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On the Statistical Modelling of Particle/Particle and Particle/Turbulence Interactions in Gas-Solid Flows

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Context

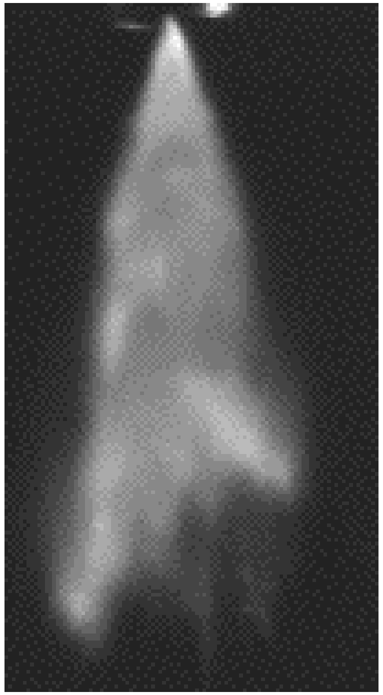
<u>Development of unsteady Euler-Euler approach for Turbulent Particulate Flows</u>

<u>Modelling of turbulent reactive two-phase flows</u>

- Fluid-particle interaction (mass, momentum and energy transfer)
- Particle-particle interaction (collision, agglomeration, attrition)
- Particle-wall interaction (inelastic bouncing with friction, deposition)

<u>Simulation of industrial applications</u>

- Coal fired furnaces
- CFB boilers
- Polymerisation reactor
- FCC riser
- IC engine (liquid fuel injection)
- Solid rocket booster
- Deposition
- ……



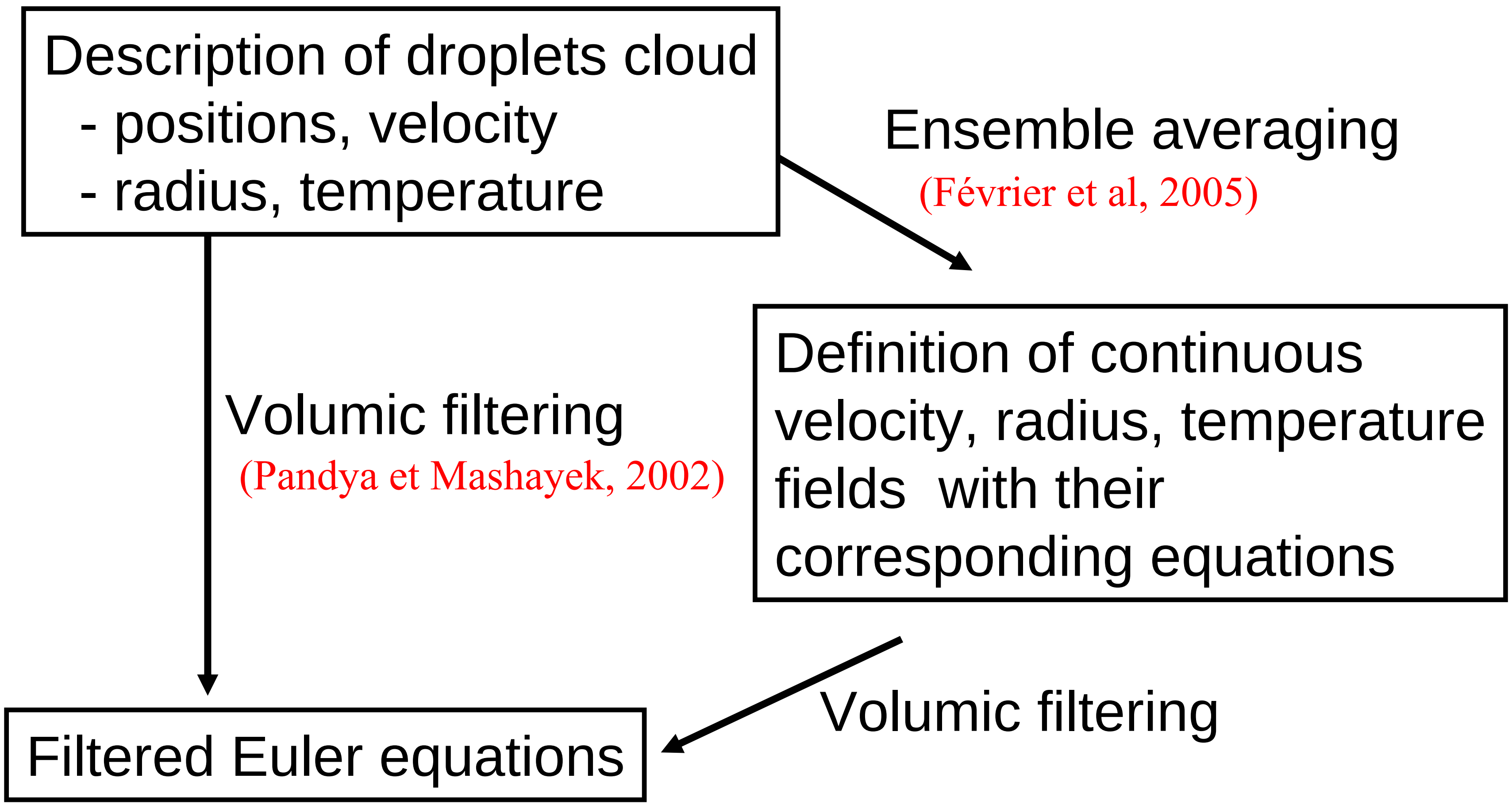
Industrial motivations

- <u>In many combustion devices, the fuel injected is liquid or solid</u>
  - The combustion "qualities" depends strongly of the spray dynamics (pulverization, dispersion, coalescence, two way coupling)

- <u>Unsteadiness appears very frequently</u>
  - Cycle to cycle dynamic variations in IC engine
  - Combustion instabilities in aircraft turbine
  - Cluster formation in circulating fluidized beds

- <u>Euler-Euler approaches should be better suited than Euler-Lagrange to handle such unsteady turbulent reacting flows</u>
  - Euler-Euler : particle continuum equations (moment approach) coupled with fluid phase averaged balance equations (LES, RANS)
  - Euler-Lagrange : discrete particle tracking coupled with fluid phase averaged balance equations (LES, RANS)

Derivation of two-fluid LES equations



Characteristic time scales

τ_p Particle relaxation time $(\approx \rho_p d_p^2 / 18\,\mu_f)$

$$\frac{du_{p,i}}{dt} = -\frac{1}{\tau_p}\left[u_{p,i} - u_{f,i}\right] + g_i$$

τ_c Inter-particle collision time

$\tau_c >> \tau_p$ very dilute flow

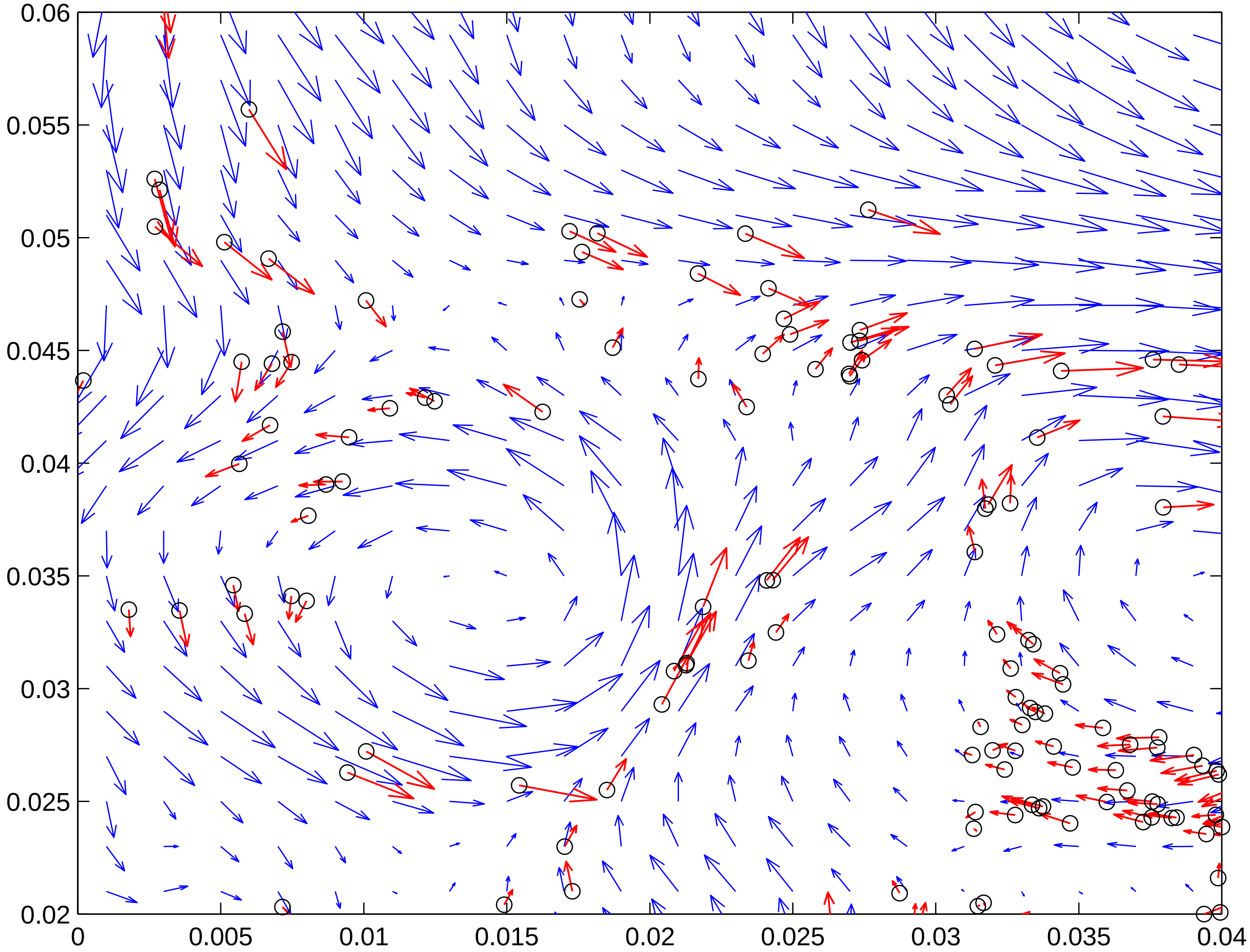
τ_η Kolmogorov time scale $(\approx \sqrt{\nu_f / \varepsilon_f})$

