Development of a multiphase PIC model for slurry flow modeling

NATIONAL ENERGY TECHNOLOGY LABORATORY

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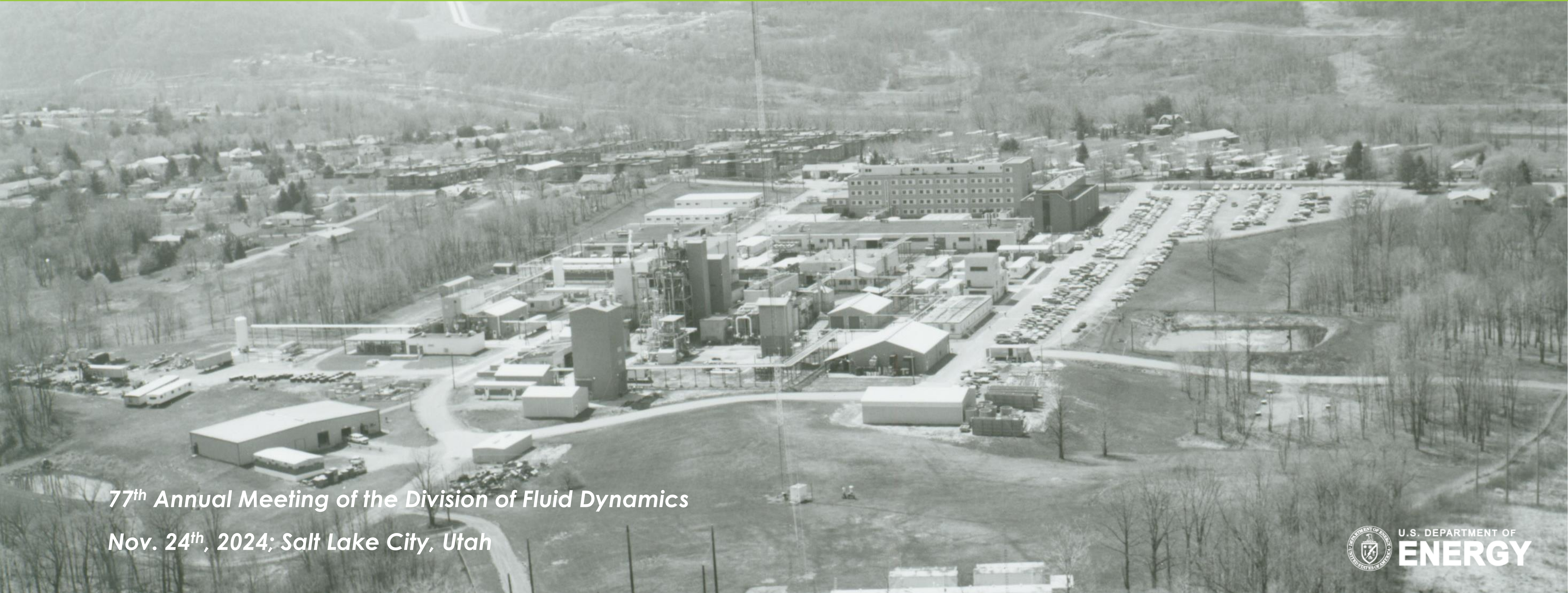

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U.S. DEPARTMENT OF ENERGY

MFIXExa overview

- MFIX-Exa is a massively-parallel, high-performance multiphase flow code
- Targeted physics: reacting gas-solid flows from dilute particle-laden to dense granular
- CFD+ high-fidelity DEM or low-fidelity PIC

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- Scaled up to 60k GPUs on OLCF's Frontier (65,535 weak scaling, 62078 challenge problem)

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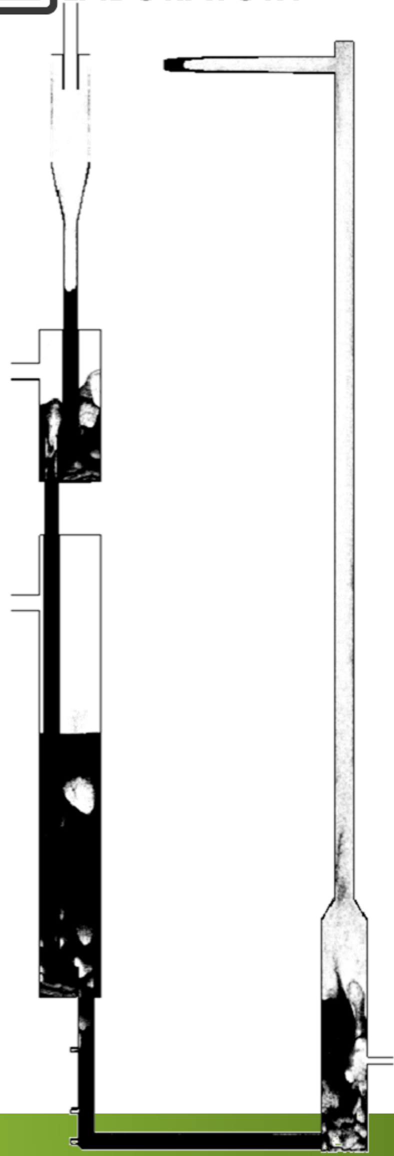
- Challenge problem: NETL's 50kW CLR

ECP EXASCALE COMPUTING PROJECT

AMReX



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problem of interest

https://www.engineeringtoolbox.com/slurry-transport-velocity-d_236.html

- Liquid fluid and solid particle slurry flow (coal liquefaction driving interest)
- Plethora of data for horizontal pipe flow which is very industrially relevant
- Start with pressure drop (head loss) vs velocity relationship
- Reference: Gillies & Shook (2000) “Modelling High Concentration Settling Slurry Flows” *Canadian J. of Chem. Eng.*, **78**, 709-716.

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Fluid: water

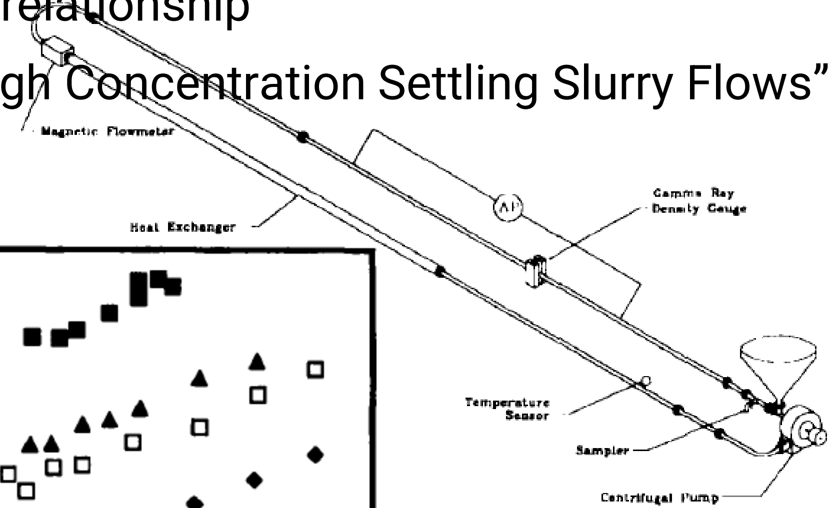
- $T = 25°\mathrm{C}$
- assume $\rho_f = 1000\ \mathrm{kg/m^3}$
- assume $\mu_f = 0.001\ \mathrm{Pa\text{-}s}$

Particles: sand

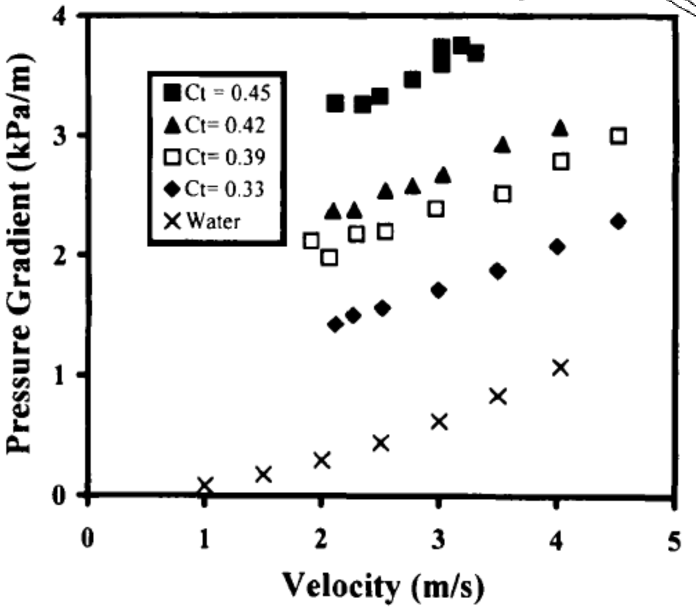
- $d_p = 420$ micron
- $\rho_p = 2655\ \mathrm{kg/m^3}$
- assume monodispersed

Pipe diameter

- $D = 10.5$, 26.4 and 49.6 cm



Schaan et al. (2000)



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previous work

Table 1
Previous numerical studies on slurry pipe flows.

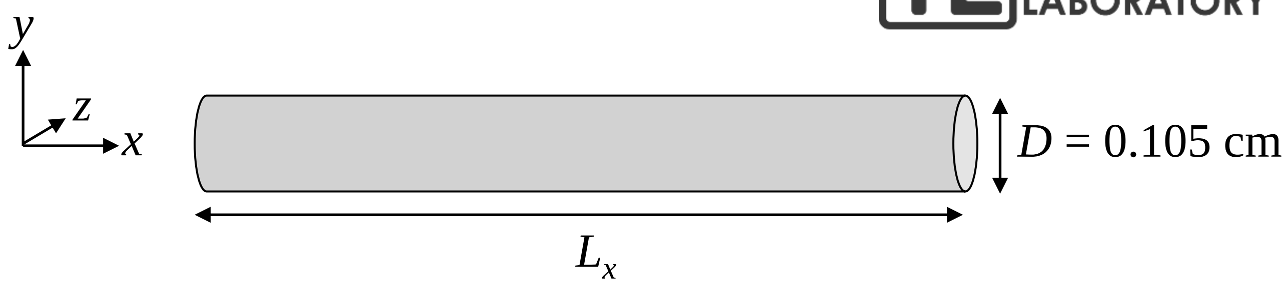
Reference	Approach	Flow regime	Fluid	Particles	ρ_p [kg/m^3]	d_p [mm]	D [mm]	V_m [m/s]	$\langle\alpha_s\rangle_A$ [−]
Capecelatro and Desjardins [17]	LES + DPM	SB, HS	Water	Sand	2650	0.165	51.5	0.83, 1.6	0.084
Arolla and Desjardins [18][a]	LES + DPM	SB, HS	Water	Sand	2650	0.280	69	–	–
Uzi and Levy [12]	RANS+DPM	MB, HS	Brine	NaCl	2150	1.0–4.0	50–100	0.6–4.0	0.05–0.30
Hernández et al. [21]	(KTGF)-TFM	HS, PS	Water	Sand	≈ 2381	0.030–0.110	22.1	1.0–3.0	0.0025–0.20
Bossio et al. [22]	(KTGF)-TFM	MB, HS, PS	Laterite	Sand	2381	0.110	26.84	0.671–4.697	0.036–0.083
Ekambara et al. [23]	KTGF-TFM	BF, FS	Water	Sand, glass beads	2470, 2650	0.090–0.500	50–500	1.5–5.5	0.08–0.45
Antaya et al. [24]	KTGF-TFM(MFM)	FS	Water	Sand	2650	0.100–0.370	51.5, 150	2.0–6.0	0.20–0.43
Hashemi et al. [25]	KTGF-TFM	–	Water	Sand	2650	0.370	265	4.0, 6.0	0.20–0.40
Kaushal et al. [26]	KTGF-TFM, MM	FS	Water	Glass beads	2470	0.125	54.9	1.0–5.0	0.30–0.50
Gopaliya and Kaushal [27]	KTGF-TFM	FS	Water	Sand	2650	0.18–2.4	53.2	1.8, 3.1	0.15–0.45
Gopaliya and Kaushal [28]	KTGF-TFM	FS	Water	Sand	2650	0.165–0.55	263	3.5–4.7	0.10–0.34
Kumar et al. [29]	KTGF-TFM	FS	Water	Iron ore	4350	0.012	105	1.35–5.11	0.0263–0.31
Singh et al. [30]	KTGF-TFM	FS	Water	Coal	1560	0.059–0.206	50–150	2–5	0.30–0.60
Roco and Balakrishnam [33]	TFM	BF, FS	Water	Sand, glass beads	–	0.165–0.580	40, 51.5	1.05–4.17	0.07–0.189
Messa et al. [35]	TFM	FS	Water	Sand, glass beads	2440, 2650	0.090–0.370	53–150	1.33–8.0	0.11–0.40
Messa et al. [36]	TFM	FS	Water	Sand, glass beads	2440, 2650	0.090–0.520	50.7–150	1.33–8.0	0.09–0.40
Messa and Malavasi [37]	TFM	MB, FS	Water	sand	≈2650	0.090–0.520	50.7–150	1.33–6.0	0.09–0.43
Messa and Malavasi [38]	TFM	FS	Water	Sand	≈2650	0.090–0.640	50–200	2.0–9.0	0.07–0.41
Chen et al. [39]	KTGF-MFM	HS, PS	Water	Coal	1465	0.065 + 0.345	25–50	0.2–5	0.38–0.538
Li et al. [40]	KTGF-MFM	MB, HS, PS	Water	Glass beads	2470	0.125 + 0.440	54.9	2.0–5.0	0.20–0.50
Li et al. [41]	KTGF-MFM	MB, HS, PS	Water	Glass beads	2470	0.125 + 0.440	54.9	2.0–4.0	0.20–0.40
Ling et al. [42]	MM	BF, FS	Water	Silica/zircon sand	2380, 4223	0.11	22.1	1.0–3.0	0.10, 0.20
Lin and Ebadian [43]	MM	BF, FS	Water	Silica/zircon sand	2380, 4223	0.11	22.1	1.0–3.0	0.10, 0.20
Silva et al. [44]	MM	SB, MB, FS	Saline water	Glass beads	2500	0.10–0.60	100	1.0–3.0	0.008–0.11

Messa & Matoušek (2020)

model setup

Model overview:

- cylindrical EB: $L_x = 8\mathrm{D}$
- periodic in x with enforced Δp_f
- no slip wall EB
- uniform grid
- boundary adjacent cut-cells
- $dx = D/16 \;\rightarrow\; W_{st} = 72.9 \;\rightarrow$ too coarse for LES
- $dx = D/32 \;\rightarrow\; W_{st} = 9.11 \;\rightarrow$ this work
- $dx = D/64 \;\rightarrow\; W_{st} = 1.14 \;\rightarrow$ why use PIC?



