} - \overline{\boldsymbol{u}_s} \right)$$

Scaled filter size

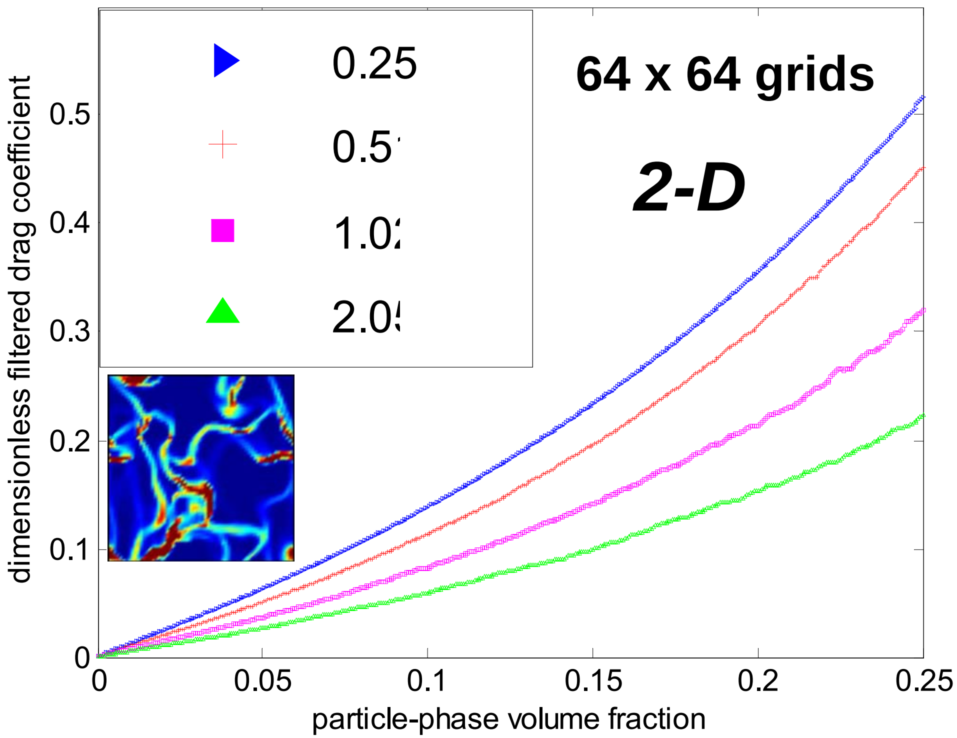
$$\frac{g\Delta}{V_t^2} = \frac{1}{Fr_\Delta}$$

All the effective quantities will depend on the choice of filter size, $\overline{\phi_s}$ and so on; such filter size dependence is present in LES of turbulent flows as well.

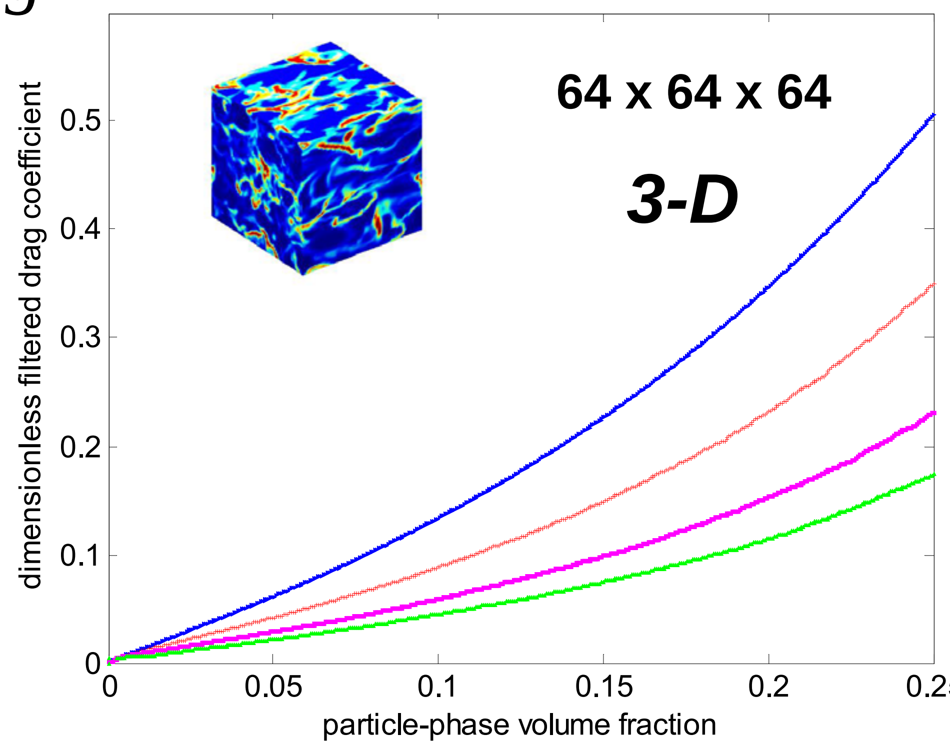
Filtered drag coefficient decreases as filter size increases for both 2-D and 3-D

