Application of a filtered Euler-Lagrange formalism to large-scale simulations of dilute and dense fluid-particle flows

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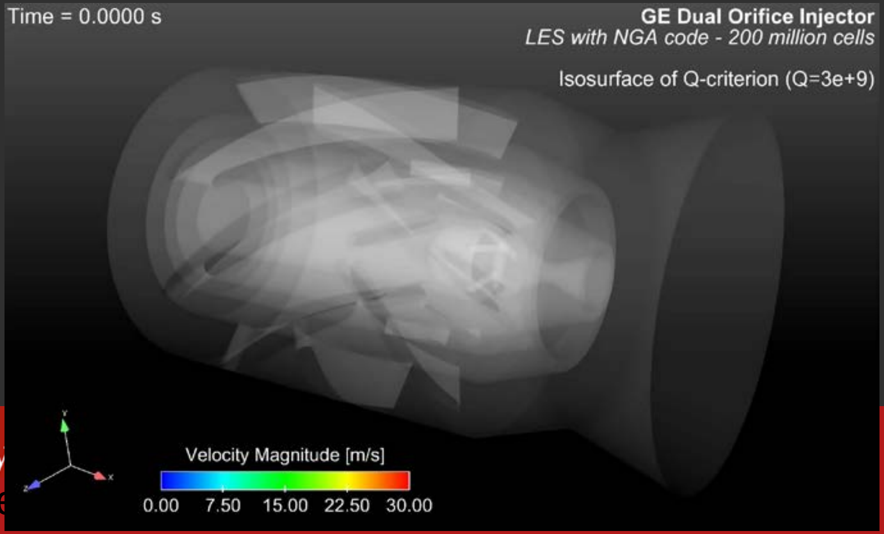
National Renewable Energy Laboratory
gratefully acknowledged

Multiphase flows in energy applications

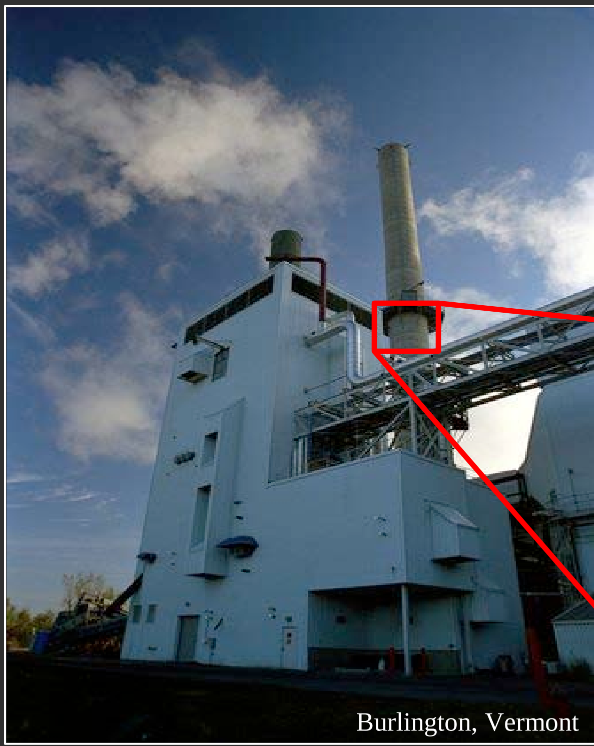
- Multi-physics and multi-scale problem
  - *Highly turbulent*
  - *Triple-phase*
  - *Complex geometries*
  - *Chemically reacting (including heat transfer + phase change)*
- Computational Thermo-Fluids Laboratory led by Dr. Olivier Desjardins
  - http://ctflab.mae.cornell.edu
  - Multi-scale and multi-physics problems
  - Phase interface tracking
  - Massively parallel computing

Chemically reacting flows
(Dr. Pepiot)

Immersed boundaries for modeling complex geometries

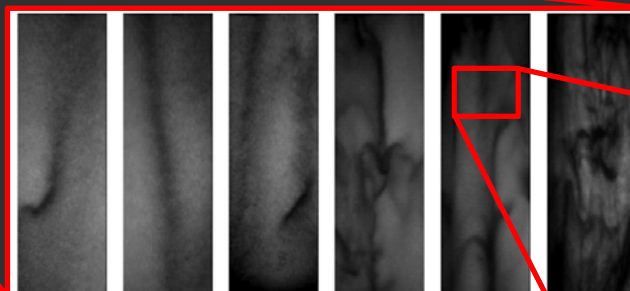


Multi-scale issue in turbulent particle-laden flows



Macroscale

- Large number of particles $\mathcal{O}(10)$
- Length scales: m



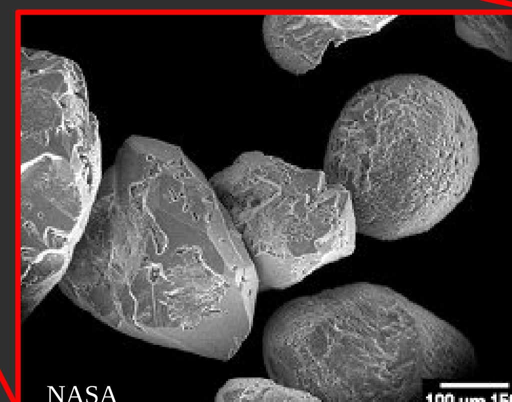
Xu & Zhu, 2011

Mesoscale

- Clustering
- Bubbling
- Particle size segregation
- Turbulence modulation

Microscale

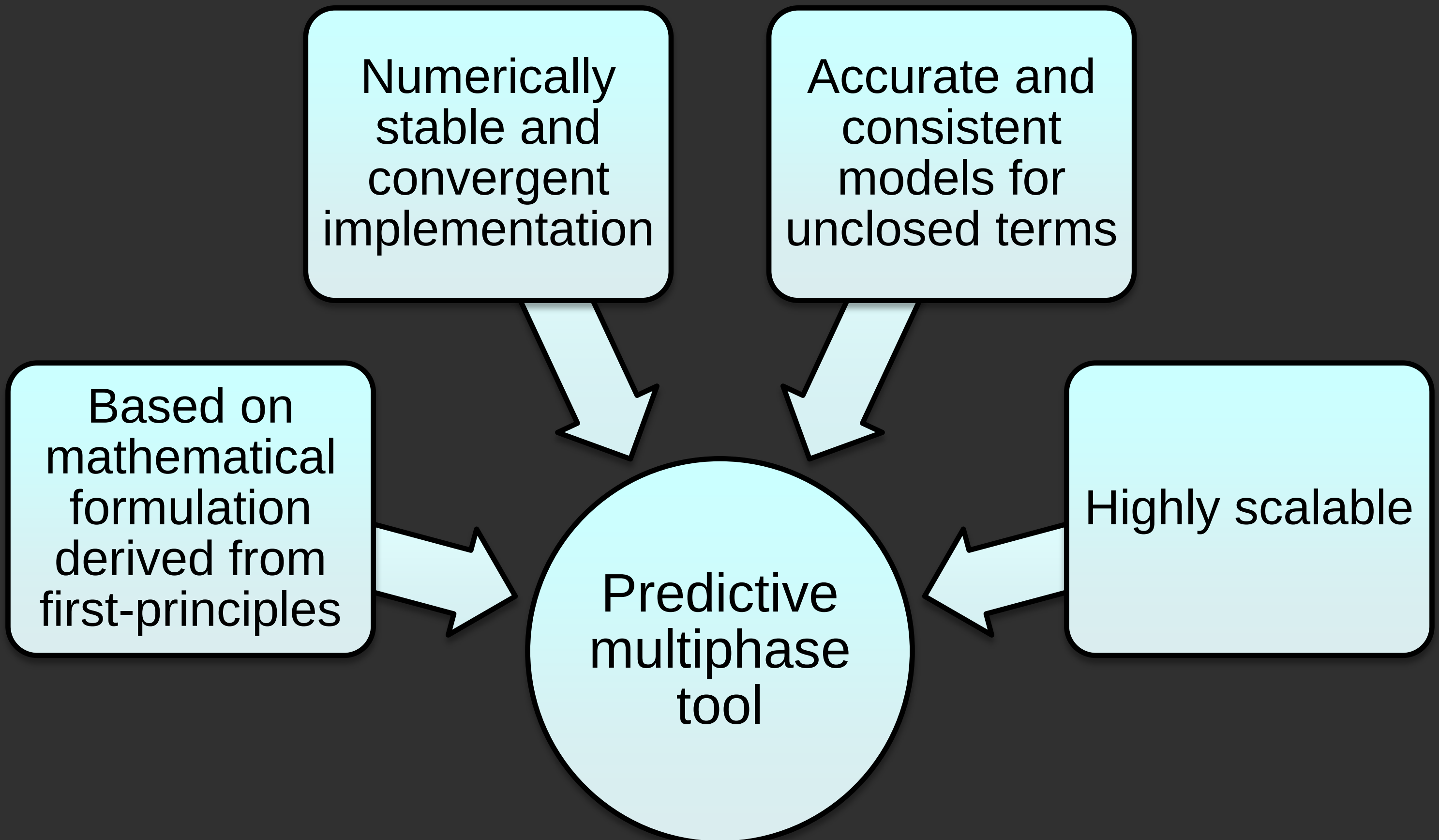
- Wakes
- Particle collisions
- Phase change



Outline

- Filtered Euler-Lagrange framework
  - Mathematical formulation
  - Numerical implementation
- Application to dense particle-laden flows
  - Gas-solid fluidized beds
  - Liquid-solid slurries
- Application to dilute particle-laden flows
  - Turbulent channel
  - Moderately-dilute riser
- Summary & conclusions

Ingredients for developing predictive multiphase tools[1]



1. S. Subramaniam, Lagrangian-Eulerian methods for multiphase flows, *IJMF*, (2013)

Mathematical formulation

First-principle equations

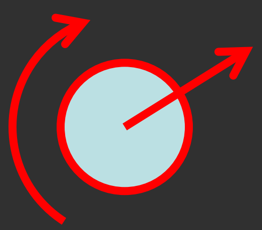
- *Gas phase:* Variable-density low-Mach Navier-Stokes equations

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

$$\frac{\partial}{\partial t}(\rho_f \boldsymbol{u}_f) + \nabla \cdot (\rho_f \boldsymbol{u}_f \otimes \boldsymbol{u}_f) = \nabla \cdot \boldsymbol{\tau} + \rho_f \boldsymbol{g}$$

$$\boldsymbol{\tau} = -p\boldsymbol{\mathcal{I}} + \mu \left[\nabla \boldsymbol{u}_f + \nabla \boldsymbol{u}_f^{\intercal} - \frac{2}{3}(\nabla \cdot \boldsymbol{u}_f)\boldsymbol{\mathcal{I}} \right]$$

- *Particles:* Newton's second law of motion



$$m_p \frac{d\boldsymbol{u}_p}{dt} = \int_{\mathcal{S}_p} \boldsymbol{\tau} \cdot \boldsymbol{n} \, dS + \boldsymbol{F}_p^{\mathrm{col}} + m_p \boldsymbol{g}$$

$$\frac{d\boldsymbol{x}_p}{dt} = \boldsymbol{u}_p$$

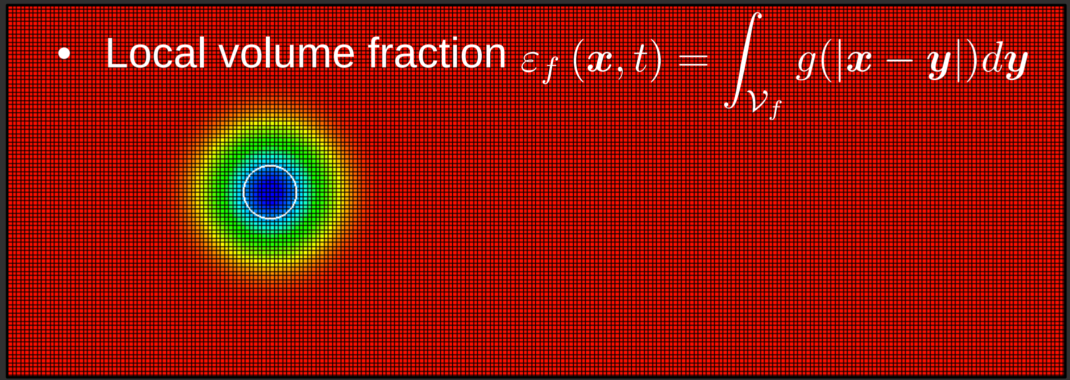
$$I_p \frac{d\boldsymbol{\omega}_p}{dt} = \int_{\mathcal{S}_p} \frac{d_p}{2} \boldsymbol{n} \times (\boldsymbol{\tau} \cdot \boldsymbol{n}) \; d\boldsymbol{y} + \sum_j \frac{d_p}{2} \boldsymbol{n} \times \boldsymbol{f}_{t,j \to p}^{\mathrm{col}}$$

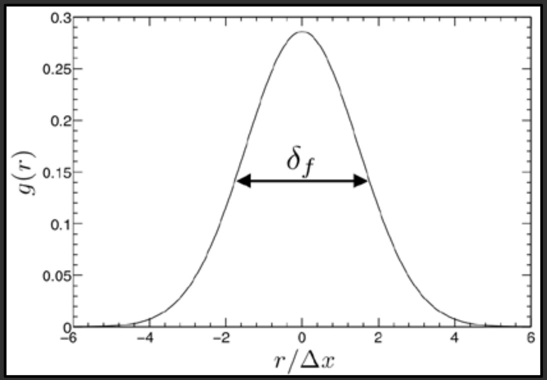
- *Boundary conditions:* no-slip and no-penetration at surface of particle
- *Collision force:* contact mechanics

