

# Modelowanie przepływów turbulentnych z fazą dyspersyjną: metoda LES i efekty podsiatkowe

**Modelling turbulent dispersed flows:  
Large-Eddy Simulation and subfilter effects**

**Jacek Pozorski**

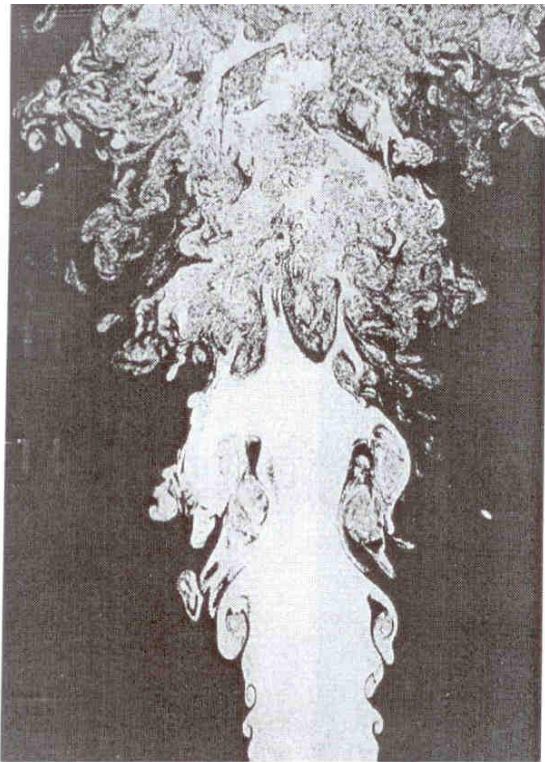
*Instytut Maszyn Przepływowych PAN w Gdańsku*



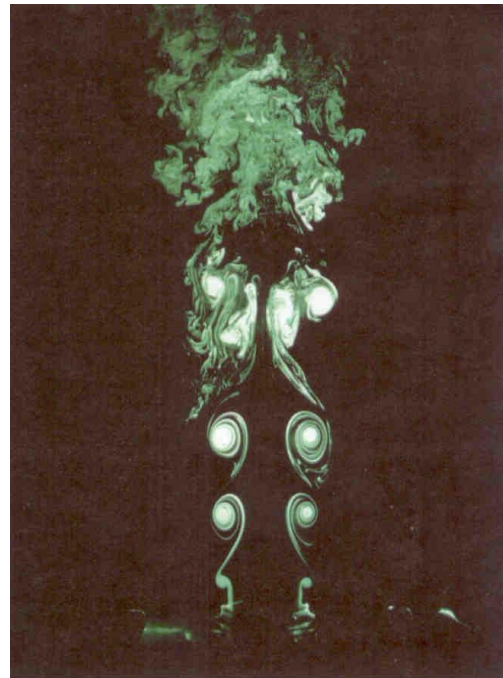
# Część I: Przepływy turbulentne wprowadzenie

Perhaps the holy grail of turbulence is *the statistical resolution of all scales* - a methodology in which representative samples of motions and processes on all scales are resolved and combined (without empiricism) in a way that remains computationally tractable at large Reynolds number."

S. B. Pope ``Ten questions concerning LES (...)"',  
New Journal of Physics **6** (2004) 35



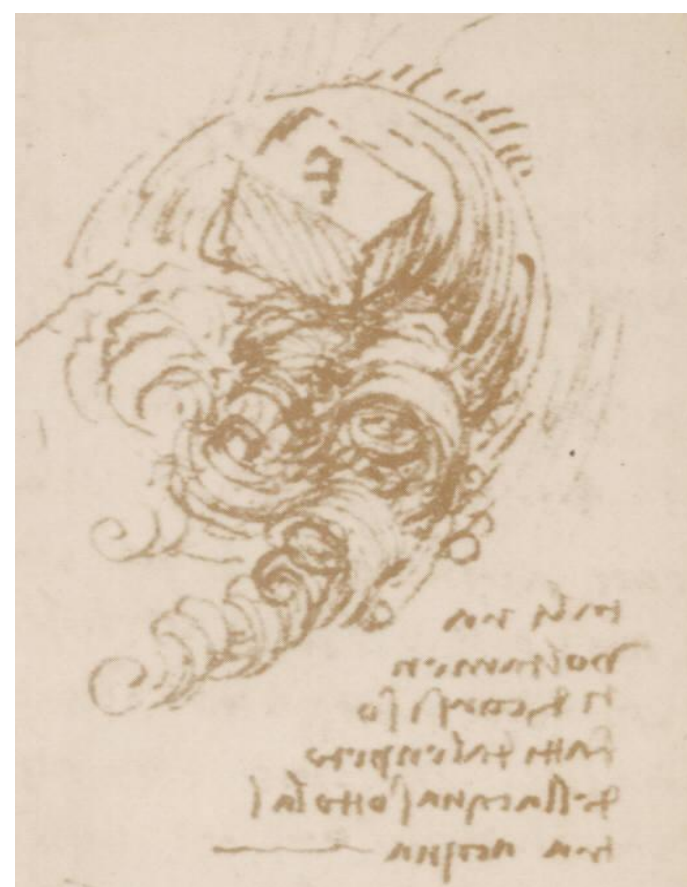
(Lesieur, 1997)



(A Gallery of Fluid Motion, 2003)

← strugi turbulentne

# A short guide to turbulence (with milestones)

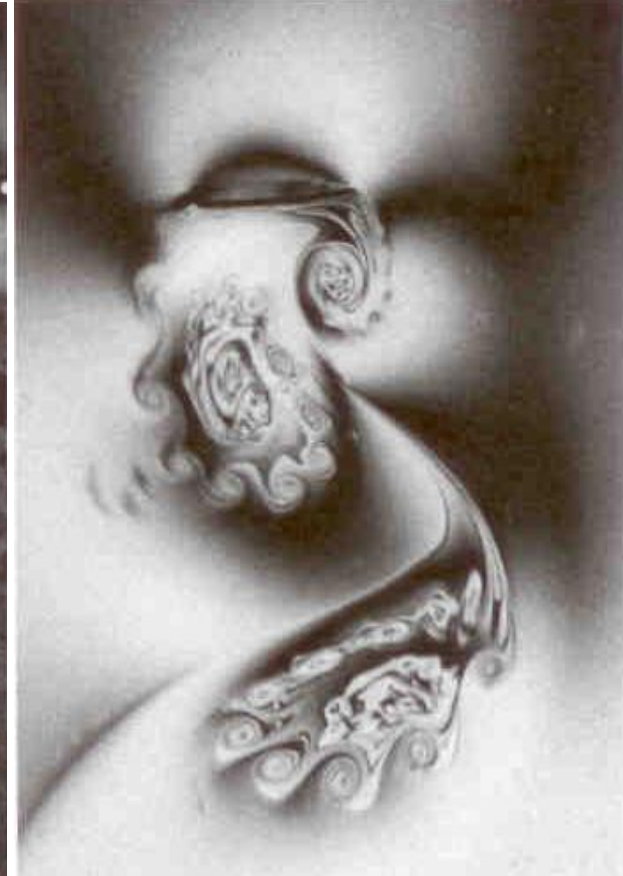


**flow past a bluff-body**

(da Vinci, around 1500)



**flow through array of rods**



**self-similar (?) flow**

(A Gallery of Fluid Motion, 2003)

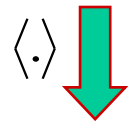
# Pierwszy kamień milowy: dekompozycja Reynoldsa

$\langle \cdot \rangle$  operator uśredniania;

$$\mathbf{U} = \langle \mathbf{U} \rangle + \mathbf{u}$$

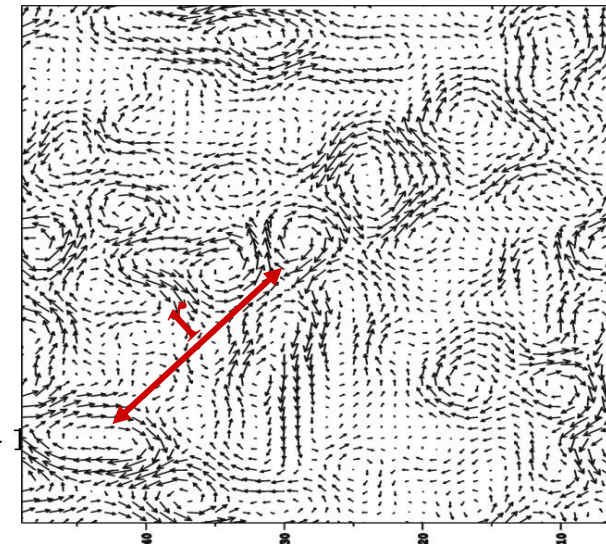
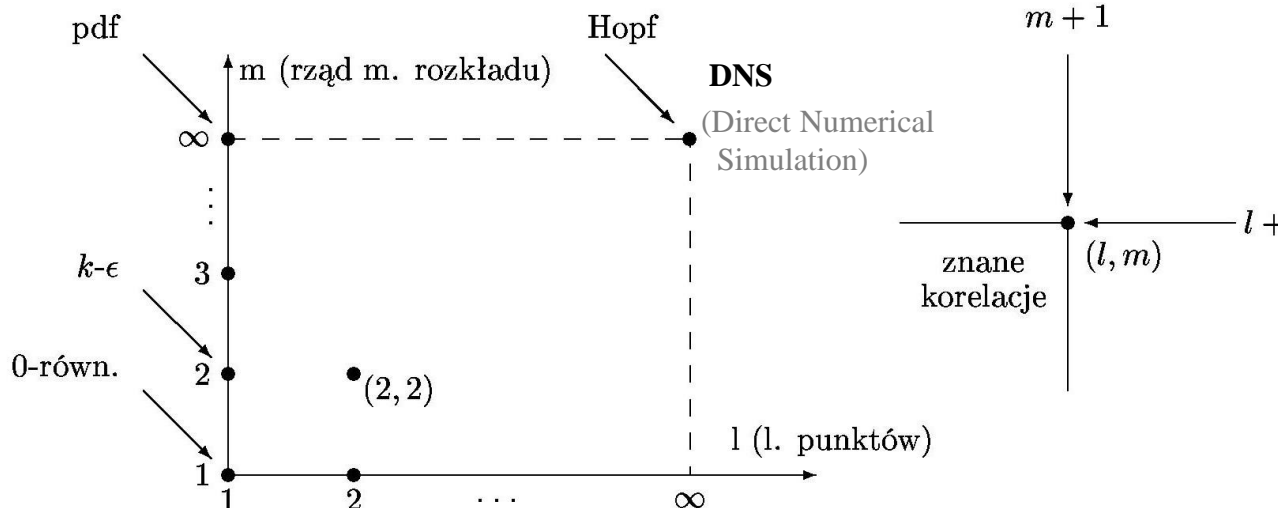
Uśrednienie równań ruchu (Reynolds, 1894)

$$\frac{\partial \mathbf{U}}{\partial t} + (\mathbf{U} \cdot \nabla) \mathbf{U} = -\frac{1}{\rho} \nabla p + \nu \nabla^2 \mathbf{U}$$



tensor naprężeń turbulentnych  $R_{ij}(\mathbf{x}) = \langle u_i(\mathbf{x})u_j(\mathbf{x}) \rangle$

$$\frac{\partial \langle \mathbf{U} \rangle}{\partial t} + (\langle \mathbf{U} \rangle \cdot \nabla) \langle \mathbf{U} \rangle = -\frac{1}{\rho} \nabla \langle p \rangle + \nu \nabla^2 \langle \mathbf{U} \rangle - Div \mathbf{R}$$



Np.  $\langle u_i(\mathbf{x})u_j(\mathbf{x} + \mathbf{r}) \rangle$   
dwupunktowy moment rozkładu  
(korelacja) drugiego rzędu

**Problem domknięcia** (gdzie jest LES?) (RANS – struktury?)

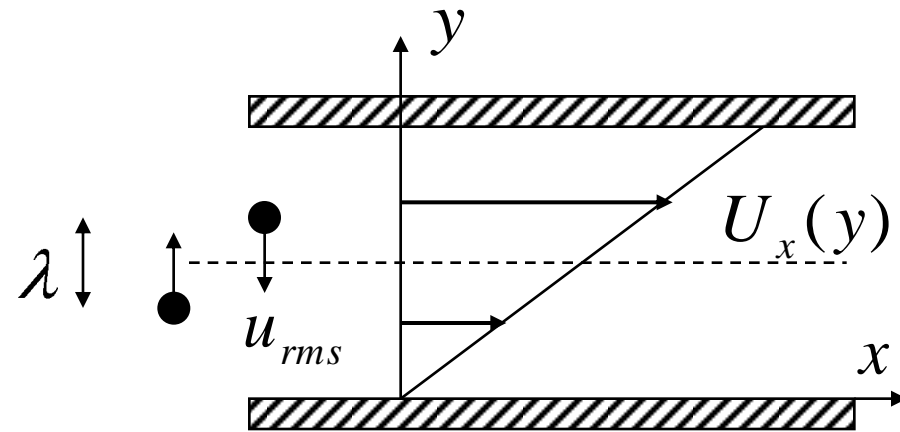


# Drugi kamień milowy: hipoteza Prandtla

Rozdział skal ruchu średniego i fluktuacji:  
analogia do teorii kinetycznej gazów

Lepkość molekularna

$$\sigma_{xy} \sim \nu \frac{\partial U_x}{\partial y} \quad \nu \sim u_{rms} \lambda$$



Hipoteza lepkości turbulentnej (Boussinesq 1877)

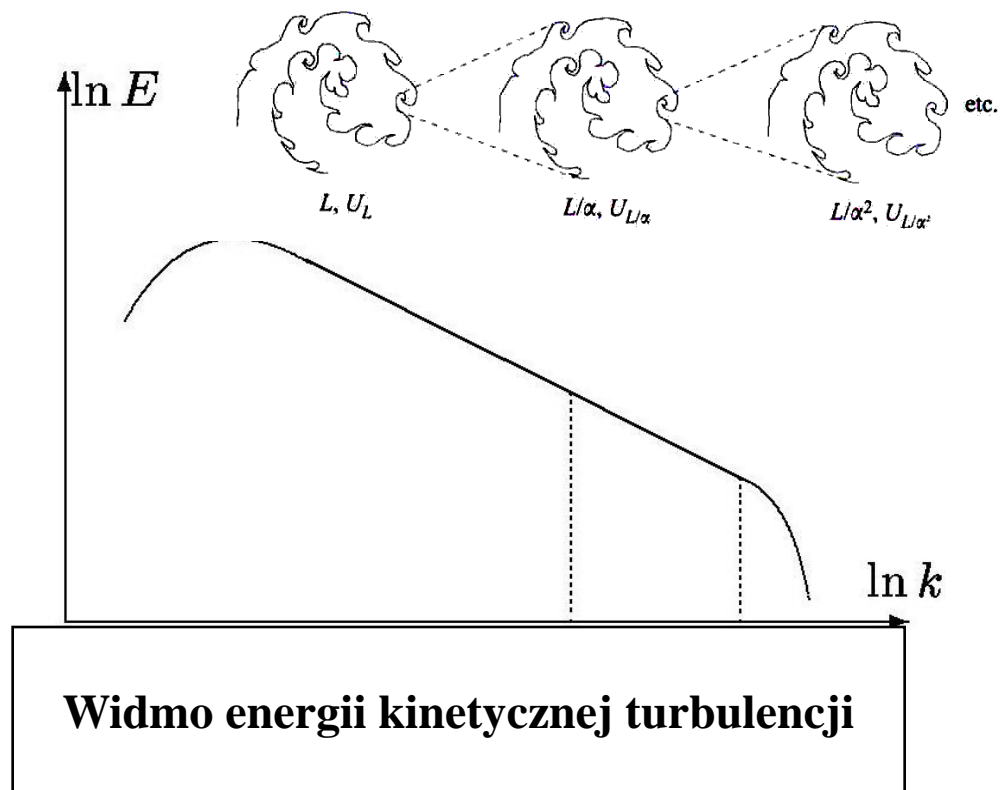
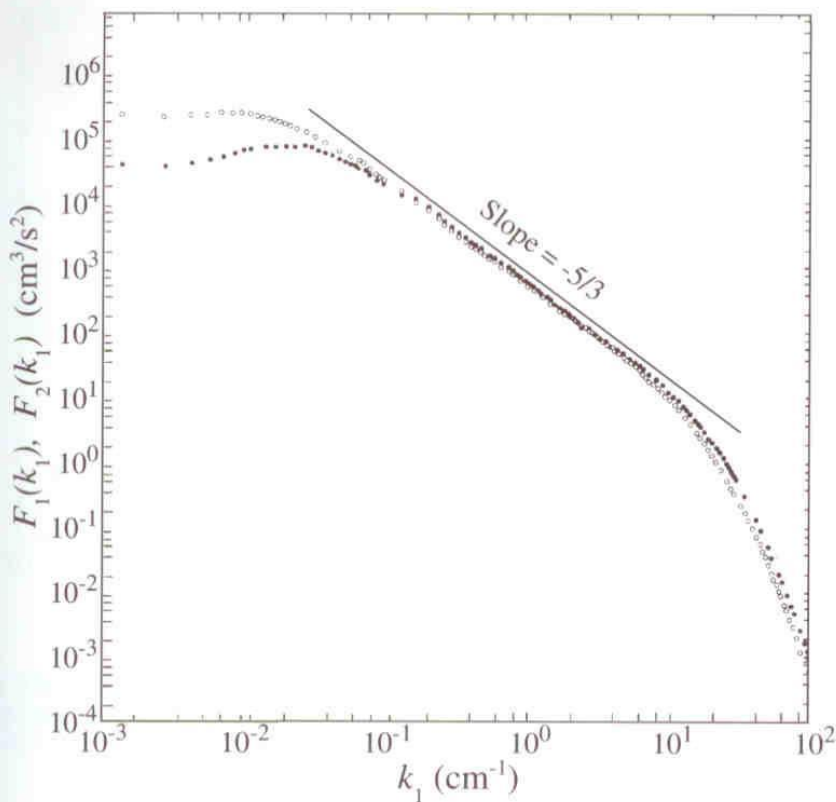
$$R_{xy} \sim \nu_t \frac{\partial \langle U_x \rangle}{\partial y} \quad \nu_t \sim ?$$

$$\nu_t \sim u' L$$

Hipoteza drogi mieszania (Prandtl 1925)

$$\nu_t \sim u' l_m; \quad u' = l_m \left| \frac{d \langle U_x \rangle}{dy} \right|; \quad l_m = \kappa y \quad (\text{rozdziel skal?})$$

# Trzeci kamień milowy: hipoteza Kołmogorowa



W „środkowym” zakresie skal:

(Kołmogorow, 1941)  $E(k) \sim \varepsilon^{2/3} k^{-5/3}$

(konstruowanie domknięć –  
*similarity models?*)

# Przepływy z fazą dyspersyjną - wprowadzenie

## Przepływ dyspersyjny:

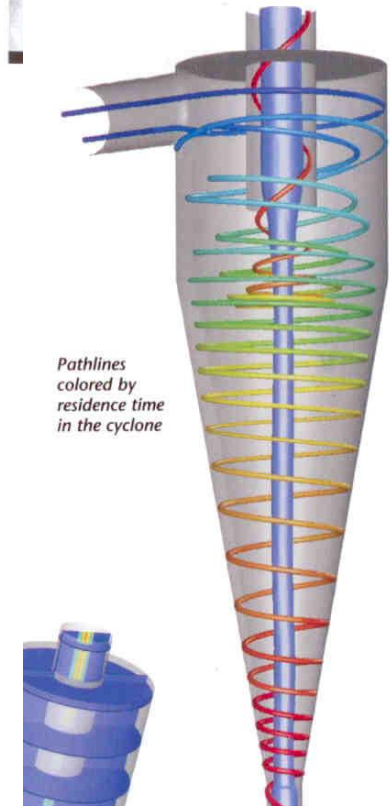
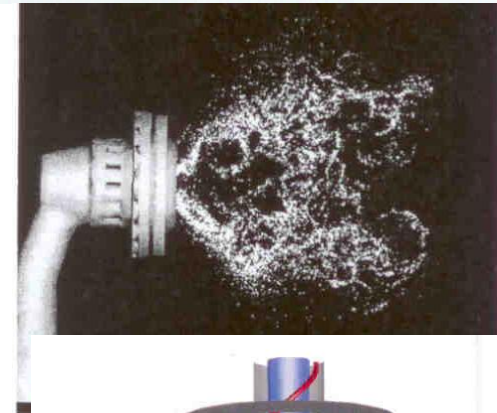
przepływ fazy nośnej (ciągłej, czyli płynu)  
z cząstkami (stałymi lub kroplami, ewent. pęcherzykami)

## Motywacje: przykłady

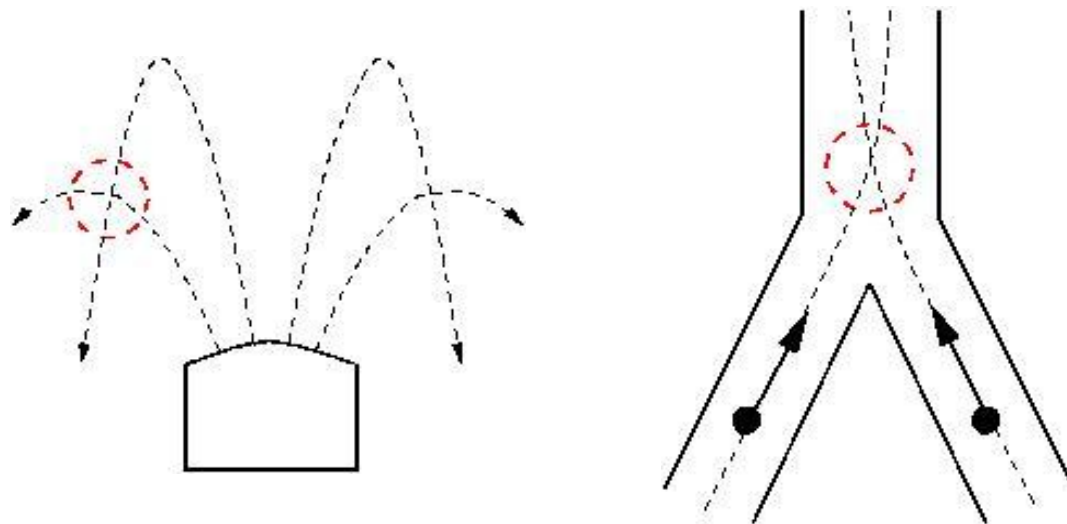
- spalanie kropeł paliwa w turbinach gazowych,
- spalanie pyłu węglowego w kotłach energetycznych,
- przepływy pary mokrej (turbiny, energetyka jądrowa)
- inżynieria chemiczna i procesowa: urządzenia i aparaty

## Motywacje: sformułowania

- model dwupłynowy (Eulerowsko-Eulerowski):
- śledzenie trajektorii cząstek (Eulerowsko-Lagrange'owski)



# Dispersed two-phase flows - computational approaches



Simple examples of dispersed flows

## Formulations:

- two-fluid model (Eulerian-Eulerian):
- particle tracking (Eulerian-Lagrangian) – applied here