$\tau_p << \tau_\eta$ "scalar" limit case

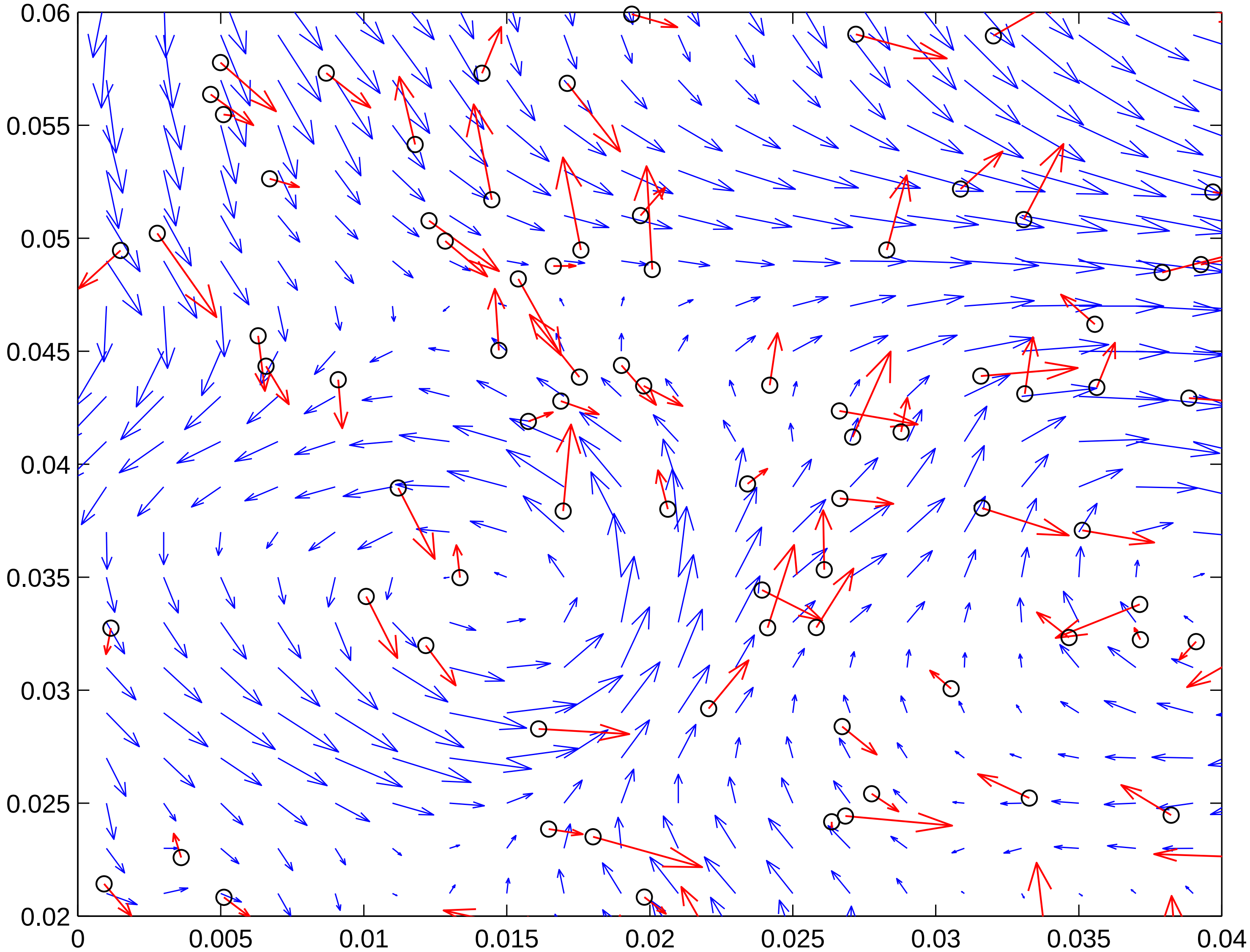
T_L^f Lagrangian integral time scale $(\approx k_f / \varepsilon_f)$

$\tau_p > T_L^f$ very inertial particle $(St = \tau_p / T_L^f)$

$T_L^{f@p}$ Fluid Lagrangian integral time scale measured along the particle paths (turbulence "viewed" by the particles)



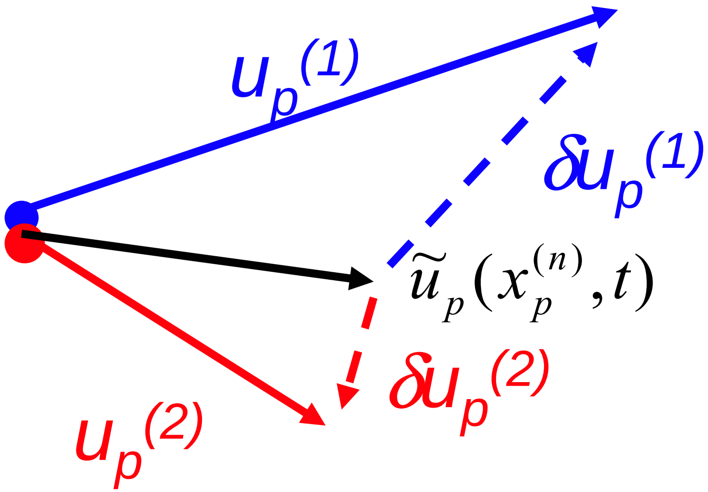
Instantaneous particle and fluid velocity distributions from DPS+DNS (one-way coupling) in homogeneous isotropic turbulent flow, particle relaxation time to fluid Lagrangian integral time scale ratio $St = 0.13$.



Instantaneous particle and fluid velocity distributions from DPS+DNS (one-way coupling) in homogeneous isotropic turbulent flow, particle relaxation time to fluid Lagrangian integral time scale ratio *St* = 2.17.
(fluid and particle velocity vectors obey different scaling)

Particle velocity partitioning

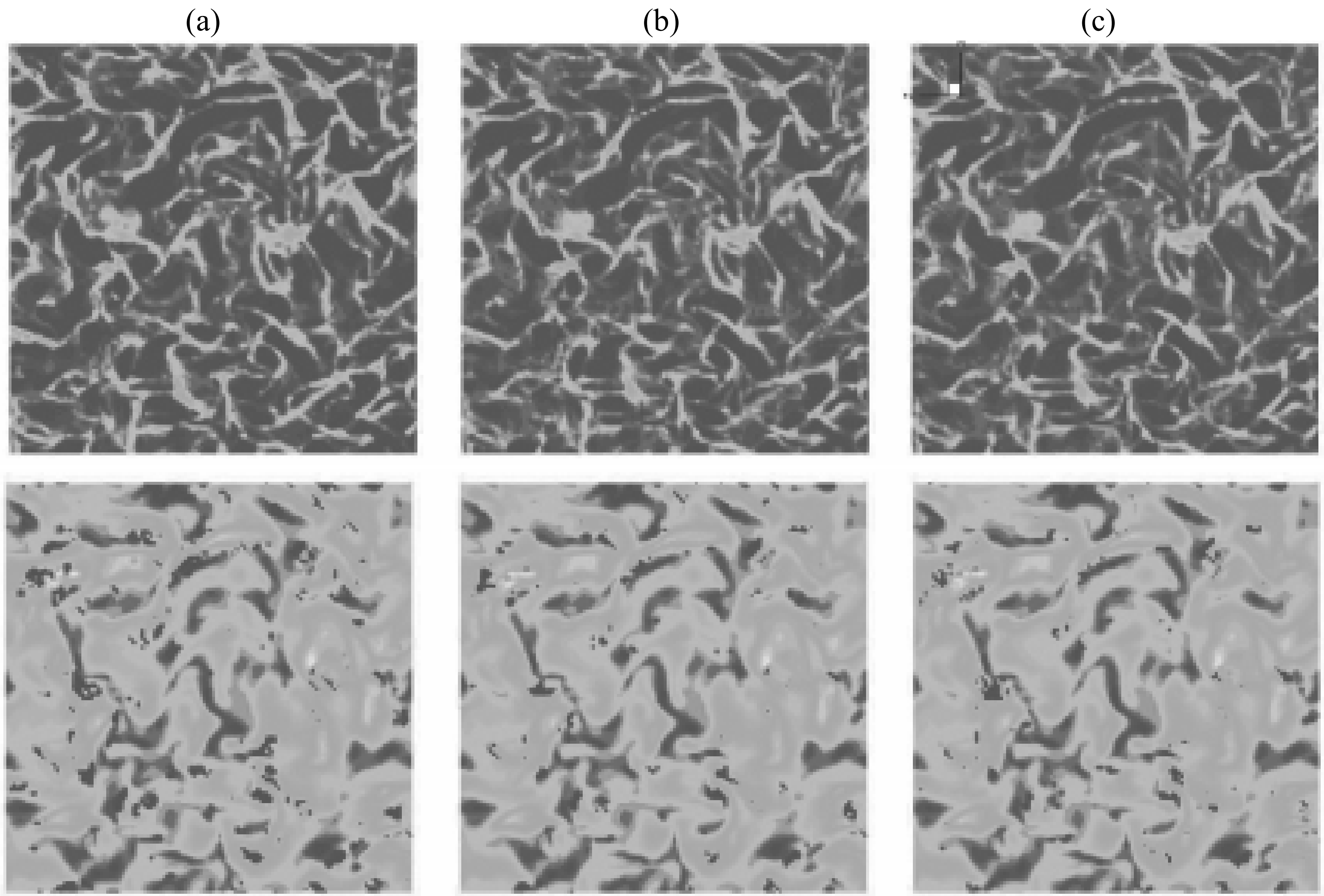
Ensemble average over the particle realizations for a given fluid flow realization (one-way coupling) $< \left| H_f \right>_p$



$$u_p^{(n)}(t) = \tilde{u}_p(x_p^{(n)}(t), t) + \delta u_p^{(n)}(t)$$

$\tilde{u}_p(x_p^{(n)}, t)$ « mesoscopic » Eulerian (correlated) particle velocity field

$\delta u_p^{(n)}(t)$ « quasi-brownian » (un-correlated) particle velocity contribution



Instantaneous fields of the particle number density (up) and mesoscopic kinetic energy (down), after the transient, for different initial conditions: (a) particle velocity equal to that of the fluid at the particle position, (b) zero particle velocity, (c) particle velocity sampled from a Gaussian distribution.

Conditional particle PDF

$\tilde{f}_p^{(1)}(\mathbf{c}_p, \mathbf{x}, t | H_f)$ conditional single particle pdf

Probable number of particles with a given translation velocity $\mathbf{u}_p^{(n)} = \mathbf{c}_p$
for the given fluid flow realization H_f

<u>Kinetic transport equation</u>

$$\frac{\partial}{\partial t}\tilde{f}_p^{(1)} + \frac{\partial}{\partial x_j}\left[c_{p,j}\tilde{f}_p^{(1)}\right] + \frac{\partial}{\partial c_{p,j}}\left[\frac{F_{p,j}}{m_p}\tilde{f}_p^{(1)}\right] = \left(\frac{\partial}{\partial t}\tilde{f}_p^{(1)}\right)_{coll}$$

$$F_{p,j} = -\frac{m_p}{\tau_p}\left[c_{p,j} - u_{f,j}\right] + m_p g_j$$ external force acting on a particle

Very dilute flows (no collision effect) :

$$\tilde{f}_p^{(2)}(\mathbf{c}_p, \mathbf{x}, \mathbf{c}'_p, \mathbf{x}', t | H_f) = \tilde{f}_p^{(1)}(\mathbf{c}_p, \mathbf{x}, t | H_f)\tilde{f}_p^{(1)}(\mathbf{c}'_p, \mathbf{x}', t | H_f)$$

Particle velocity moments

$$\tilde{n}_p(\mathbf{x},t) = \int f_p^{(1)}(\mathbf{c}_p,\mathbf{x},t \,|\, H_f)\,d\mathbf{c}_p$$

Mesoscopic particle number density

$$\tilde{\mathbf{u}}_p(\mathbf{x},t) = \frac{1}{\tilde{n}_p}\int \mathbf{c}_p f_p^{(1)}(\mathbf{c}_p,\mathbf{x},t \,|\, H_f)\,d\mathbf{c}_p$$

Mesoscopic (correlated) particle velocity

$$\delta\theta_p = \frac{1}{2\tilde{n}_p}\int (c_{p,i} - \tilde{u}_{p,i})^2 f_p^{(1)} d\mathbf{c}_p$$

Quasi-Brownian (random un-correlated) particle kinetic energy

Particle moment transport equations can be derived directly by integration from the pdf kinetic equation

(analogy with kinetic theory of dilute gases or dry granular media)

Mesoscopic transport equations

Particle number density transport equation

$$\frac{\partial}{\partial t}\tilde{n}_p + \frac{\partial}{\partial x_i}\tilde{n}_p\tilde{u}_{p,i} = 0$$

Particle mesoscopic velocity transport equation

$$\frac{\partial}{\partial t}\tilde{n}_p\tilde{u}_{p,i} + \frac{\partial}{\partial x_j}\tilde{n}_p\tilde{u}_{p,i}\tilde{u}_{p,j} = \tilde{n}_p g_i - \frac{\tilde{n}_p}{\tilde{\tau}_p}\left[\tilde{u}_{p,i} - \tilde{u}_{f,i}\right] \boxed{-\frac{\partial}{\partial x_j}\tilde{n}_p\delta\tilde{\sigma}_{p,ij}}$$

$$\delta\tilde{\sigma}_{p,ij} =< \delta u_{p,i}\delta u_{p,j}\Big| H_f >_p$$

mesoscopic stress due to the quasi-Brownian velocity components

Particle quasi-Brownian kinetic energy transport equation $\tilde{n}_p\delta\theta_p = \delta\tilde{\sigma}_{p,ii}/2$

$$\frac{\partial}{\partial t}\tilde{n}_p\delta\theta_p + \frac{\partial}{\partial x_i}\tilde{n}_p\tilde{u}_{p,i}\delta\theta_p = -\frac{\tilde{n}_p}{\tilde{\tau}_p}\delta\theta - \tilde{n}_p\delta\tilde{\sigma}_{p,ij}\frac{\partial\tilde{u}_{p,i}}{\partial x_j} \boxed{-\frac{\partial}{\partial x_j}\tilde{n}_p\tilde{Q}_{p,ij}} - \tilde{n}_p\delta\varepsilon_p$$