$$\frac{\beta_{eff} V_t}{\rho_s g}$$

Domain size = 16 x 16



16 x 16 x 16



Example: 75 μm; 1500 kg/m^3; domain size = 8 cm

$$\frac{g\Delta}{V_t^{\,2}} = \frac{1}{Fr_\Delta}$$

$$\frac{1}{Fr_\Delta} = 2 \;\Rightarrow\; \Delta = 1cm$$

Dependence of the filtered drag coefficient on resolution (2-D)

Domain size

=132x132 (dim.less)

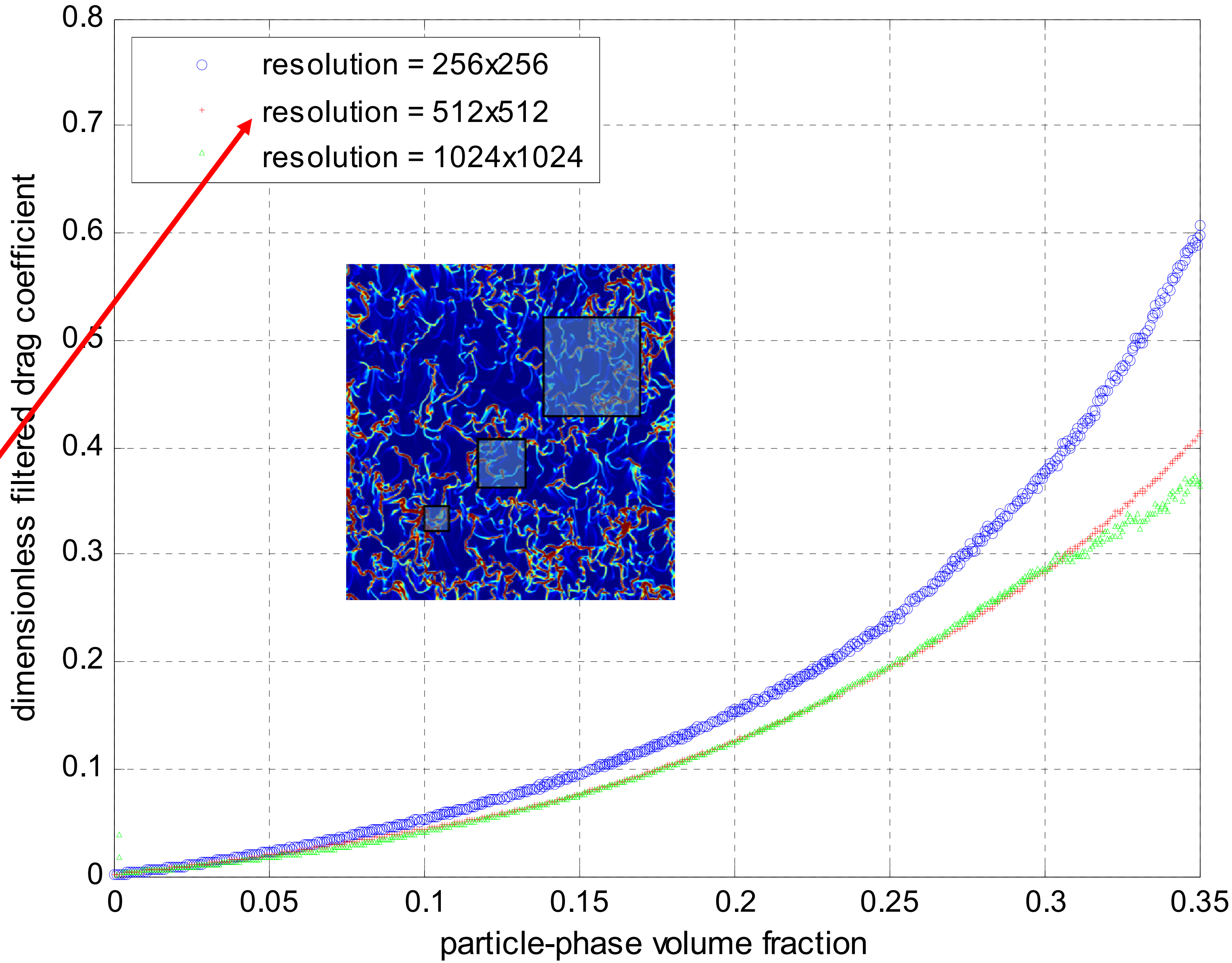
= 64 cm x 64 cm

Filter size

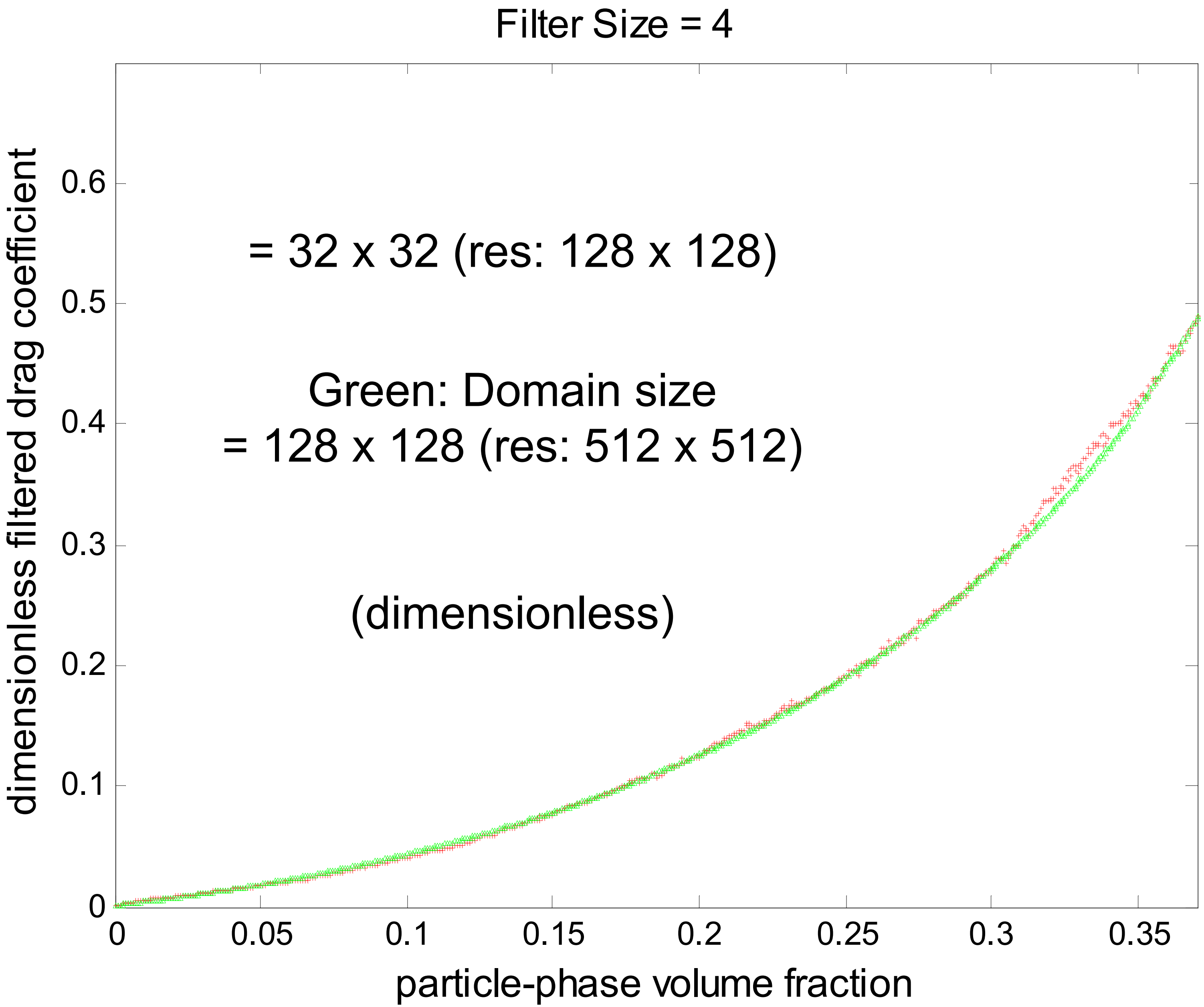
= 4 (dim.less)