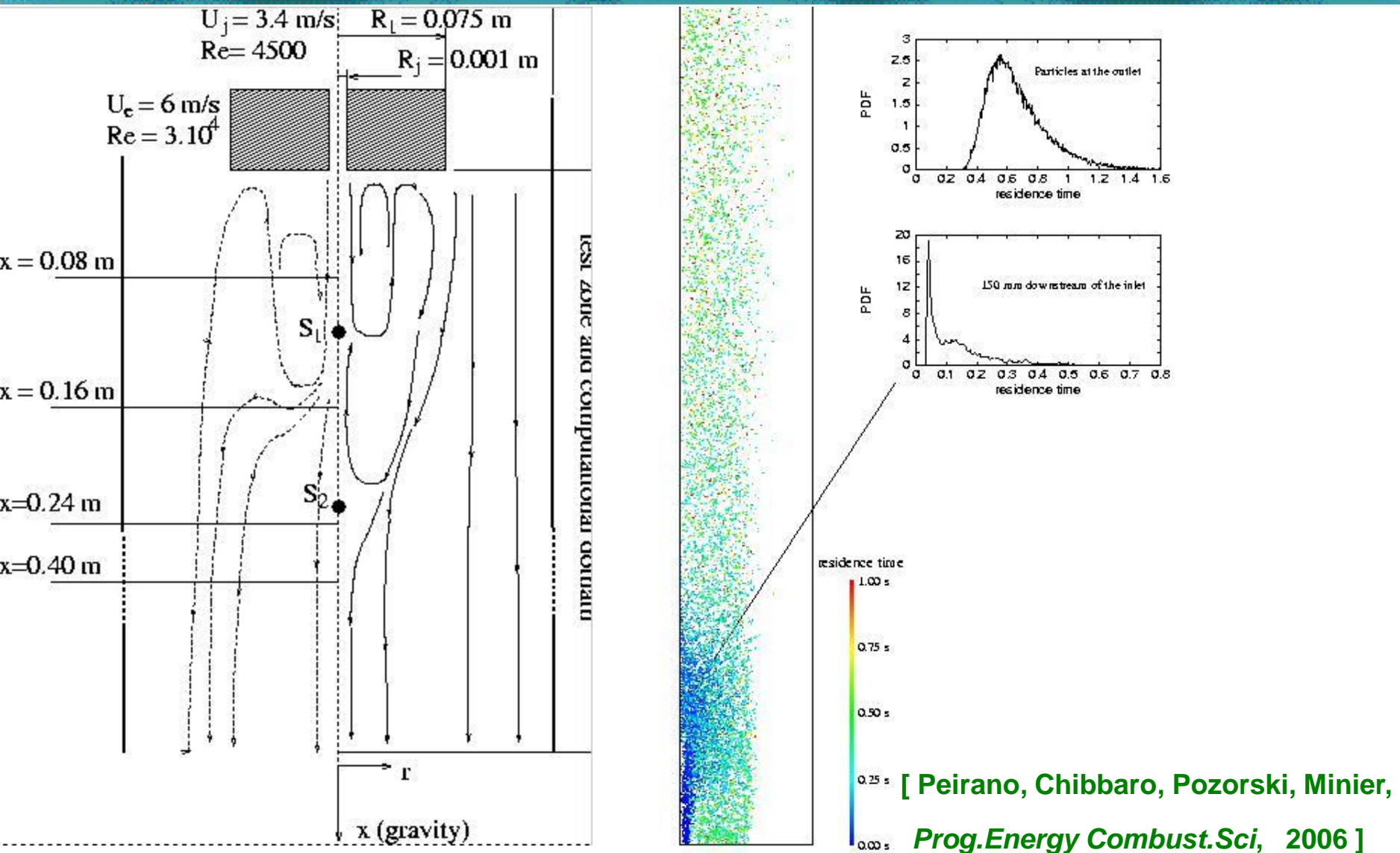
Remarks: - statistical vs. instantaneous fluid flow resolution

- inadequacy of gradient hypotheses  
(based on local equilibrium assumption)

$$\vec{j}_m = -D_t \nabla n_p$$



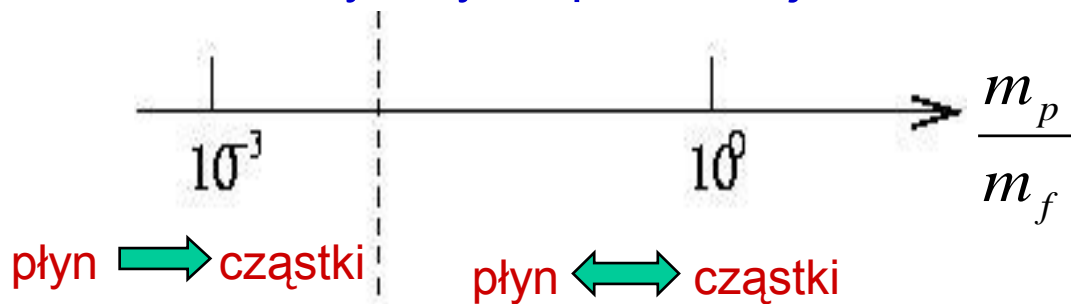
# Efektywność podejścia Eulera-Lagrange'a (cd.)



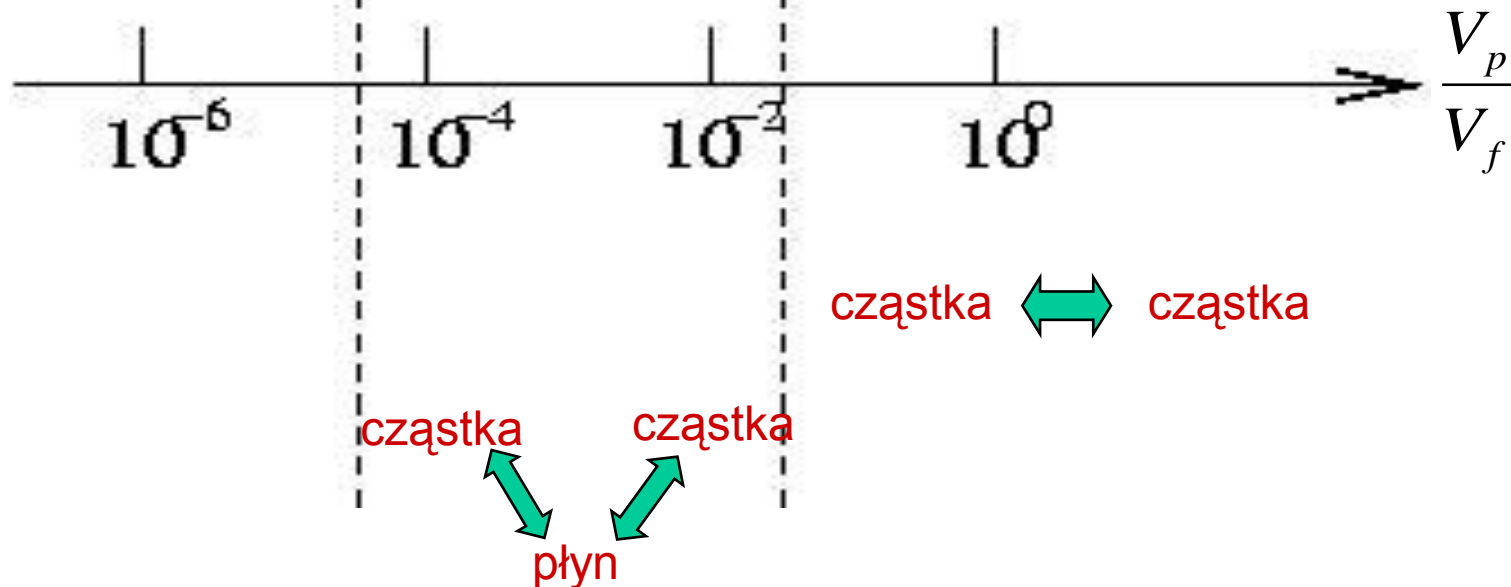
# Obliczenia dyspersyjnych przepływów wielofazowych

Udział masy fazy rozproszonej:

cząstki ciężkie:  $\frac{\rho_p}{\rho_f} \approx 10^3$



Udział objętościowy fazy rozproszonej:



# Opis dyspersyjnych przepływów dwufazowych

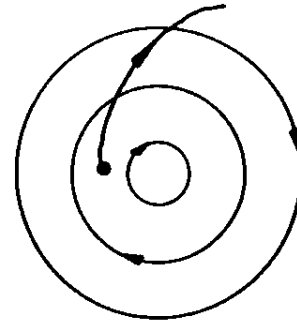
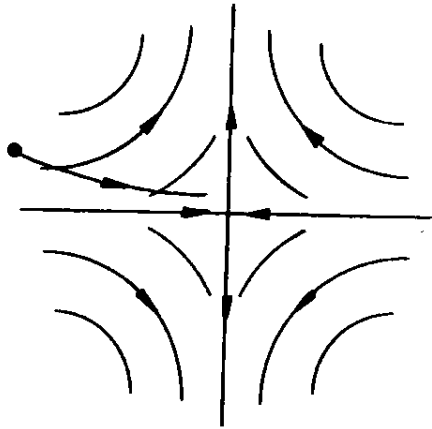
## Fizyka zjawisk:

- **ruch cząstek:** siła oporu, nośna, historii, itd.
- **oddziaływania cząstka-ścianka:** uderzenie/odbicie, separacja
- przemiany fazowe: odparowanie kropeł lub kondensacja
- zderzenia cząstek, niestabilności hydrodynamiczne powierzchni kropeł
- efekty ściśliwości (w przepływach gaz-ciecz): zjawiska falowe, zadławienie

## Problemy modelowania:

- **wpływ turbulencji fazy nośnej na cząstki** oraz *vice versa*
- warunki brzegowe na ścianie (modele dwupłynowe), **separacja**
- przemiany fazowe (nukleacja, *flashing*, nierównowaga termodynamiczna)
- atomizacja strugi, rozpad i koalescencja kropeł, rozkład wielkości cząstek

# Korelacja położenia cząstek z polem przepływu



$$2S_{ij} = U_{i,j} + U_{j,i}$$

$$2\Omega_{ij} = U_{i,j} - U_{j,i}$$

strefa ścinania (obszar siodłowy)

wir

$$|S| \gg |\Omega|$$

$$|\Omega| \gg |S|$$

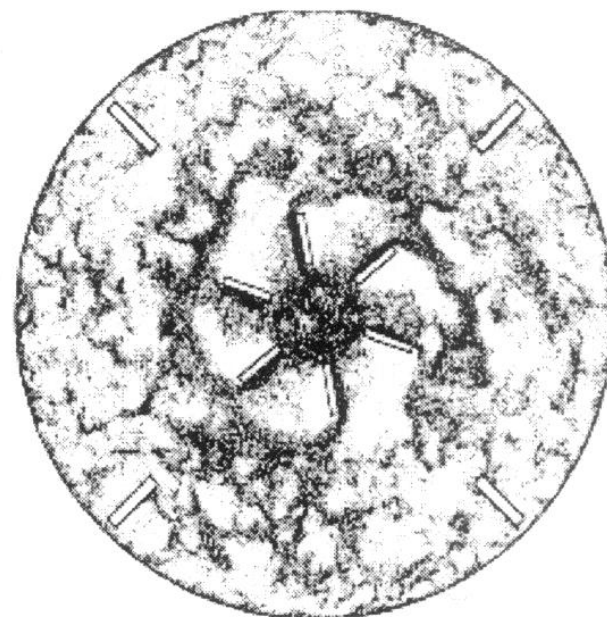
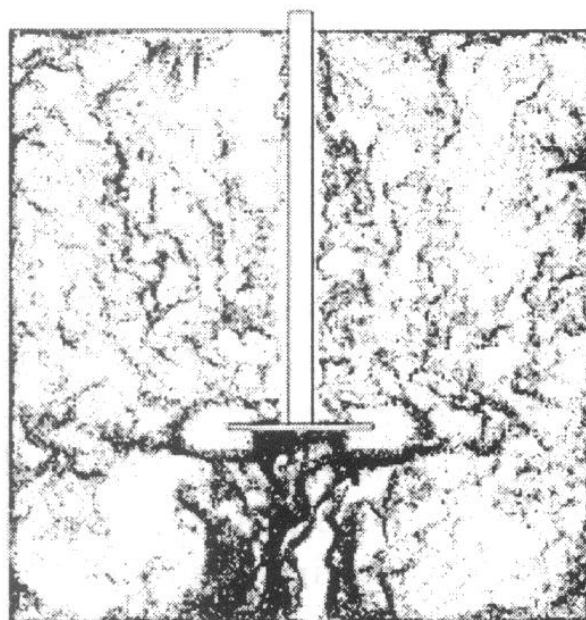
## Struktury pola przepływu

drugi niezmiennik tensora gradientu prędkości:

$$Q = S_{ij}S_{ij} - \Omega_{ij}\Omega_{ji}$$

## Nierównomierność koncentracji cząstek

W przepływach dyspersyjnych, położenia cząstek są skorelowane ze strukturami przepływu (obszary siodłowe, wiry)



*Przepływ z fazą dyspersyjną w reaktorze zbiornikowym*



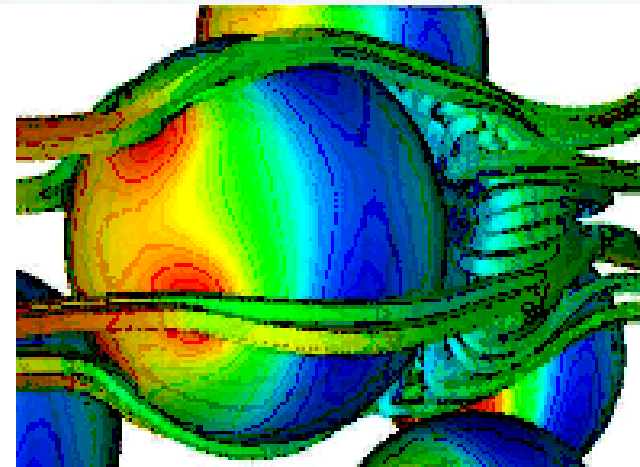
# Siły działające na cząstkę w przepływie

## Równanie ruchu cząstki

Boussinesq-Basset-Oseen (XIX/XX w.),  
Maxey & Riley (1983)

$$\frac{\pi d^3}{6} \rho_p \frac{d\mathbf{v}_p}{dt} = \mathbf{F}_d + \mathbf{F}_p + \mathbf{F}_b + \mathbf{F}_a + \mathbf{F}_h,$$

gdzie



$$\mathbf{F}_d = 3\pi d \rho_f \nu (\mathbf{v} - \mathbf{v}_p)$$

– siła oporu lepkiego

$$\mathbf{F}_p = \frac{\pi d^3}{6} \rho_f \frac{D\mathbf{v}}{Dt}$$

– siła gradientu ciśnienia

$$\mathbf{F}_b = \frac{\pi d^3}{6} (\rho_p - \rho_f) \mathbf{g}$$

– siła wyporu (grawitacji)

$$\mathbf{F}_a = \frac{\pi d^3}{12} \rho_f \left( \frac{D\mathbf{v}}{Dt} - \frac{d\mathbf{v}_p}{dt} \right)$$

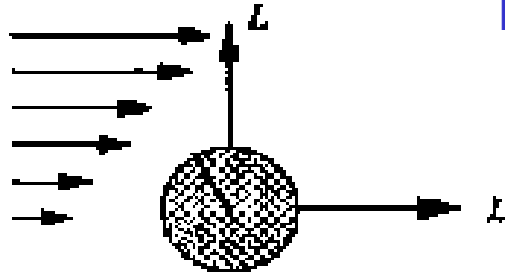
– składnik masy dołączonej

$$\mathbf{F}_h = \frac{3}{2} d^2 \rho_f \sqrt{\pi \nu} \int_{-\infty}^t \frac{d(\mathbf{v} - \mathbf{v}_p)}{d\tau} \frac{d\tau}{\sqrt{t - \tau}}$$

– składnik Bassetta (historii)

# Particle equation of motion (drag and lift only)

$$\frac{4}{3} \pi r_p^3 \rho_p \frac{d\mathbf{U}_p}{dt} = \mathbf{F}_d + \mathbf{F}_l$$



heavy particles:  $\frac{\rho_p}{\rho_f} \approx 10^3$

$$\mathbf{V}_s = \mathbf{U}_f - \mathbf{V}_p$$

particle Reynolds number:

$$\text{Re}_p = \frac{2r_p V_s}{\nu_f}$$

particle Reynolds number (shear-based):

$$\text{Re}_G = \frac{(2r_p)^2 G}{\nu_f}$$

for  $\text{Re}_p \ll 1$  (Stokes)  $C_d = \frac{24}{\text{Re}_p}$

$$F_l = -\frac{9}{\pi} \mu r_p^2 |\mathbf{V}_s| (|G|/\nu)^{1/2} \text{sgn}(G) J(\varepsilon) \quad \text{where} \quad \varepsilon = \frac{\text{Re}_G^{1/2}}{\text{Re}_p} = \frac{(|G|\nu)^{1/2}}{|\mathbf{V}_s|}$$

for  $\text{Re}_p, \text{Re}_G \ll 1, \text{Re}_p \ll \text{Re}_G^{1/2}$  (Saffman)  $J = 2.255$

## Obliczenia dyspersyjnych przepływów turbulentnych

**DNS jest kosztowne obliczeniowo** (nawet w przybliżeniu cząstek punktowych),  
a niezwykle kosztowne dla cząstek o skończonych obszarach traktowanych  
jako ruchome granice obszaru obliczeniowego (Tryggvason et al., Balachandar & Bagchi, 2000+)

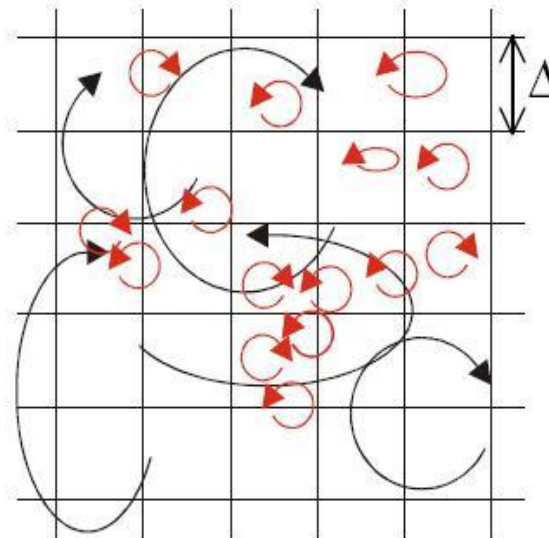
**RANS nie może odtworzyć cech strukturalnych przepływów z cząstkami**

(np. korelacji położień cząstek z chwilowymi strukturami przepływu)

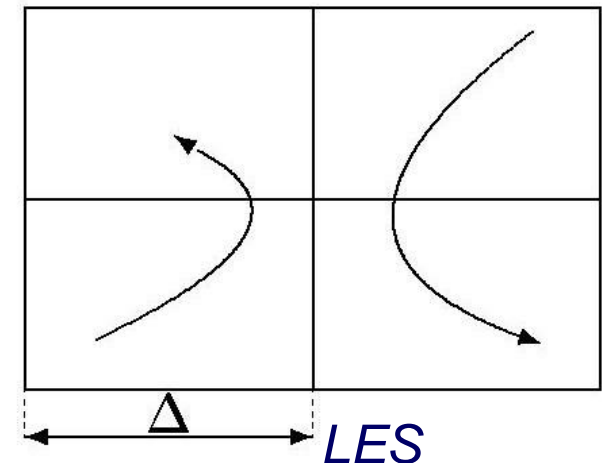
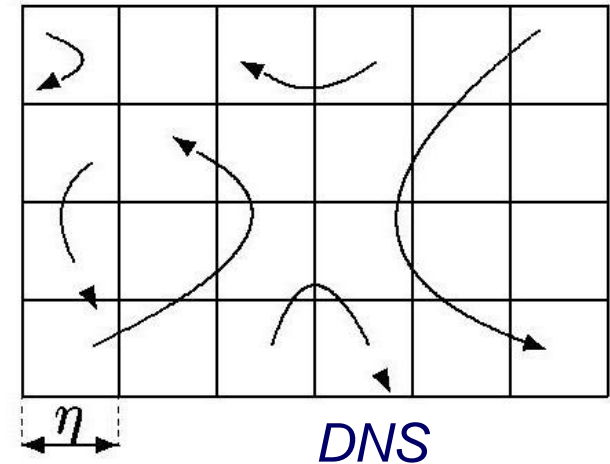
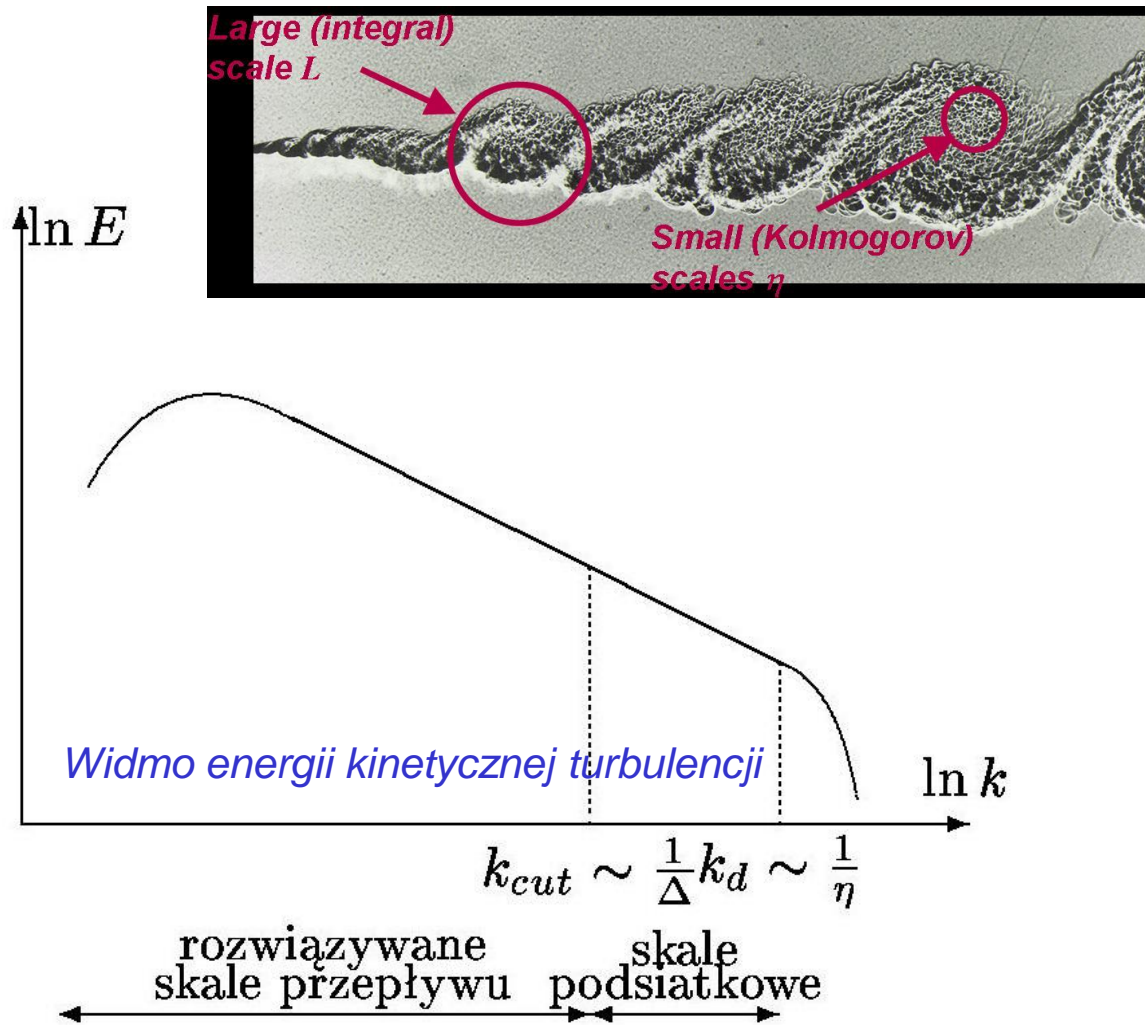
**Remedium: częściowe rozwiązanie chwilowych pól przepływu**