$\delta\varepsilon_p$ kinetic energy dissipation by inelastic particle-particle collision

Particle and fluid-particle velocity correlations

Whole particle turbulent kinetic energy

$$q_p^2 = \tilde{q}_p^2 + \delta q_p^2 \qquad q_{fp} = \tilde{q}_{fp} = < \tilde{n}_p \tilde{u}'_{p,i} u'_{f,i} > / < \tilde{n}_p >$$

$< . >$ ensemble average over all turbulent fluid flow realizations

Mean mesoscopic Eulerian (correlated) particle turbulent kinetic energy

$$2\tilde{q}_p^2 = < \tilde{u}'_{p,i} \tilde{u}'_{p,i} >_p = < \tilde{n}_p \tilde{u}'_{p,i} \tilde{u}'_{p,i} > / < \tilde{n}_p >$$

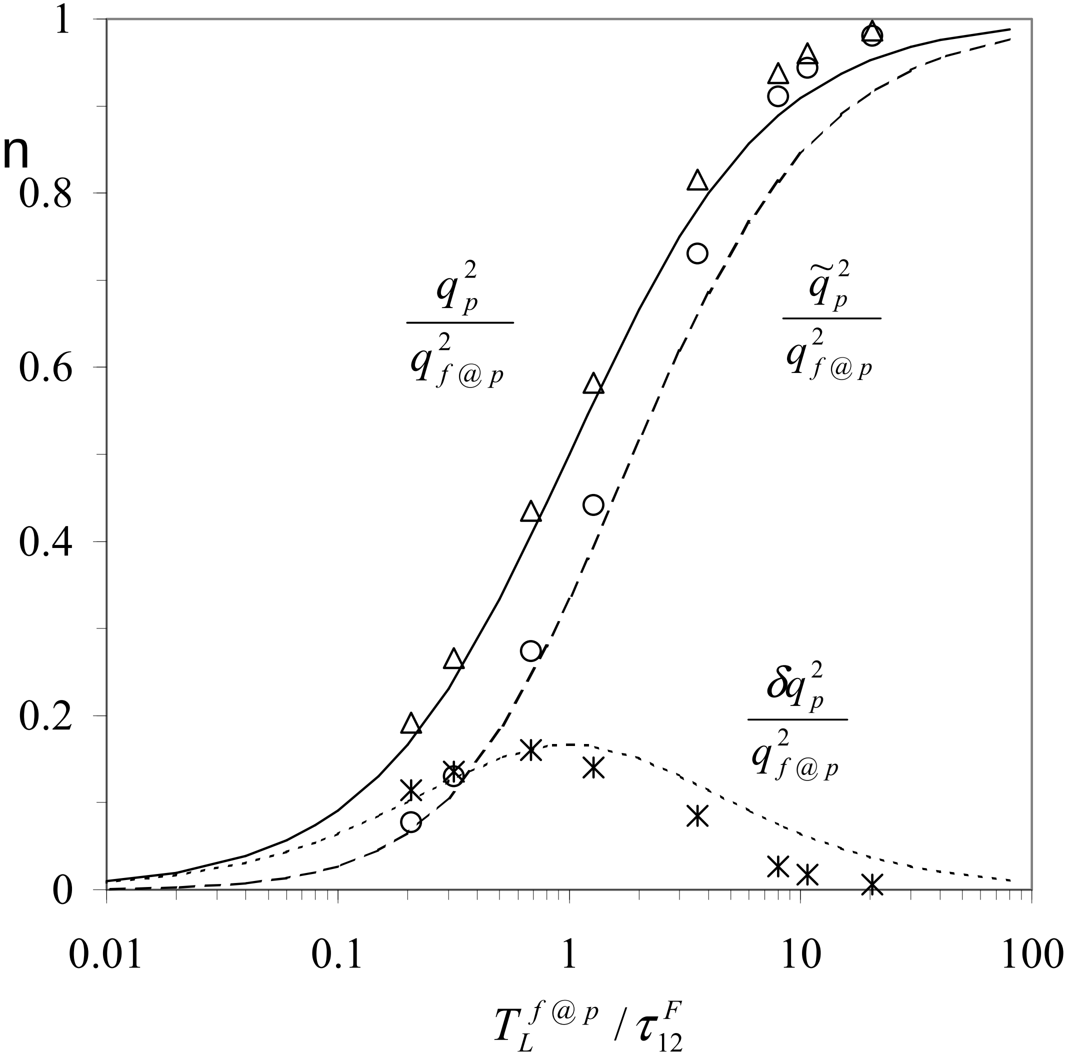
Mean “quasi-Brownian” (un-correlated) particle kinetic energy

$$\delta q_p^2 = < \delta u_{p,i} \delta u_{p,i} >_p / 2 = < \tilde{n}_p \delta \theta_p > / < \tilde{n}_p >$$

Tchen-Hinze’s theory (homogeneous isotropic turbulence) :

$$q_p^2 = q_{fp} / 2 \qquad q_{fp} = 2 \frac{\eta_r}{1 + \eta_r} q_f^2 \qquad \eta_r = T_L^{f@p} / \tau_{fp}^F$$

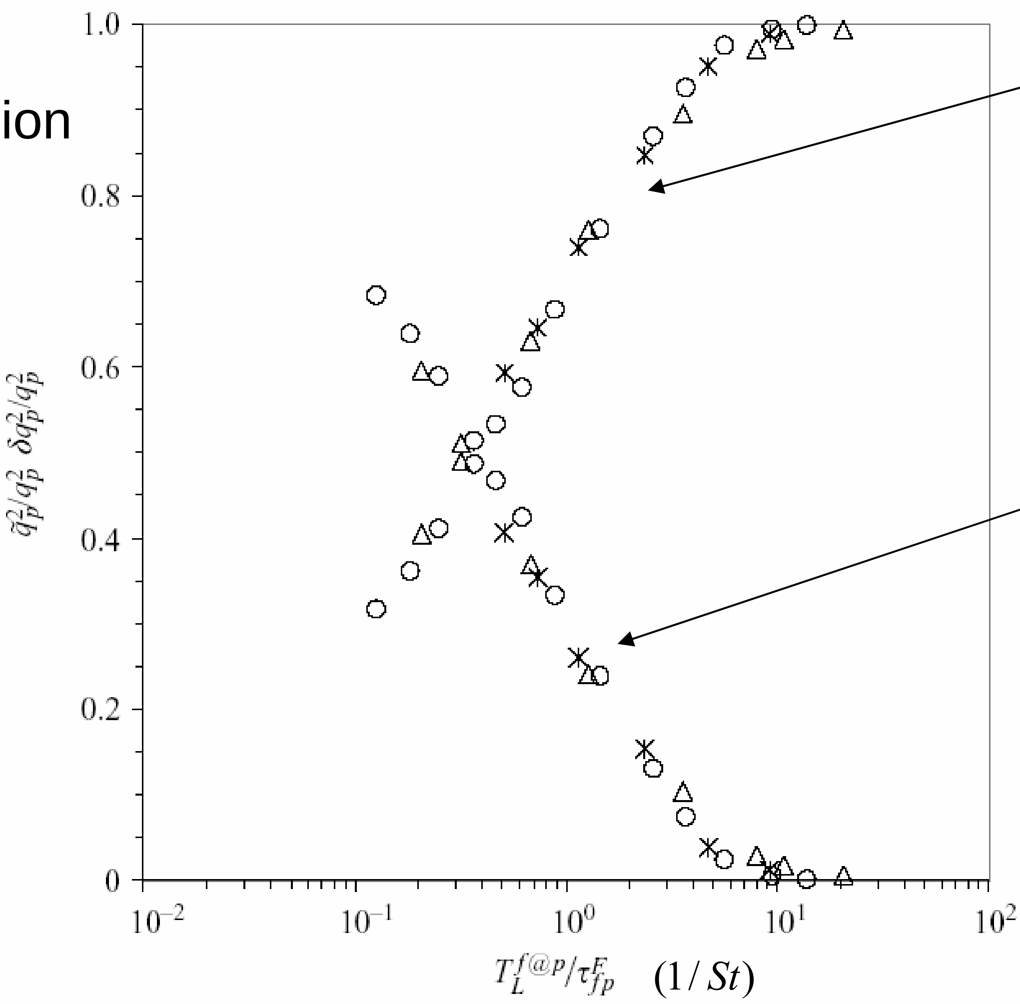
Homogeneous isotropic forced turbulence
(DPS/LES)
without collision



Whole particle kinetic energy, mean mesoscopic Eulerian particle kinetic energy and mean quasi-Brownian kinetic energy, for non-settling particles suspended in homogeneous isotropic turbulence from LES at Re_L=700. (—) Tchen-Hinze's theory

Homogeneous isotropic forced turbulence

(DPS/LES)
without collision



$$\widetilde{q}_p^2 = \frac{<\widetilde{n}_p \widetilde{u}'_{p,i}\,\widetilde{u}'_{p,i}>}{2<\widetilde{n}_p>}$$

Kinetic energy of the correlated motion

$$\delta q_p^2 = \frac{<\widetilde{n}_p \delta\theta_p>}{<\widetilde{n}_p>}$$

Kinetic energy of the un-correlated motion

○ Re_L : 110 (DNS)

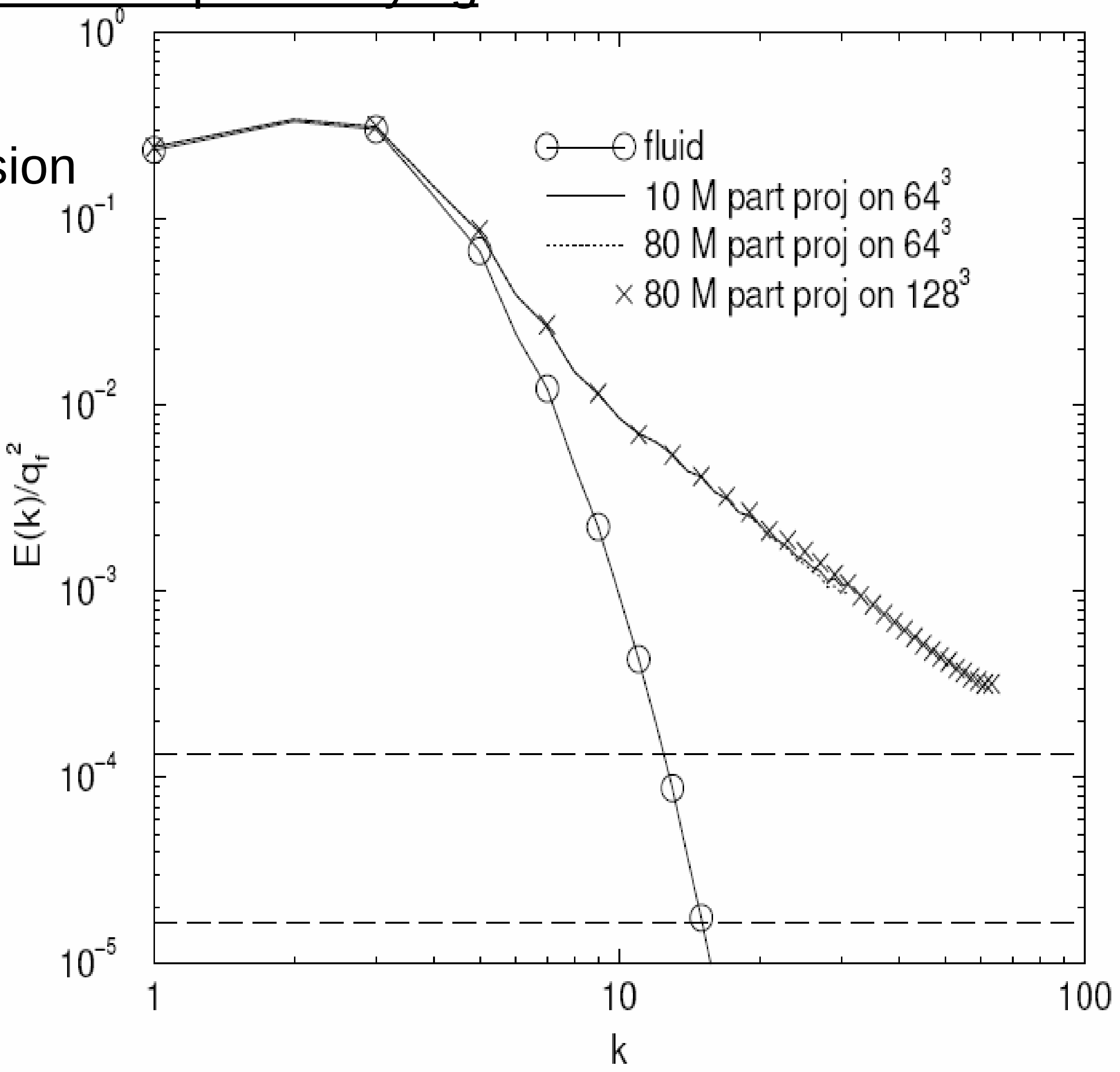
✱ Re_L : 140 (DNS)

