Direct numerical simulations of particles in turbulence Lecture I

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International school
Fluctuations and Turbulence in the
Microphysics and Dynamics of Clouds
Porquerolles, Sep. 2-10, 2010

Distributed
European
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Where innovation starts

Aim & TOC

- **Lecture I**
  - Numerical methods for fluid
  - Numerical methods for particles
- Lecture II
  - Physical modeling
  - Validation
  - iCFDdatabase

Motivation(s)

Eyjafjallajökull eruption

http://earthobservatory.nasa.gov

Volcanic ash over Europe ?

http://upload.wikimedia.org/wikipedia/commons/a/a7/Eyjafjallaj%C3%B6kull_volcanic_ash_17_April_2010.png

Rain Drops, Cloud Droplets, and CCN

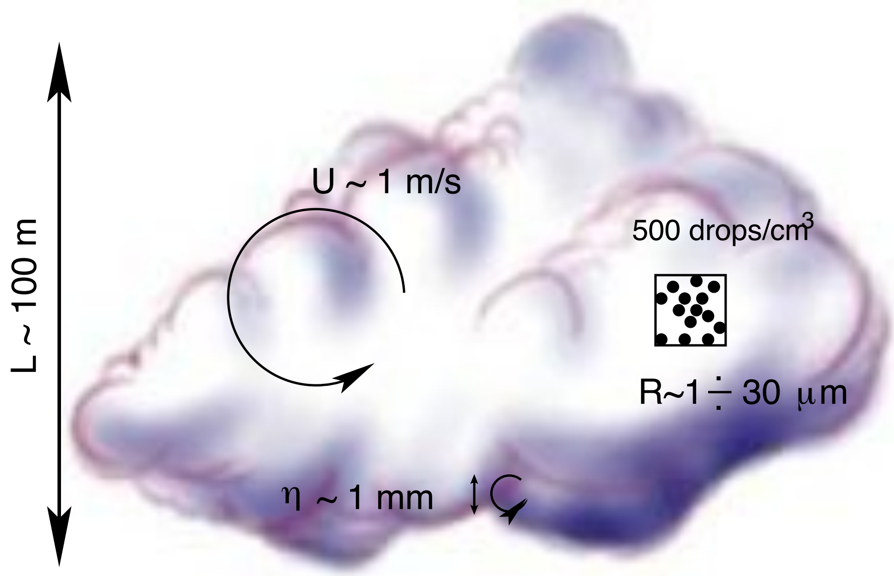
Raind drop size
2mm

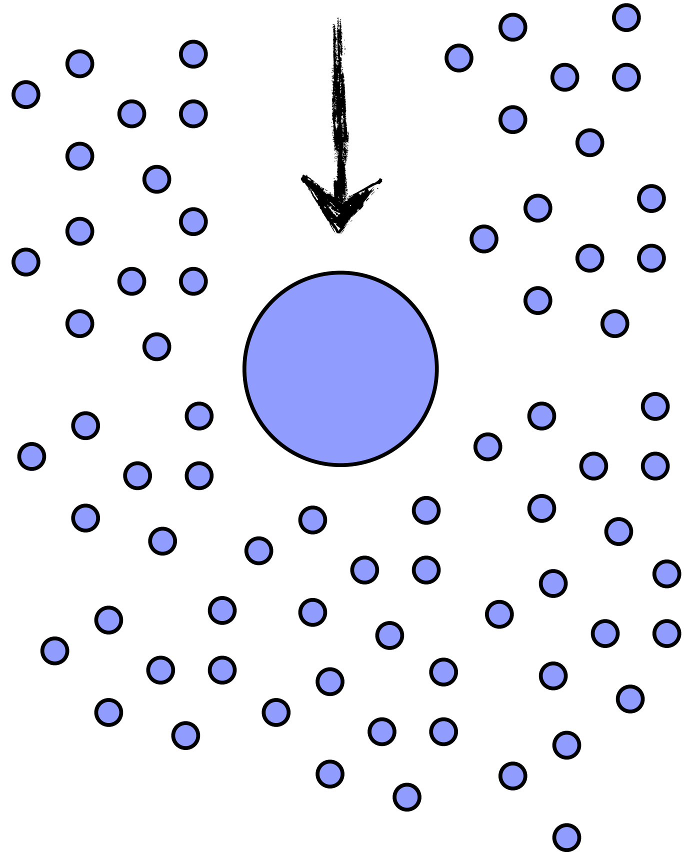
Droplet size
0.02mm

CCN size
2micron

Aerosol particles: 1micron - 0.1mm

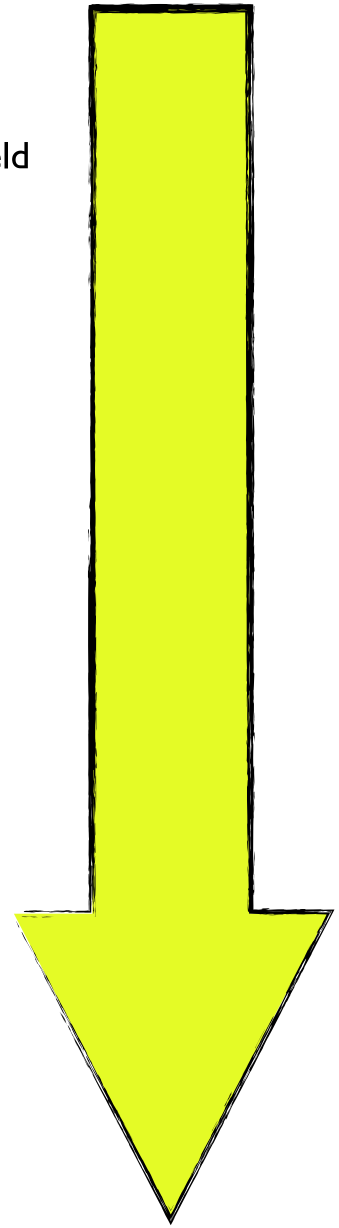
Clouds



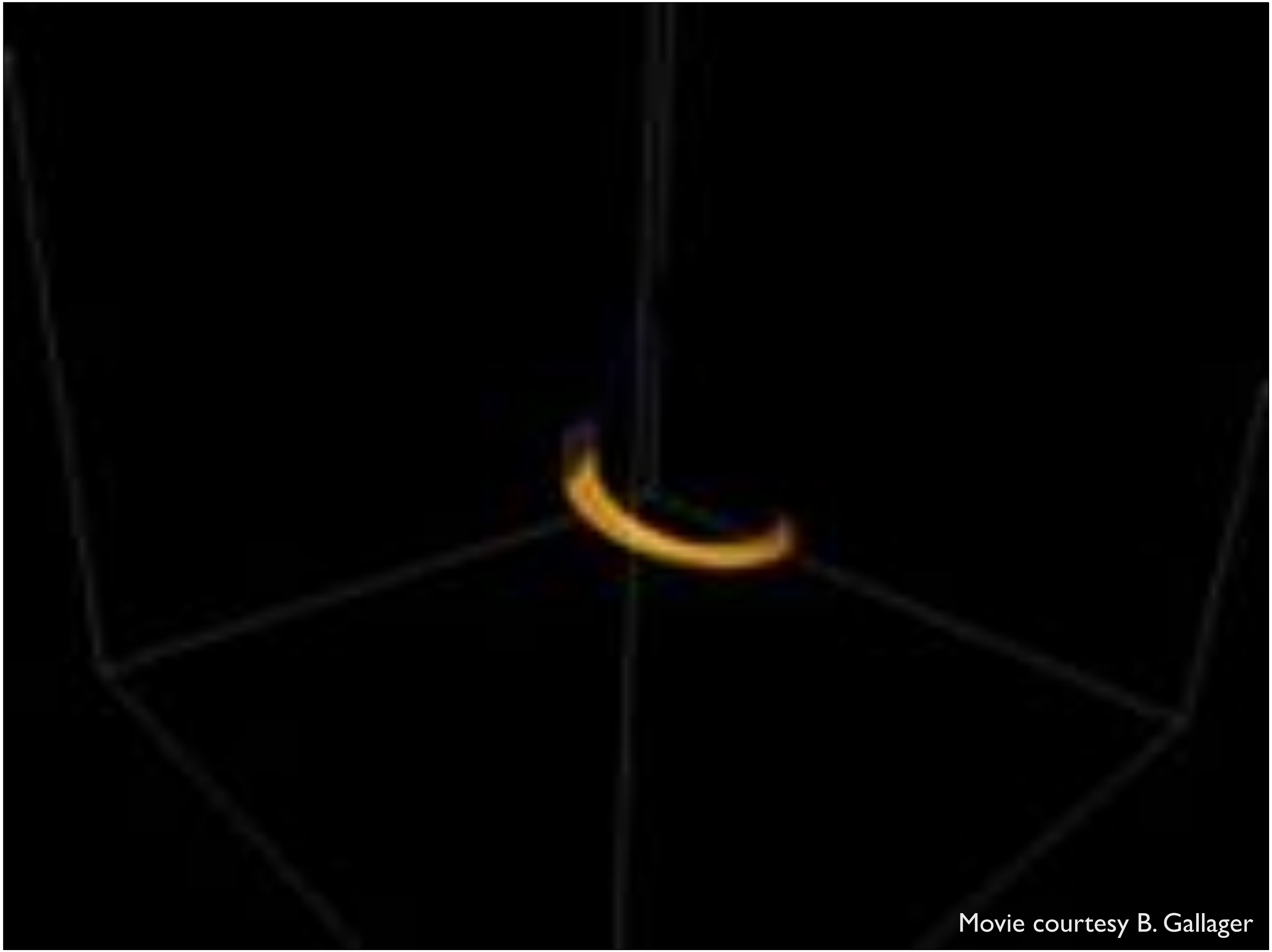


Particles (complications route):

- **Neutrally buoyant case**
  - Smaller that the dissipative scale of turbulence and with same density of advecting field
- **Heavy particle case**
  - Smaller that the dissipative scale of turbulence but with density much higher that advecting field
  - One way coupling
  - Two way coupling
- **Generic density contrast case**
  - One way coupling
  - Two way and four way coupling (collisions)
- **Non idealized particles**
  - Finite particle size, non spherical geometry case
- **Thermal effects** (both stable and unstable conditions)
- **Intrinsic dynamics** ("reaction" i.e.droplet in clouds)
  - Radii growth
  - Coalescence

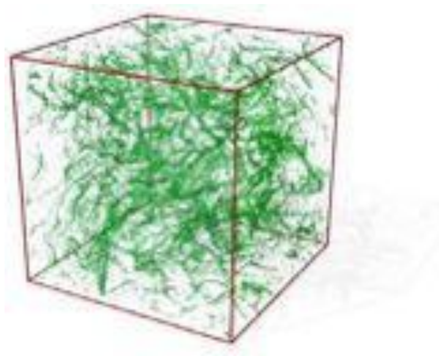


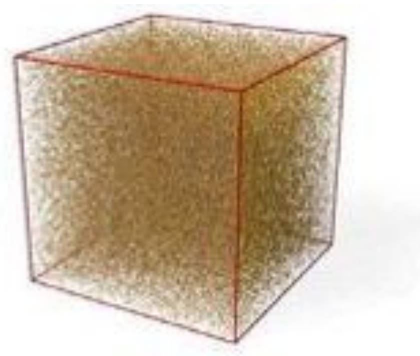
Numerics vs. experiments ?

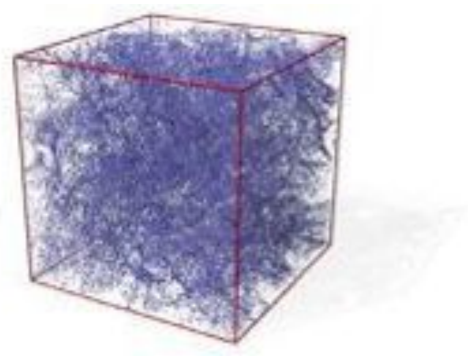

Movie courtesy B. Gallager

Numerical simulations

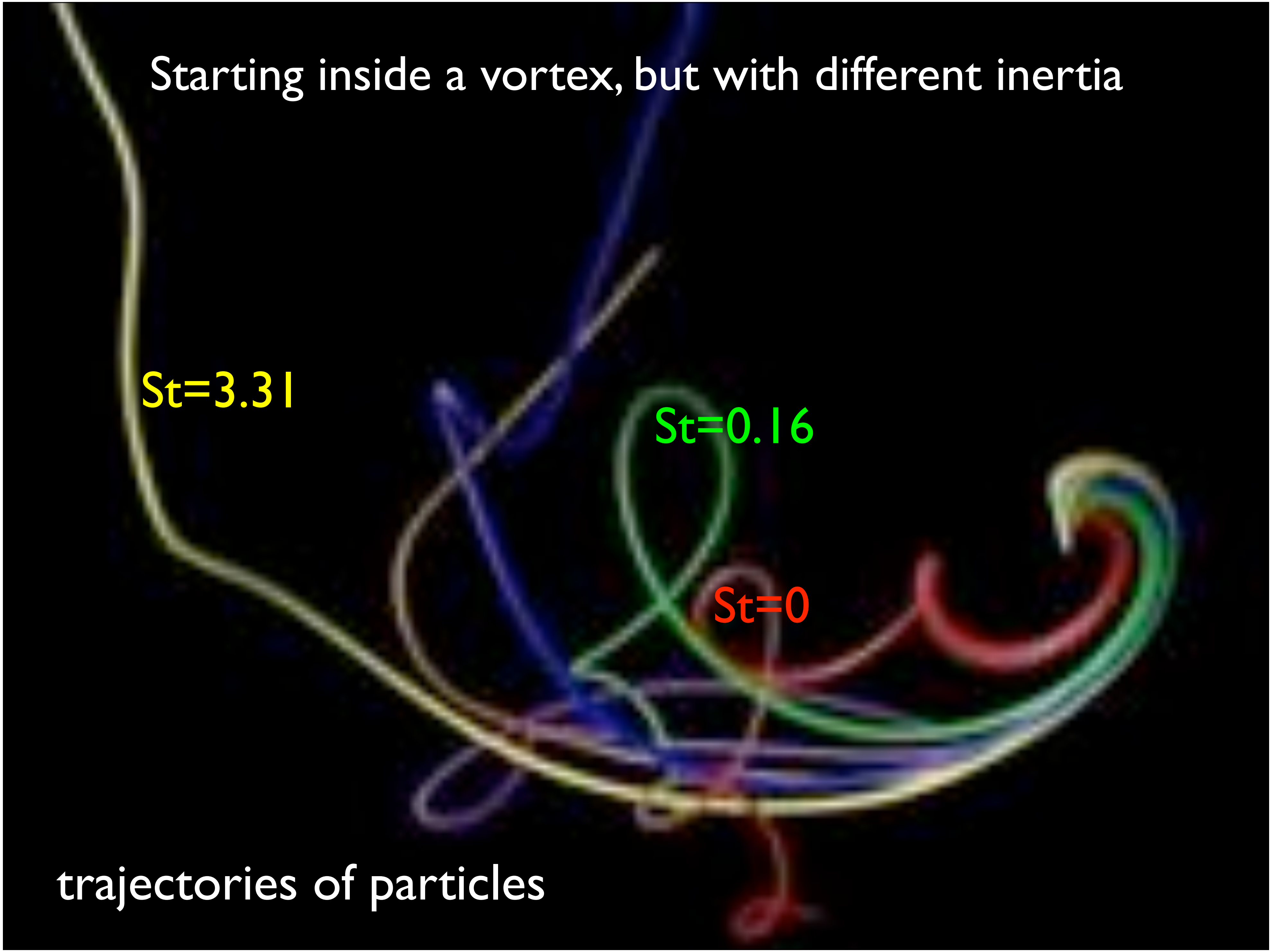
Numerical simulations of particles in turbulence





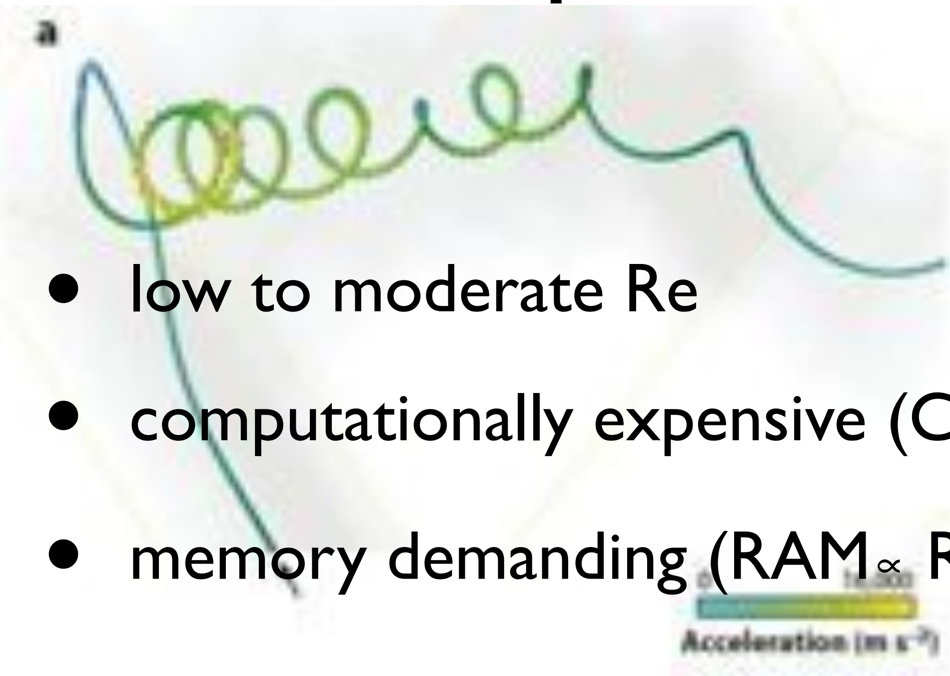


Starting inside a vortex, but with different inertia

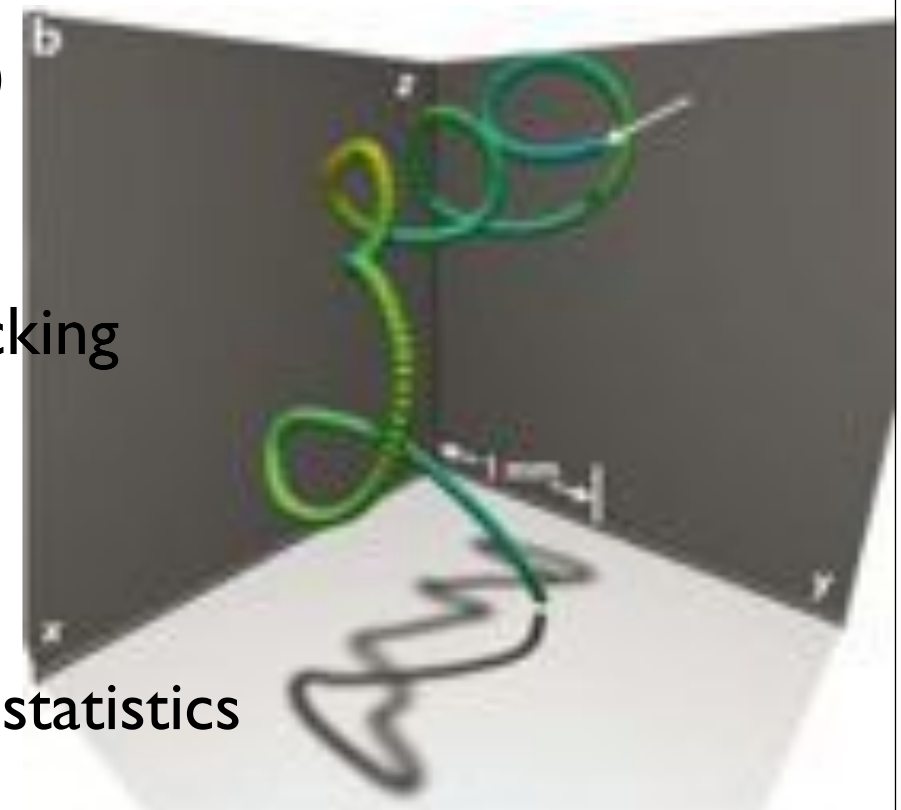


trajectories of particles

More quantitative: EXP vs DNS



- low to moderate Re
- computationally expensive (CPU time $\propto R_\lambda^6$)
- memory demanding (RAM $\propto R_\lambda^{9/2}$)



- high time resolution and long tracking
- large Lagrangian statistics
- multiparticle tracking
- simultaneous Eulerian-Lagrangian statistics

Example of databases

mp0806.cineca.it/icfd.php

iCFDdatabase2

http://mp0806.cineca.it/icfd.php

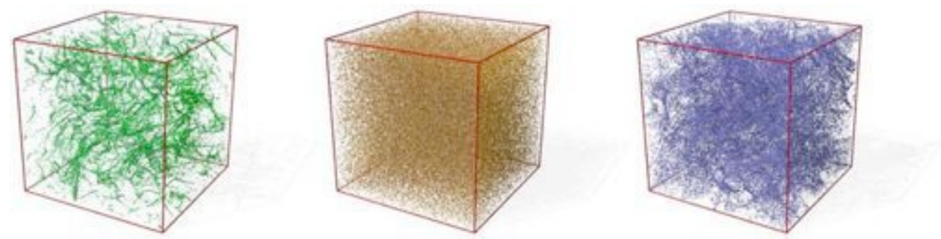
512^3 DNS tracers & heavy & light

N	Re_λ	η	L	T_L	τ_η	T	δx	N_p
512	183	0.01	3.14	2.1	0.048	5	0.012	$1\cdot 10^8$

Pseudo spectral code - dealiased 2/3 rule - normal viscosity - 100 millions of passive tracers & heavy/light particles- code fully parallelized with MPI+FFTW - Platform IBM SP5 1.9 GHz - 30000 cpu hours - duration of the run: 30 days.

64 different particles classes (ß,St)

bubble tracer heavy

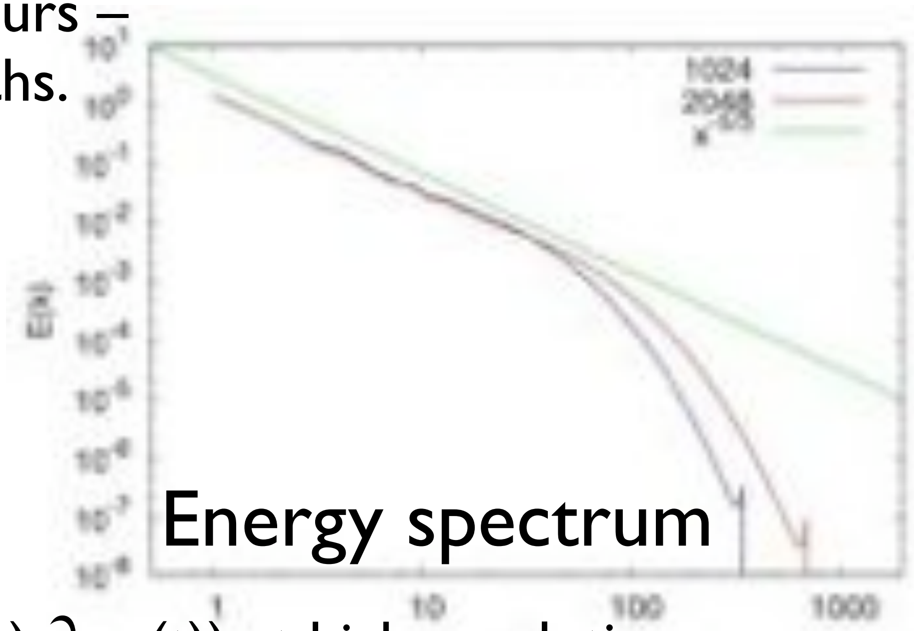


Lagrangian database $(x(t), v(t), u(t), \partial_i u_j\,(t))$ at high resolution

2048^3 DNS with tracers & heavy

N	Re_λ	η	L	T_L	τ_η	T	δx	N_p
2048	400	0.0025	3.14	1.8	0.02	5.9	0.003	$2\cdot 10^9$

Pseudo spectral code - dealiased 2/3 rule - normal viscosity - 2 billions of passive tracers & heavy particles- code fully parallelized with MPI+FFTW - Platform SGI Altix 4700 - 400000 cpu hours – duration of the run: 40 days over 3 months.

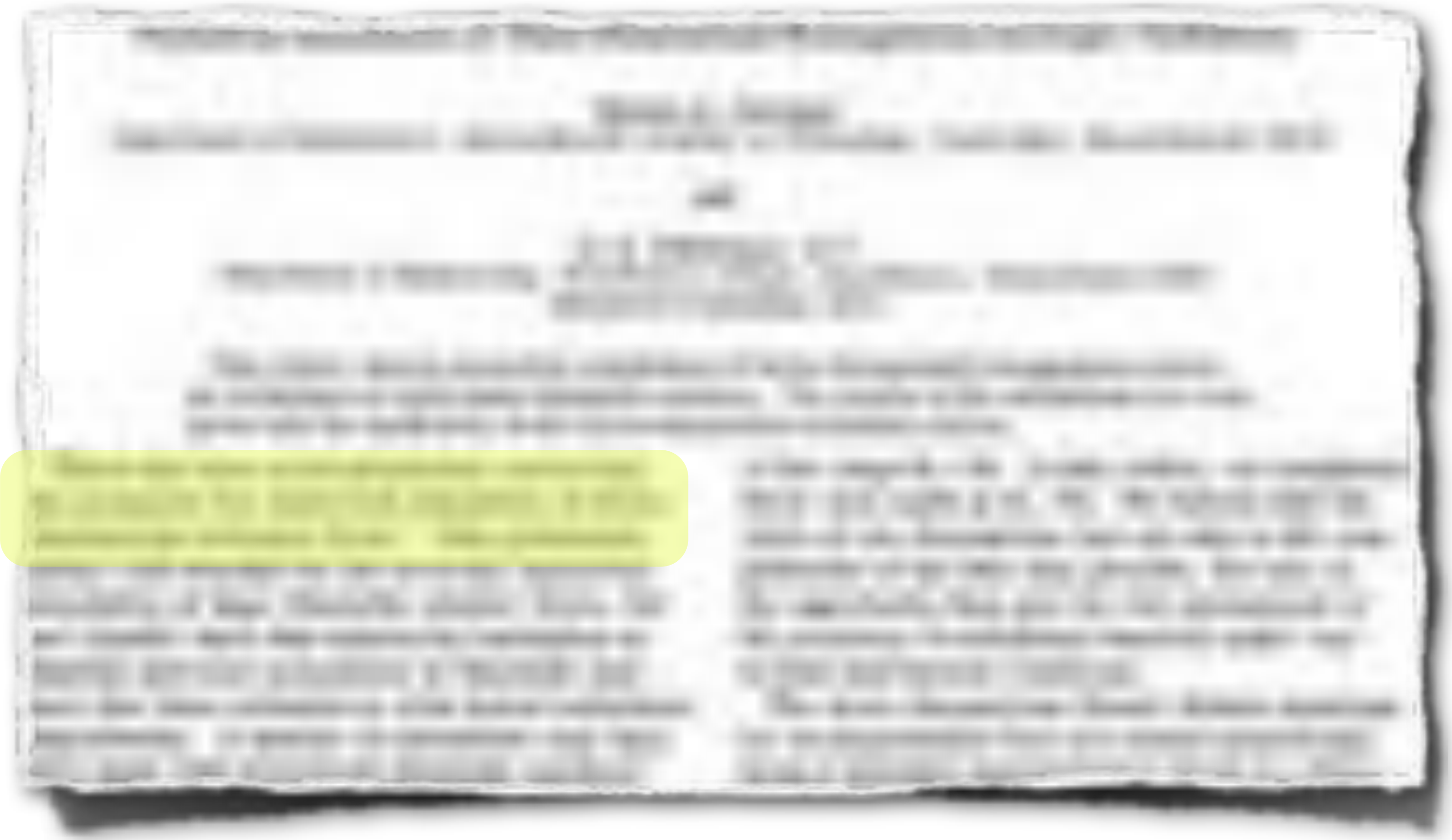


Lagrangian database $(x(t),v(t),u(t),\partial_i u_j\ (t))$ at high resolution

Few words about the past...

... to learn about the future !