→ **LES (ang. large eddy simulation), CVS (metody falkowe) lub POD**

+ przybliżenie cząstek punktowych



# Metoda symulacji dużych wirów: LES (ang. *Large Eddy Simulation*)

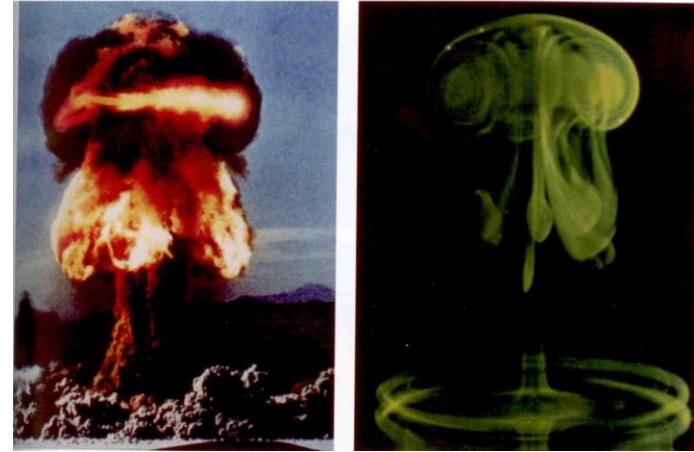


Uwaga: modelowanie LES przepływów złożonych fizycznie (reaktywne, 2F)

# Metoda LES: podstawy

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{U}) = S_\rho$$

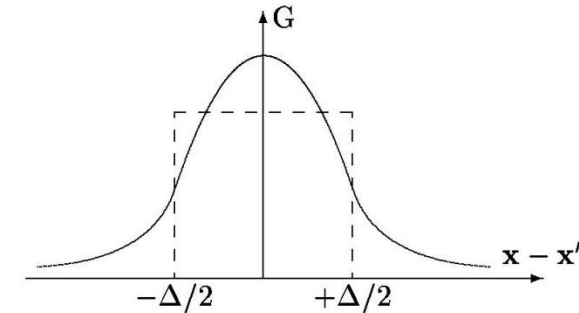
$$\frac{\partial \mathbf{U}}{\partial t} + (\mathbf{U} \cdot \nabla) \mathbf{U} = -\frac{1}{\rho} \nabla p + \nu \Delta \mathbf{U} + S_U$$



Zmienne wielkoskalowe (filtrowane):

$$\tilde{U}_i(x) = \int G(x - x') U_i(x') dx',$$

$$\text{Supp}(G) \sim \Delta = \frac{1}{k_{cut}}$$



Dynamikę dużych wirów opisuje filtrowane r-nie N-S:

$$\frac{\partial \tilde{\mathbf{U}}}{\partial t} + (\tilde{\mathbf{U}} \cdot \nabla) \tilde{\mathbf{U}} = -\frac{1}{\rho} \nabla \tilde{p} + \nu \Delta \tilde{\mathbf{U}} + \nabla \cdot \mathbf{T} + \tilde{S}_U$$

Tensor naprężeń podsiatkowych  $\mathbf{T}$  wymaga domknięcia (tu: Smagorinski)

$$T_{ij} = \frac{1}{3} \delta_{ij} T_{kk} - 2\nu_{SGS} S_{ij}, \quad \nu_{SGS} = C_S^2 \Delta^2 (S_{ij} S_{ij})^{1/2}$$



# metoda LES dla przepływów z fazą dyspersyjną

## dwojakie znaczenie filtrowania

\* Wyznaczanie pól przepływu w turbulencji swobodnej i przyściennej:

z definicji, pomija się fluktuacje podsiatkowe

\* Przepływy dwufazowe z fazą rozproszoną:

fluktuacje podsiatkowe wielkości przepływowych  
mogą mieć znaczenie (konieczność modelowania)

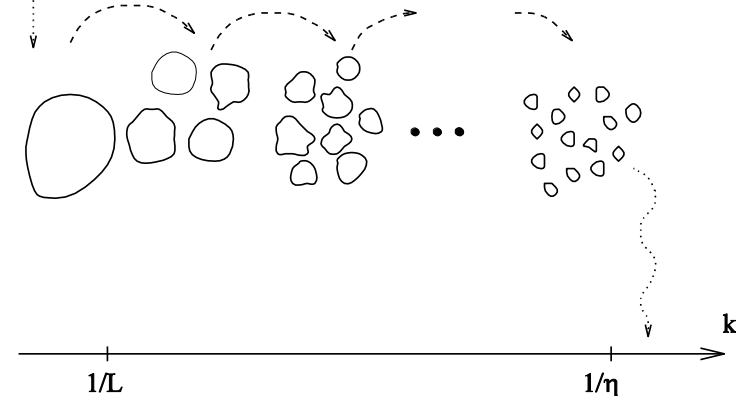
- W ogólności, cząstki „filtrują” skalę przepływu  
(reagują na skale rzędu czasu relaksacji pędu)

- W LES, cząstki poruszają się w filtrowanym  
polu prędkości (dużych skal)

niektóre statystyki ruchu cząstek bardziej

wrażliwe na efekty podsiatkowe

(nierównomierność koncentracji, częstość zderzeń)



*Szkic kaskady energii*

# Reconstruction of SGS flow velocity in particle-laden flows

In particle equation of motion,  
fluid velocity at particle location is needed:

- tri-linear interpolation (results presented)
- second-order interpolation, cf. Squires (2007)

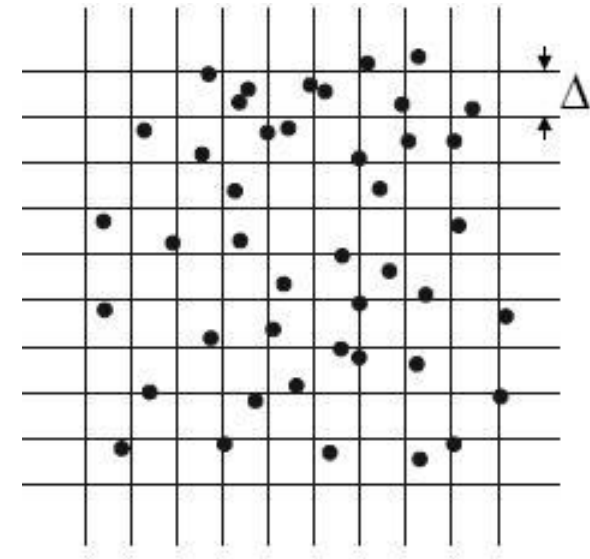
- DNS 
$$\mathbf{U}^* = \mathbf{U}(\mathbf{x}_p, t) = \tilde{\mathbf{U}} + \mathbf{u}'$$

- LES with no SGS particle dispersion

$$\mathbf{U}^* = \tilde{\mathbf{U}}(\mathbf{x}_p, t)$$

- modelled/reconstructed SGS fluid velocity fluctuations  
along particle trajectories, i.e.  $\mathbf{u}'$

LES filtering impacts on: pref.conc., slip vel. → collision rate  
particle tke → wall deposition  
slip vel., rel.temp. → cooling/heating, evaporation



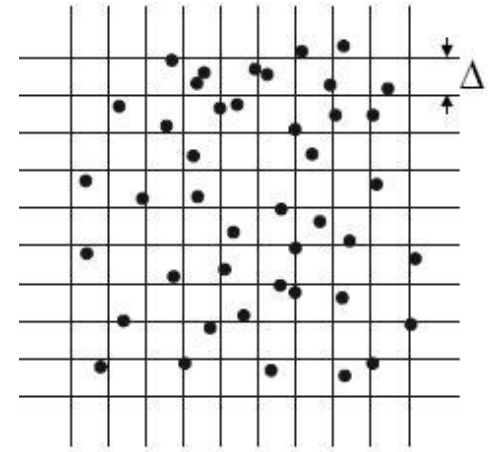
# Reconstruction of SGS flow velocity in particle-laden flows

„functional” approaches: (in line with effective diffusivity concept for fluid LES):  
modelling the impact of subfilter scales on resolved ones

## - *stochastic diffusion model*

(Pozorski et al. 2004, Shotorban & Mashayek 2006):

Langevin eq. for fluid velocity along particle trajectories



„structural” approaches: resolving (part of) subfilter velocity field

- *approximate deconvolution* (Kleiser et al. 2001, Kuerten & Vreman 2005)
- *linear-eddy model* (Kerstein 1990s): triplet map
- *fractal reconstruction* (Scotti & Meneveau 1999; Salvetti & Soldati 2006)

# Reconstruction of subfilter field (cntd.)

## Structural approaches:

- 1) *Approximate deconvolution* (Kleiser et al. 2001, Kuerten PoF 2006)

$$\tilde{\mathbf{U}} = \mathbf{G} * \mathbf{U} \quad \longrightarrow \quad \mathbf{U} = \mathbf{G}^{-1} * \tilde{\mathbf{U}}$$

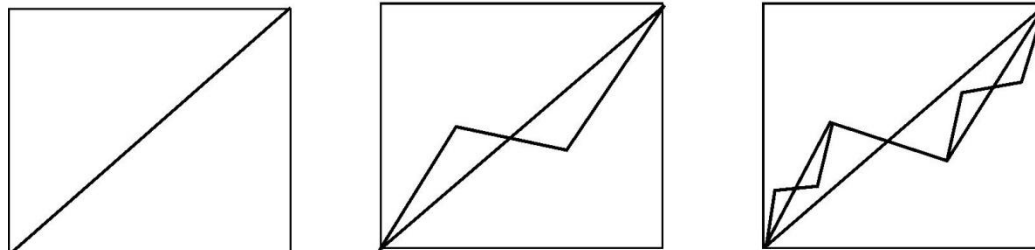
truncated van Cittert series expansion:

$$U_i = \sum_{m=0}^M (1 - \mathbf{G})^m * \tilde{U}_i = \tilde{U}_i + (\tilde{U}_i - \tilde{\tilde{U}}_i) + \dots$$

- 2) *Linear-eddy model* (Kerstein 1990s): triplet map

- 3) *Fractal reconstruction* (Scotti & Meneveau 1999)

two-parameter, 1D affine velocity transformation



# SGS particle dispersion model: Langevin-type eq.

## Functional approach:

Langevin eq. for SGS fluid velocity along particle trajectories

$$d\mathbf{u}_i^* = -\frac{\mathbf{u}_i^*}{\tau_L^*} dt + \sqrt{\frac{4k_{sg}}{3\tau_L^*}} dW_i$$

Estimation of SGS fluid kinetic energy  $k_{sg}$  (Yoshizawa, 1982; Moin *et al.*, 1991):

$$k_r = C_I \bar{\Delta}^2 |\bar{S}|^2 \quad \text{where} \quad |\bar{S}| = (2\bar{S}_{ij}\bar{S}_{ij})^{1/2}$$

analogously to  $C_G$ , dynamic procedure applied to solve for  $C_I$

$$C_I = \frac{1}{2} \frac{\langle \widehat{\bar{U}_k \bar{U}_k} - \widehat{\bar{U}_k} \widehat{\bar{U}_k} \rangle_{av}}{\langle \bar{\Delta}^2 |\bar{S}|^2 - \widehat{\bar{\Delta}^2} |\widehat{\bar{S}}|^2 \rangle_{av}}$$

Estimation of the SGS fluid time scale:

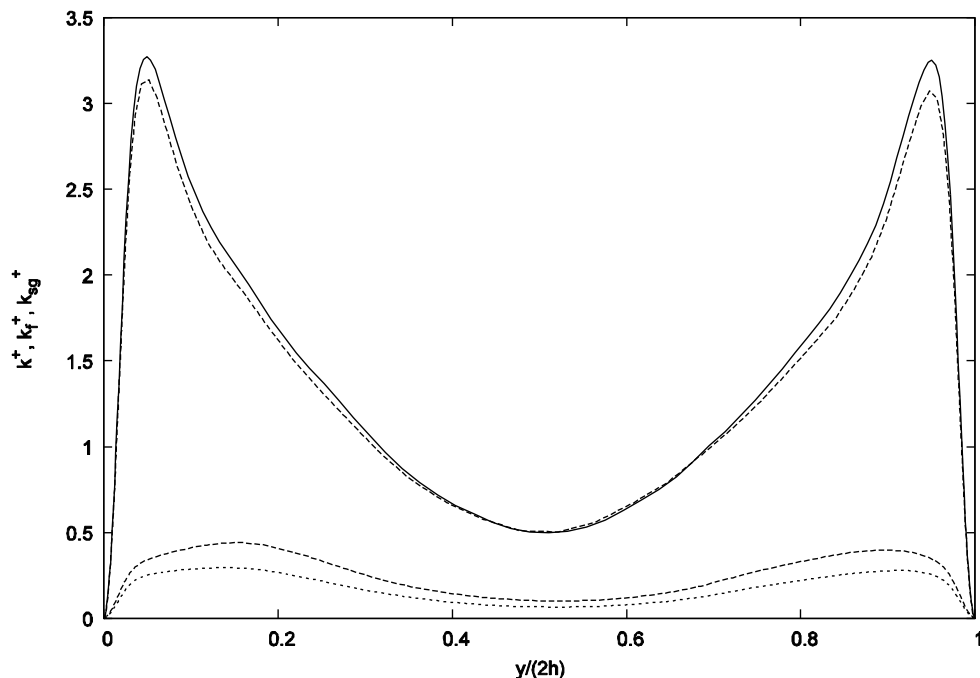
$$\tau_L^* = C_{sg} \frac{\bar{\Delta}}{\sigma_{sg}} \quad \sigma_{sg} = \sqrt{\frac{2}{3} k_{sg}}$$



# Energia kinetyczna skal podsiatkowych w LES

## Obliczenia przepływu turbulentnego w kanale

solver CFD FASTEST (kod opracowany na politechnice w Darmstadt)



## Obliczenia DNS oraz *a priori* LES

[J.Pozorski & T.Wacławczyk, 2006]

# Dynamika cząstek w przepływie turbulentnym

## Równania ruchu cząstek:

(cząstki punktowe  
o skończonej masie)

$$\frac{d\mathbf{x}_p}{dt} = \mathbf{U}_p$$

$$\frac{d\mathbf{U}_p}{dt} = \frac{\mathbf{U}_f^* - \mathbf{U}_p}{\tau_p^e} + \mathbf{g}$$

czas relaksacji pędu cząstek:

$$\tau_p = \frac{\rho_p \frac{d_p^2}{18\nu_f}}{\rho_f}$$

$$\tau_p^e = \tau_p / f_D \quad f_D = 1 + 0.15 Re_p^{0.687}$$

- obliczenia DNS

$$\mathbf{U}^* = \mathbf{U}(\mathbf{x}_p, t) = \tilde{\mathbf{U}} + \mathbf{u}'$$

- LES bez dyspersji podsiatkowej

$$\mathbf{U}^* = \tilde{\mathbf{U}}(\mathbf{x}_p, t)$$

- model rekonstrukcji fluktuacji podsiatkowych prędkości płynu

wzdłuż trajektorii cząstek, i.e.  $\mathbf{u}'$

# DNS oraz *a priori* LES przepływu dwufazowego

-DNS turbulencji izotropowej

(na siatce 96\*96\*96) przy

$$Re_{\lambda} = 40$$

- modelowanie Lagrange'owskie ruchu

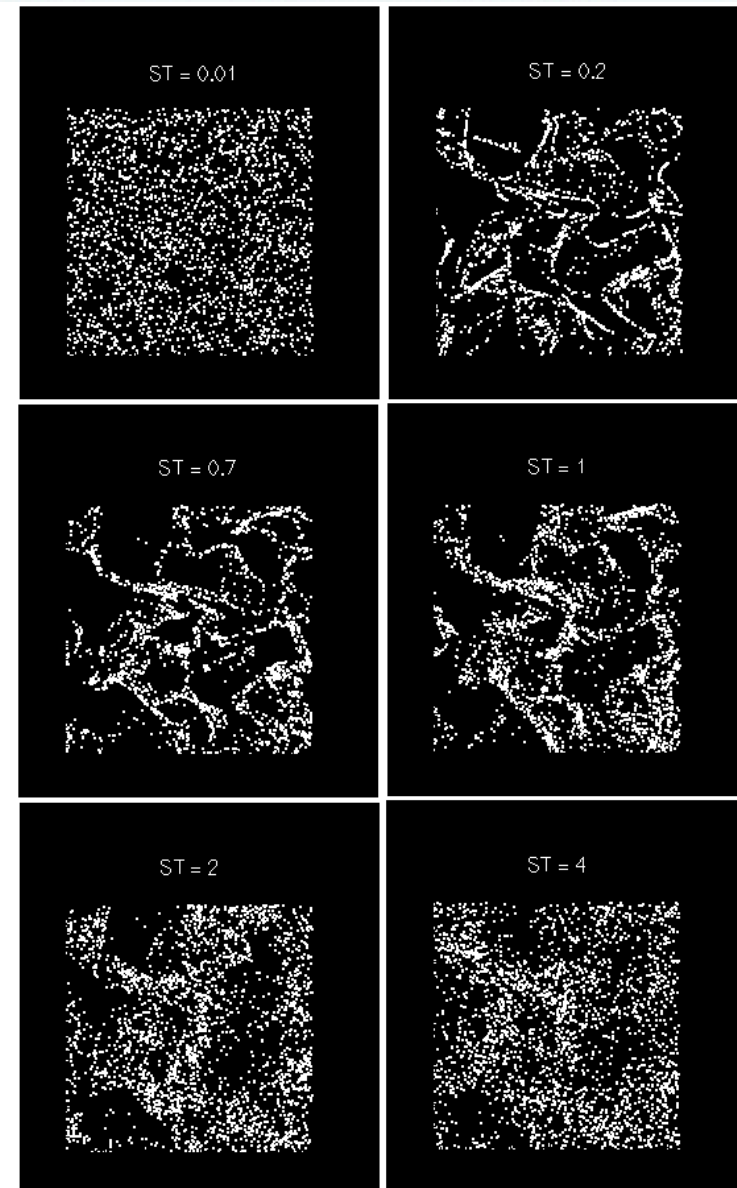
cząstek dla różnych liczb Stokesa

$$St = \frac{\tau_p}{\tau_{\eta}}$$

- nierównomierność koncentracji cząstek dla

$$0.2 < St < 2$$

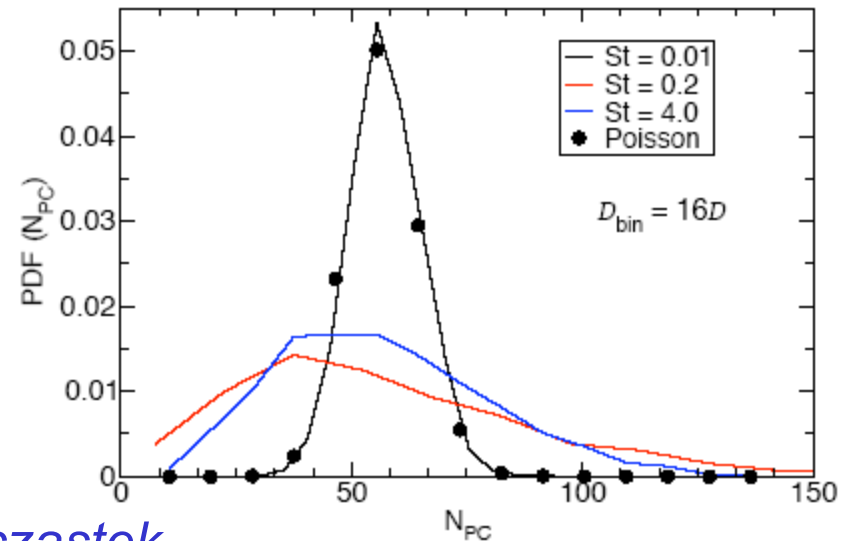
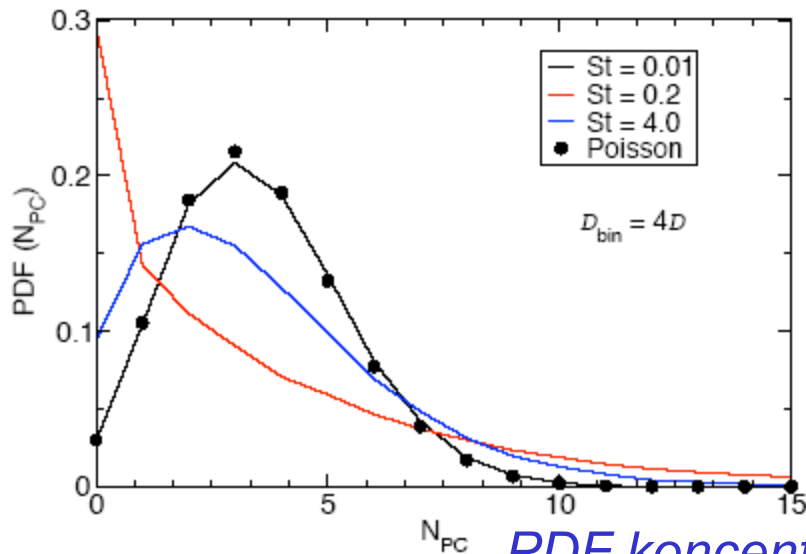
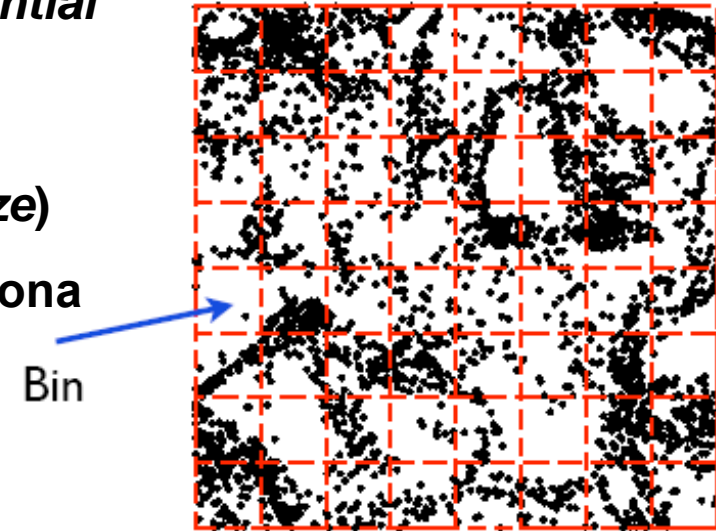
*(Pozorski, Apte & Raman 2004)*