Mathematical formulation

Volume-filtered description[2]

- Objective: formulate equations for particle-laden flows that allow $\Delta x \gg d_p$
- Introduce local volume filter based on convolution product with kernel[3] $g(r)$
  - $\delta_f \gg d_p$: enabling the use of microscale models
  - $\delta_f \ll \mathcal{L}_{meso}$: mesoscale structures are fully resolved
- Local volume fraction $\varepsilon_f(\boldsymbol{x},t) = \int_{\mathcal{V}_f} g(|\boldsymbol{x}-\boldsymbol{y}|)d\boldsymbol{y}$





- Allows to define filtered variable $\overline{\boldsymbol{a}}$ from point variable $\boldsymbol{a}$

$$\varepsilon_f \overline{\boldsymbol{a}}(\boldsymbol{x},t) = \int_{\mathcal{V}_f} \boldsymbol{a}(\boldsymbol{y},t)\, g(|\boldsymbol{x}-\boldsymbol{y}|)d\boldsymbol{y}$$

$$\boldsymbol{a} = \overline{\boldsymbol{a}} + \boldsymbol{a}'$$

2. Capecelatro & Desjardins, An Euler-Lagrange strategy for simulating particle-laden flows, *JCP*, (2012)
3. 3. T. Anderson, R. Jackson, Fluid mechanical description of fluidized beds, (1967)

Mathematical formulation

Volume-filtering the Navier-Stokes equations

- Continuity

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

- Momentum

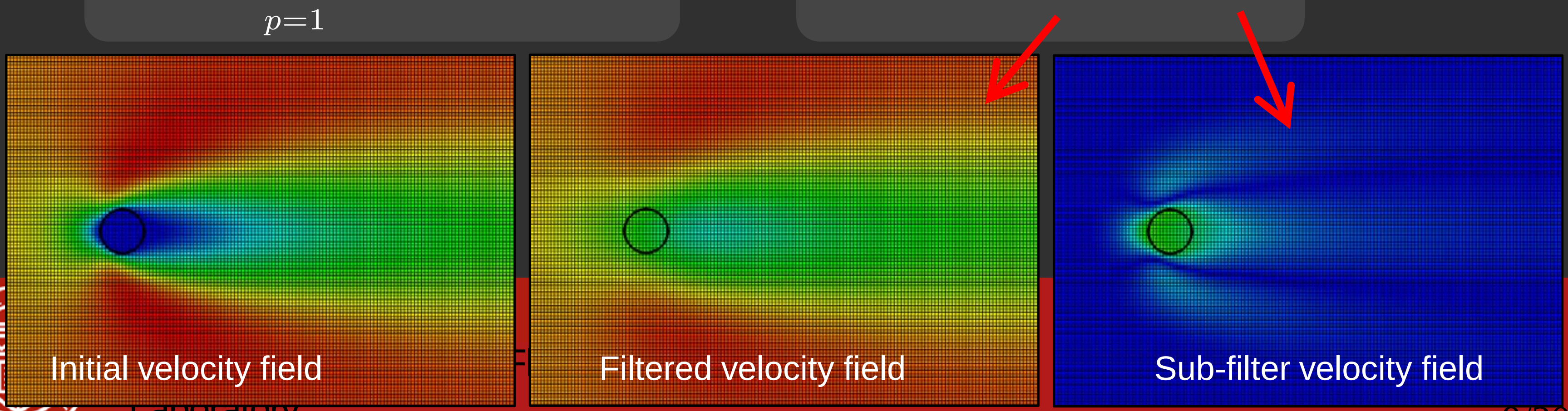
$$\frac{\partial}{\partial t}\left(\varepsilon_f \rho_f \overline{\boldsymbol{u}_f}\right) + \nabla \cdot \left(\varepsilon_f \rho_f \overline{\boldsymbol{u}_f} \otimes \overline{\boldsymbol{u}_f}\right) = \nabla \cdot \left(\overline{\boldsymbol{\tau}} - \underline{\boldsymbol{R}_u}\right) + \varepsilon_f \rho_f \boldsymbol{g} - \underline{\boldsymbol{F}^{\text{inter}}}$$

$$\overline{\boldsymbol{\tau}} = -\overline{p}\boldsymbol{\mathcal{I}} + \mu\left[\nabla\overline{\boldsymbol{u}_f} + \overline{\boldsymbol{u}_f}^{\mathsf{T}} - \frac{2}{3}\left(\nabla \cdot \overline{\boldsymbol{u}_f}\right)\boldsymbol{\mathcal{I}}\right] + \underline{\boldsymbol{R}_\mu}$$

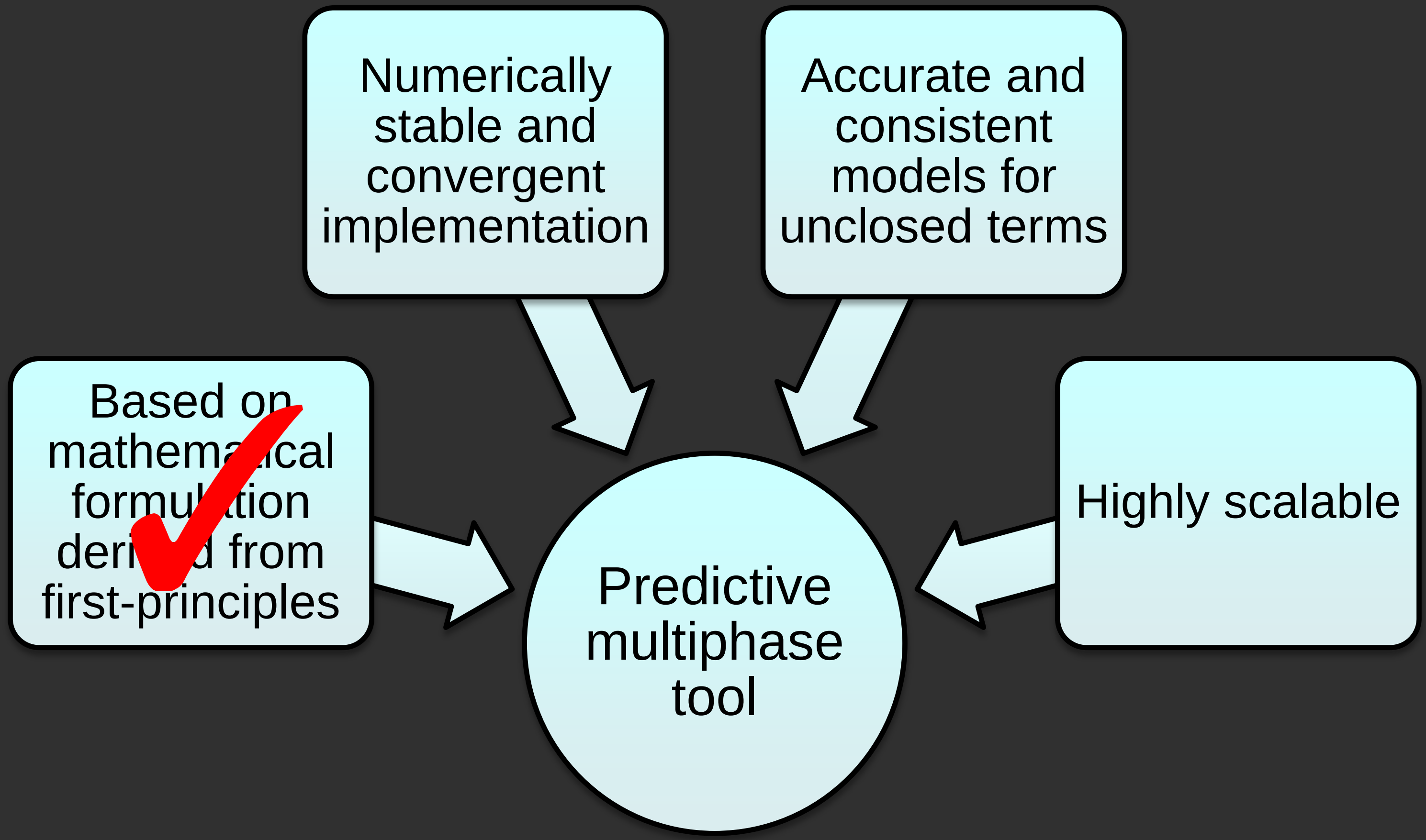
- Interphase exchange

$$\boldsymbol{F}^{\text{inter}} = \sum_{p=1}^{n_p} g\left(|\boldsymbol{x} - \boldsymbol{x}_p|\right) \boldsymbol{f}_p^{\text{inter}}$$

$$\boldsymbol{f}_p^{\text{inter}} \approx \mathcal{V}_p \nabla \cdot \overline{\boldsymbol{\tau}} + \boldsymbol{f}_p^{\text{drag}}$$



Ingredients for developing predictive multiphase tools[1]

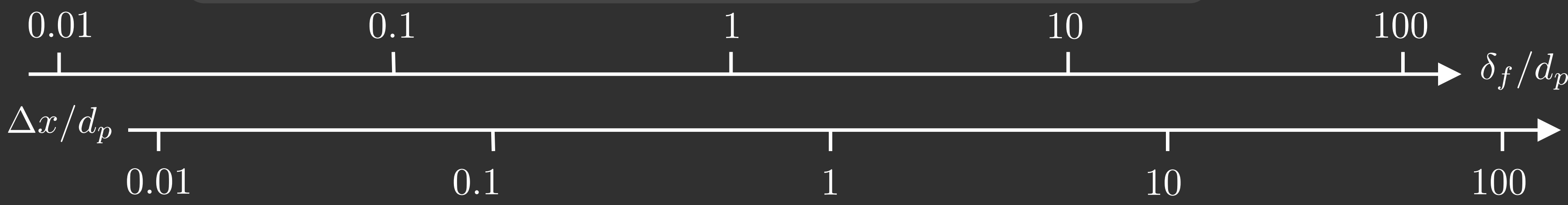


1. S. Subramaniam, Lagrangian-Eulerian methods for multiphase flows, *IJMF*, (2013)

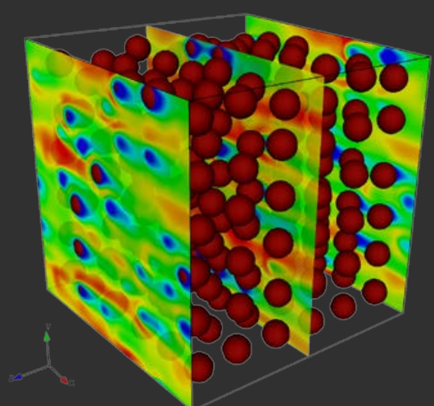
Consistent framework from point-particle to full DNS

- Accurate solution of the equations requires $\Delta x \ll \delta_f$
- Model closures depend on δ_f
- What is the appropriate choice for δ_f ?

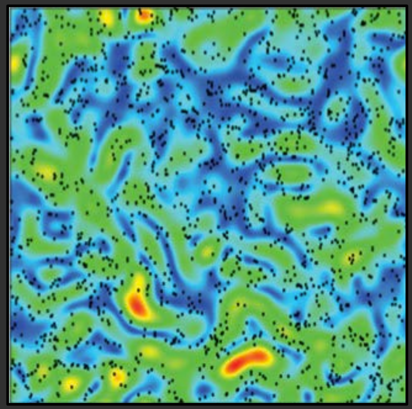
$$\int_{\mathcal{V}_f} \nabla \cdot \boldsymbol{\tau} g(|\boldsymbol{x}-\boldsymbol{y}|) d\boldsymbol{y} = \nabla \cdot (\varepsilon_f \overline{\boldsymbol{\tau}}) - \sum_{p=1}^{n_p} \int_{\mathcal{S}_p} \boldsymbol{n} \cdot \boldsymbol{\tau} g(|\boldsymbol{x}-\boldsymbol{y}|) d\boldsymbol{y}$$



Fully-resolved DNS | Point-particle



- Microscale models might break down
- Cannot resolve boundary layers



Ray & Collins, 2011

Consistent framework from point-particle to full DNS

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- Model closures depend on δ_f
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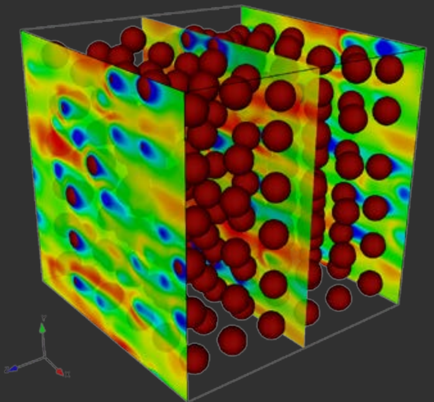
$$\int_{\mathcal{V}_f} \nabla \cdot \boldsymbol{\tau} g(|\boldsymbol{x}-\boldsymbol{y}|)d\boldsymbol{y} = \nabla \cdot (\varepsilon_f \overline{\boldsymbol{\tau}}) - \sum_{p=1}^{n_p} \int_{\mathcal{S}_p}$$