Numerical simulations



- Orszag and Patterson. Numerical Simulation of Three-Dimensional Homogeneous Isotropic Turbulence. Physical review letters (1972) vol. 28 (2) pp. 76-79

The cost of computing

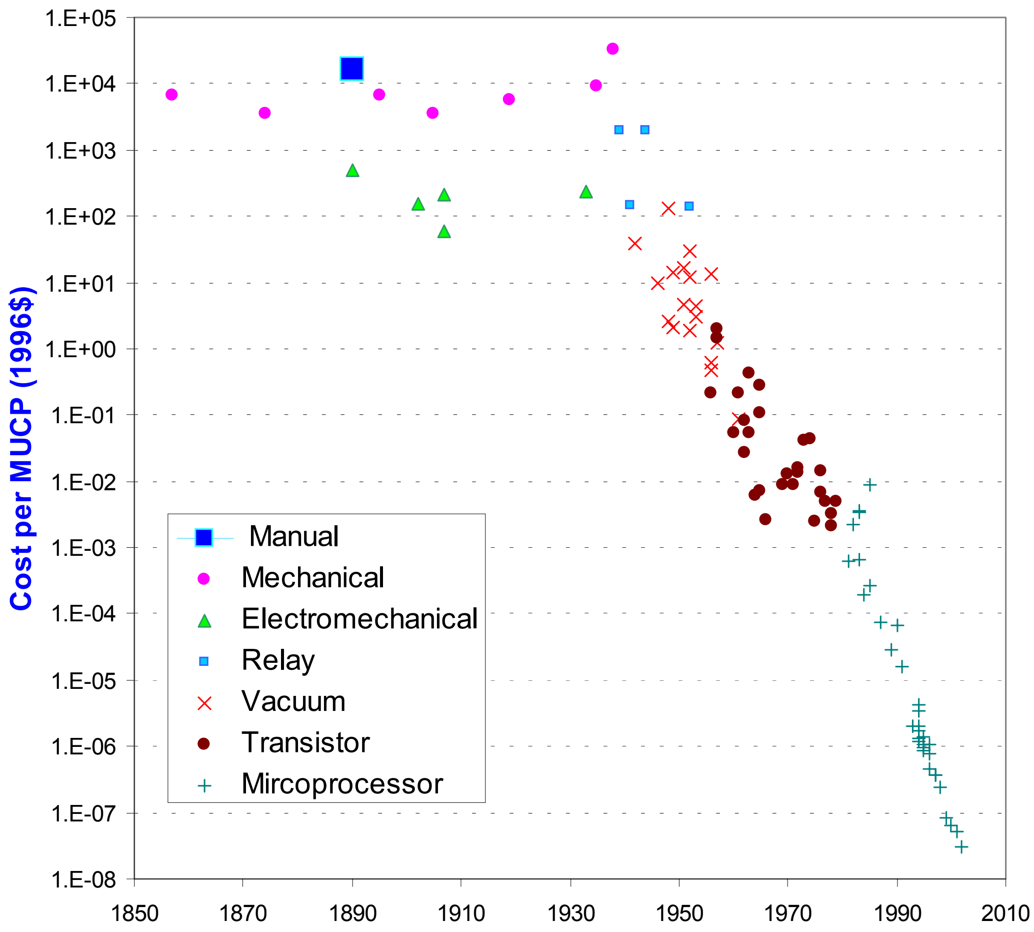


Figure 2. **The cost of computer power for different technologies**

Nordhaus. The Progress of Computing. SSRN eLibrary (2001)

Performance development

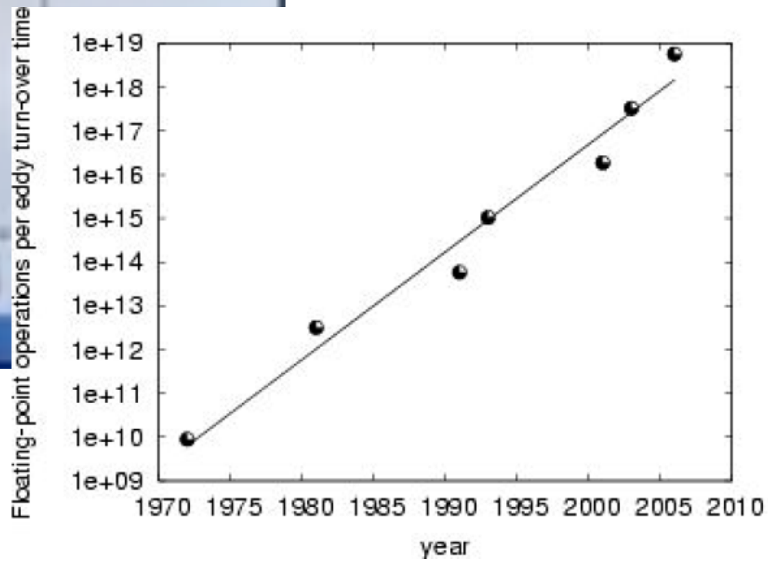


Figure 4. The number of floating-point operations performed for the computation of one eddy turn-over-time $\propto N^4 \log_2 N$. The solid line is the least-squares fit $\propto 2^{year/1.25}$.

Celani. The frontiers of computing in turbulence: challenges and perspectives. J Turbul (2007) vol. 8 pp. N34

State-of-the-art vs. year

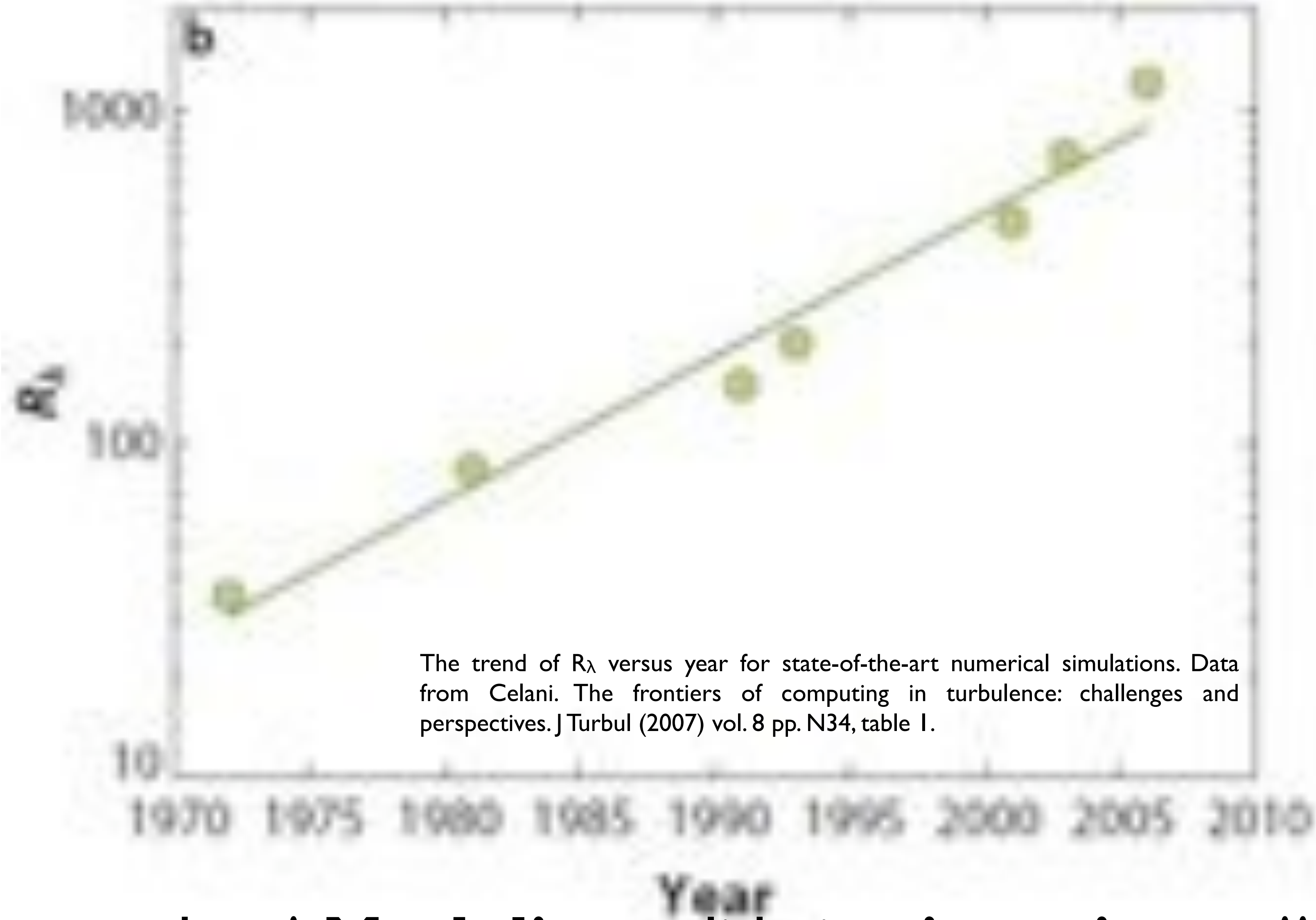
The frontiers of computing in turbulence: challenges and perspectives 5

Table 1. Progress in computing homogeneous isotropic turbulence

Year	N	R_λ	Reference
1972	32	35	Orszag & Patterson, Phys. Rev. Lett. **28**, 76
1981	128	84	Rogallo, NASA Report 1981, Phys. Rev. Lett. **58**, 547
1991	256	150	Vincent & Meneguzzi, J. Fluid Mech. **25**, 1; Sanada, Phys. Rev. A **44**, 6480
1993	512	200	She *et al*., Phys. Rev. Lett. **70**, 3251
2001	1024	460	Gotoh & Fukuyama, Phys. Rev. Lett. **86**, 3775
2003	2048	730	Kaneda *et al*., Phys. Fluids **15** L21
2006	4096	1200	Kaneda & Ishihara, J. of Turb. **7**, N20

Celani. The frontiers of computing in turbulence: challenges and perspectives. J Turbul (2007) vol. 8 pp. N34

Scale up of DNS (promising !)



The trend of R_λ versus year for state-of-the-art numerical simulations. Data from Celani. The frontiers of computing in turbulence: challenges and perspectives. J Turbul (2007) vol. 8 pp. N34, table 1.

...but ! **Modeling** validation **is an issue** !!

Celani. The frontiers of computing in turbulence: challenges and perspectives. J Turbul (2007) vol. 8 pp. N34

Bigger computers are important

www.top500.org

but green computers are better...

Green500 Rank	MFLOPS/W	Site*	Computer*	Total Power (kW)
[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
[illegible]	[illegible]	[illegible]	[illegible]	[illegible]

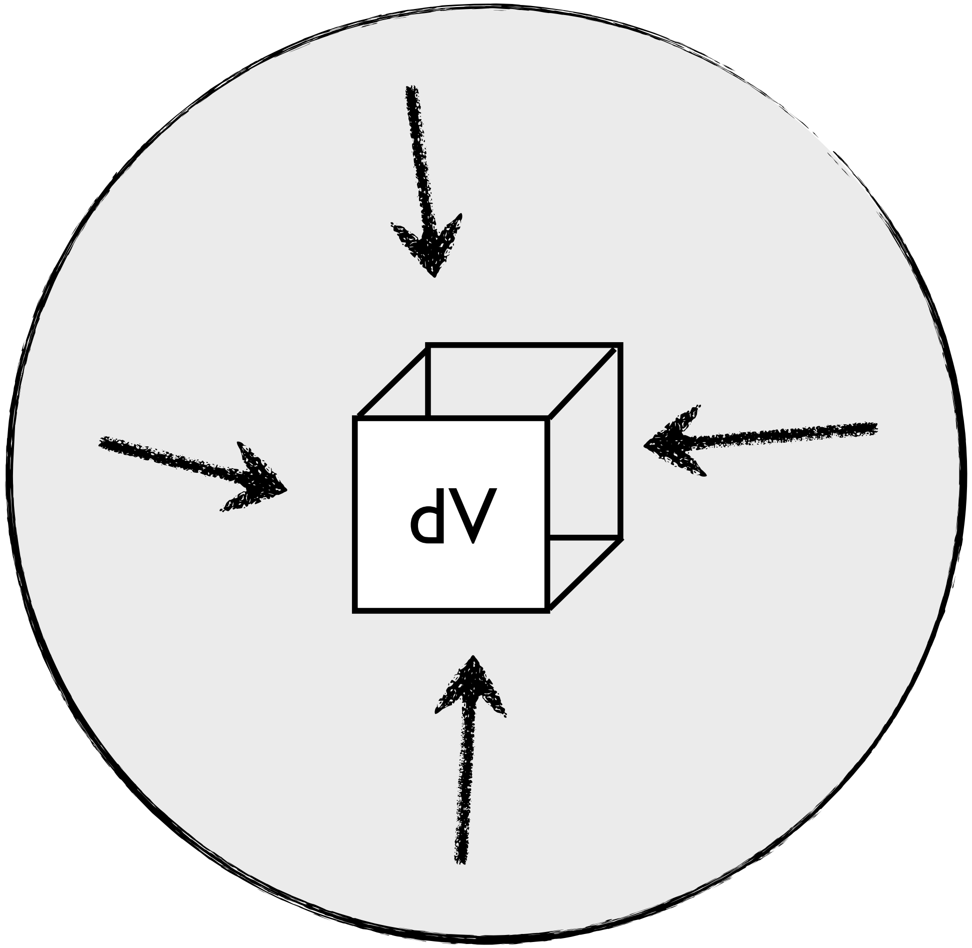
http://www.green500.org/

Equation of motion for a viscous fluid

$$\boldsymbol{F} = m\boldsymbol{a}$$

Internal forces

External forces

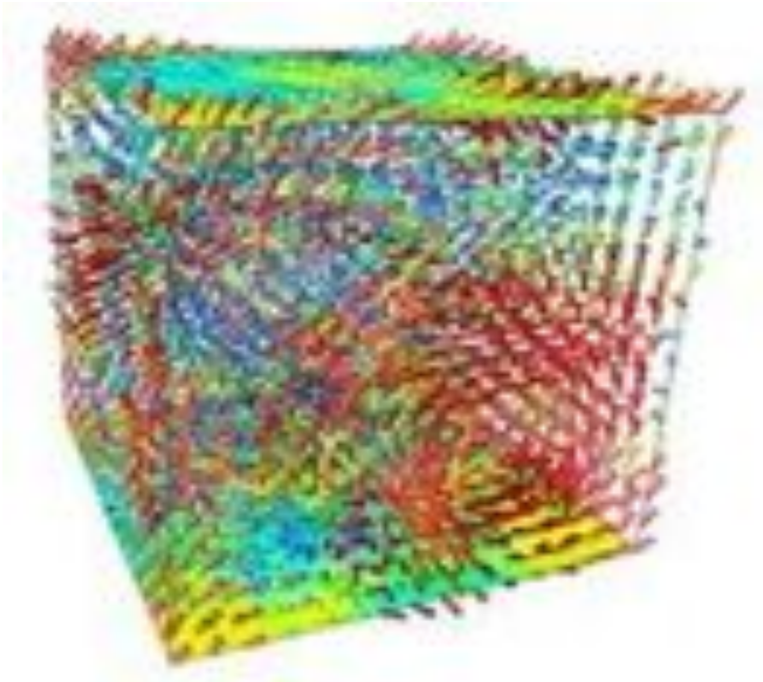


Equation of motion for a viscous fluid

$$m\mathbf{a} = \boldsymbol{f}$$

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

$$\frac{D\boldsymbol{u}}{Dt}$$



$$\boldsymbol{u}_L(t|\boldsymbol{x}_0, t_0) \equiv \boldsymbol{u}_E(\boldsymbol{x}(t|x_0, t_0), t)$$

$$\frac{d\boldsymbol{u}_L}{dt}(t|\boldsymbol{x}_0, t_0) \equiv \frac{d\boldsymbol{u}_E(\boldsymbol{x}(t|x_0, t_0), t)}{dt} = \frac{\partial \mathbf{u}_E}{\partial t} + \mathbf{u}_E \cdot \nabla \mathbf{u}_E$$

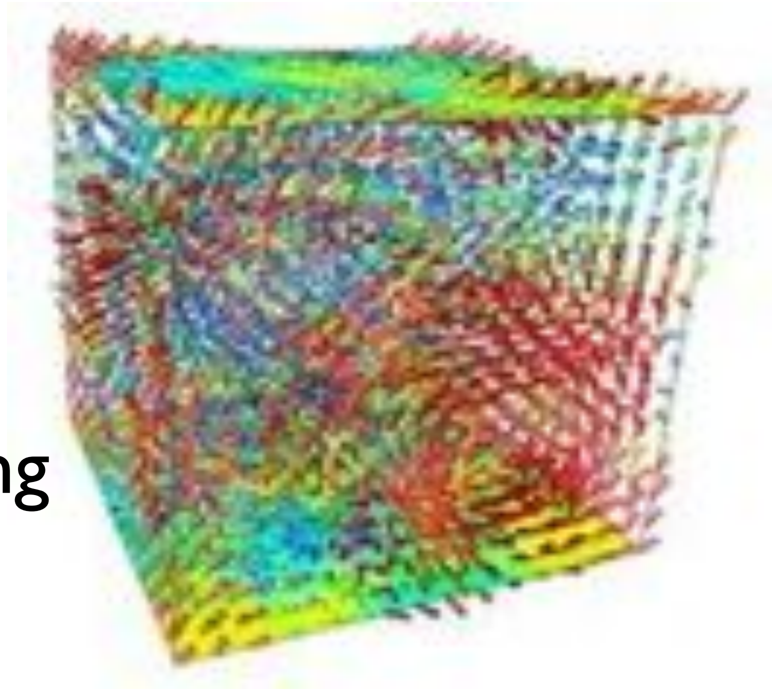
$$\nabla \cdot \mathbf{u} = 0$$

Equation of motion for a viscous fluid

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

Pressure is a Lagrangian multiplier to impose zero divergence

$$\nabla \cdot \mathbf{u} = 0$$



Pressure is computationally annoying as it propagate with infinite speed (all-to-all communication)

Equations for turbulence

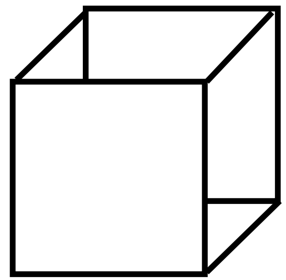
Whatever the geometry, some forcing must be present to inject energy in the (otherwise purely dissipative) system

$$m\mathbf{a} = \boldsymbol{f}$$

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = -\frac{1}{\rho} \nabla p + \nu \nabla^2 \mathbf{u} + \boldsymbol{f}(\boldsymbol{x}, t)$$

$$\nabla \cdot \mathbf{u} = 0$$

dV

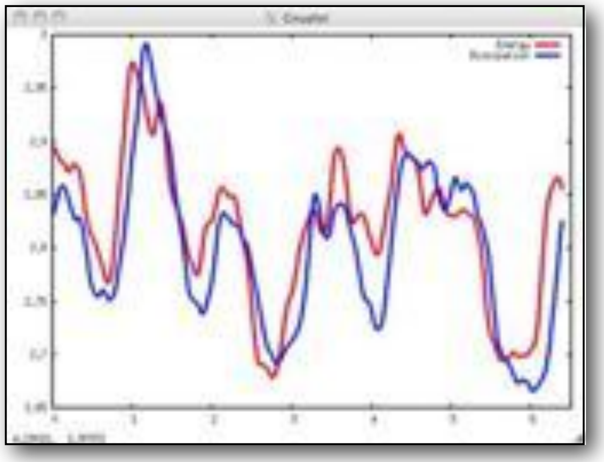


Stationary state

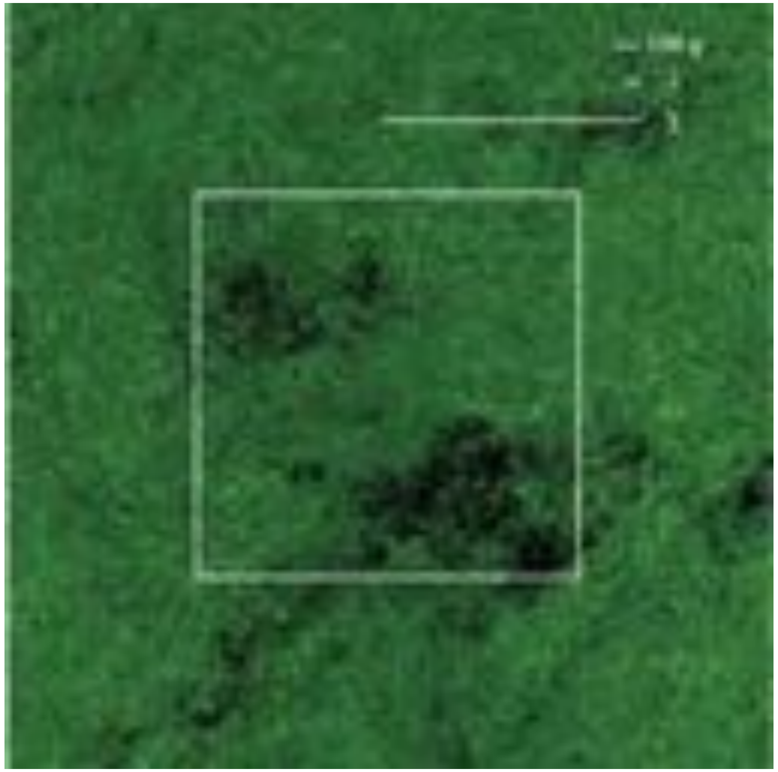
$\langle \boldsymbol{f} \cdot \boldsymbol{u} \rangle$

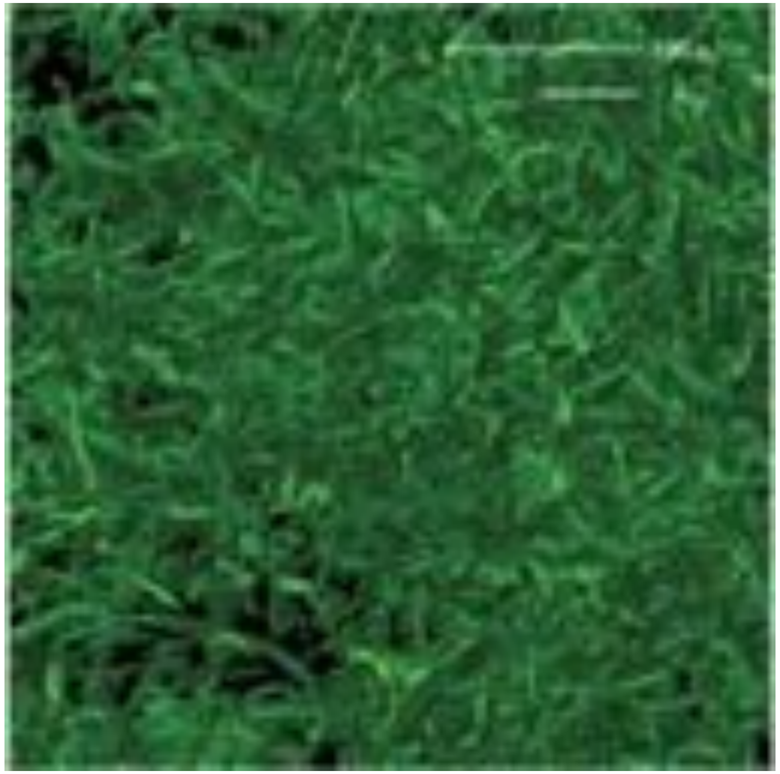
inertial range

$\nu \langle \boldsymbol{u} \cdot \Delta \boldsymbol{u} \rangle$



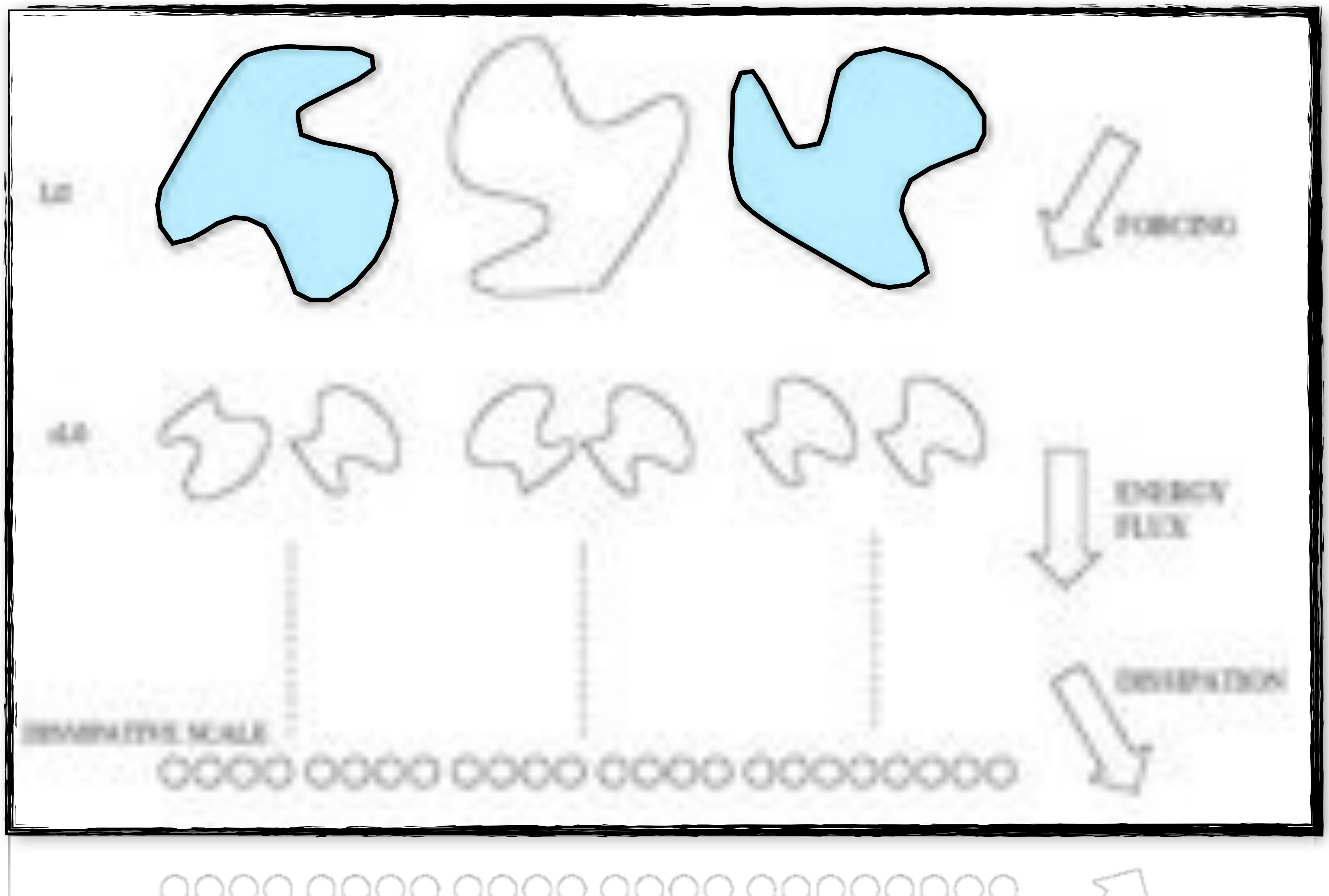
Vortex filament





Ishihara et al. Small-scale statistics in high-resolution direct numerical simulation of turbulence: Reynolds number dependence of one-point velocity gradient statistics. J Fluid Mech (2007) vol. 592 pp. 335-366

K41 in a nutshell and its computational consequences



Eulerian turbulence

$$\partial_t \boldsymbol{v} + \boldsymbol{v} \cdot \nabla \boldsymbol{v} = -\nabla p + \nu \Delta \boldsymbol{v} + \boldsymbol{f}$$

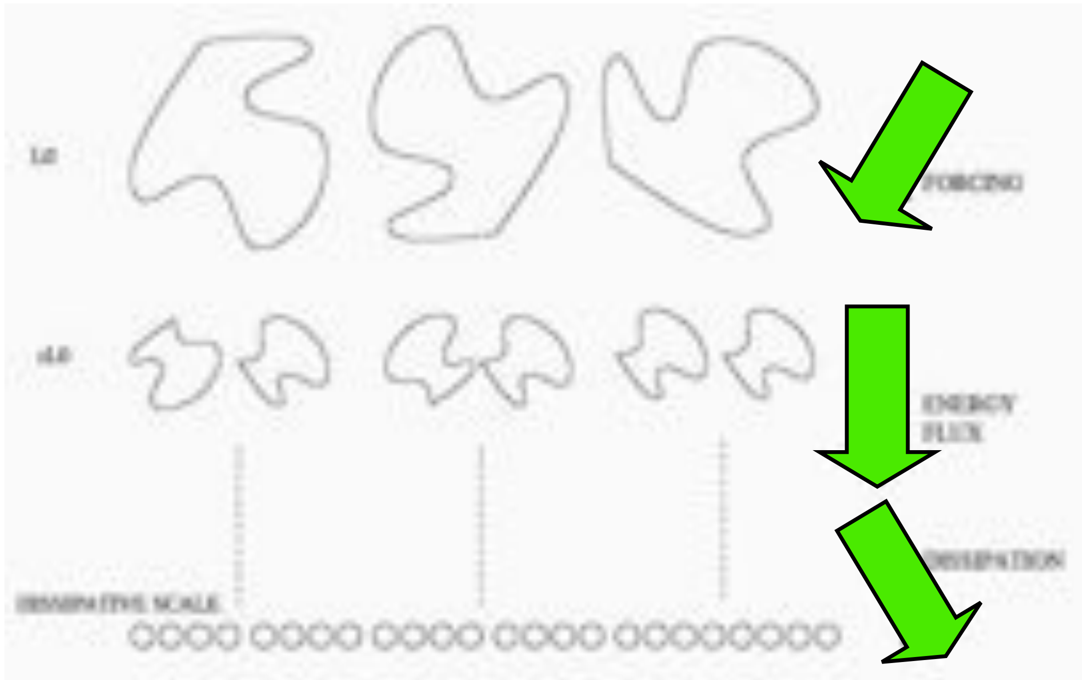
$$\partial \cdot \boldsymbol{v} = 0$$

$$Re = \frac{L_0 v}{\nu}$$

$$\eta \ll r \ll L_0$$

Inertial range

Energy flux



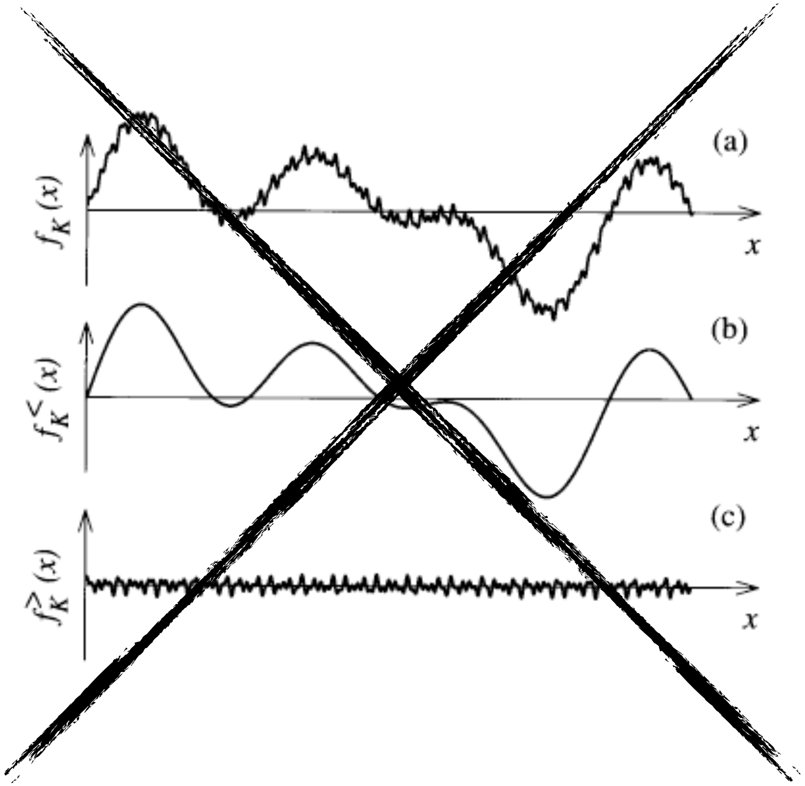
$$\eta = (\nu^3/\varepsilon)^{1/4} \quad \tau_\eta = (\nu/\varepsilon)^{1/2}$$

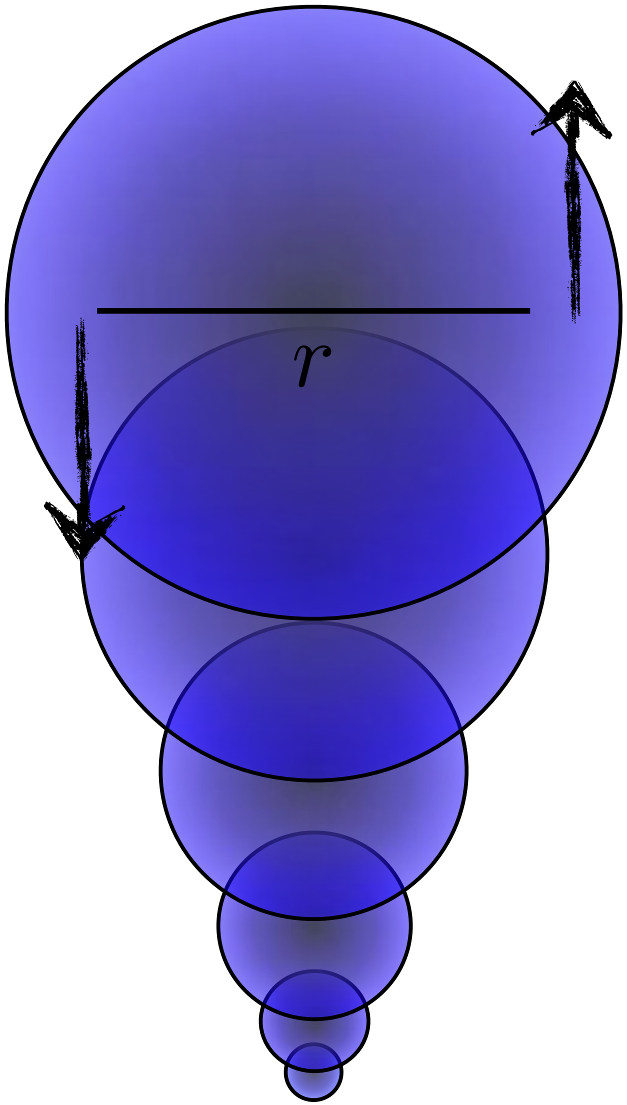
Phenomenology of K41

- Remember: Goal is to **study** computationally the **universal properties** of fluid dynamic turbulence
- Theoretically it is expected that for large enough ***Re*** numbers an inertial range develop
- The **inertial range** is expected to be **universal**, i.e. independent from the forcing (and dissipation?) mechanisms
- Computationally: need to separate the forced range and dissipative scales as much as possible !