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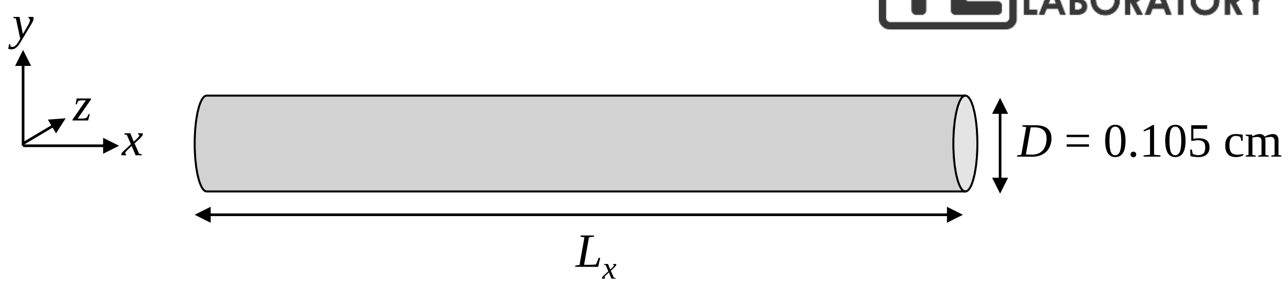

Nomenclature:

- "bulk" fluid velocity

$$\langle\langle u_f \rangle\rangle = \frac{\langle \varepsilon_f u_f \rangle}{\langle \varepsilon_f \rangle} = \frac{\frac{1}{\pi R^2 L_x} \int \varepsilon_f u_f \, dV}{\frac{1}{\pi R^2 L_x} \int \varepsilon_f \, dV}$$

$$\langle\langle\langle u_f \rangle\rangle\rangle = \frac{1}{\delta t} \int \langle\langle u_f \rangle\rangle \, dt$$

governing equations

“base model”

Lagrangian: discrete particles as *parcels*

$$\frac{d\boldsymbol{x}_i}{dt} = \boldsymbol{u}_i \quad \text{and} \quad m_i \frac{d\boldsymbol{u}_i}{dt} = m_i \boldsymbol{g} + \frac{V_p}{\varepsilon_p} \nabla \tau_p + \boldsymbol{F}_{fi}$$

Eulerian: continuous fluid

$$\nabla \cdot \varepsilon_f \boldsymbol{u}_f = 0 \quad \text{and} \quad \rho_f \left(\frac{\partial \varepsilon_f \boldsymbol{u}_f}{\partial t} + \nabla \cdot \varepsilon_f \boldsymbol{u}_f \boldsymbol{u}_f \right) = -\varepsilon_f \nabla \pi_f + \nabla \cdot \boldsymbol{\tau}_f + \boldsymbol{M}_{pf} + \rho_f \varepsilon_f \boldsymbol{g}$$

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$$\mu_f \longrightarrow \mu_{eff} = \mu_f + \mu_t + \mu_s$$

governing equations

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governing equations

$F_{fi} = (-\nabla \tau_f) V_p$

$+ F_D$

$F_D \propto u_R^2$, C_D = Gidaspow

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$F_{fi} = (-\nabla \tau_f) V_p + F_D + F_{vm}$

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$F_{fi} = (-\nabla \tau_f) V_p + F_D + F_{VM} + F_L + ?\ F_{TD} \rightarrow \propto k \nabla \varepsilon_f$

$F_D \propto u_R^2,\ C_D = \text{Gidaspow}$; $F_{VM} \propto \frac{du_i}{dt} - \frac{Du_f}{Dt},\ C_{VM} = 0.5$; $F_L \rightarrow \propto u_R \times \nabla \times u_f$

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$N_{St} \approx 10$, probably not.

$N_{St} > 100,000\ldots$ maybe

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$N_{St} > 100,000\ldots$ maybe

Lagrangian: discrete particles as *parcels*

$$\frac{d\boldsymbol{x}_i}{dt} = \boldsymbol{u}_i \quad \text{and} \quad m_i \frac{d\boldsymbol{u}_i}{dt} = m_i \boldsymbol{g} + \frac{V_p}{\varepsilon_p} \nabla \tau_p + \boldsymbol{F}_{fi}$$

transfer

Eulerian: continuous fluid

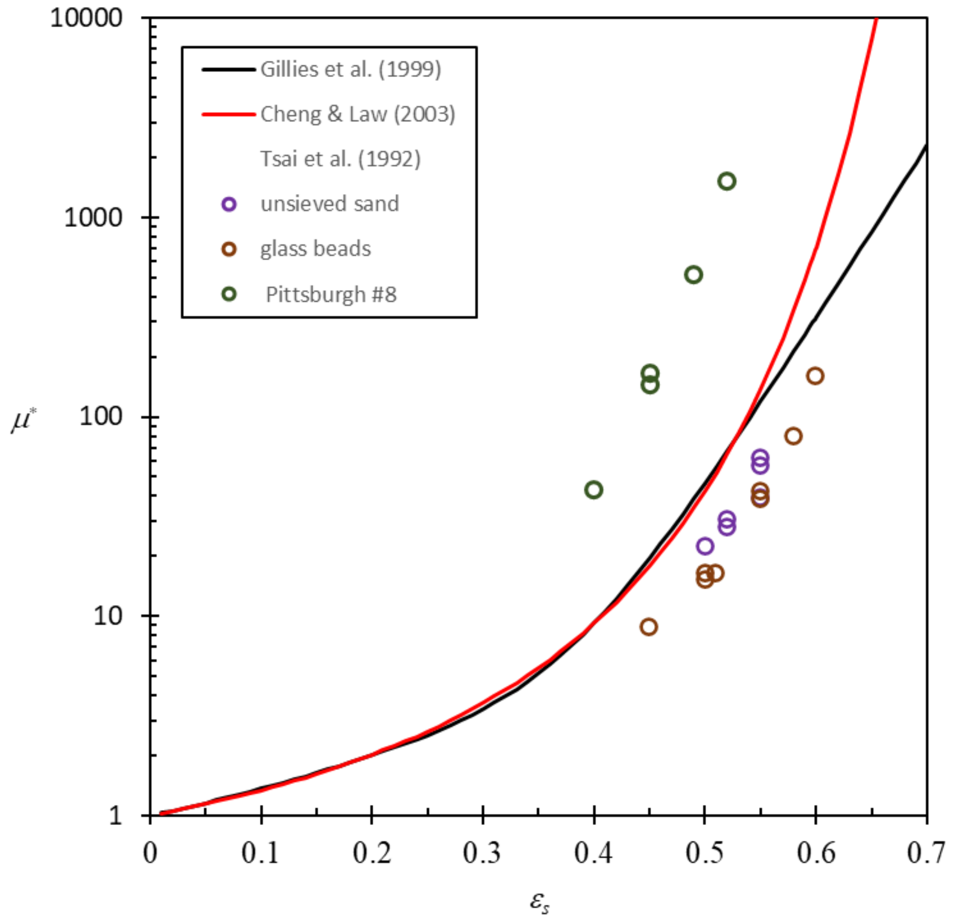
$$\nabla \cdot \varepsilon_f \boldsymbol{u}_f = 0 \quad \text{and} \quad \rho_f \left(\frac{\partial \varepsilon_f \boldsymbol{u}_f}{\partial t} + \nabla \cdot \varepsilon_f \boldsymbol{u}_f \boldsymbol{u}_f \right) = -\varepsilon_f \nabla \pi_f + \nabla \cdot \boldsymbol{\tau}_f + \boldsymbol{M}_{pf} + \rho_f \varepsilon_f \boldsymbol{g}$$

$\mu_f \to \mu_{eff} = \mu_f + \mu_t + \mu_s$

μ_t = Smagorinsky

$\mu_s = \mu(\varepsilon_p) = \{$ Einstein, Brinkman, Gibilaro, Roscoe, Krieger & Dougherty, Cheng & Law, etc.

suspension viscosity



Suspension viscosity model:

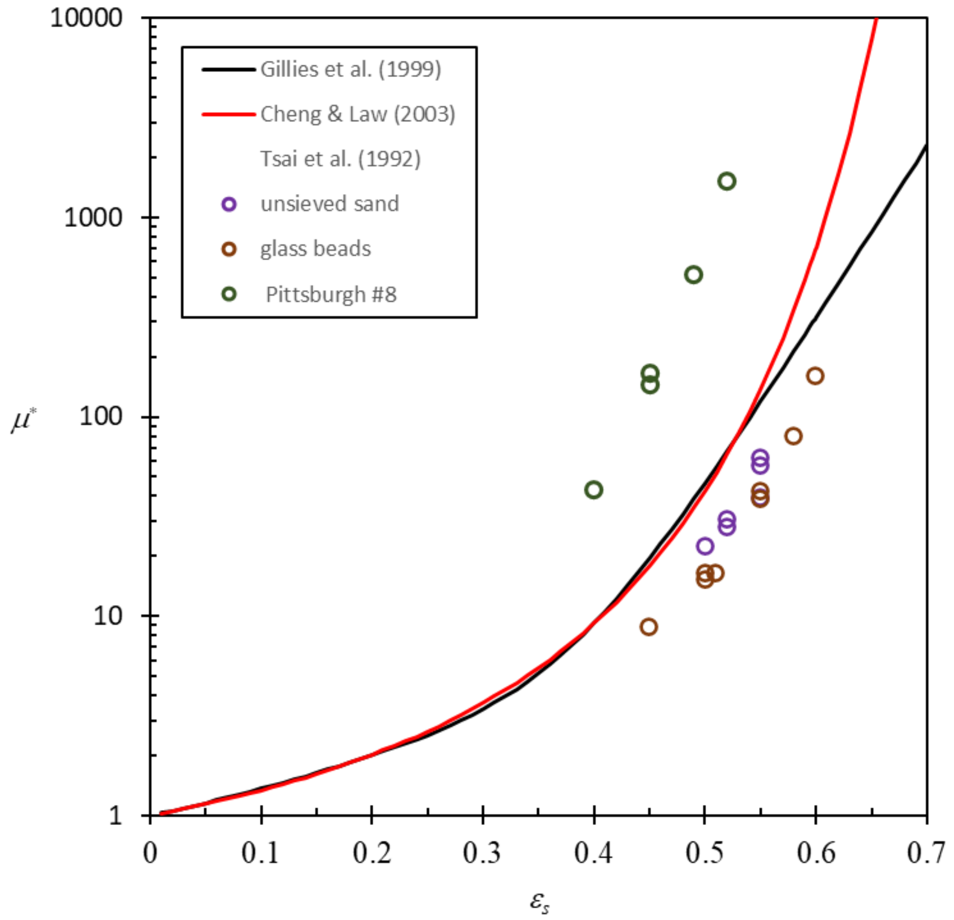
- Gillies et al. (1999)

$$\mu^* = 1 + 2.5\varepsilon_f + 10\varepsilon_f^2 + 0.0019e^{20\varepsilon_f}$$

- Cheng & Law (2003)

$$\mu^* = \exp\left[\frac{2.5}{\beta}\left(\frac{1}{(1-\varepsilon_f)^\beta} - 1\right)\right]$$

suspension viscosity



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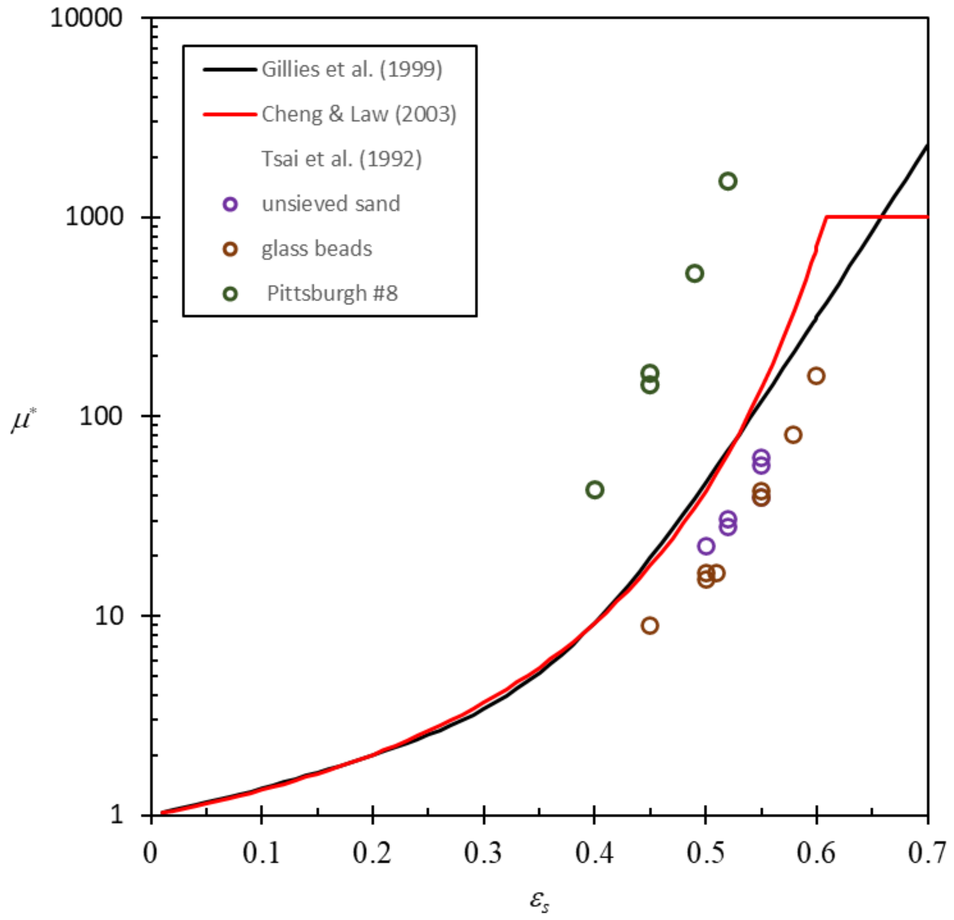
Solids stress model:

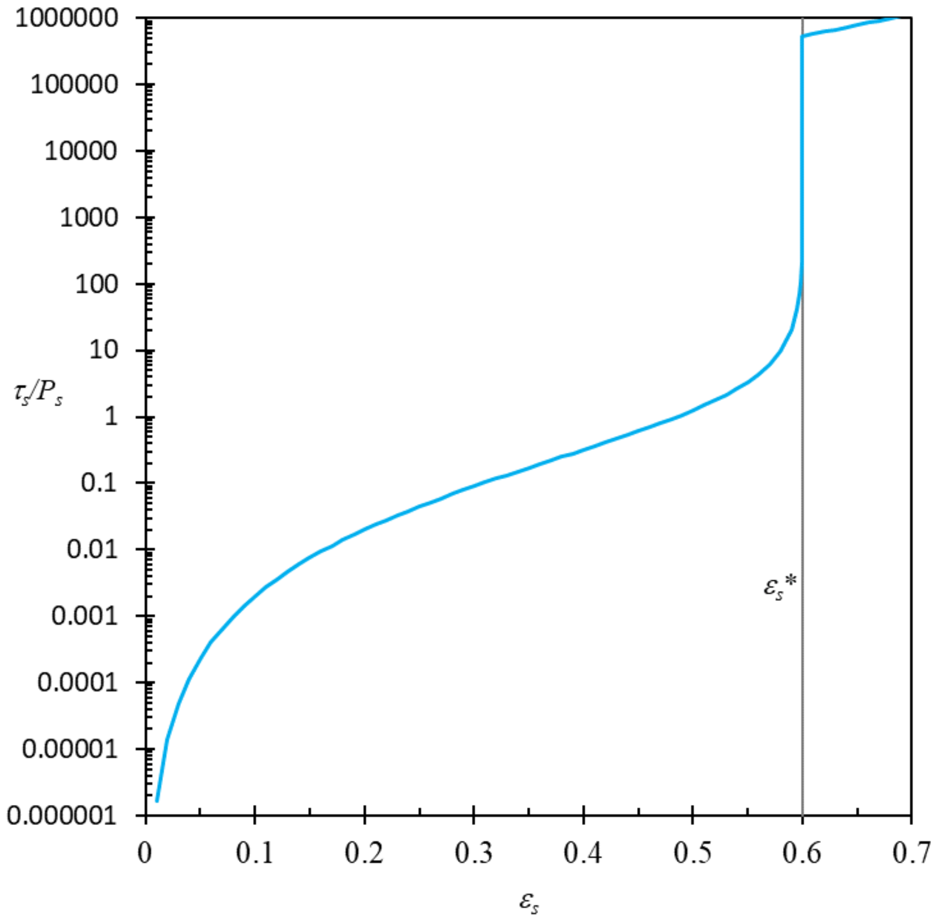
- Snider (2001), Harris & Crighton (1994)

$$\tau_s = \frac{P_s \varepsilon_s^\beta}{\max\left[(\varepsilon_s^* - \varepsilon_s), \epsilon(1-\varepsilon_s)\right]}$$

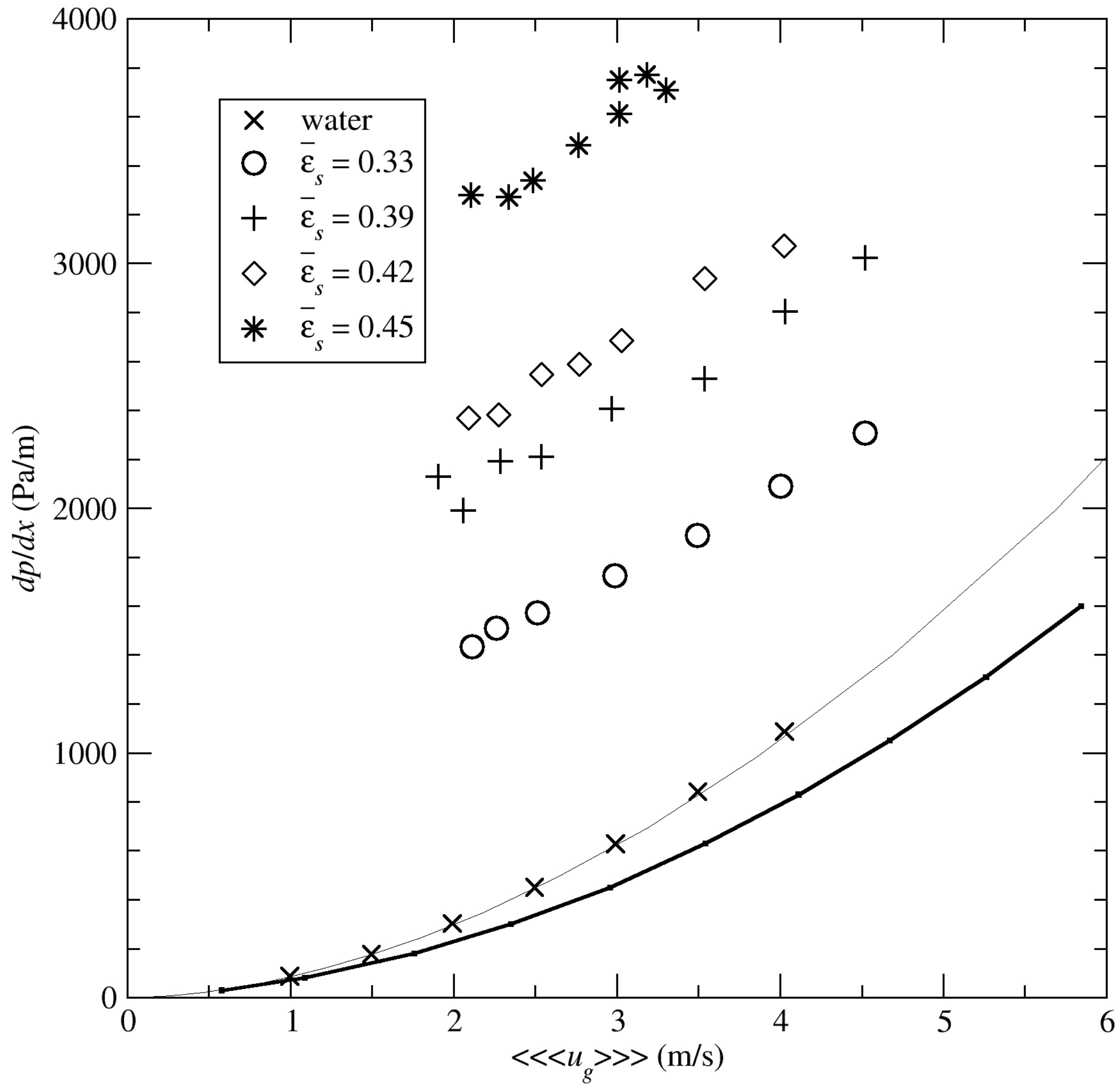
$$P_s = 100,\ \beta = 3,\ \epsilon = 10^{-6}$$

suspension viscosity





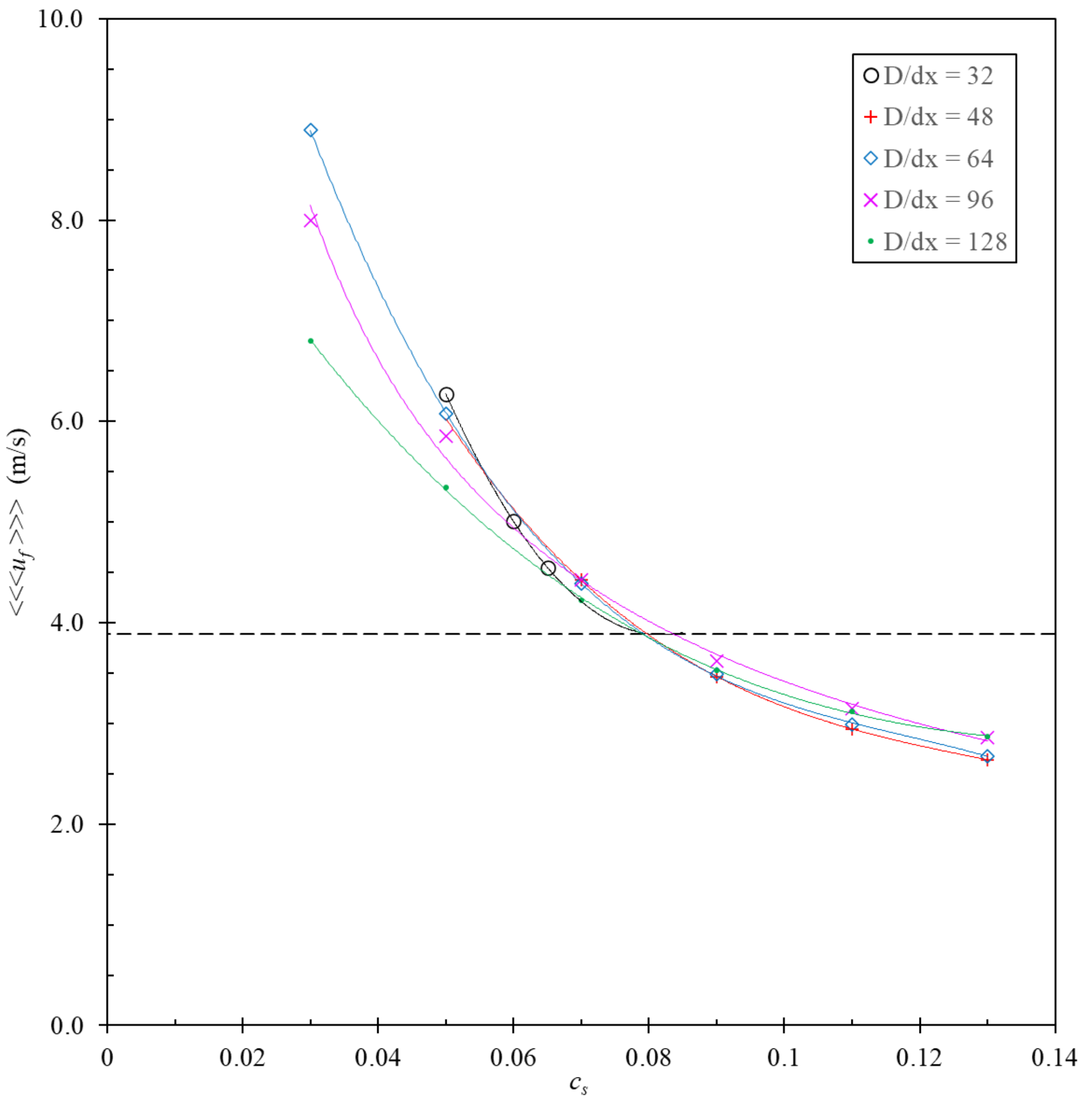
results



Darcy's law (Superpipe fit)