△ Re_L : 700 (LES)

Mean mesocsopic Eulerian particle kinetic energy and mean quasi-Brownian kinetic energy, for non-settling particles suspended in homogeneous isotropic turbulence

Homogeneous isotropic decaying turbulence

(DPS/LES)
without collision



Mesoscopic energy spectrum from DPS/DNS results with 10^7 and $8\ 10^7$ particles
Computed on 64^3 and 128^3 grids with a Gaussian projector.
Decaying isotropic turbulence with $St_0 = 0.53$ after about 4 T_E ($St = \tau_p / T_E$).

Particle-laden channel flow (DPS/LES)
without collision

with collision

Streamwise
velocity correlations

Wall-normal
velocity correlations

Spanwise
velocity correlations

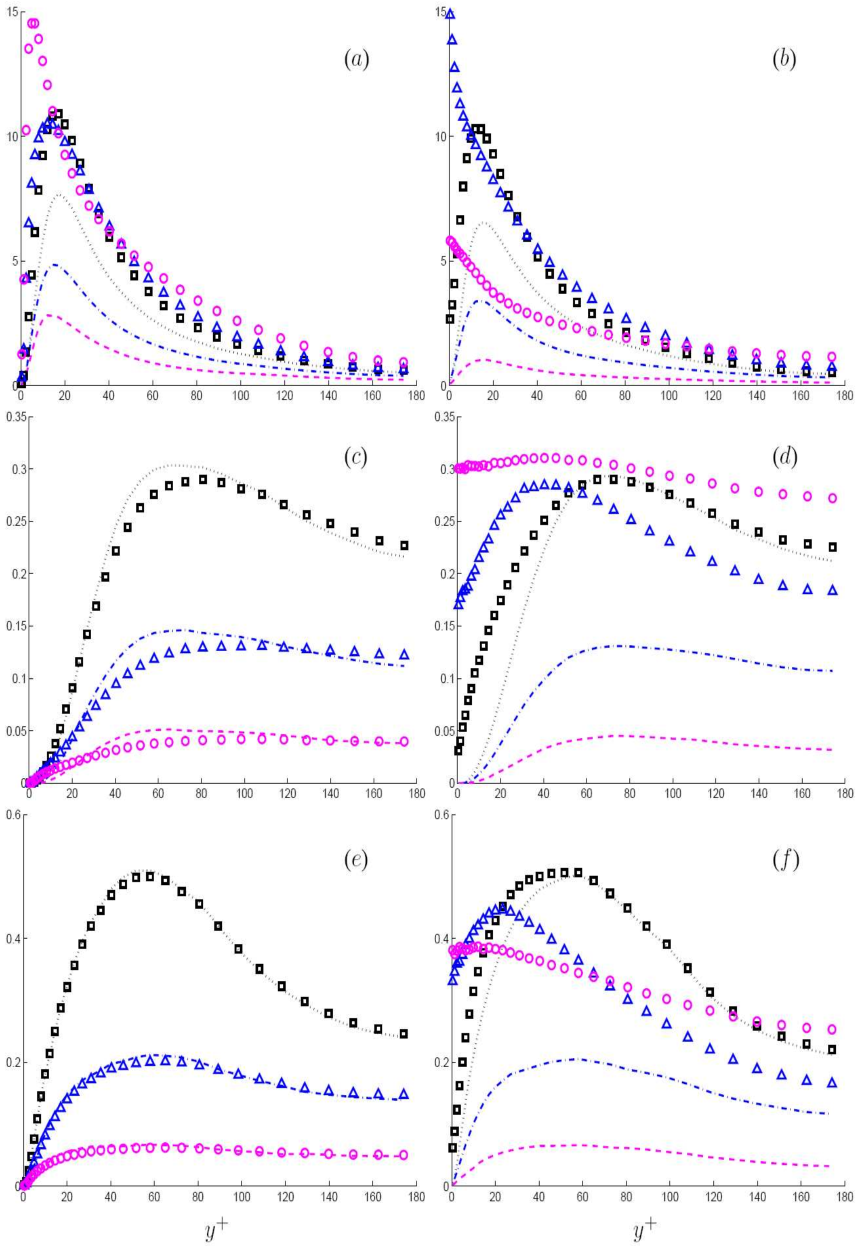


Figure 3: Components of the fluid-particle and particle-particle velocity correlation. Fluid-particle correlation: ········ $St = 0.1625$; —·— $St = 0.65$; ---- $St = 2.60$. Particle-particle correlation: ◻ $St = 0.1625$; △ $St = 0.65$; ○ $St = 2.60$. Left-hand frames from simulations without inter-particle collisions, right-hand frames from simulations with inter-particle collisions. (a) and (b) streamwise component; (c) and (d) wall-normal component; (e) and (f) spanwise component;

Particle-laden channel flow (DPS/LES)

without collision

with collision

Streamwise velocity correlations

Wall-normal velocity correlations

Spanwise velocity correlations

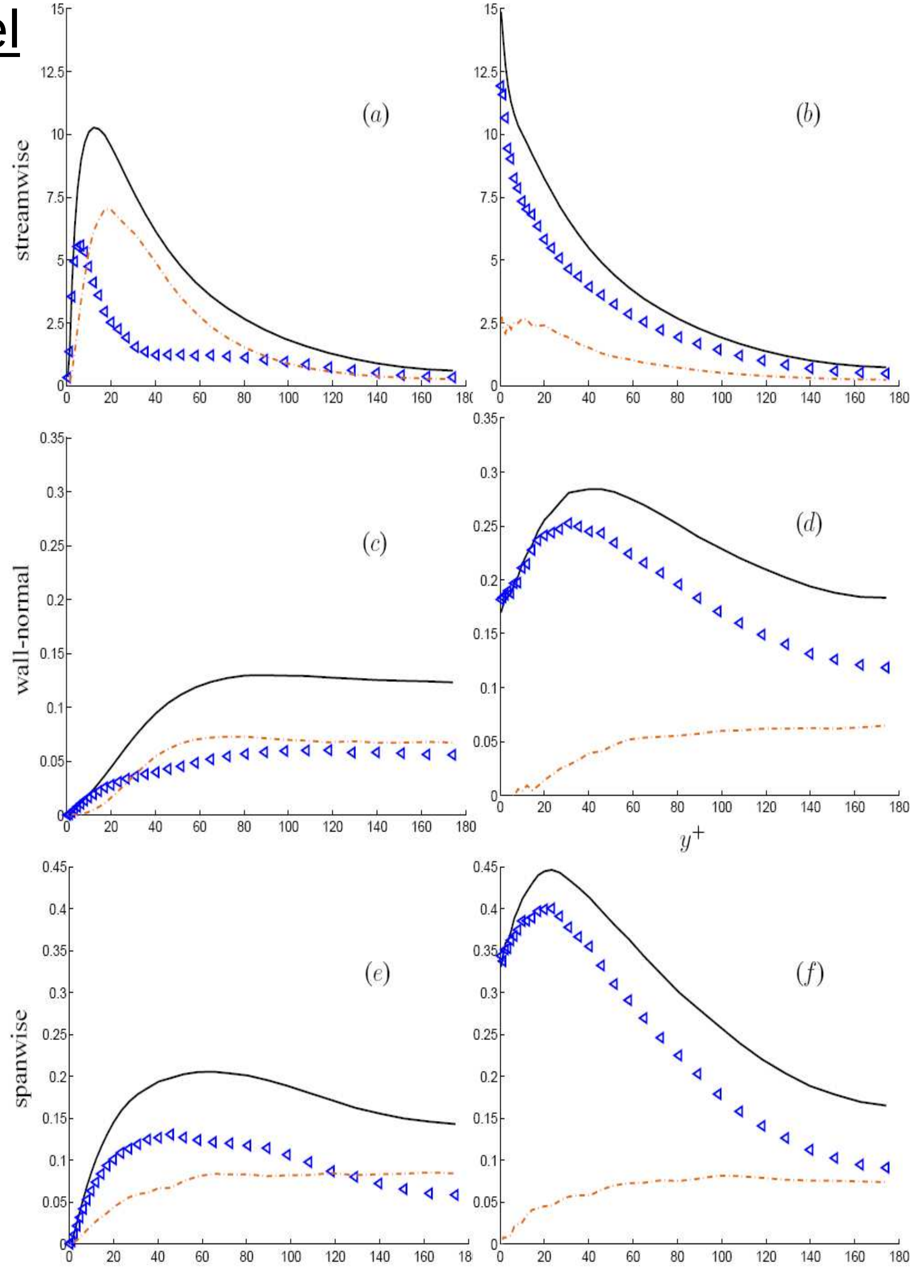


Figure 7: Partitioning of the particle velocity fluctuations, $St = 0.65$. —— total velocity variance; —·— correlated component; ◁ random-uncorrelated component. Left-hand frames from simulations without inter-particle collisions, right-hand frames from simulations with inter-particle collisions. (a) and (b) streamwise component; (c) and (d) wall-normal component; (e) and (f) spanwise component.

Simulation of decaying particle-laden turbulence

DPS reference computation (IMFT) :