Time scales in turbulence

$$\tau(r) = \frac{r}{\delta u(r)}$$





Eddy turnover times

K41 in a nutshell and its computational consequences

Mean field model for fluid-dynamics turbulence

$$\langle \delta u^3(r) \rangle = -\frac{4}{5}\varepsilon \cdot r$$

$$Re(r) = \frac{\delta u(r) \cdot r}{\nu} \xrightarrow{\text{K41}} 1 = \frac{\eta^{4/3}\varepsilon^{1/3}}{\nu}$$

$$\eta = \left(\frac{\nu^3}{\varepsilon}\right)^{1/4}$$

Reynolds number and all that

Reynolds number $$Re = \frac{u \cdot L}{\nu}$$

Taylor's Reynolds number $$R_\lambda \equiv \frac{u_{rms}\lambda}{\nu}$$

Taylor scale $$\frac{1}{\lambda^2} \equiv \frac{\langle(\partial_1 u_1)^2\rangle}{u_{rms}^2}$$

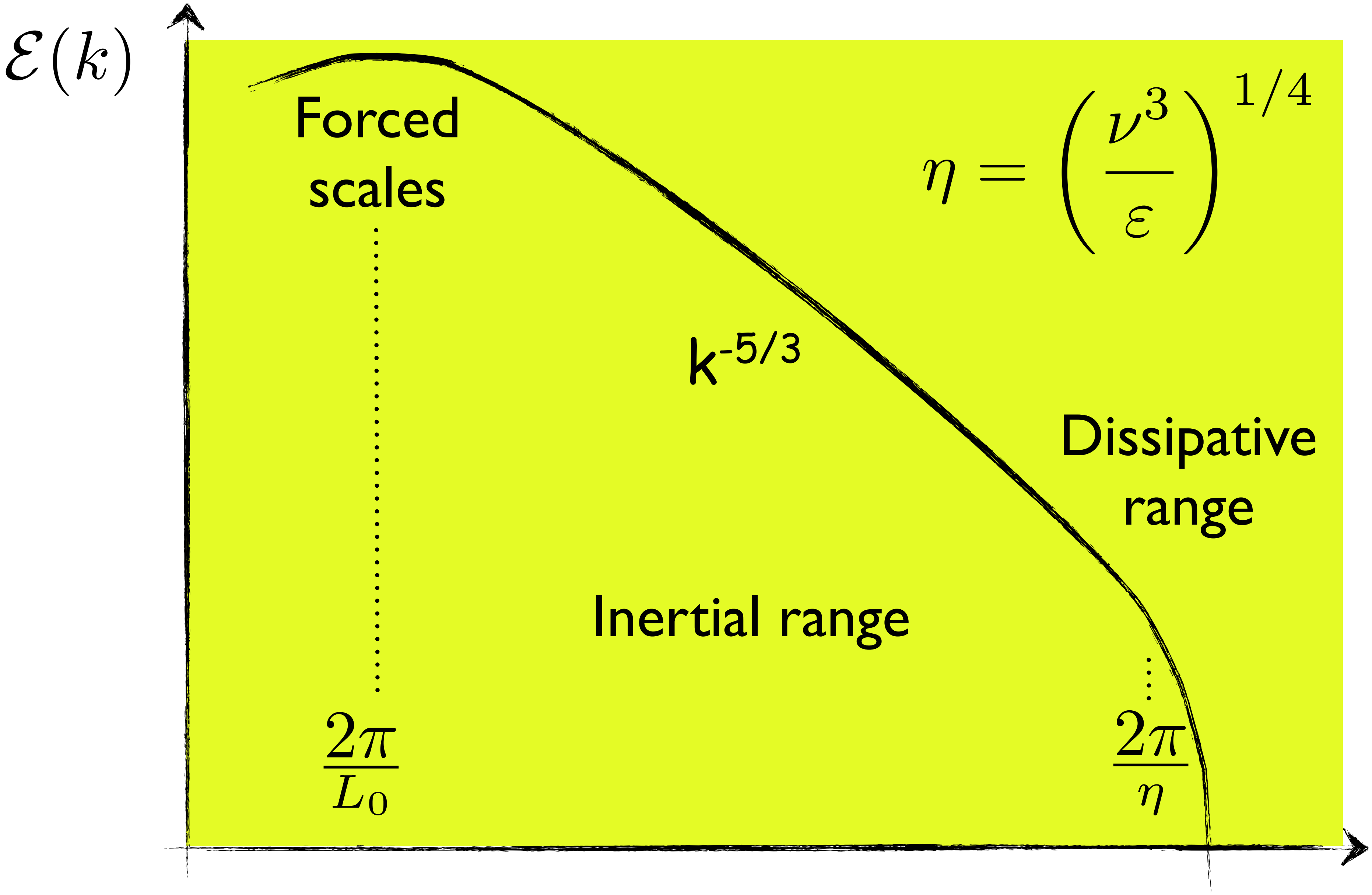
$$Re(r) = \frac{\delta u(r) \cdot r}{\nu} \longrightarrow 1 = \frac{\eta^{4/3}\varepsilon^{1/3}}{\nu}$$

Dimensional estimate for end of the cascade

dissipative or Kolmogorov scale

$$\eta = \left(\frac{\nu^3}{\varepsilon}\right)^{1/4}$$

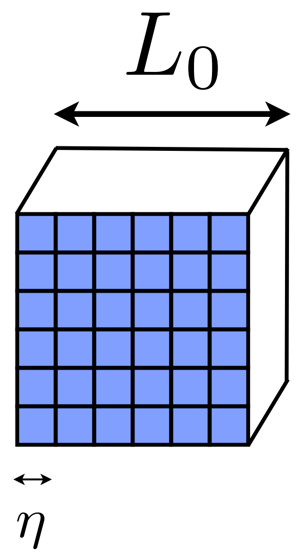
Length scales in turbulence



Computational cost

$$\eta = \left(\frac{\nu^3}{\varepsilon}\right)^{1/4} \qquad \frac{L_0}{\eta} \sim Re^{3/4}$$

$$N \equiv \left(\frac{L_0}{\eta}\right)^3 \sim Re^{9/4}$$

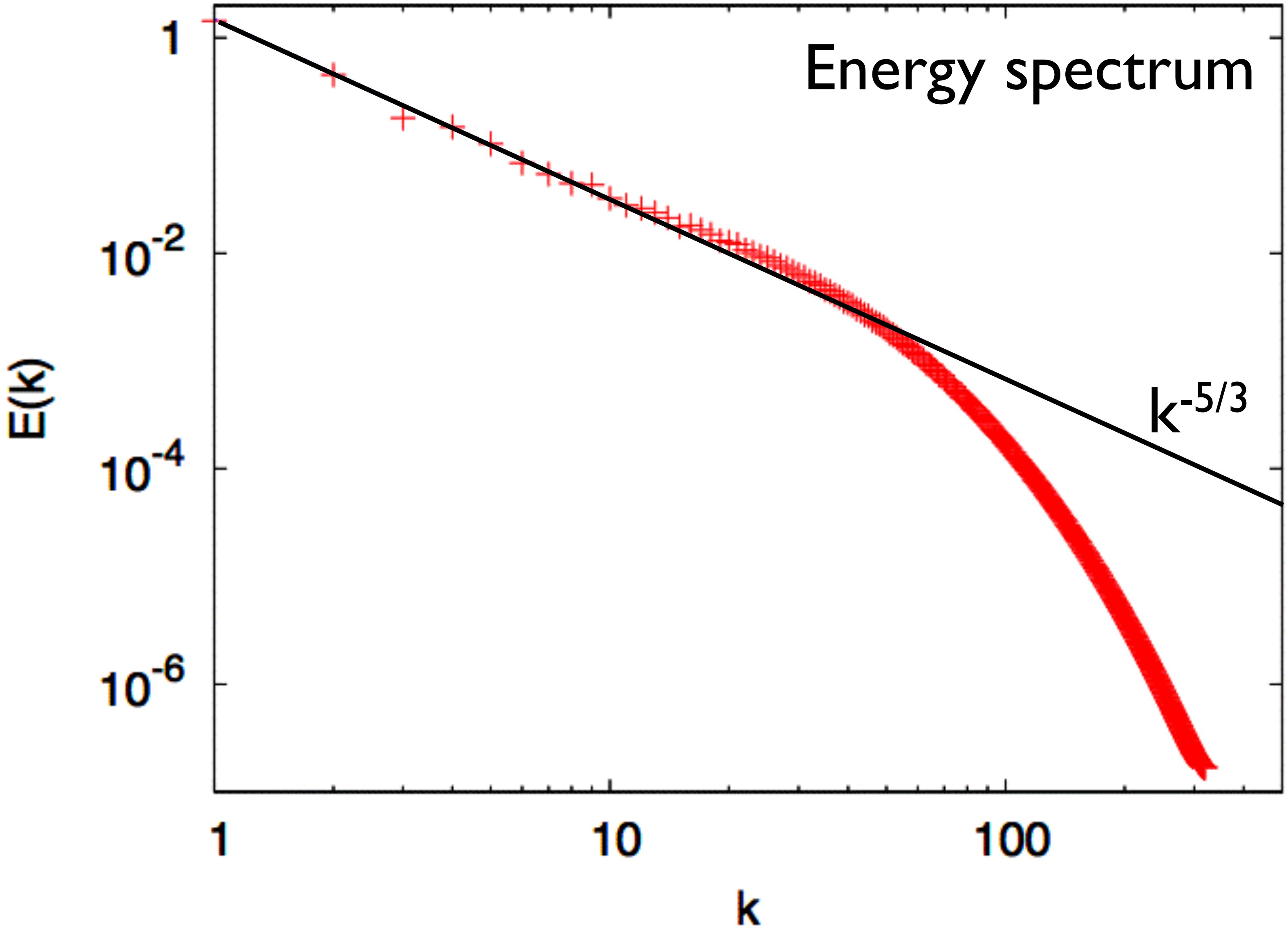


$$flops \propto \left(\frac{L_0}{\eta}\right)^3 \frac{T_0}{dt} \sim Re^3$$

These degrees of freedom are all necessary !

They all constitute the physics of the inertial range

Energy spectrum

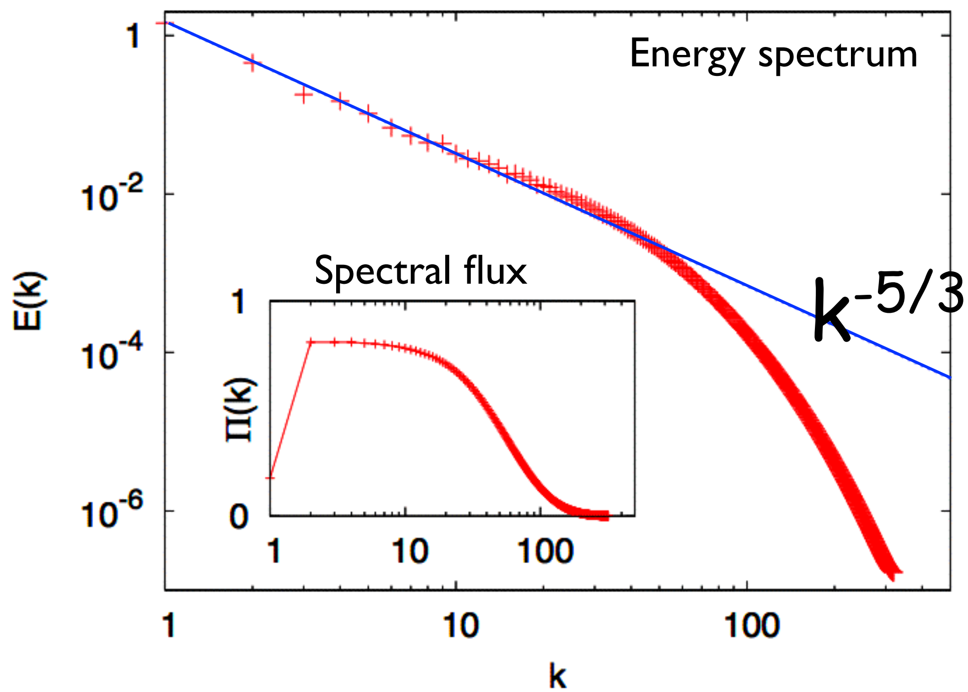


512^3 & 1024^3 DNS+tracers

N	Re_λ	η	L	T_L	τ_η	T	δx	N_p
512	183	0.01	3.14	2.1	0.048	5	0.012	$0.96\ 10^6$
1024	284	0.005	3.14	1.8	0.033	4.4	0.006	$1.92\ 10^6$

Pseudo spectral code - dealiased 2/3 rule - normal viscosity - 2 millions of passive tracers- code fully parallelized with MPI+FFTW - Platform IBM SP4 (sust. Performance 150Mflops/proc) - 50000 cpu hours - duration of the run: 40 days

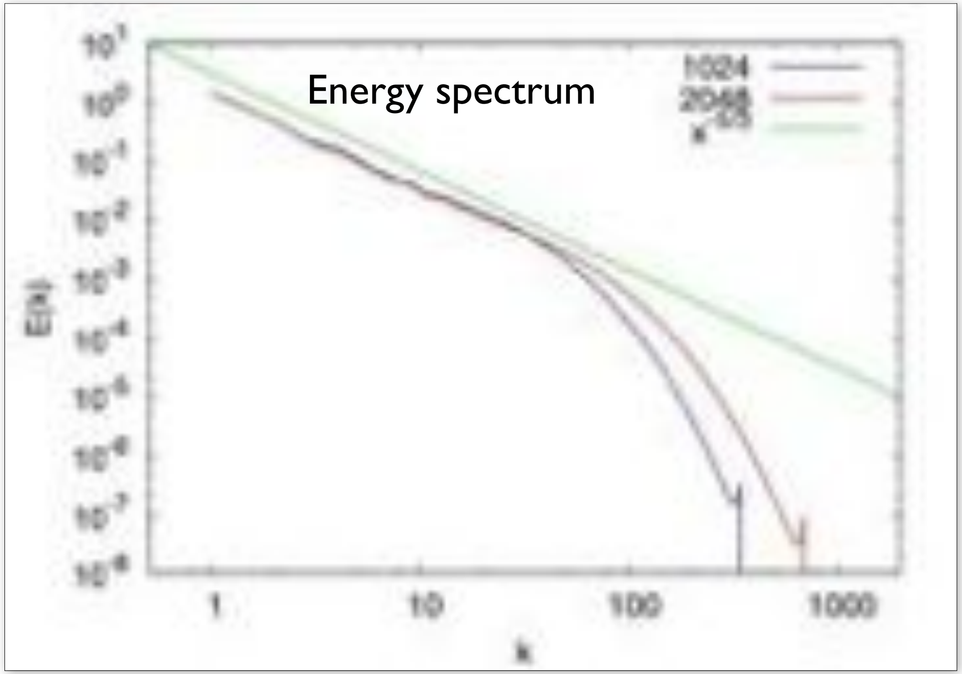
Lagrangian database
$(x(t),v(t),a(t)=-\nabla p+\nu\Delta u)$
with high temporal resolution



2048^3 DNS with tracers & heavy

N	Re_λ	η	L	T_L	τ_η	T	δx	N_p
2048	400	0.0025	3.14	1.8	0.02	5.9	0.003	$2\ 10^9$

Pseudo spectral code - dealiased [illegible] - normal viscosity - 2 billions of passive tracers & heavy particles- code fully parallelized with MPI+FFTW - Platform SGI Altix 4700 - 400000 cpu hours - duration of the run: 40 days over 3 months.



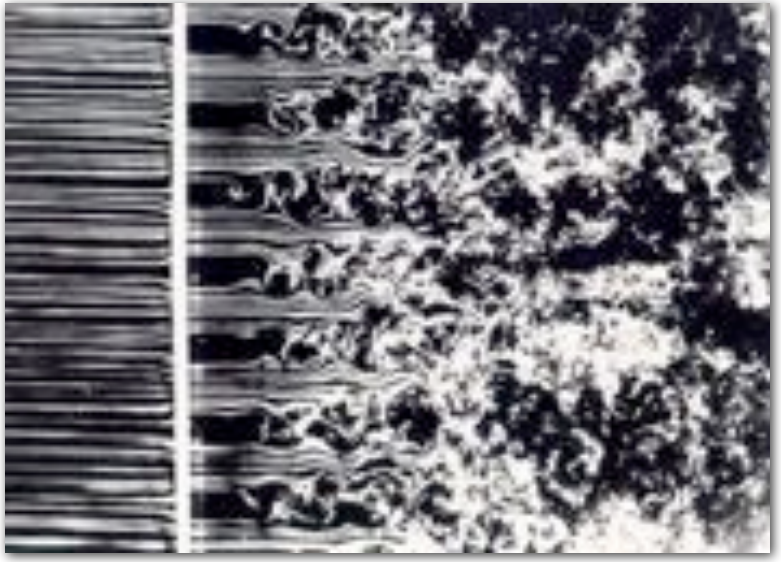
Lagrangian database $(x(t), v(t), u(t), \partial_i u_j (t))$ at high resolution

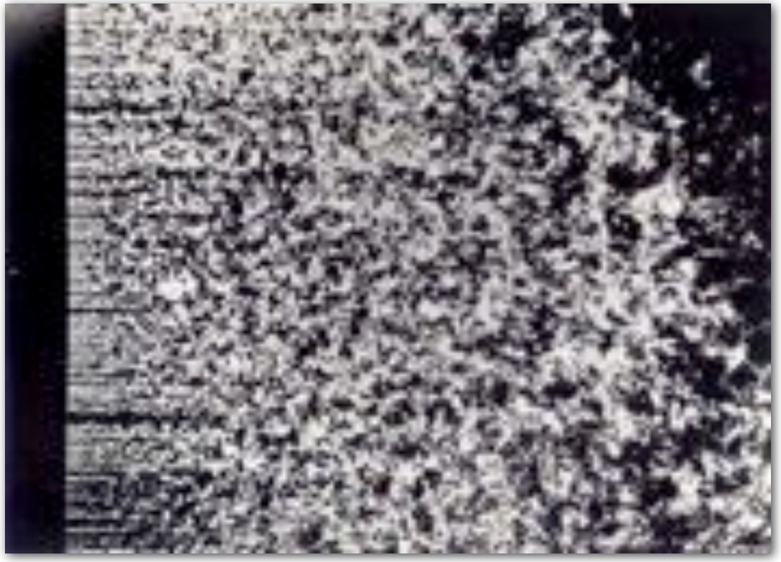
Non homogeneous systems ?

- In non homogeneous system the situation **may be better**. Large volume may have smaller Re numbers.
- However to exploit such computational saving, the numeric methods is more involved and expensive than spectral methods.
- Technical problem(s):
  - grid refinement...
  - adaptive grid refinement...

Fully developed turbulence

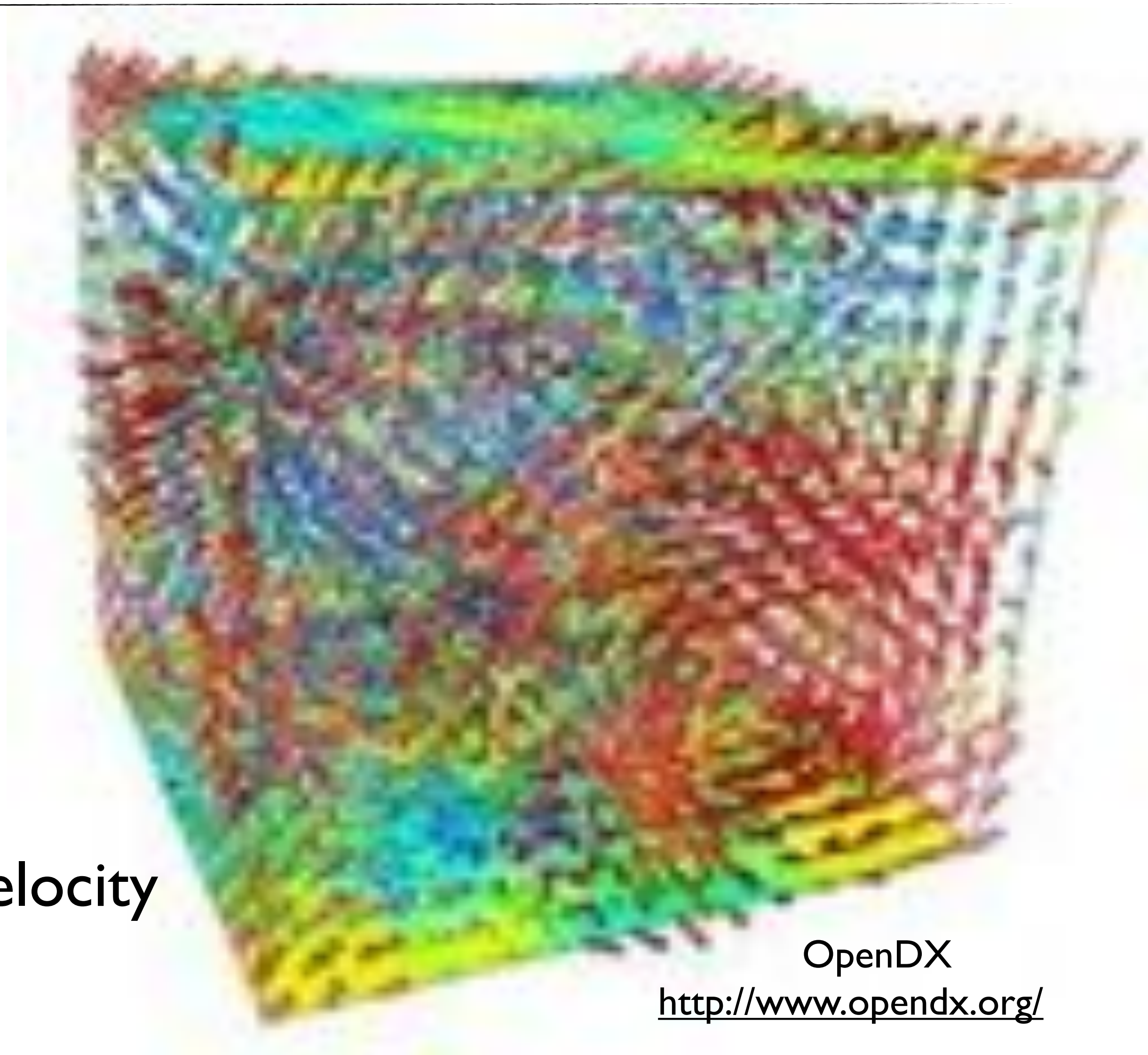
- What is the **conceptually simplest** instance of **turbulent flow** ? Homogeneous and Isotropic !
- **Fully developed**: all symmetries of the problem are recovered in statistical sense





http://fdrc.iit.edu/research/nagibResearch.php

Definitions



OpenDX
http://www.opendx.org/

- u(x,t) Eulerian fluid velocity
- p(x,t) Pressure field
- v(t) Lagrangian velocity of a particle at time t

Eulerian vs. Lagrangian description

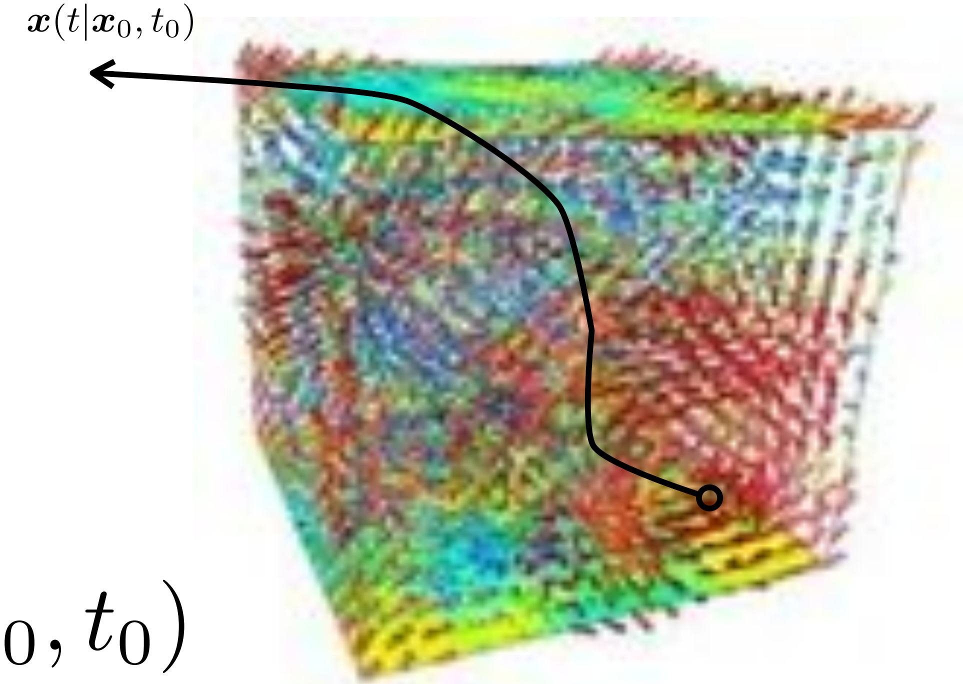
Particle position $\boldsymbol{x}(t|\boldsymbol{x}_0, t_0)$

Lagrangian velocity field $\boldsymbol{u}_L(t|\boldsymbol{x}_0, t_0)$

$$\frac{d\boldsymbol{x}}{dt}(t|\boldsymbol{x}_0, t_0) \equiv \boldsymbol{u}_L(t|\boldsymbol{x}_0, t_0)$$

Euerian velocity field

$\boldsymbol{u}_E(\boldsymbol{x}, t)$



$$\boldsymbol{u}_L(t|\boldsymbol{x}_0, t_0) \equiv \boldsymbol{u}_E(\boldsymbol{x}(t|x_0, t_0)$$

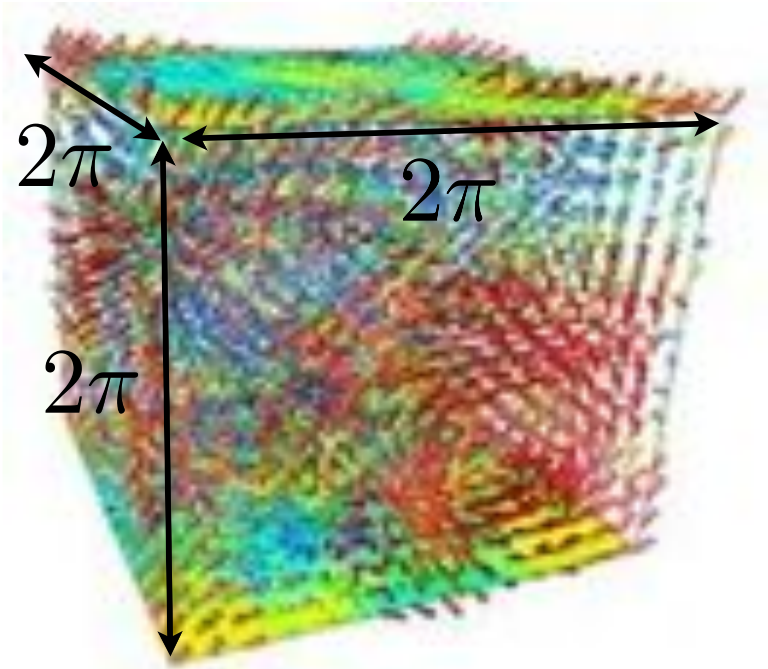
Advantages of periodicity

Homogeneous system ?