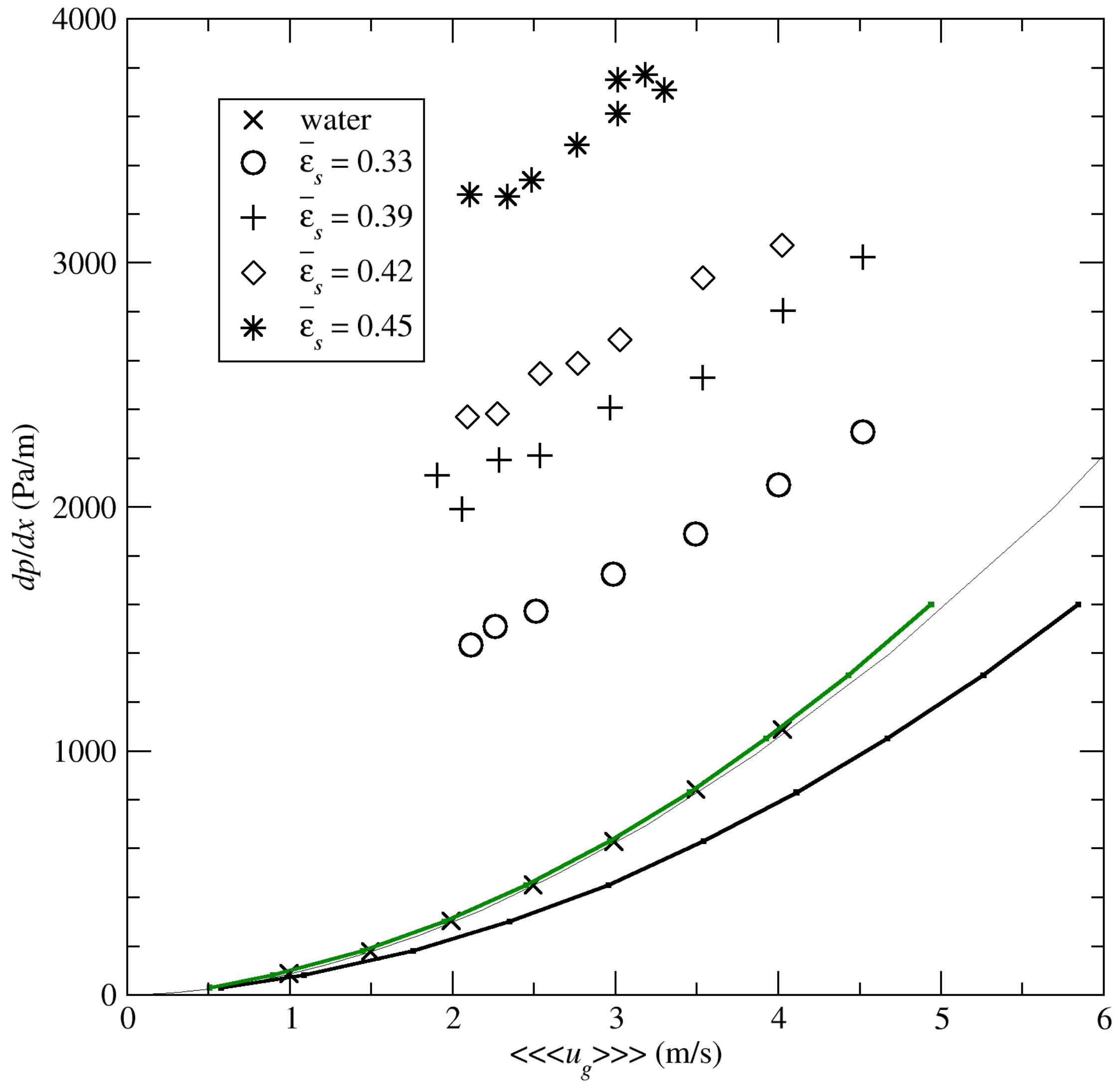
$c_s = 0.065$

Smagorinsky constant



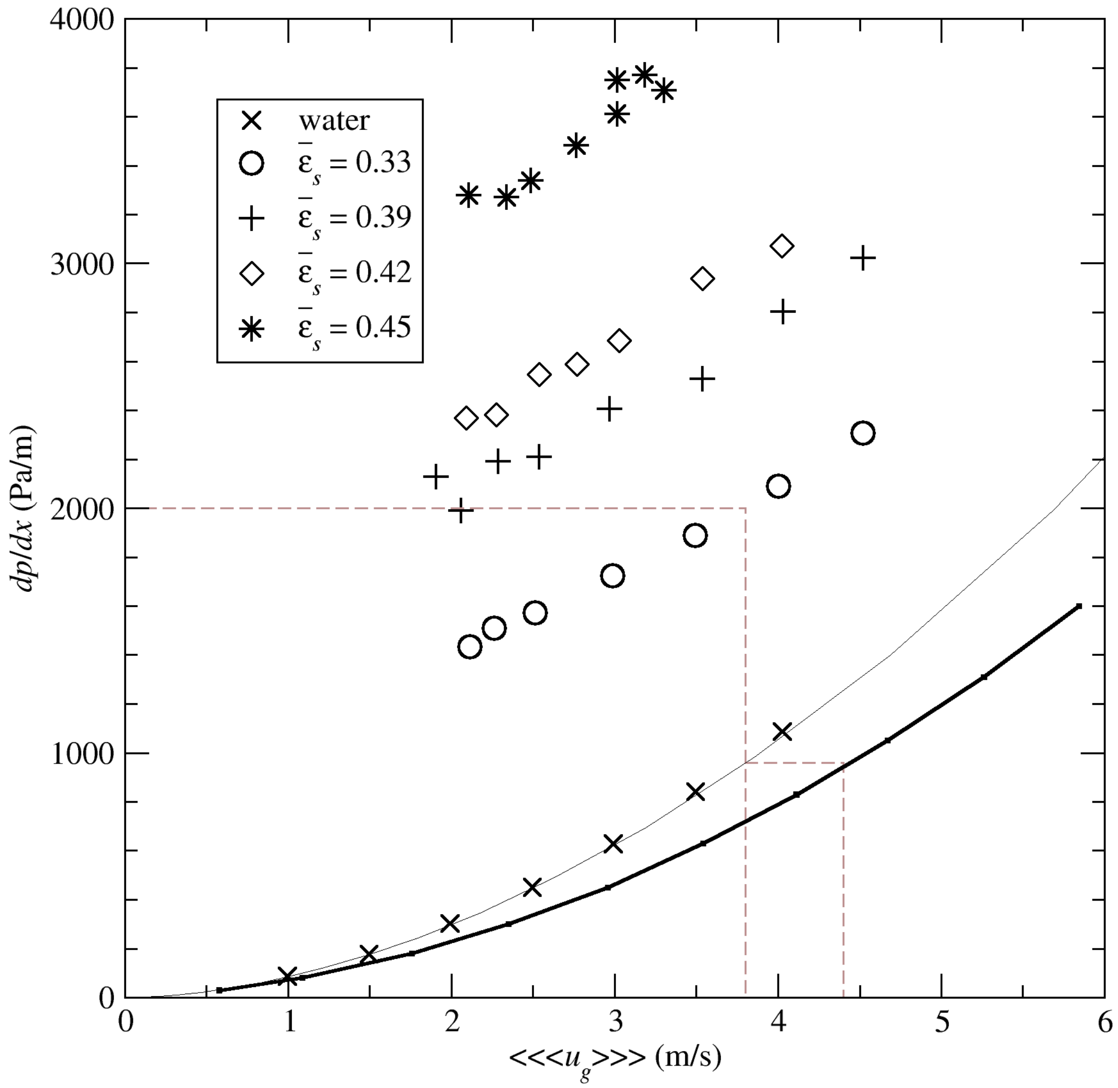
For a wide range of resolutions, we find that a constant of $c_s = 0.08$ is ideal, but this is too diffusive for this coarse grid

results



$dx = D/64$ and $c_s = 0.08$

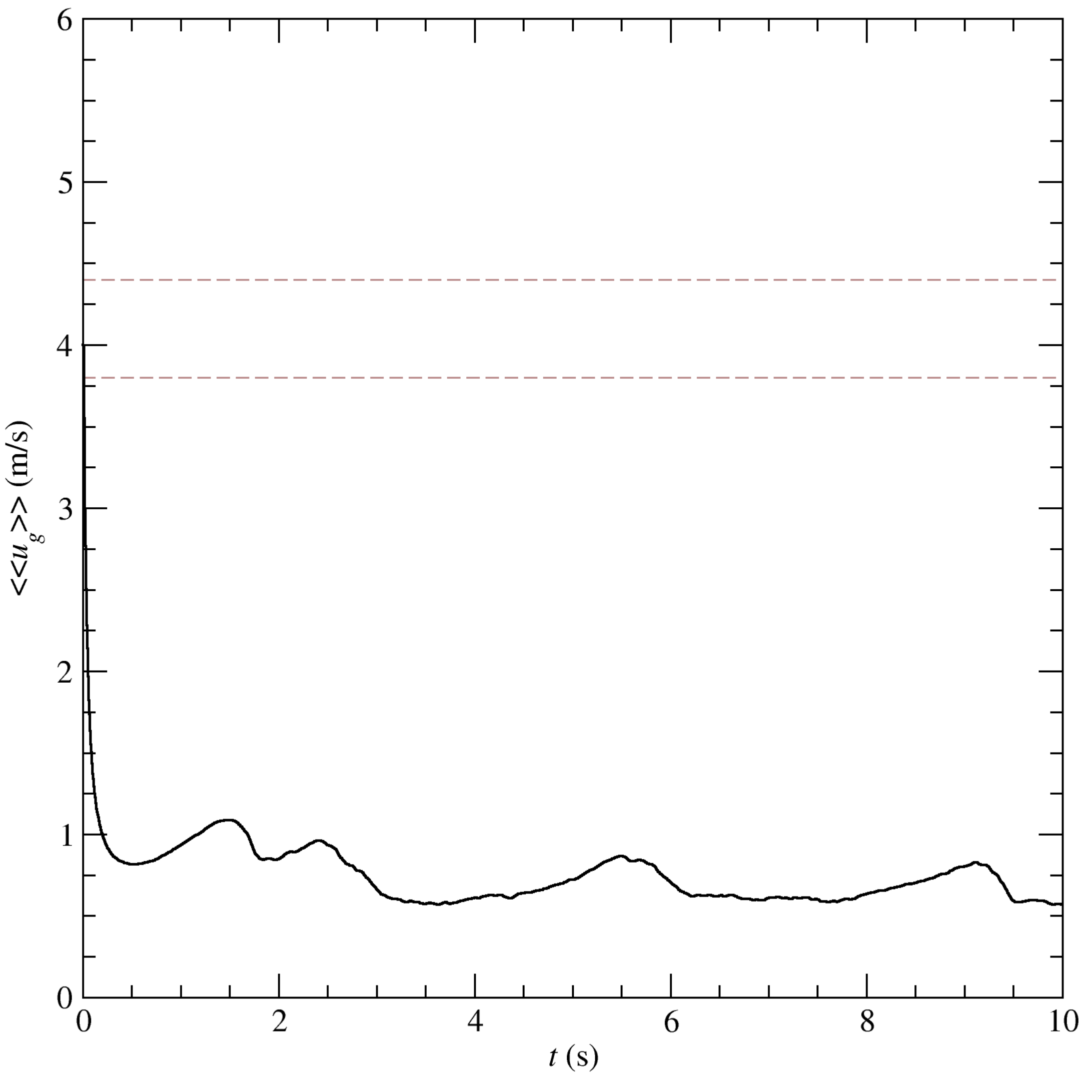
results



set: $dp/dx = 2000$ Pa/s

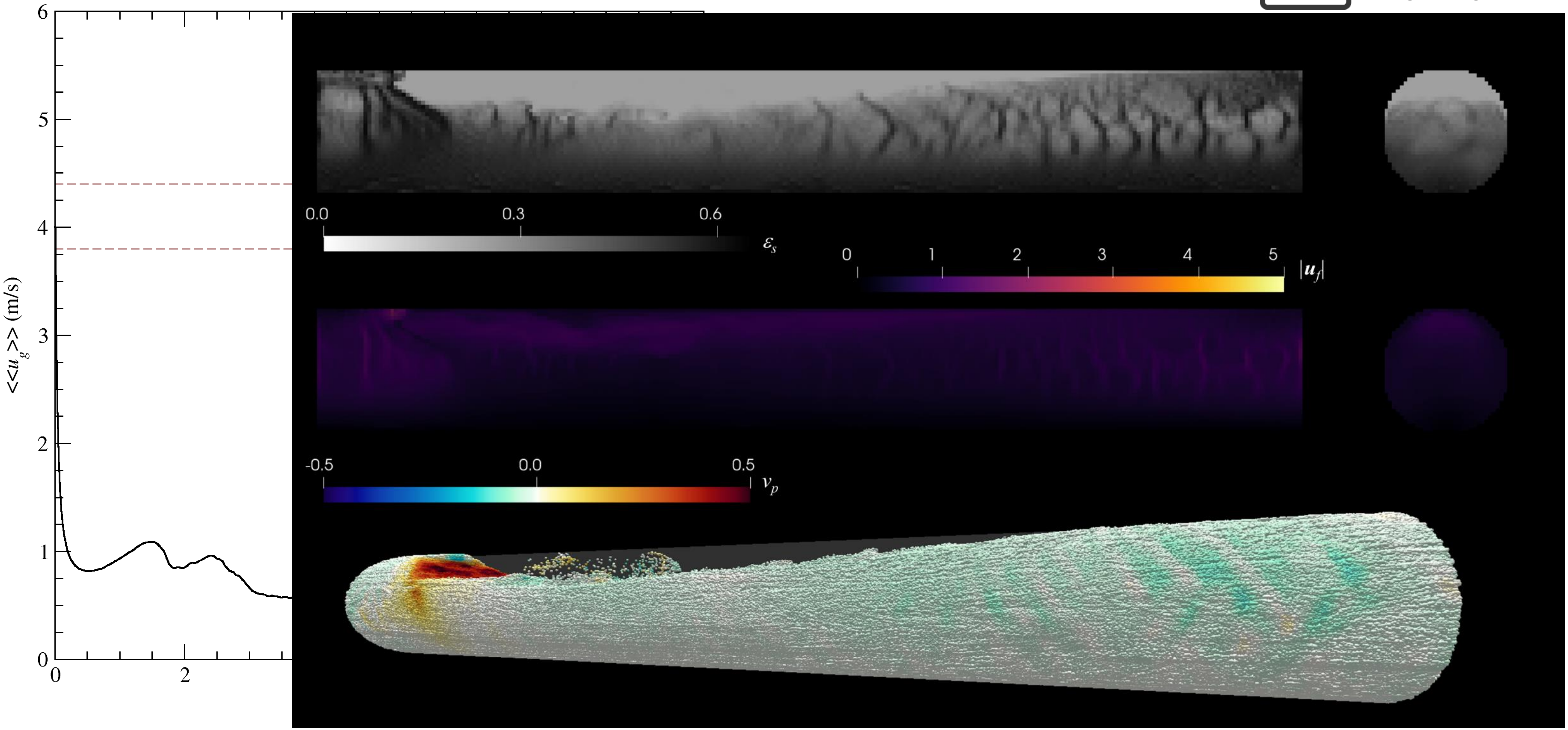
target bulk velocity: 3.8 ~ 5 m/s

results

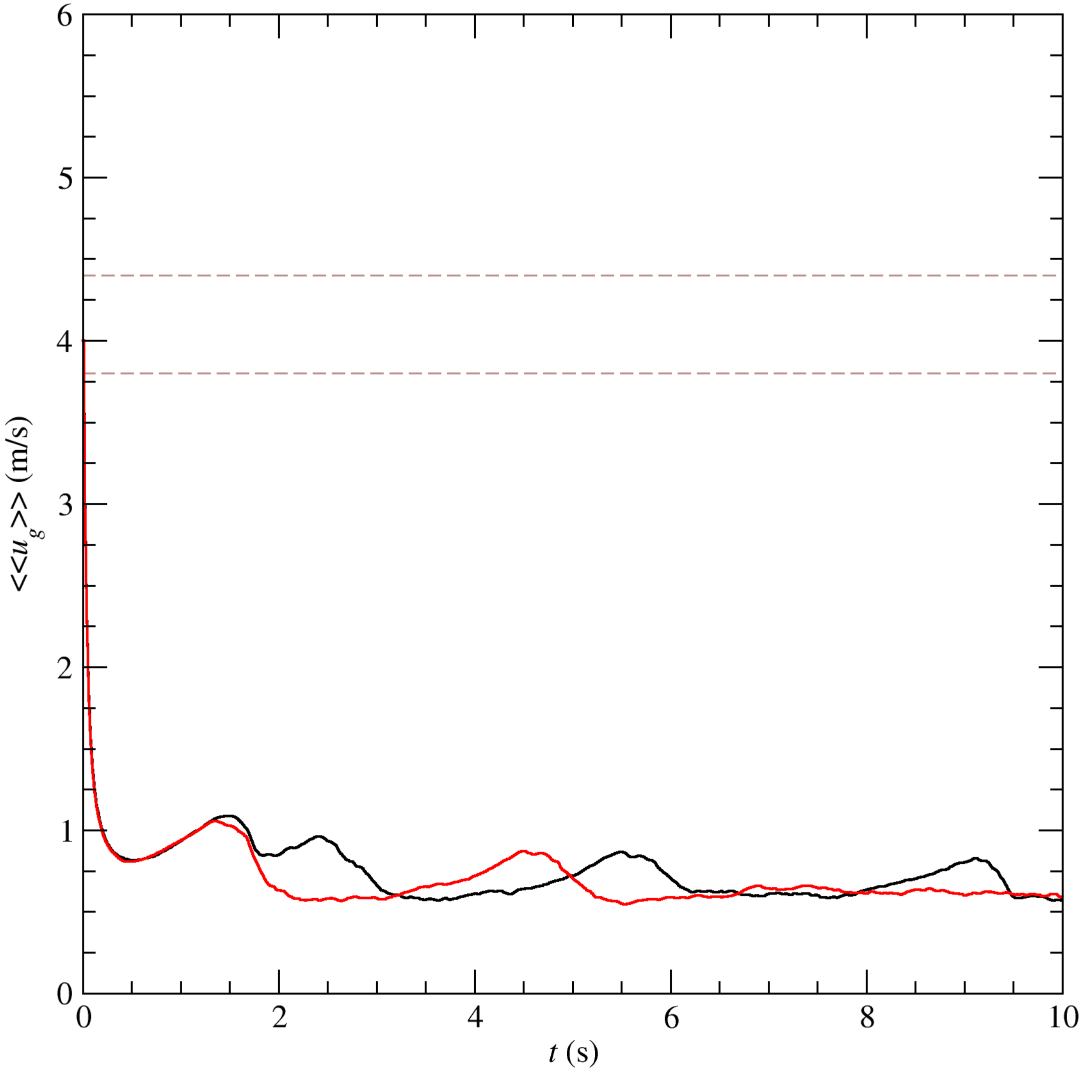


"base model"