mesh 64^3

10.4 10^6 particles

code NTMIX: structured, MPI, domain decomposition

6th order in space, RK in time

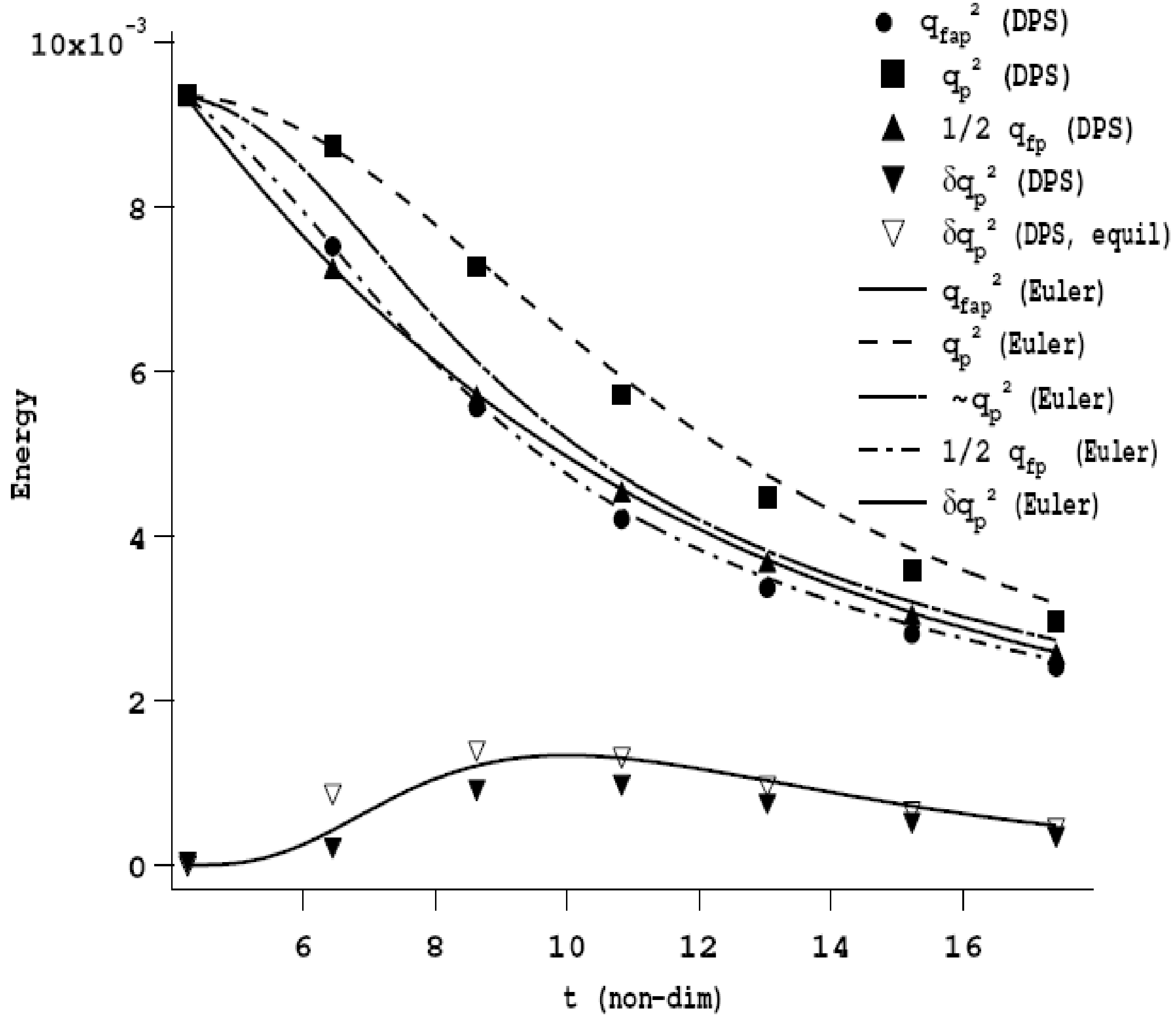
Eulerian-Eulerian computation (CERFACS) :

meshes: 64^3 (262144), 128^3 (2097152), 192^3 (7077888)

code AVBP: hybrid, MPI, domain decomposition

2nd order in space, FV, Lax Wendroff,RK

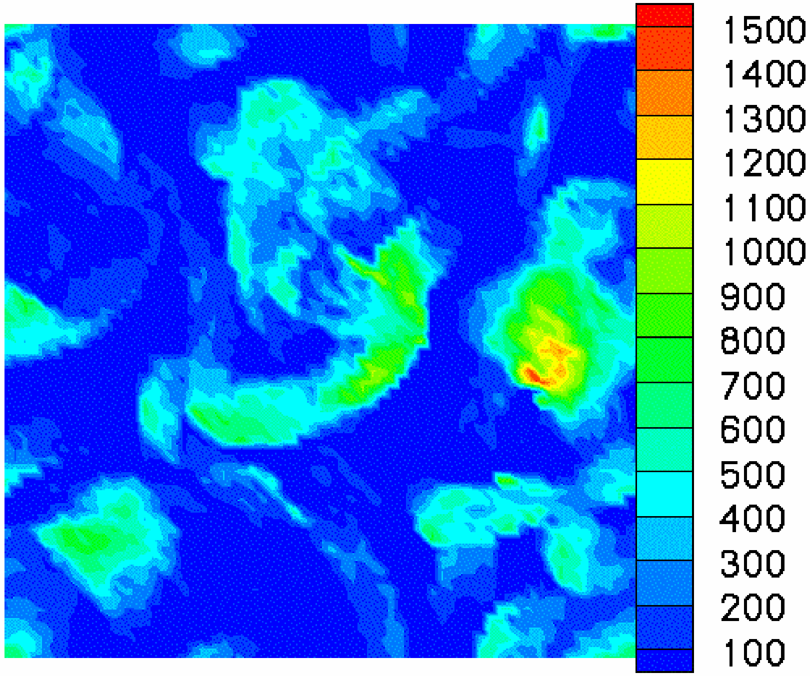
3rd order in space & time, FE, TTGC



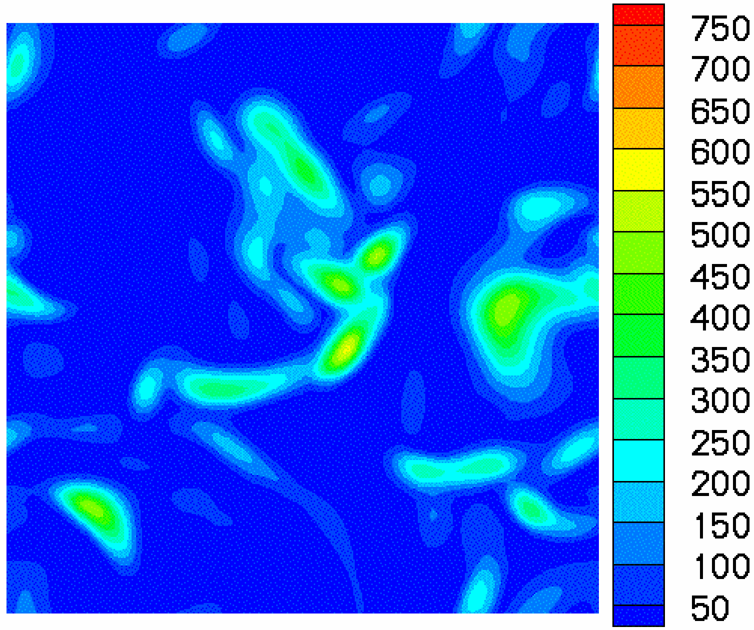
Particle and fluid-particle velocity correlations from DPS/DNS results
<u>Decaying isotropic turbulence</u> with St0= 0.53 (St= τ_p / T_E).

Simulation of decaying particle-laden turbulence

NTMIX: DPS



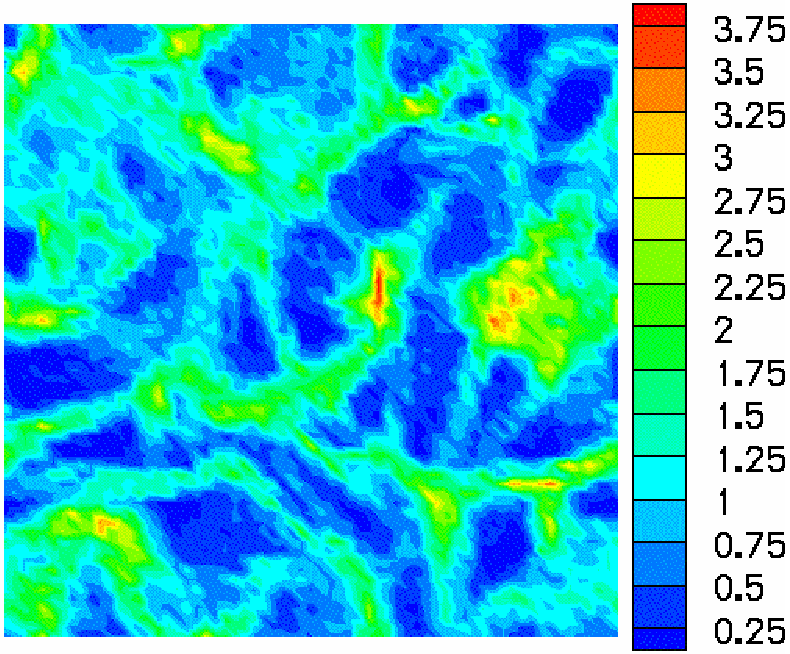
AVBP: Euler Euler



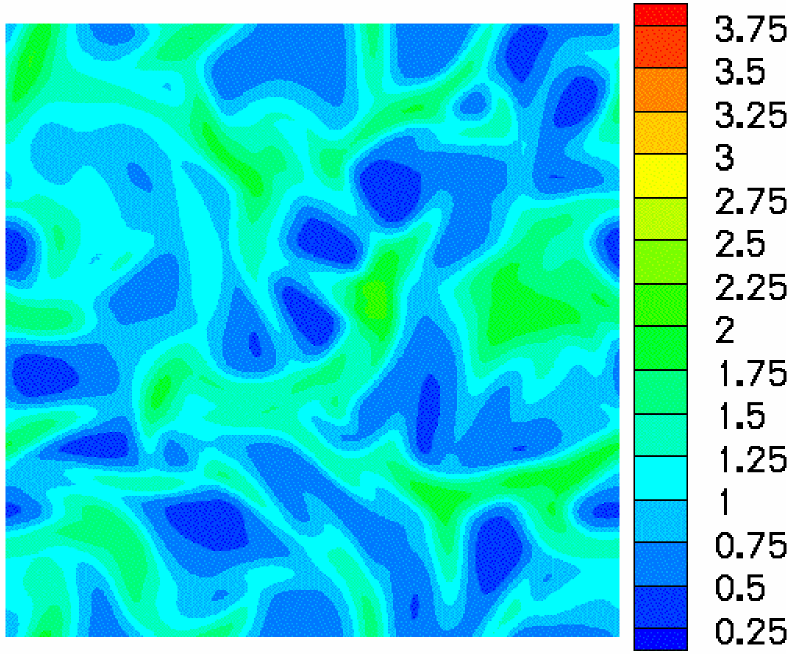
Quasi-Brownian kinetic energy: QBE

Simulation of decaying particle-laden turbulence

NTMIX: DPS



AVBP: Euler Euler



Normalized particle number density

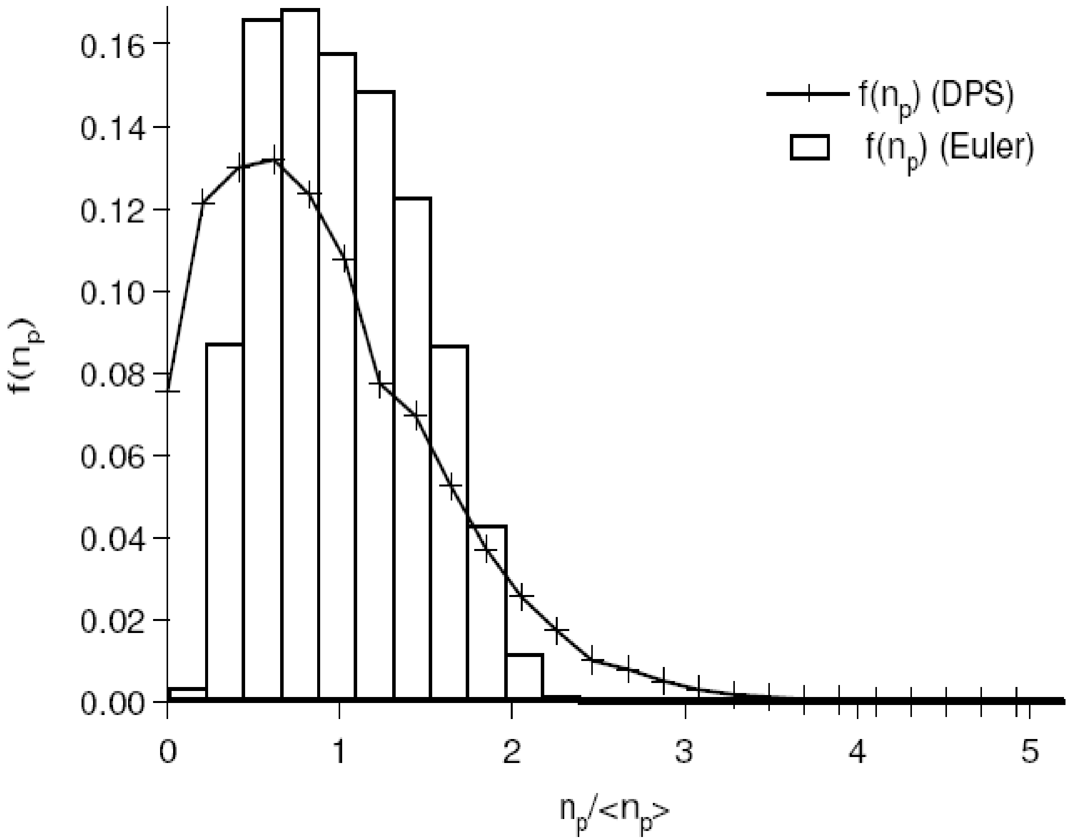


Fig. 19. Comparison of DPS and Eulerian number density PDF for the test case St =0.53 at t=10.8.