→ Periodic boundary conditions..

$$\phi(\boldsymbol{x} + \boldsymbol{n}L, t) = \phi(\boldsymbol{x}, t)$$

$\boldsymbol{n}$ integer vector



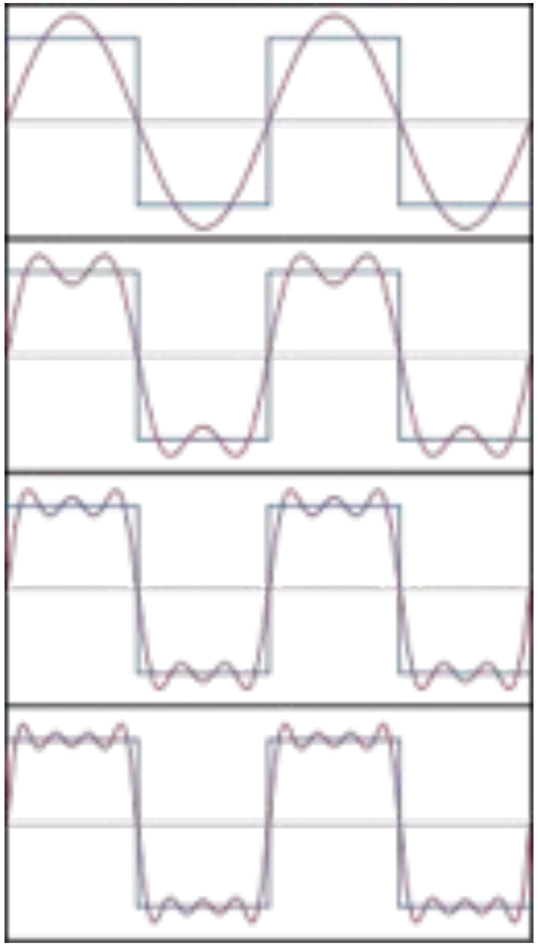
→ Periodic function ?
Fourier series !

Fourier series

$$\boldsymbol{k} \in \frac{2\pi}{L}\boldsymbol{Z}^3$$

$$\psi(\boldsymbol{r}) = \sum_{\boldsymbol{k}} e^{i\boldsymbol{k}\cdot\boldsymbol{r}}\hat{\psi}_{\boldsymbol{k}}$$

$$\hat{\psi}_{\boldsymbol{k}} = \frac{1}{L^3}\int e^{-i\boldsymbol{k}\cdot\boldsymbol{r}}\psi(\boldsymbol{r})$$



Wikipedia: In mathematics, a **Fourier series** decomposes any periodic function or periodic signal into the sum of a (possibly infinite) set of simple oscillating functions, namely sines and cosines (or complex exponentials).

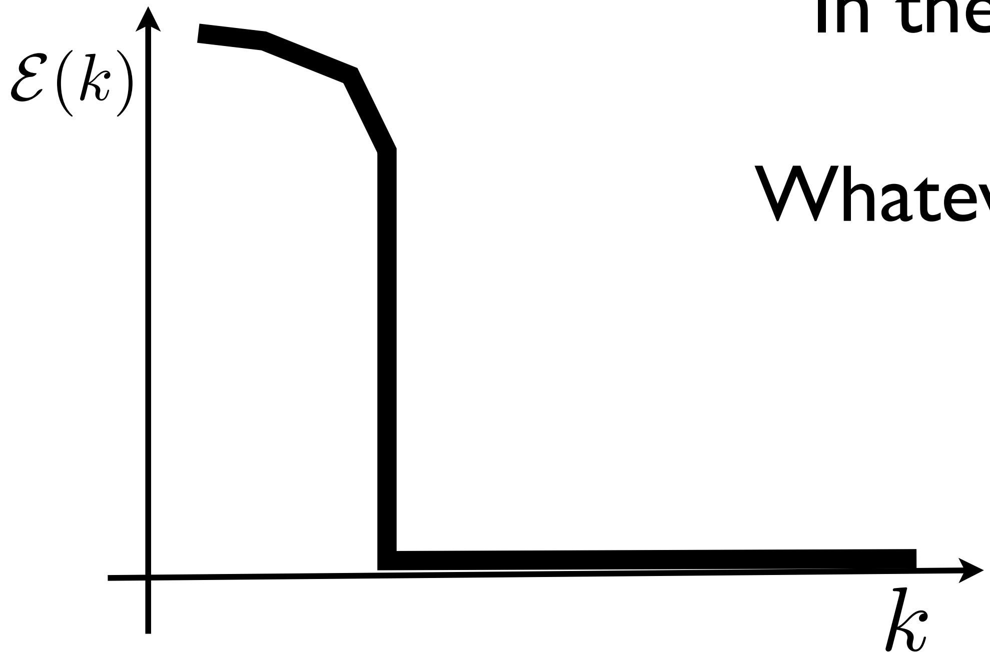
Pseudo-spectral method

- Spectral: Discretize the fields on a Fourier series
- Evaluate the terms local in Fourier space
- Pseudo-spectral: Evaluate the convolution term in real space, then move back to Fourier space

Pseudo-spectral method

- Chebyshev and Fourier Spectral Methods, Second Edition, John P. Boyd, DOVER Publications, Inc. (2000)
- Canuto et al. Spectral Methods in Fluid Dynamics. Book (1988)
- Rogallo. Numerical Experiments in Homogeneous Turbulence. NASA Tech. Memo. (1981) vol. 81315 pp. 1-92

Eulerian initialization



In the end not very important

Whatever will let your simulation go will do...

but:

Forcing only one mode will not do !

Triadic interaction needs at least to mode to transfer energy

Depending on the forcing scheme used, one may need to fill in energy into several shells not to run in troubles...

Small scales: Hyper-viscosity and resolution

How to make "more room" for inertial range ?

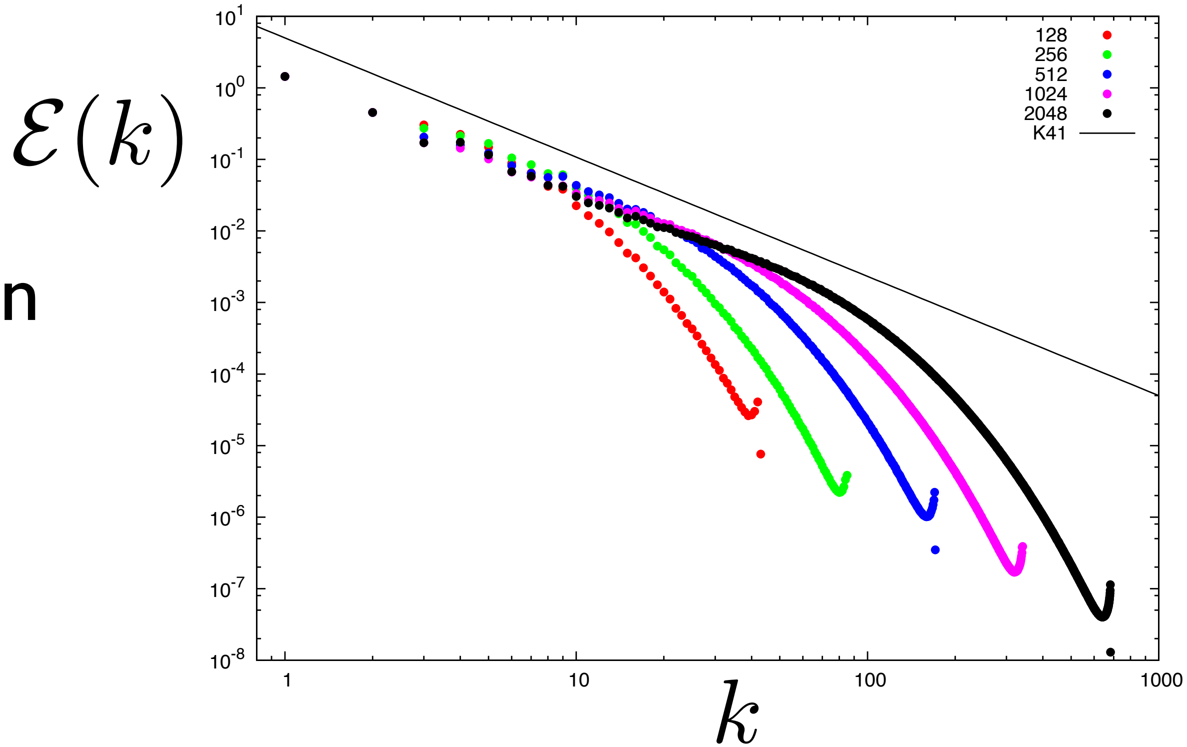
$$\partial_t \boldsymbol{u} + \boldsymbol{u} \cdot \boldsymbol{\nabla} \boldsymbol{u} = -\boldsymbol{\nabla} p + \nu \Delta \boldsymbol{u} + \boldsymbol{f}$$

$$\alpha \leq 1$$

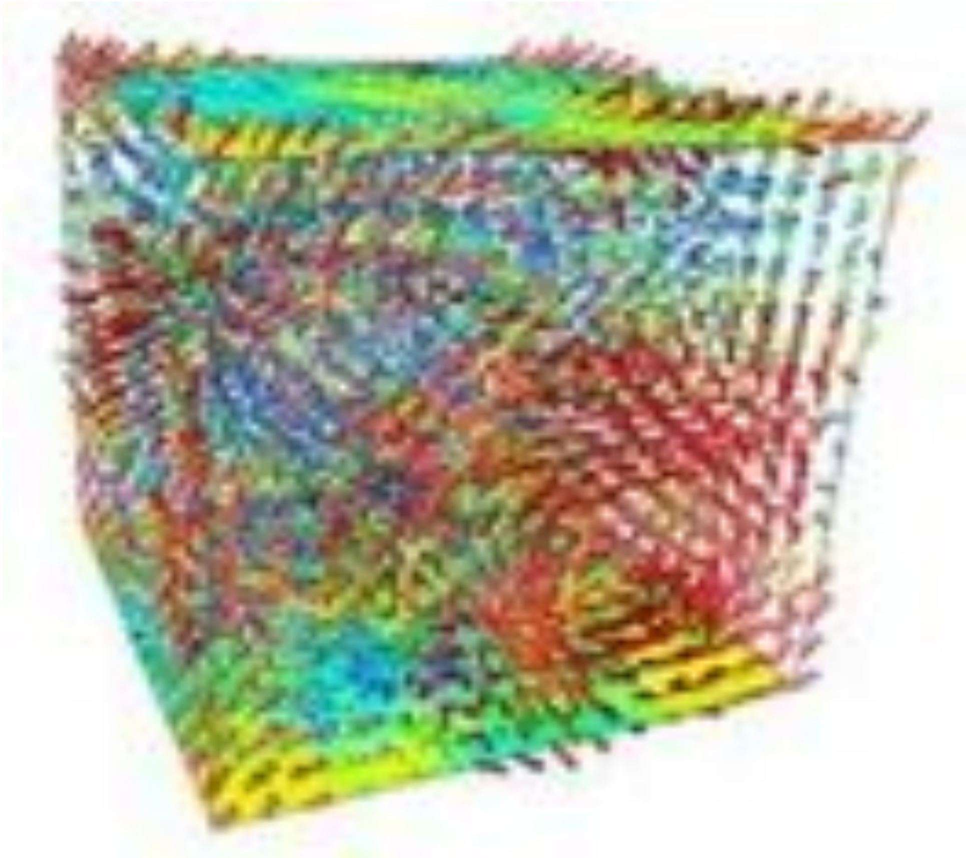
$$\nu_\alpha \Delta^\alpha \boldsymbol{u}$$

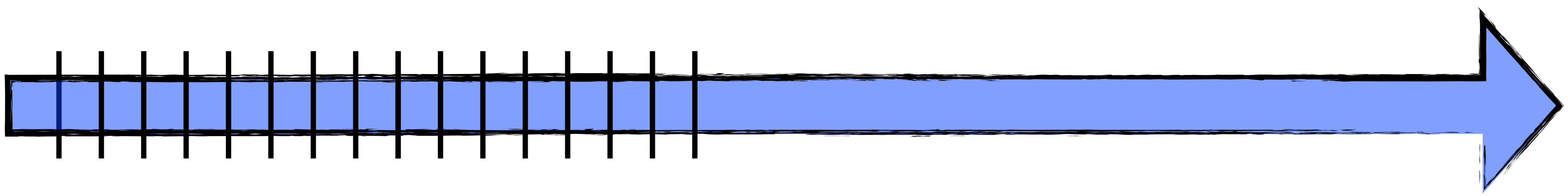
Small scale resolution

$$\eta k_{max}$$



Integration scheme





Treatment of Pressure

Helmholtz Theorem

$$\nabla^2 p = -\nabla \cdot (\mathbf{u} \cdot \nabla \mathbf{u})$$

$$\mathbf{u} = \nabla\phi + \nabla \times \mathbf{b}$$

Vector potential **b**

Transversal component $\boldsymbol{\nabla} \times \boldsymbol{b}$

Longitudinal component $\boldsymbol{\nabla}\phi$

$\nabla \cdot \mathbf{u} = 0$ ⇒ $\boldsymbol{\nabla}\phi = 0$

$$\boldsymbol{\omega} = \nabla \times \mathbf{u} \qquad \boldsymbol{\omega} = \boldsymbol{\nabla} \times \boldsymbol{\nabla} \times \boldsymbol{b} = -\Delta \boldsymbol{b}$$

$$\boldsymbol{b} = -\Delta^{-1}\boldsymbol{\omega}$$

Going to Fourier

$$\boldsymbol{\nabla} \longrightarrow -i\boldsymbol{k}$$

$$\boldsymbol{\nabla}^2 \longrightarrow -\boldsymbol{k}^2$$

Treatment of Pressure (Fourier)

Helmholtz Theorem

$$\mathbf{u} = \nabla\phi + \nabla \times \mathbf{b} \longrightarrow \boldsymbol{u}(\boldsymbol{k}) = -i\boldsymbol{k} \times \hat{\boldsymbol{b}}(\boldsymbol{k})$$

$$\boldsymbol{u}(\boldsymbol{r}) = \boldsymbol{u}^*(\boldsymbol{r}) \qquad \hat{\boldsymbol{u}}(\boldsymbol{k}) = \hat{\boldsymbol{u}}^*(-\boldsymbol{k})$$

Implication on memory storage requirements

$$\boldsymbol{\omega} = \nabla \times \mathbf{u} \qquad \boldsymbol{\omega} = \boldsymbol{\nabla} \times \boldsymbol{\nabla} \times \boldsymbol{b} = -\Delta \boldsymbol{b}$$

$$\boldsymbol{b} = -\Delta^{-1}\boldsymbol{\omega}$$

Equation in Fourier space

$$\nabla^2 p = -\nabla \cdot (\mathbf{u} \cdot \nabla \mathbf{u})$$

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

$$\partial_t \left(|\mathbf{k}|^2 \hat{\mathbf{b}}_{\mathbf{k}} \right) = i\mathbf{k} \times \mathcal{F}(\mathbf{u} \times \boldsymbol{\omega})_{\mathbf{k}} - \nu |\mathbf{k}|^4 \hat{\mathbf{b}}_{\mathbf{k}}$$

Equation in Fourier space

$$\partial_t \left(|\mathbf{k}|^2 \hat{\mathbf{b}}_{\mathbf{k}} \right) = i\mathbf{k} \times \mathcal{F}(\mathbf{u} \times \boldsymbol{\omega})_{\mathbf{k}} - \nu |\mathbf{k}|^4 \hat{\mathbf{b}}_{\mathbf{k}}$$

Non linear term (NLT) is a convolution in Fourier space

$\longrightarrow$ in real space NTL is a scalar product

$$\mathcal{F}(\mathbf{u} \times \boldsymbol{\omega})_{\mathbf{k}}$$

Fourier		Real		Fourier
$\boldsymbol{k}$	$\longrightarrow$	$\boldsymbol{x}$	$\longrightarrow$	$\boldsymbol{k}$

Pseudo-spectral method

Time marching

$$\partial_t \hat{\mathbf{b}}_{\mathbf{k}} = \frac{i\mathbf{k}}{|\mathbf{k}|^2} \times \mathcal{F}(\mathbf{u} \times \boldsymbol{\omega})_{\mathbf{k}} - \nu |\mathbf{k}|^2 \hat{\mathbf{b}}_{\mathbf{k}}$$

$$\mathbf{N}_{\mathbf{k}} = (N_{1\mathbf{k}}, N_{2\mathbf{k}}, N_{3\mathbf{k}}) = \frac{i\mathbf{k}}{|\mathbf{k}|^2} \times \mathcal{F}(\mathbf{u} \times \boldsymbol{\omega})_{\mathbf{k}}$$

Time marching

$$\partial_t \hat{\boldsymbol{b}}_{\mathbf{k}} + \nu \boldsymbol{k}^2 \hat{\boldsymbol{b}}_{\mathbf{k}} = N_{\mathbf{k}}$$

$$\tilde{\boldsymbol{b}}_{\mathbf{k}} = G(t)\hat{\boldsymbol{b}}_{\mathbf{k}} \qquad \partial_t \tilde{\boldsymbol{b}}_{\mathbf{k}} = G(t) N_{\mathbf{k}}$$

$$G(t) = \exp\left(\nu \boldsymbol{k}^2 t\right)$$ Viscous term exactly integrated

$$\tilde{\boldsymbol{b}}_{\mathbf{k}}^{n+1} = \tilde{\boldsymbol{b}}_{\mathbf{k}}^{n} + \frac{dt}{2}\left[3G(t^n)N_{\boldsymbol{k}}^n - G(t^{n-1})N_{\boldsymbol{k}}^{n-1}\right]$$

$$\hat{\boldsymbol{b}}_{\mathbf{k}}^{n+1} = G(t^{n+1})^{-1}\left\{G(t^n)\hat{\boldsymbol{b}}_{\mathbf{k}}^{n} + \frac{dt}{2}\left[3G(t^n)N_{\boldsymbol{k}}^n - G(t^{n-1})N_{\boldsymbol{k}}^{n-1}\right]\right\}$$

Adams-Bashforth 2nd order

Forcing schemes

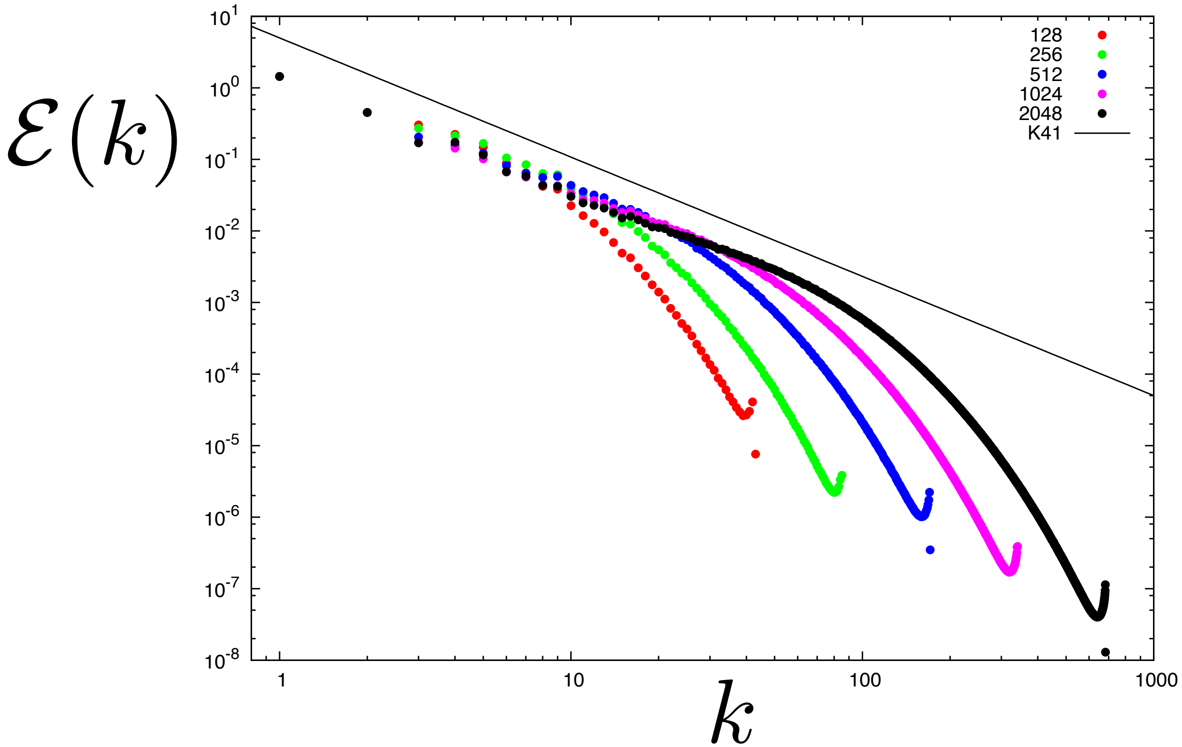
- Many possibilities... non unique choice, i.e. non universality at large scales.
- *Inertial range turbulence* is universal with respect to the forcing **but**:
  - Different forcing may affect more or less directly and severely the extension of the inertial range
  - Different forcing may make the large scales more or less isotropic

The role of forcing

Singular limit $Re \to \infty \quad \neq \quad \nu = 0$

$$\langle \boldsymbol{f} \cdot \boldsymbol{u} \rangle = -\nu \left\langle \boldsymbol{u} \cdot \nabla^2 \boldsymbol{u} \right\rangle = \varepsilon(\nu)$$

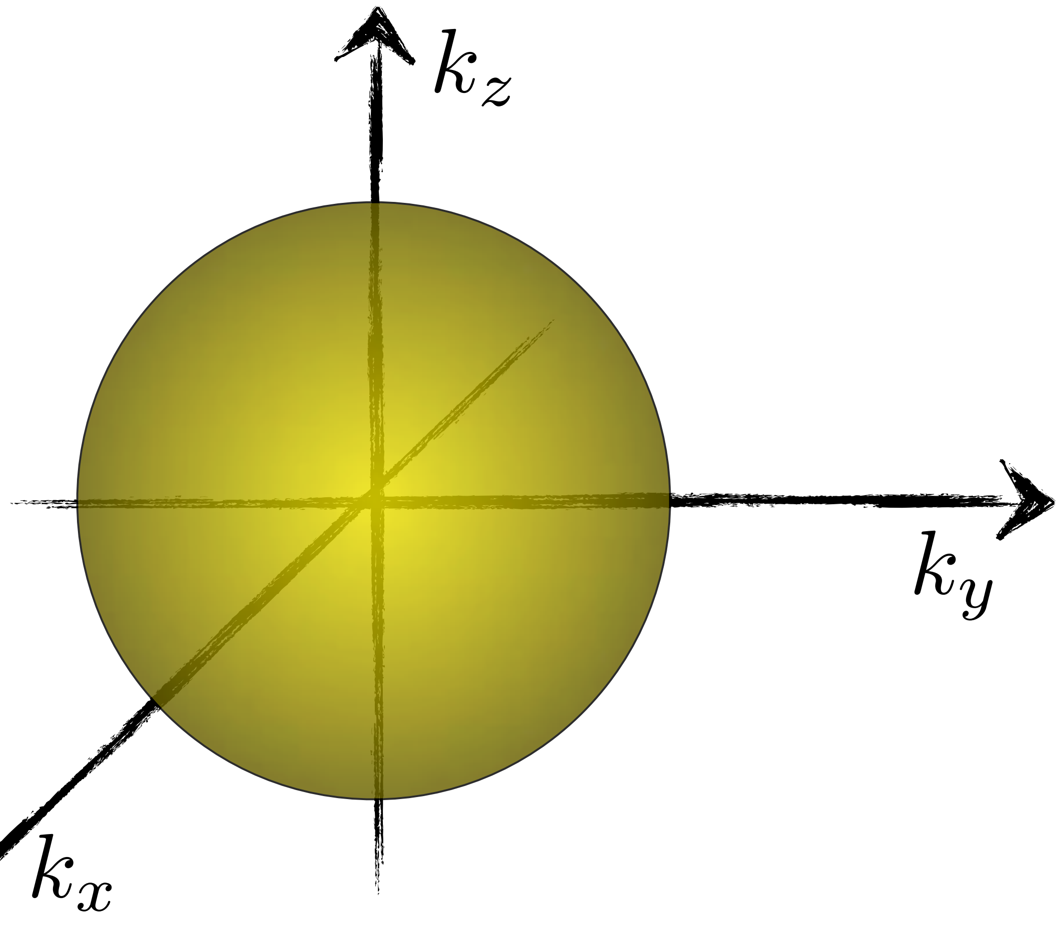
$$\lim_{\nu \to 0} \varepsilon(\nu) = \varepsilon > 0$$



$$\frac{dE}{dt} = \langle \boldsymbol{u} \cdot \boldsymbol{f} \rangle - \nu \left\langle |\boldsymbol{\nabla} \boldsymbol{u}|^2 \right\rangle \simeq 0$$

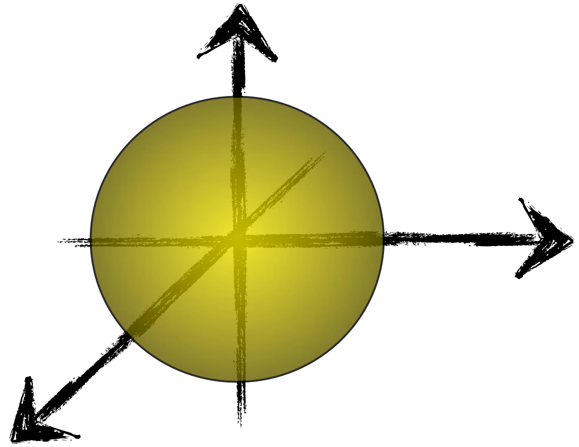
Forced wavenumber in a shell

$\boldsymbol{K}_f : |\boldsymbol{k}| \leq k_t$ (e.g. $k_t = 2$)



Frozen amplitude

$\boldsymbol{K}_f : |\boldsymbol{k}| \leq k_t$ (e.g. $k_t = 2$)



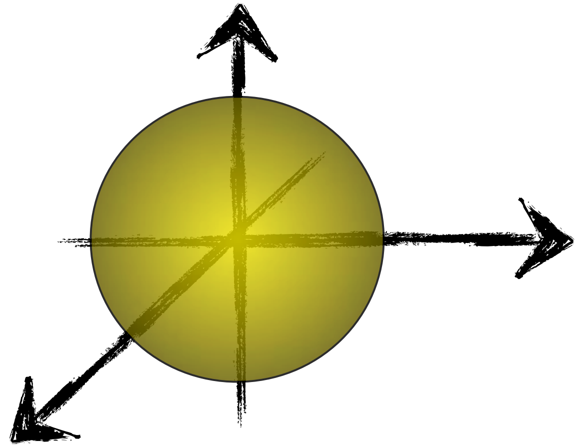
shell of small wavenumbers

$$\boldsymbol{u}(\boldsymbol{k}, t) \equiv \boldsymbol{u}_0(\boldsymbol{k}) \qquad \boldsymbol{k} \in \boldsymbol{K}_f$$

Constant energy input

$\boldsymbol{K}_f : |\boldsymbol{k}| \leq k_t$ (e.g. $k_t = 2$)

shell of small wavenumbers



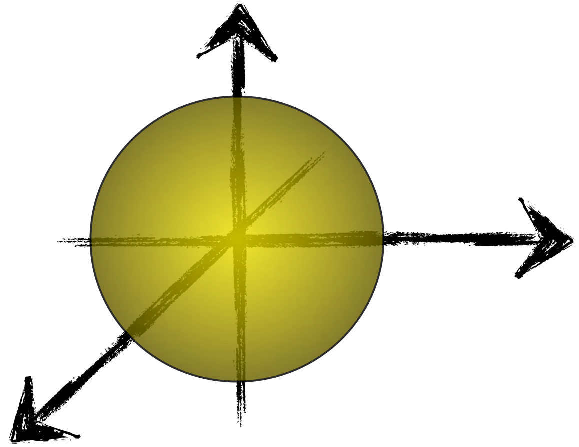
$$\boldsymbol{f}(\boldsymbol{k},t) = \varepsilon \cdot \frac{\boldsymbol{u}(\boldsymbol{k},t)}{\sum_{\boldsymbol{k}\in\boldsymbol{K}_f} |\boldsymbol{u}(\boldsymbol{k},t)|^2}$$

$$\boldsymbol{k} \in \boldsymbol{K}_f$$

$$\boldsymbol{u}\boldsymbol{f}(\boldsymbol{k},t) = \varepsilon \cdot \frac{|\boldsymbol{u}(\boldsymbol{k},t)|^2}{\sum_{\boldsymbol{k}\in\boldsymbol{K}_f} |\boldsymbol{u}(\boldsymbol{k},t)|^2} \qquad \sum_{\boldsymbol{k}\in\boldsymbol{K}_f} \boldsymbol{u}\boldsymbol{f}(\boldsymbol{k},t) = \varepsilon \cdot \frac{\sum_{\boldsymbol{k}\in\boldsymbol{K}_f} |\boldsymbol{u}(\boldsymbol{k},t)|^2}{\sum_{\boldsymbol{k}\in\boldsymbol{K}_f} |\boldsymbol{u}(\boldsymbol{k},t)|^2} = \varepsilon$$

Appended modes

$\boldsymbol{K}_f : |\boldsymbol{k}| \leq k_t$ (e.g. $k_t = 2$)



shell of small wavenumbers

Rescale amplitude to keep energy fixed in a shell of small wavenumbers

$$\boldsymbol{u}_k \longrightarrow \alpha \boldsymbol{u}_k \qquad \boldsymbol{k} \in \boldsymbol{K}_f$$