# DNS turbulencji z cząstkami: rozkład przestrzenny

- nierównomierność rozkładu cząstek (ang. *preferential concentration*) szacowana na podstawie PDF ich gęstości/koncentracji (ang. *bin-counting*)
- PDF zależy od  $St$  oraz rozdzielczości (ang. *bin size*)
- równomierną koncentrację opisuje rozkład Poissona

$$f_P(n) = \frac{e^{-\lambda}}{n!} \lambda^n \quad \lambda = \langle N_{PC} \rangle$$

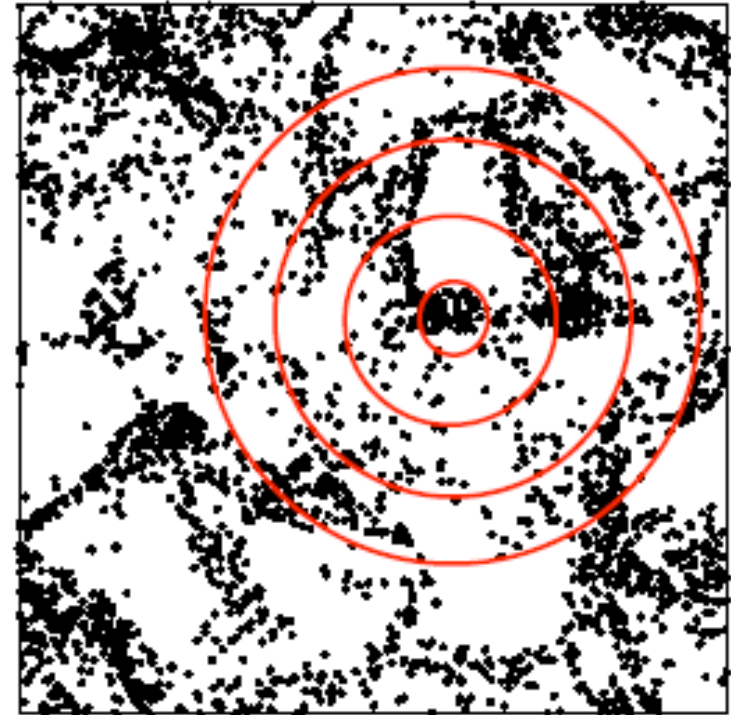


PDF koncentracji cząstek

# DNS przepływu z cząstkami: wynikowe RDF

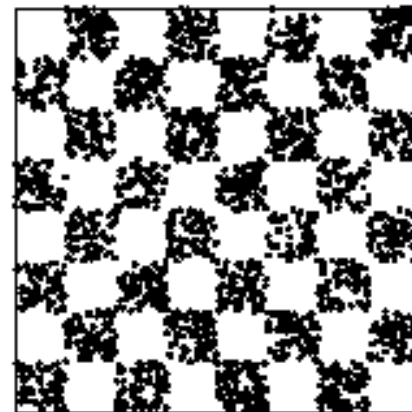
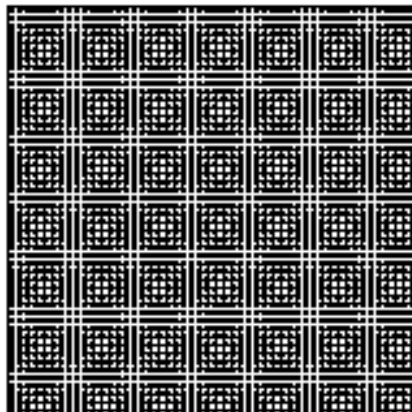
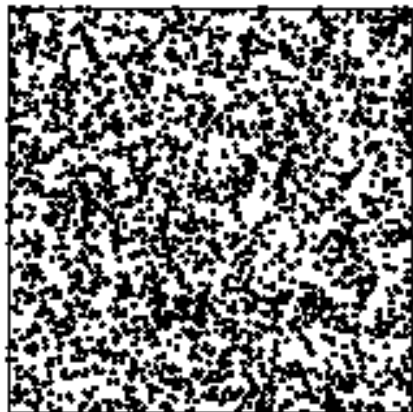
- nierównomierność koncentracji cząstek w obszarze przepływu szacowana za pomocą radialnej funkcji rozkładu (ang. RDF - *radial distribution function*)

$g(r)dr$  jest liczbą cząstek w powłoce kulistej  $(r, r + dr)$

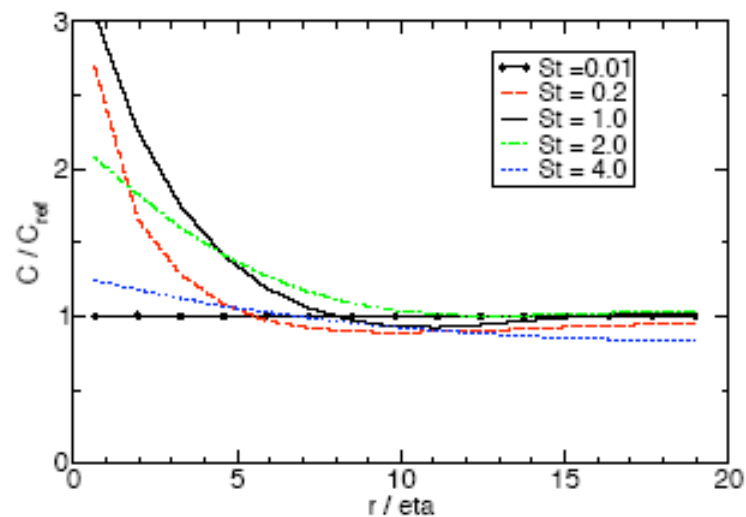
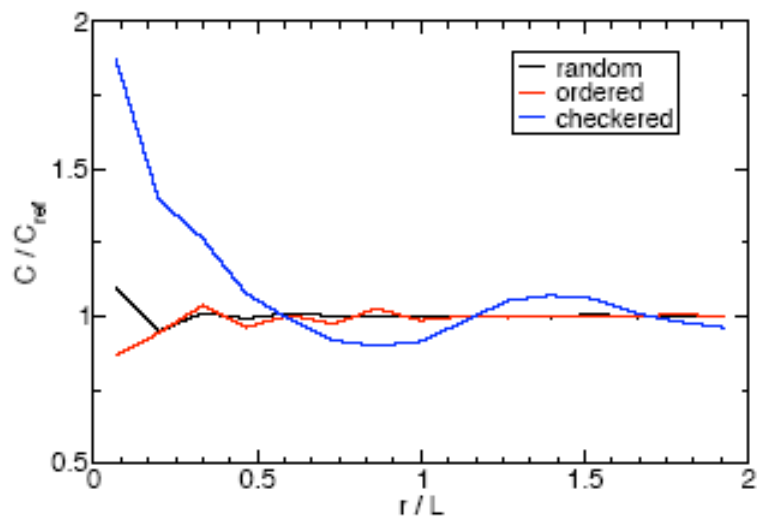


- RDF stanowi miarę nierównomierności rozkładu cząstek
- RDF daje oszacowanie skali korelacji przestrzennej

# Nierównomierność koncentracji cząstek: RDF



*Testy dla różnych rozkładów cząstek*



*RDF: nierównomierność rozkładu i skala długości*



# Turbulencja z cząstkami: model dyspersji podsiatkowej

→ DNS oraz *a priori* LES turbulencji z cząstkami

$$k_{resolved} \approx 0.65 k_{DNS}$$

→ uwzględnienie wpływu fluktuacji podsiatkowych  
pola prędkości LES na ruch cząstek

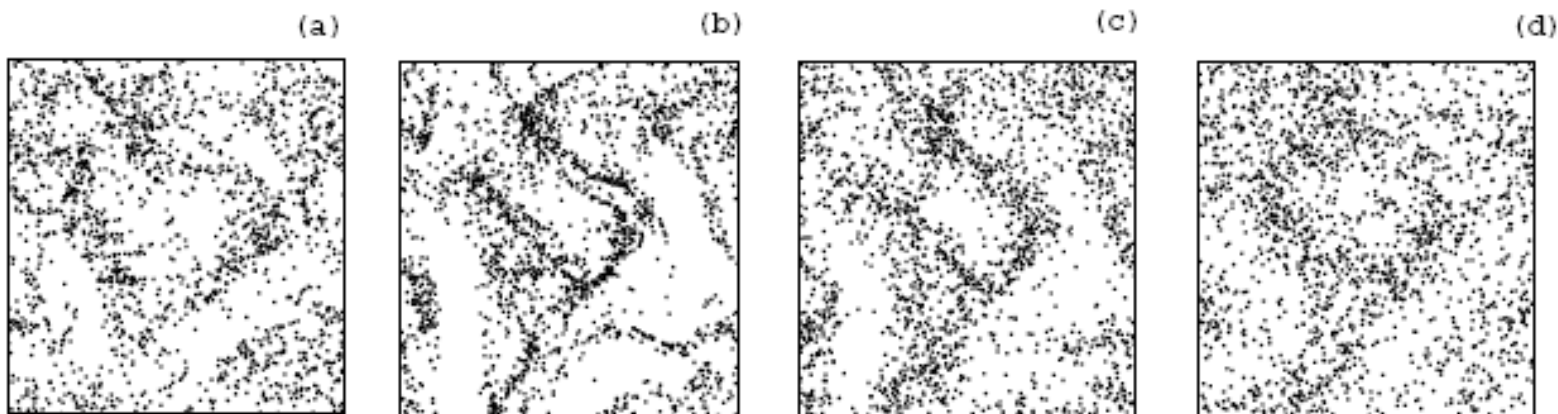
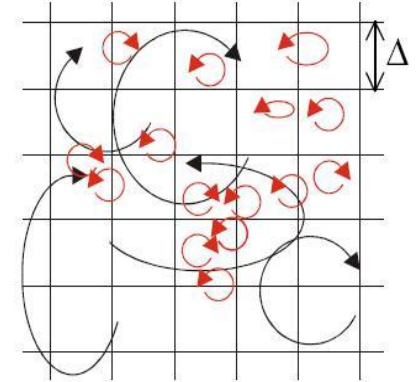


FIGURE 9. Snapshots of particle positions; runs for particles of  $St = 2$ . a) DNS; b) *a priori* LES with no FPT model; c) *a priori* LES with FPT model and  $C=0.05$ ; d) DNS for  $St = 4$ .

→ **wyniki obliczeń** jakościowo poprawne dla cząstek o większej bezwładności

## LES of dispersed flows – examples of results

Results from regular particle-laden LES  
and LES with subfilter dispersion modelling

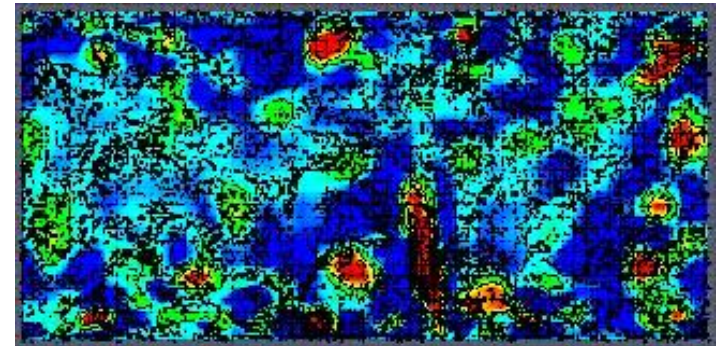


### 1) Turbulent channel flow

(also with particle wall separation)

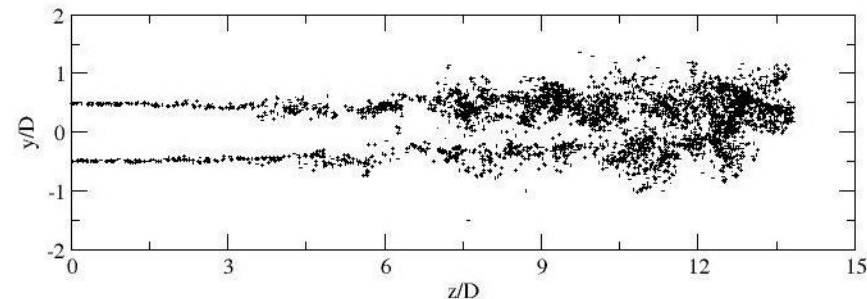
### 2) Non-isothermal channel

(heated/cooled and isoflux)



### 3) Jet flows

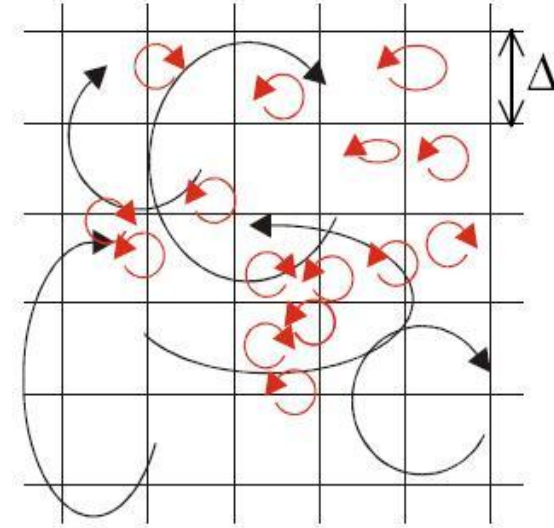
(single axisymmetric and coaxial jets)



# LES for fluid: reminder on governing equations

Dynamics of large-eddy motion (filtered N-S eq.):

$$\frac{\partial \bar{U}_i}{\partial t} + \bar{U}_j \frac{\partial \bar{U}_i}{\partial x_j} = -\frac{1}{\rho} \frac{\partial \bar{p}}{\partial x_i} + \nu \nabla^2 \bar{U}_i - \frac{\partial \tau_{ij}}{\partial x_j}$$



Closure of the SGS stress tensor: **dynamic model (Germano & Lilly)**

$$\tau_{ij}^d = -2\nu_r \bar{S}_{ij} \text{ where } \nu_r = C_G \bar{\Delta}^2 |\bar{S}|$$

Temperature treated as a passive scalar (filtered energy eq.):

$$\frac{\partial \bar{T}_f}{\partial t} + \bar{U}_{f,i} \frac{\partial \bar{T}_f}{\partial x_i} = \frac{\partial}{\partial x_i} \left[ \left( \frac{\nu_f}{\text{Pr}} + \frac{\nu_t}{\text{Pr}_t} \right) \frac{\partial \bar{T}_f}{\partial x_i} \right]$$

## LES and particle solvers

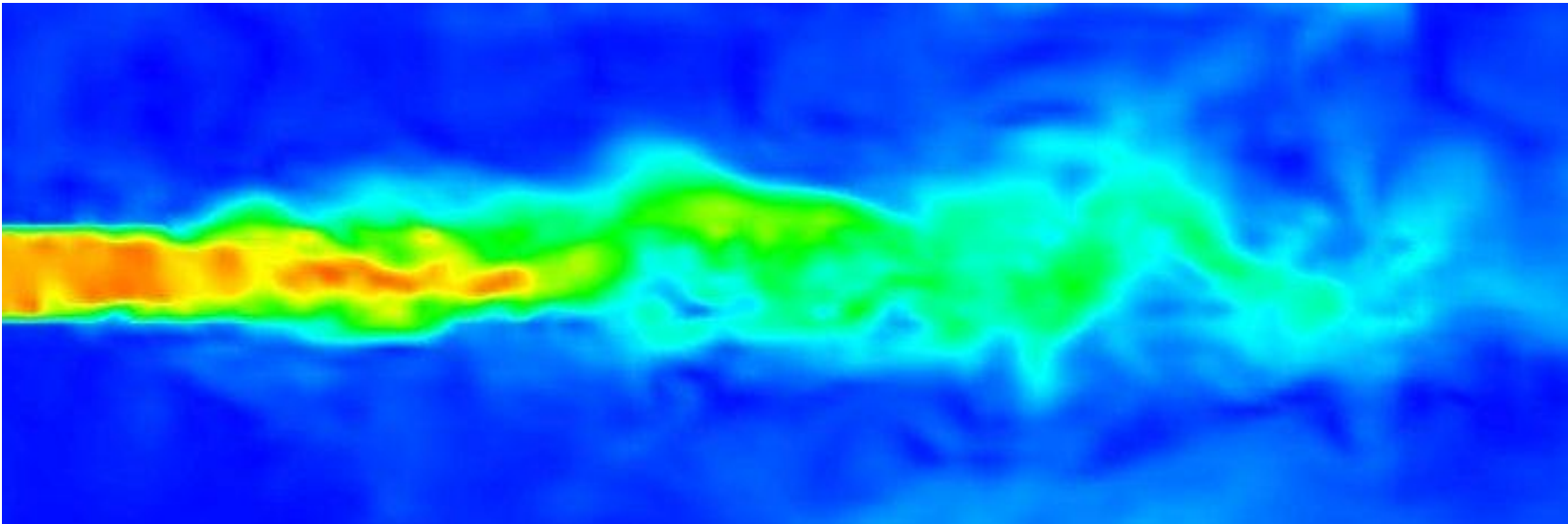
**FASTEST3D** : academic LES code (Darmstadt, Germany)

-finite volume, second-order accuracy, dynamic (Germano) SGS stress model

**SAILOR** : monoblock, spectral LES code (TU Częstochowa, Poland) – single jet only

**PTSOLV** : particle solver (in-house)

- Lagrangian tracking, one-way coupled to fluid LES (dilute regime)



*Velocity magnitude: Eulerian LES computed with FASTEST3D code*

# Summary of evolution equations

## for particle velocity and temperature (point-particle approximation)

particle velocity  $U_p$ ;      fluid velocity  $U_f$ ;      in LES:  $U_f = \bar{U}_f + u_f$

fluid velocity along particle trajectory:  $U_f^* = U_f(x_p, t)$ ,      or       $U_f^* = \bar{U}_f(x_p, t) + u_f^*$

fluid temperature seen by particles:  $T_f^* = T_f(x_p, t)$ ,      in general       $T_f^* = \bar{T}_f(x_p, t) + \theta_f^*$

$$\begin{aligned}\frac{dx_p}{dt} &= U_p \\ \frac{dU_p}{dt} &= f_D \frac{U_f^* - U_p}{\tau_p} \\ \frac{dT_p}{dt} &= f_\theta \frac{T_f^* - T_p}{\tau_\theta}\end{aligned}$$

the particle momentum and thermal relaxation times, respectively:

$$\tau_p = \frac{\rho_p}{\rho_f} \frac{d_p^2}{18\nu_f}, \quad \tau_\theta = \frac{\rho_p c_p}{\rho_f c_f} \frac{d_p^2}{12\alpha_f}$$

moreover,  $f_D = 1 + 0.15 Re_p^{0.687}$       and       $f_\theta = Nu/2 = 1 + 0.3 Re_p^{1/2} Pr^{1/3}$

(correction factor  $f_\theta$  taken from the Ranz-Marshall correlation for the Nusselt number)

# LES results for non-isothermal particle-laden turbulent channel flow

**Flow case:** turbulent channel flow at  $Re_\tau = 150$  (benchmark of COST Action LES-AID)

- domain size in streamwise ( $x$ ), wall-normal ( $y$ ) and spanwise ( $z$ ) directions:

$$4\pi h \times 2h \times (4/3)\pi h$$

- discretisation:  $64 \times 84 \times 64$  FV meshes

- the mesh: uniform with  $\Delta x^+ = 29.5$ ,  $\Delta z^+ = 9.8$ ,

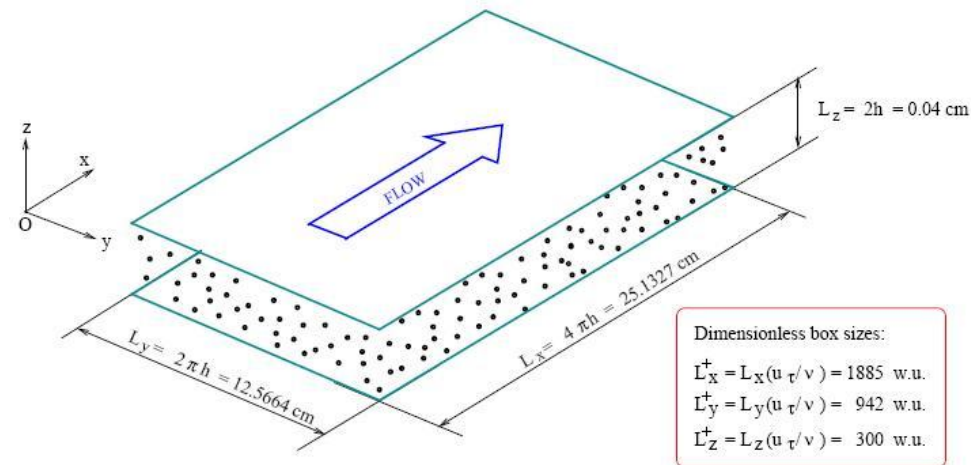
$$\Delta y^+ = 0.17 \text{ at the wall up to } \Delta y^+ = 10 \text{ at the CL}$$

DNS data available for particle dynamics:

[Marchioli, Soldati, Kuerten et al., ICMF 2007]

also, for temperature of particles:

[Jaszczur & Portela, QLES 2007]

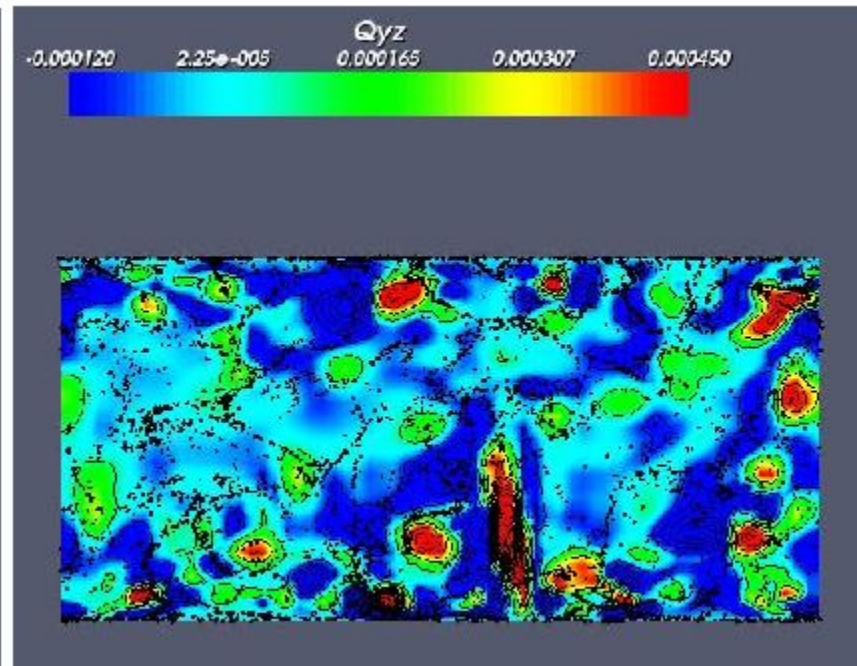
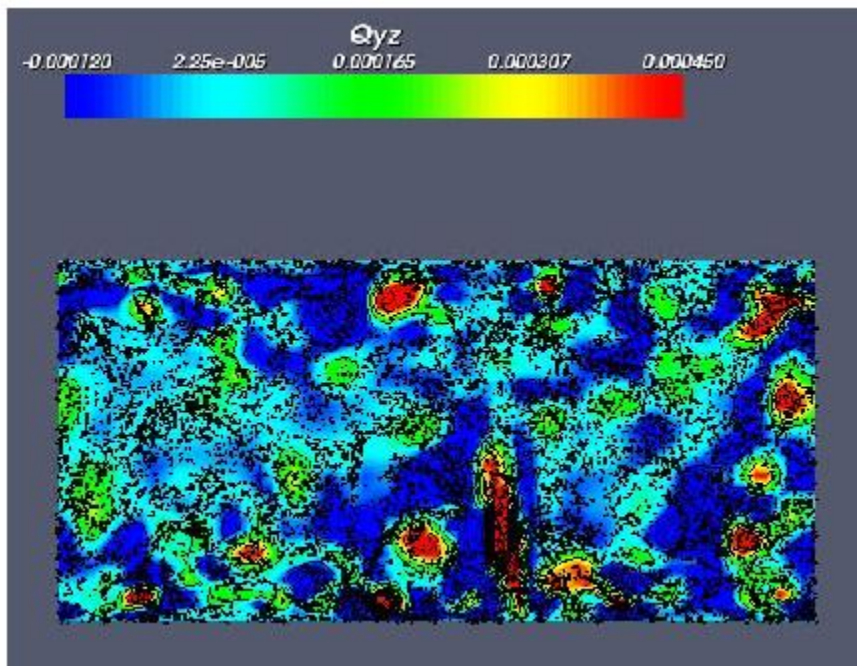


for **non-isothermal** channel flow: either isothermperature (heated/cooled)  
or isoflux wall b.c.;  $Pr=0.71$  (air)