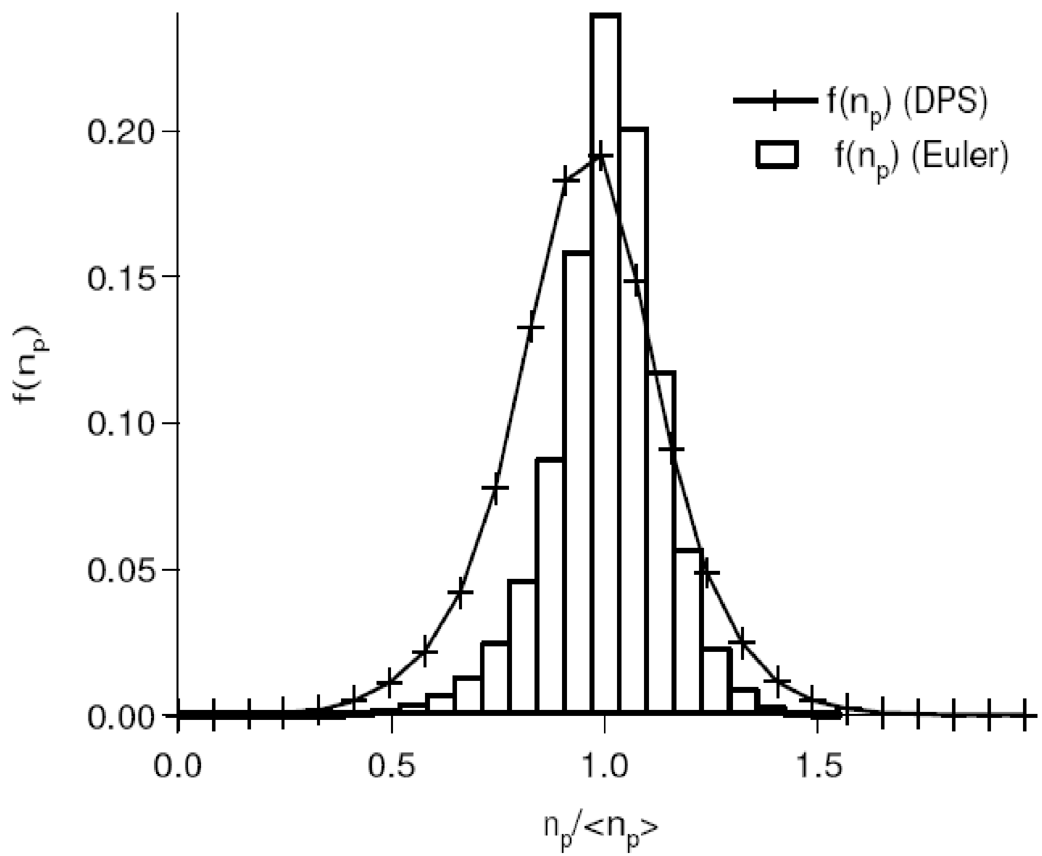
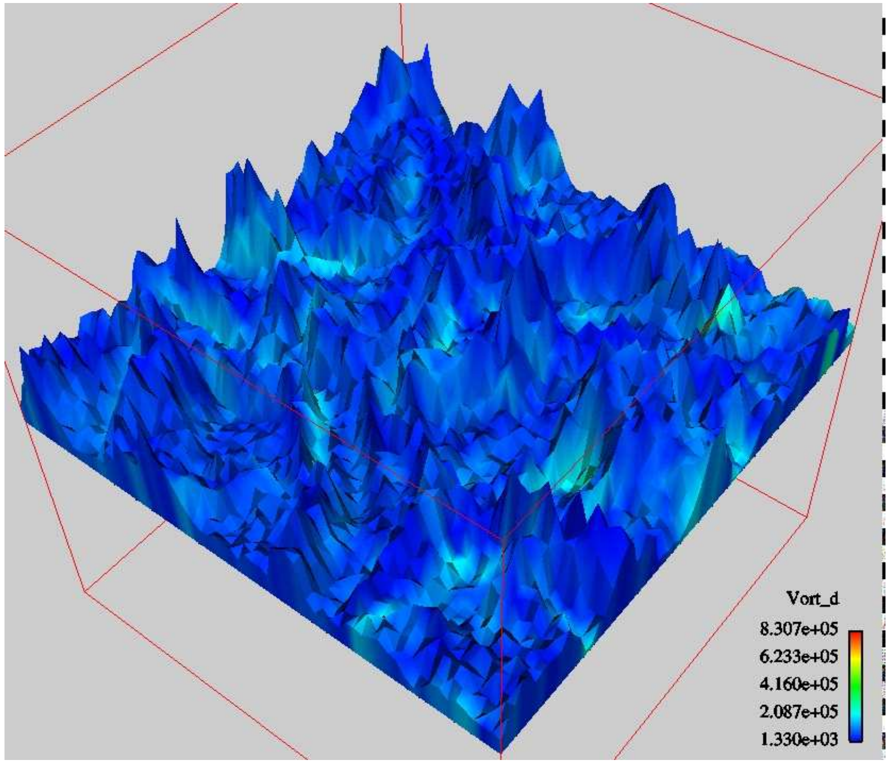


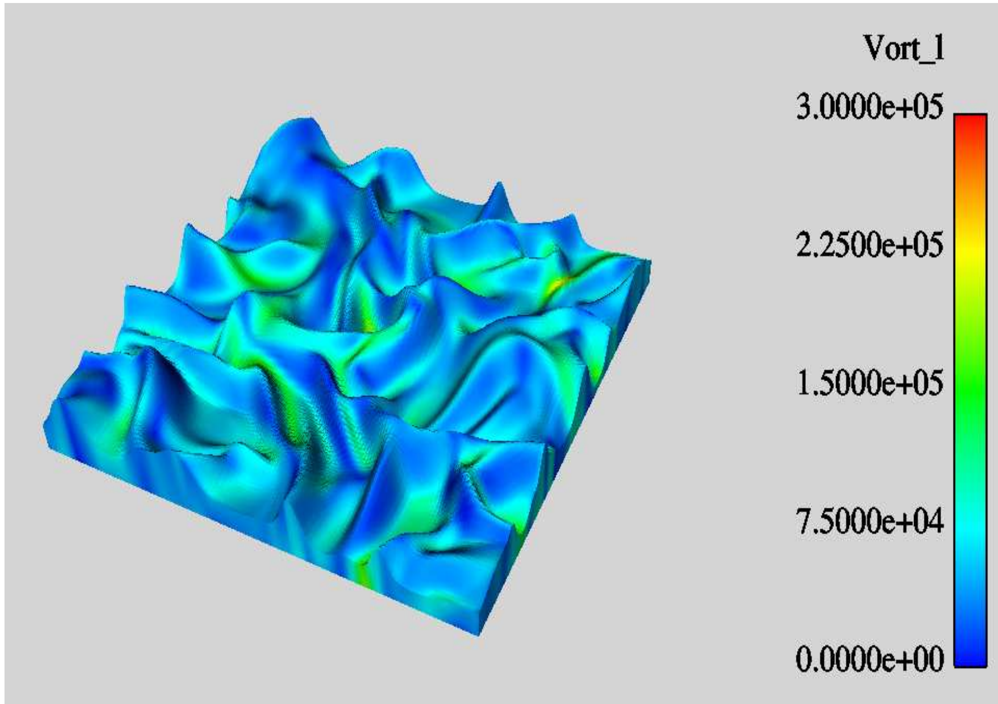
Fig. 15. Comparison of volume filtered DPS and Eulerian number density PDF for the test case with St = 0.042 at t=10.8.

Simulation of decaying particle-laden turbulence

NTMIX: DPS



AVBP: Euler Euler



Elevated surface of particle number density

LES of the correlated motion

- Favre spatial filtering

$$\hat{n}_p(x) = \int G_{\Delta filter}(x-y)\tilde{n}_p(y)dy$$

$$\overline{\tilde{n}_p \varphi} = \hat{n}_p \hat{\varphi}$$

With $G_{\Delta f}$: filter kernel of characteristic length Δ_f

- Filtered momentum equation of the correlated motion

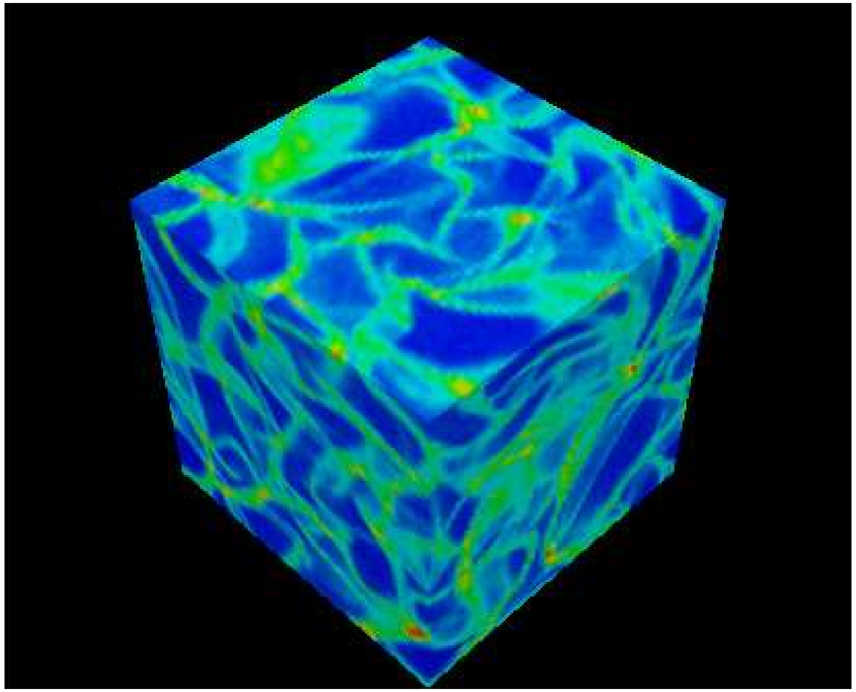
$$\frac{\partial}{\partial t}\hat{n}_p \hat{u}_{p,i} + \frac{\partial}{\partial x_j}\hat{n}_p \hat{u}_{p,j}\hat{u}_{p,i} = -\frac{\hat{n}_p}{\tau_p}(\hat{u}_{p,i} - \hat{u}_{f@p,i}) - \frac{\partial}{\partial x_j}\hat{n}_p \widehat{< \delta u_{p,i}\delta u_{p,j} >_p} - \frac{\partial}{\partial x_j} T_{SGS,ij}$$

$$T_{SGS,ij} = \widehat{\tilde{n}_p \tilde{u}_{p,i}\tilde{u}_{p,j}} - \hat{n}_p \hat{u}_{p,i}\hat{u}_{p,j}$$

Need models

Simulation conditions

- DNS+DPS
  - 6^{th} order in space
  - 3^{rd} order Runge-Kutta in time
  - 4^{th} order Lagrange for interpolation
- Free Decaying turbulence (homogeneous and isotropic)
  - 64^3 grid point cubic box with periodic BC
  - Particles randomly embedded
  - Number of particles: 10 and 80 M



