Closures for Coarse-Grid Simulation of Fluidized Gas-Particle Flows

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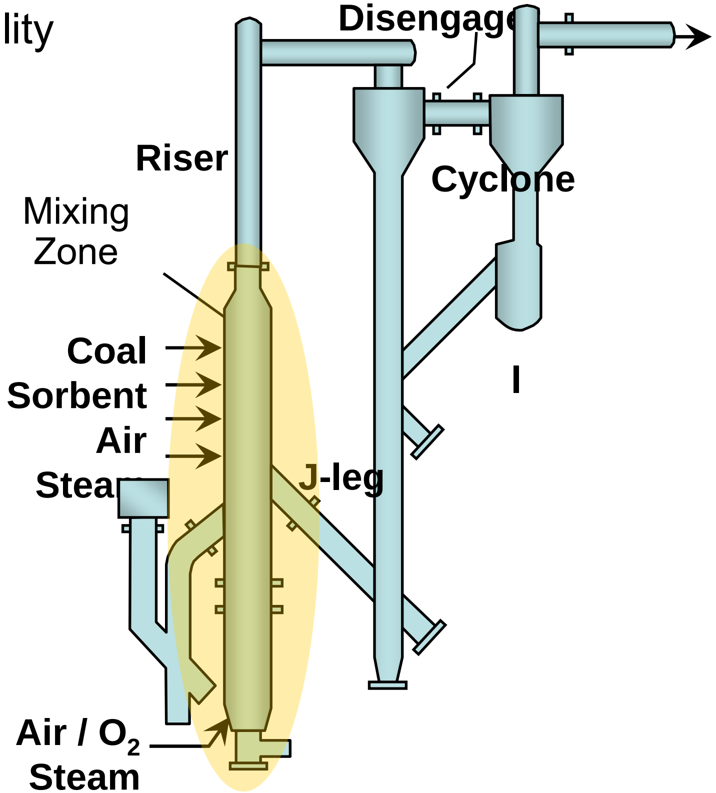
Outline

- *The Problem and Project Objectives*
- *Principal results thus far*
- *Summary*

Advanced Coal Gasification Technology

Power Systems Development Facility
Wilsonville, Alabama



Demonstration Scale

- Air and oxygen blown operation
- Coal Feed Rate ~5000 lbs/hr
- Bituminous and Sub-bituminous
- Pressure (250 psi)

Commercial Scale

- Air and oxygen blown operation
- Coal Feed Rate ~250,000 lbs/hr
- Bituminous and Sub-bituminous
- Pressure (465 psi)

Chris Guenther, NETL

NETL

DOE – NETL; KBR; Southern Co; Siemens – Westinghouse
Electric Power Res. Inst.; Peabody Holding Co.; Southern Res. Inst.

Characteristics of flows in turbulent fluidized beds & fast fluidized beds

- Up to ~ 30 vol% particles, with particle size distribution
- Persistent density and velocity fluctuations
  - Wide range of spatial scales
  - Wide range of frequencies
  - Macroscopically inhomogeneous structures, such as radial segregation of particles in risers (core-annular flow)
- Particle-particle collisions
- Too many particles to track individually
- Model in terms of local-average variables in locally-averaged equations of motion (“two-fluid models”)

