Exact Regularized Point Particle method for particle laden flows in the two-way coupling regime

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in collaboration with

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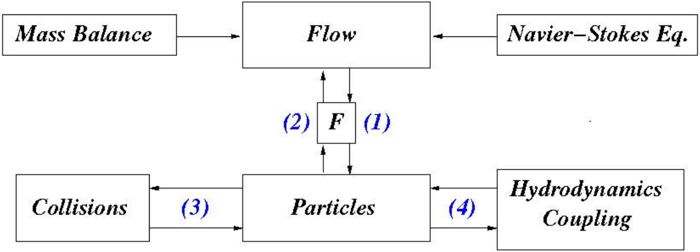
Dynamics of Particles in Flows
Fundamentals and Applications
Stockholm

Fluid-particles interaction



- (1) one-way coupling
- (1) + (2) two-way coupling
- (1) + (2) + (3) + (4) four-way coupling

- beyond the one-way coupling $\cdots\cdots$
  - $\Rightarrow$ turbulence modulation in the *two-way coupling regime*
  - $\Rightarrow$ develope innovative momentum coupling methods

Particle In Cell approach (PIC) [Crowe et al. *J. Fluid Eng.* (1977)]

- Eulerian description (fluid) & Lagrangian tracking (particles) [e.g. Eaton *Int. J. Mult. Flow*]

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla \pi + \nu \nabla^2 \mathbf{u} - \frac{1}{\rho_f} \sum_p \mathbf{D_p(t)} \delta \left[\mathbf{x} - \mathbf{x_p(t)} \right]$$

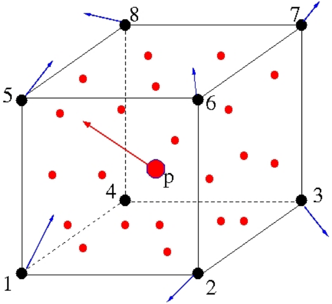
- The *back-reaction* **F** is singular: average on the cell ΔV_{cell}

$$\mathbf{F}(\mathbf{x}_p) = \frac{1}{\Delta V_{cell}} \frac{1}{\rho_f} \mathbf{D}_p$$

equivalent to $\{\mathbf{F}(\mathbf{x}_q)\}_{q=1,8}$

$$\sum_{q=1}^{8} \mathbf{F}(\mathbf{x}_q) = \mathbf{F}(\mathbf{x}_p)$$

$$\sum_{q=1}^{8} (\mathbf{x}_q - \mathbf{x}_p) \times \mathbf{F}(\mathbf{x}_q) = 0$$

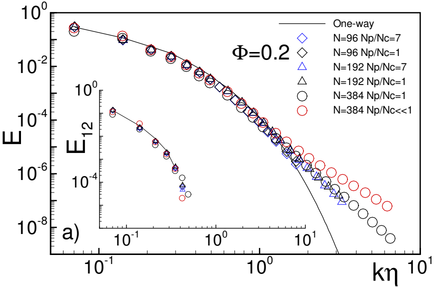


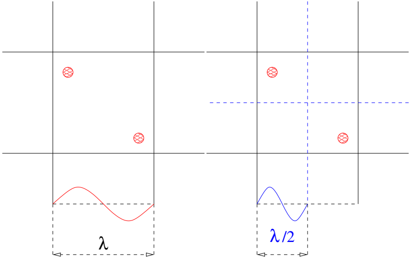
- The mass load $\Phi = M_p/M_f$ controlls the momentum

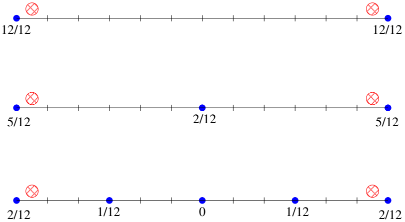
PIC: numerical issues

The *tails* *of the spectra* *hardly decay* *when* $N_p/N_c \ll 1$

- fine grids require a large number of particles
- grid dependent forcing
- limitations on the mass load







P.G., F. Picano, G. Sardina, C.M. Casciola, JFM **715** (2013)