## Correlation of particle location with fluid velocity

$$Q = S_{ij}S_{ij} - \Omega_{ij}\Omega_{ji}$$



Particle Stokes number: a)  $St=2$  , b)  $St=10$

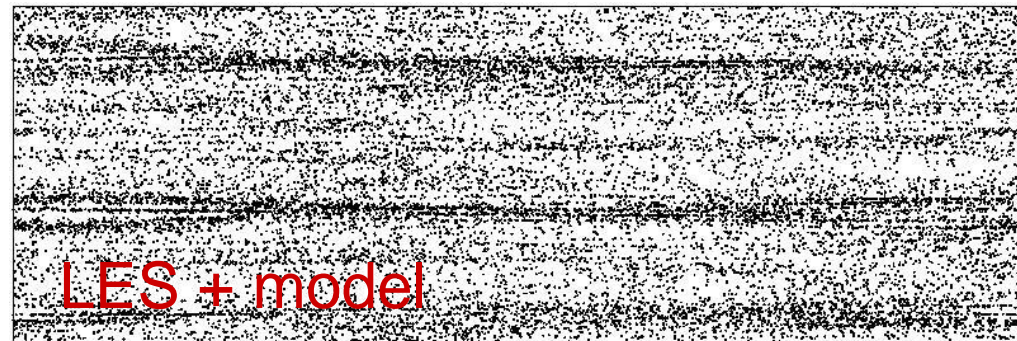
$$St = \frac{\tau_p}{(v / u_\tau^2)} = \tau_p^+$$

# Particle-laden channel flow: particle locations

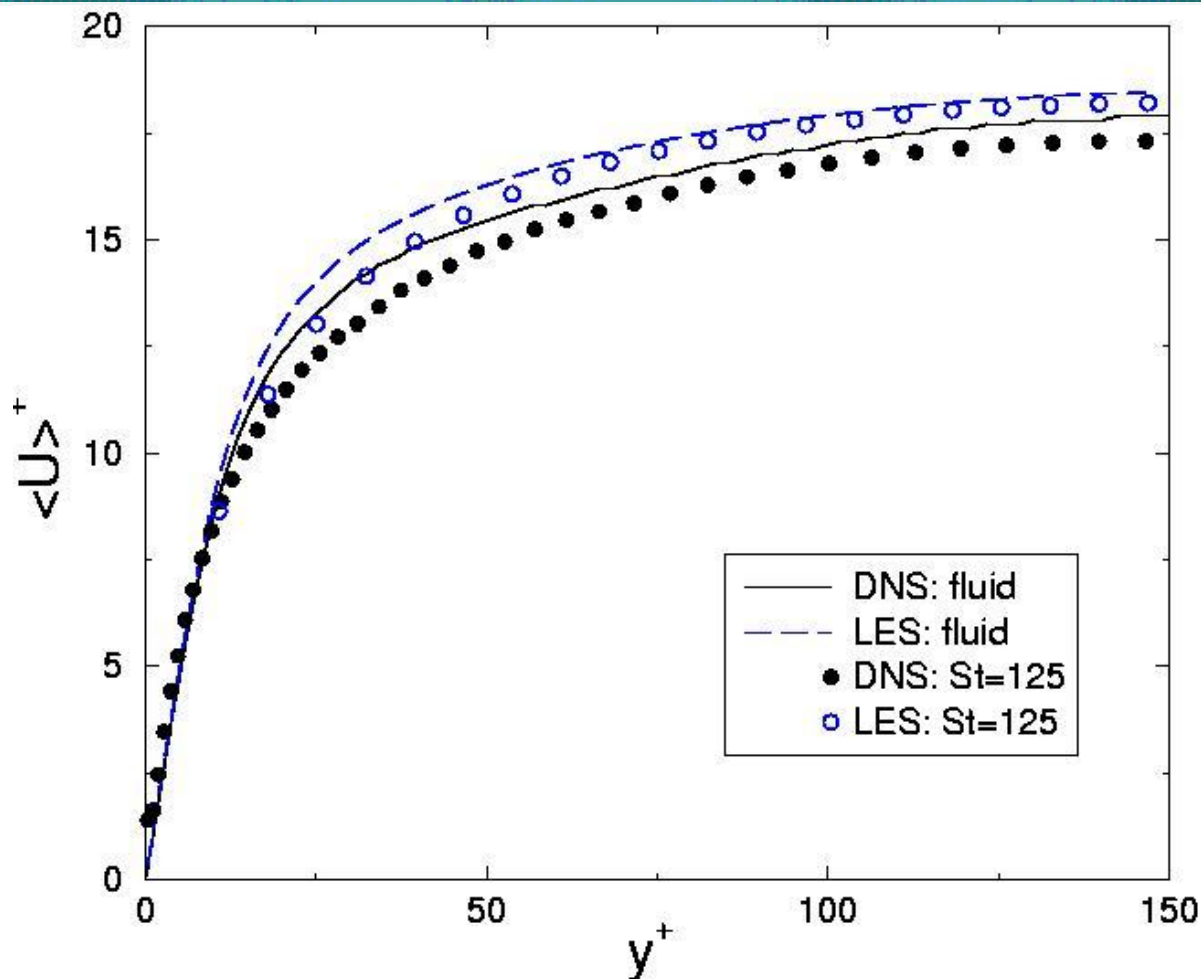
Near-wall layer:  $0.5 < y^+ < 5$

- DNS,
- LES + no model,
- LES + Langevin eq.  
for SGS particle dispersion

particles of  $St=25$



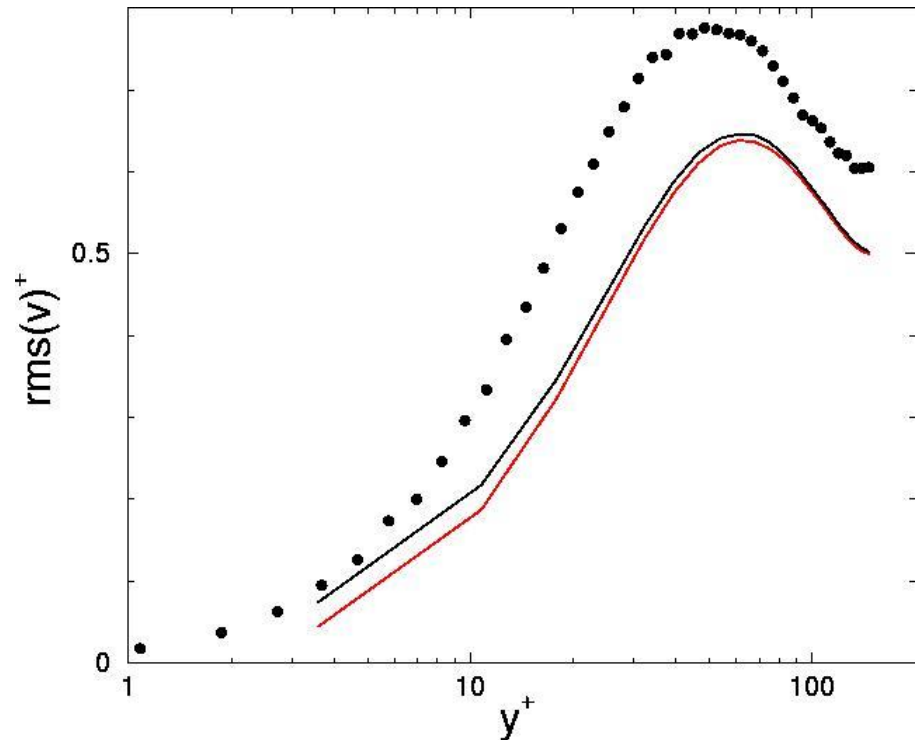
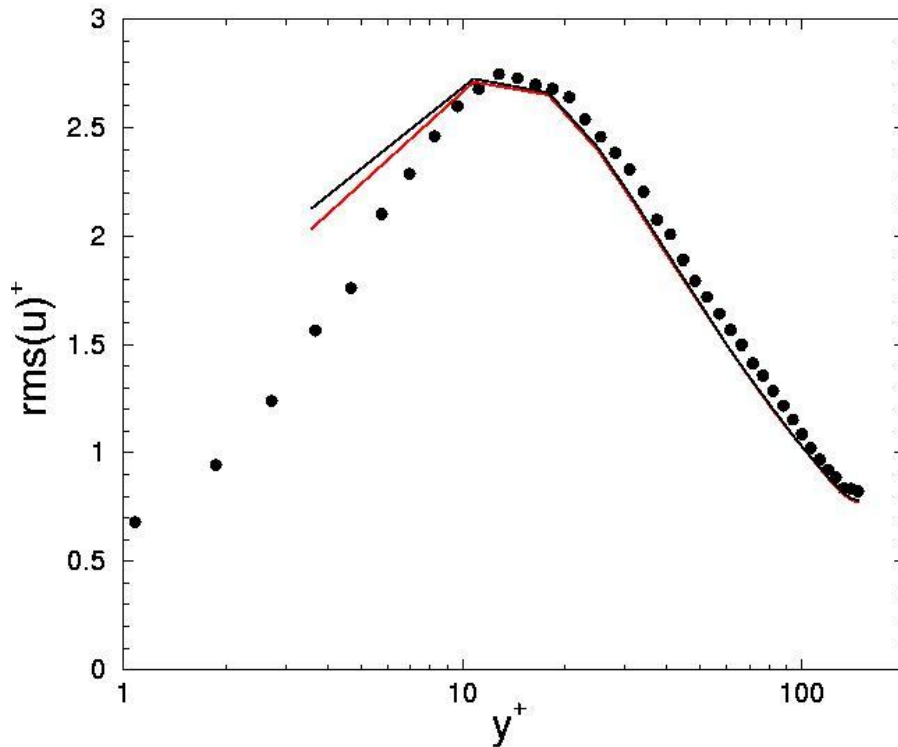
# Channel flow: particle velocity statistics



Mean velocity profile for particles of  $St=125$   
 Reference data (●): DNS of Marchioli & Soldati  
 ([cfd.cineca.it/CFD/repository](http://cfd.cineca.it/CFD/repository))



# Channel flow: intensity of particle velocity fluctuations



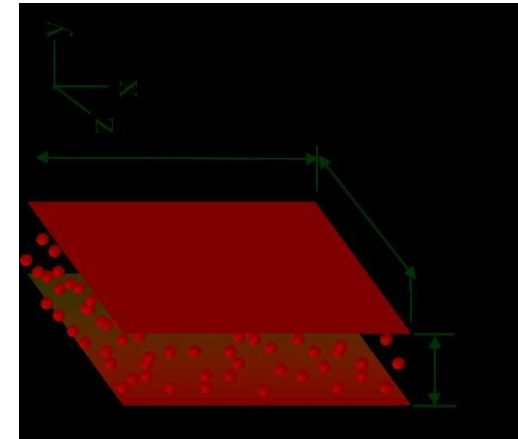
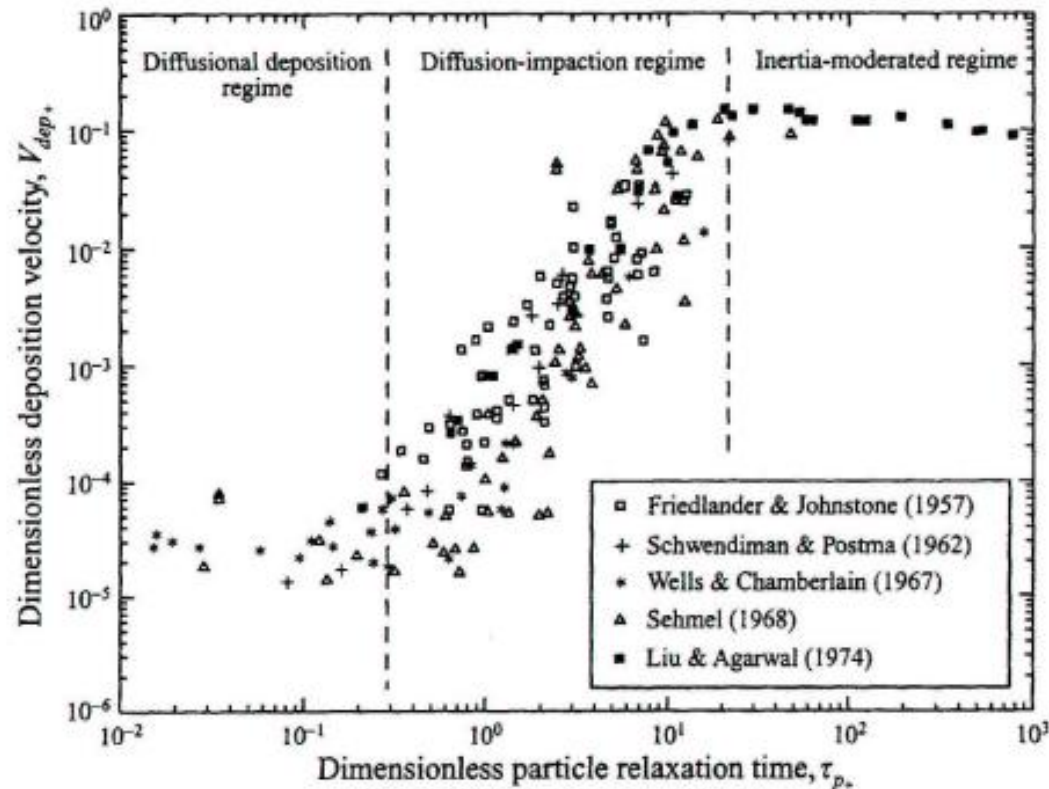
Particle rms velocity: a) streamwise, b) wall-normal. Particles of  $St=1$ .  
Symbols: DNS reference data; red lines: LES; black lines:  
LES with stochastic SGS particle dispersion model.

# Particle separation from turbulent flow

## Deposition velocity

(mass flux of separating particles):

$$V_{dep}^+ = \frac{J_w}{\rho_{dp} u_\tau} = \frac{n_{dep}}{n_{tot}} \frac{\Delta L / \Delta t}{u_\tau}$$

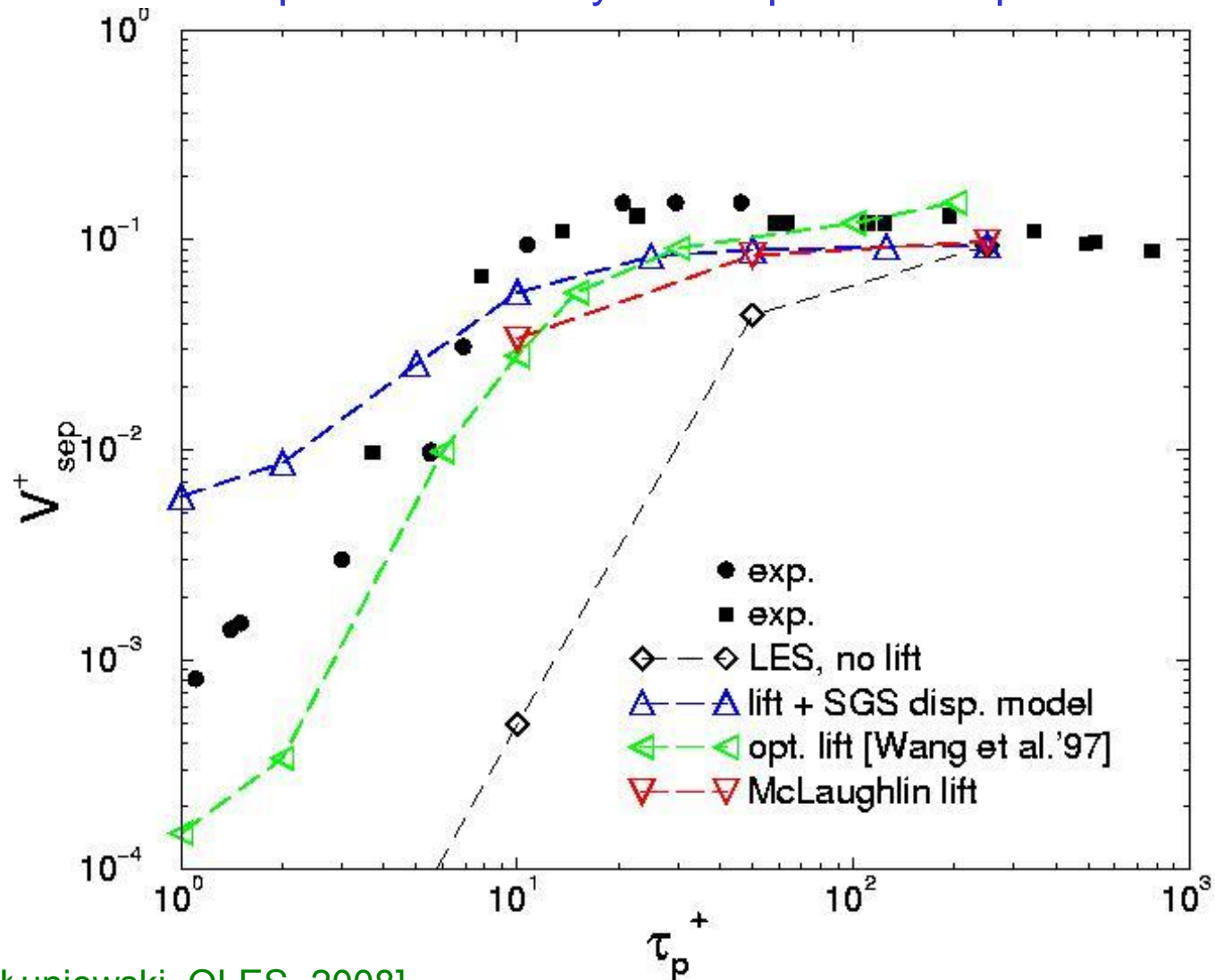


← experimental data  
for turbulent pipe flow

[Young & Leeming, JFM 1997]

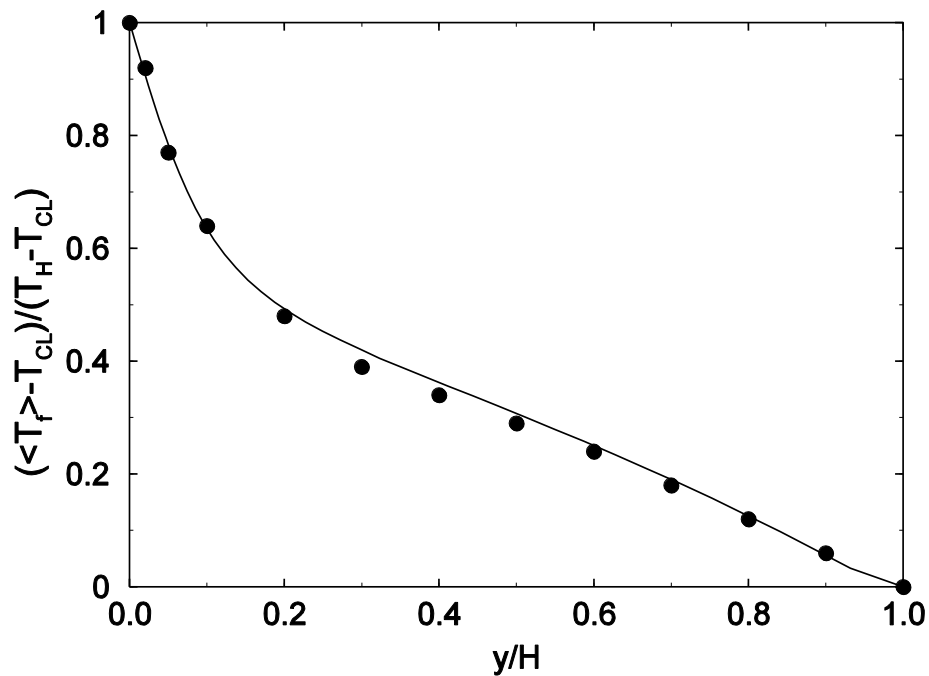
# Particle wall deposition (cntd.)