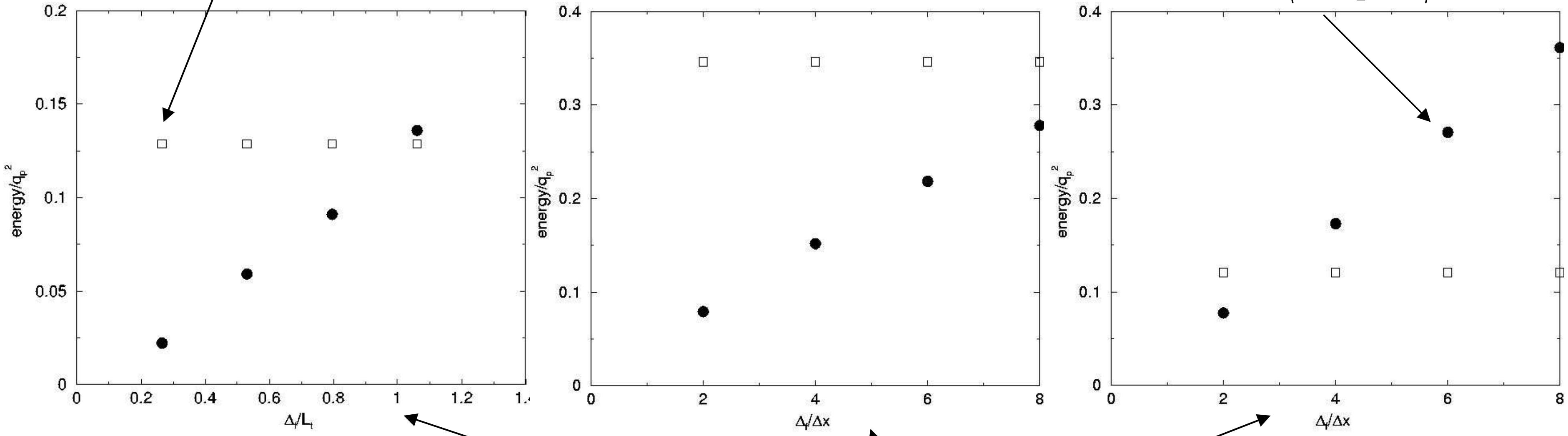
Case A: 64^3,10^7 particles

Cases:	A	B	C
Re_t	6,6	40	40
St	1.1	1.1	0.47

Relative influence of the mean sub-grid correlated and uncorrelated energies

$$\delta\breve{\theta}_p = \frac{1}{2}\widehat{\left\langle \delta u_{p,i}\delta u_{p,i} \right\rangle_p}$$

$$\frac{1}{3}\left\langle \frac{T_{SGS,kk}}{\overline{\breve{n}}_p} \right\rangle$$



Cases:	A	B	C
Re_t	6,6	40	40
St	1.1	1.1	0.47

Modeling of $T_{SGS,ij}$

- Compressible gaseous turbulence subgrid stress models
  - Fluid subgrid stress: $T_{f,ij} = \overline{\rho}(\widehat{u_{f,i}u_{f,j}} - u_{f,i}u_{f,j})$
  - Viscosity model: $T_{f,ij} = P_{SGS}\delta_{ij} - \upsilon_{SGS}S^*_{f,ij}$

$$S_{f,ij} = \tfrac{1}{2}\left(\frac{\partial \hat{u}_{f,i}}{\partial x_j} + \frac{\partial \hat{u}_{f,j}}{\partial x_i}\right)$$

(Moin et al, 1991)

$$S^*_{f,ij} = S_{f,ij} - \tfrac{1}{3}S_{f,kk}\delta_{ij}$$

$$P_{SGS} = 2C_l\overline{\rho}_f\Delta_f^2\left|S_f\right|^2$$

$$\upsilon_{SGS} = 2C_s\overline{\rho}_f\Delta_f^2\left|S_f\right|$$

C_l and C_s are dynamically evaluated

$C_l \in$ [0.0025-0.009] and $C_s \in$ [0.008-0.014]

Modeling of $T_{SGS,ij}$

- Mixed Model (Erlebacher et al, 1992):
- Triple decomposition $T_{f,ij} = L_{ij} + C_{ij} + R_{ij}$
  - Leonard term — No modelling
  - Cross term — Scale similarity model
  - Reynolds term — Yoshizawa+ Smagorinsky model

- Adaptation to dispersed flow

$$\rho_f \Rightarrow \breve{n}_p \quad u_f \Rightarrow \breve{u}_p$$

A priori testing of particle sub-grid scales models

ε_{SGS}^{I} ■ : Exact

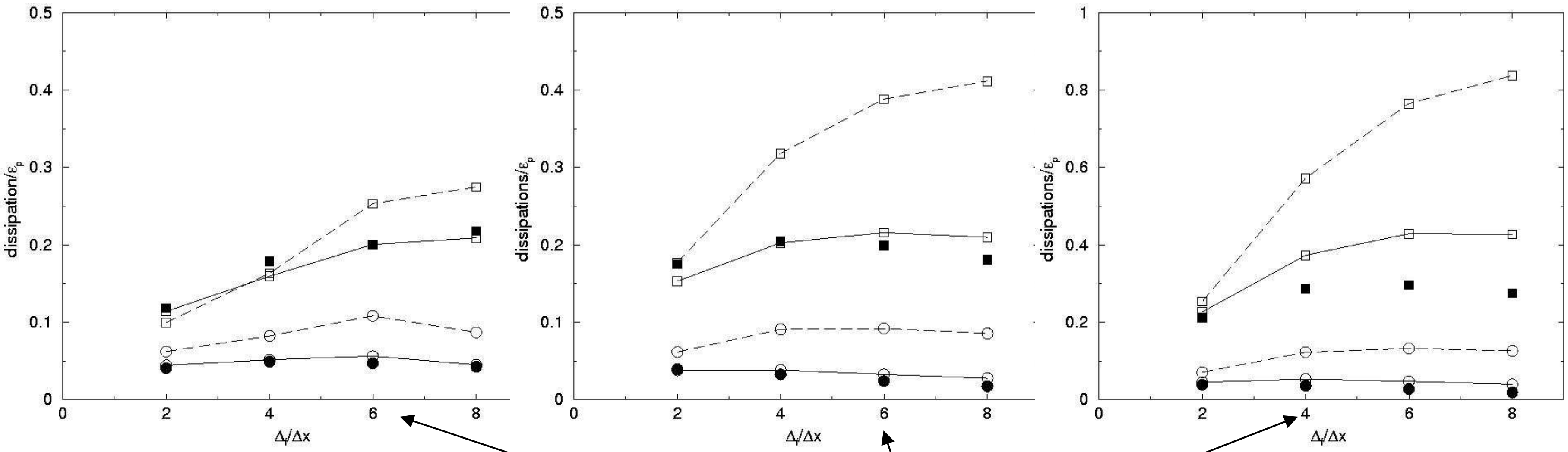
□– – □ : Viscosity

□——□ : Mixed

ε_{SGS}^{II} ●: Exact

○– – ○ : Viscosity

○——○ : Mixed



Cases:	A	B	C
Re_t	6,6	40	40
St	1.1	1.1	0.47

	C_S	C_l
Viscosity	0.02	0.012
Mixed	0.0085	0.0033

Modeling of $\widehat{\left\langle \delta u_{p,i}\delta u_{p,j}\right\rangle_p}$

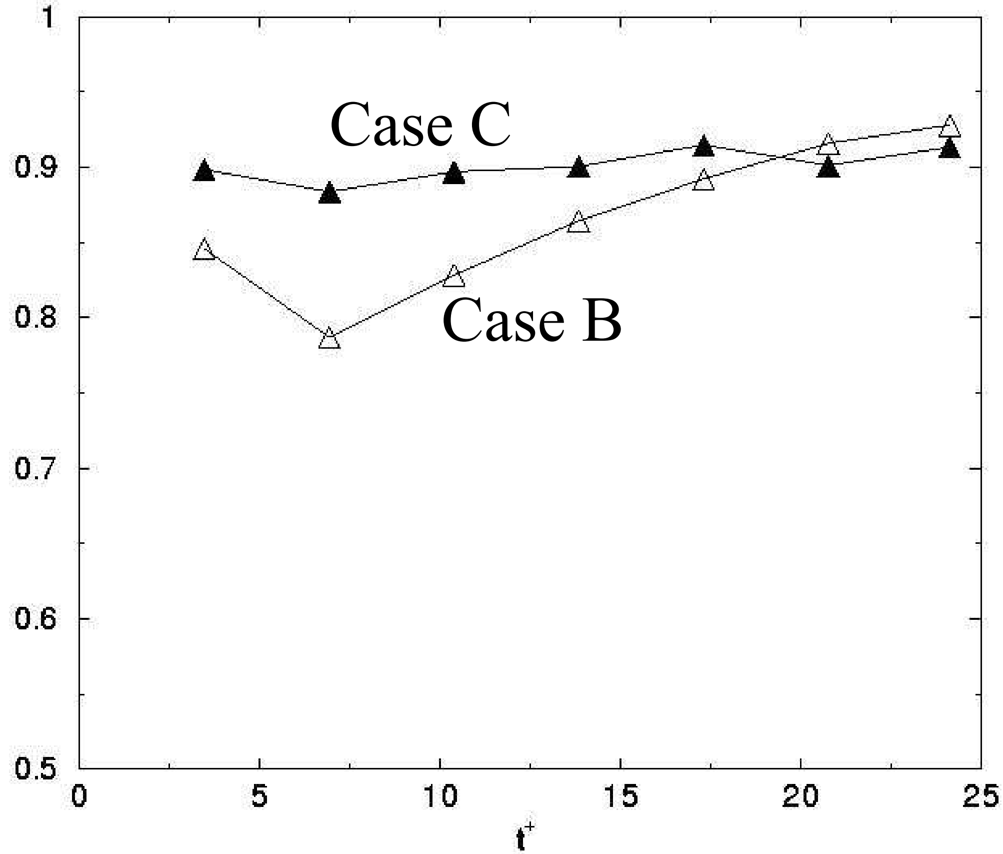
$$\widehat{\left\langle \delta u_{p,i}\delta u_{p,j}\right\rangle_p} = \hat{\breve{\tau}}_{p,ij} - \frac{2}{3}\overline{\breve{n}_p}\,\delta\hat{\breve{\theta}}_p\,\delta_{ij}$$

- Viscosity model for filtered $\hat{\breve{\tau}}_{ij}$

$$\hat{\breve{\tau}}_{ij} = \hat{\breve{\mu}}\left(\frac{\partial \hat{\breve{u}}_{p,i}}{\partial x_j} + \frac{\partial \hat{\breve{u}}_{p,j}}{\partial x_i} - \frac{2}{3}\frac{\partial \hat{\breve{u}}_{p,k}}{\partial x_k}\delta_{ij}\right)$$

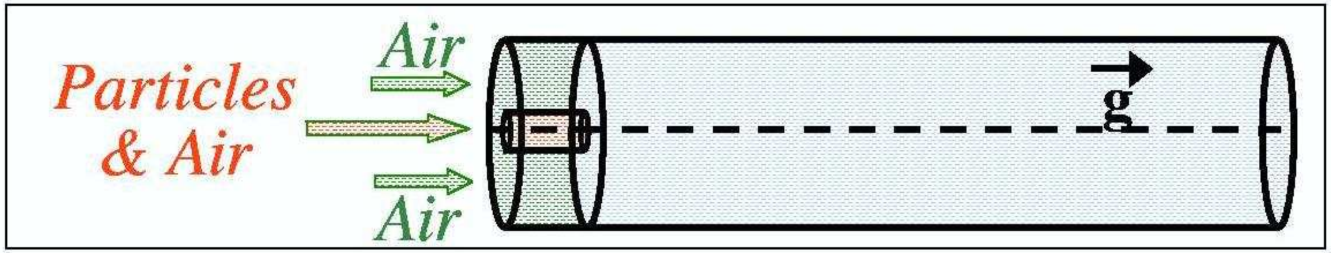
$$\hat{\breve{\mu}} = \frac{\hat{\breve{n}}_p}{3}\tau_p\delta\hat{\breve{\theta}}_p$$