- Drag model of Tenneti et al. (2011)
- Soft-sphere collision model (Cundall & Strack 1979)
- Lagrangian Dynamic Smagorinsky SGS model of Meneveau et al. (2000)
- Effective viscosity (Gibilaro 2007)

0.01 0.1 1

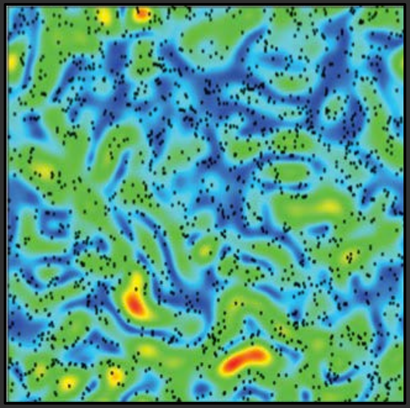
$\Delta x / d_p$: 0.01 0.1 1 10 100

Fully-resolved DNS | Push modeling limits | Point-particle



- Microscale models might break down
- Cannot resolve boundary layers

- Better capture turbulence and mesoscale dynamics
- Can handle large number of particles

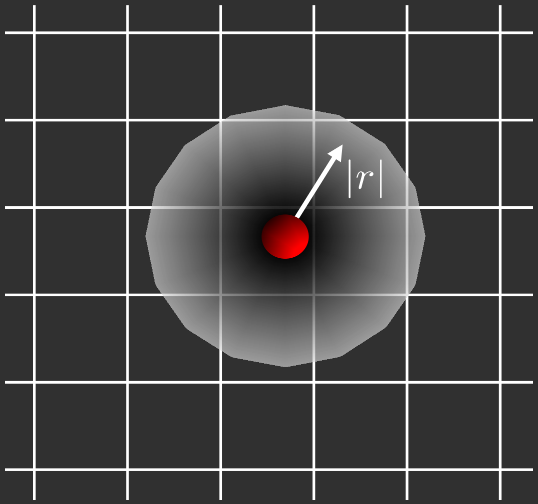


Ray & Collins, 2011

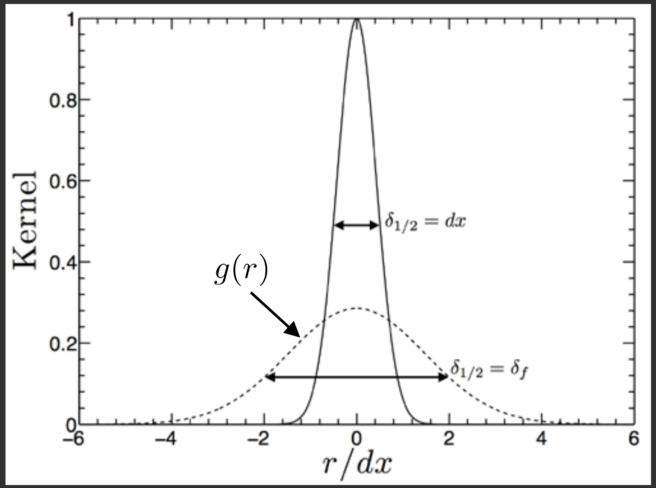
Numerical implementation

Filter discretization

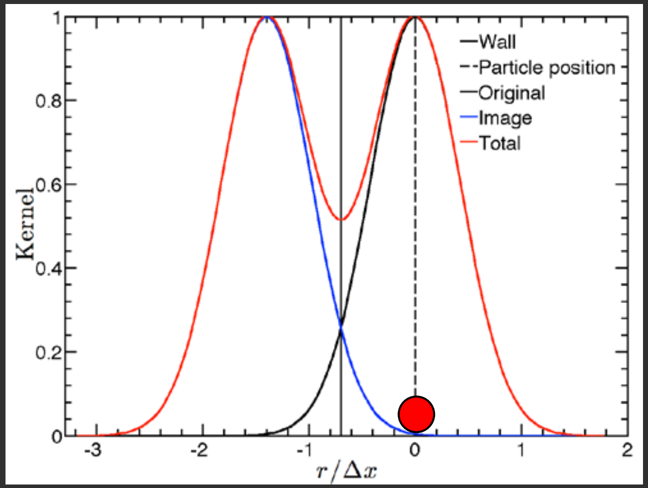
- Direct implementation becomes too expensive
- Filter based on the convolution of mollification and Laplacian smoothing[2]
  1. Mollification: transfer particle data to neighboring cells
  2. Diffusion: smooth data with specified width
- Fully conservative, implicit treatment
- Special care is needed at the walls



Particle influence on mesh



Two-step filter



Near-wall treatment

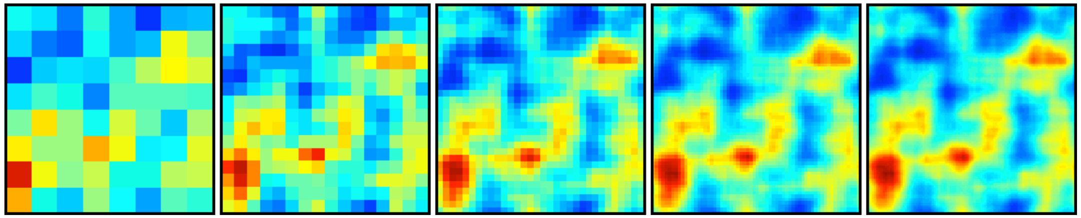
2. Capecelatro & Desjardins, An Euler-Lagrange strategy for simulating particle-laden flows, *JCP*, (2012)

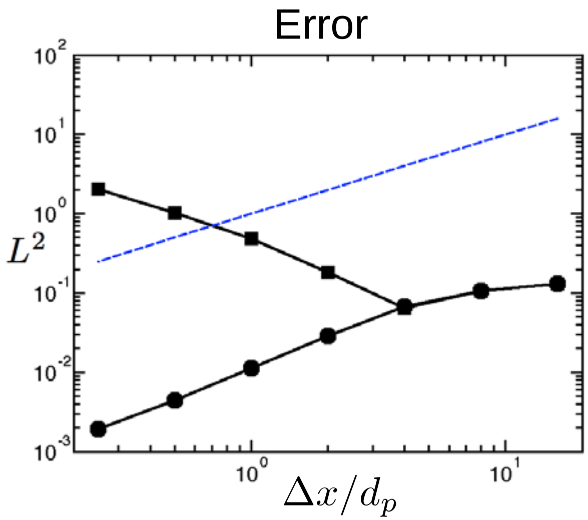
Numerical implementation

Filter discretizatio…

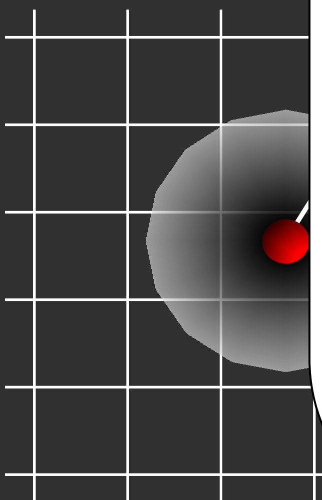
- Direct…
- Filte… …othing[2]
  1. …
  2. …
- Full…
- Spe…

Filter width δ_f is independent of the mesh size



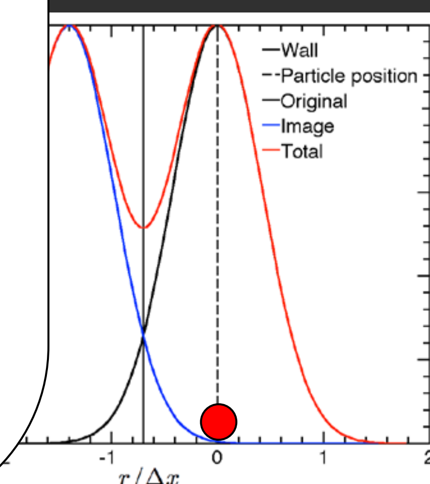


1st-order (- -)
Single-step (■)
Two-step (●)



Particle influence on mesh

Two-step filter



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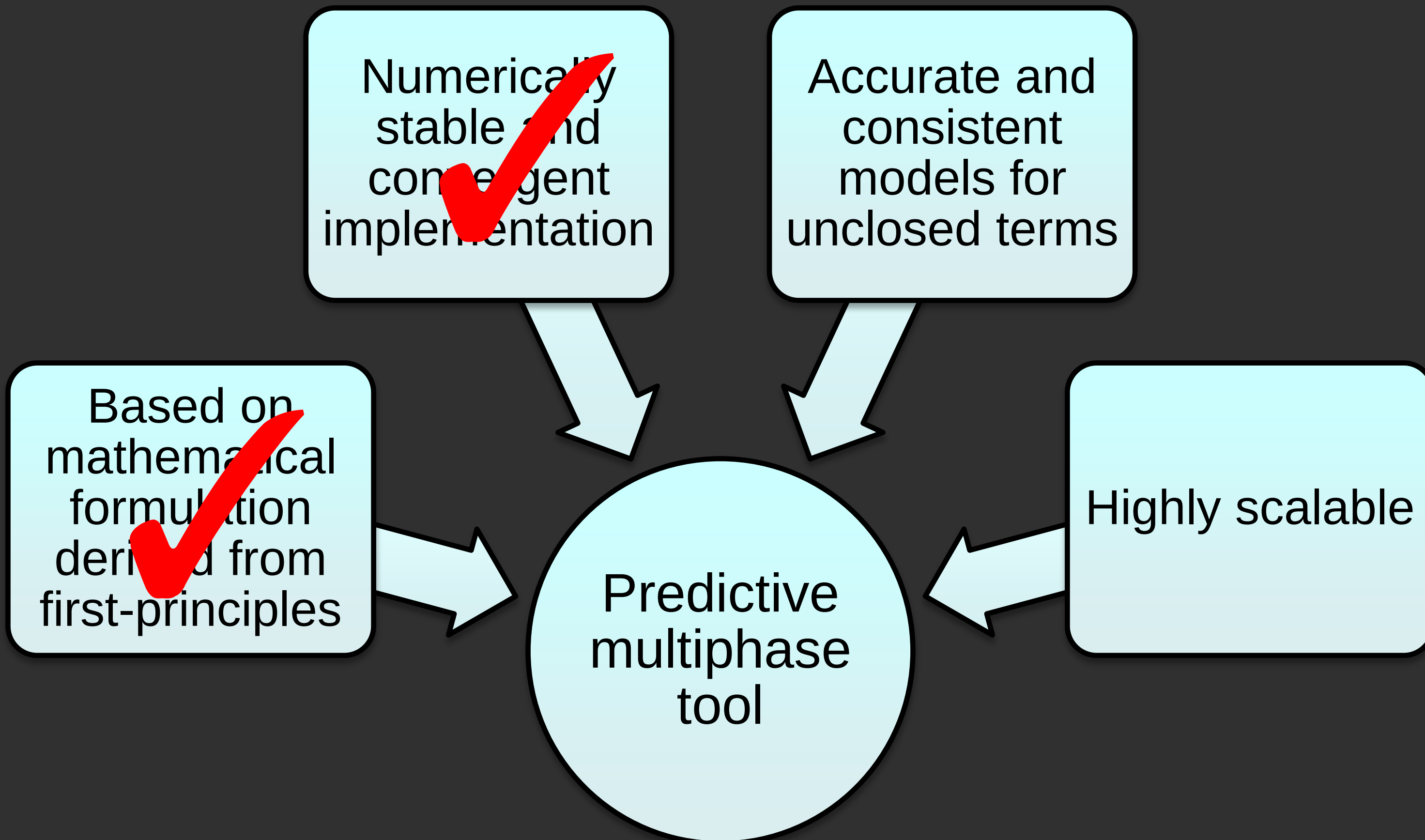
Ingredients for developing predictive multiphase tools[1]