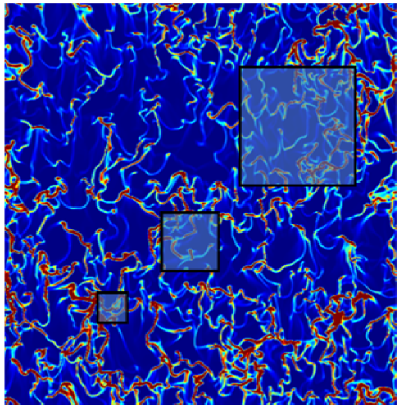
= 2 cm

Corresponds to 1/8 cm

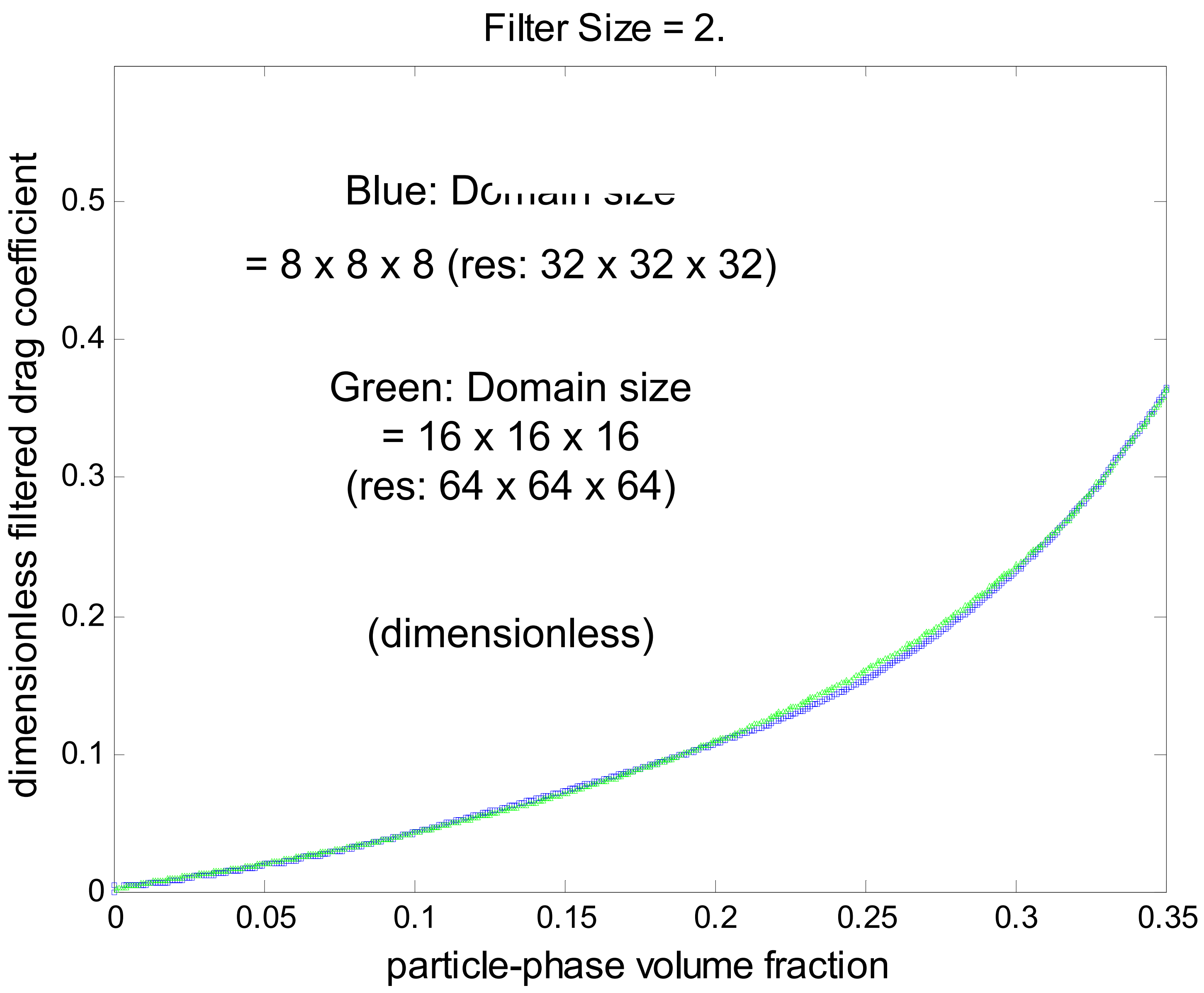


Filtered drag coefficient is