Two-fluid model equations: uniformly sized particles

Continuity equations

Solids

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

Fluid

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

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

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

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

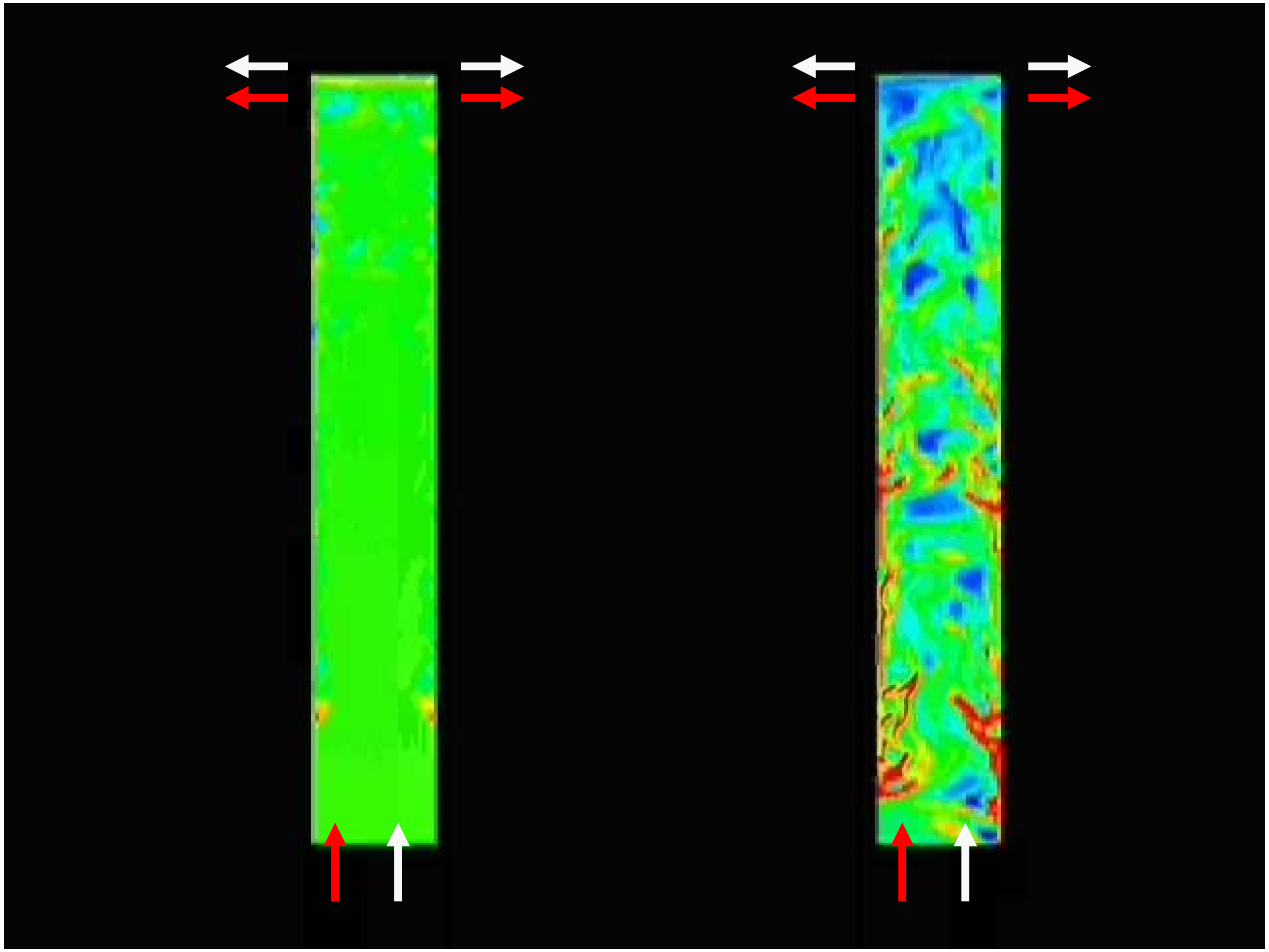
30 m tall

76 cm channel width

75μm particles

2 cm grid

2-D simulations



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

What I get

What I expect based on experimental data

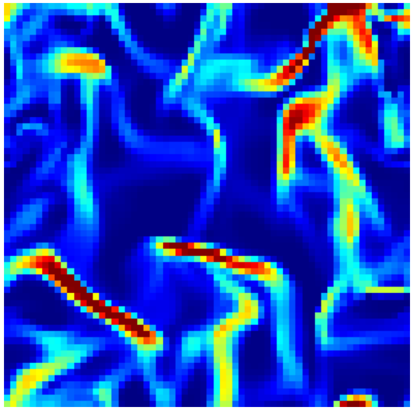
75 µm particles in air

with MFIX

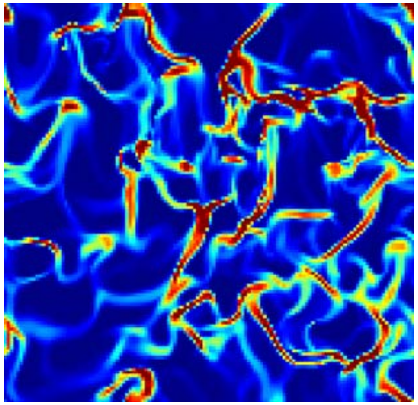
(Multiphase Flow with Interphase eXchanges)

Average particle volume fraction: 0.05

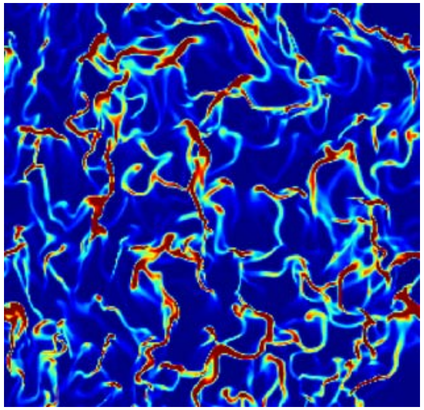
2D Domain size : 64 cm x 64 cm



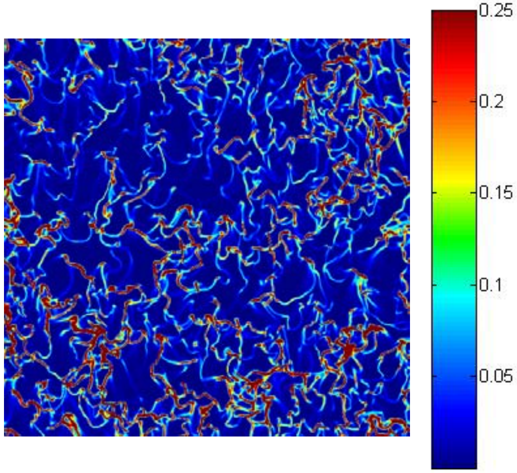
64 x 64



128 x 128



256 x 256



512 x 512

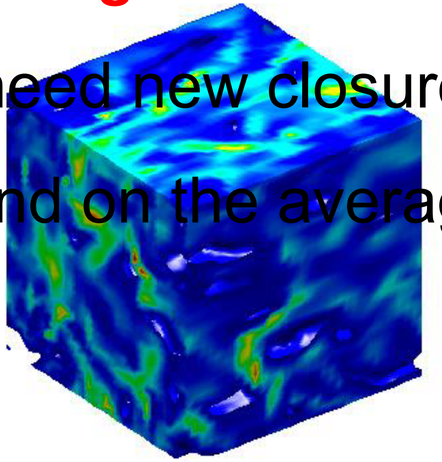
3D Domain size : 8 cm x 8 cm x 8 cm

For coarse grid simulations:

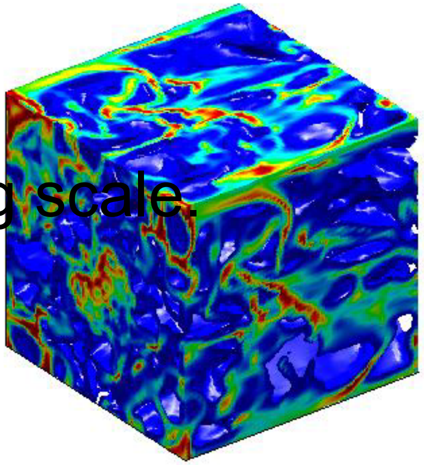
We need new closures

that will depend on the averaging scale.

16x16x16

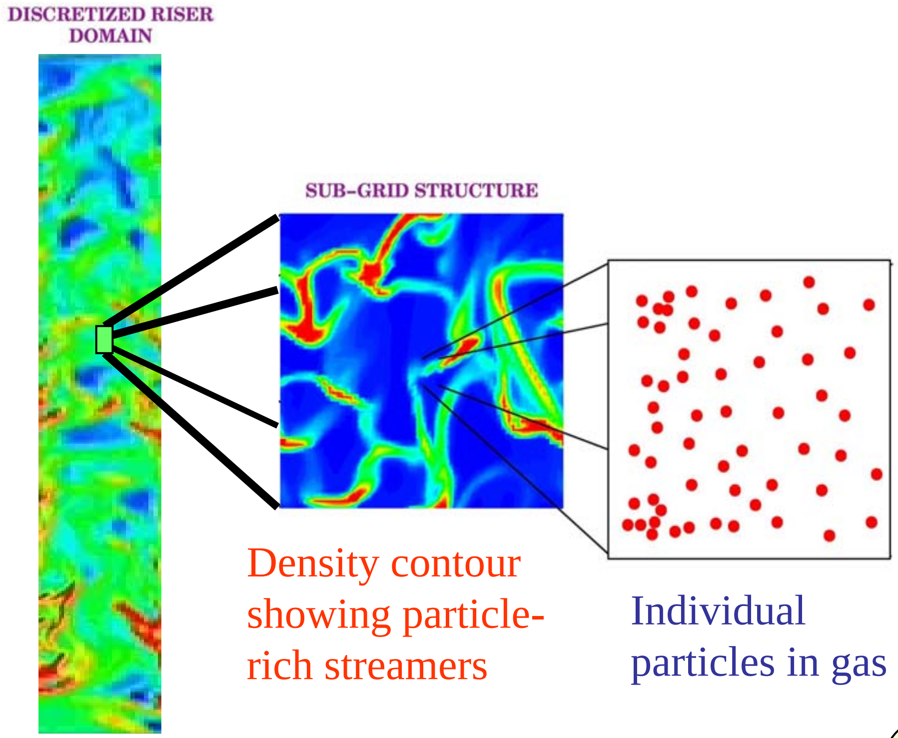


32x32x32



64x64x64

Project Objective: Coarse-grained equations



Density contour showing particle-rich streamers

Individual particles in gas

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

Single-phase turbulent Flows

- Eddies with a wide range of length and time scales
- Too expensive to resolve all the eddies through Direct Numerical Simulation of the Navier-Stokes Equations
- Approach: Simulate the large eddies and model the smaller eddies – Large Eddy Simulations
- Filtered Navier Stokes equations
- Unresolved eddies – effective transport properties: viscosity, diffusivities