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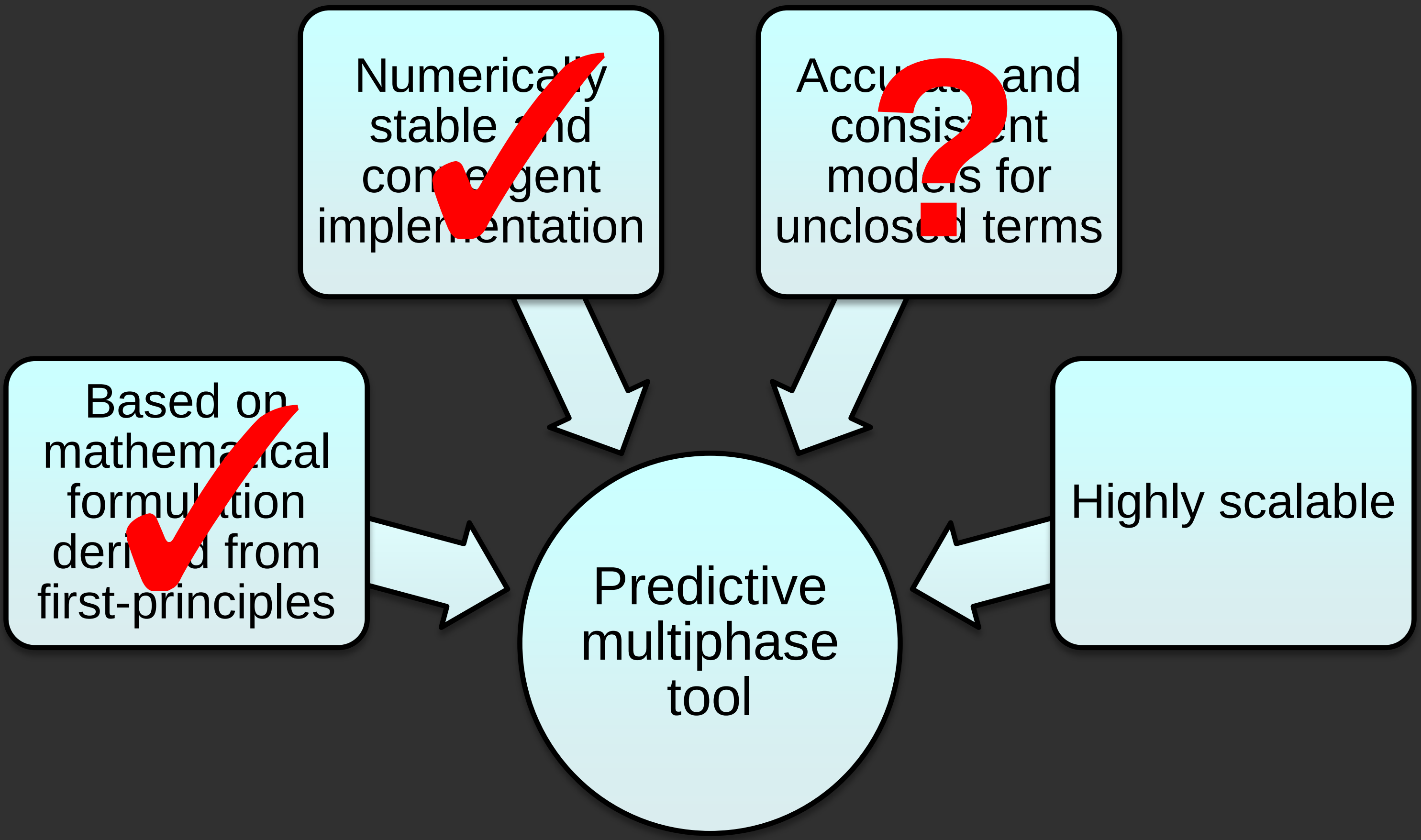


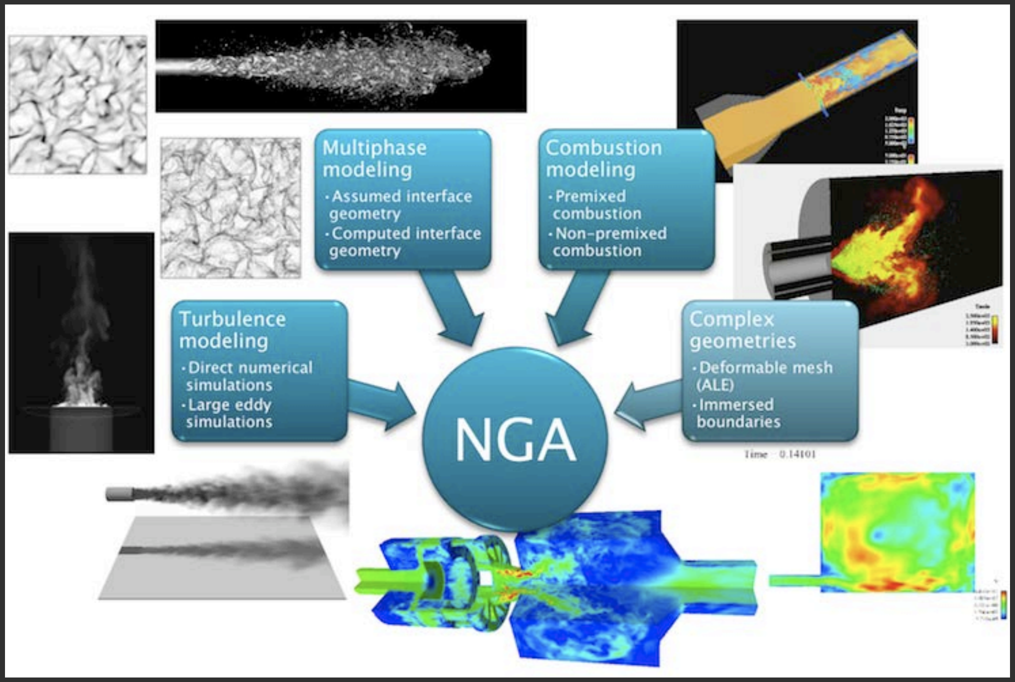
1. S. Subramaniam, Lagrangian-Eulerian methods for multiphase flows, *IJMF*, (2013)

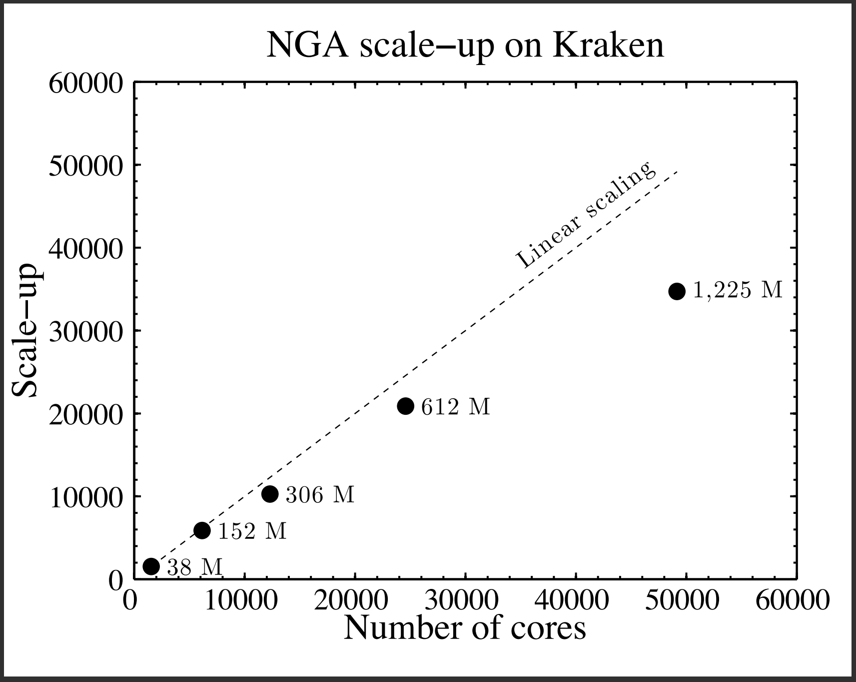
Numerical implementation

Computational platform

NGA[4]

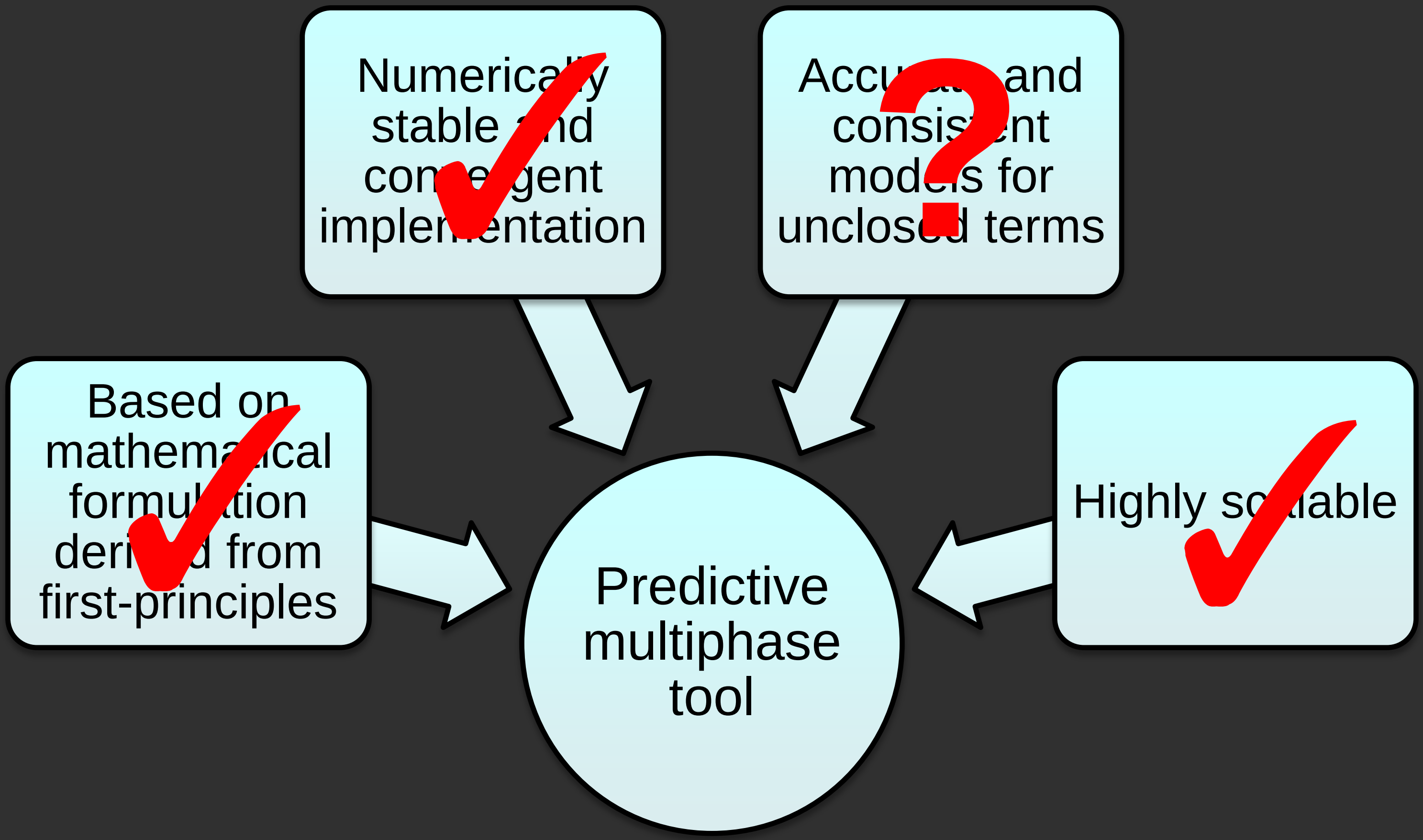
- Arbitrarily high-order multi-physics DNS/LES code
- Conservation of mass, momentum, and kinetic energy
- Highly scalable





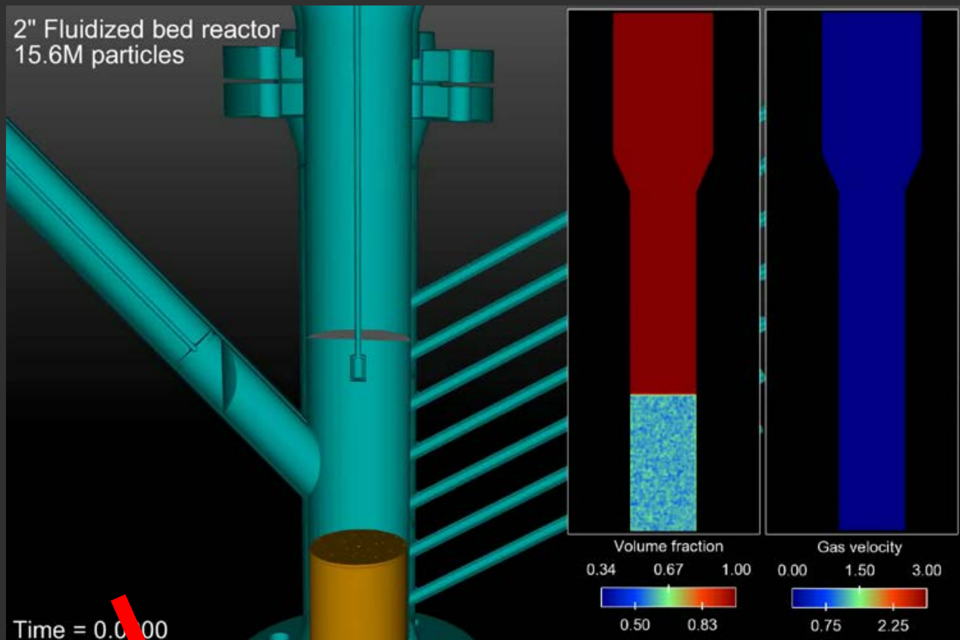
4. O. Desjardins, G. Blanquart, G. Balarac, H. Pitsch, High order conservative finite difference scheme for variable density low Mach number turbulent flows, *JCP* (2008)

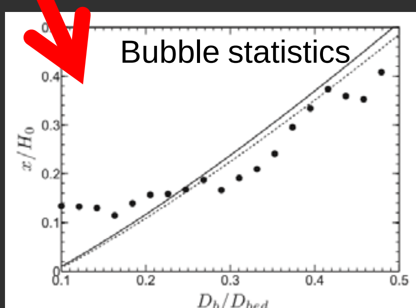
Ingredients for developing predictive multiphase tools[1]