independent of domain size (2-D)





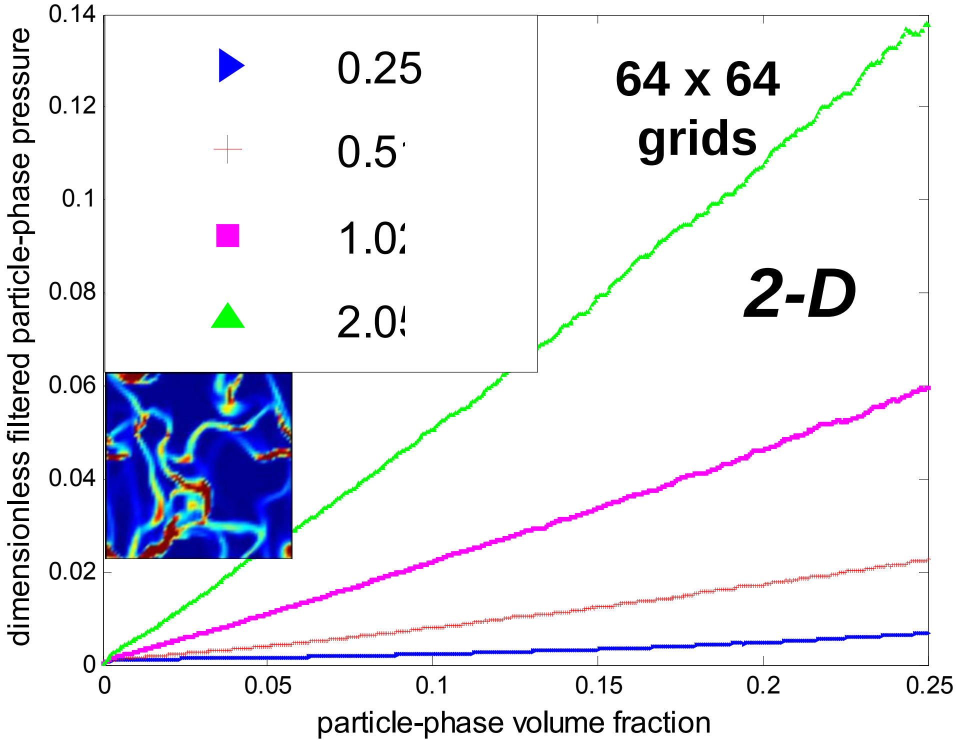
Filtered drag coefficient is independent of domain size (3-D)