Project Objectives

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 → Filtered two-fluid model

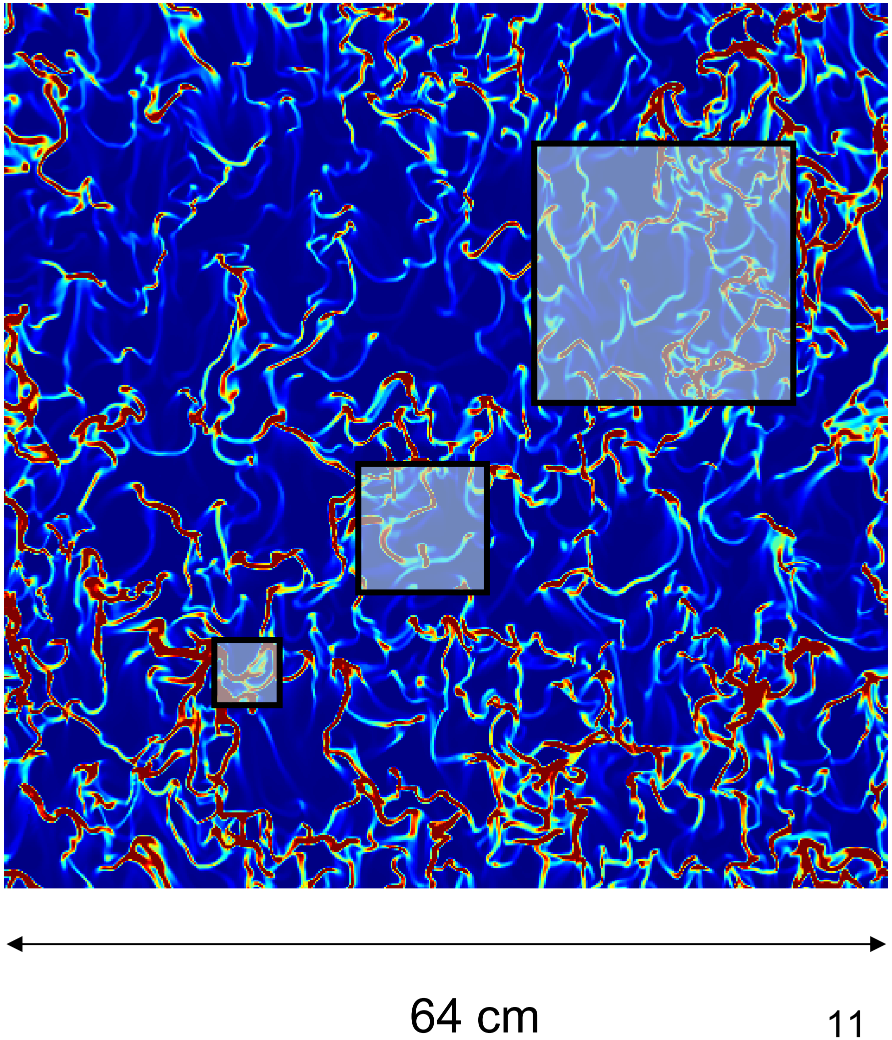
Modified constitutive relations

- Construct constitutive models that filter over meso-scale structures that occur over length scales of 100 – 1000 particle diameters
- Validate filtered models

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

- Snapshot of particle volume fraction field – kinetic theory based two-fluid model.
- 75 μm particles in air
- 512 x 512 cells
- The average particle volume fraction in the domain = 0.05
- Squares of different sizes illustrate **filters** of different sizes.

$$\Delta_{grid} << \Delta_{filter} << \Delta_{domain}$$

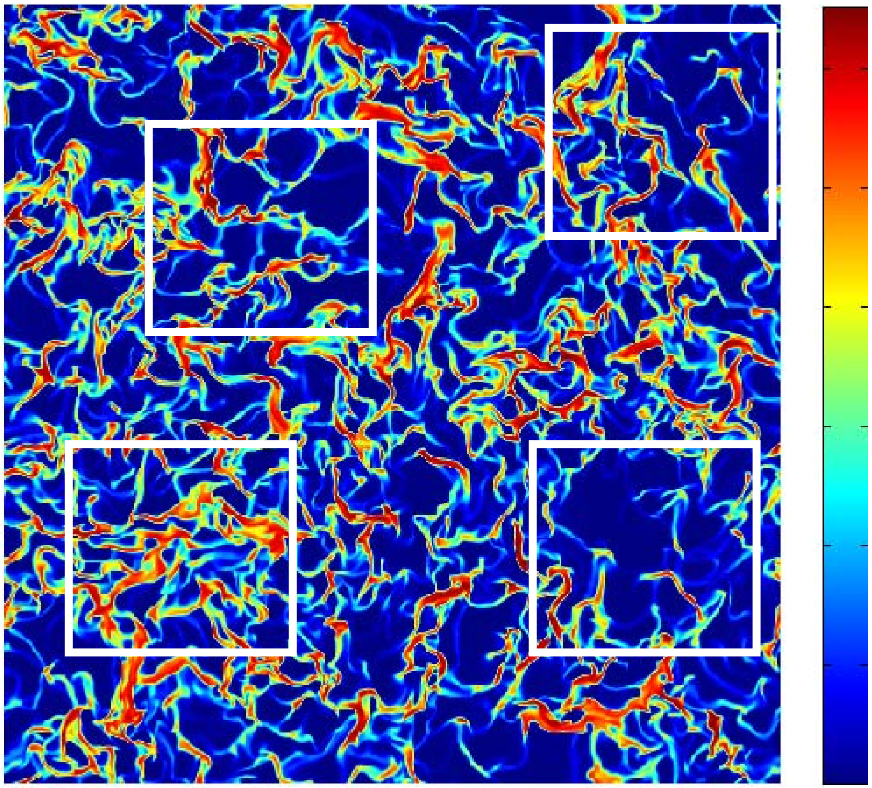


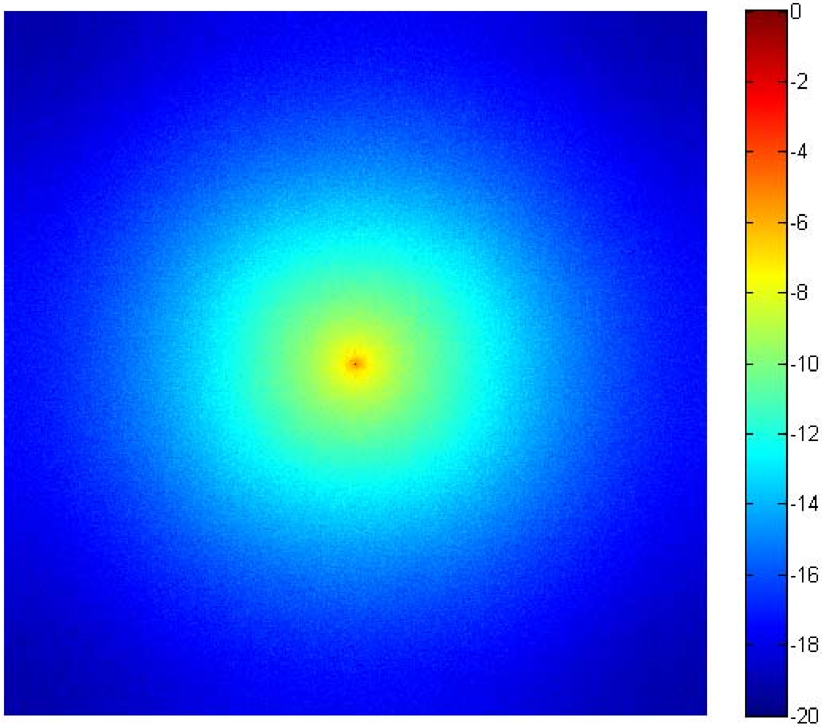
Completed tasks

- Performed highly resolved 2-D and 3-D simulations of a kinetic theory based microscopic two-fluid model for uniformly sized particles, and construct closures for filtered drag coefficient, filtered particle phase pressure and filtered gas & particle phase viscosities.