results

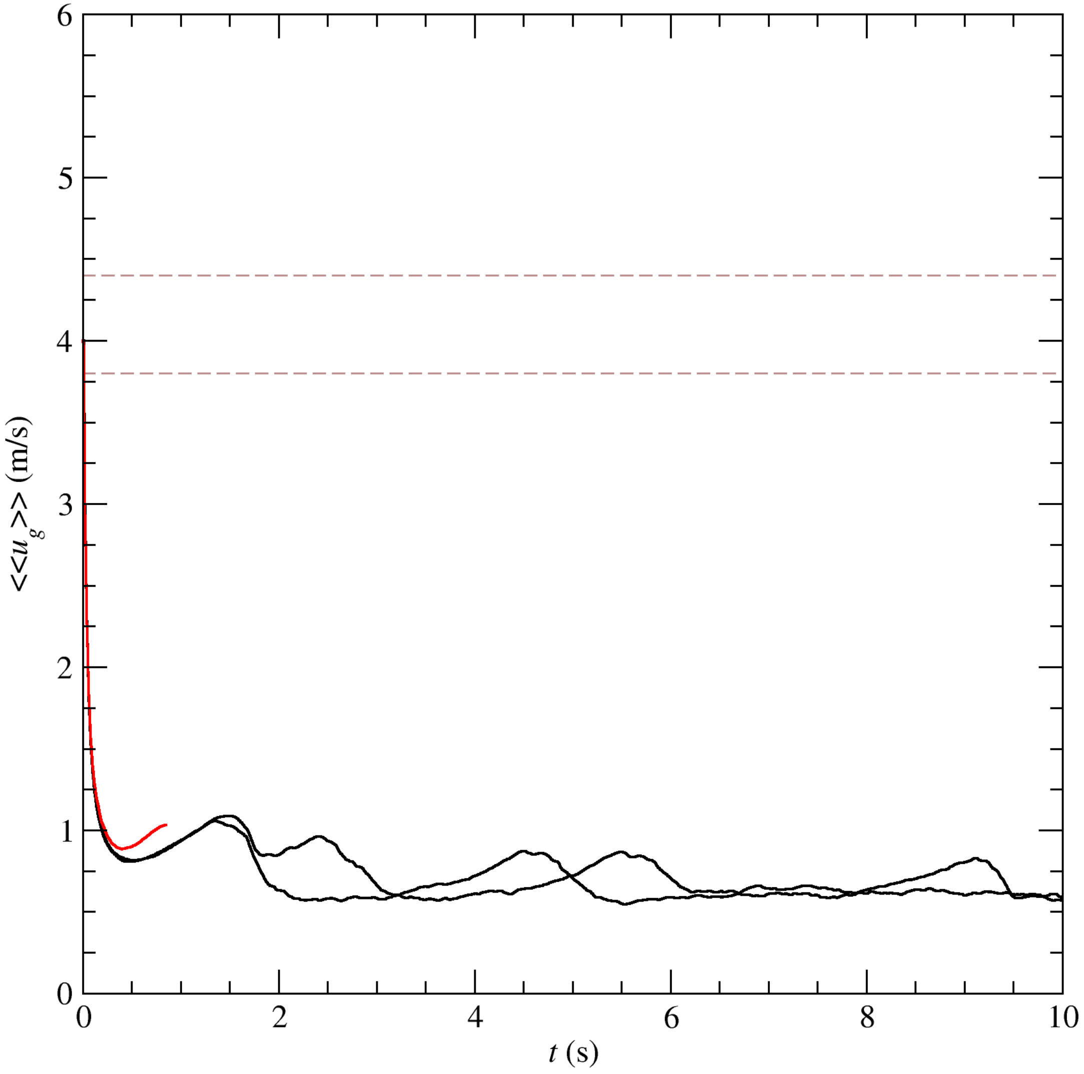


results



w/ Smagorinsky

results

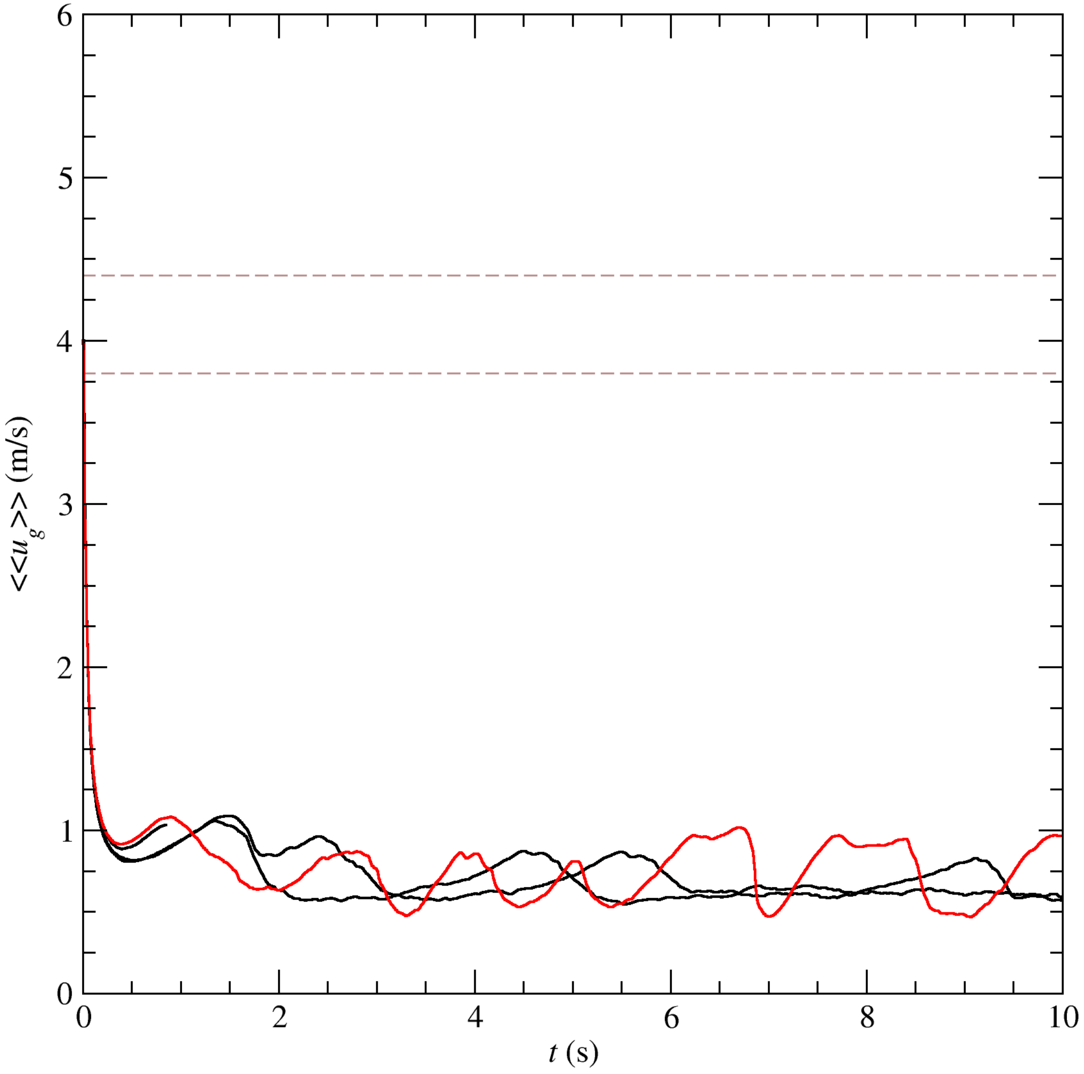


w/ Smagorinsky

+

μ_s = Chang & Law

results



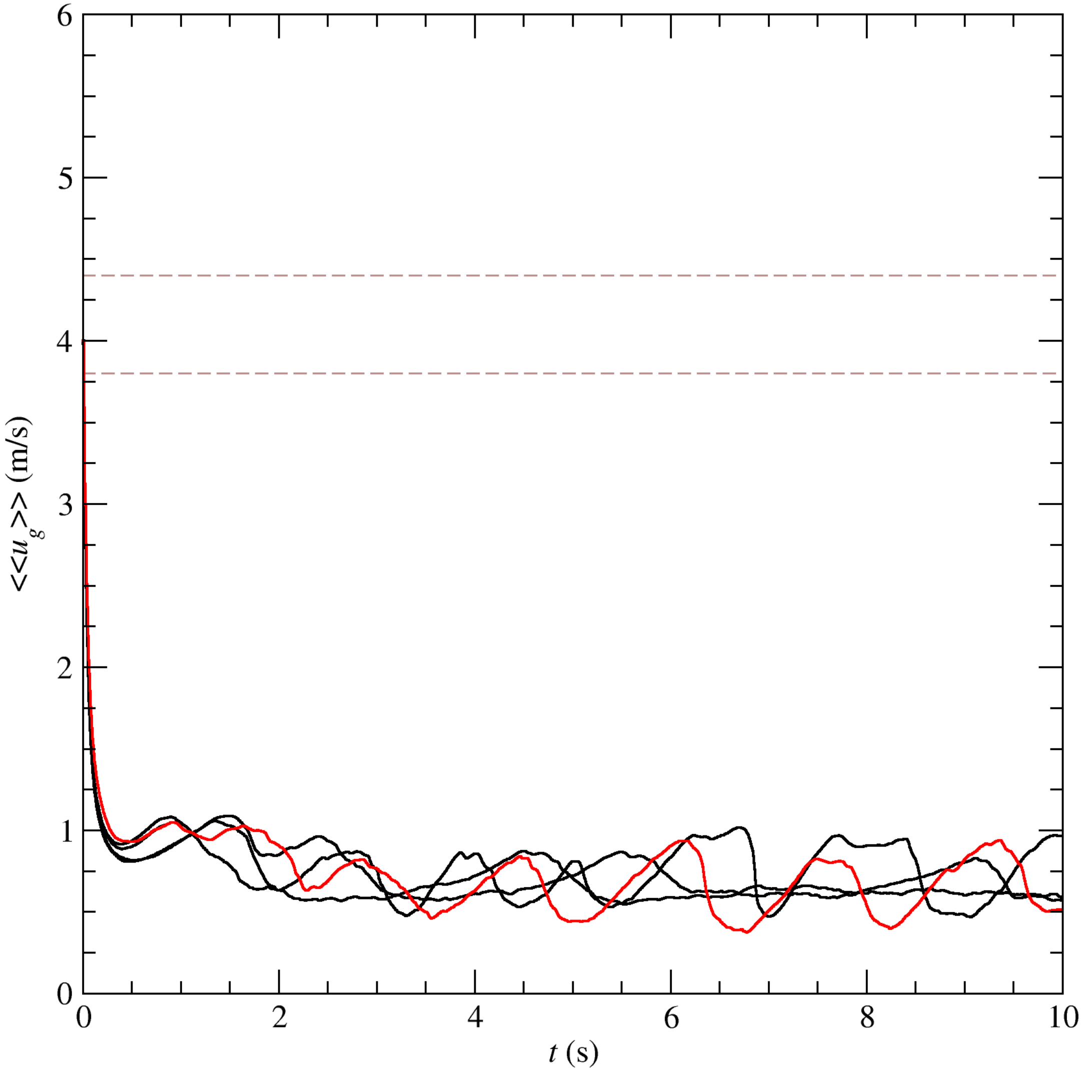
w/ Smagorinsky

+

μ_s = Chog & Law

w/ limiter

results



w/ Smagorinsky

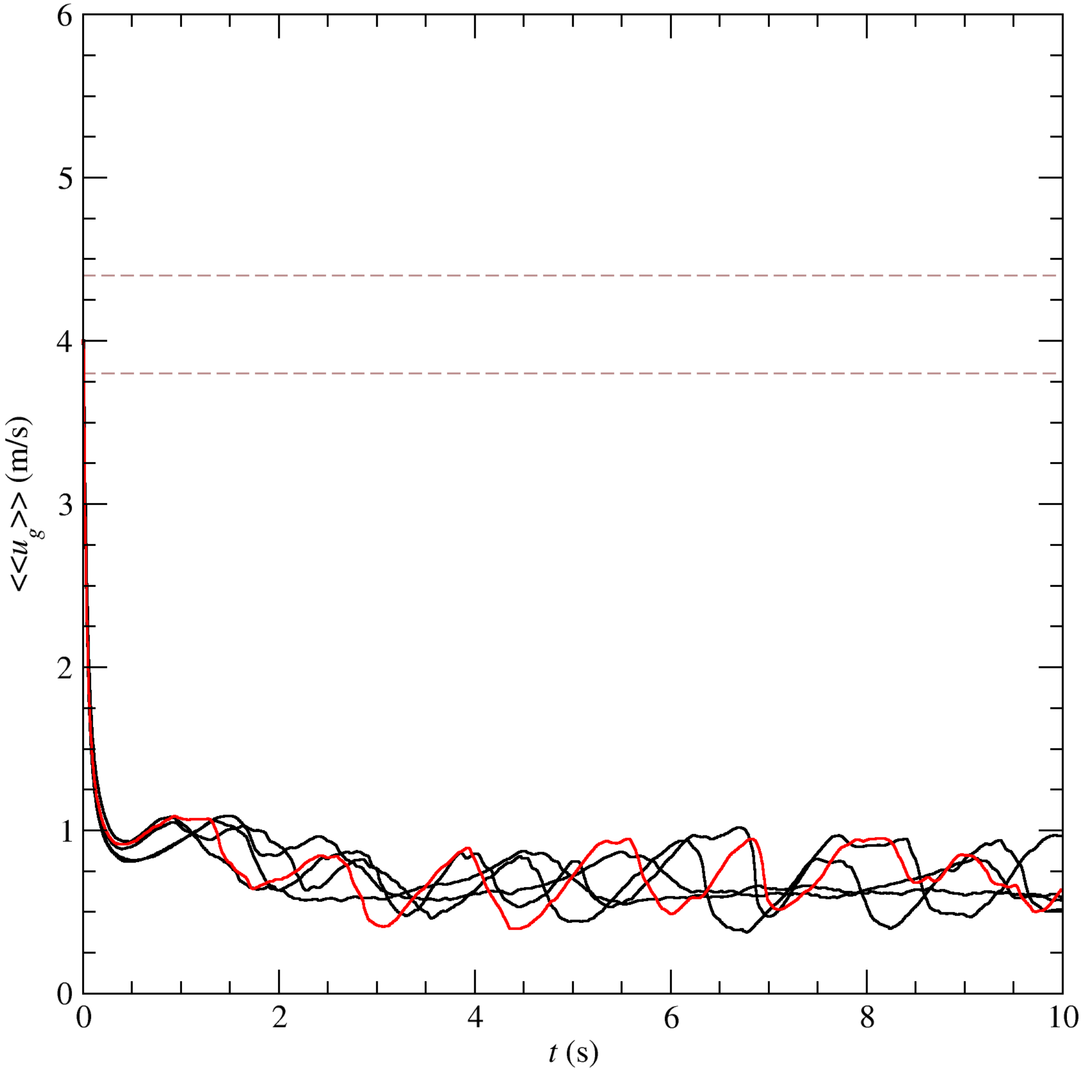
+

μ_s = Chap & Law w/ limiter

+

DNS drag law

results



w/ Smagorinsky

+

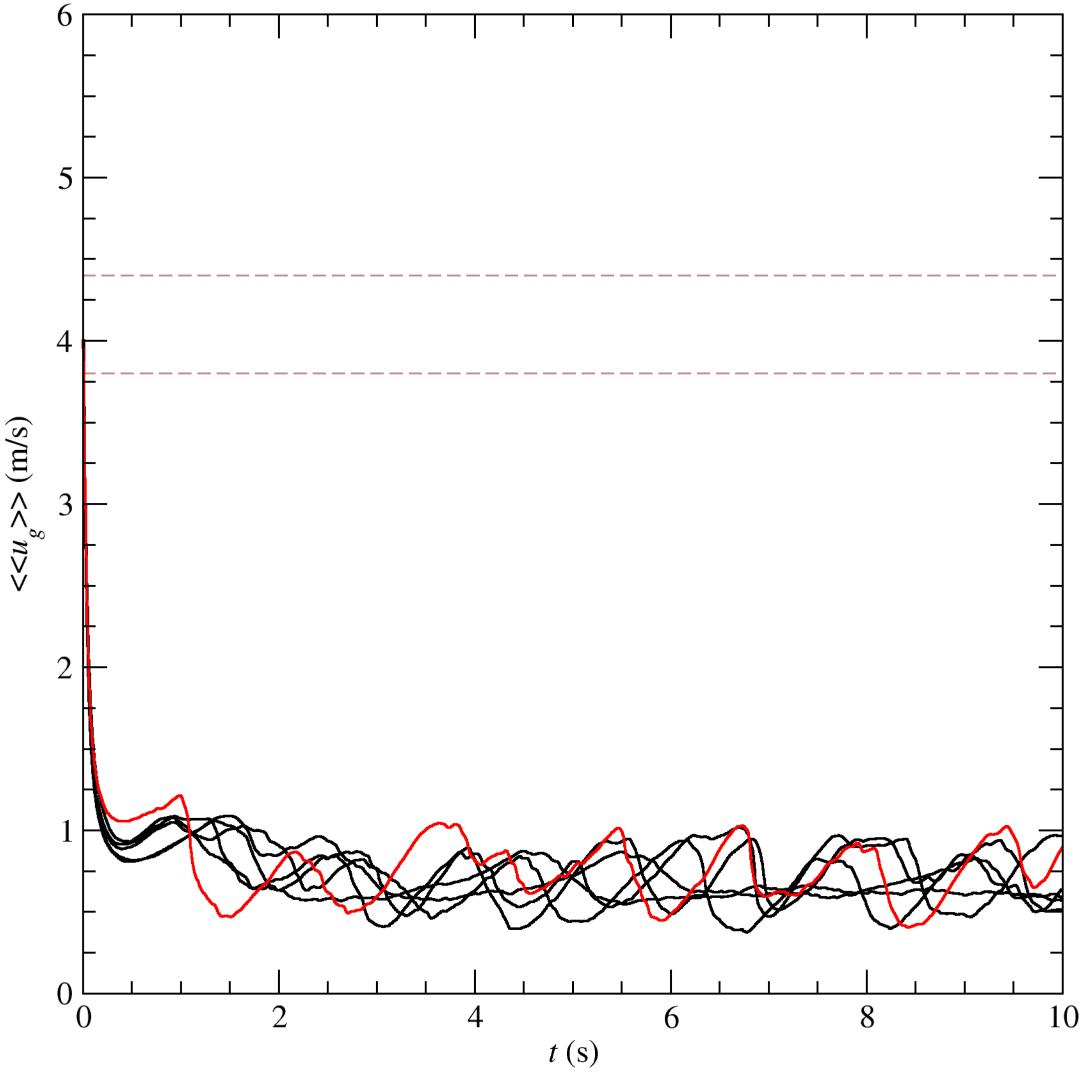
μ_s = Chapman & Law
w/ limiter

+

~~DNS drag law~~

$(\nabla\cdot\tau_f)\phi_f$

results