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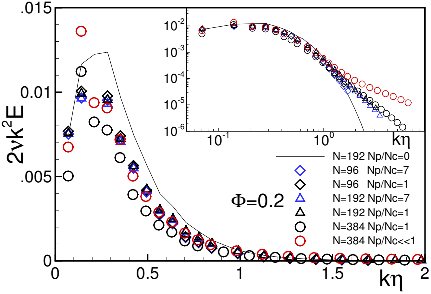
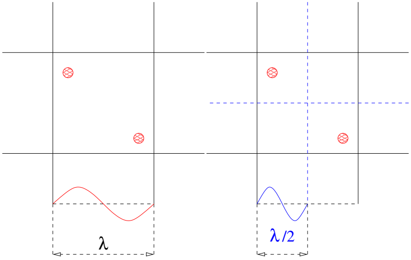
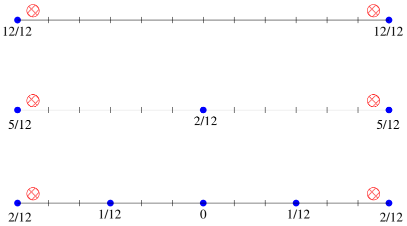
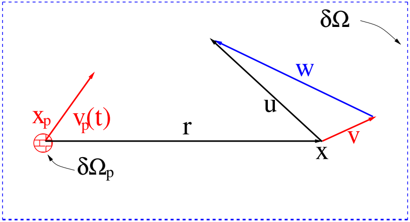






P.G., F. Picano, G. Sardina, C.M. Casciola, JFM **715** (2013)

Exact Regularized Point Particle (ERPP) method



$$\begin{cases} \dfrac{\partial \mathbf{u}}{\partial t} + \mathbf{u}\cdot\nabla\mathbf{u} = -\nabla p + \nu\nabla^2\mathbf{u} \\ \mathbf{u}|_{\partial\Omega_p} = \mathbf{v}_p; \quad \mathbf{u}|_{\partial\Omega} = \mathbf{u}_{wall} \\ \mathbf{u}(\mathbf{x}, t_n) = \mathbf{u}_0(\mathbf{x}) \end{cases}$$

Decompose the (incompressible) fluid velocity $\mathbf{u}$ in a background flow $\mathbf{w}$ and a perturbation $\mathbf{v}$, namely $\mathbf{u} = \mathbf{w} + \mathbf{v}$

$$\begin{cases} \dfrac{\partial \mathbf{w}}{\partial t} + \mathbf{u}\cdot\nabla\mathbf{u} = -\nabla \pi + \nu\nabla^2\mathbf{w} \\ \mathbf{w}|_{\partial\Omega} = \mathbf{u}_{wall} - \mathbf{v}|_{\partial\Omega} \\ \mathbf{w}(\mathbf{x}, t_n) = \mathbf{u}_0(\mathbf{x}) \end{cases}$$

$$\begin{cases} \dfrac{\partial \mathbf{v}}{\partial t} = -\nabla \tilde{p} + \nu\nabla^2\mathbf{v} \\ \mathbf{v}|_{\partial\Omega_p} = \mathbf{v}_p - \mathbf{w}|_{\partial\Omega_p} \\ \mathbf{v}(\mathbf{x}, t_n) = 0 \end{cases}$$

Perturbation $\mathbf{v}$ *described in terms of unsteady Stokes equations*

P.G., F. Picano, G. Sardina, C.M. Casciola, submitted to JFM, http://arxiv.org/abs/1405.6969

ERPP: perturbation field

Exact solution of the unsteady Stokes problem

$$v_i(\mathbf{x},t) = \int_0^t d\tau \int_{\partial\Omega} t_j(\boldsymbol{\xi},\tau) G_{ij}(\mathbf{x},\boldsymbol{\xi},t,\tau) - v_j(\boldsymbol{\xi},\tau)\mathcal{T}_{ijk}(\mathbf{x},\boldsymbol{\xi},t,\tau) n_k(\boldsymbol{\xi})\, dS$$

G_{ij} the *unsteady Stokeslet*; $\mathcal{T}_{ijk}$ the associated stress tensor

For *small particles* the *far field* disturbance is estimated in terms of multipole expansion [Kim & Karilla, Microfluidics, (2000)]

$$v_i(\mathbf{x},t) \simeq -\int_0^t D_j(\tau) G_{ij}(\mathbf{x},\mathbf{x}_p,t,\tau)\, d\tau$$

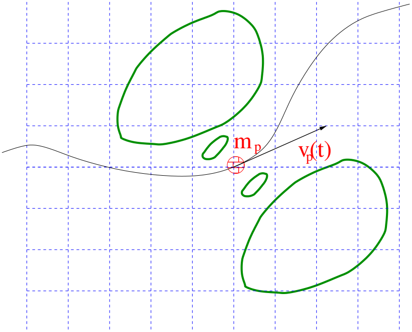
with $\mathbf{D}(\tau)$ hyrodynamic force, i.e. the Stokes Drag ($\cdots$ or more [Maxey & Riley, (1983); Gatignol (1983)])

ERPP: vorticity

Eulerian *far field* disturbance $\mathbf{v}(\mathbf{x}, t)$ described by the unsteady singularly forced Stokes equation

$$\frac{\partial \mathbf{v}}{\partial t} - \nu \nabla^2 \mathbf{v} + \nabla \tilde{p} = -\frac{\mathbf{D}(t)}{\rho_f} \, \delta \left[\mathbf{x} - \mathbf{x}_p(t) \right]$$

How to regularize the solution of the disturbance field?