- Igci et al., AICHE J., **54**, 1431 (2008).

Kinetic Theory Based Model





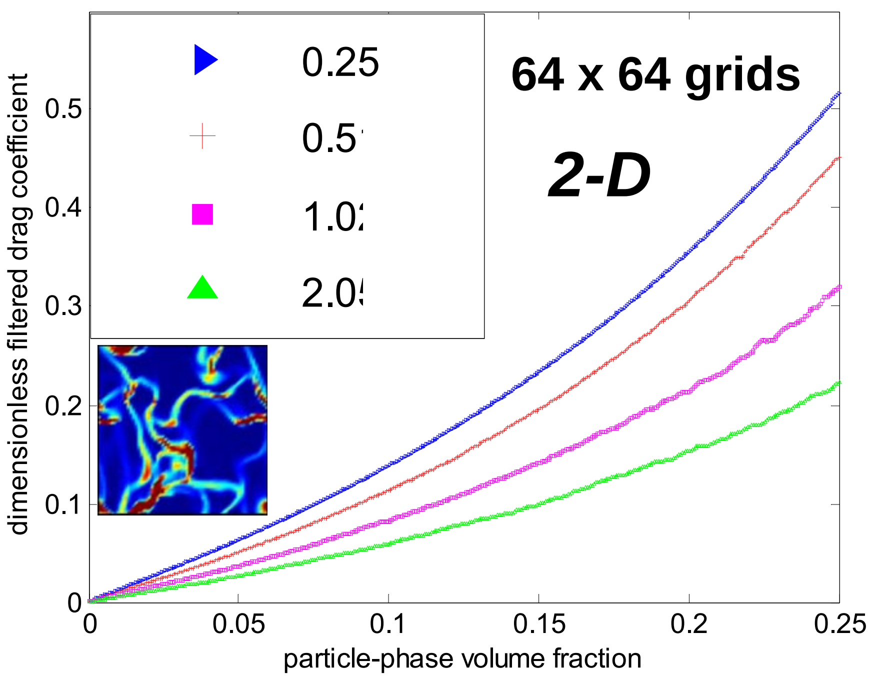
Power spectra

Meso-scale structures are statistically isotropic

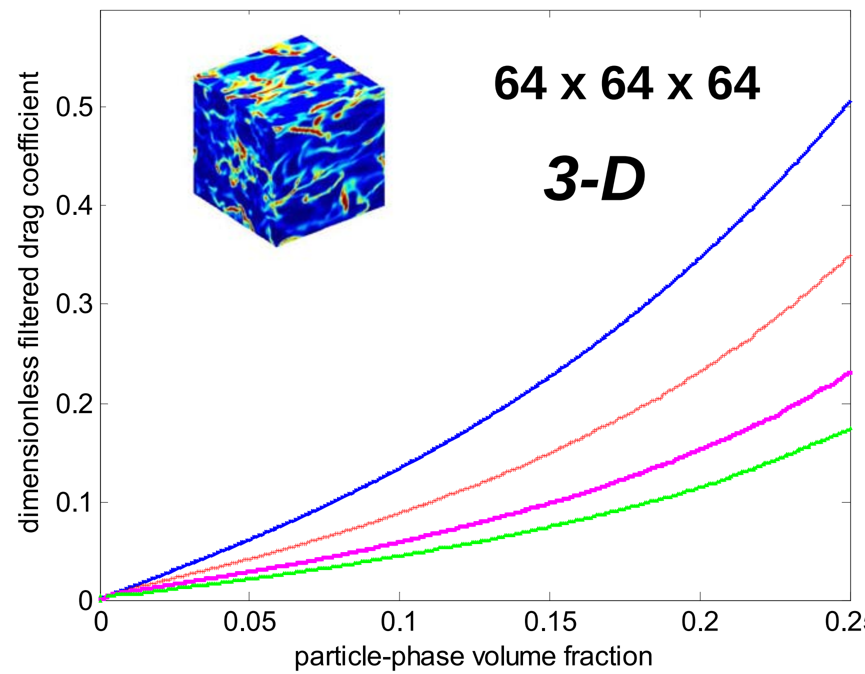
Filtered drag coefficient decreases as filter size increases for both 2-D and 3-D

$$\frac{\beta V_t}{\rho_s g}$$

Domain size = 16 x 16



16 x 16 x 16



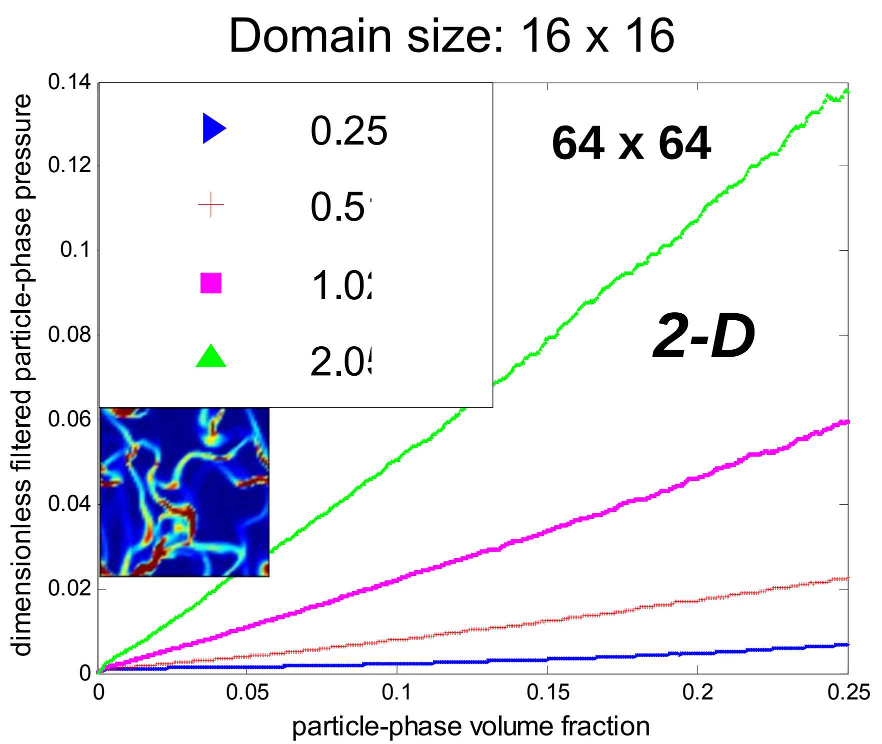
Example: 75 μm; 1500 kg/m^3; domain size = 8 cm