w/ Smagorinsky

+

μ_s = Chapman & Law w/ limiter

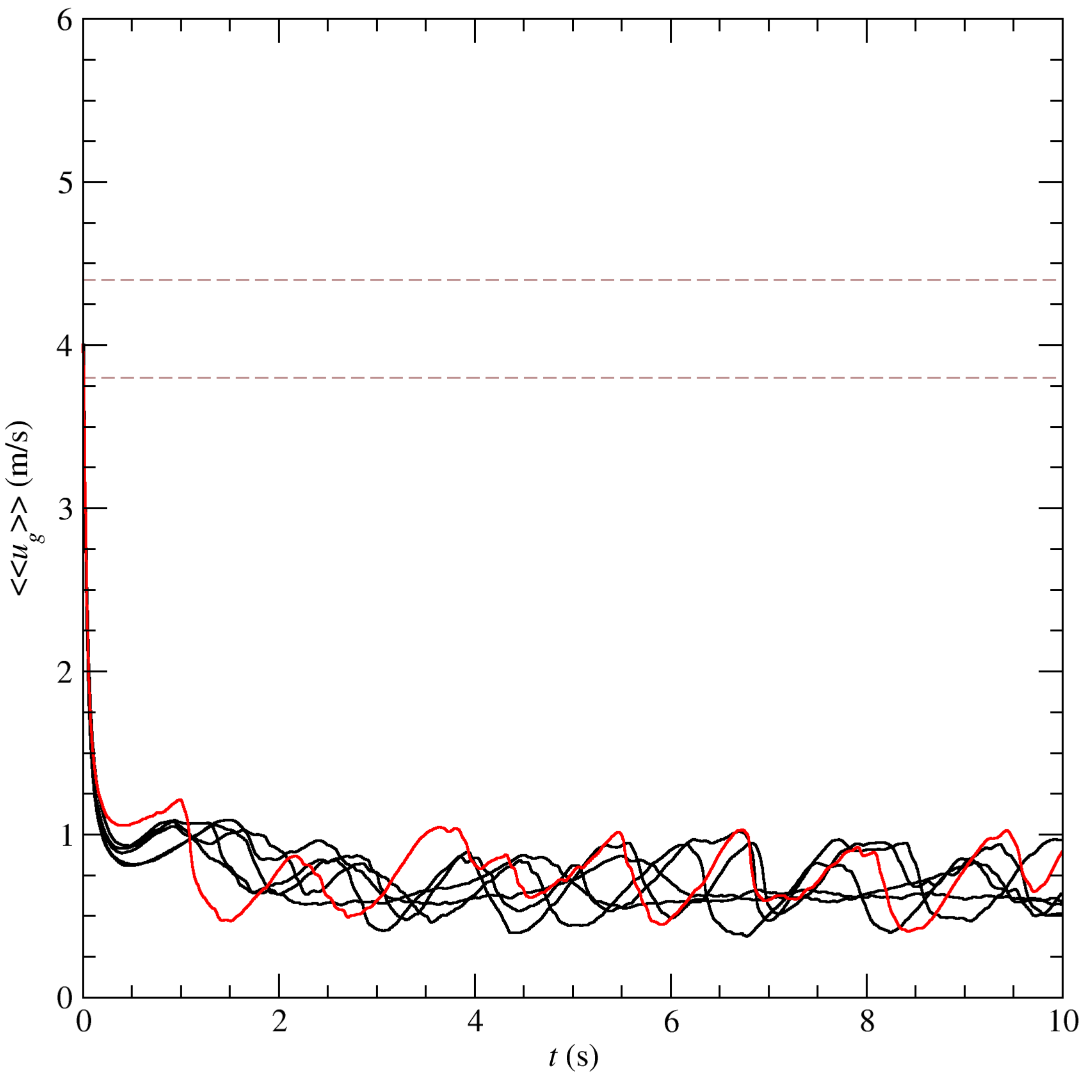
+

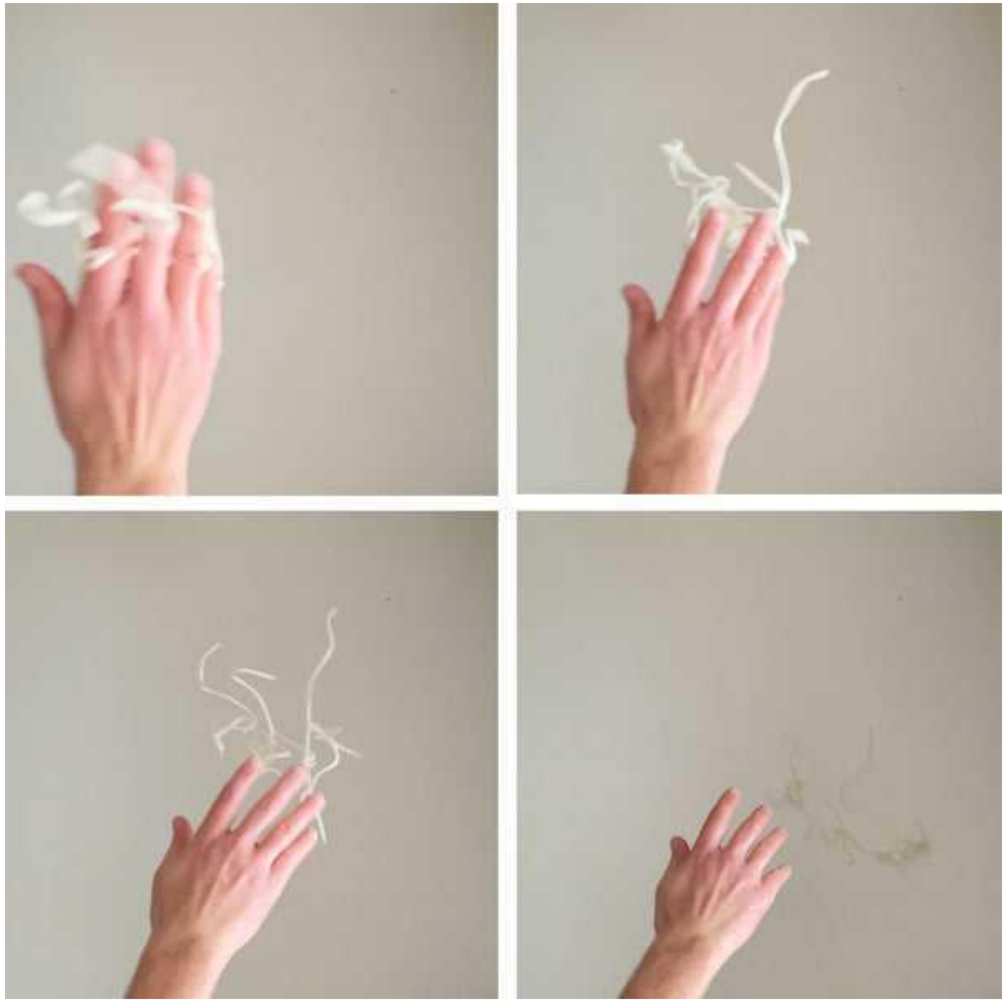
~~DNS drag law~~

~~[illegible]~~

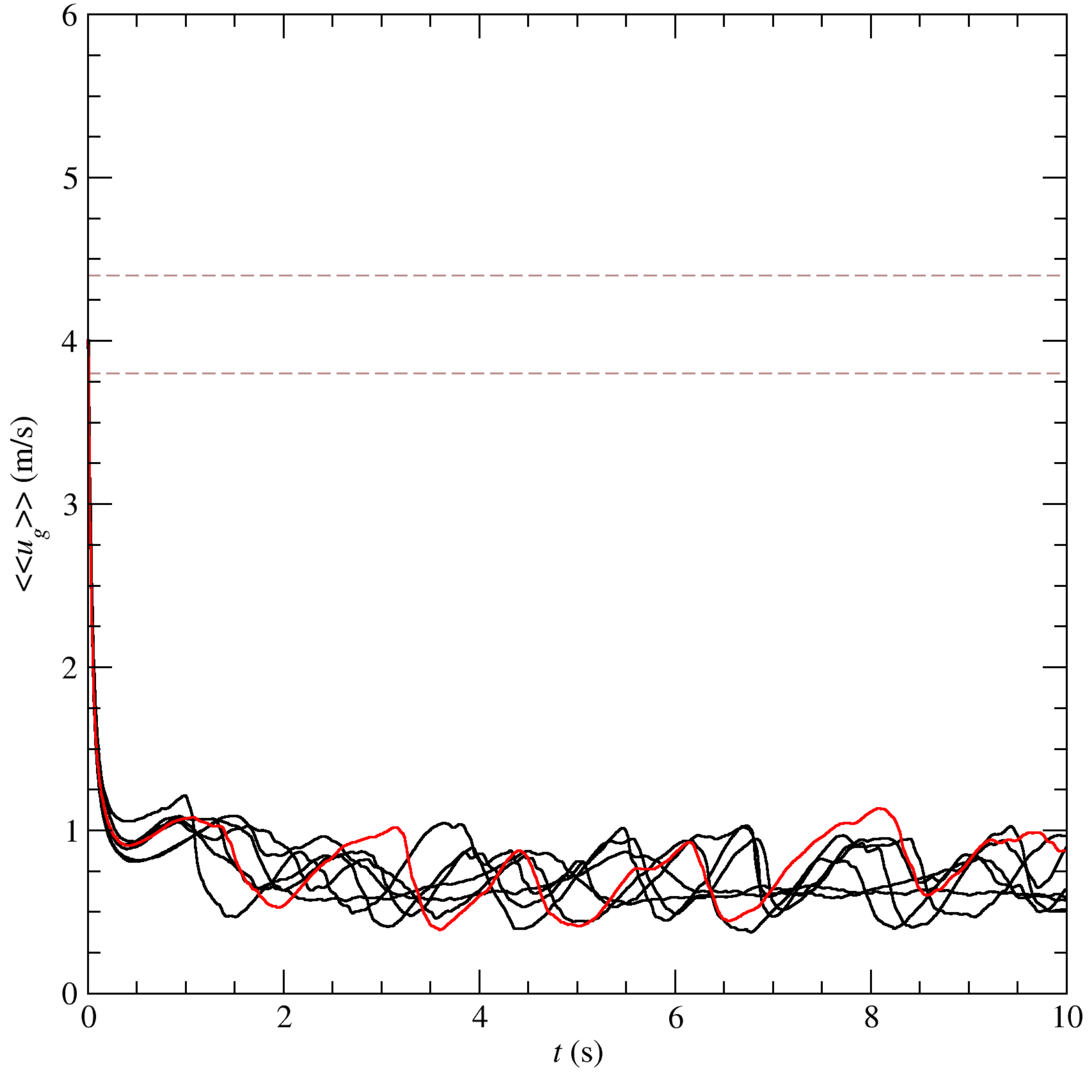
virtual mass

results



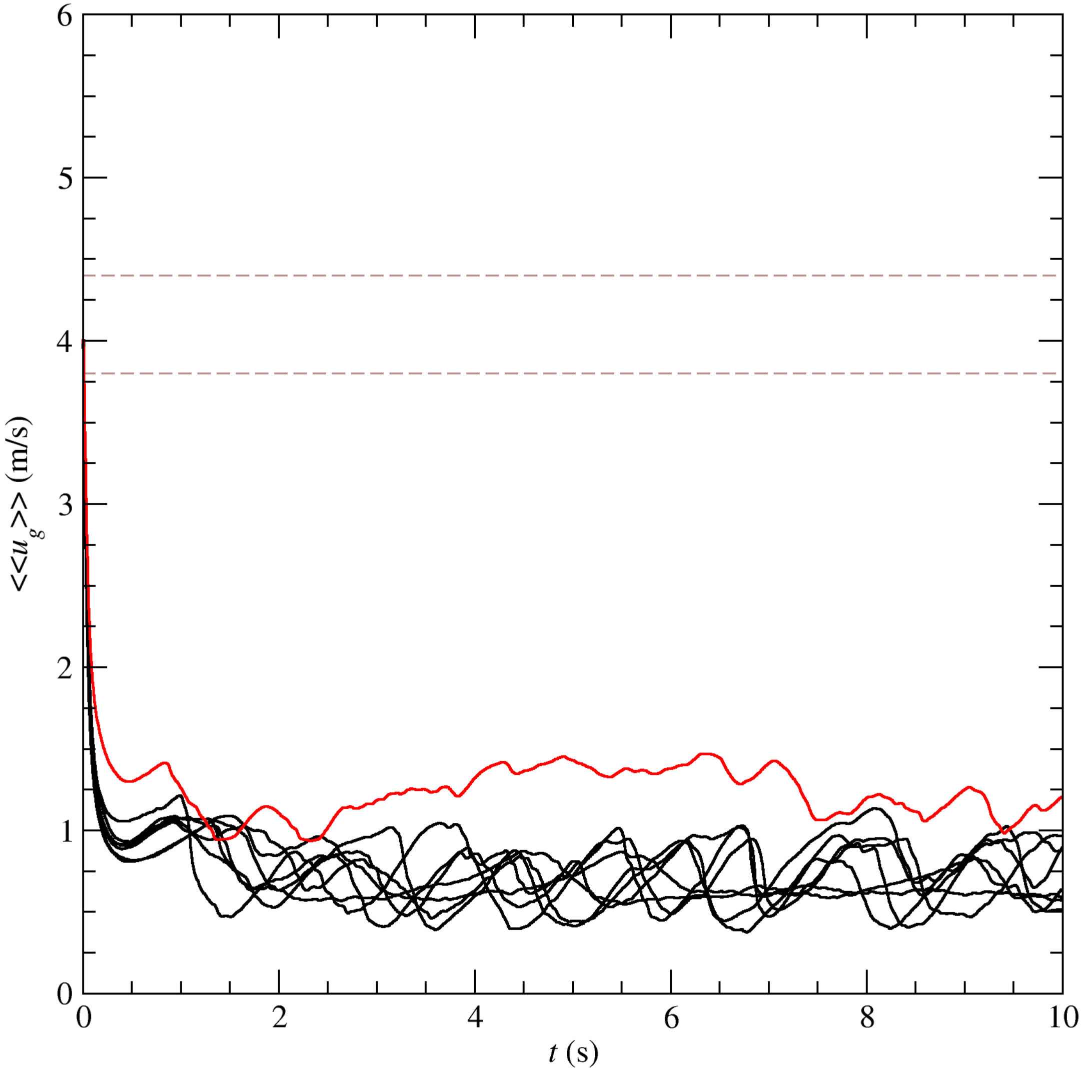


results



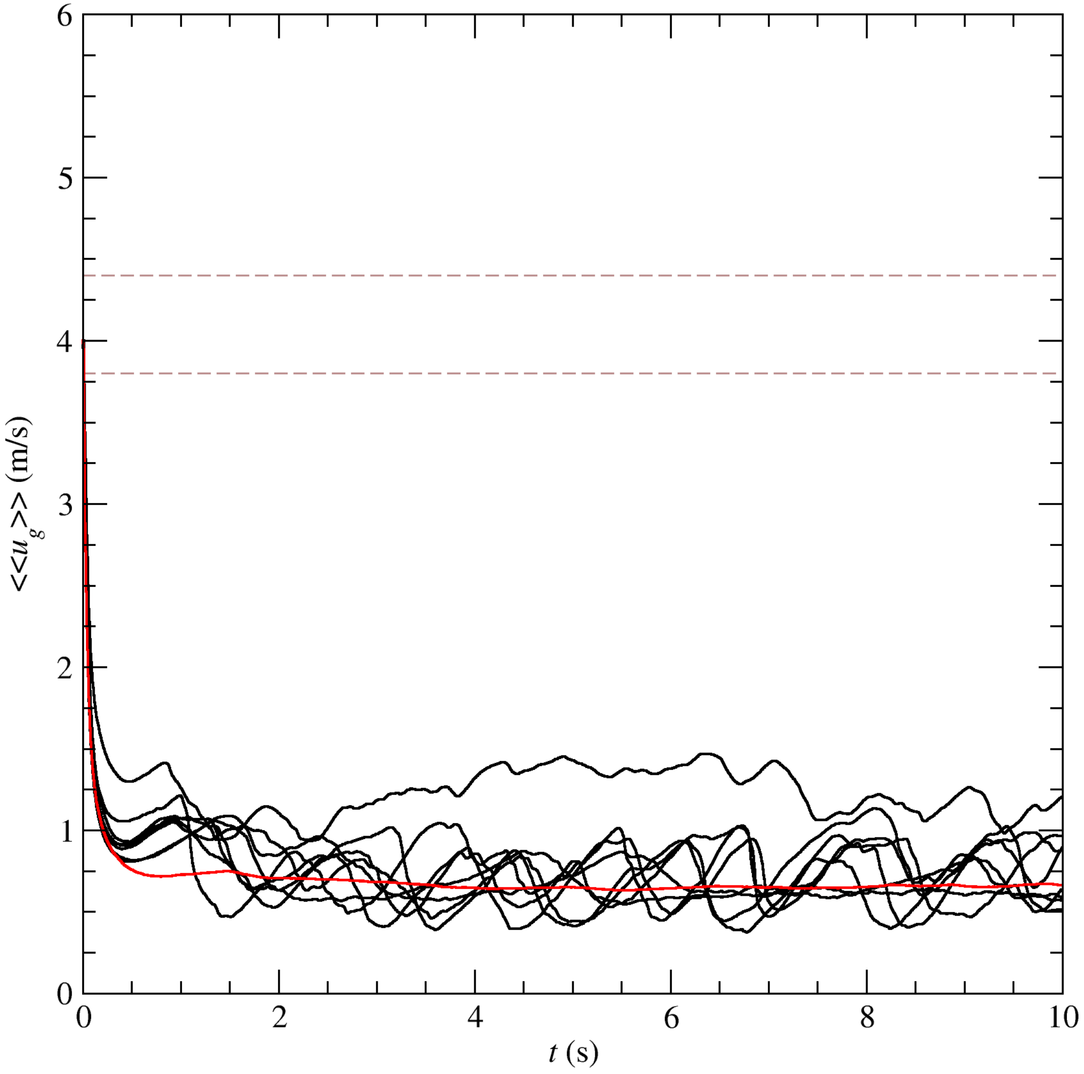
w/ Smagorinsky
+
μ_s = Chapman & Law
w/ limiter
+
~~DNS drag law~~
~~$(\nabla \cdot \tau_f) / \epsilon_f$~~
~~virtual mass~~
Flux Redist

results



w/ Smagorinsky
+
μ_s = Chap & Law
w/ limiter
+
~~DNS drag law~~