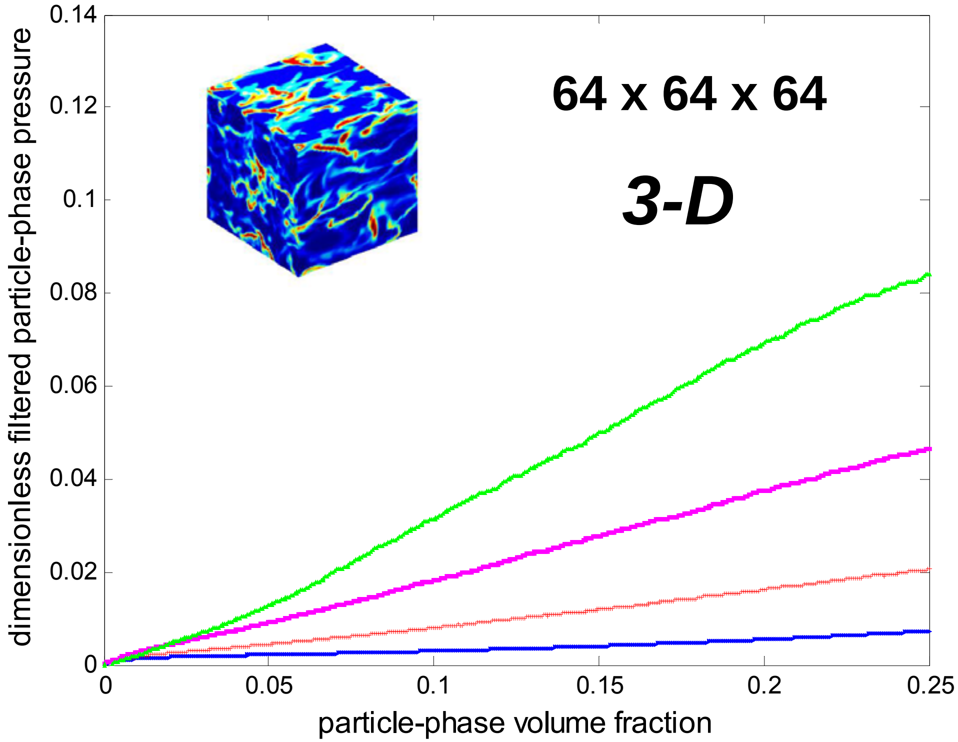
Filtered particle phase pressure increases as filter size increases for both 2-D and 3-D

$$\frac{p_{s,eff}}{\rho_s V_t^2}$$

Domain size: 16 x 16



16 x 16 x 16



Example: 75 μm; 1500 kg/m^3; domain size = 8 cm

$$\frac{g\Delta}{V_t^2} = \frac{1}{Fr_\Delta}$$

$$\frac{1}{Fr_\Delta} = 2 \Rightarrow \Delta = 1cm$$

Filtered particle phase pressure increases as filter size increases for both 2-D and 3-D

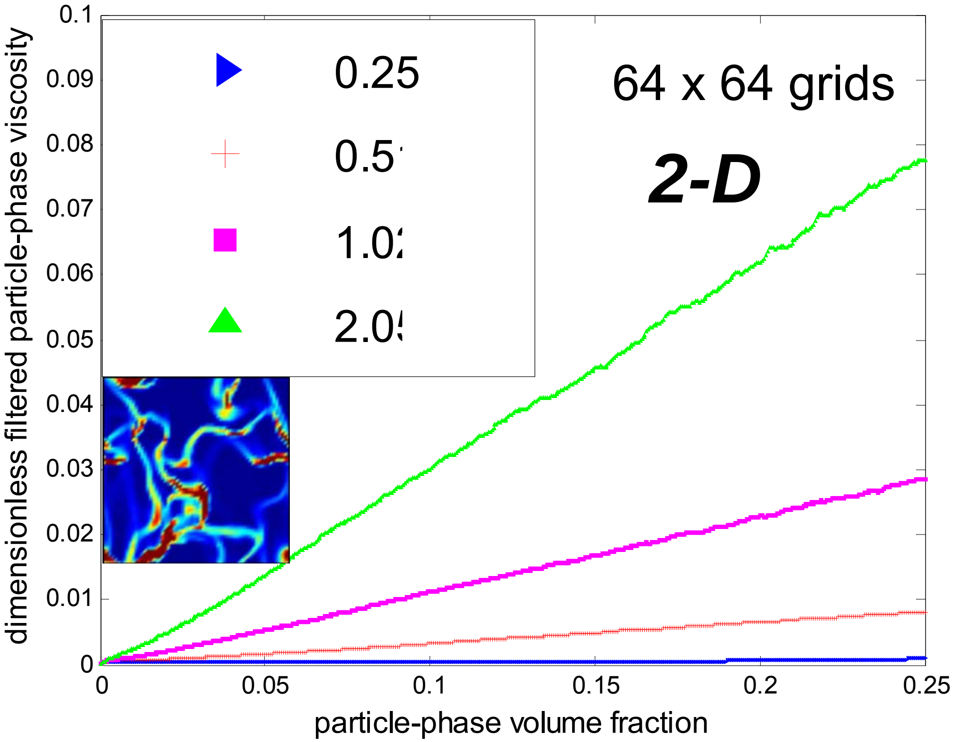
$$\rho_s \overline{\phi_s \mathbf{u}'_s \mathbf{u}'_s} + \underbrace{\overline{\boldsymbol{\sigma}_s}}_{\text{from kinetic theory}} = p_{s,eff}\mathbf{I} + 2\mu_{s,eff}\boldsymbol{S}$$