LES computation of deposition velocity: SGS particle dispersion + lift force

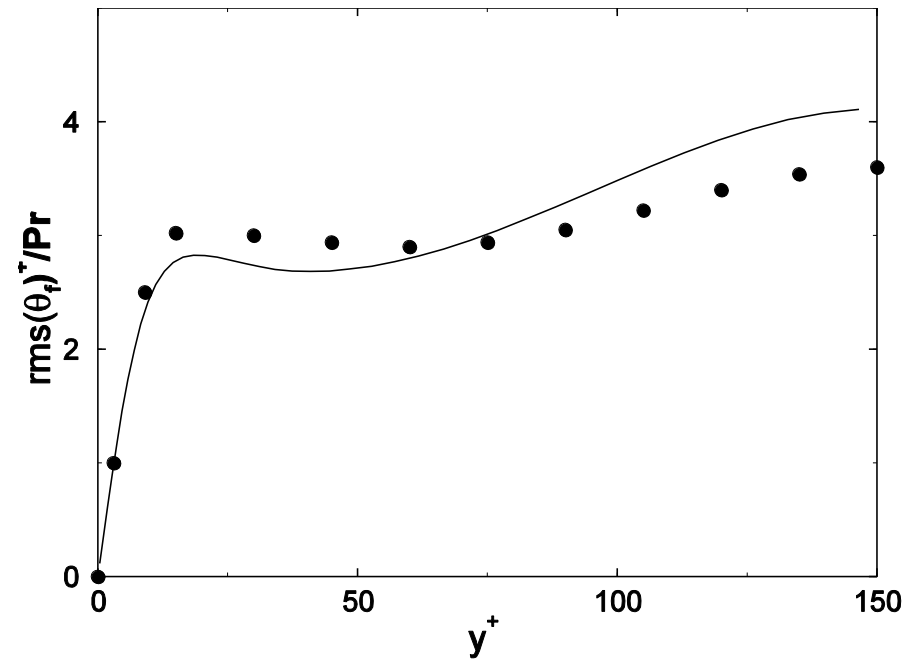




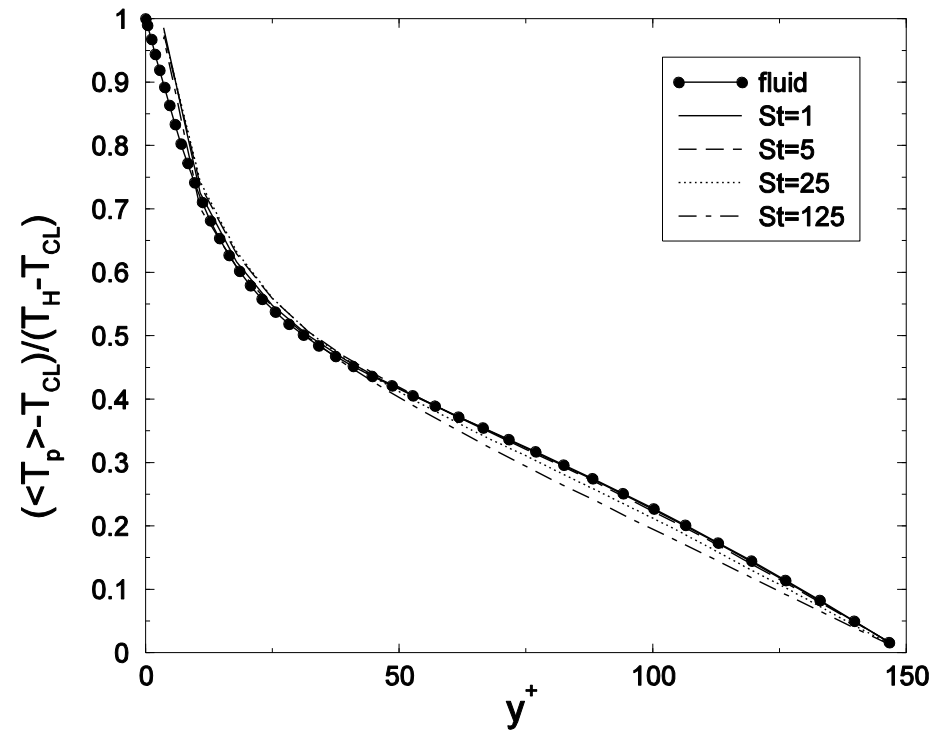
# Heated/cooled channel flow: fluid temperature statistics



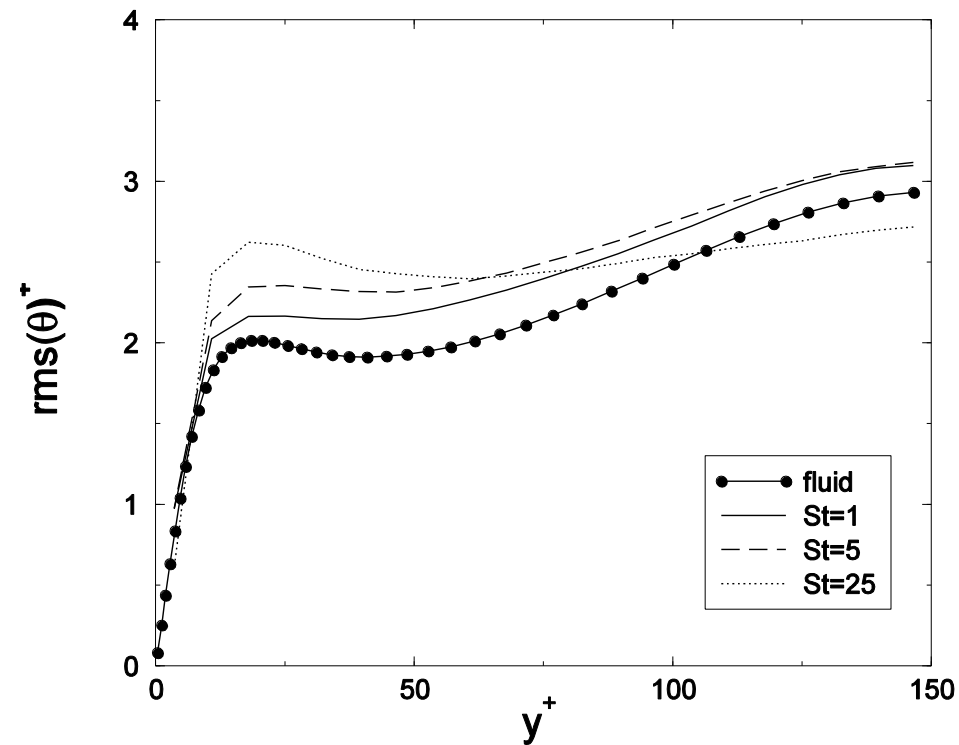
Mean temperature profile; temperature r.m.s.



# Heated/cooled channel flow: fluid and particle statistics

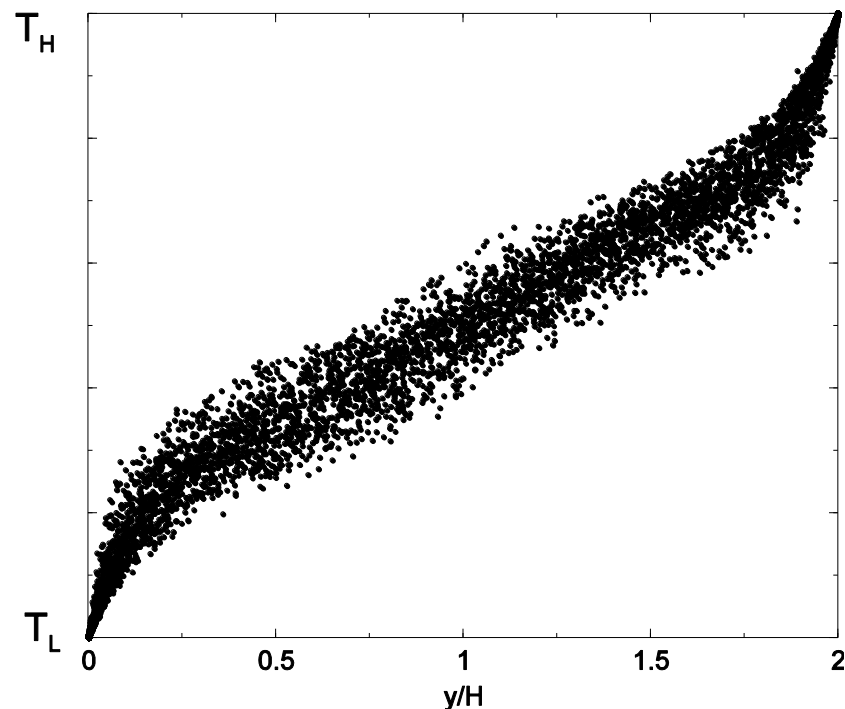
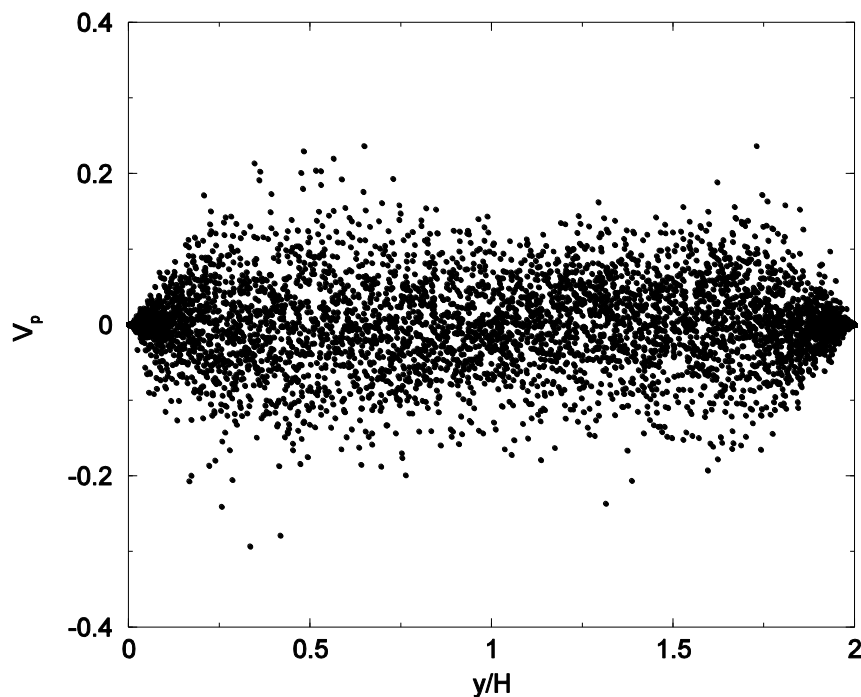


Mean temperature profile;



temperature r.m.s.

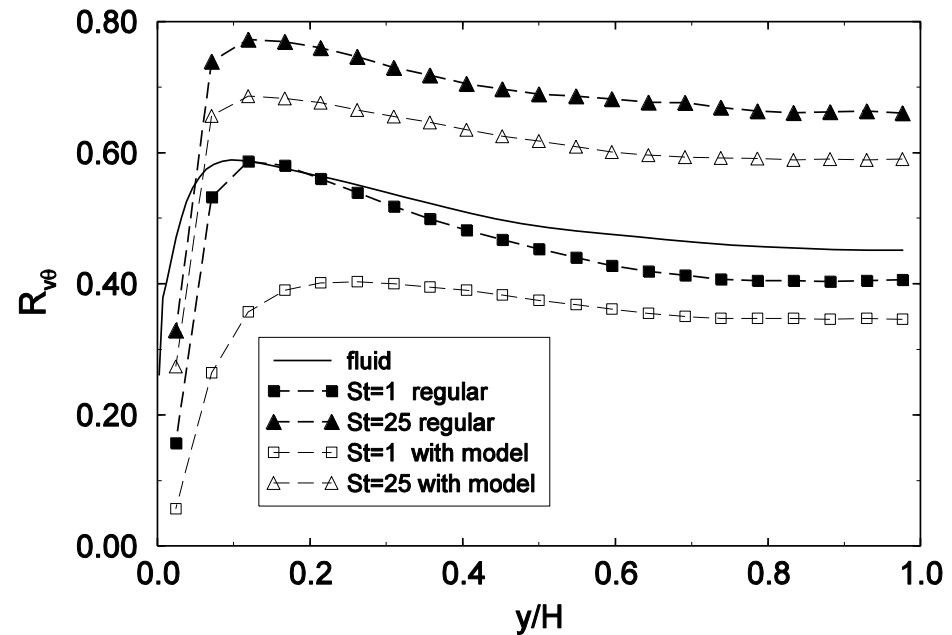
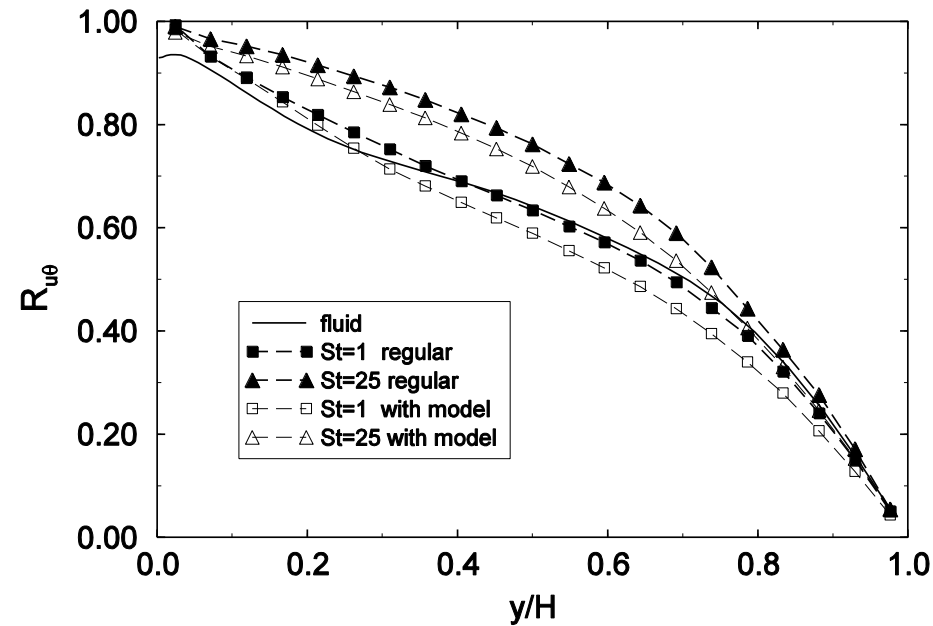
## Heated/cooled channel flow: scatter plots for particles of $St=5$



(a) particle wall-normal velocity, (b) particle temperature

...scalar boundedness constraint should be preserved  
if a model for SGS temperature fluctuation is attempted

# Heated/cooled channel flow: particle velocity-temperature correlation coefficients



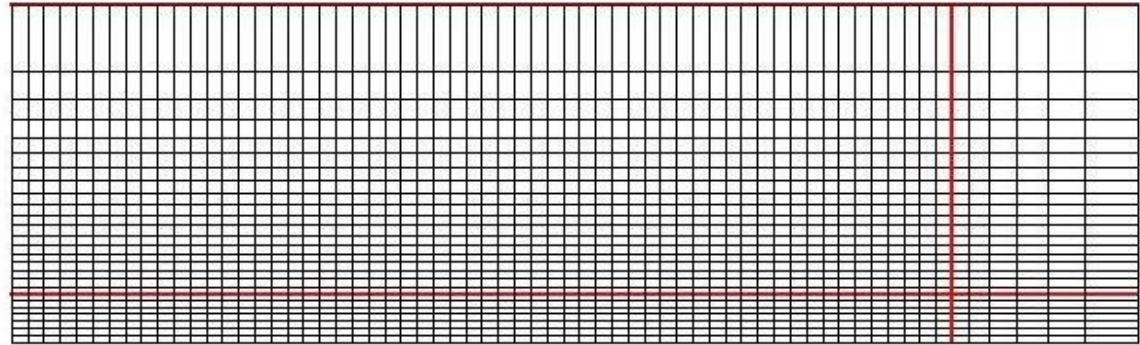
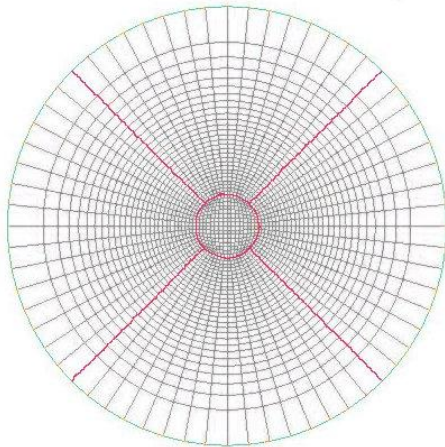
Velocity-temperature correlation: a) streamwise, b) wall-normal  
Solid lines: regular LES; dot-dashed lines: LES with SGS dispersion model

# LES results for particle-laden axisymmetric and coaxial jets

Benchmark problem, experimental data available

[Hishida et al., JCMF 2000]

$$\text{Re}_J = u_z^J D / \nu = 27500$$



**present LES:**

computational domain:  
( $r, \theta, z$ ):  $3.5D \times 2\pi \times 18D$

Inlet b.c.: 
$$U_z = \frac{u_z^J}{2} \left( 1 + \tanh \left[ 7.5 \left( 1 - \frac{R}{R_J} \right) \right] \right)$$

Outlet b.c.: 
$$\frac{\partial U_z}{\partial t} + U_c \frac{\partial U_z}{\partial z} = 0$$

Block-structured grid: total ~200 000 cells;

**Central part:** „O-grid” of  $15 \times 15 \times 130$  cells

**Outer part:** 4 regular  $(r, \theta, z)$  blocks  
of  $20 \times 15 \times 130$  cells

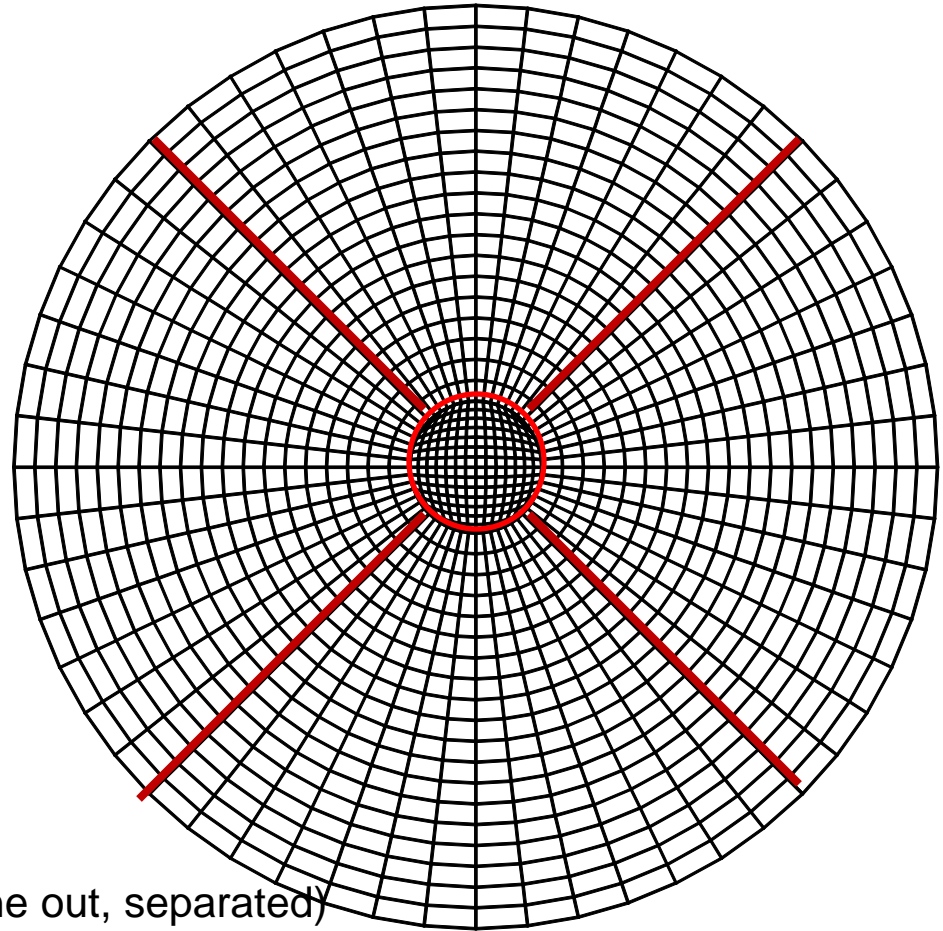
parallel comp. with domain decomposition

### → Efficient update of particle data arrays:

- particle localisation : global (b.c.)  
and local (within blocks)
- particle „exchange” between processors  
(parallel computing, MPI library)
- handling new (inlet) and „dead” particles (gone out, separated)

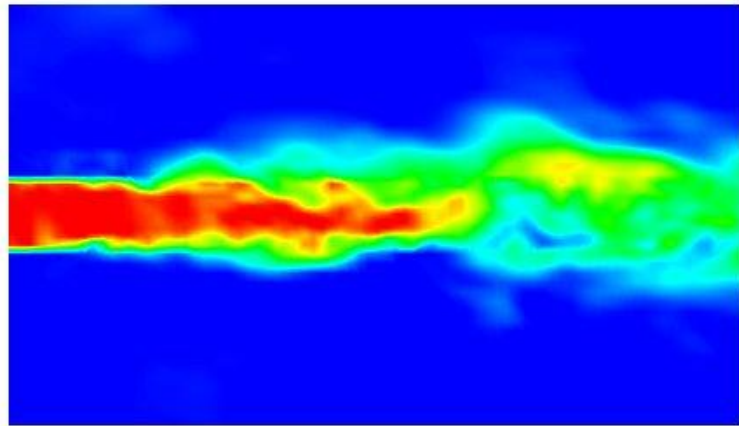
### → Fluid velocity interpolation at particles:

- „quarter-blocks” - linear interpolation on regular  $(r, \theta)$  meshes
- „O-grid” – interpolation using tabulated (pre-computed) fine grid



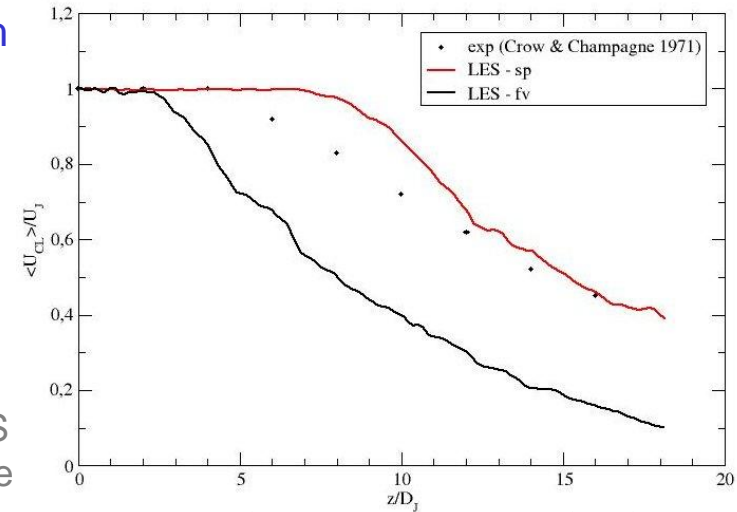


# LES for fluid: streamwise (axial) velocity statistics



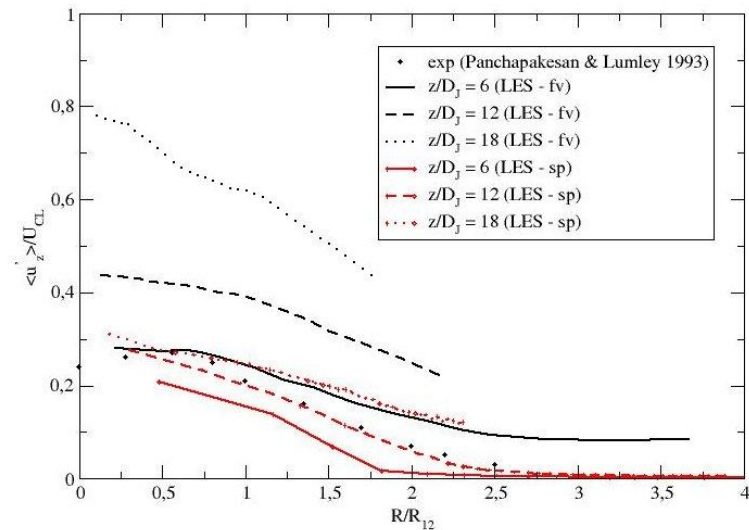
- potential core length  
- effects of i.c. & b.c.