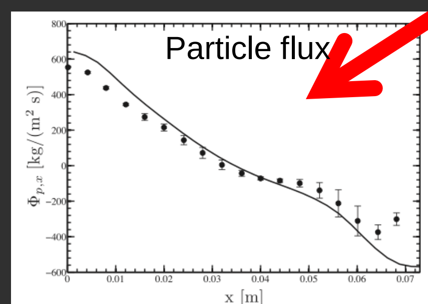


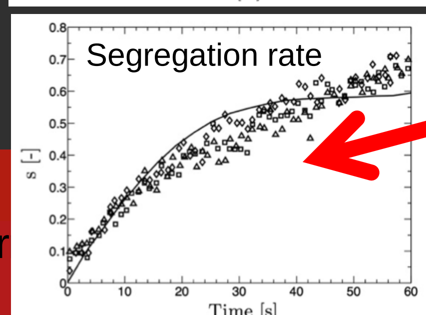
1. S. Subramaniam, Lagrangian-Eulerian methods for multiphase flows, *IJMF*, (2013)

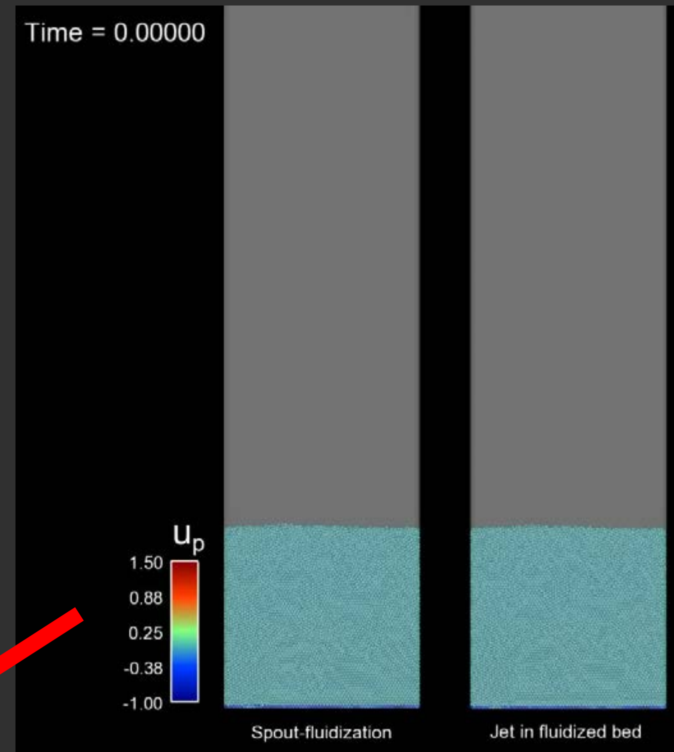
Application to dense gas-solid flows[2]

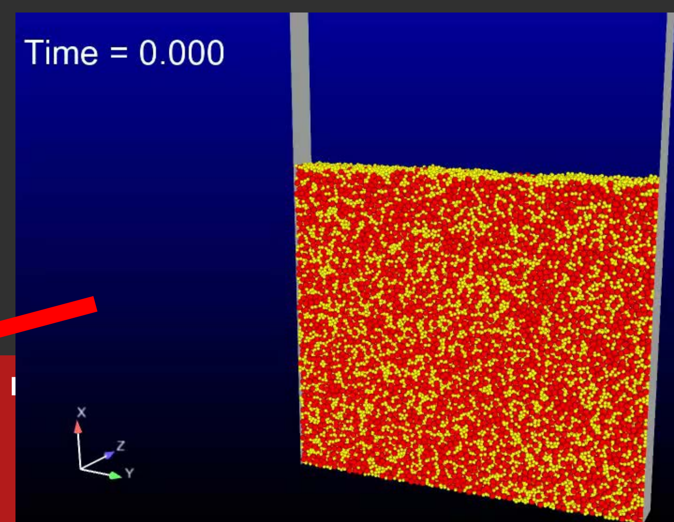








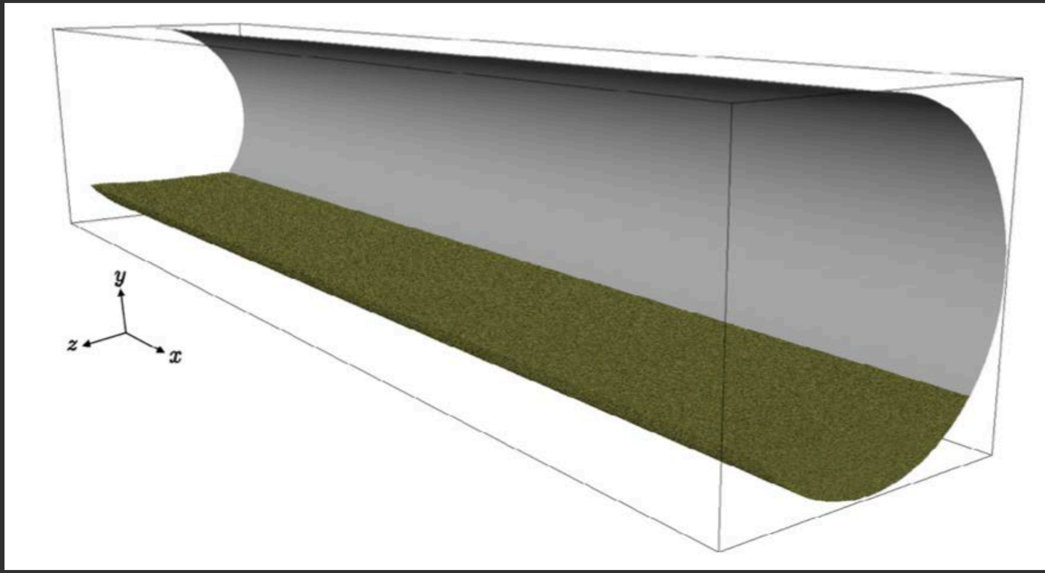


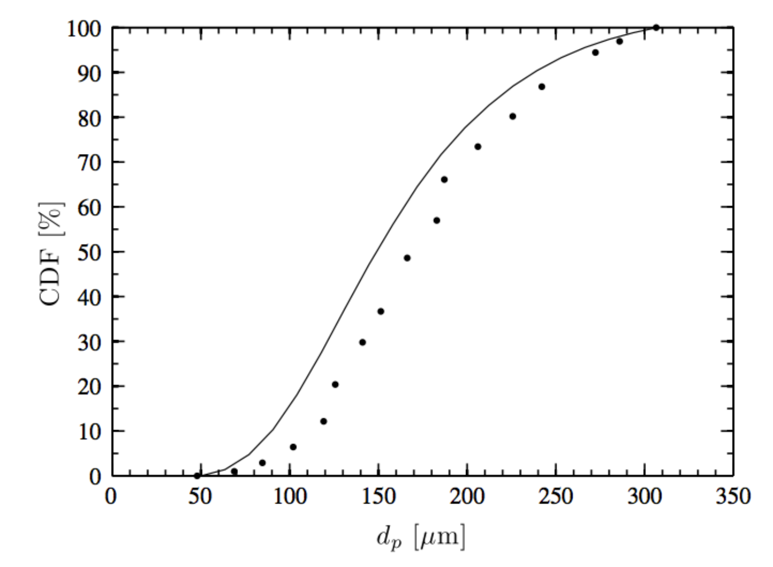


n I … flows, *JCP*, (2012)

Application to liquid-solid slurries[5]

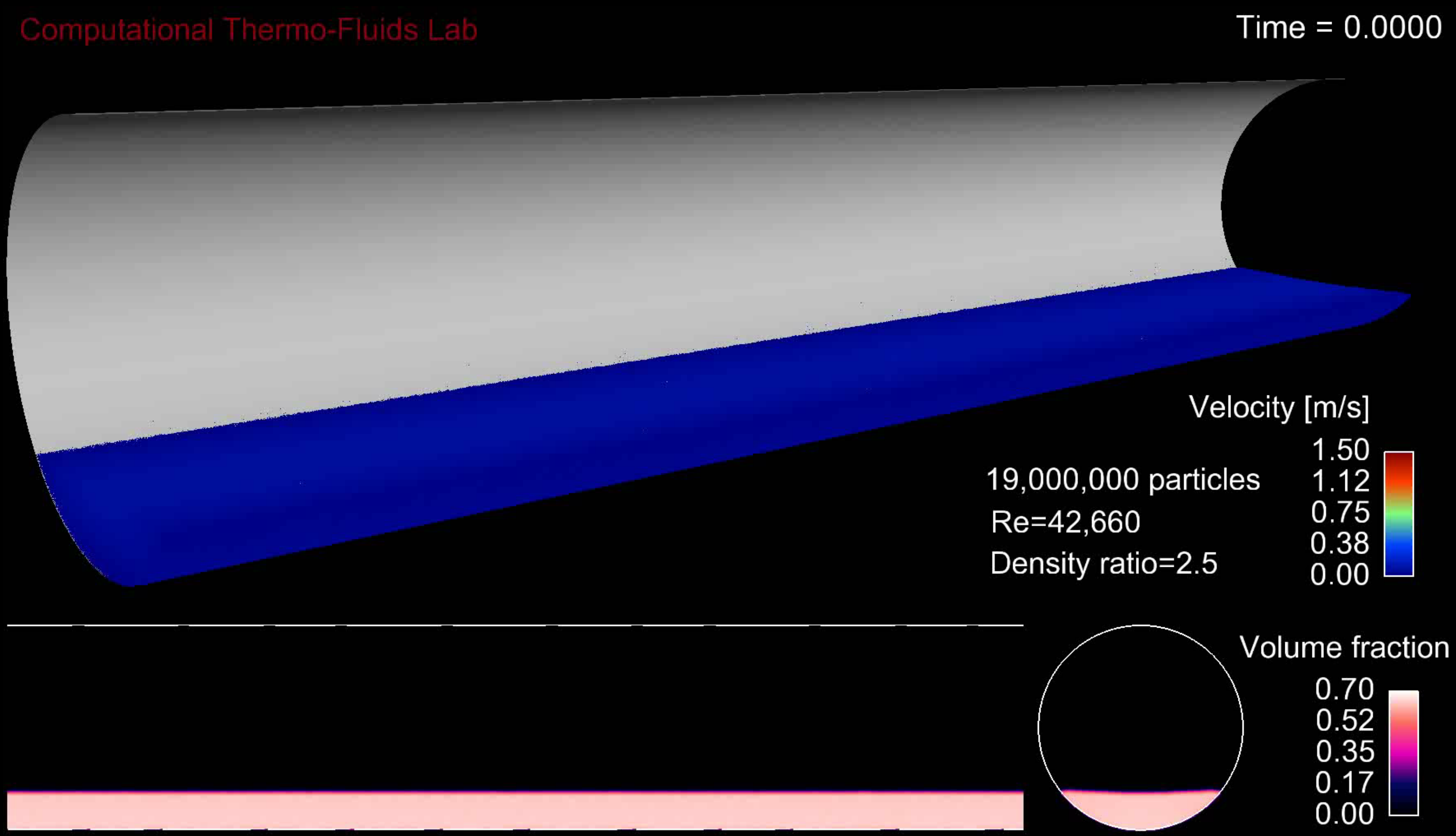
- Compared with experiments by Roco & Balakrishnam (1985)
- Two cases simulated
  - Re=85,000 (above critical deposition velocity)
  - Re=42,660 (below critical deposition velocity)
- Force liquid mass flow rate in a periodic pipe
- 768 x 156 x 156 mesh
- 19 M polydisperse particles



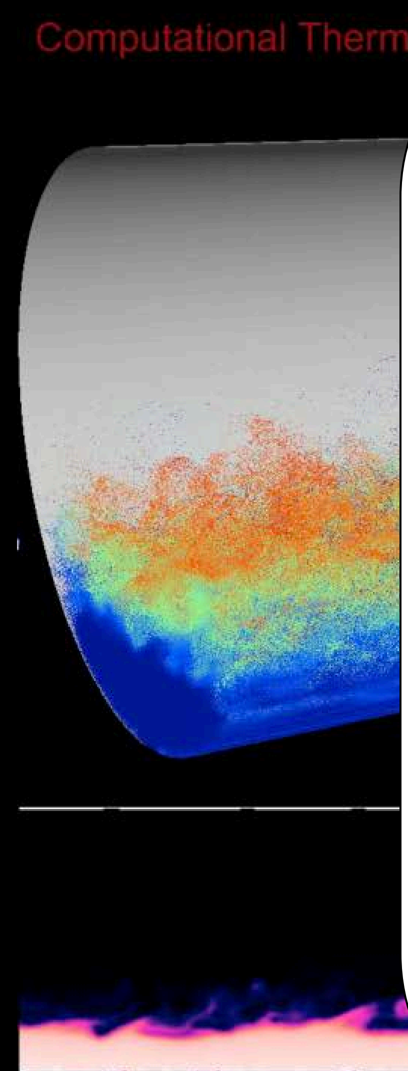


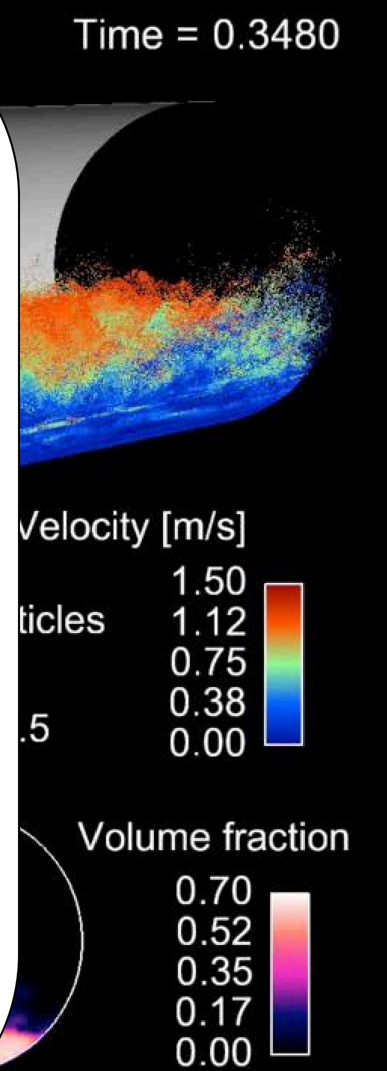
5. Capecelatro & Desjardins, Eulerian-Lagrangian modeling of turbulent liquid-solid slurries in horizontal pipes, *IJMF* (2013)