Physics of the coupling

The vorticity, once generated along the particle trajectory, is diffused by viscosity and then injected into the Eulerian grid

vorticity generated by the particle $\Rightarrow$ Eulerian Navier–Stokes solver

ERPP: vorticity diffusion

Why vorticity? $\Rightarrow$ Diffusion equation

$$\partial_t \boldsymbol{\zeta} - \nu \nabla^2 \boldsymbol{\zeta} = \frac{\mathbf{D}(t)}{\rho_f} \times \nabla \delta \left[\mathbf{x} - \mathbf{x}_p(t) \right]$$

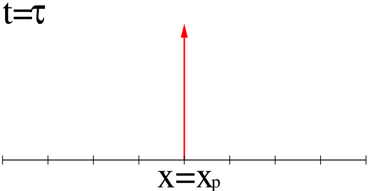
Fundamental solution

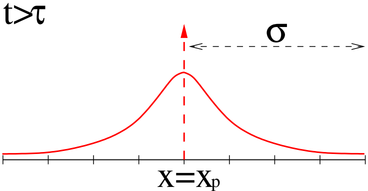
$$\partial_t g - \nu \nabla^2 g = \delta \left(\mathbf{x} - \mathbf{x}_p \right) \delta(t - \tau)$$

$$g(\mathbf{x}, \mathbf{x}_p, t, \tau) = \frac{1}{\left(2\pi\sigma^2\right)^{3/2}} \exp\left(\frac{-\|\mathbf{x} - \mathbf{x}_p\|^2}{2\sigma^2} \right), \quad \sigma(t-\tau) = \sqrt{2\nu(t-\tau)}$$

For $t > \tau$ the solution is both

- *regular*, e.g. $g \in C^\infty$
- *local*, i.e decays more than exponentially





ERPP: vorticity regularization

- *Analytical solution* expressed as a convolution with the fundamental solution of the diffusion equation

$$\boldsymbol{\zeta}(\mathbf{x},t) = \frac{1}{\rho_f}\int_0^t \mathbf{D}(\tau) \times \nabla g\left[\mathbf{x}-\mathbf{x}_p(\tau), t-\tau\right] d\tau$$

- For $\tau \simeq t$, $g(\mathbf{x}, \mathbf{x}_p, t, \tau)$ tends to behave as badly as the Dirac delta function $\Rightarrow$ split $\boldsymbol{\zeta} = \boldsymbol{\zeta}_{Regular} + \boldsymbol{\zeta}_{Singular}$

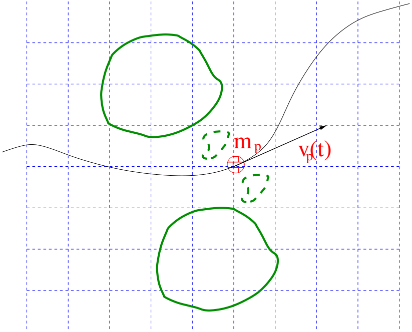
- The regularization procedure adopts a temporal cut-off ϵ_R

$$\boldsymbol{\zeta}_R(\mathbf{x},t) = \frac{1}{\rho_f}\int_0^{t-\epsilon_R} \mathbf{D}(\tau) \times \nabla g\left[\mathbf{x}-\mathbf{x}_p(\tau), t-\tau\right] d\tau$$

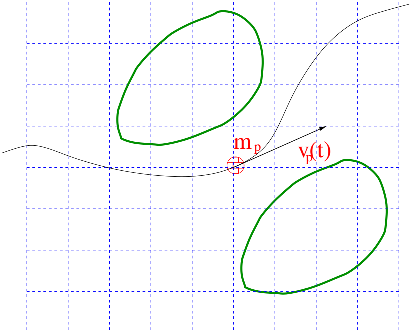
$\Rightarrow$ Regularized field $\boldsymbol{\zeta}_R$ everywhere smooth and characterized by the smallest spatial scale $\sigma_R = \sqrt{2\nu\epsilon_R}$

ERPP: a cartoon

complete field



regularized field



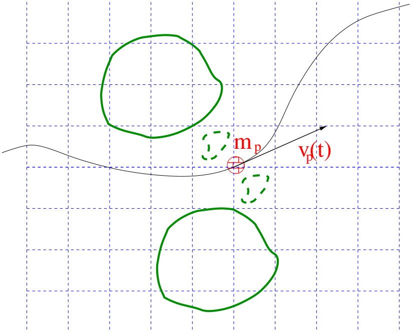
$$\boldsymbol{\zeta}(\mathbf{x},t) = \frac{1}{\rho_f}\int_0^t \mathbf{D}(\tau) \times \nabla g \, d\tau$$

$$\boldsymbol{\zeta}_R(\mathbf{x},t) = \frac{1}{\rho_f}\int_0^{t-\epsilon_R} \mathbf{D}(\tau) \times \nabla g \, d\tau$$