Correlation between exact and modeled term

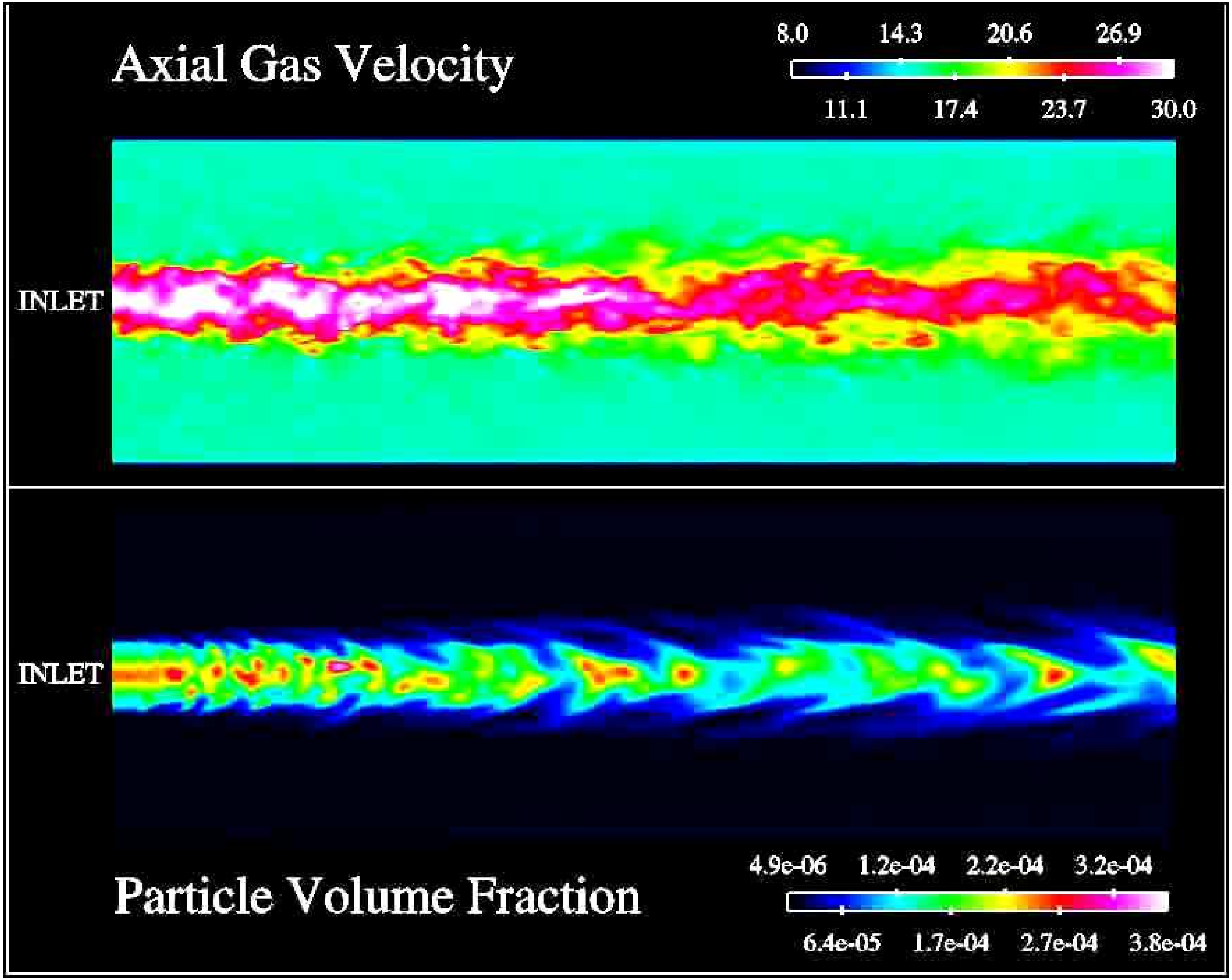


Euler-Euler LES of particle laden jet

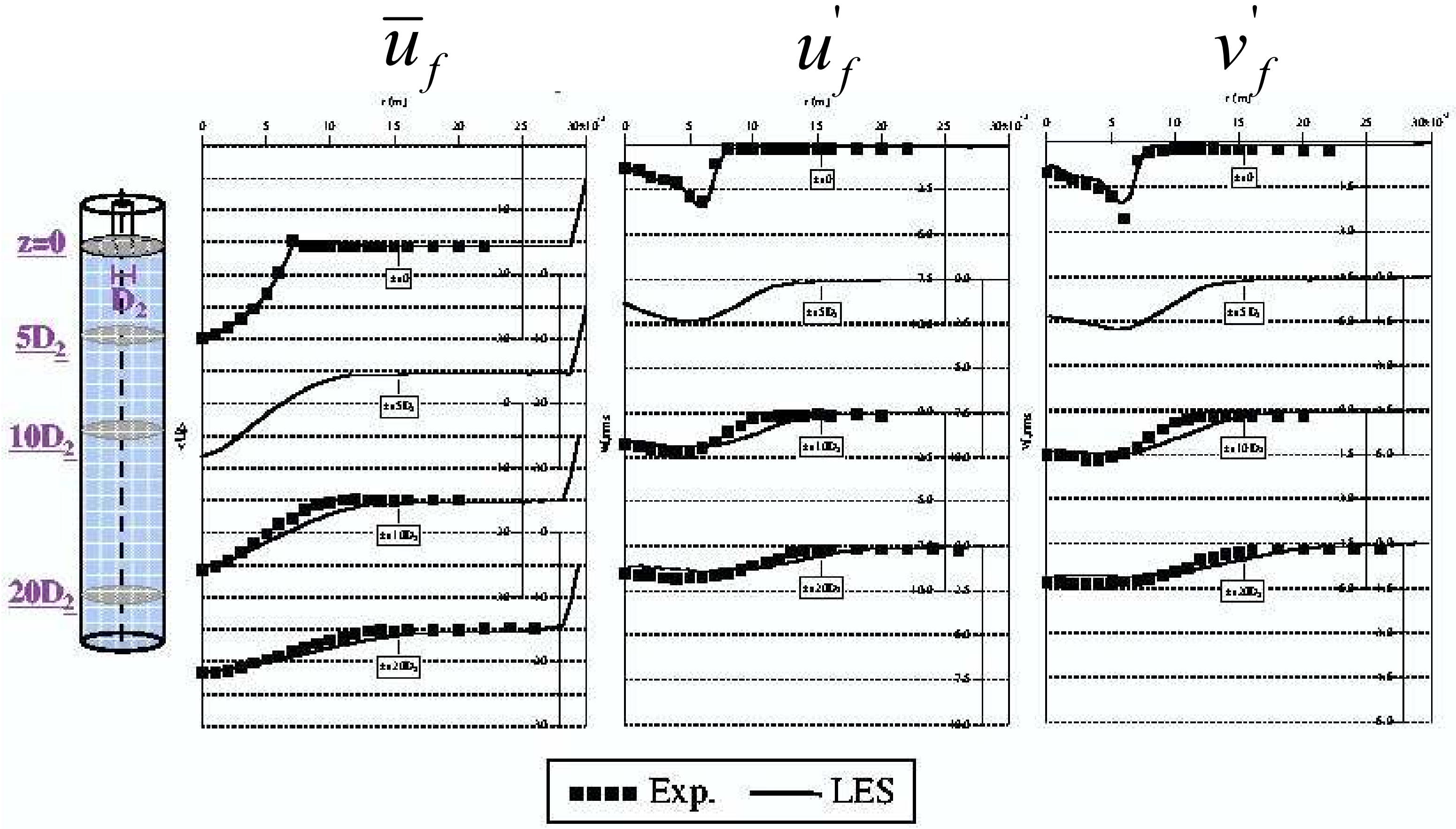
- Turbulent co-axial jet (Hishida et al, 1987)
- dilute flow (no two way couplings)
- St ~ 0.4



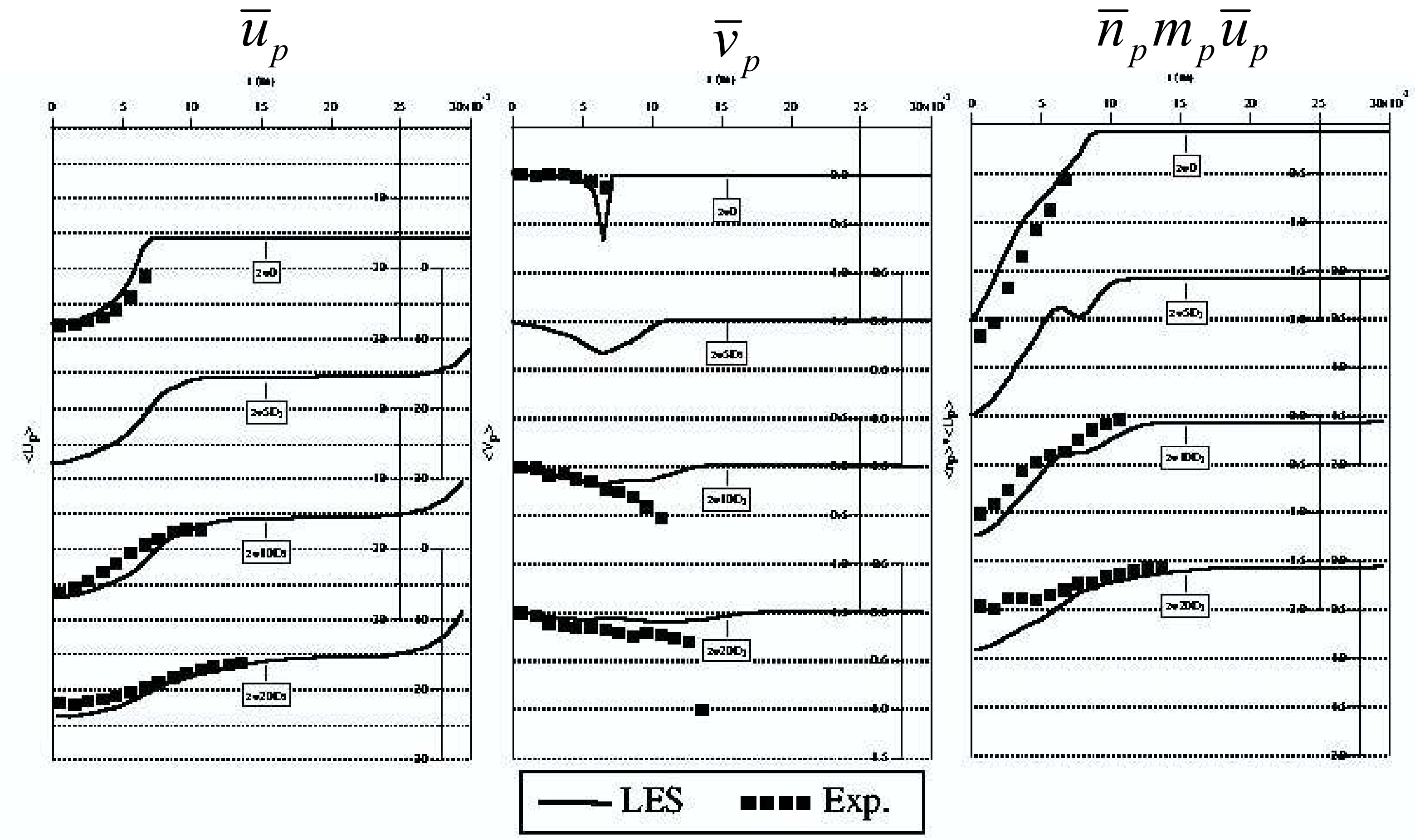
- Model:
  - Gas: Wales
  - Particles : viscosity model for $T_{SGS,ij}$ (C_l=0.012, C_s=0.02)
  - No model for $\widehat{\langle \delta u_{p,i} \delta u_{p,j} \rangle_p}$
- Numeric:
  - TTGC (3rd order)
  - Non-Reflecting BC for the gaz
  - Turbulence injection
  - Appropriated injection for particles


Axial Gas Velocity
8.0
14.3
20.6
26.9
11.1
17.4
23.7
30.0
INLET
INLET
Particle Volume Fraction
4.9e-06
1.2e-04
2.2e-04
3.2e-04
6.4e-05
1.7e-04
2.7e-04
3.8e-04

Euler-Euler LES of particle laden jets



Euler-Euler LES of particle laden jets



Conclusion and Perspectives

Conditional average with respect to the fluid flow realization allows to separate the particle velocity in an instantaneous mesoscopic Eulerian velocity field and a quasi-Brownian distribution.

Local instantaneous transport equations can be derived for the mesoscopic Eulerian velocity field and should allow to perform two-fluid DNS but closure assumptions are needed for modelling the effects of the quasi-Brownian motion (kinetic energy and viscosity).

Such partitioning should be very interesting to improve the understanding and modelling of particle-particle collision in dilute turbulent flows and modification of the turbulence spectrum by inertial particles.

Euler LES transport equations and closure models for the dispersed phase may be derived by spatial filtering from the mesoscopic approach