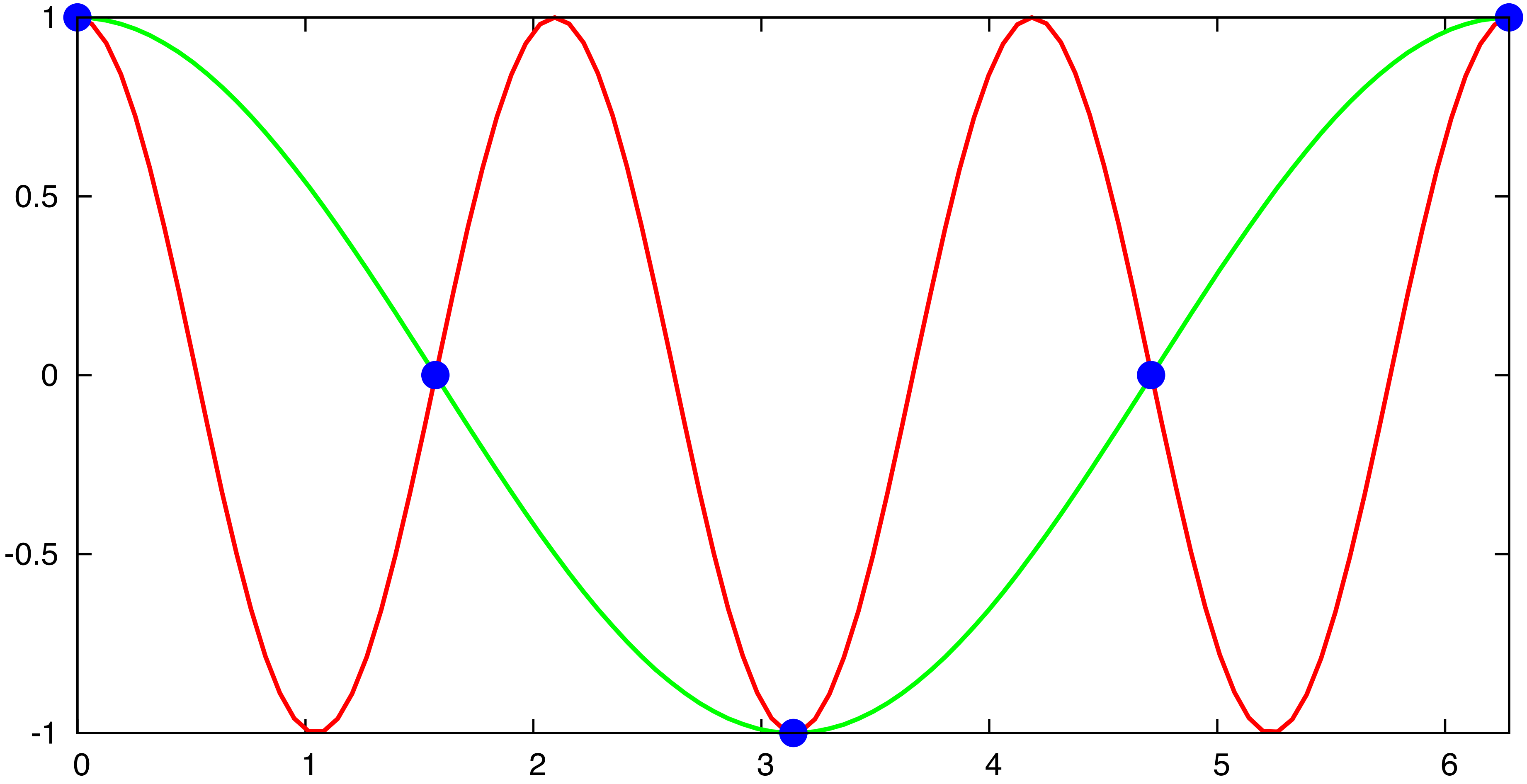
$$\mathcal{E}_{k_c} \equiv \sum_{|\boldsymbol{k}|<k_c} |\boldsymbol{u}_k|^2 \qquad \overline{\mathcal{E}}_{k_c} \equiv \alpha^2 \sum_{|\boldsymbol{k}|<k_c} |\boldsymbol{u}_k|^2$$

Aliasing

"Blowup of an aliased, non-energy-conserving model is God's way of protecting you from believing a bad simulation." J. P. Boyd

- from P. Boyd. Chebyshev and Fourier spectral methods. Second edition (Revised). (2001) pp. 668

Problem with NLT: aliasing



$$[\psi^1(\boldsymbol{r})\psi^2(\boldsymbol{r})] = \left(\sum_{\boldsymbol{k}=-K}^{+K} e^{i\boldsymbol{k}\cdot\boldsymbol{r}}\hat{\psi}^1_{\boldsymbol{k}}\right)\left(\sum_{\boldsymbol{k}=-K}^{+K} e^{i\boldsymbol{k}\cdot\boldsymbol{r}}\hat{\psi}^2_{\boldsymbol{k}}\right) = \sum_{\boldsymbol{k}=-2K}^{\boldsymbol{k}=2K} \phi_{\boldsymbol{k}} e^{i\boldsymbol{k}\cdot r}$$

Spectral blocking & 2/3 rule

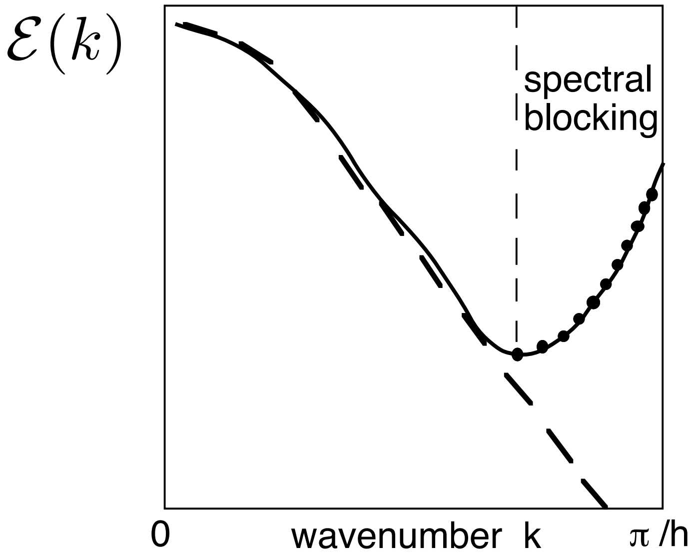
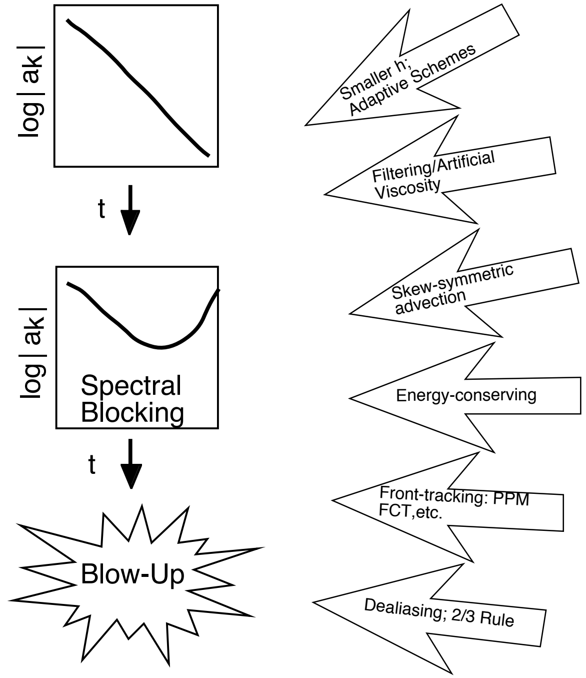


Figure 11.3: Schematic of "spectral blocking". Dashed line: logarithm of the absolute values of Fourier coefficients ("spectrum") at $t = 0$. Solid: spectrum at a later time. The dashed vertical dividing line is the boundary in wavenumber between the decreasing part of the spectrum and the unphysical region where the amplitude increases with k due to numerical noise and aliasing. The corrupted coefficients are marked with disks.



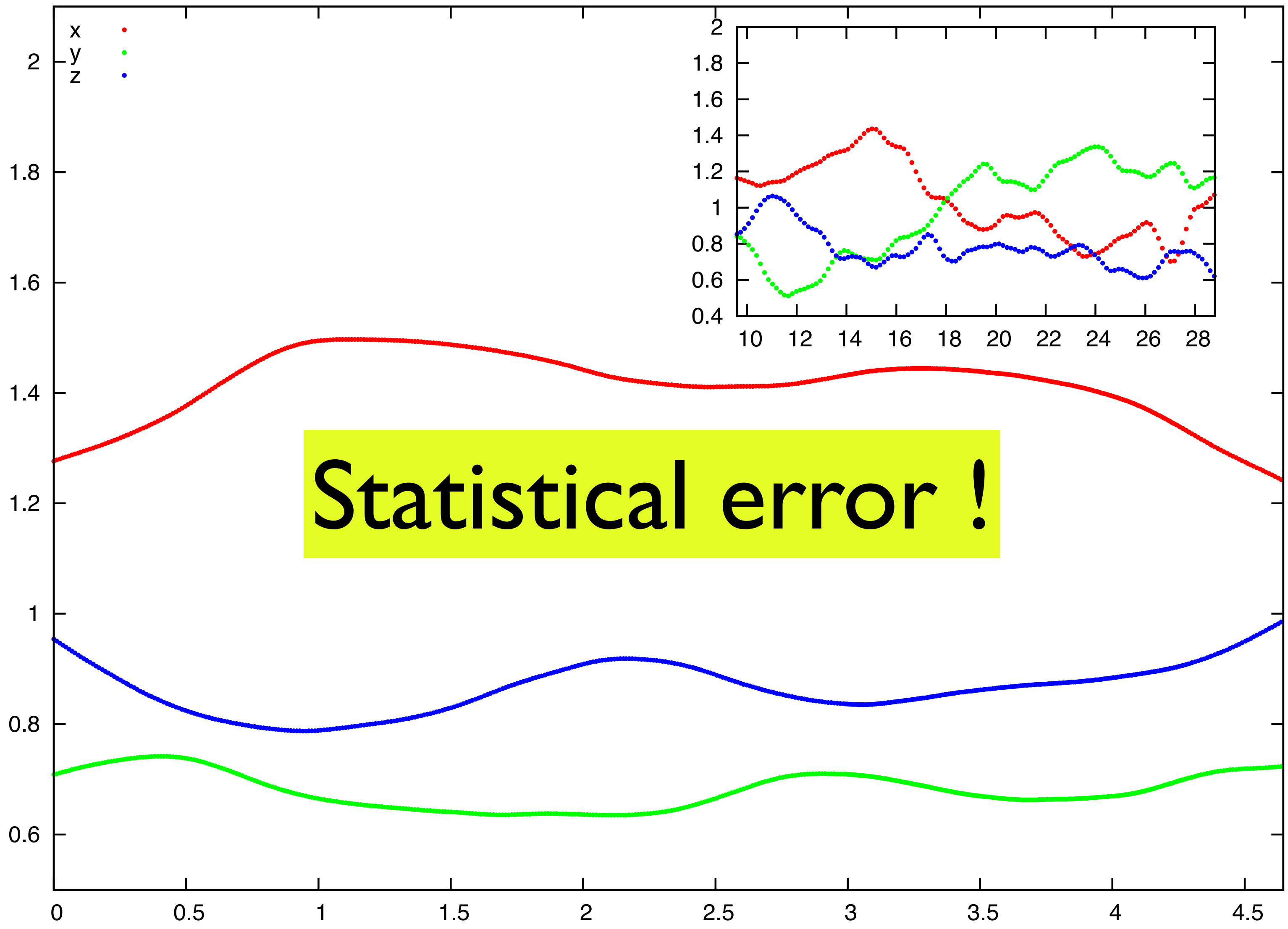
Solution

pad to zero amplitudes for modes $$k \in \left[\frac{2}{3}k_{max}, k_{max}\right]$$

P. Boyd. Chebyshev and Fourier spectral methods.
Second edition (Revised). (2001) pp. 668

Handling non idealities in an ideal system

Deviation from ideality: Isotropy



Is this a sphere ?

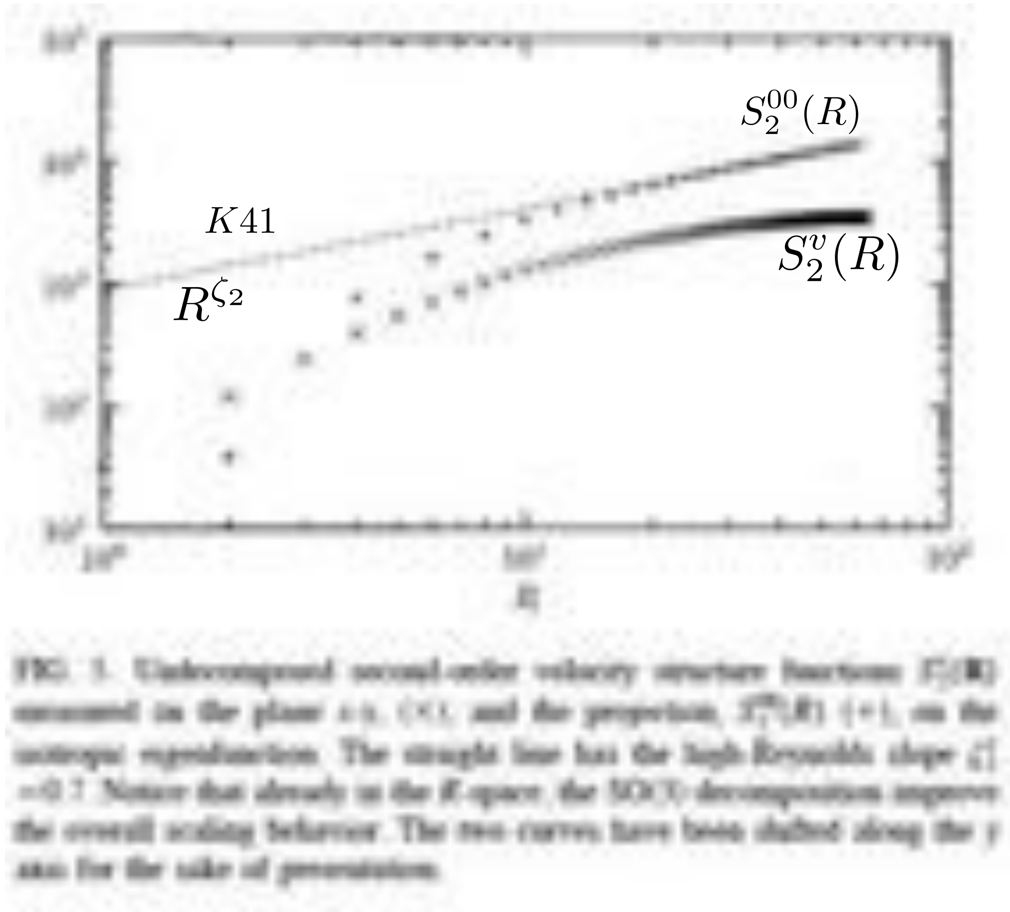
Systematic error !

$$S_p(\boldsymbol{r}) \equiv \langle (u(\boldsymbol{x}+\boldsymbol{r}) - u(\boldsymbol{x}))^p \rangle$$

$$S^p_{l,m}(|\boldsymbol{r}|) \equiv \int d\Omega S_p(\boldsymbol{r}) Y_{lm}(\hat{\boldsymbol{r}})$$

... maybe

Systematic error !



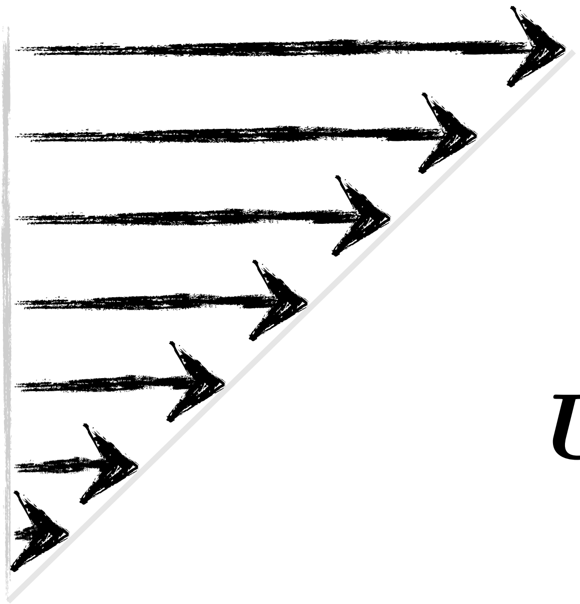
Biferale et al. Statistics of pressure and of pressure-velocity correlations in isotropic turbulence. Phys Fluids (2000) vol. 12 (7) pp. 1836-1842

Something more fancy...

out of a cubic box !

Shear turbulence

A more complex realization:
homogeneous and **non isotropic** flow



$$\boldsymbol{U} = (Sy, 0, 0)$$

$$D_t\mathbf{u} + Sy\partial_x\mathbf{u} + Su_y\hat{e}_x = -\nabla p + \nu\nabla^2\mathbf{u}$$

Deforming grid

$$
\begin{aligned}
x' &= x - Sty \\
y' &= y \\
z' &= z
\end{aligned}
$$

$$
\begin{aligned}
\frac{\partial}{\partial t} &= \frac{\partial}{\partial t'} - Sy\frac{\partial}{\partial x'} \\
\frac{\partial}{\partial x} &= \frac{\partial}{\partial x'} \\
\frac{\partial}{\partial y} &= \frac{\partial}{\partial y'} - St\frac{\partial}{\partial x'} \\
\frac{\partial}{\partial x} &= \frac{\partial}{\partial x'}
\end{aligned}
$$

Remeshing ?

Equations in the deforming grid

$$D_t \mathbf{u} + S u_y \hat{e}_x = -\nabla p + \nu \nabla^2 \mathbf{u}$$

$$\boldsymbol{\nabla} \cdot \mathbf{u} = 0$$

$$\begin{aligned} \nabla &= (\partial_x, \partial_y - St\partial_x, \partial_z) \\ \nabla^2 &= \partial_{xx} + [\partial_{yy} + (St)^2 \partial_{xx} - 2St\partial_{xy}] + \partial_{zz} \end{aligned}$$

$$\begin{aligned} \hat{\nabla}_k &= (\iota k_x, \iota(k_y - Stk_x), \iota k_z) \\ \hat{\nabla}^2{}_k &= -(k_x^2 + (k_y - Stk_x)^2 + k_z^2) \end{aligned}$$

Equation for shear

$$
\begin{aligned}
\partial_t \hat{\mathbf{u}} &= \widehat{(\mathbf{u} \times \omega)} + \hat{\nabla}^2{}_k \mathbf{u} - \hat{\nabla}_k p - S\hat{v}\hat{e}_x \\
\hat{\nabla}_k \hat{\mathbf{u}} &= 0
\end{aligned}
$$

Usual integration scheme...

Energy vs enstrophy

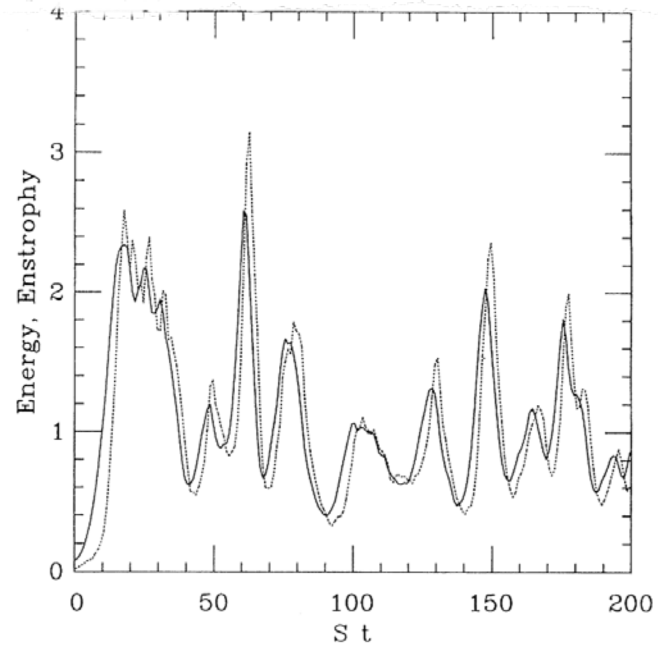
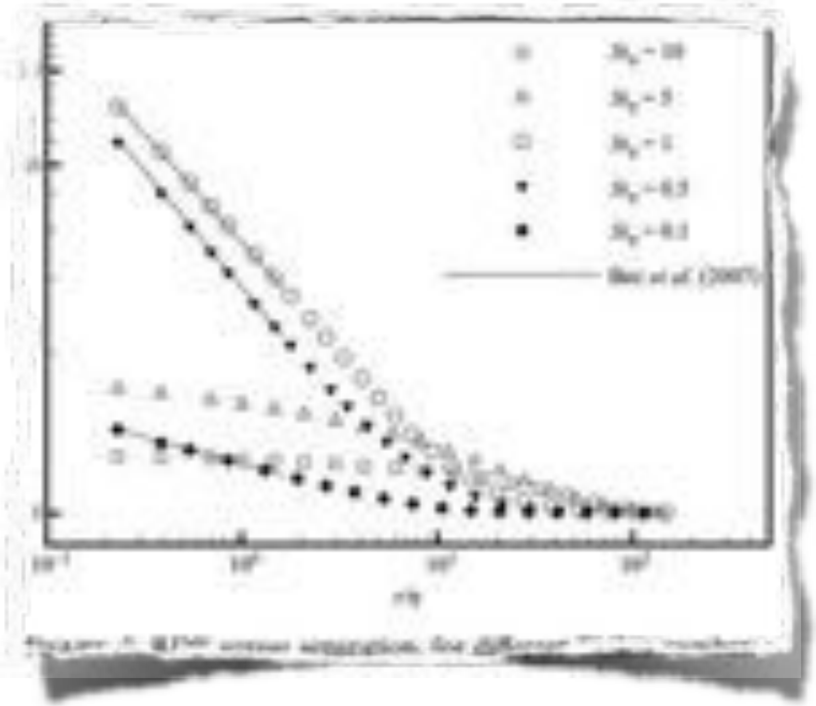
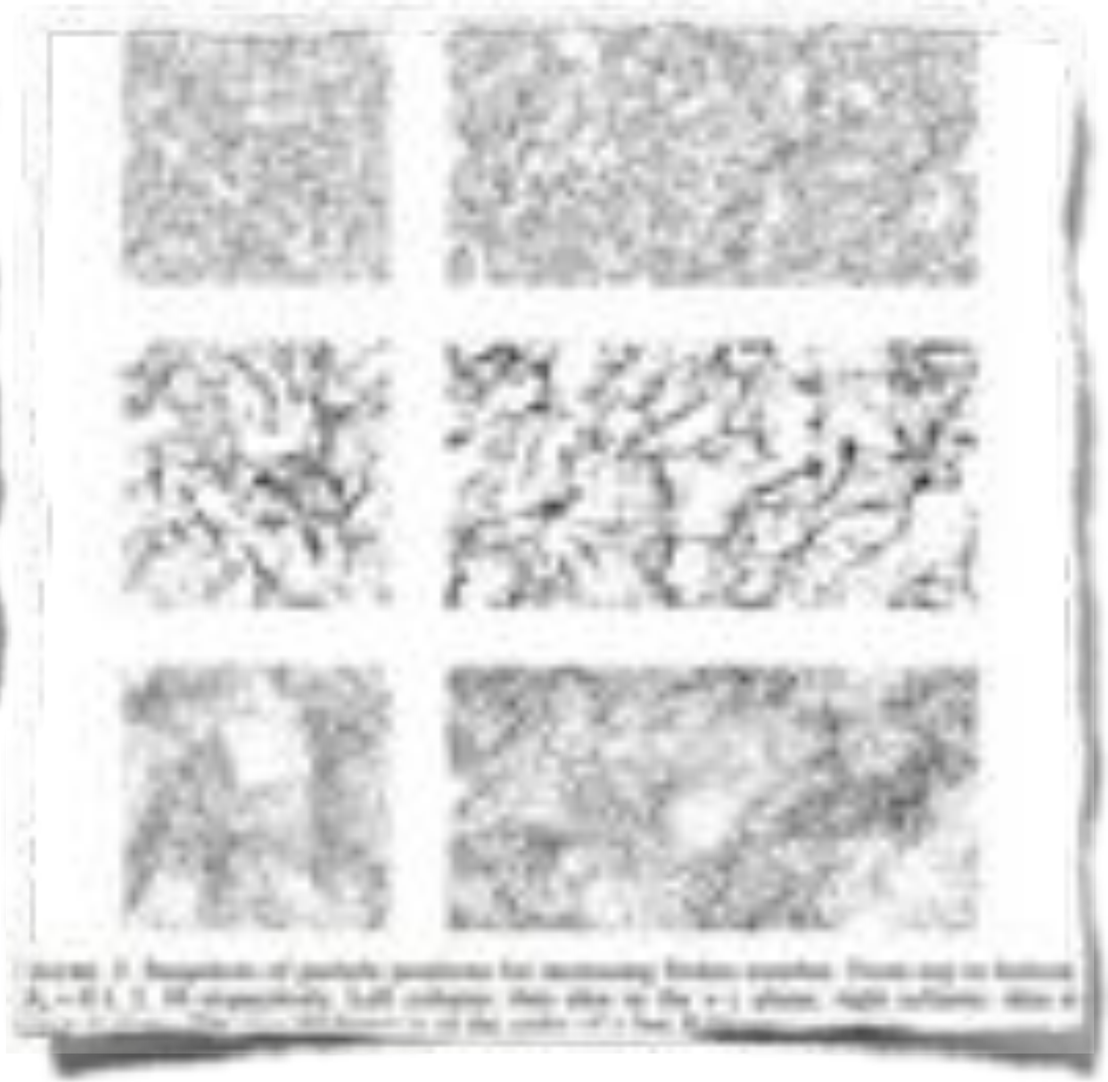


FIG. 2. Energy fluctuations (full line), and enstrophy fluctuations (dotted line), as a function of time for our run 3. Both quantities have been divided by their rms: $\langle u^2/2 \rangle = 1.85$ and $\langle \omega^2 \rangle = 49.26$. Spikes in kinetic energy are followed by spikes in enstrophy (i.e., dissipation). The level of the fluctuations is about 50% and roughly independent of the Reynolds number

Pumir and Shraiman. Persistent Small Scale Anisotropy in Homogeneous Shear Flows.
Physical review letters (1995) vol. 75 (17) pp. 3114

Particles in shear flow





Gualtieri et al. Anisotropic clustering of inertial particles in homogeneous shear flow.
J Fluid Mech (2009) vol. 629 pp. 25-39

DNS computational cost

Memory issues

- Memory occupancy:
- 3 (arrays) x SizeX x SizeY x SizeZ x 3 (velocity components) x (4 or 8 bytes, single or double)
- + eventual work array needed by FFT
- (in place FFTs)
- Eventual arrays for additional measurements

e.g. $A_{ij} = (\partial_i v_j)$

MPI - Message Passing Interface

Np processors, each need to allocate M/Np

Data structure

```
u[x][y][z].{vx,vy,vz}

cu[x][y][z].{vx,vy,vz}.{re,im}
```

*Direction **x** split on processors*
*Direction **z** complexified by the FFT*

*The inverse transform (from x to k space) has to be normalized dividing by Nx*Ny*Nz.*

Computational cost

- Mflops = 5 N $\log_2(N)$ / (time for one FFT in microseconds) / 2 for real-data FFTs
- Rule of the thumb: In spectral code FFTs takes “roughly” 50% of full computational time
- Checkpoint and restart negligible
- Heavy I/O can have an impact but usually when it hits on performance, hits on disk space first.
- Lagrangian integration usually negligible as long as particle density if much smaller than grid point density
- Additional “innocent” measurements which imply extra FFTs hit hard, but usually diluted as not performed at each time step

conclusion...

... should better have a **good** FFT !

FFT: fftw

- http://www.fftw.org/
- Features
- FFTW 3.2.2 is the latest official version of FFTW (refer to the release notes to find out what is new). Subscribe to the fftw-announce mailing list to receive announcements of future updates. Here is a list of some of FFTW's more interesting features:

Speed. (Supports SSE/SSE2/3dNow!/Altivec, since version 3.0.)
Both one-dimensional and multi-dimensional transforms.
Arbitrary-size transforms. (Sizes with small prime factors are best, but FFTW uses O(N log N) algorithms even for prime sizes.)
Fast transforms of purely real input or output data.
Transforms of real even/odd data: the discrete cosine transform (DCT) and the discrete sine transform (DST), types I-IV. (Version 3.0 or later.)
Efficient handling of multiple, strided transforms. (This lets you do things like transform multiple arrays at once, transform one dimension of a multi-dimensional array, or transform one field of a multi-component array.)
Parallel transforms: parallelized code for platforms with Cilk or for SMP machines with some flavor of threads (e.g. POSIX). An MPI version for distributed-memory transforms is also available, currently only as part of FFTW 2.1.5. FFTW 3.2.2 includes support for Cell processors.
Portable to any platform with a C compiler. Documentation in HTML and other formats.
Both C and Fortran interfaces.
Free software, released under the GNU General Public License (GPL, see FFTW license). (Non-free licenses may also be purchased from MIT, for users who do not want their programs protected by the GPL. Contact us for details.) (Also see the FAQ.)