$\Rightarrow$ Vorticity at scales smaller that σ_R is not neglected but injected at later times

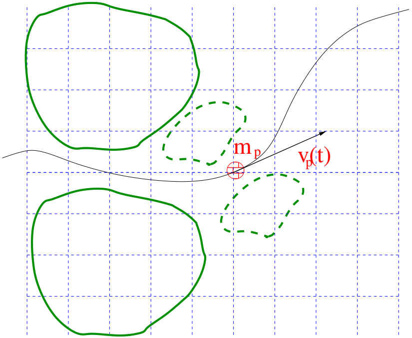
ERPP: a cartoon

complete field



$$\boldsymbol{\zeta}(\mathbf{x},t) = \frac{1}{\rho_f}\int_0^t \mathbf{D}(\tau) \times \nabla g \, d\tau$$

regularized field at later times



$$\boldsymbol{\zeta}_R(\mathbf{x},t) = \frac{1}{\rho_f}\int_0^{t-\epsilon_R} \mathbf{D}(\tau) \times \nabla g \, d\tau$$

$\Rightarrow$ Vorticity at scales smaller that σ_R is not neglected but injected at later times

ERPP: coupling with the carrier phase

- The regular component of the vorticity field $\boldsymbol{\zeta}_R$ satisfy

$$\frac{\partial \boldsymbol{\zeta}_R}{\partial t} - \nu \nabla^2 \boldsymbol{\zeta}_R = \frac{1}{\rho_f} \nabla \times \mathbf{D}(t-\epsilon_R) g\left[\mathbf{x} - \mathbf{x}_p(t-\epsilon_R), \epsilon_R\right]$$

- The regular (perturbation) velocity field $\mathbf{v}_R$ follows as

$$\frac{\partial \mathbf{v}_R}{\partial t} - \nu \nabla^2 \mathbf{v}_R = -\frac{1}{\rho_f} \mathbf{D}(t-\epsilon_R) g\left[\mathbf{x} - \mathbf{x}_p(t-\epsilon_R), \epsilon_R\right]$$

- The fluid velocity $\mathbf{u} = \mathbf{w} + \mathbf{v}_R$ is then given by

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla p + \nu \nabla^2 \mathbf{u} - \sum_{p=1}^{N_p} \frac{\mathbf{D}_p(t-\epsilon_R)}{\rho_f} g\left[\mathbf{x} - \mathbf{x}_p(t-\epsilon_R), \epsilon_R\right]$$

- Remarks
  - simply add an extra term in any $N-S$ solver
  - the function g is *local* in space $\Rightarrow$ *computational efficiency*

Particles Dynamics & Hydrodynamic force

- Diluted small particles

$$\frac{d\mathbf{x}_p}{dt} = \mathbf{v}_p\,; \quad m_p \frac{d\mathbf{v}_p}{dt} = \mathbf{D}_p(t) + (m_p - m_f)\,\mathbf{g}$$

- Hydrodynamic force

[Maxey & Riley, *PoF* (1983); Gatignol, *J. Mec. Theor. et appl.* (1983)]

$$\begin{aligned}
\mathbf{D}_p(t) &= 6\pi\mu a_p \left[\tilde{\mathbf{u}}(\mathbf{x}_p, t) - \mathbf{v}_p(t)\right] \\
&+ m_f \left.\frac{D\tilde{\mathbf{u}}}{Dt}\right|_{x_p} + \frac{1}{2} m_f \frac{d}{dt}\left[\tilde{\mathbf{u}}(\mathbf{x}_p, t) - \mathbf{v}_p(t)\right] \\
&+ 6\pi\mu a_p^2 \int_0^t d\tau\, \frac{1}{\left[\pi\nu\,(t-\tau)\right]^{1/2}} \frac{d}{d\tau}\left[\tilde{\mathbf{u}}(\mathbf{x}_p, \tau) - \mathbf{v}_p(\tau)\right]
\end{aligned}$$

$\Rightarrow$ $\tilde{\mathbf{u}}(\mathbf{x}_p, t)$ fluid velocity at $\mathbf{x}_p$ *in absence of the particle*

Particles Dynamics & Hydrodynamic force

- Removal of the self-disturbance $\mathbf{v}_{pth}$ from $\mathbf{u}(\mathbf{x}, t)$

$$\tilde{\mathbf{u}}(\mathbf{x}_p, t) = \mathbf{u}(\mathbf{x}_p, t) - \mathbf{v}_{pth}\left[\mathbf{x}_p(t) - \mathbf{x}_p(t_n); Dt\right]$$