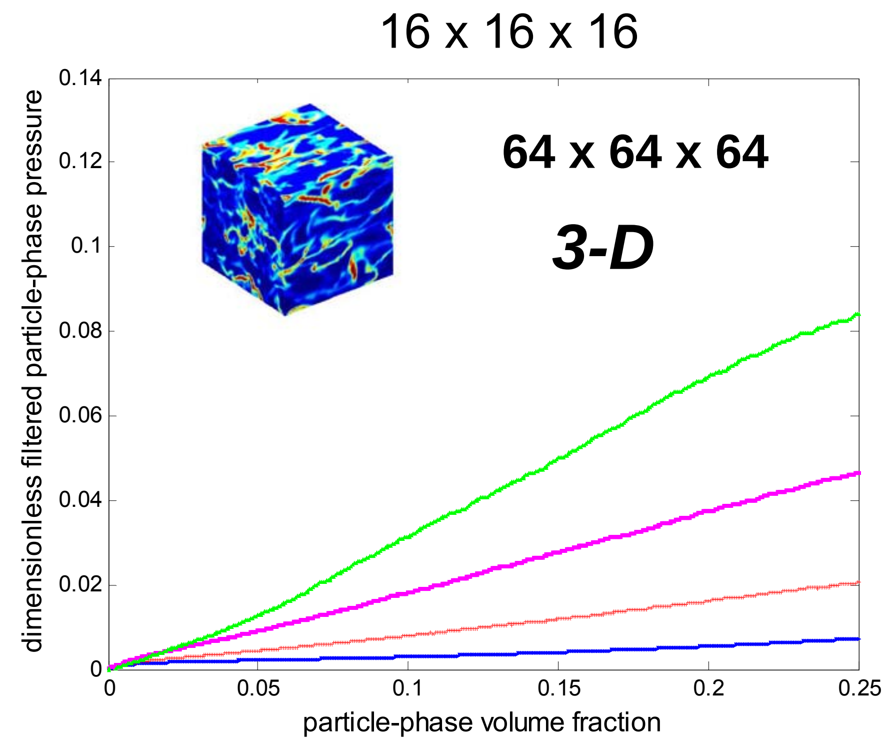
$$\frac{g\Delta}{V_t^2} = \frac{1}{Fr_h}$$

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

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

$$\frac{p_s}{\rho_s V_t^2}$$





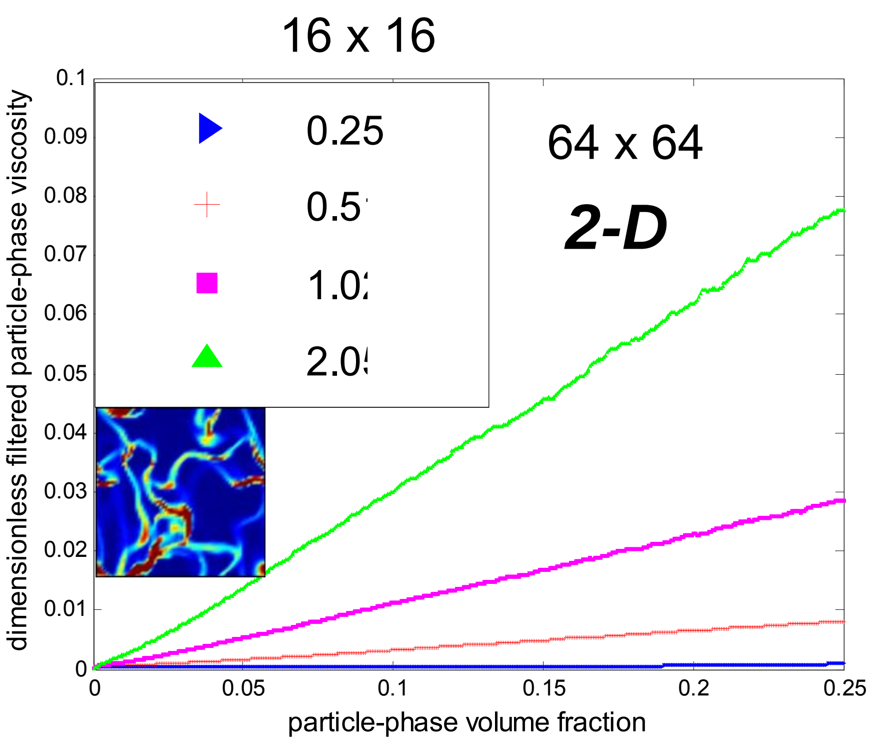
Example: 75 μm; 1500 kg/m³; domain size = 8 cm

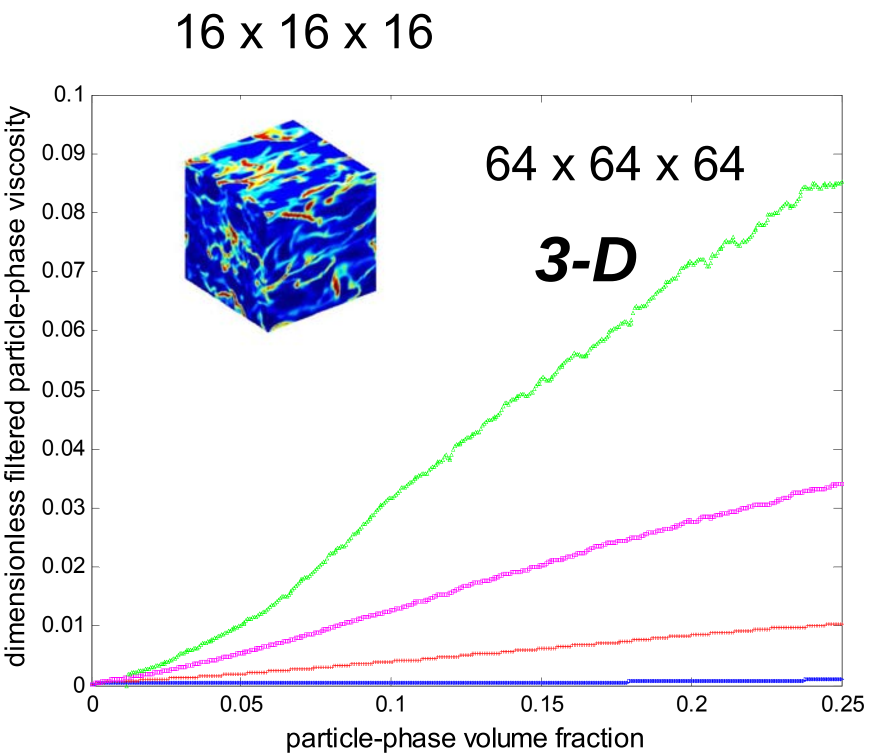
$$\frac{g\Delta}{V_t^2} = \frac{1}{Fr_h}$$