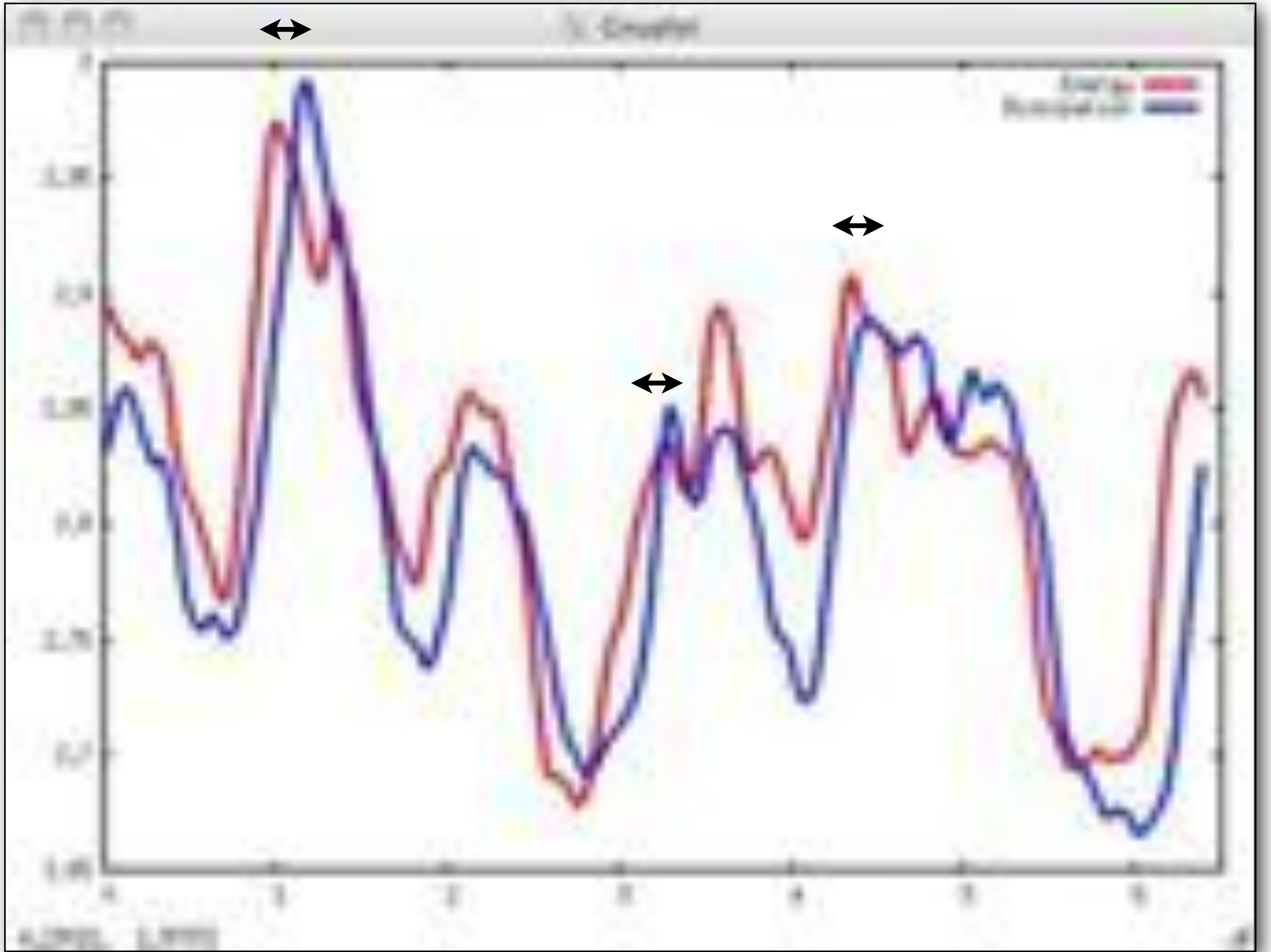
FFT: p3dfft

- http://www.sdsc.edu/us/resources/p3dfft/
- Features (v. 2.3)

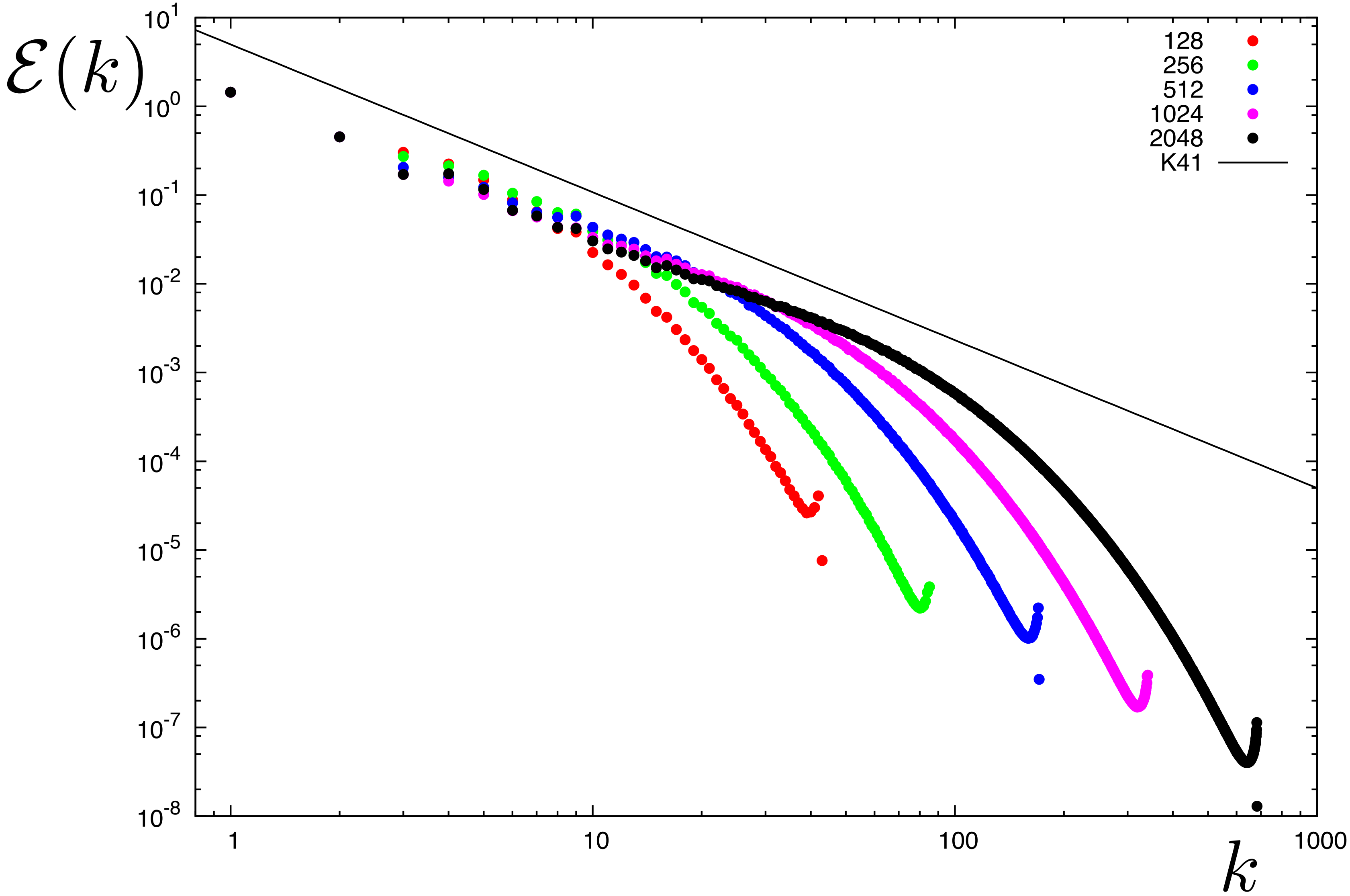
Highly scalable parallel implementation with 2D data decomposition.
Optimized for parallel communication and CPU performance.
Built on top of established 1D FFT libraries (FFTW or ESSL).
Fortran and C interfaces.
Example programs provided.
Extra feature: ghost cell operations for nearest-neighbor communication

How to control a simulation ?

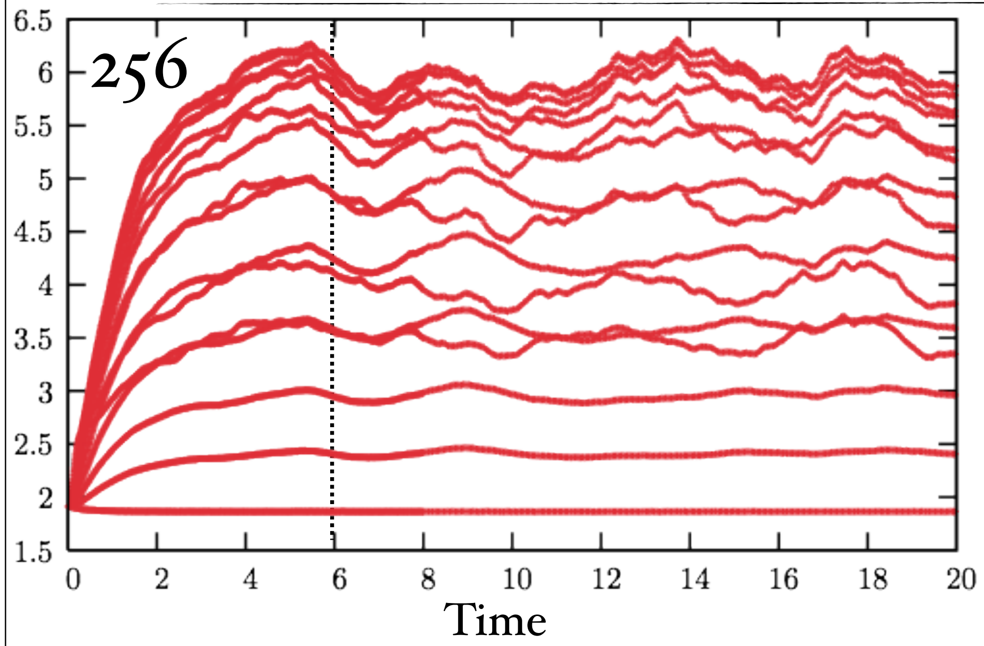
How to check for turbulence ?

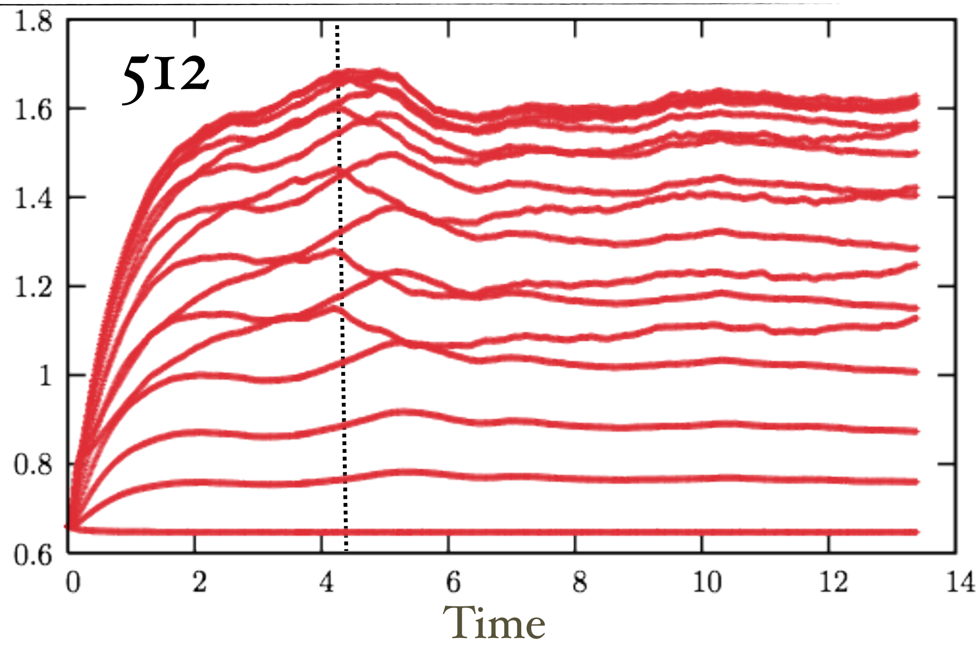


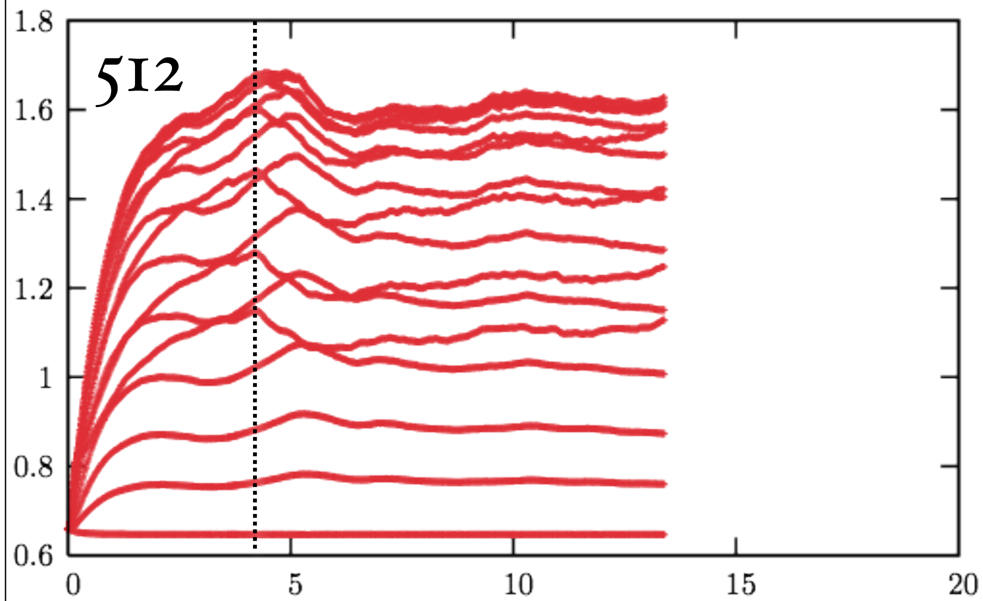
Spectra vs. resolution



Thermalization of particles







$$\mathcal{C}^p(L) = \left\langle \left[\int_{-L/2}^{L/2} c(\boldsymbol{x}+\boldsymbol{y}) d^3y \right]^p \right\rangle$$

- Transient (chapter 0)
- Stationary regime (chapter 1)
- Plots repr. d^2 vs. time

Tracers

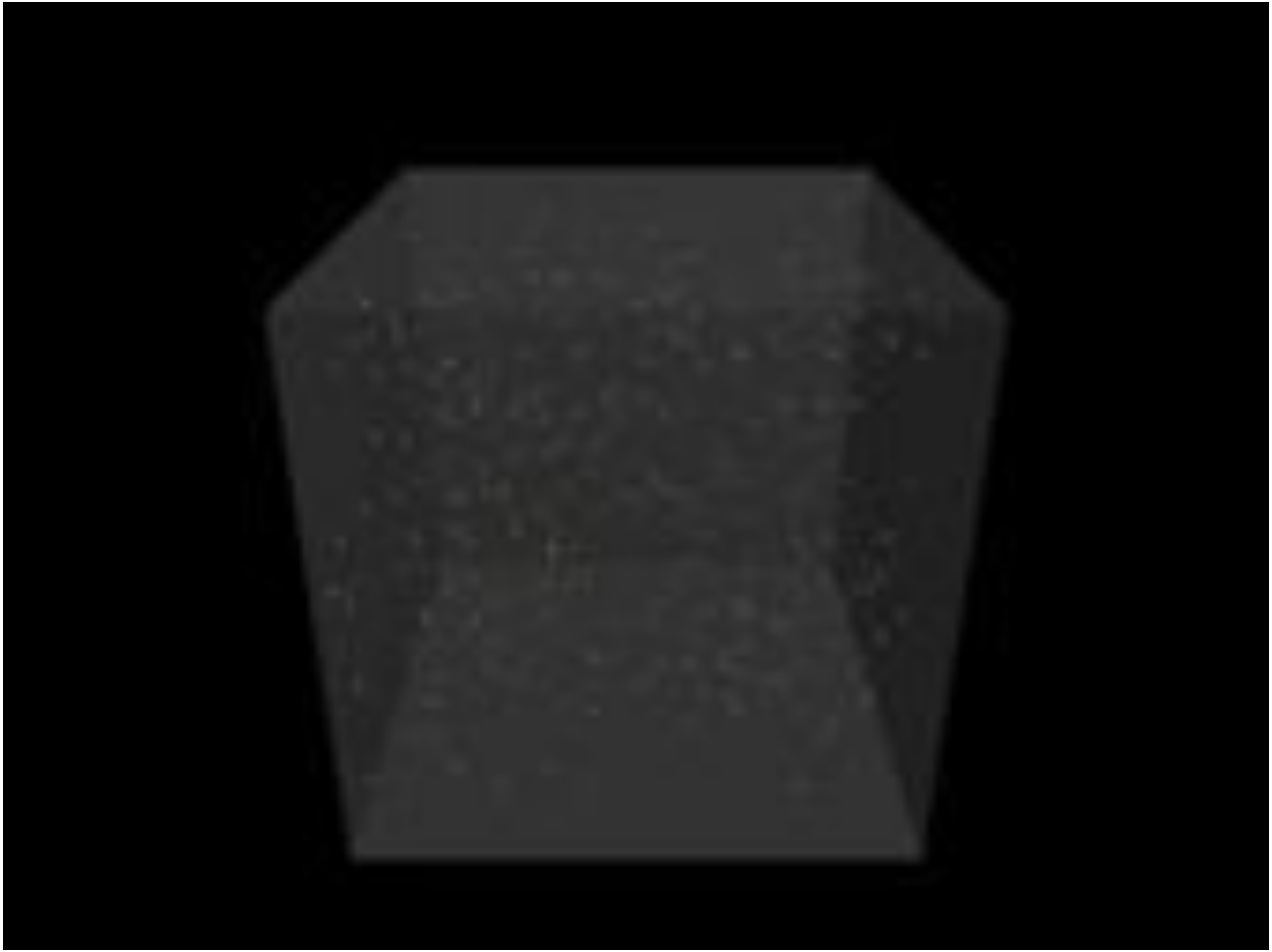
Particles small "enough" can be described as "neutral" tracers.

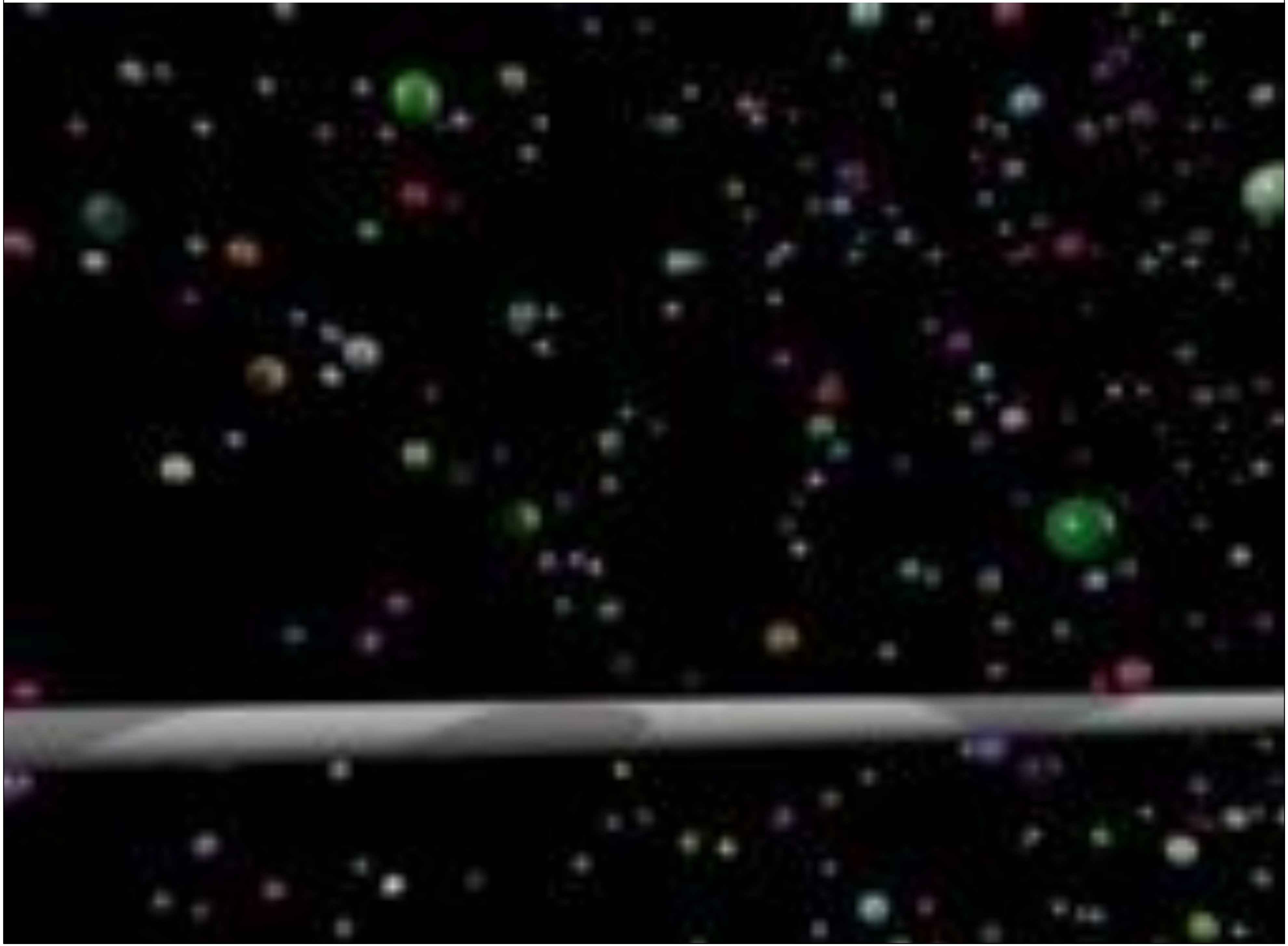
No modeling needed !!

Equation of motion of tracer is:

$$\frac{d\boldsymbol{x}}{dt}(t|\boldsymbol{x}_0, t_0) \equiv \boldsymbol{u}_L(t|\boldsymbol{x}_0, t_0)$$

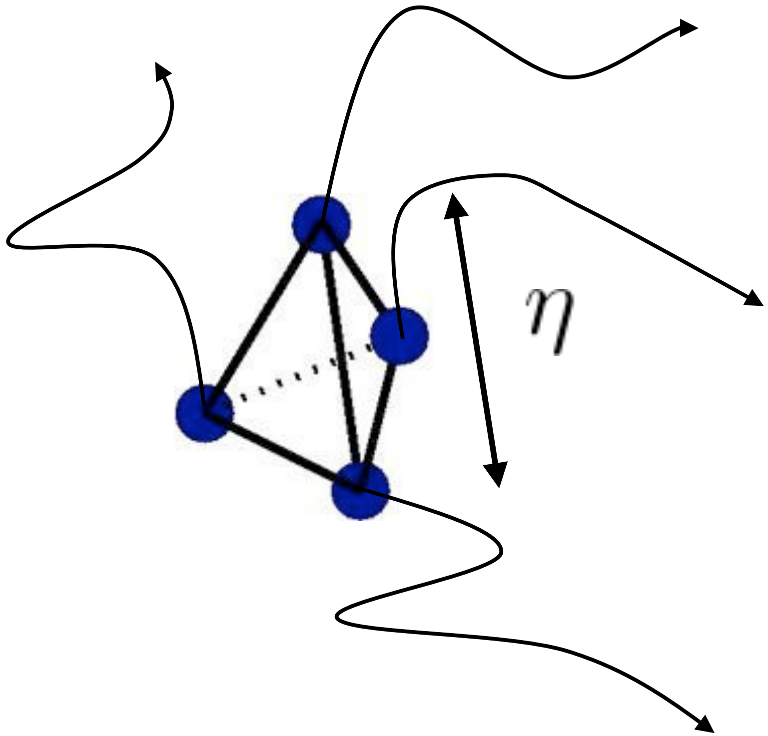
$$\boldsymbol{u}_L(t|\boldsymbol{x}_0, t_0) \equiv \boldsymbol{u}_E(\boldsymbol{x}(t|x_0, t_0), t)$$





Neutrally buoyant tracers: starting config

Starting configuration:
Homogeneous distribution of tetrads divided into 5 classes (regular + irregular shapes). In such a way one can study the single particle statistic, separation of pair and deformation and growth of volumes.



Starting position

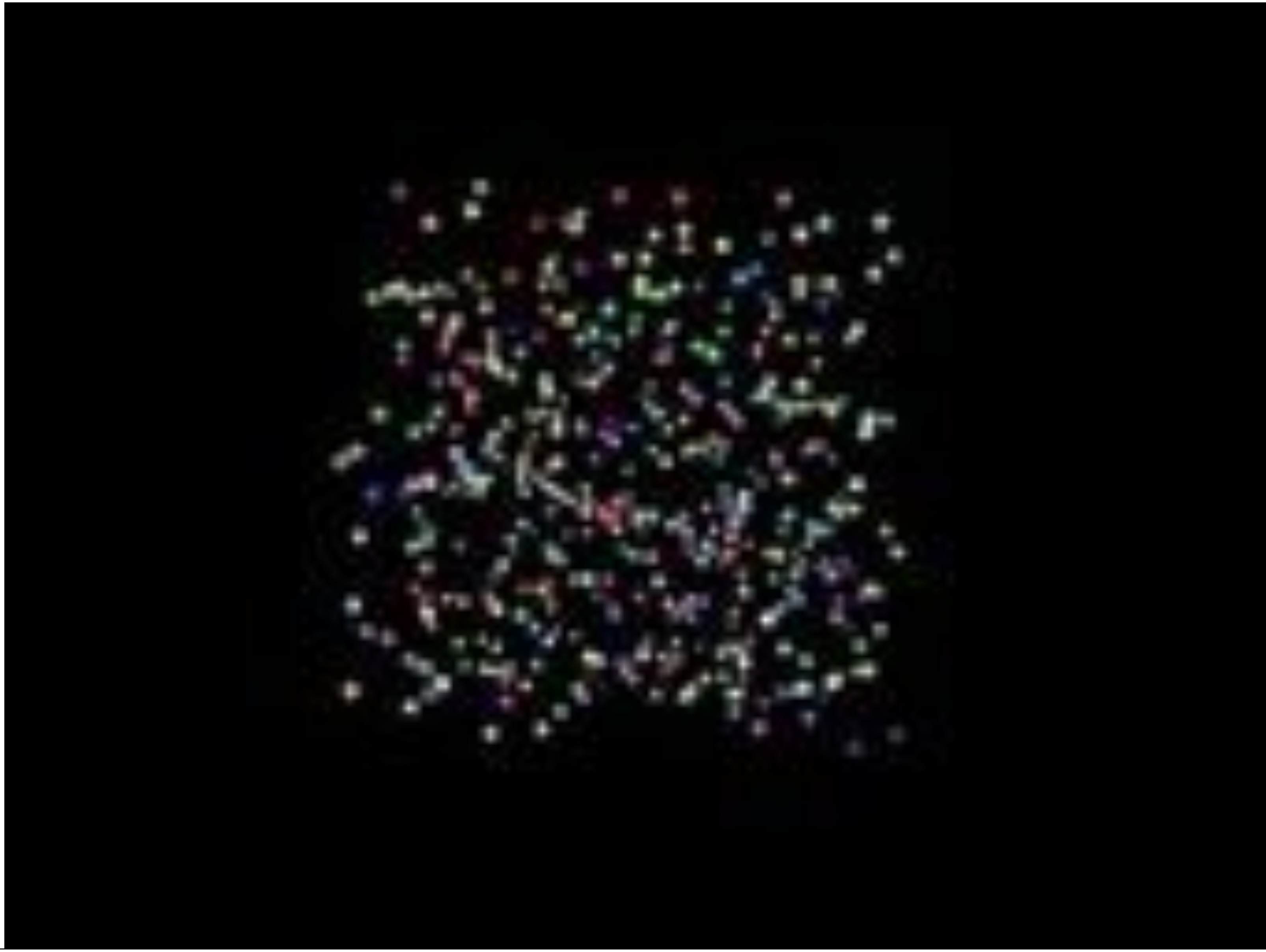
Starting time

$$\boldsymbol{x}_L(t) = \boldsymbol{x}(t; \boldsymbol{x}_0, t_0)$$
$$\boldsymbol{v}_L(t) = \dot{\boldsymbol{x}}_L(t) = \boldsymbol{v}_E(\boldsymbol{x}(t); t)$$

Equation of motion!!