- Self-disturbance velocity evaluated in closed form

$$\mathbf{v}(\mathbf{r}, Dt) = \frac{1}{\left(2\pi\sigma^2\right)^{3/2}}\left\{\left[e^{-\eta^2} - \frac{f(\eta)}{2\eta^3}\right]\mathbf{D}_p^n - \left(\mathbf{D}_p^n \cdot \hat{\mathbf{r}}\right)\left[e^{-\eta^2} - \frac{3f(\eta)}{2\eta^3}\right]\hat{\mathbf{r}}\right\}$$

where

$$\mathbf{r} = \mathbf{x}(t) - \mathbf{x}_p(t_n); \qquad \eta = r/\sqrt{2}\sigma; \qquad \sigma = \sqrt{2\nu(\epsilon_R + Dt)}$$

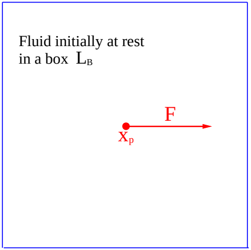
and

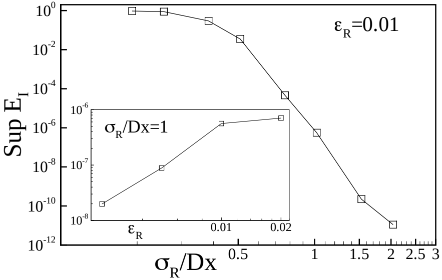
$$f(\eta) = \frac{\sqrt{\pi}}{2}\mathrm{erf}(\eta) - \eta e^{-\eta^2}$$

Concentrated force at a fixed point

- the impulse increases linearly in time, $I(t) = |\mathbf{F}|\, t$
- exact solution for the perturbation field

$$u(\mathbf{r},t) = \frac{1}{4\pi\mu r}\left[\left(\frac{1}{2\eta_t^2} - 1\right)\mathrm{erf}\left(\eta_t\right) - \frac{1}{\sqrt{\pi}\eta_t}e^{-\eta_t^2} + 1\right]; \quad \eta_t = r/\sqrt{4\nu t}$$





$\Rightarrow$ The impulse converges w.r.t. σ_R/Dx and ϵ_R

Concentrated force at a fixed point

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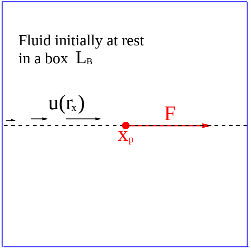
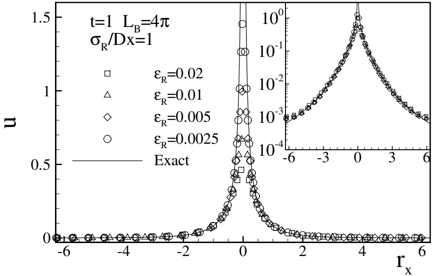
- exact solution for the perturbation field

$$u(\mathbf{r},t) = \frac{1}{4\pi\mu r}\left[\left(\frac{1}{2\eta_t^2} - 1\right)\operatorname{erf}(\eta_t) - \frac{1}{\sqrt{\pi}\eta_t} e^{-\eta_t^2} + 1\right]; \quad \eta_t = r/\sqrt{4\nu t}$$



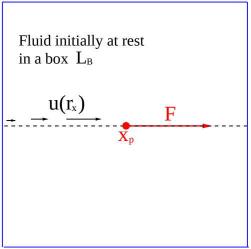


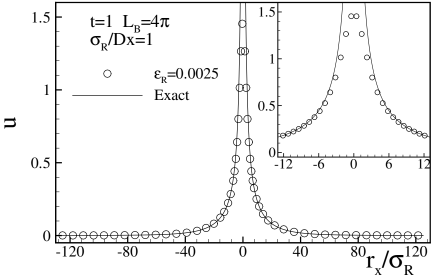
$\Rightarrow$ The far field is independent on ϵ_R

Concentrated force at a fixed point

- the impulse increases linearly in time, $I(t) = |\mathbf{F}|\, t$
- exact solution for the perturbation field

$$u(\mathbf{r},t) = \frac{1}{4\pi\mu r}\left[\left(\frac{1}{2\eta_t^2} - 1\right)\operatorname{erf}(\eta_t) - \frac{1}{\sqrt{\pi}\eta_t}e^{-\eta_t^2} + 1\right]; \quad \eta_t = r/\sqrt{4\nu t}$$