**Axial velocity:**  
*close-up of the near field (up to  $z=10D$ )*

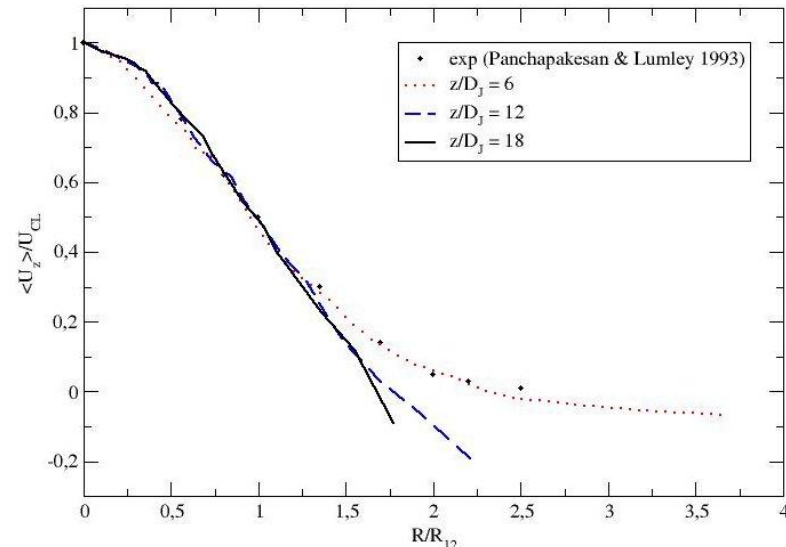


- fv: Finite-Volume LES  
- sp: spectral LES code

*Downstream decay of mean axial velocity at jet centerline*

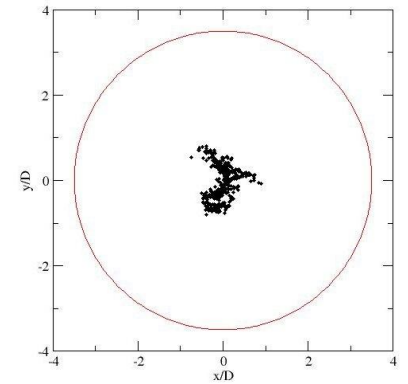
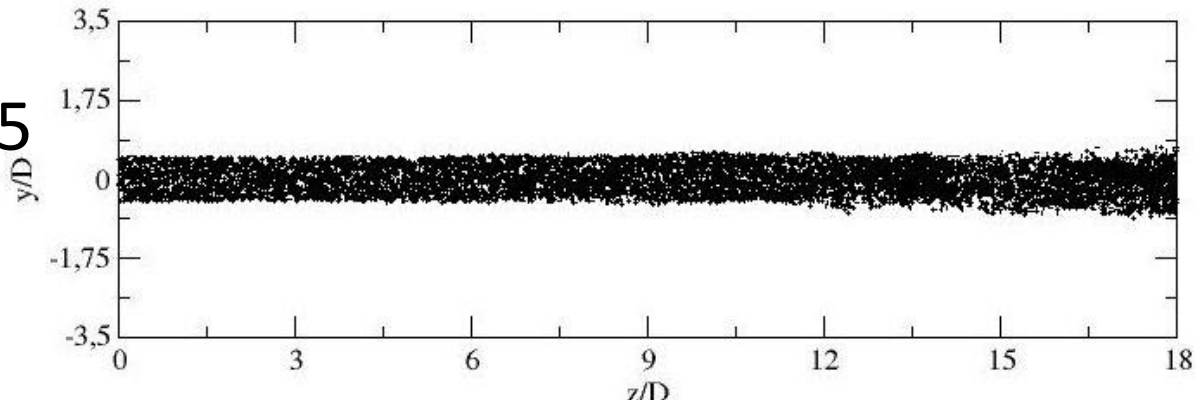


*Mean and rms axial velocity profiles*

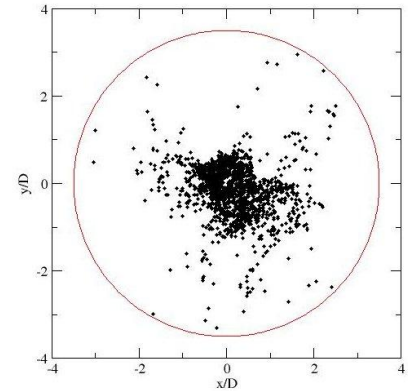
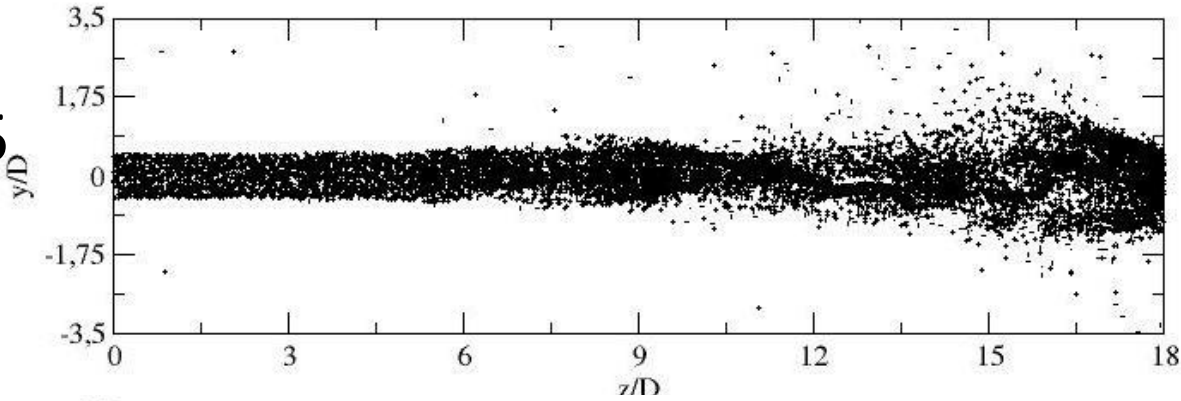


# Axisymmetric jet: particle number and patterns

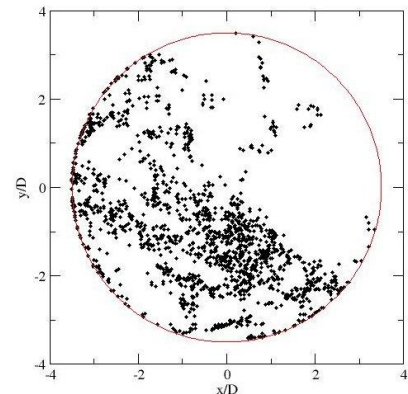
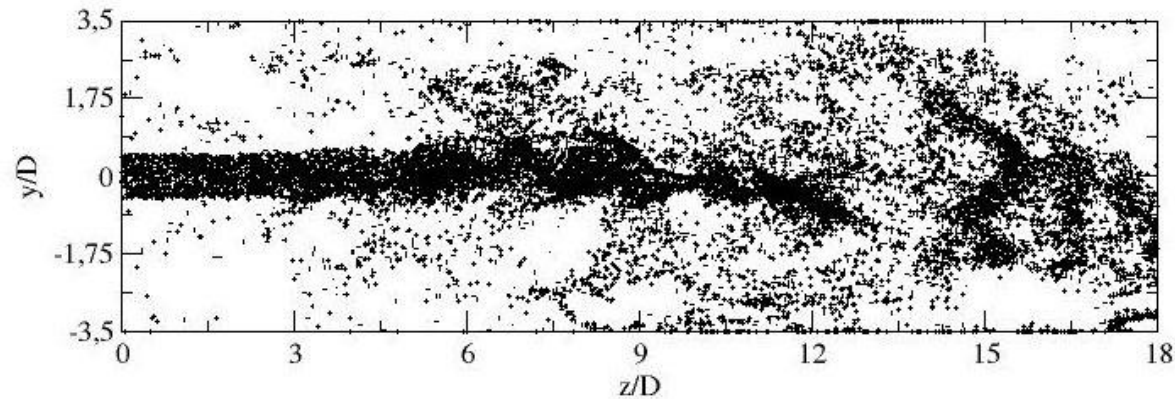
St=125



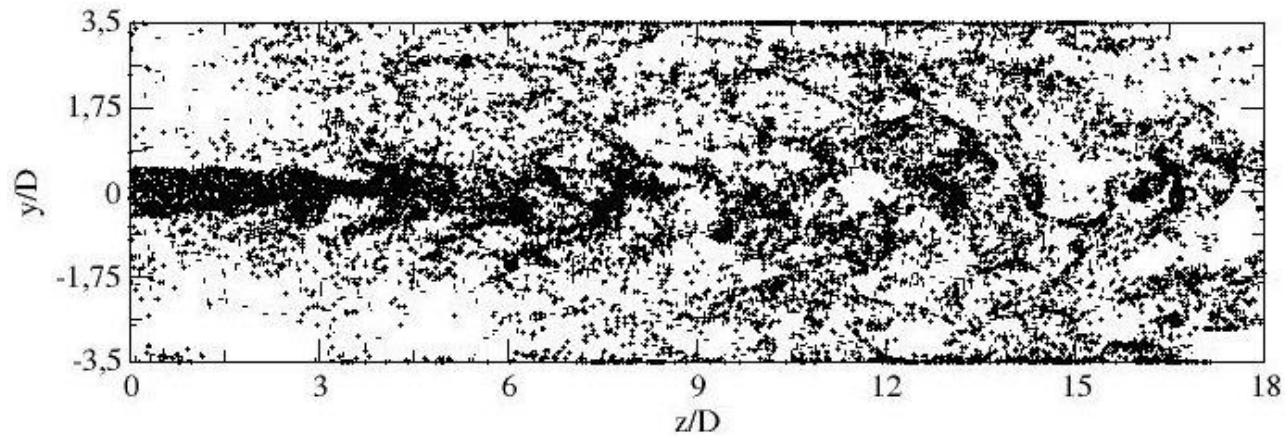
St=25



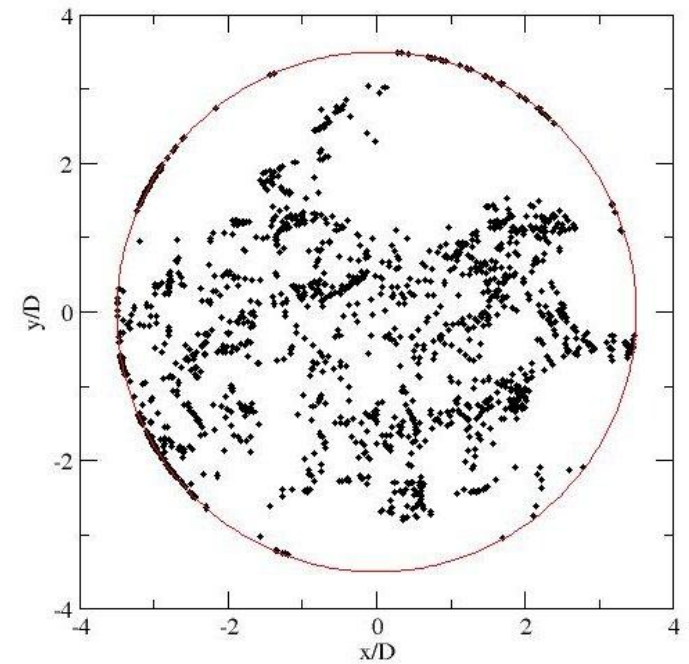
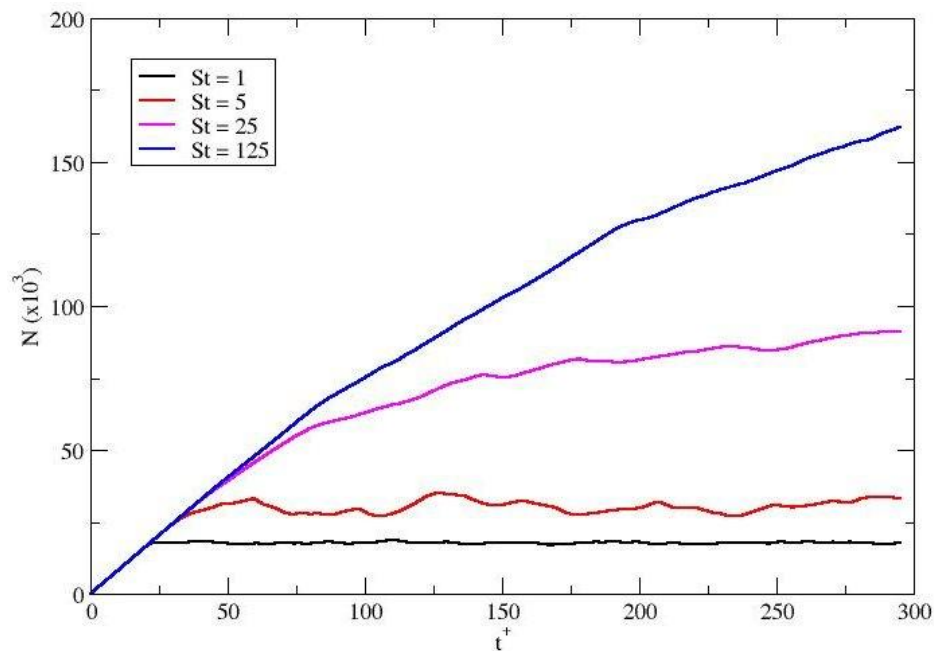
St=5



# Axisymmetric jet: particle number and patterns



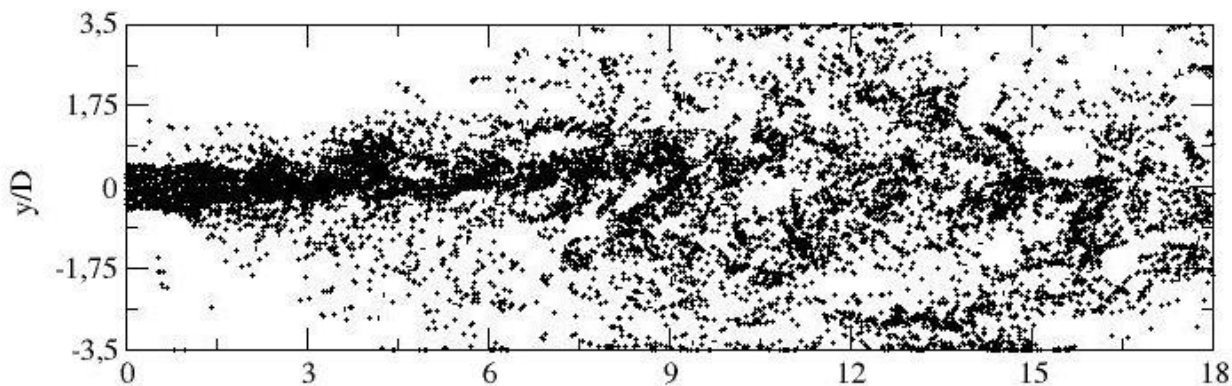
St=1



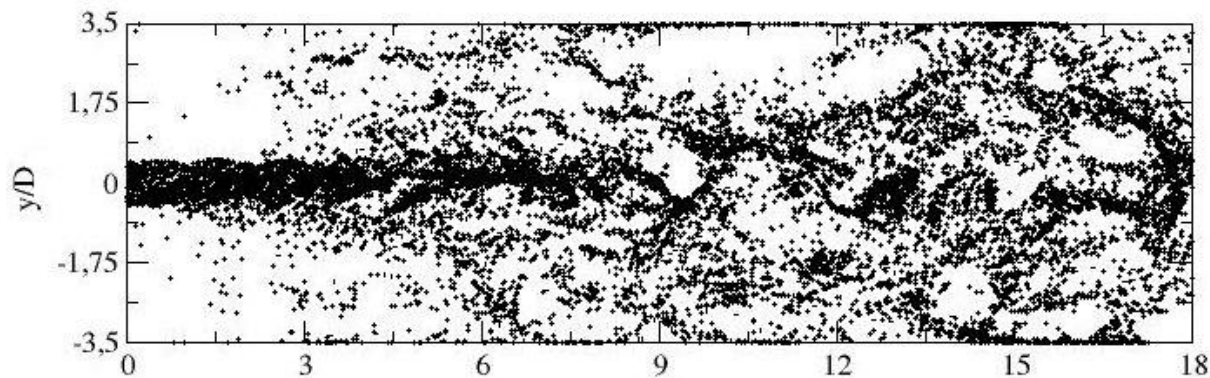


# Axisymmetric jet: particles of $St=1$

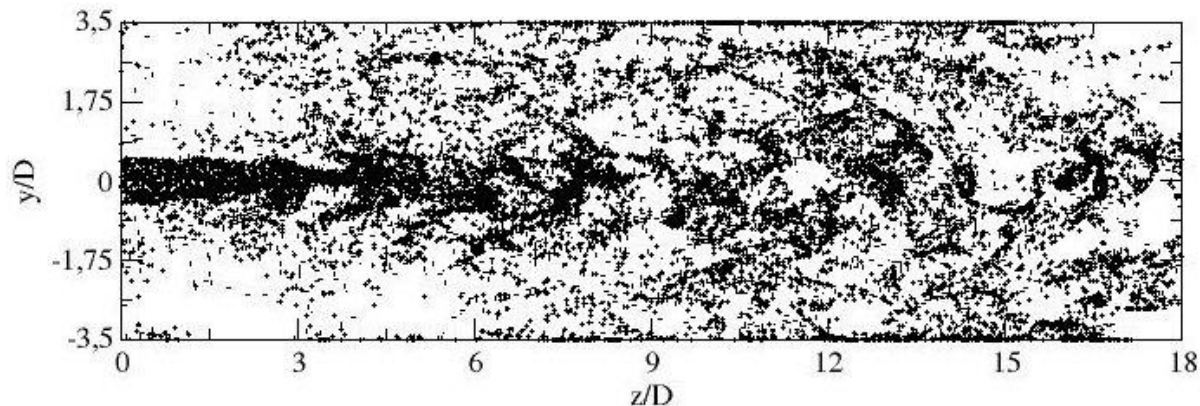
$t^+ = 100$



$t^+ = 200$

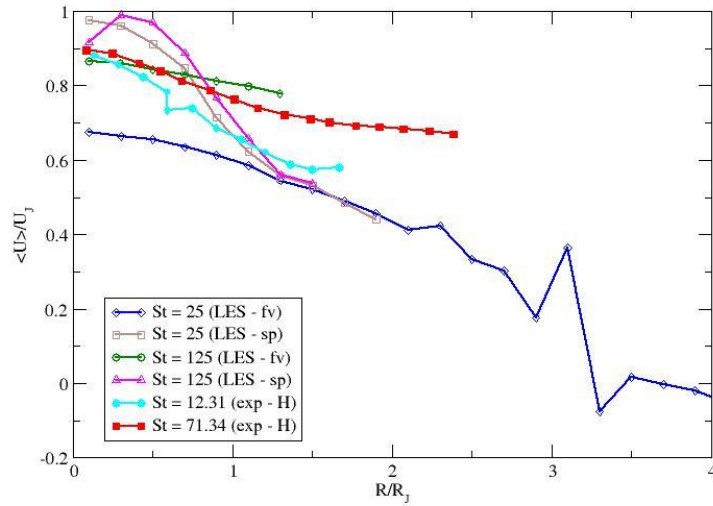


$t^+ = 300$

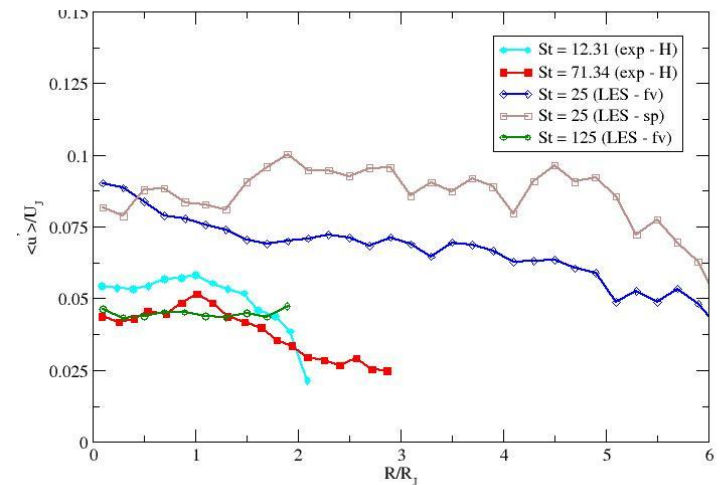
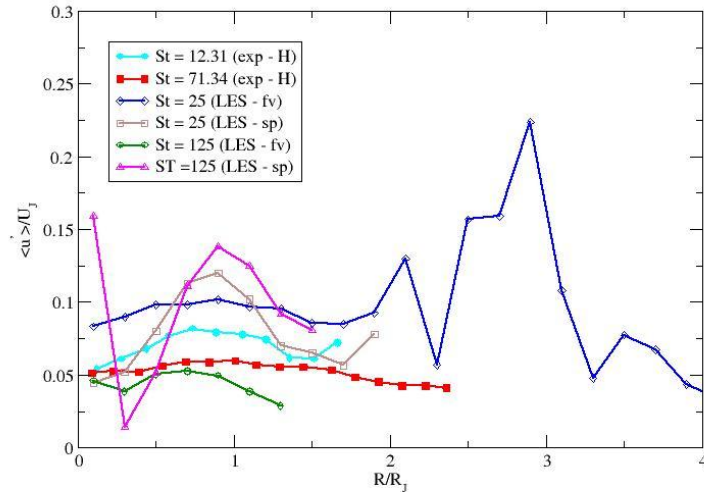
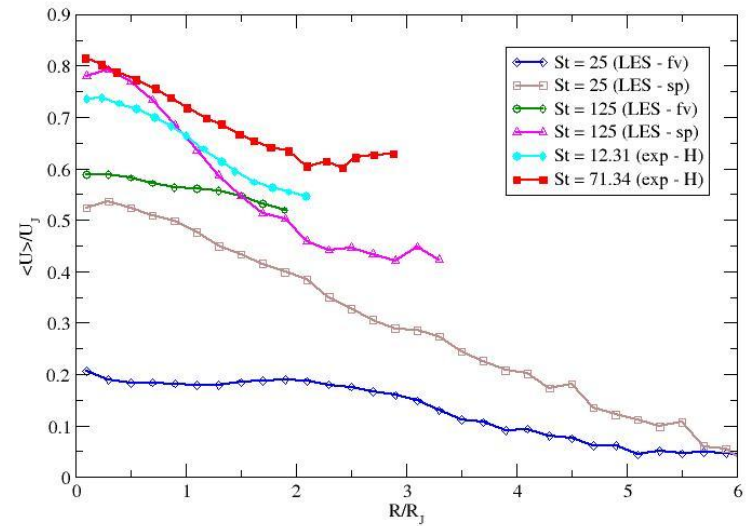


# Axisymmetric jet: particle statistics (axial)

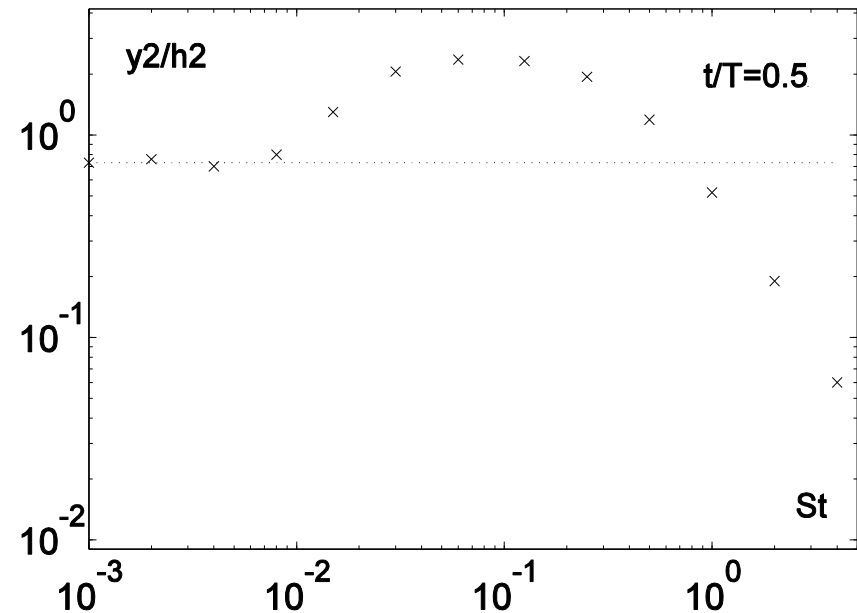
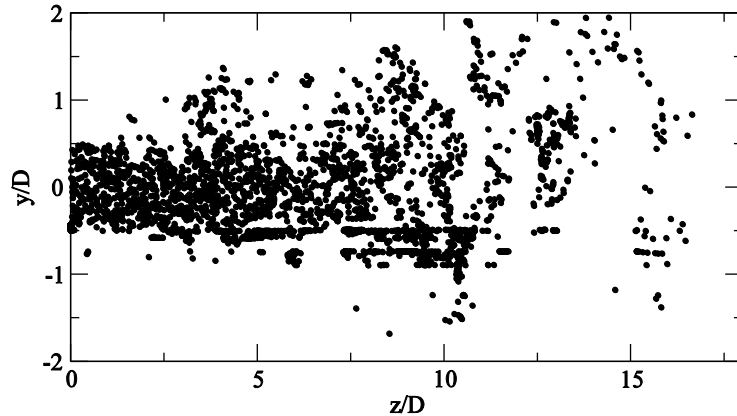
$z/D = 10$