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

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

$$\frac{\mu_s g}{\rho_s V_t^3}$$





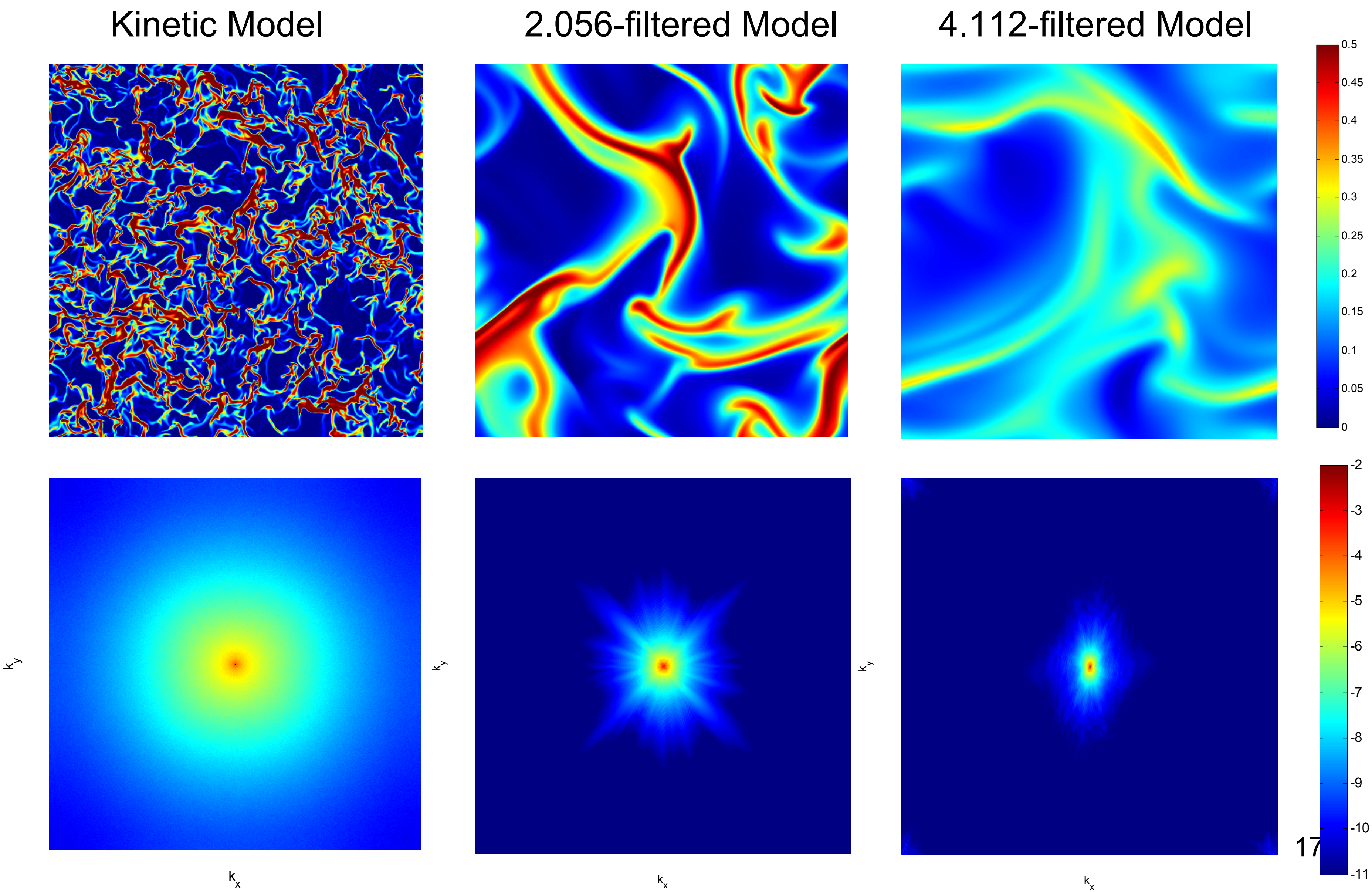
Example: 75 μm; 1500 kg/m^3; domain size = 8 cm

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

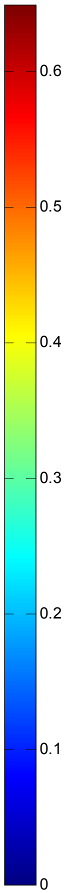
$$\frac{1}{Fr_h} = 2 \Rightarrow \Delta = 1cm$$

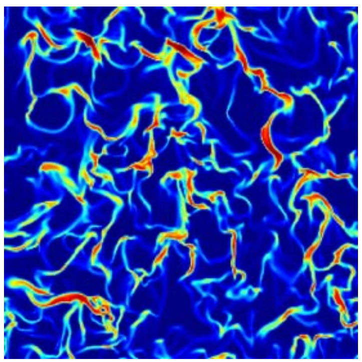
Filtering removes fine structures!

Highly resolved test problem



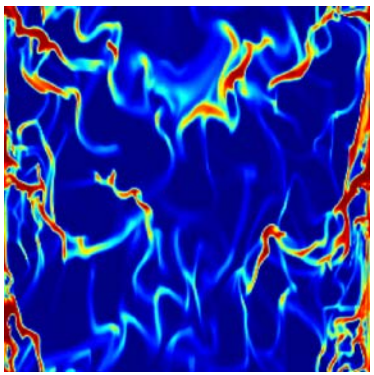
Two-fluid model simulations with side walls





Periodic BC in both directions (a.k.a. “Doubly periodic”)

$$\langle \phi_s \rangle = 0.10.$$



Partial-slip side walls

Periodic BC in the vertical direction

As filter size increases, the boundary condition for the both phases goes towards <u>free slip.</u>