$\Rightarrow$ After few σ_R the exact solution is approached

Settling from rest under gravity

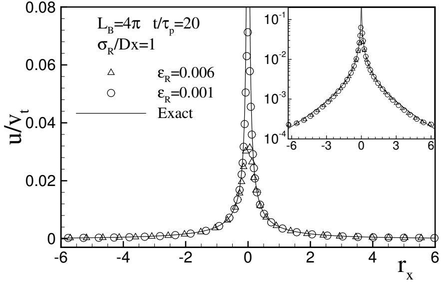
$$\frac{d\mathbf{x}_p}{dt} = \mathbf{v}_p$$
$$m_p \frac{d\mathbf{v}_p}{dt} = m_p \mathbf{g} + \mathbf{D}_p$$

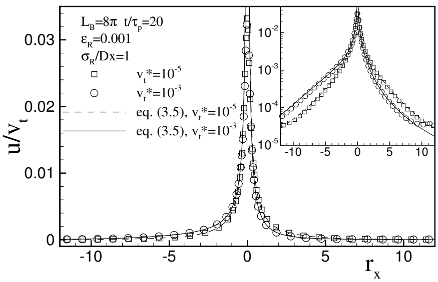
$$\mathbf{D}_p = -6\pi\mu a_p \, \mathbf{v}_p(t)$$

Exact solution

$$\mathbf{u}(\mathbf{x},t) = \int_0^t \mathbf{G}\left[\mathbf{x} - \mathbf{x}_p(\tau), t-\tau\right] \cdot \mathbf{D}_p(\tau)\, d\tau$$

(quadrature formula)





$\Rightarrow$ Note the fore-and-aft symmetry breaking at high v_t

Settling from rest under gravity

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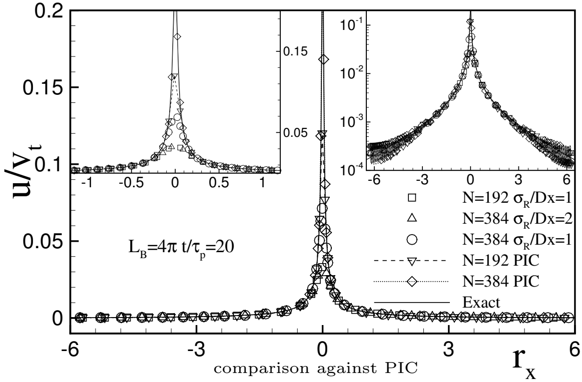


comparison against PIC

Settling from rest under gravity

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

$$m_p \frac{d\mathbf{v}_p}{dt} = m_p \mathbf{g} + \mathbf{D}_p$$

$$\mathbf{D}_p = 6\pi\mu a_p \left[\tilde{\mathbf{u}}(\mathbf{x}_p, t) - \mathbf{v}_p(t)\right]$$

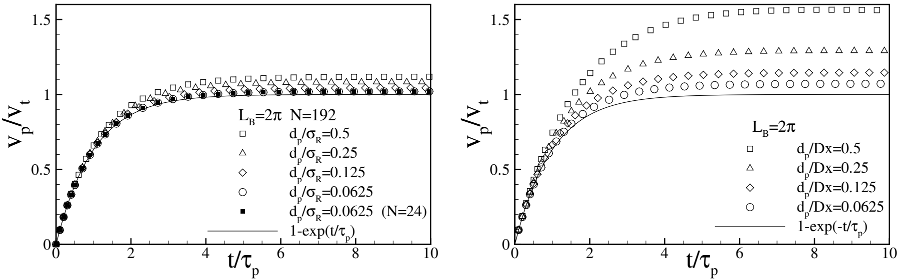
Self-induced disturbance removed

Exact solution

$$v_p = v_t \left(1 - e^{-t/\tau_p}\right)$$

ERPP

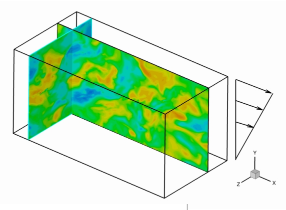
PIC

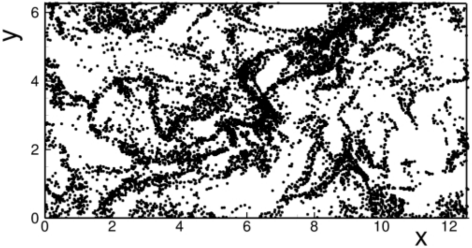


$\Rightarrow$ Terminal velocity better captured by the ERPP

Turbulent Flows: Homogeneos shear flow

$Re_\lambda = 50$
$St_\eta = 1,\ \Phi = 0.4$
$N_p = 2.200.000$
$d_p/\eta = 0.1$





- Remarks about turbulent simulations
  - regularization scale $\sigma_R = \eta$
  - the feedback field is everywhere *smooth*