Application to liquid-solid slurries

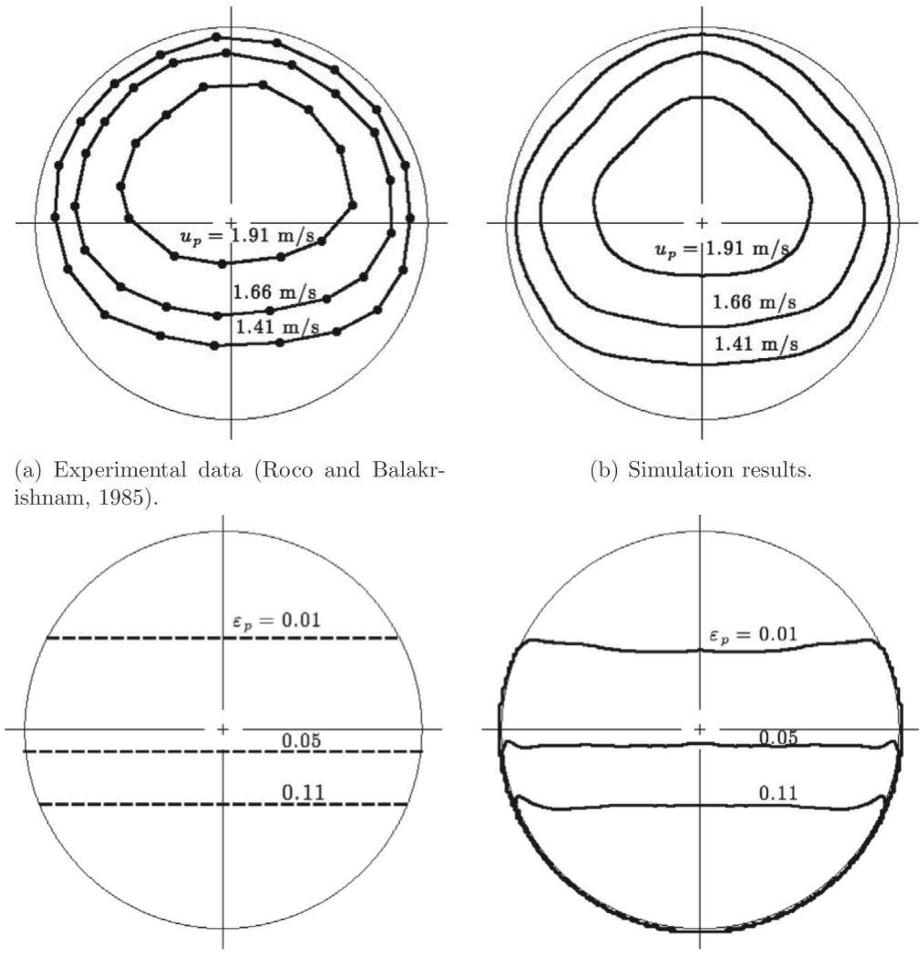


Application to liquid-solid slurries





Excellent agreement with experiments



(a) Experimental data (Roco and Balakrishnam, 1985). (b) Simulation results.

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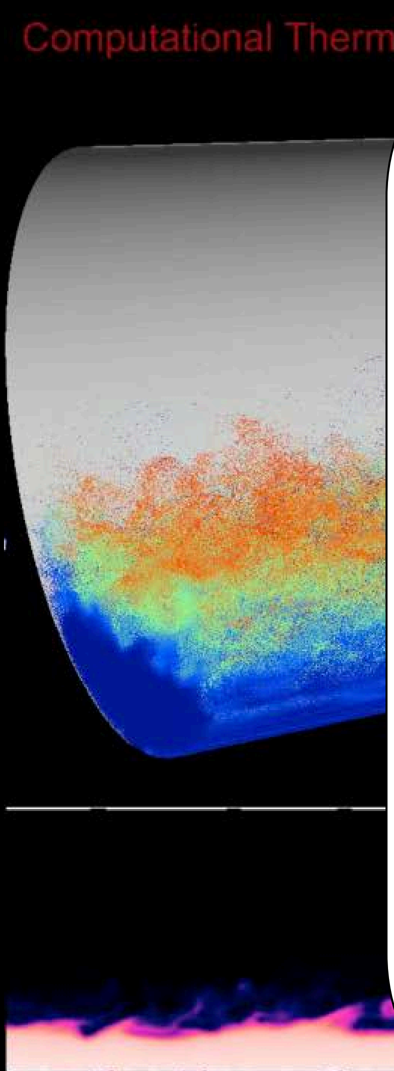
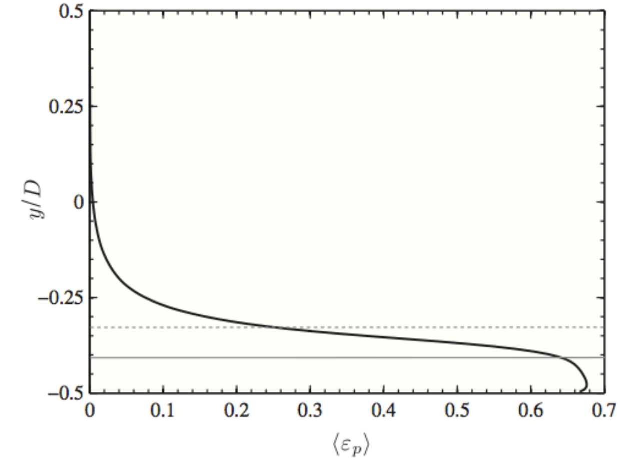
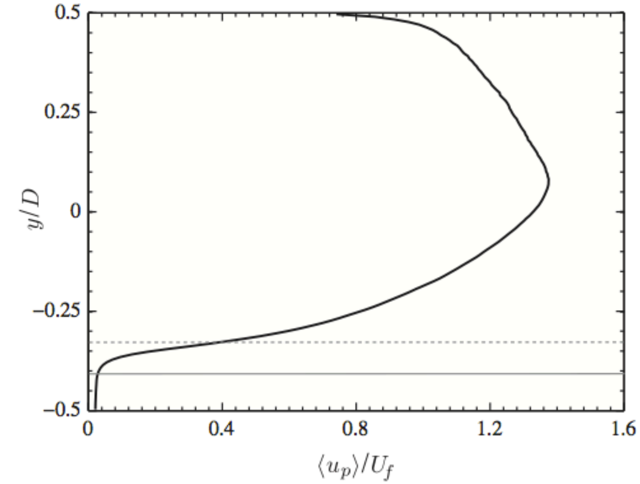
Application to liquid-solid slurries



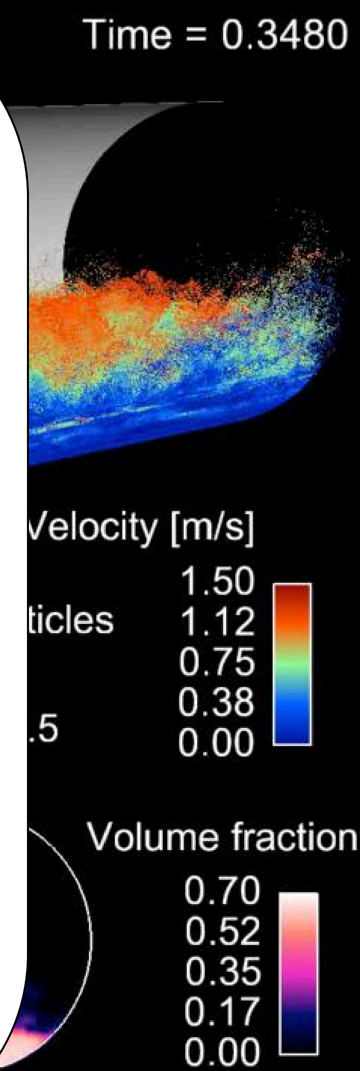
Capable of predicting onset of bed formation



(a) Solid concentration profile.



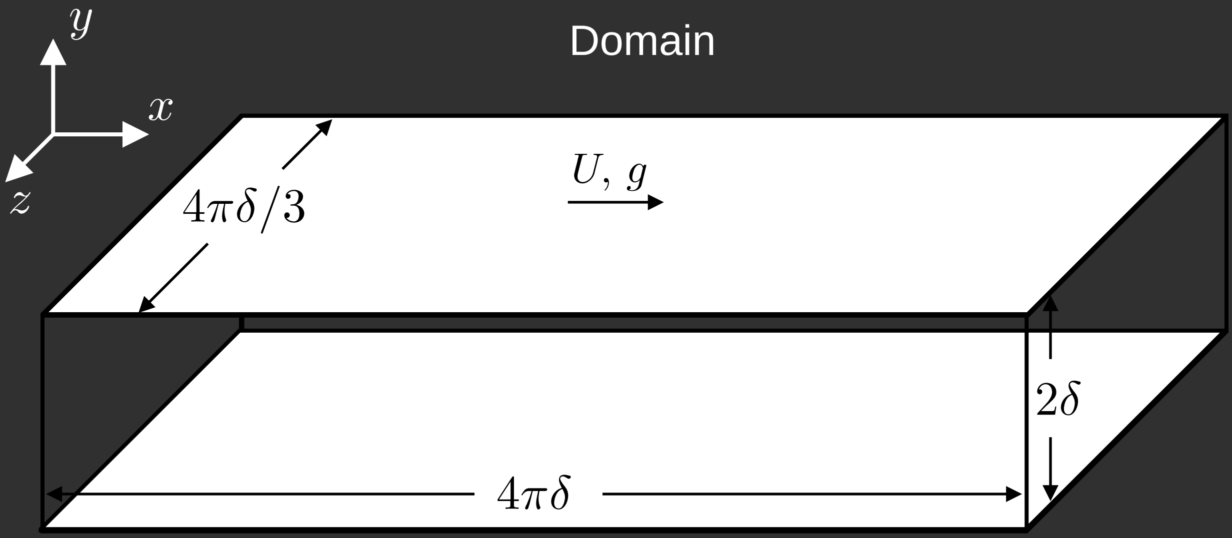
(b) Solid velocity profile.