<u>Dimensionless domain size</u>: 65.792 x 65.792

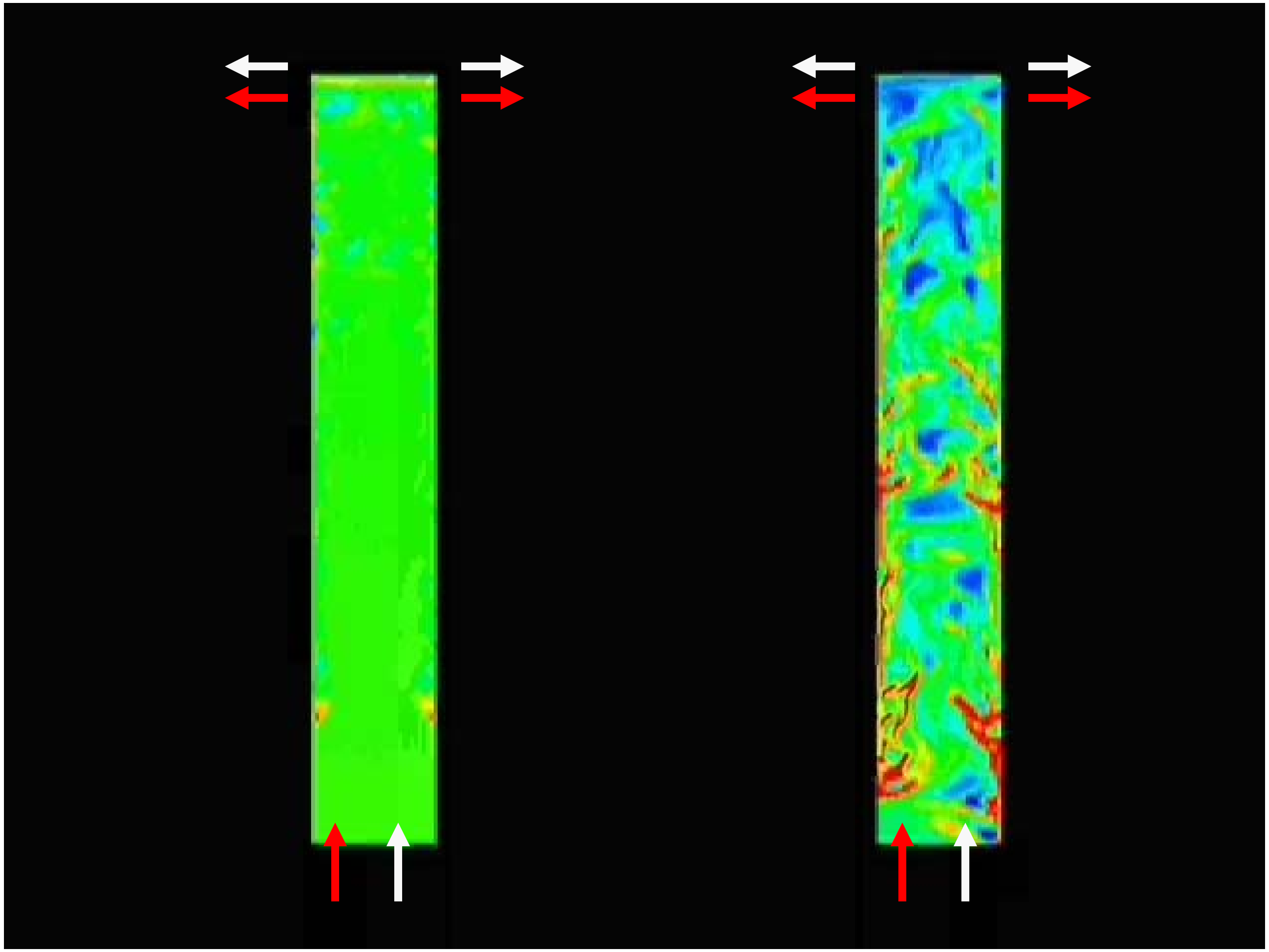
<u>Resolution:</u> 256 x 256

Solution of discretized form of the microscopic and the filtered equations of motion

30 m tall

76 cm channel width

2 cm grid

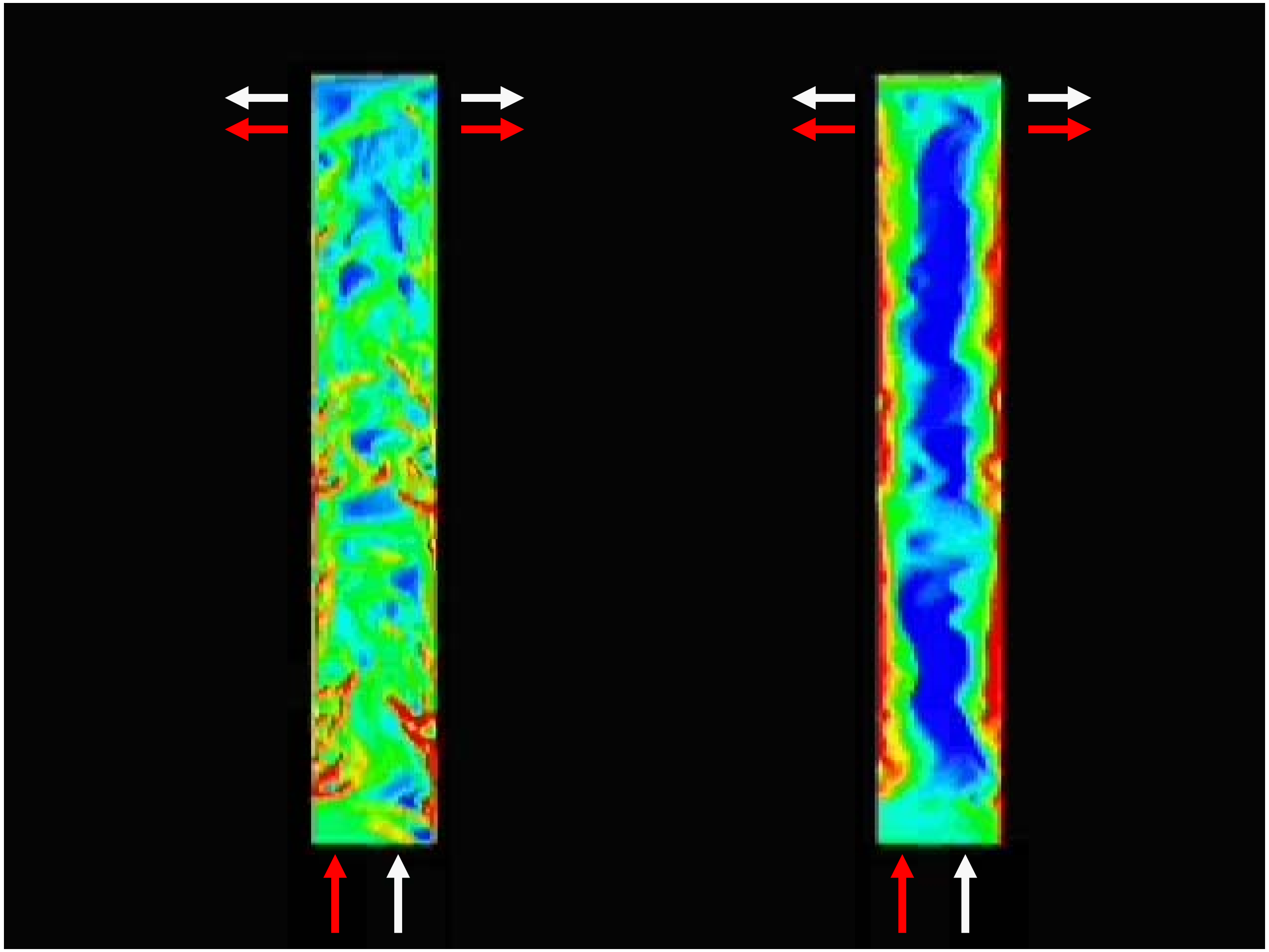


Gas velocity = 6 m/s
Solids flux = 220 kg/m2.s

Kinetic theory

Filtered equations

Solution of discretized form of the filtered equations of motion



Particle volume fraction Vertical velocity

Summary

- Through highly resolved simulations of *any* two-fluid model, one can extract closures for the corresponding filtered two-fluid model. We have demonstrated this for a kinetic theory based two-fluid model.

- The drag law and the effective stresses which should be used in the filtered equations vary systematically with filter size.

- Two-dimensional and three-dimensional analyses yield similar statistical information.

- The test problem shows that the “filtered equations” approach has promise.