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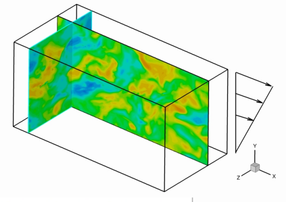

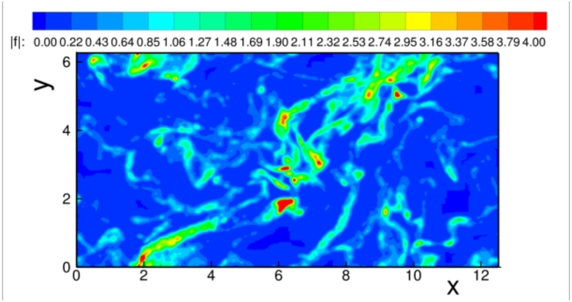

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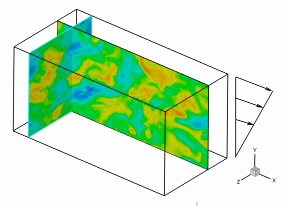
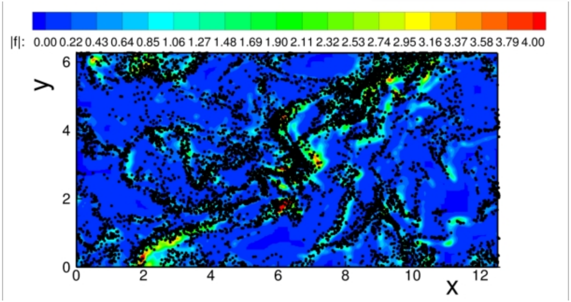
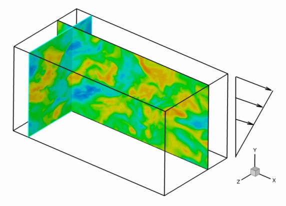




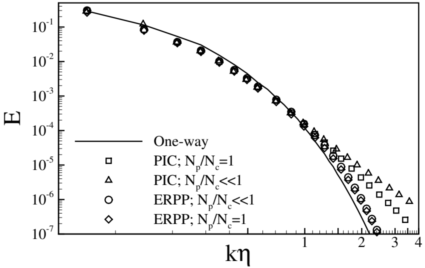
- Remarks about turbulent simulations
  - regularization scale $\sigma_R = \eta$
  - the feedback field is everywhere *smooth*

Turbulent Flows: Homogeneos shear flow

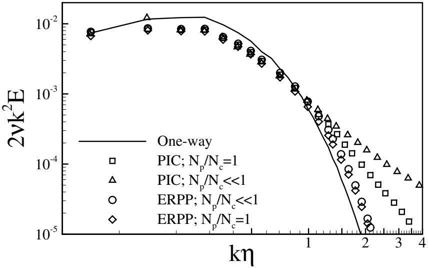
$Re_\lambda = 50$
$St_\eta = 1,\ \Phi = 0.4$
$N_p = 2.200.000$
$d_p/\eta = 0.1$



Energy spectrum



Dissipation spectrum

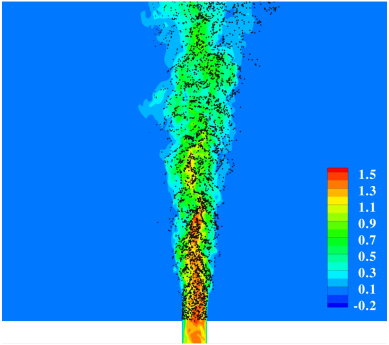


- Remarks
  - $E(k)$ and $2\nu\, k^2\, E(k)$ nicely smooth at small scales
  - ERPP prediction independent on N_p/N_c

Turbulent Jet

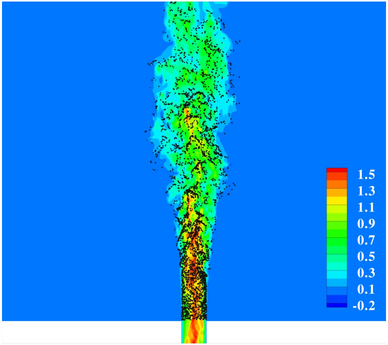
- $Re = U_b D/\nu = 3000$, domain $2\pi \times 50\,R \times 60\,R$
- $\Phi = 0.3 \Rightarrow$ about $N_p = 500.000$ at steady state