Application to dilute channel flows

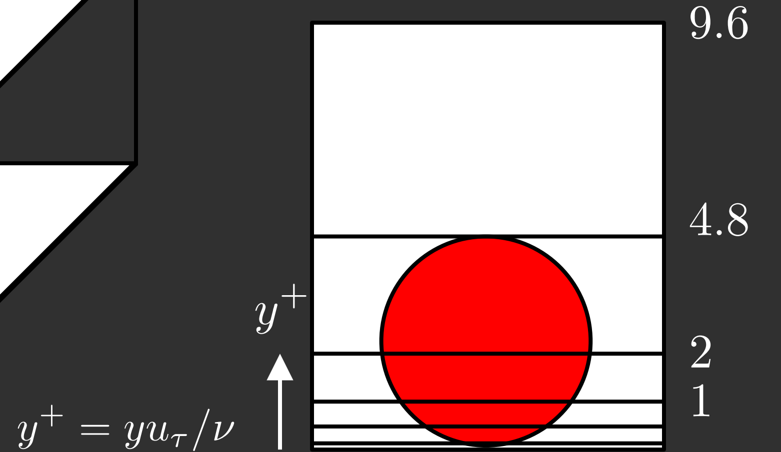
Simulation configuration

Domain



Mesh: 1000 x 272 x 320

$\Delta x^+ = 8 \quad \Delta y^+ = 4.8 \quad \Delta z^+ = 8$



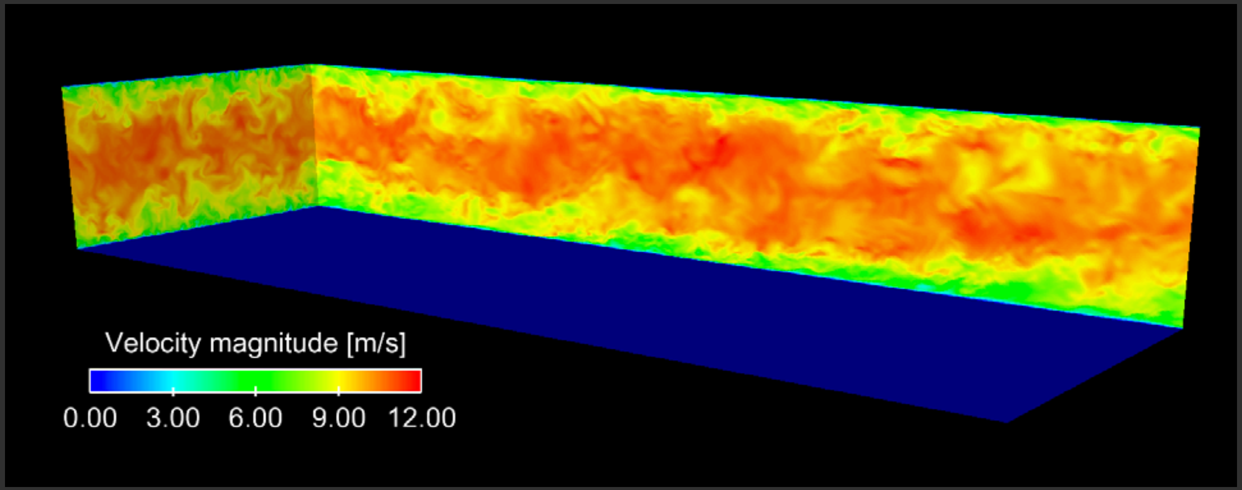
Experimental parameters

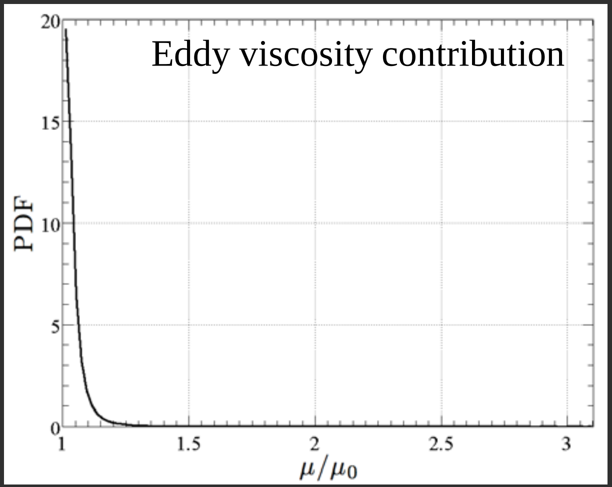
- δ = 2 cm
- $Re_{2\delta}$ = 13,850
- Bulk velocity = 9.2 m/s
- Centerline velocity, U_{cl} = 10.5
- Particle diameter = 150 μm
- Particle density = 2,500 kg/m^3
- St = 50

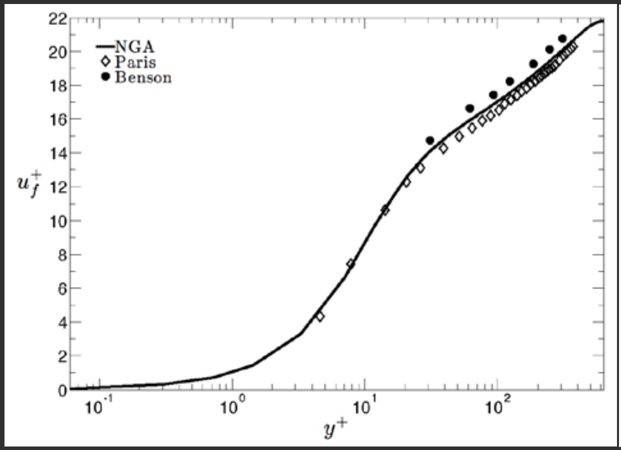
	Re_τ	ϕ	Wall boundary condition
Paris & Eaton (2001)	644	0.2	Rough
Benson & Eaton (2003)	617	0.15	Smooth
NGA	630	0.15	Smooth

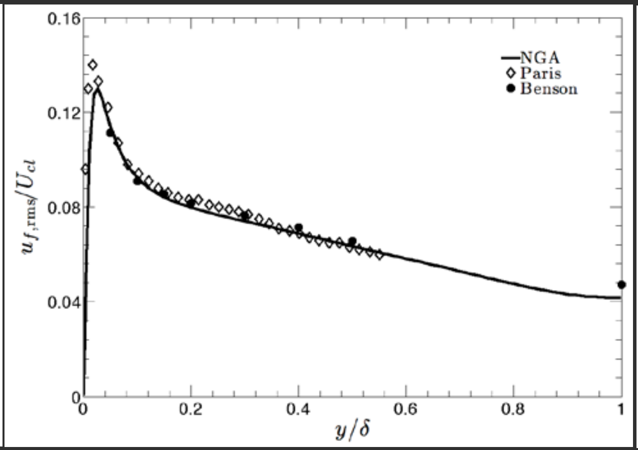
Application to dilute channel flows

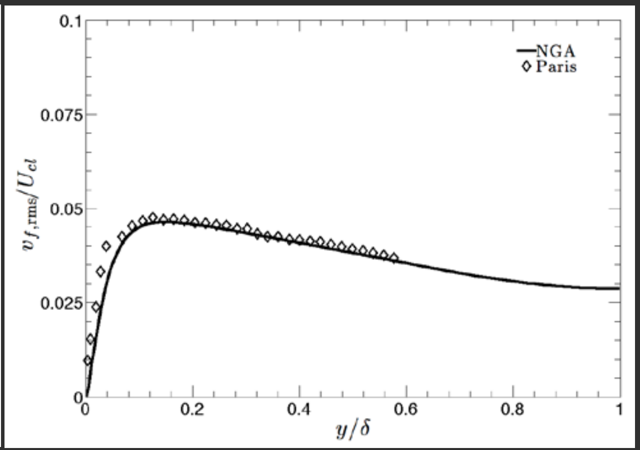
Single-phase channel flow











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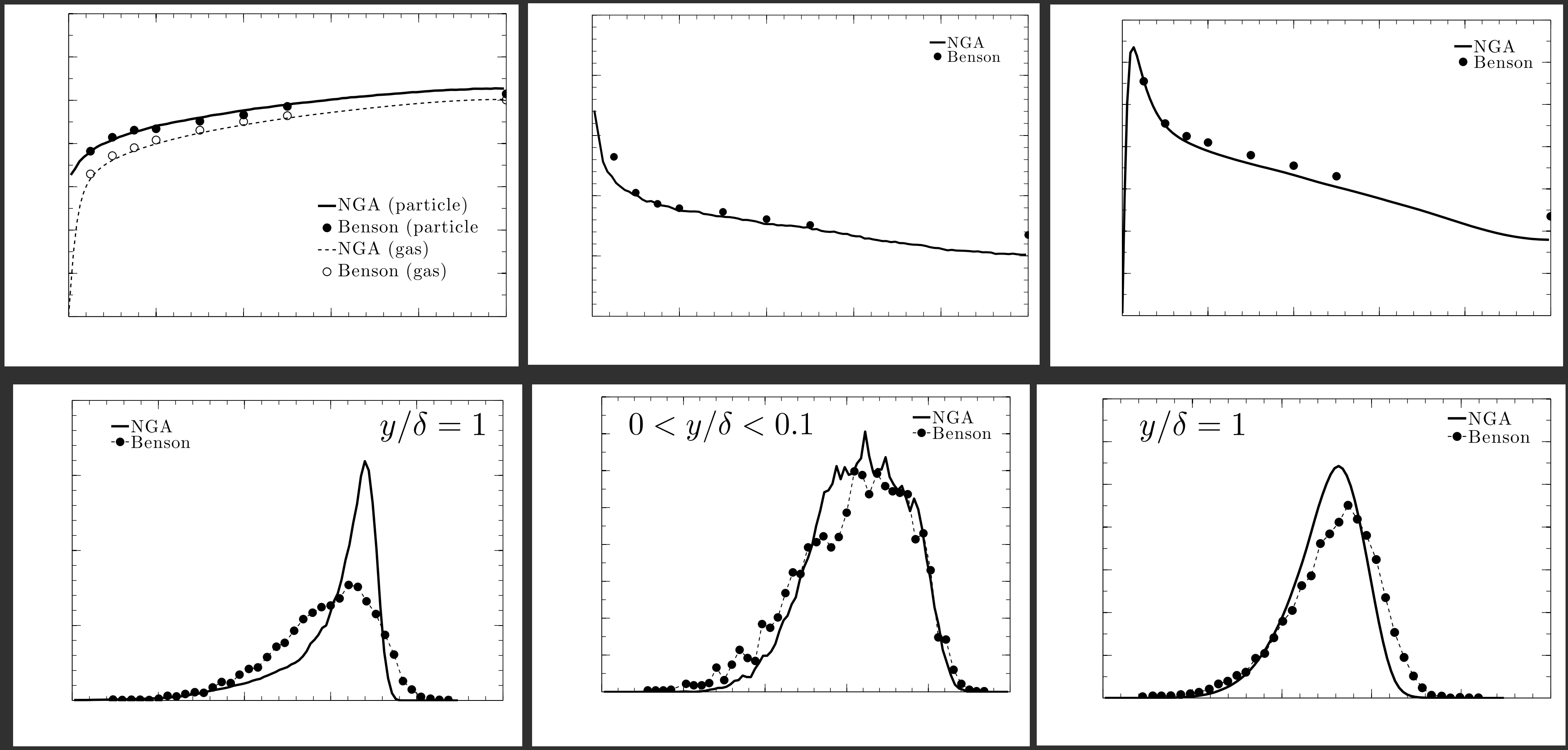
Application to dilute channel flows

Particle-laden channel

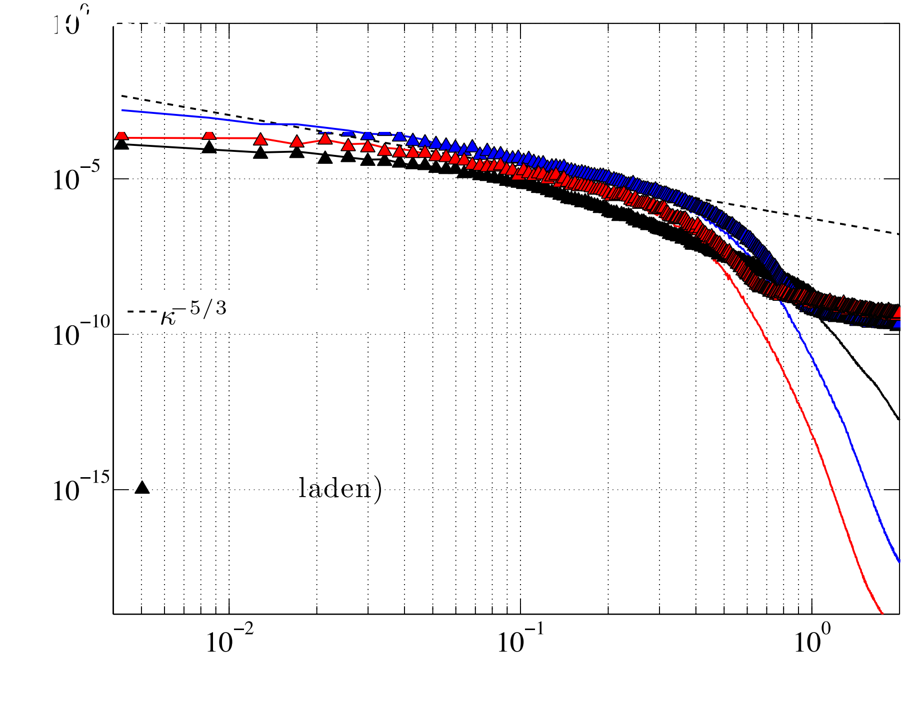


Application to dilute channel flows

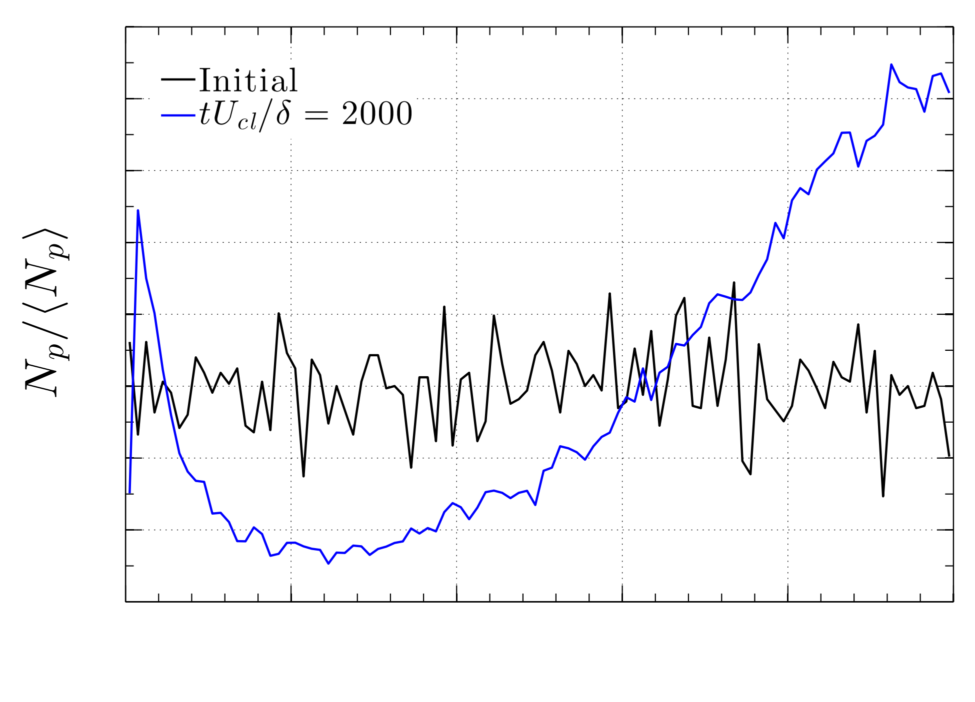
Particle-laden channel

Turbulence modulation & preferential concentration due to non-uniform interphase coupling