~~$(\nabla \cdot \tau_f)\, \epsilon_p$~~
~~virtual mass~~
~~Flux Correct~~
Method of Lines

results



w/ Smagorinsky

\+

μ_s = Chapman & Law w/ limiter

\+

~~DNS drag law~~

~~$(V_s \cdot \tau_f) \rho_p$~~

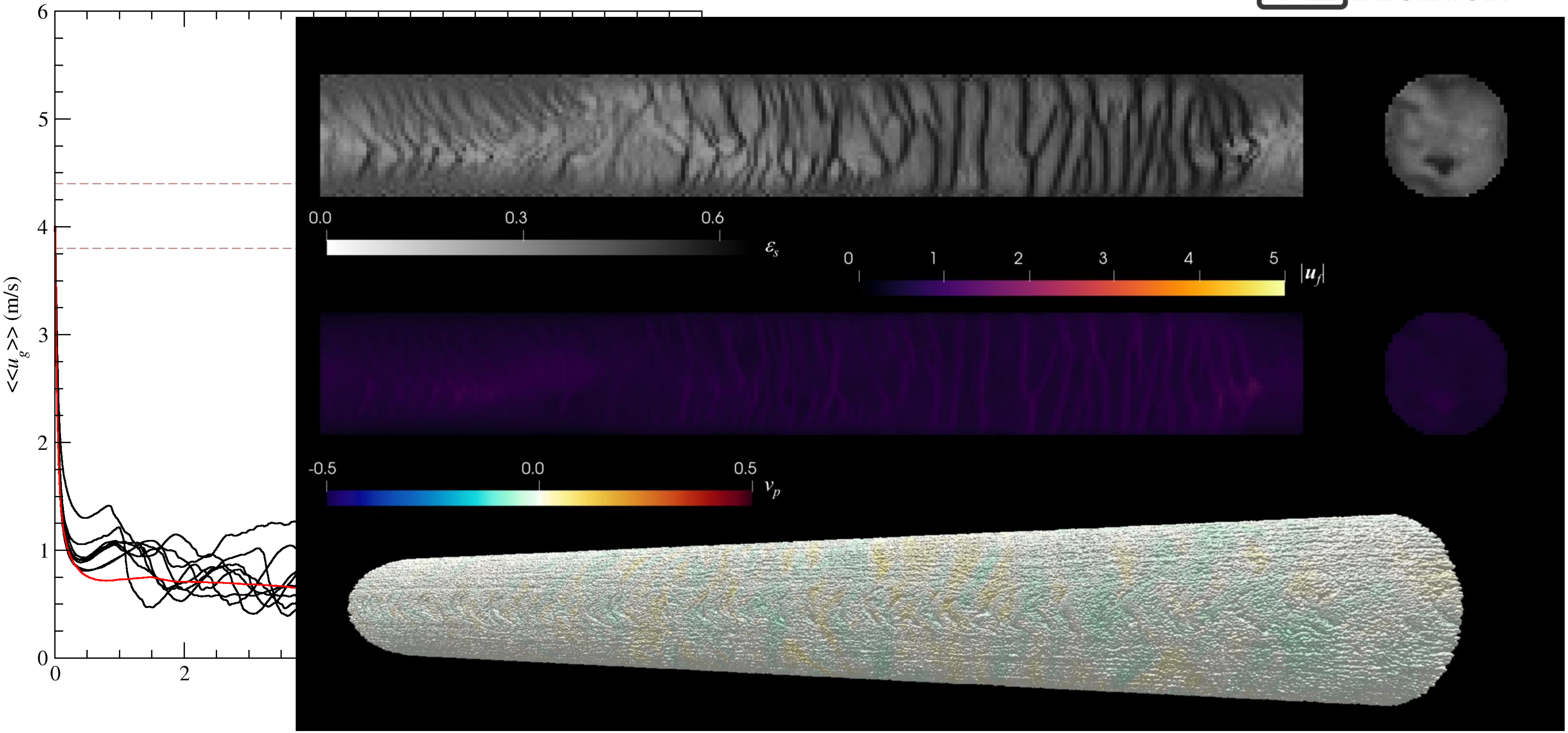
~~virtual mass~~

~~Flux Correct~~

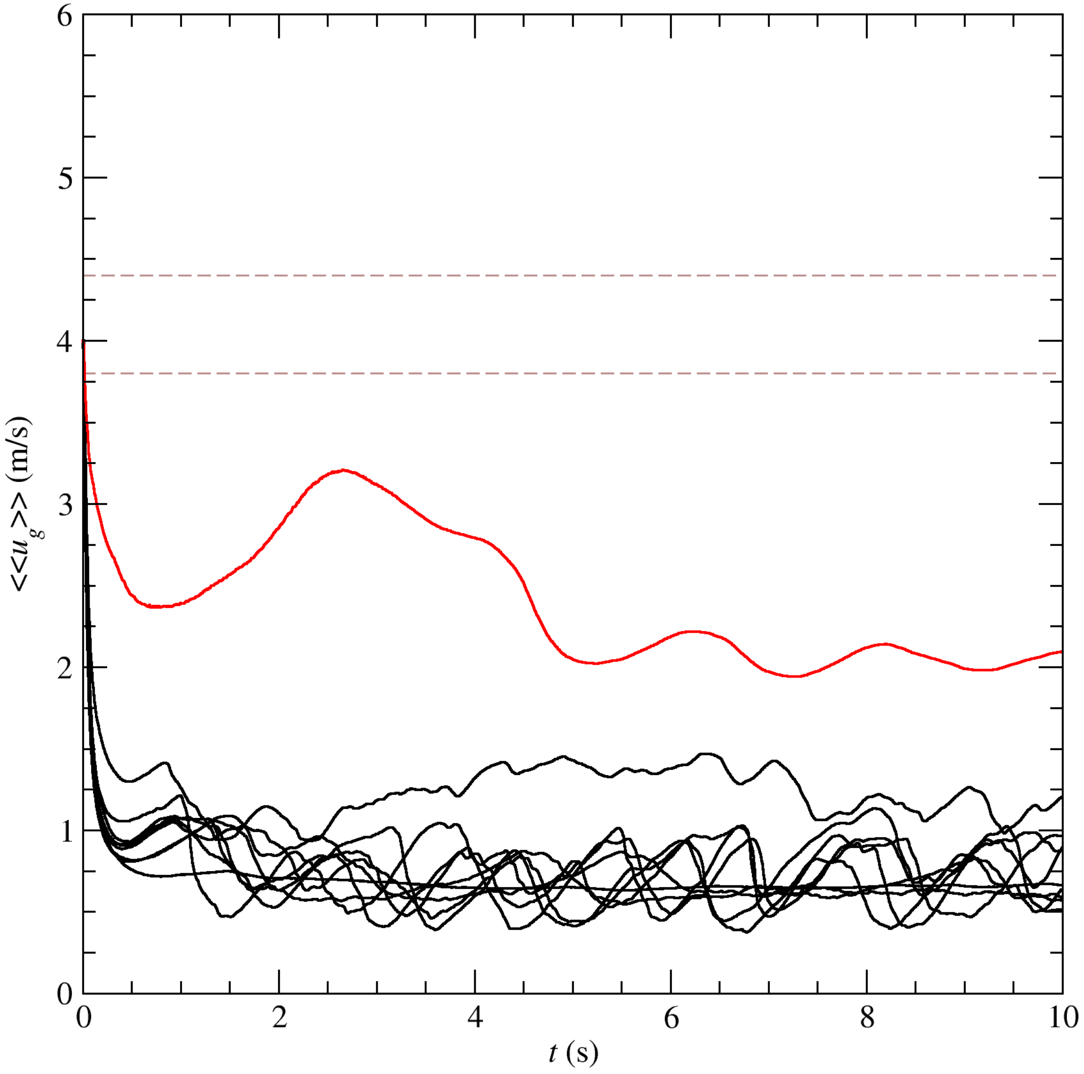
~~Method of Lines~~

no gravity !

results



results



w/ Smagorinsky
+
μ_s = Chapman & Law
w/ limiter
+
~~DNS drag law~~
~~$(\nabla \cdot \tau_f)\,\phi_p$~~
~~virtual mass~~
~~Flux Corrected~~
~~Method of Lines~~
~~no gravity~~ !