- The effective pressure in 3-D is smaller than that in 2-D (smaller by 40%)
- The effective pressure increases nearly linearly with filter size
- Effective pressure is by and large due to the mesoscale velocity fluctuations once the filter size exceeds 1 cm for FCC particles.
- This means that it may not be necessary to consider a filtered granular energy equation, if we use a large enough filter size

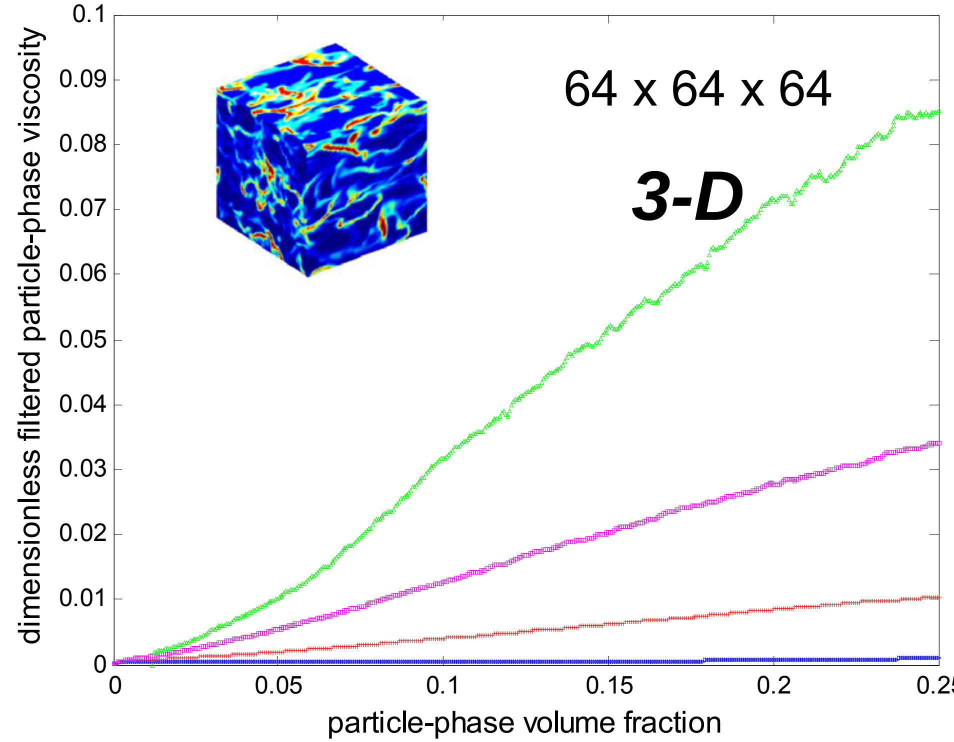
Filtered particle phase viscosity increases as filter size increases for both 2-D and 3-D

$$\frac{\mu_{s,eff}\, g}{\rho_s V_t^3}$$

Domain size = 16 x 16



16 x 16 x 16



Example: 75 μm; 1500 kg/m^3; domain size = 8 cm

$$\frac{g\Delta}{V_t^2} = \frac{1}{Fr_\Delta}$$

$$\frac{1}{Fr_\Delta} = 2 \Rightarrow \Delta = 1cm$$

Filtered particle phase viscosity increases as filter size increases for both 2-D and 3-D

$$\rho_s \overline{\phi_s \mathbf{u}_s' \mathbf{u}_s'} + \underbrace{\overline{\boldsymbol{\sigma}_s}}_{\text{from kinetic theory}} = p_{s,eff}\mathbf{I} + 2\mu_{s,eff}\boldsymbol{S}$$

- The effective viscosity in 3-D and 2-D are comparable
- The effective viscosity ~ (filter size)$^{1.5\text{–}1.6}$
- Effective viscosity is by and large due to the mesoscale velocity fluctuations once the filter size exceeds 1 cm for FCC particles.
- This means that it may not be necessary to consider a filtered granular energy equation