Project Goals: Year 3

- Validate the filtered two-fluid model equations against experimental data

Acknowledgments

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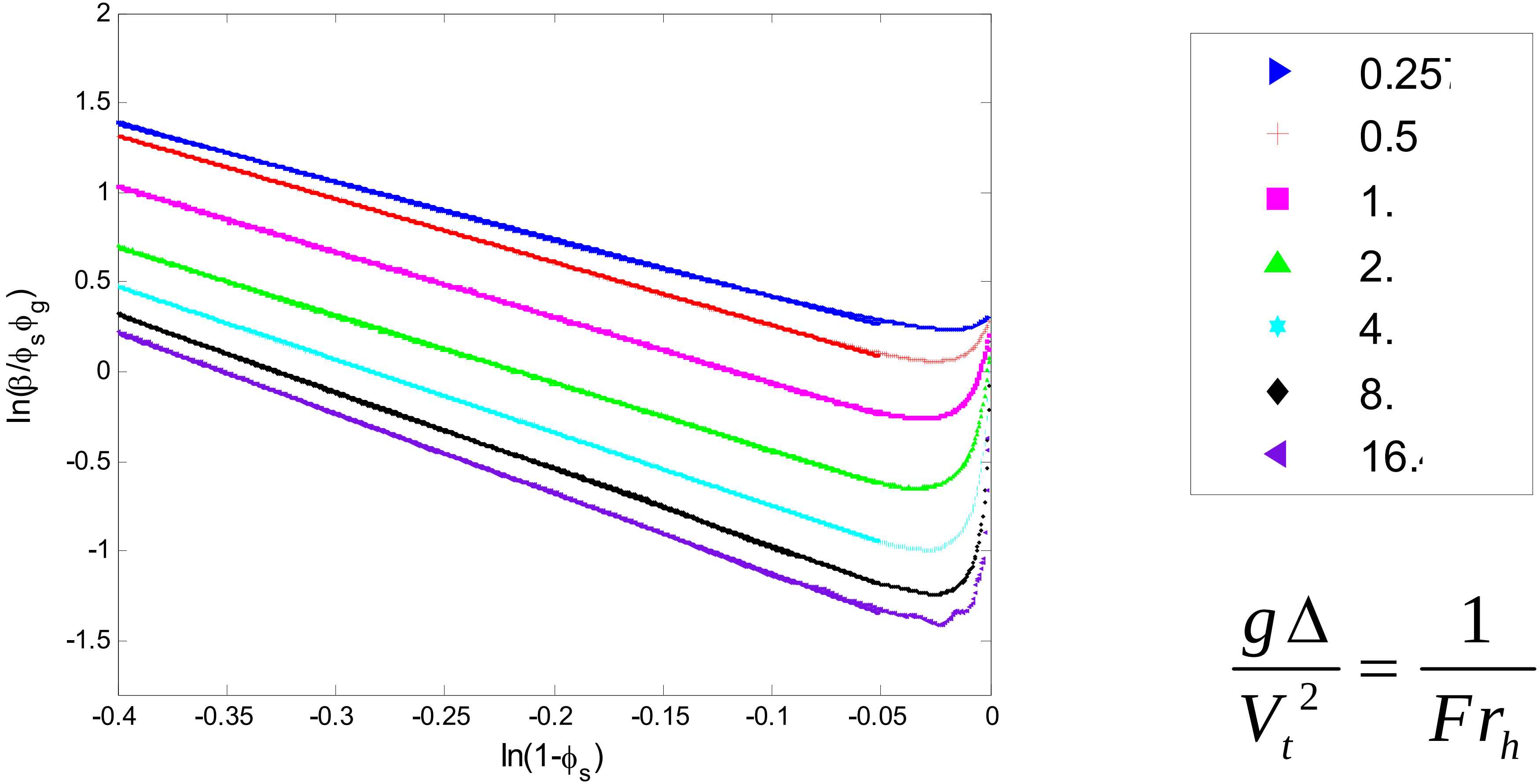
Sofiane Benyahia (Fluent)

Variation of filtered drag coefficient with filter size 2-D

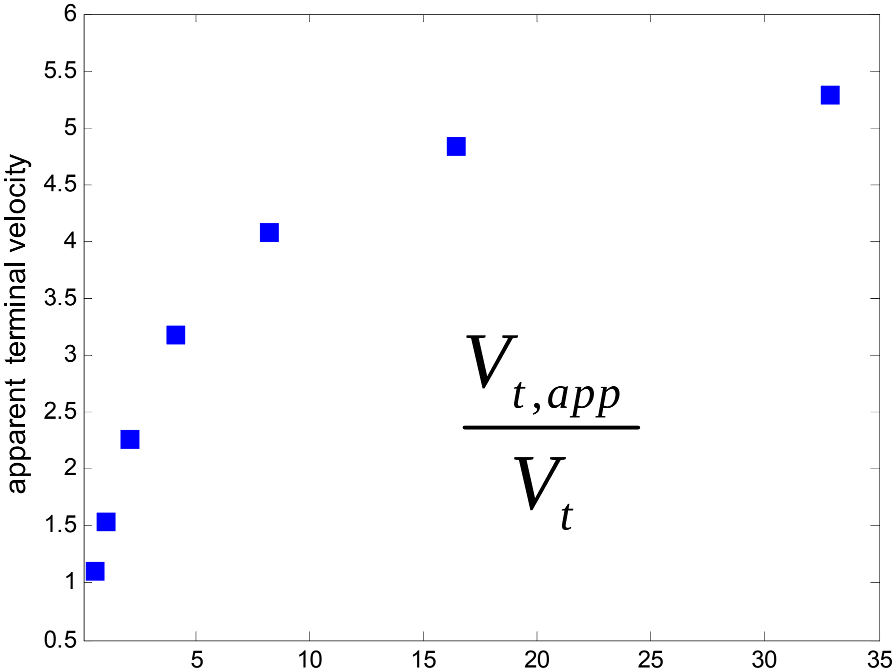
$$\frac{\beta V_t}{\rho_s g \phi_s (1-\phi_s)}$$

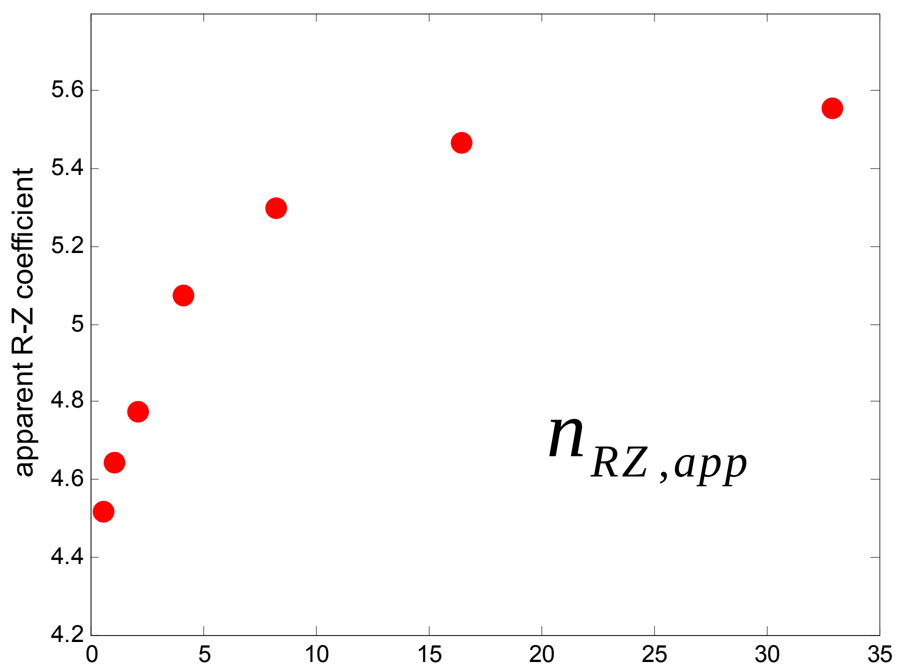


$$\frac{g\Delta}{V_t^2} = \frac{1}{Fr_h}$$

Filtered drag coefficient 2-D

$$\beta = \frac{\rho_s g \phi_s}{V_{t,app}\left(1-\phi_s\right)^{n_{RZ,app}-2}}$$





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