$z/D = 20$



# Comment on „anomalous” particle dispersion



Effects of fluid-particle velocity correlation:

- \* for intermediate inertia, cross-stream particle dispersion is faster than that of Lagrangian fluid particles

- \* relationship to turbophoresis and preferential concentration

*Wake flow: mean-square dispersion*

*[Pozorski 1995]*

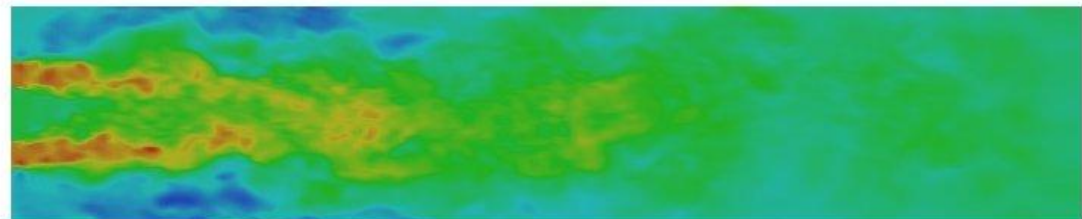
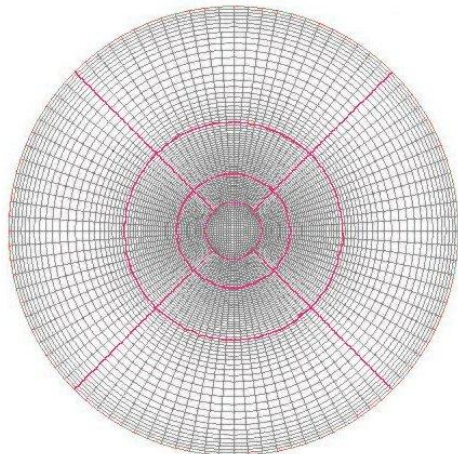
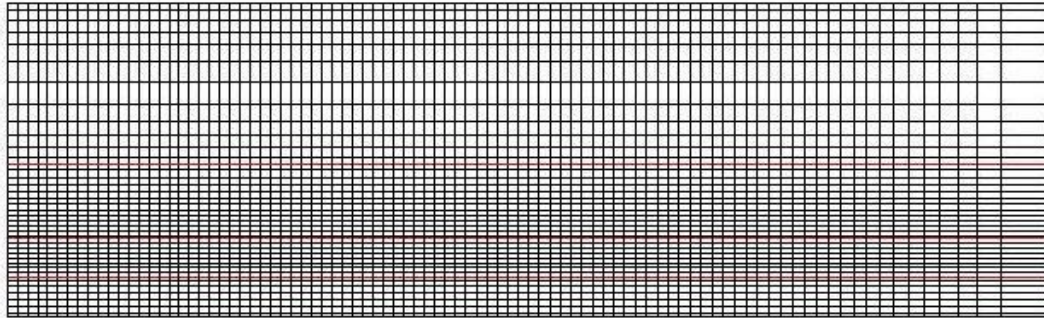
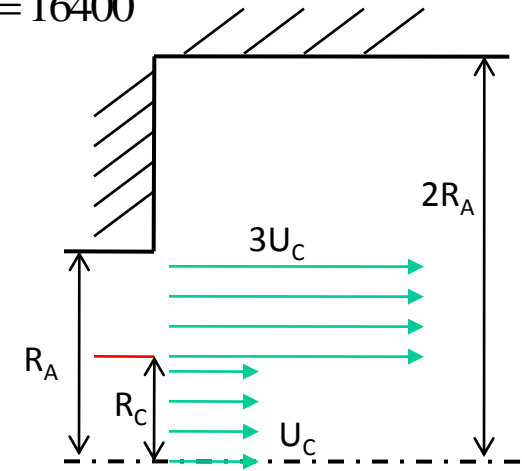


# Coaxial jets

$$Re = u_z^C (R_{\max} - R_A) / \nu = 16400$$

$$\text{Inlet: } \lambda = \frac{U_A}{U_C} = 3 \quad \lambda_A = \frac{\pi(R_A^2 - R_C^2)}{\pi R_C^2} = 2.72$$

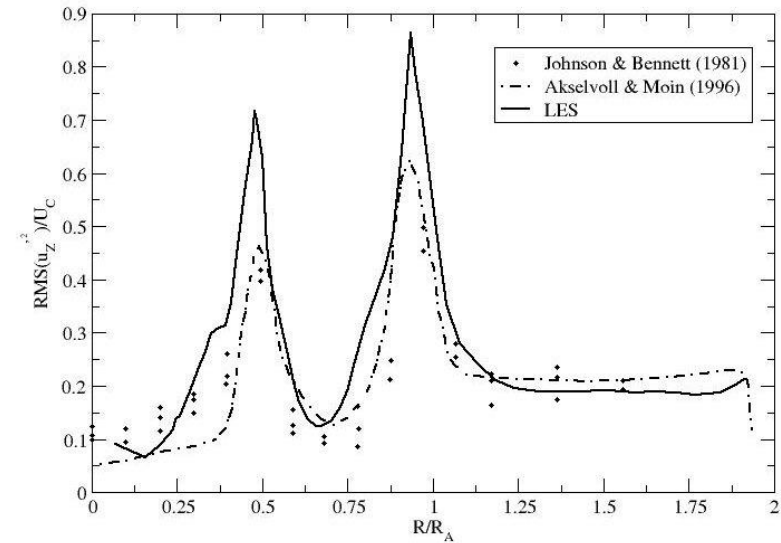
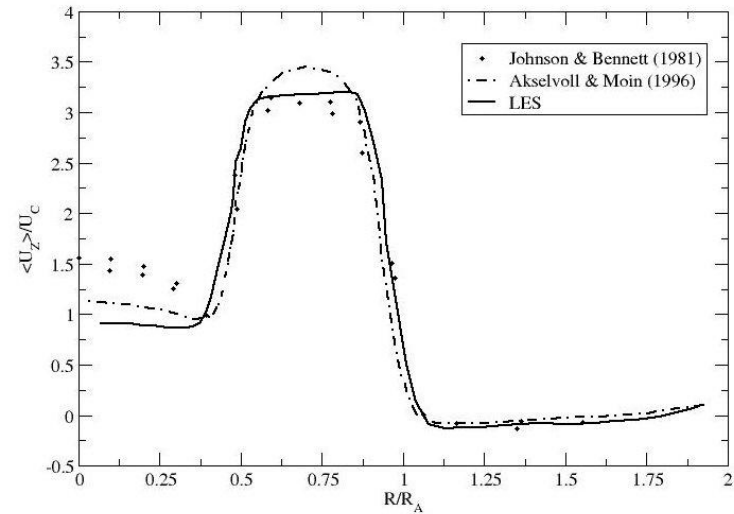
$$\text{Outlet b.c.: } \frac{\partial U_z}{\partial t} + U_C \frac{\partial U_z}{\partial z} = 0$$



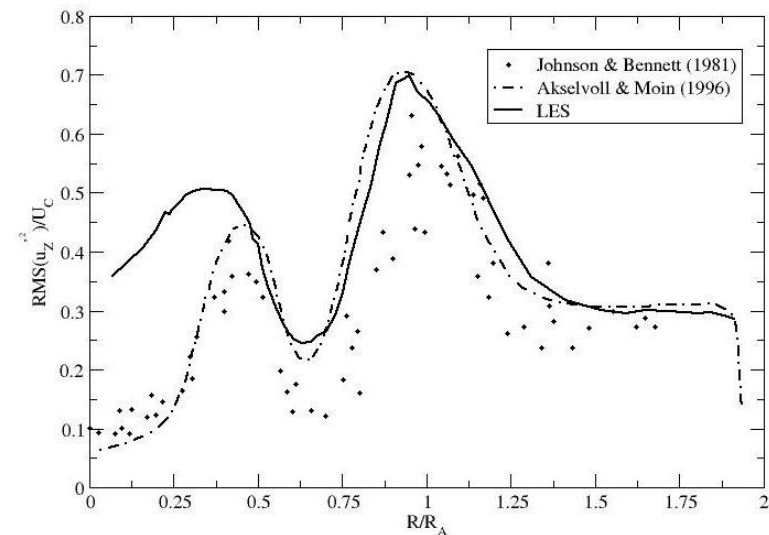
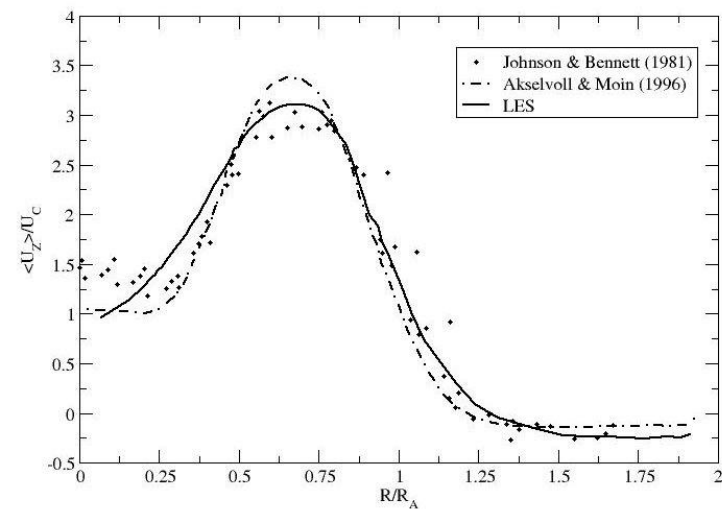
# Coaxial jets: fluid statistics

## mean and r.m.s streamwise velocity profiles

$z/D = 0.22$

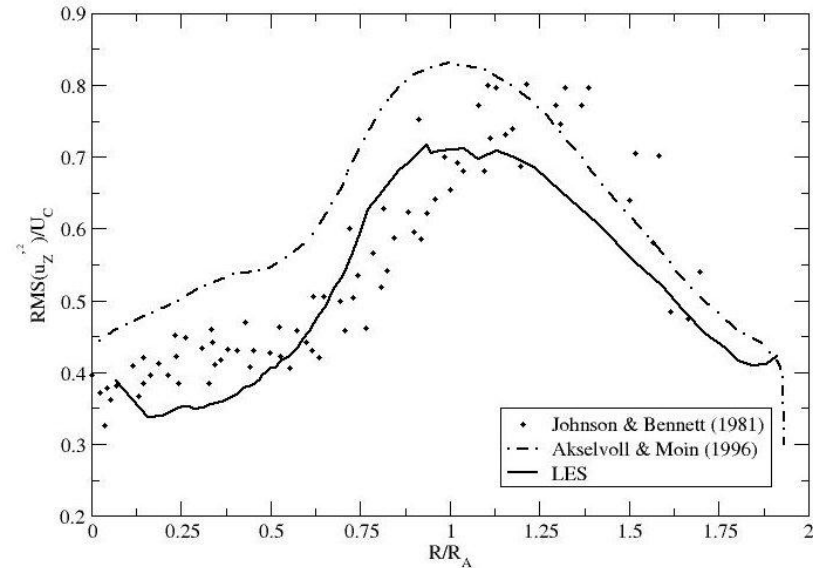
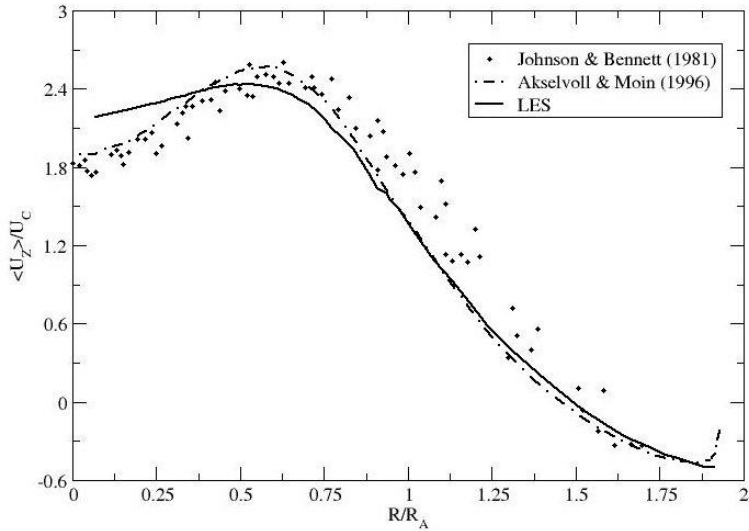


$z/D = 0.87$

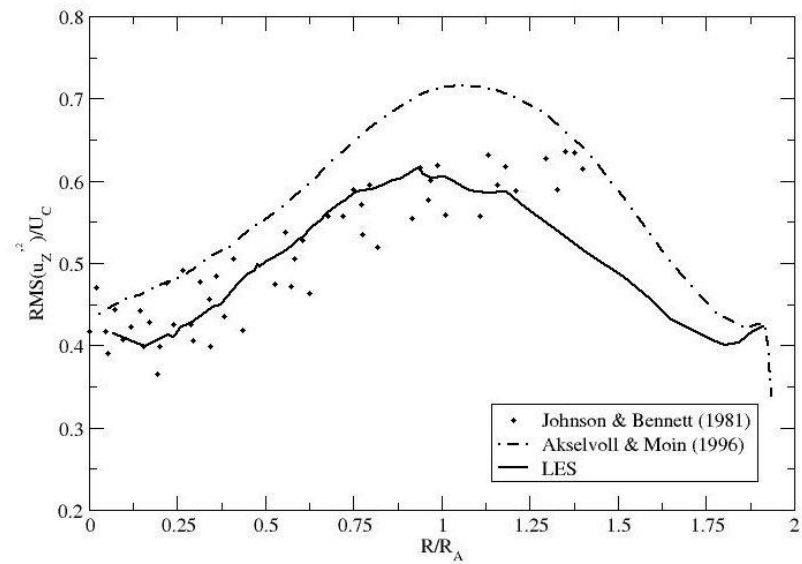
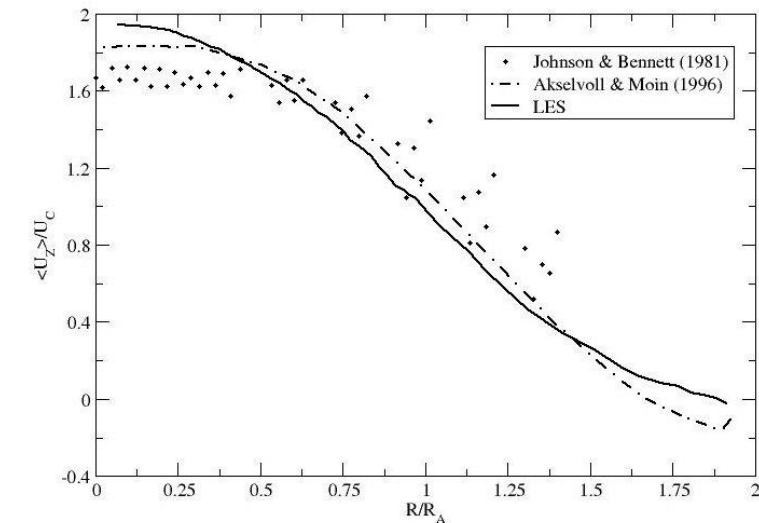


# Coaxial jets: fluid statistics (cntd.)

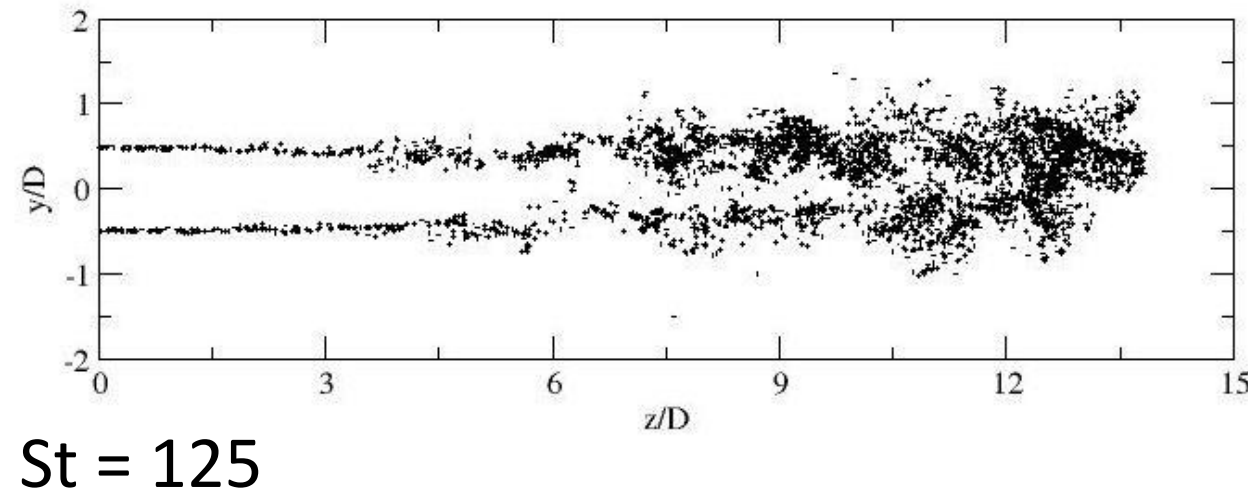
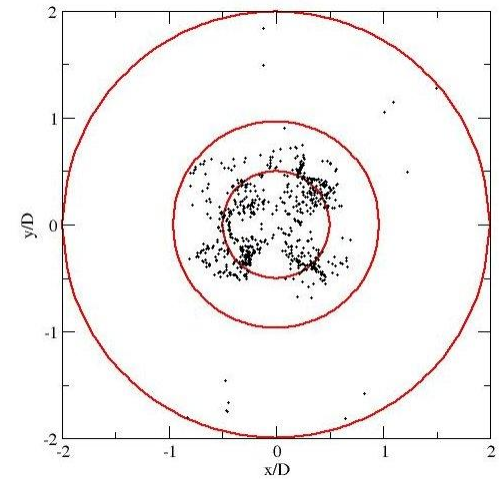
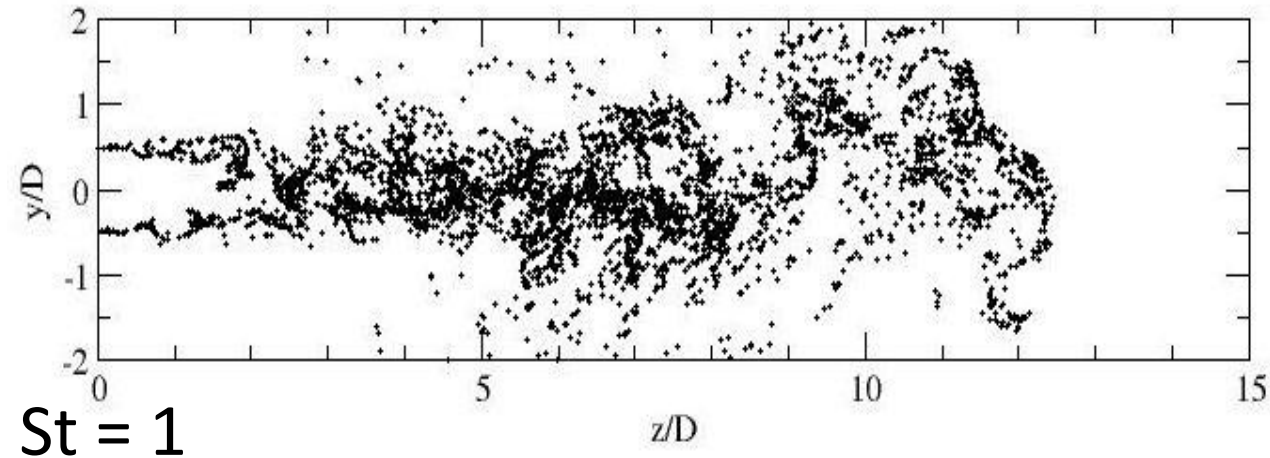
$z/D = 2.58$



$z/D = 4.3$



# Coaxial jets: particle snapshots



quantitative comparison with  
exp. of (Fan,Zhao & Jin, 1996)  
is worked on

## Summary of Part III (results)

### → Channel flows:

- statistics of particle velocity and temperature computed
- stochastic model for SGS particle dispersion included

### → Jet flows:

- parallel implementation developed
- effect of flow domain tested; single axisymmetric and coaxial jets computed
- statistics of fluid and some particle classes gathered

### → Next-term objectives:

- heated channel: compute more thermal statistics, compare with DNS  
[Jaszczur & Portela, 2007]
- coaxial jets: develop inflow b.c. to compare particle results with experiment  
[Hishida, 2000]
- LES of jet flow with particle heating and evaporation

(towards combustion)



## Conclusion: perspectives for further work

### → Modelling of flow-particle interactions:

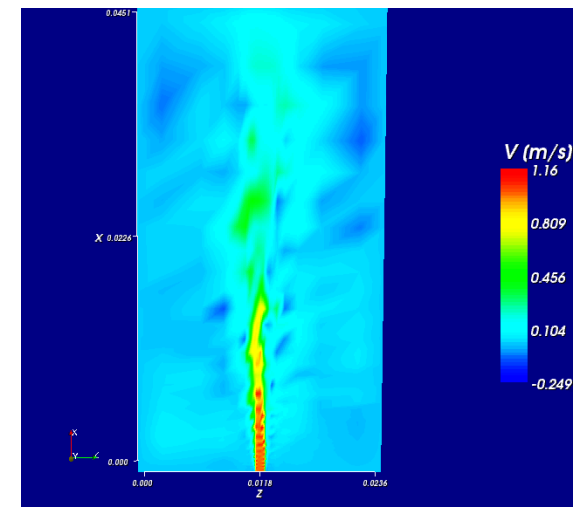
- mass and energy coupling ( $F \leftrightarrow P$ : evaporation, condensation, combustion)
- momentum coupling ( $F \rightarrow P$ : preferential concentration,  $P \rightarrow F$ : SGS stress)
- structural changes: complex  $\rightarrow$  disperse (liquid jet atomisation)

### → Sub-filter models, theoretical developments:

- subgrid-scale particle dispersion: stochastic and structural models
- Filtered Density Function (FDF) formalism for polydispersed flows

### → Applications :

- coaxial particle/droplet – laden jets with swirl, burners





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