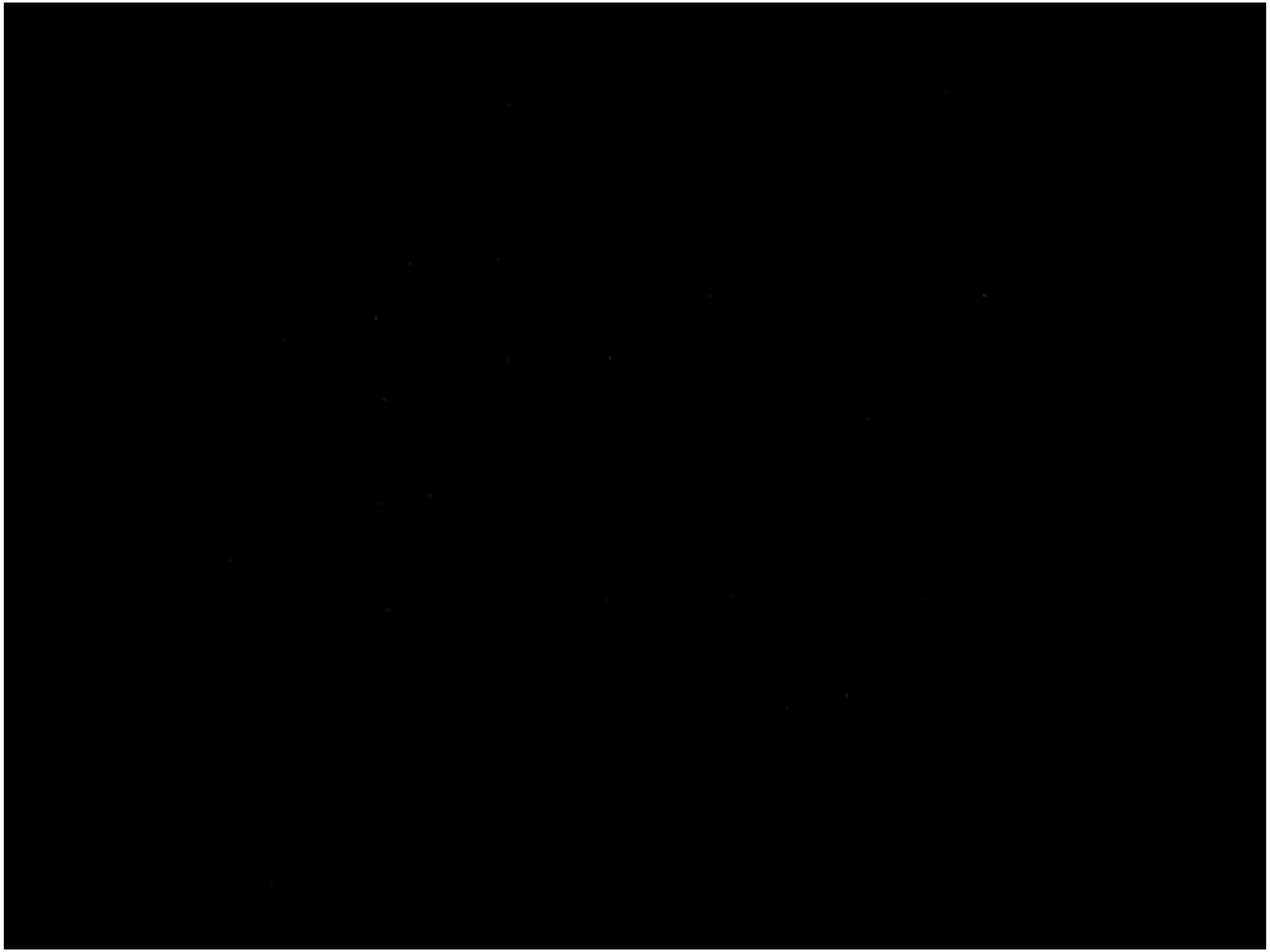
Numerical relative dispersion

evolution of 5×10^5 particle pairs starting from $R(0) \approx \eta$



Evolution of shapes in turbulence

Evolution of ~10^5 tetrahedra starting from the Kolmogorov scale with regular shape



Interpolation

Basic observations

- Need to move particles
- Particles moves out-of-grid
  - Need to know the fluid velocity at particle position

- Solution: interpolation

Fluid tracer

- Yeung and Pope. An algorithm for tracking fluid particles in numerical simulations of homogeneous turbulence. J. Comput. Phys. (1988) vol. 79 pp. 373-416
- Lalescu et al. Implementation of high order spline interpolations for tracking test particles in discretized fields. Journal of Computational Physics (2010) vol. 229 (17) pp. 5862-5869

Spectral (exact) interpolation

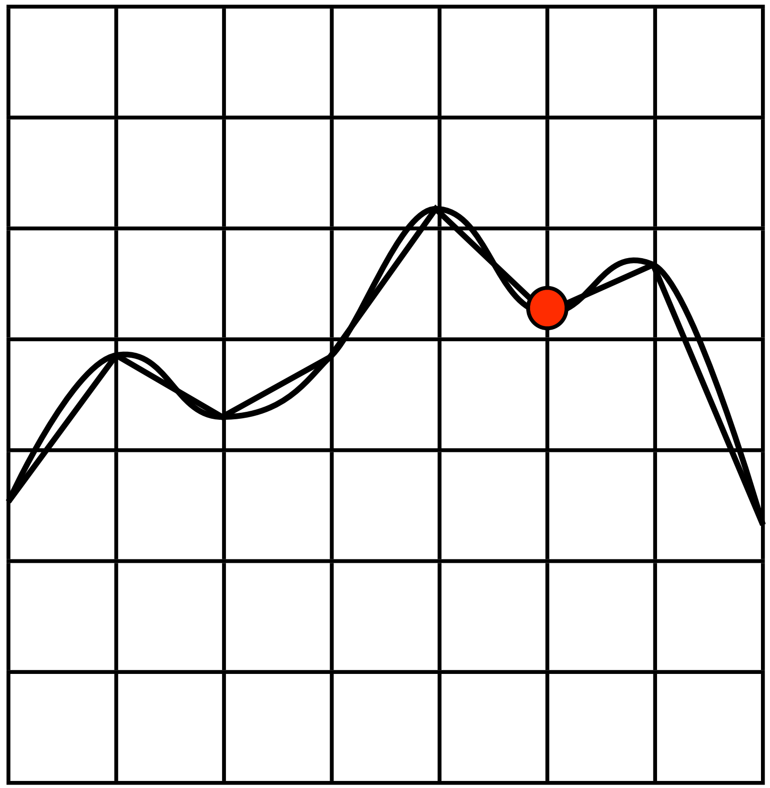
$$\boldsymbol{v}(t) = \boldsymbol{u}(\boldsymbol{x}(t), t)$$

$$\boldsymbol{u}(\boldsymbol{x}(t), t) = \sum_{\boldsymbol{k}} e^{i\boldsymbol{k}\cdot\boldsymbol{x}(t)} \hat{\boldsymbol{u}}_{\boldsymbol{k}}(t_n)$$

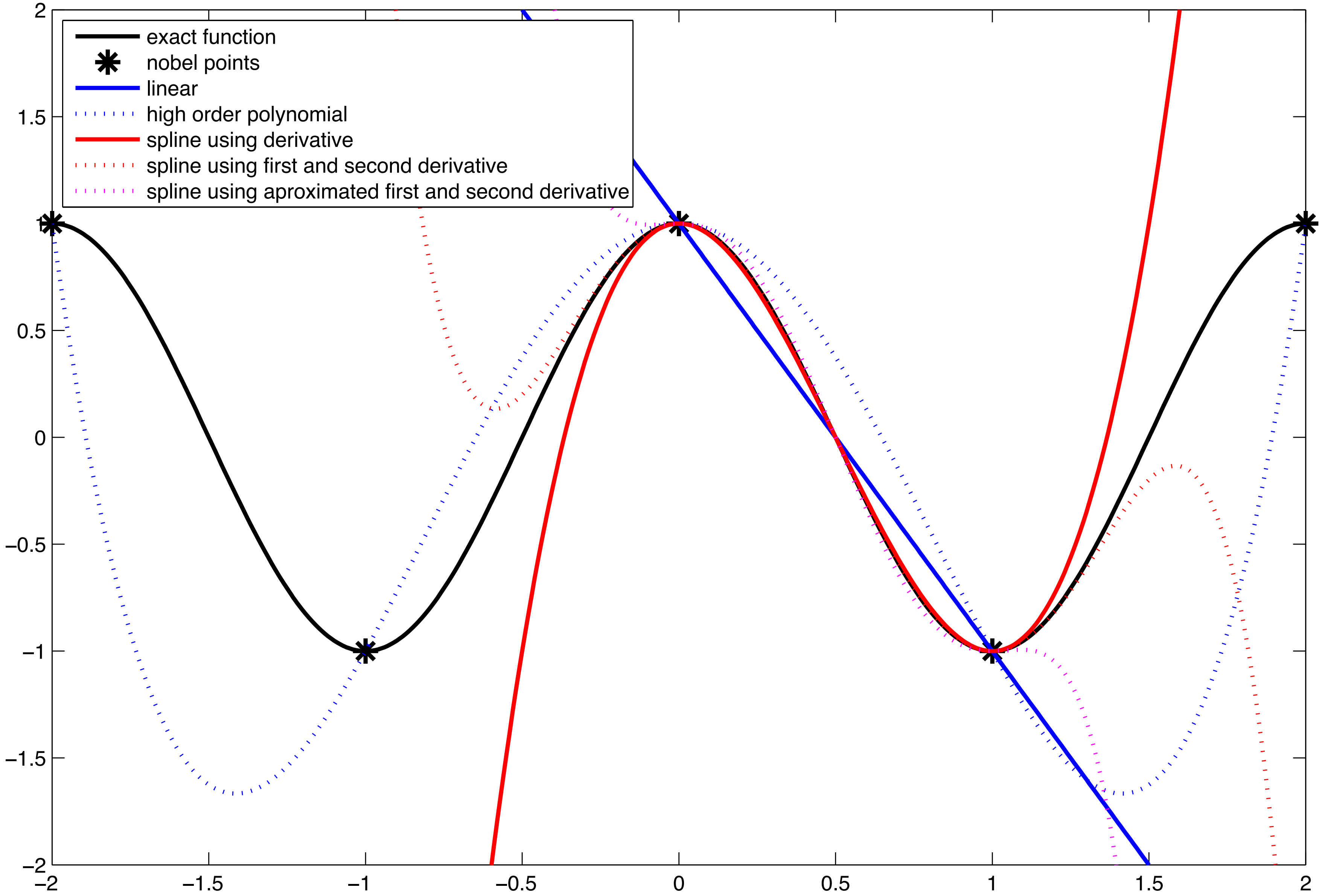
Computational cost $\qquad N_p N^3 \ln(N)$

Many choice...

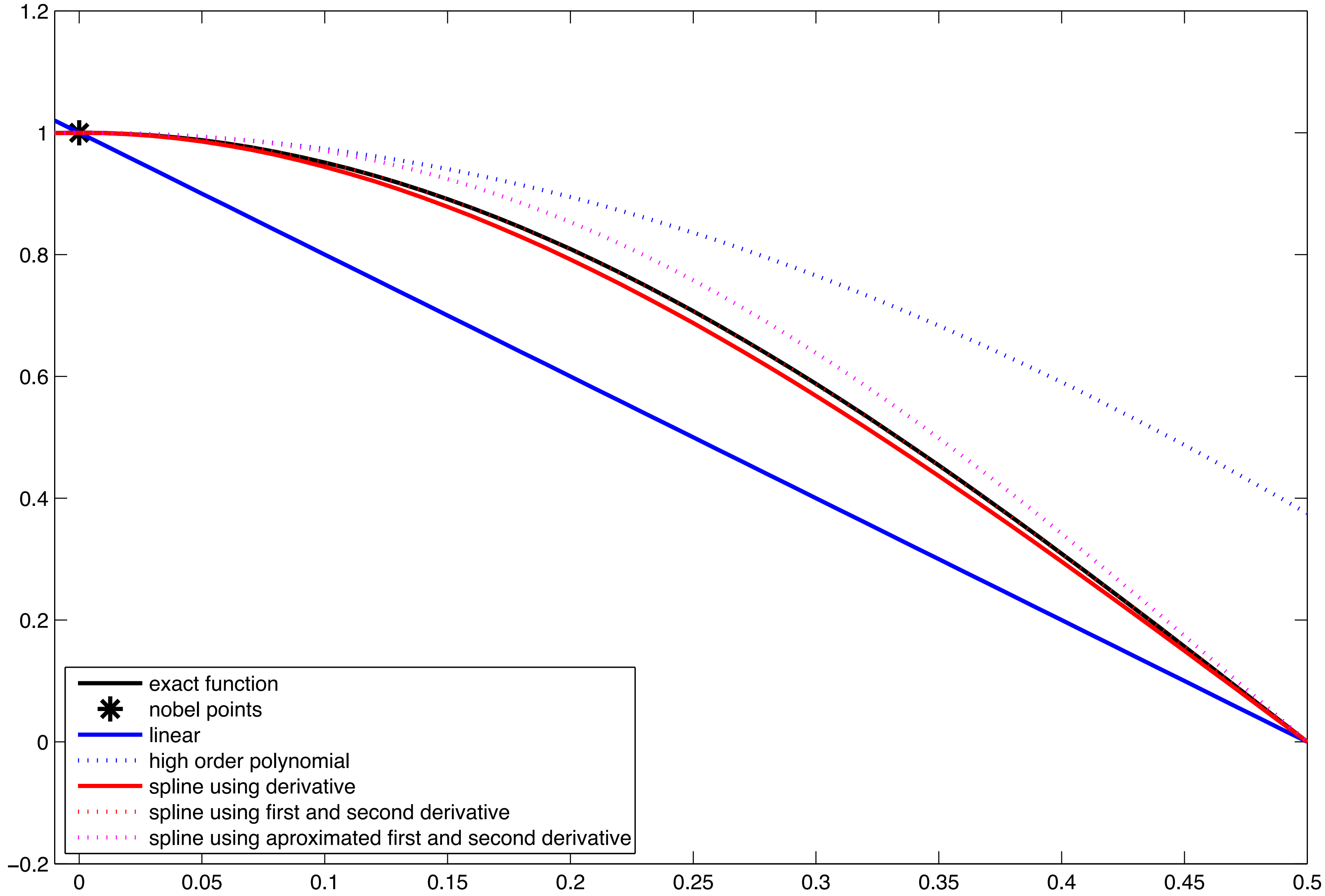
- Linear
- Polynomial order k
- Derivative at extreme of interval



A visual example...



A visual example...



Evolution of (real?) particles

Equation of motion (anticipation)

$$
\begin{aligned}
\frac{d\mathbf{v}}{dt} &= \beta\left[\frac{D\mathbf{u}}{Dt}\right]_V + \frac{3\nu\beta}{{r_p}^2}\left([\mathbf{u}]_S - \mathbf{v}\right) \\
&+ \frac{3\beta}{r_p}\int_{t-t_h}^{t}\left(\frac{\nu}{\pi(t-\tau)}\right)^{\frac{1}{2}}\frac{d}{d\tau}\left([\mathbf{u}]_S - \mathbf{v}\right)d\tau \\
&+ c_{Re_p}\frac{3\nu\beta}{{r_p}^2}\left([\mathbf{u}]_S - \mathbf{v}\right) + \left(1 - \frac{3\ \rho_f}{\rho_f + 2\ \rho_p}\right)\ \mathbf{g}
\end{aligned}
$$

$$\beta \equiv \frac{3\ \rho_f}{(\rho_f + 2\ \rho_p)}$$

$$c_{Re_p} = 0.15 \cdot Re_p^{0.687} \qquad Re_p < 1000$$

Effective compressibility

$$\frac{d\boldsymbol{v}(t)}{dt} = -\frac{1}{\tau}\left(\boldsymbol{v}(t) - \boldsymbol{u}(\boldsymbol{x},t)\right)$$

$$\boldsymbol{v}(t) = \boldsymbol{u}(\boldsymbol{x},t) - \tau\frac{d\boldsymbol{v}(t)}{dt} \sim \tau\boldsymbol{a}$$

$$\boxed{\boldsymbol{\nabla}\cdot\boldsymbol{v}(t) \simeq \tau\boldsymbol{\nabla}\left(\boldsymbol{u}\cdot\boldsymbol{\nabla}\boldsymbol{u}\right)}$$

Statistical role of singularities ??

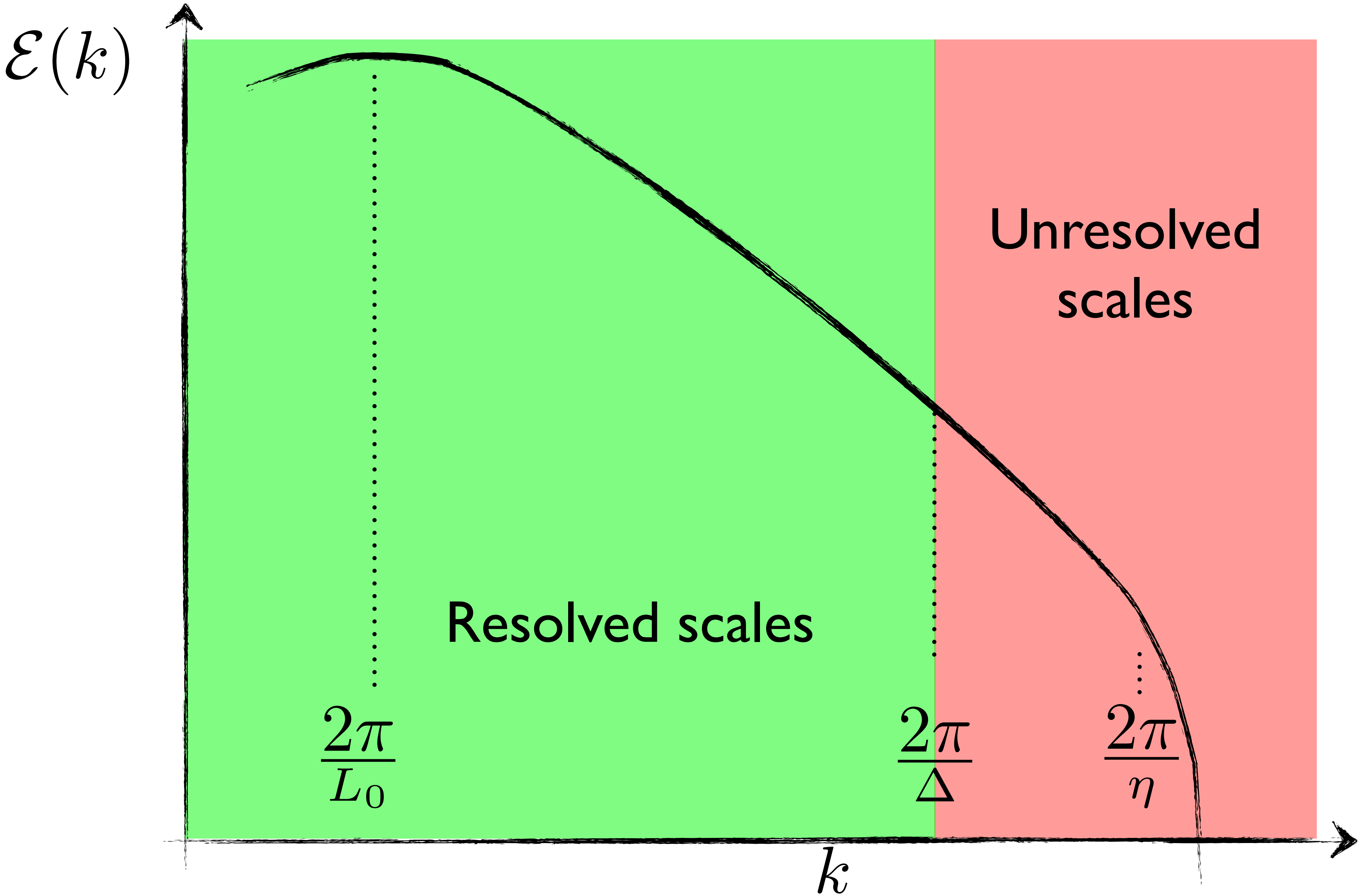
How to save ?

- Simulations of particles in turbulence can be very expensive in terms of time and resources allocated

- How to save ? Two ideas...

  - Save on computing the Eulerian field
    - **Large Eddy Simulation**
  - Save on computing the particles
    - **Eulerian-Eulerian description**

Large Eddy Simulation: LES



Particle in under-resolved field

- Evolution of particles in a velocity field which "resolves" only the larger scales (LES)

- Is this possible at all ?

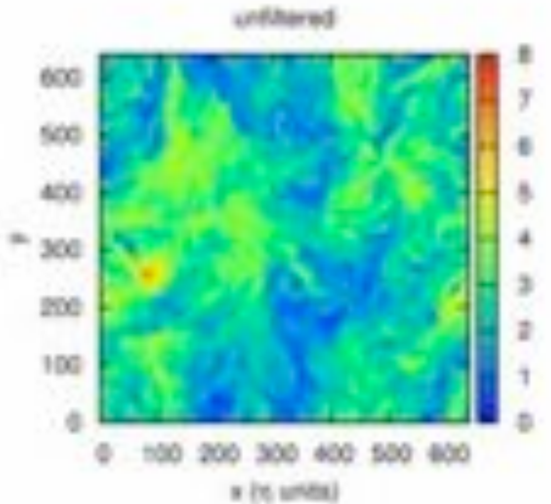
- What are the errors and how to quantify them ?

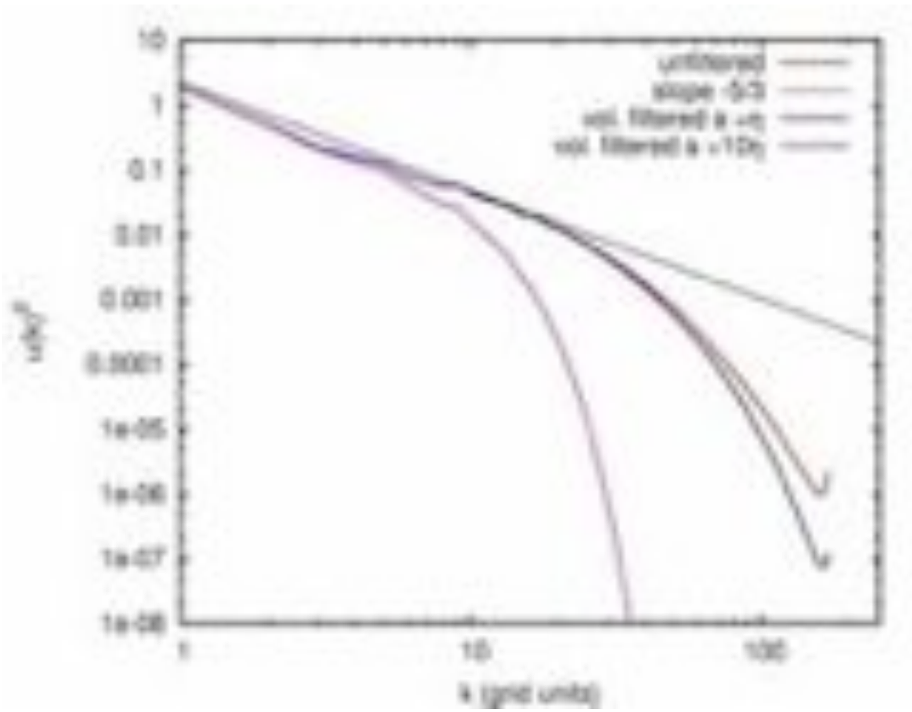
  E. Calzavarini, A. Donini, V. Lavezzo, C. Marchioli, E. Pitton, A. Soldati and F. Toschi "On the Error Estimate in Sub-Grid Models for Particles in Turbulent Flows" Proceedings DLES8 2010

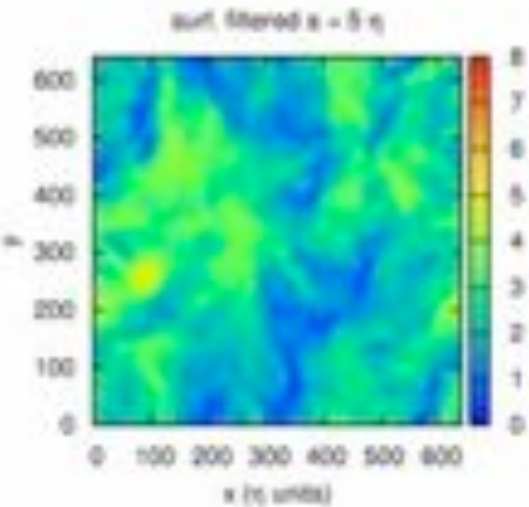
- Need for models ?

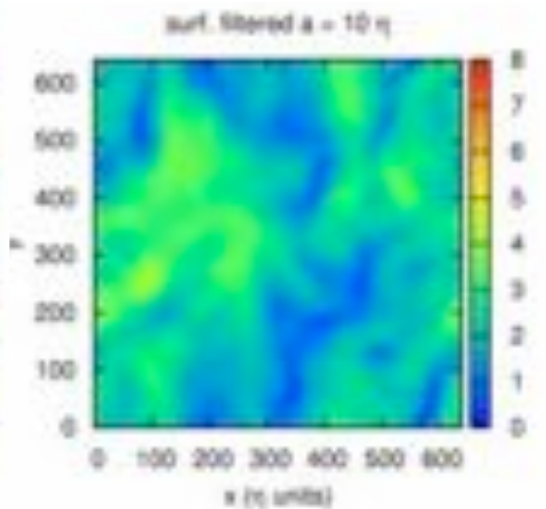
Description of the simulation

Filtering effect on a section of the velocity field



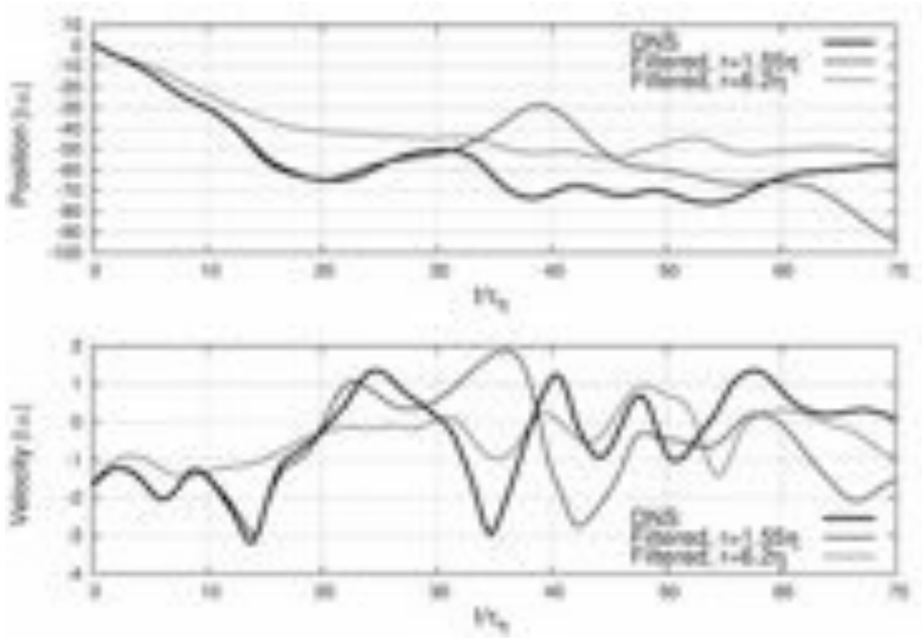






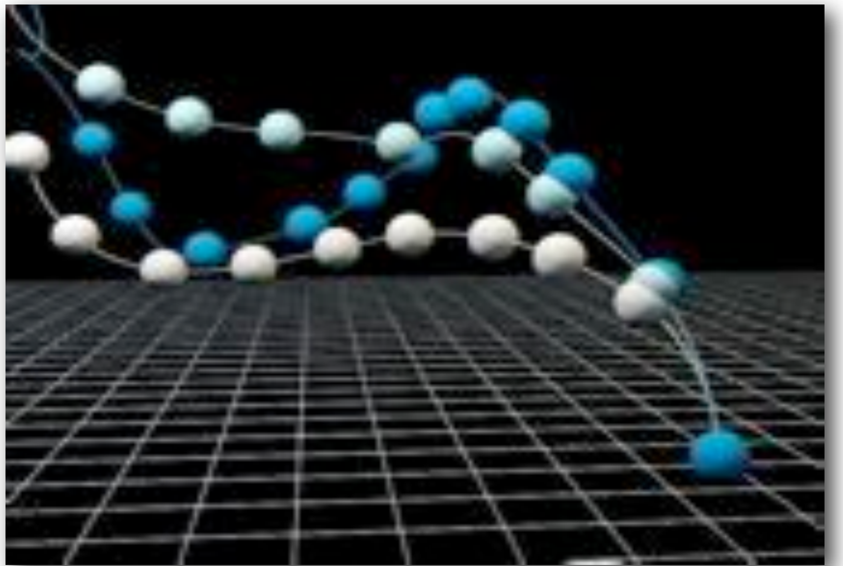
Filtering effect on the energy spectra.

Single particle analysis



An example of trajectory and velocity of a typical particle. Every curve corresponds to a different filtering amplitude.

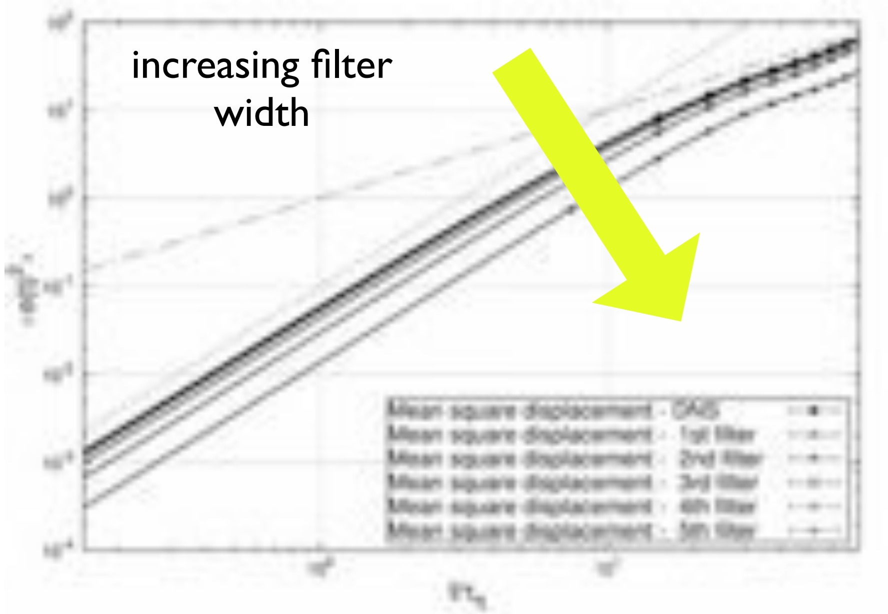
Increasing the filter width the particle sees a "smoother" velocity field.
Larger the filter the sooner the trajectory and velocity become "uncorrelated" with the "real" (i.e. DNS) ones.