$\frac{\partial \epsilon_f}{\partial t} \neq 0$

governing equations

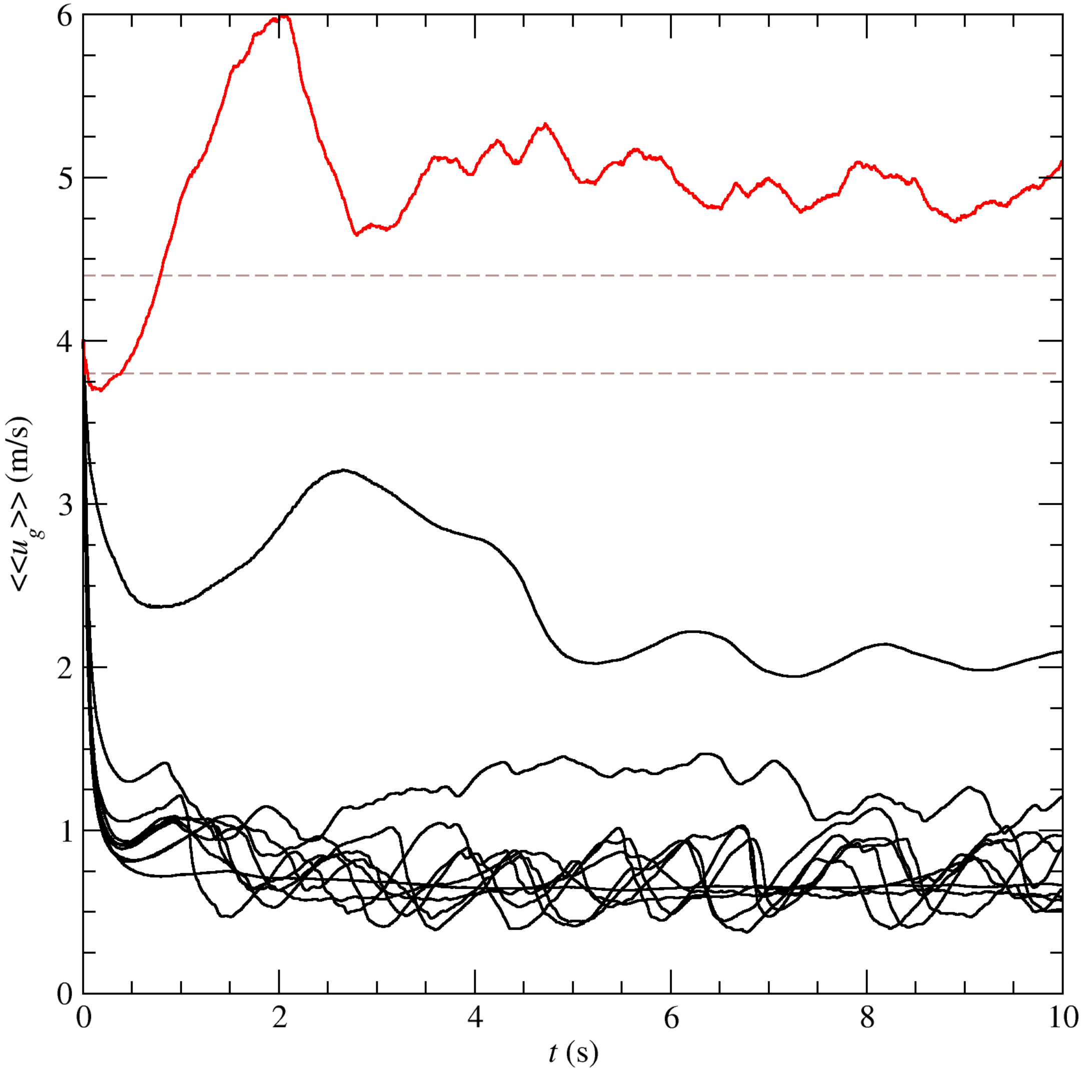
Lagrangian: discrete particles as *parcels*

$$\frac{d\boldsymbol{x}_i}{dt} = \boldsymbol{u}_i \quad \text{and} \quad m_i \frac{d\boldsymbol{u}_i}{dt} = m_i \boldsymbol{g} + \frac{V_p}{\varepsilon_p} \nabla \tau_p + \boldsymbol{F}_{fi}$$

Eulerian: continuous fluid

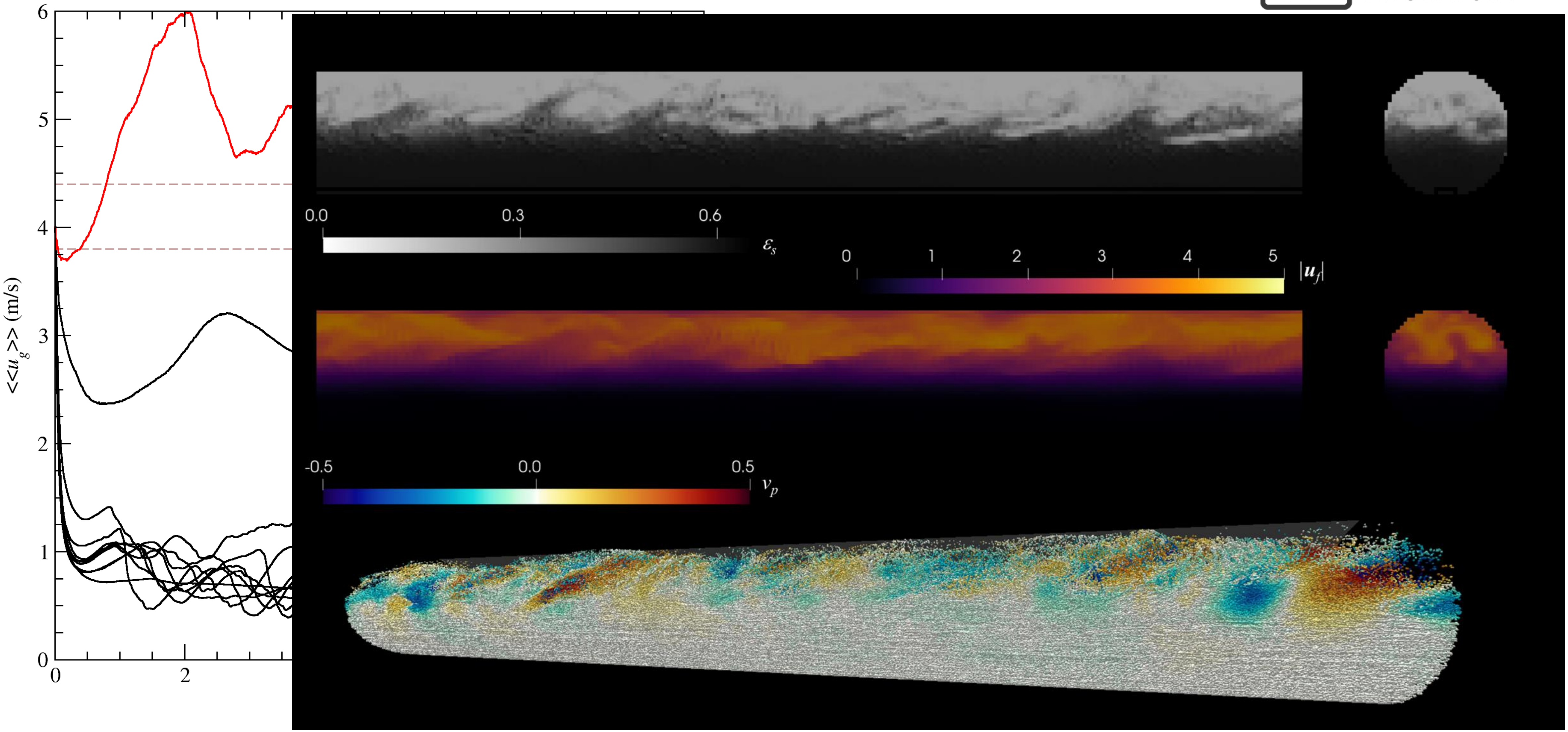
$$\nabla \cdot \varepsilon_f \boldsymbol{u}_f = 0 \quad \text{and} \quad \rho_f \left(\frac{\partial \varepsilon_f \boldsymbol{u}_f}{\partial t} + \nabla \cdot \varepsilon_f \boldsymbol{u}_f \boldsymbol{u}_f \right) = -\varepsilon_f \nabla \pi_f + \nabla \cdot \boldsymbol{\tau}_f + \boldsymbol{M}_{pf} + \rho_f \varepsilon_f \boldsymbol{g}$$

results

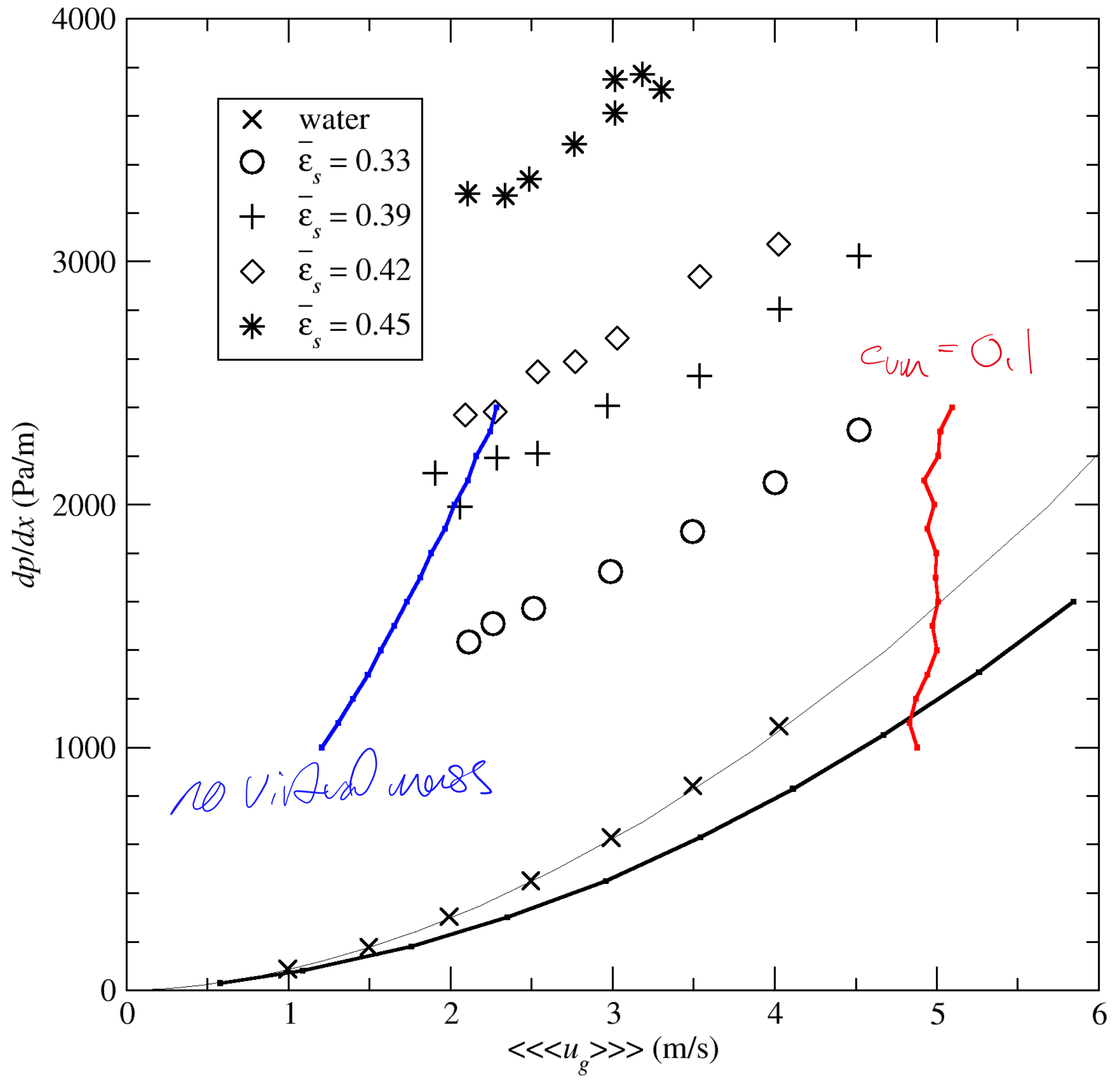


w/ Smagorinsky
+
μ_s = Chapman & Law
w/ limiter
+
virtual mass (C_{vm} = 0.1)
+ $(\nabla \cdot \tau_f)\epsilon_f$
+ $\frac{\partial \epsilon_f}{\partial t} \neq 0$

results



results



bound the data but we have a lot of work left to do

summary & conclusions (are there any?)

- Developing a multiphase PIC model for slurry flow with MFIX-Exa
- "Switching" from gas-solid to liquid-solid is non-trivial
- Previously neglected void fraction transient term is important to include in the divergence constraint
- Unclear why virtual mass seems to have such a significant influence on quasi-steady pipe flow (need to validate implementation!)
- Still need to add lift force
- Much more work left to do!

thanks!

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