One-way



particles & axial velocity

Two-way

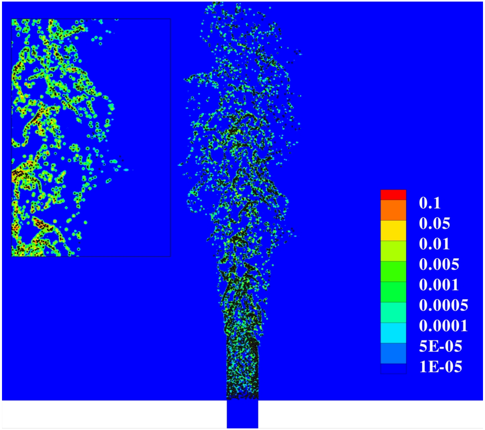


particles & axial velocity

$\Rightarrow$ potential core almost doubled in the two-way regime

Turbulent Jet

particles & feedback on the fluid



- smooth back-reaction at turbulent/laminar interface
  - entrainment
  - evaporation rate in case of liquid droplets

Final remarks

Exact Regularized Point Particle method

- perturbation field due to the particles
  - based on physical arguments ⇒ *Unsteady Stokes Solutions*
  - local ⇒ efficient algorithms
  - smooth ⇒ few particles e.g. *turbulent jets*
- easy to implement
- overcomes several drawbacks of the PIC approach

P.G., F. Picano, G. Sardina, C.M. Casciola J. Phys. Conf. Ser. **318** (2011)

P.G., F. Picano, G. Sardina, C.M. Casciola, submitted to JFM, `http://arxiv.org/abs/1405.6969`

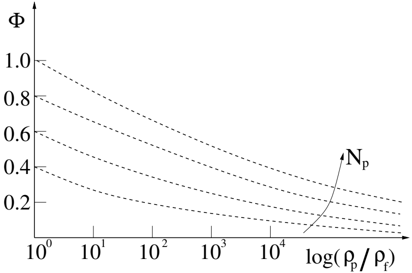
P.G., F. Battista, F. Picano, C.M. Casciola, in preparation

Credits: PRACE-2IP project (FP7 RI-283493)
Cost Action MP0806 *Particles in Turbulence*
ERC grant *BIC*
Nordita

Remarks about the mass load Φ

Six dimensionless parameters $\left\{ Re_0;\ St_\eta;\ \dfrac{\rho_p}{\rho_f};\ \dfrac{d_p}{\eta};\ \Phi;\ N_p \right\}$

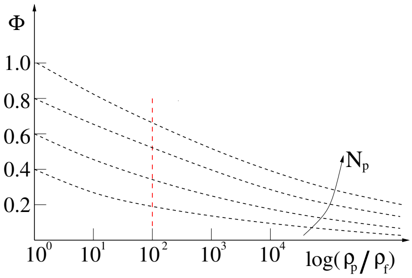
$$St_\eta = \frac{1}{18}\frac{\rho_p}{\rho_f}\left(\frac{d_p}{\eta}\right)^2 \qquad \Phi = 9\sqrt{2}\pi\, N_p\, \frac{St_\eta^{3/2}}{Re_0^{9/4}\ (\rho_p/\rho_f)^{1/2}}$$



Remarks about the mass load Φ

In experiments or numerics fix $\left\{ Re_0;\ St_\eta;\ \dfrac{\rho_p}{\rho_f};\ \dfrac{d_p}{\eta};\ \Phi;\ N_p \right\}$

$$St_\eta = \frac{1}{18}\frac{\rho_p}{\rho_f}\left(\frac{d_p}{\eta}\right)^2 \qquad \Phi = 9\sqrt{2}\pi\, N_p\, \frac{St_\eta^{3/2}}{Re_0^{9/4}\,(\rho_p/\rho_f)^{1/2}}$$



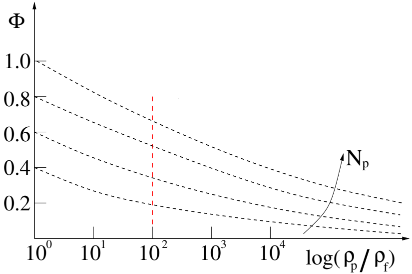
In the ERPP

- smooth perturbation field
- N_p can be modified safely
- *adjust Φ by changing N_p*

Remarks about the mass load Φ

In experiments or numerics fix $\left\{ Re_0;\ St_\eta;\ \frac{\rho_p}{\rho_f};\ \frac{d_p}{\eta};\ \Phi;\ N_p \right\}$

$$St_\eta = \frac{1}{18}\frac{\rho_p}{\rho_f}\left(\frac{d_p}{\eta}\right)^2 \qquad \Phi = 9\sqrt{2}\pi\,\frac{N_p}{N_c}\,\frac{St_\eta^{3/2}}{(\rho_p/\rho_f)^{1/2}}$$



In the PIC

- $N_p/N_c \geq 1$ to achieve a smooth forcing
- $N_c \propto Re_0^{9/4}$ is fixed
- *Φ can not be changed anymore!*