1D kinetic energy



Particle number density

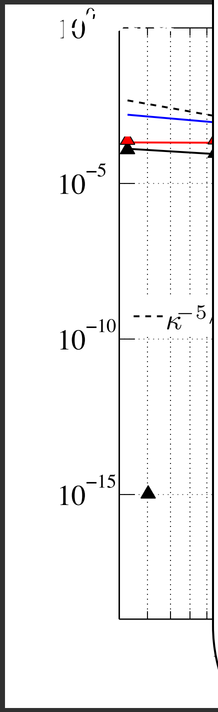


Application to dilute channel flows

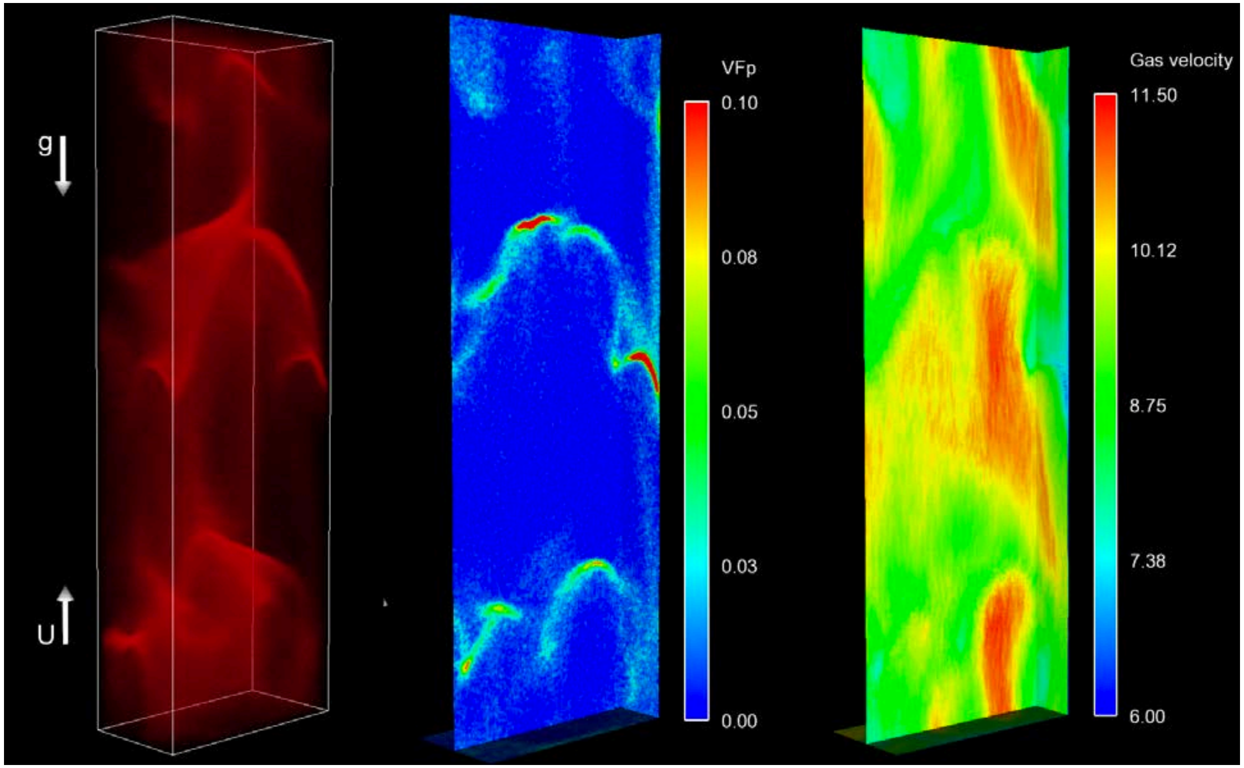
Particle-laden channel

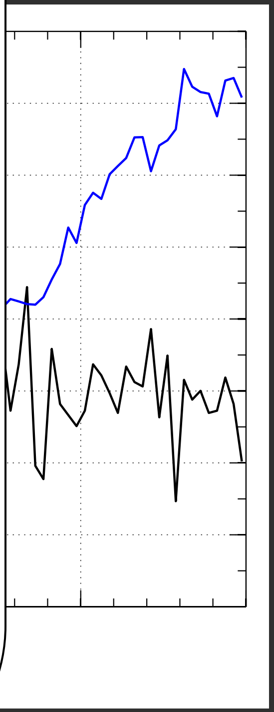
Turbulence r ... **pling**

1D kinetic



Extend to moderately-dilute flows





Application to risers

- Dimensional analysis

$$\text{Fr} = U/\sqrt{g d_p} \qquad \text{Ar} = \rho_s \rho_f d_p^3 g/\mu^2 \qquad D/d_p$$

- Experimental observations (Noymer & Glicksman, 2000)
  - Clusters fall very close to the walls (~100 μm)
  - Clusters located within hydrodynamic boundary layer
  - Cluster fall velocity independent of inflow conditions

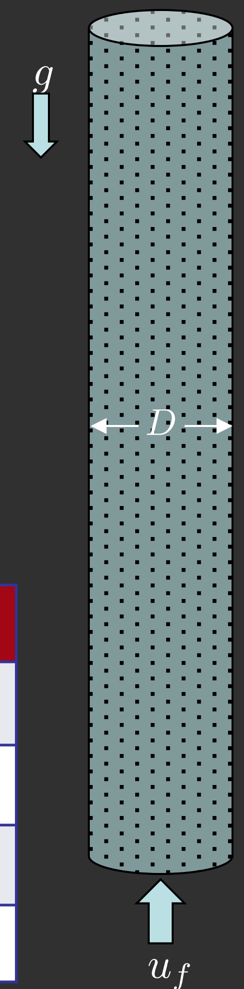
$$\frac{u_{cl}}{u_{mf}} = \frac{1000}{\sqrt{\text{Ar}}} \qquad u_{mf} = 0.00075 \frac{\rho_s g d_p^2}{\mu}$$

$$u_{cl} = 0.75 \sqrt{\frac{\rho_s}{\rho_f} g d_p}$$

- Simulation parameters
  - 3D pipe geometry (immersed boundaries)
  - Periodic in vertical direction
  - 760,000 particles
  - Mesh: 800x83x83

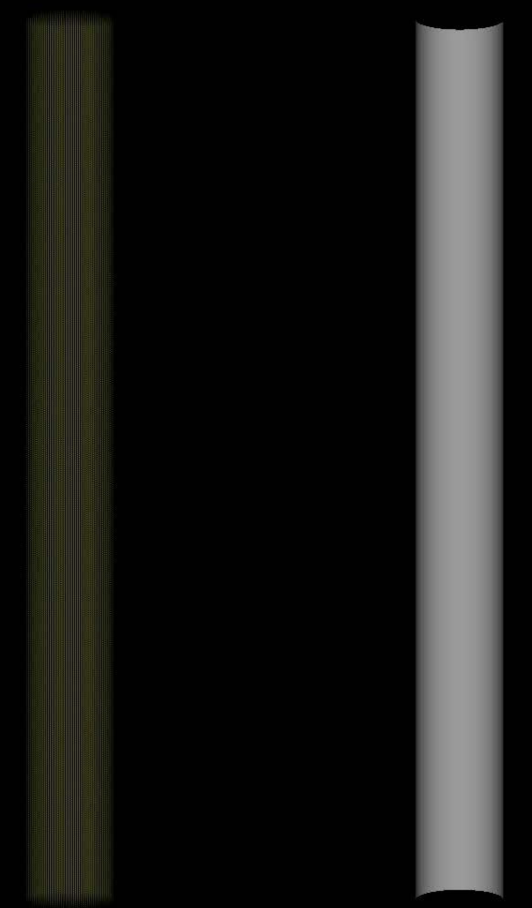
Simulation cases

	Case 1	Case 2	Case 3	Case 4	Case 5
Ar	50	100	500	2500	12500
D/d_p	320	150	150	150	150
$\langle \varepsilon_p \rangle$	0.15%	1.5%	1.5%	1.5%	1.5%
ρ_p/ρ_f	2500	2500	2500	2500	2500



Application to risers

Case 4: Ar=2500

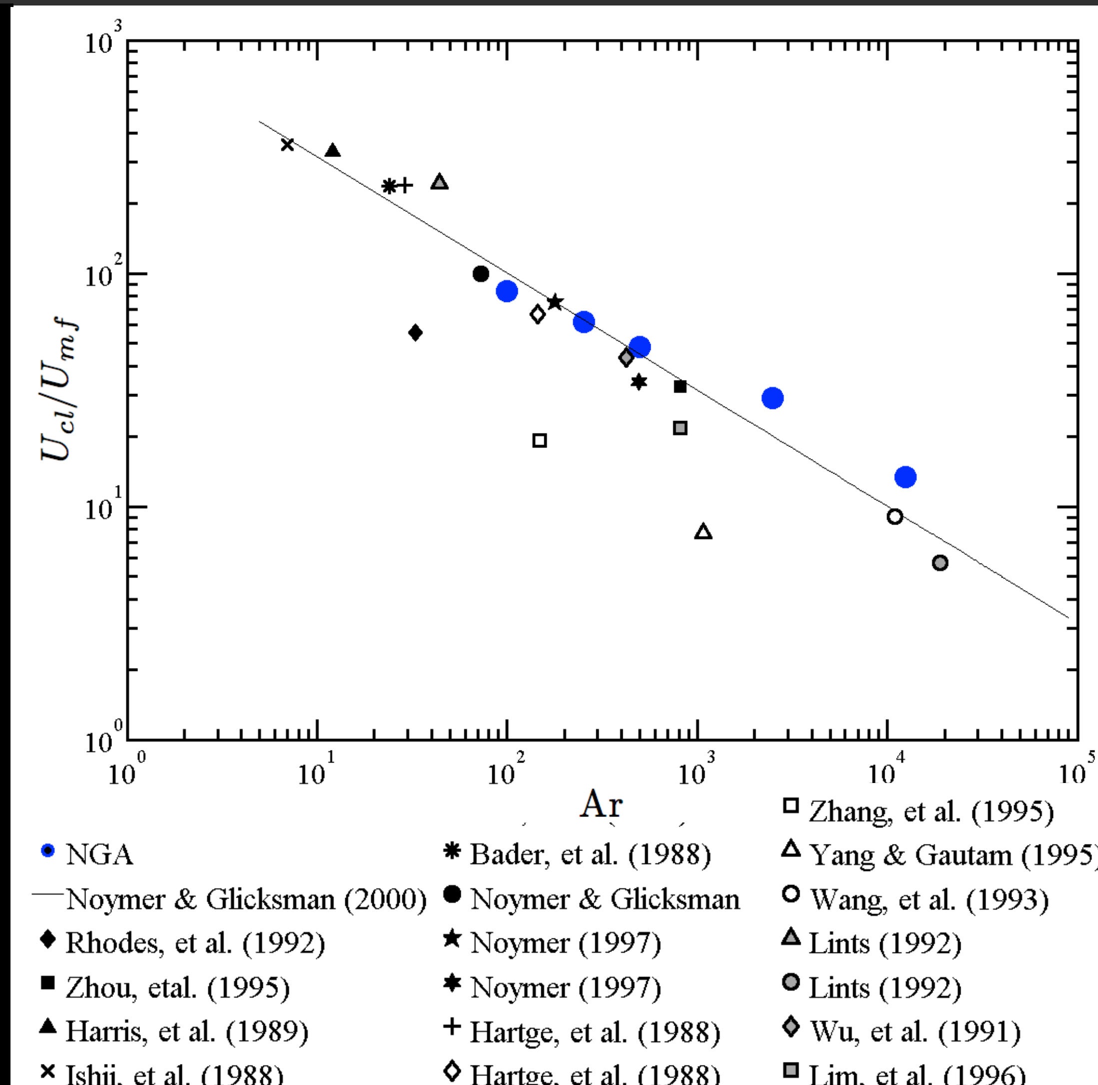


Particle position

Iso-surface of particle concentration (ε_p=3σ)

Cluster fall velocity

- Computed from tracking of identified cluster structures
- Compared to experimental correlation of Noymer & Glicksman (2000)



Conclusions

- Volume filtered formalism provides a consistent framework from point-particle to fully resolved simulations
- Pushing the validity of classical microscale models to finer meshes yields excellent results
- The proposed framework can capture a range of phenomenon including
  - Clustering
  - Bubbling
  - Segregation in particle size
  - Preferential concentration
- Looking forward
  - Study intermediate values of particle diameter to mesh size ratio ($1 \lesssim d_p/\Delta x \lesssim 10$)
  - Implement sharper / higher accuracy filters
  - Use this framework to provide closure for RANS modeling:

R.O. Fox, J. Capecelatro, O. Desjardins
Validation of a Multiphase Turbulence Model Using Mesoscale DNS of Gravity-Driven Gas-Particle Flow. 11:50-12:10 PM