Mean square displacement

In isotropic turbulence of zero mean velocity, the first non-vanishing statistical moment is the the variance of displacement:

$$\sigma_X^2(t) = \langle \sum_{i=1}^{3} (x_i(\boldsymbol{x}_0, t_0 | t) - x_{0i})^2 \rangle$$

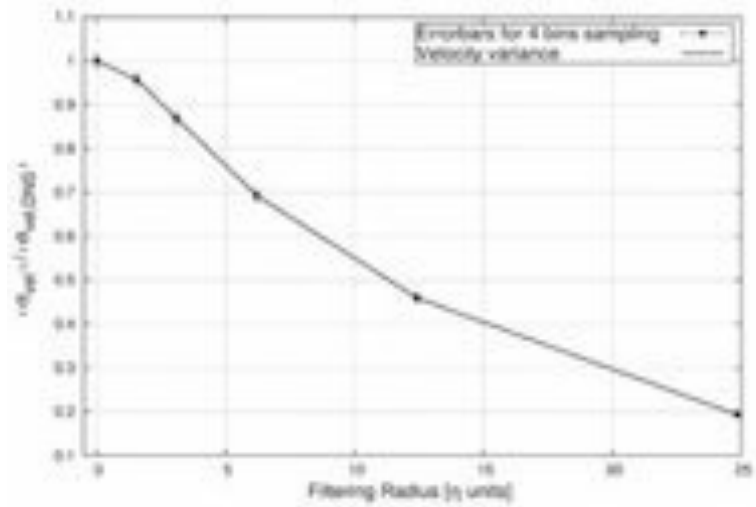


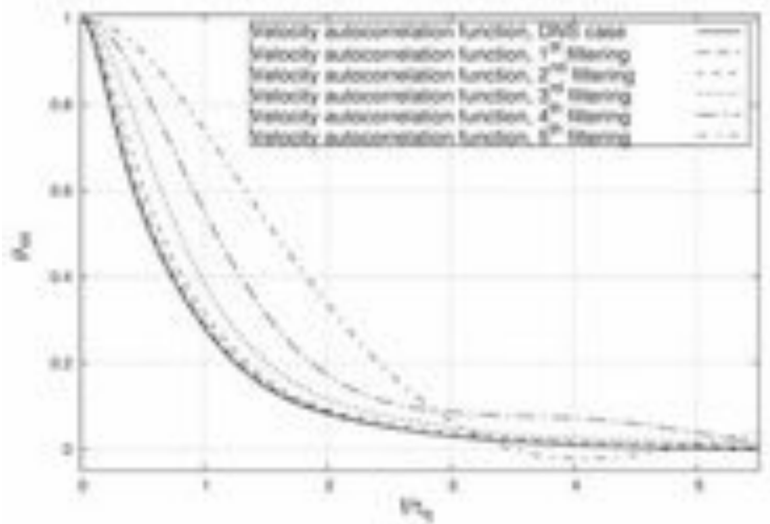
Taylor's theory: two asymptotic results:

$$\begin{cases} \sigma_X(t) = \sigma_V t \\ \sigma_X(t) = \sigma_V (2T_L t)^{1/2} \end{cases}$$

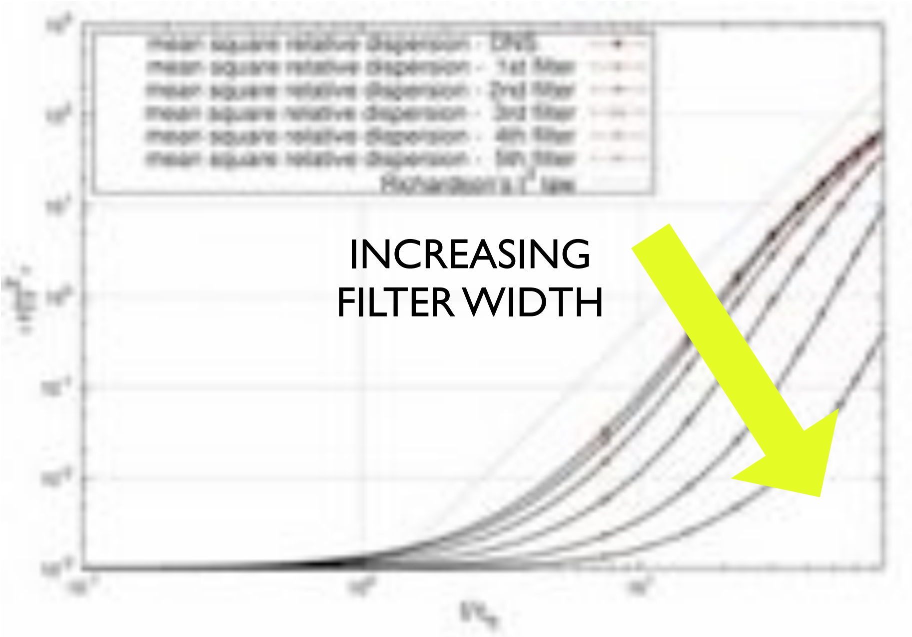
$\sigma_V^2 = \langle V_i V_i \rangle$ Velocity variance

$T_L = \int_0^\infty \rho_v(\tau) d\tau$ Lagrangian integral time

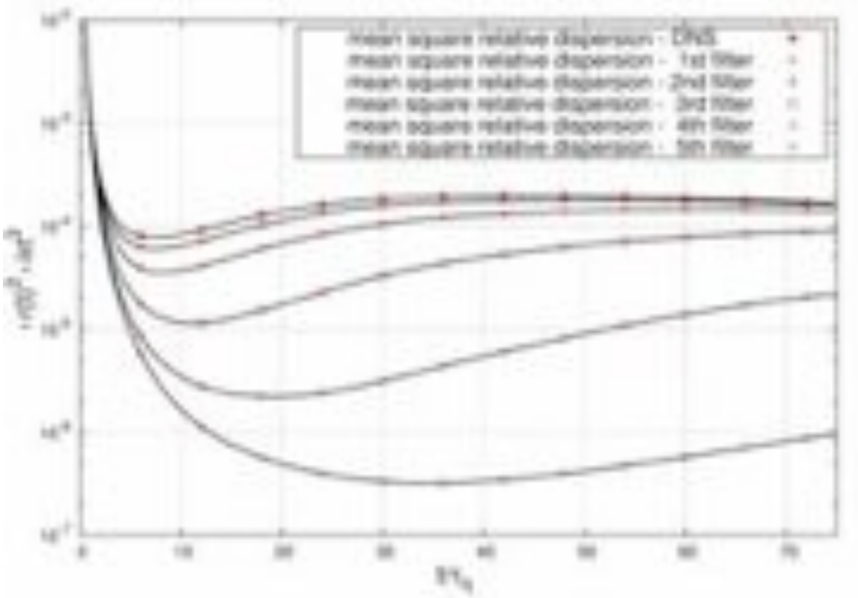




Mean Square Relative Dispersion - HIT



Curves compensated with Richardson's law:



Given the separation distance:

$$\boldsymbol{r}(t) = \boldsymbol{r}^{(1)}(t) - \boldsymbol{r}^{(2)}(t) \qquad r = |\boldsymbol{r}|$$

Richarson's model predictions the scaling law:

$$\langle r^2 \rangle = g \varepsilon t^3$$

Where g is the Richardson's universal constant.

Filtered dispersion is somewhat delayed, making LES less efficient than DNS in predicting the dispersion.

Dispersion is under-predicted by LES.

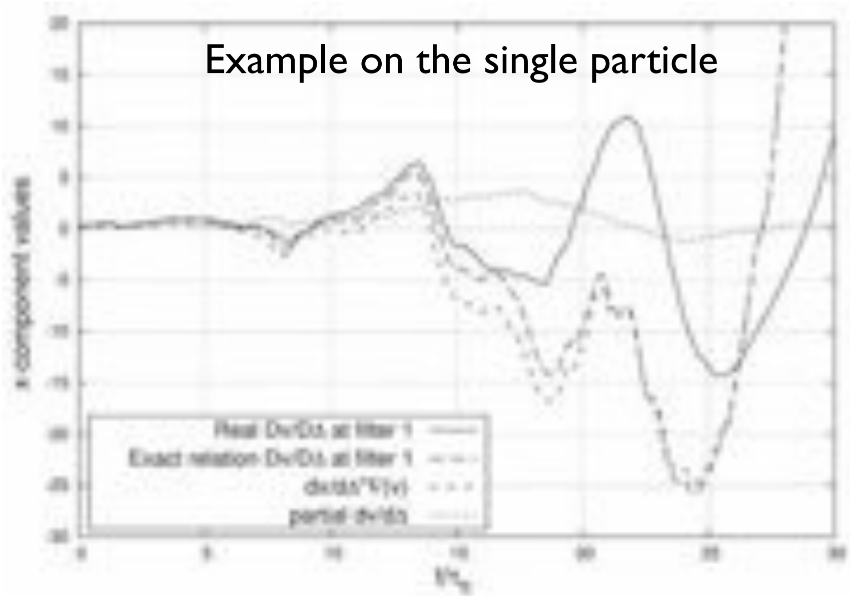
Exact Relation

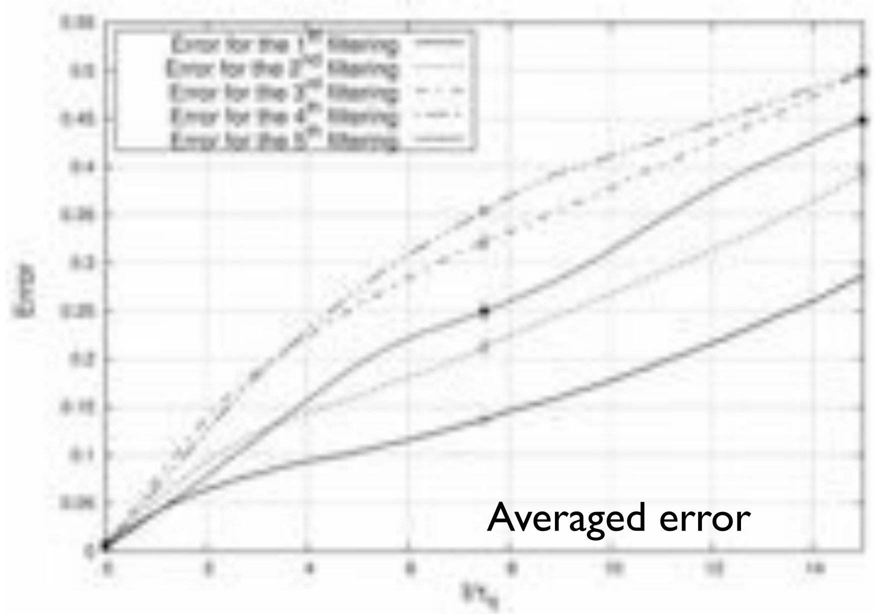
LES error on dispersion is caused by:
1. The **filtered** velocity field
2. The fact that the particle is evolving in a trajectory that is almost no more correlated with the DNS one.

$$\frac{d}{d\Delta}\boldsymbol{v}_{\Delta}(\boldsymbol{x}_{\Delta}(t),t) = \frac{\partial \boldsymbol{u}_{\Delta}}{\partial \Delta} + \frac{\partial \boldsymbol{x}_{\Delta}(t)}{\partial \Delta} \cdot \nabla \boldsymbol{u}_{\Delta}(\boldsymbol{x}_{\Delta}(t),t)$$

And evaluating the error between the two members

$$e = \left| \frac{\left(\frac{d\boldsymbol{v}_{\Delta}}{d\Delta}\right)_{\Delta i+\delta} - \left(\frac{d\boldsymbol{v}_{\Delta}}{d\Delta}\right)_{\Delta(i+1)}}{\frac{\left(\frac{d\boldsymbol{v}_{\Delta}}{d\Delta}\right)_{\Delta i+\delta} + \left(\frac{d\boldsymbol{v}_{\Delta}}{d\Delta}\right)_{\Delta(i+1)}}{2}} \right|$$

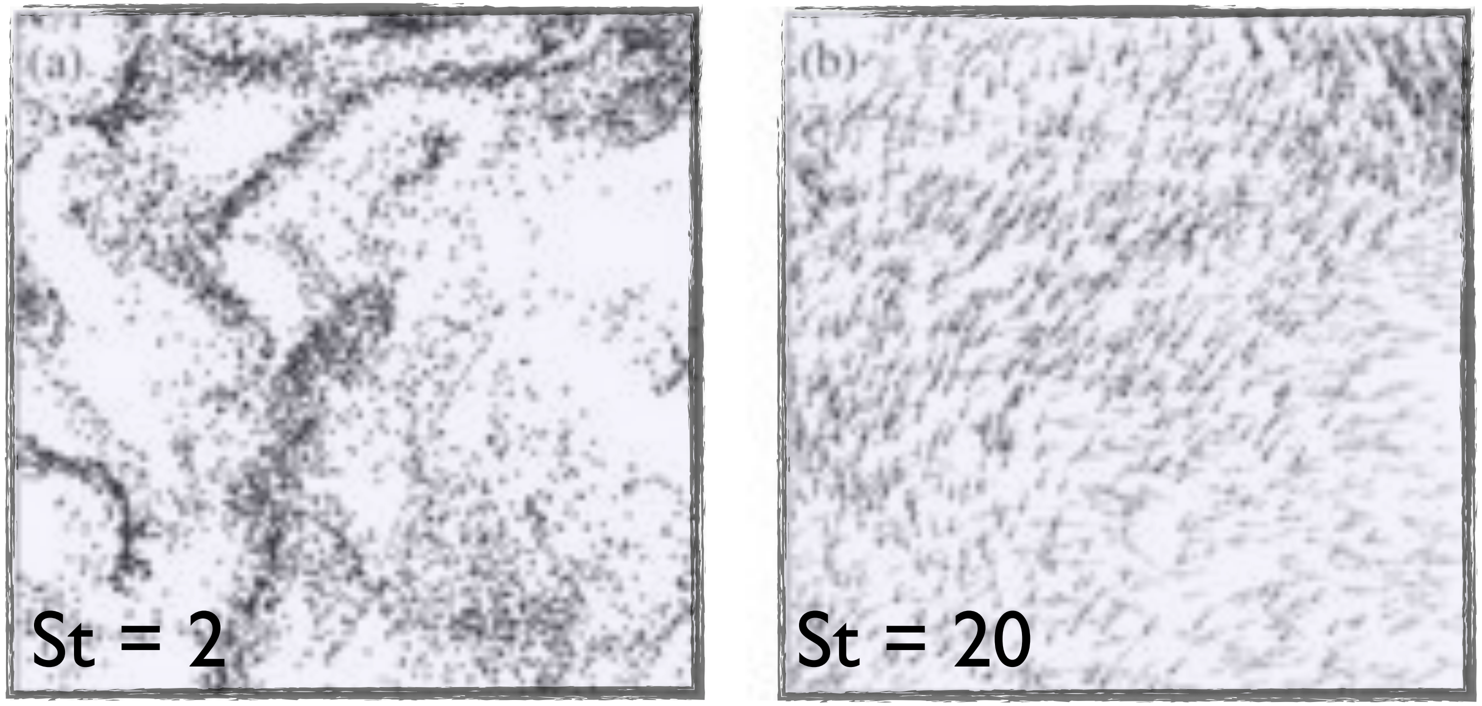




Two fluid description ?

see e.g. Boffetta et al. The Eulerian description of dilute collisionless suspension. EPL (2007) vol. 78 (1) pp. 14001

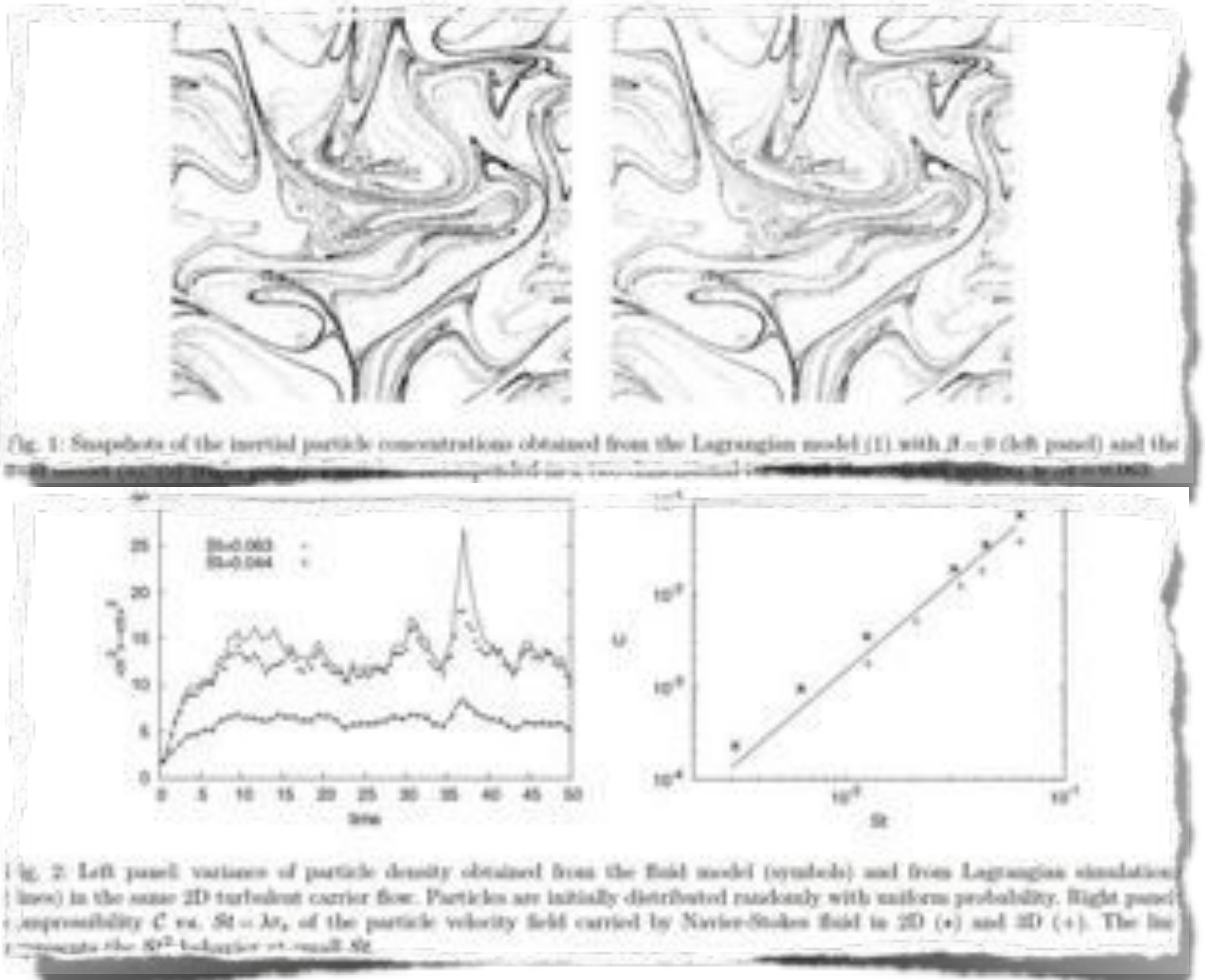
Caustics and "particle velocity field"



(a) Snapshot of the position of particles for St = 2 in a slice of size 5η x 100 η x 100 η for Reλ≈ 400.

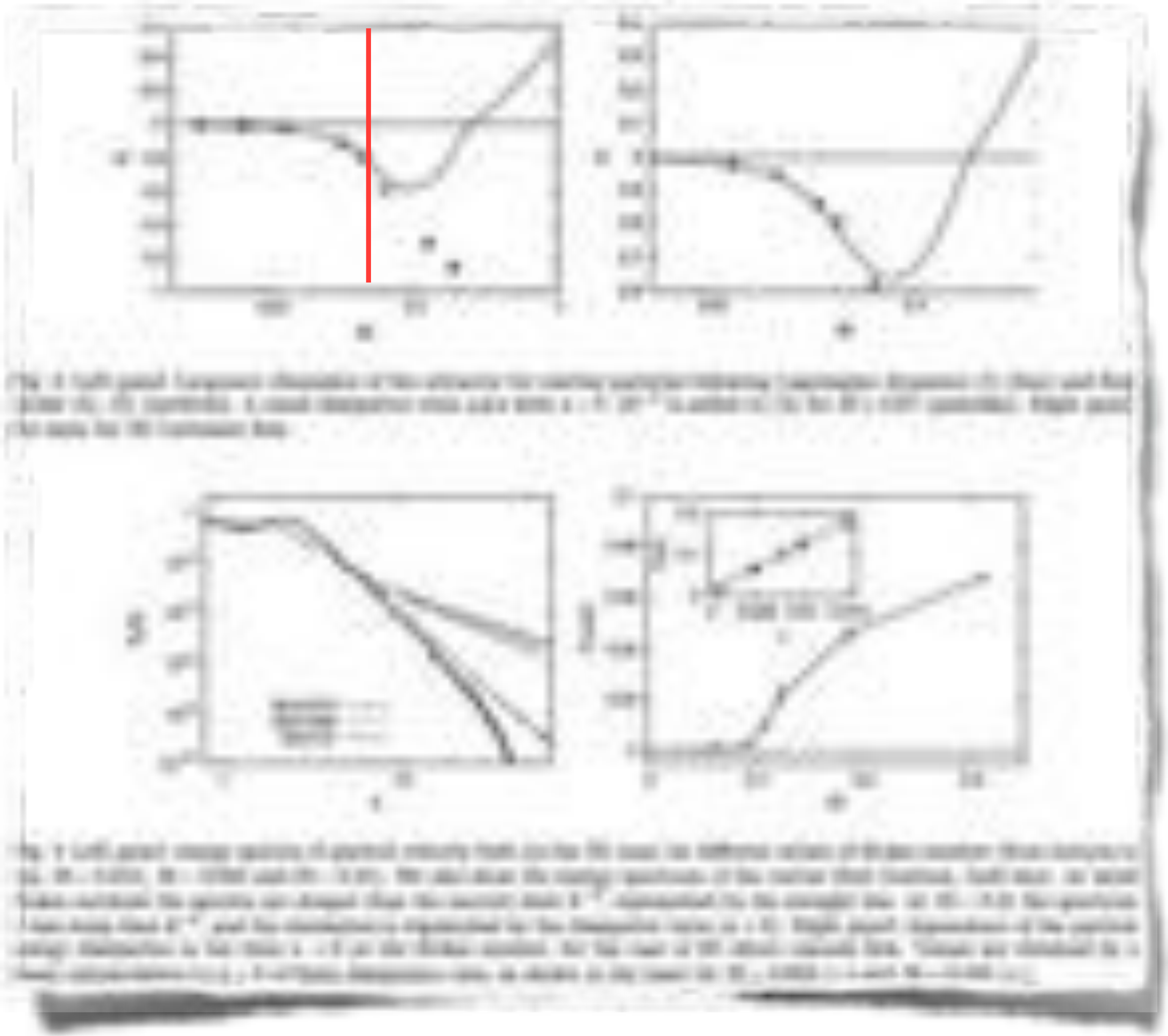
(b) Particle velocity field in the same slice for a larger Stokes, St = 20, showing the existence of regions where particles have different velocities (highlighted by gray and black arrows, respectively).

Eulerian vs. Lagrangian



Boffetta et al. The Eulerian description of dilute collisionless suspension. EPL (2007) vol. 78 (1) pp. 14001

Eulerian vs. Lagrangian



Boffetta et al. The Eulerian description of dilute collisionless suspension. EPL (2007) vol. 78 (1) pp. 14001

The end.

Direct numerical simulations of particles in turbulence
Lecture II

Federico Toschi - *http://www.phys.tue.nl/toschi*

International school
Fluctuations and Turbulence in the
Microphysics and Dynamics of Clouds
Porquerolles, France Sep. 2-10, 2010

Distributed European Infrastructure for Supercomputing Applications

cost

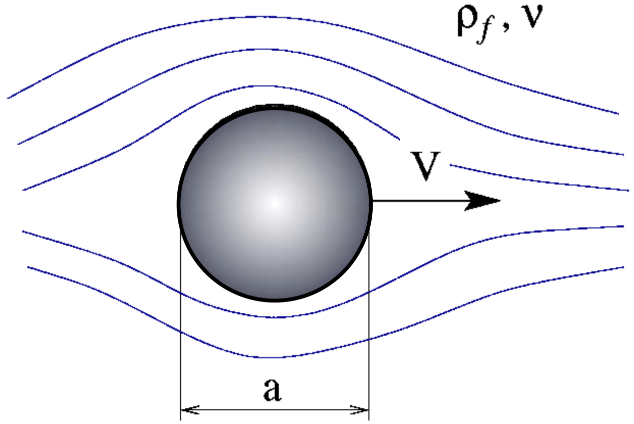
TU/e Technische Universiteit Eindhoven University of Technology

Where innovation starts

Aim & TOC

- Lecture I
  - Numerical methods for fluid
  - Numerical methods for particles
- **Lecture II**
  - Physical modeling
  - Validation
  - iCFDdatabase

Forces on a particle



Minimal bibliography

- Maxey MR, Riley JJ. Equation of motion for a small rigid sphere in a nonuniform flow. Phys Fluids 1983;26(4):883–889.
- Gatignol R. The faxén formulae for a rigid particle in an unsteady non- uniform stokes flow. J Mecanique Theorique et Applique´ e 1983;1(2):143– 160.
- Auton T, Hunt J, Prud'homme M. The force exerted on a body in inviscid unsteady non-uniform rotational flow. J Fluid Mech 1988;197:241–257.
- Lovalenti PM, Brady JF. The hydrodynamic force on a rigid particle undergoing arbitrary time-dependent motion at small reynolds number. J Fluid Mech 1993;545:561–605.

Particle model

- Computational model which allow to treat particles as *pointwise* (from the *computational* point of view)
- Phenomenological forces
- Validation against experiments and fully resolved simulations

Equation of motion

$$
\begin{aligned}
\frac{d\mathbf{v}}{dt} &= \beta\left[\frac{D\mathbf{u}}{Dt}\right]_V + \frac{3\nu\beta}{{r_p}^2}\left([\mathbf{u}]_S - \mathbf{v}\right) \\
&+ \frac{3\beta}{r_p}\int_{t-t_h}^{t}\left(\frac{\nu}{\pi(t-\tau)}\right)^{\frac{1}{2}}\frac{d}{d\tau}\left([\mathbf{u}]_S - \mathbf{v}\right)d\tau \\
&+ c_{Re_p}\frac{3\nu\beta}{{r_p}^2}\left([\mathbf{u}]_S - \mathbf{v}\right) + \left(1 - \frac{3\ \rho_f}{\rho_f + 2\ \rho_p}\right)\ \mathbf{g}
\end{aligned}
$$

r_p particle radius

g gravity acceleration

"density ratio"

$$\beta \equiv \frac{3\ \rho_f}{(\rho_f + 2\ \rho_p)}$$

Equation of motion

$$\frac{d\mathbf{v}}{dt} = \beta\left[\frac{D\mathbf{u}}{Dt}\right]_V + \frac{3\nu\beta}{{r_p}^2}\left([\mathbf{u}]_S - \mathbf{v}\right)$$
$$+ \frac{3\beta}{r_p}\int_{t-t_h}^{t}\left(\frac{\nu}{\pi(t-\tau)}\right)^{\frac{1}{2}}\frac{d}{d\tau}\left([\mathbf{u}]_S - \mathbf{v}\right)d\tau$$
$$+ c_{Re_p}\frac{3\nu\beta}{{r_p}^2}\left([\mathbf{u}]_S - \mathbf{v}\right) + \left(1 - \frac{3\,\rho_f}{\rho_f + 2\,\rho_p}\right)\mathbf{g}$$

Particle radius r_p

Particle diameter $d_p = 2r_p$

$$Re_p \equiv |[\mathbf{u}]_S - \mathbf{v}|\,d_p/\nu \qquad \beta \equiv \frac{3\,\rho_f}{(\rho_f + 2\,\rho_p)}$$

Faxen correction - I

$$\frac{d\mathbf{v}}{dt} = \beta\left[\frac{D\mathbf{u}}{Dt}\right]_V + \frac{3\nu\beta}{{r_p}^2}\left([\mathbf{u}]_S - \mathbf{v}\right)$$

$$+ \frac{3\beta}{r_p}\int_{t-t_h}^{t}\left(\frac{\nu}{\pi(t-\tau)}\right)^{\frac{1}{2}}\frac{d}{d\tau}\left([\mathbf{u}]_S - \mathbf{v}\right)d\tau$$

$$+ c_{Re_p}\frac{3\nu\beta}{{r_p}^2}\left([\mathbf{u}]_S - \mathbf{v}\right) + \left(1 - \frac{3\ \rho_f}{\rho_f + 2\ \rho_p}\right)\ \mathbf{g}$$

$$\left[\frac{D\mathbf{u}}{Dt}\right]_V = (4/3\ \pi r_p^3)^{-1}\int_V \frac{D\mathbf{u}}{Dt}(\mathbf{x},\mathbf{t})\ \mathbf{d^3x}$$

$$[\mathbf{u}]_S = (4\pi r_p^2)^{-1}\int_S \mathbf{u}(\mathbf{x},\mathbf{t})\ \mathbf{d^2x}$$

Faxen correction - II

$$\left[\frac{D\mathbf{u}}{Dt}(\mathbf{x},\mathbf{t})\right]_V \simeq \int\int\int_{\frac{-L}{2}}^{\frac{+L}{2}} G(\mathbf{x}')\ \frac{\mathbf{Du}}{\mathbf{Dt}}(\mathbf{x}-\mathbf{x}',\mathbf{t})\ \mathbf{d^3x}'$$

$$[\mathbf{u}(\mathbf{x},\mathbf{t})]_S = \frac{1}{3r_p^2}\frac{d}{dr_p}\left(r_p^3\ [\mathbf{u}(\mathbf{x},\mathbf{t})]_V\right) = \mathcal{DFT}^{\ -1}\left[\left(1-\sigma^2\mathbf{k^2}/\mathbf{3}\right)\tilde{G}(\mathbf{k})\ \tilde{\mathbf{u}}(\mathbf{k},\mathbf{t})\right].$$

$$\tilde{G}(\mathbf{k}) = \exp\left(\frac{-\sigma^2\mathbf{k}^2}{2}\right)$$

$$\downarrow \quad \sigma \equiv r_p/\sqrt{5}$$

$$\tilde{G}(\mathbf{k}) \simeq 1 - \left(\frac{r_p^2}{10}\right)\mathbf{k}^2 + \mathcal{O}(r_p^4)$$

$$\mathbf{u} + \left(\frac{r_p^2}{10}\right)\Delta\mathbf{u} + \mathcal{O}(r_p^4)$$

iCFDdatabase: FAT

Fluid tracer

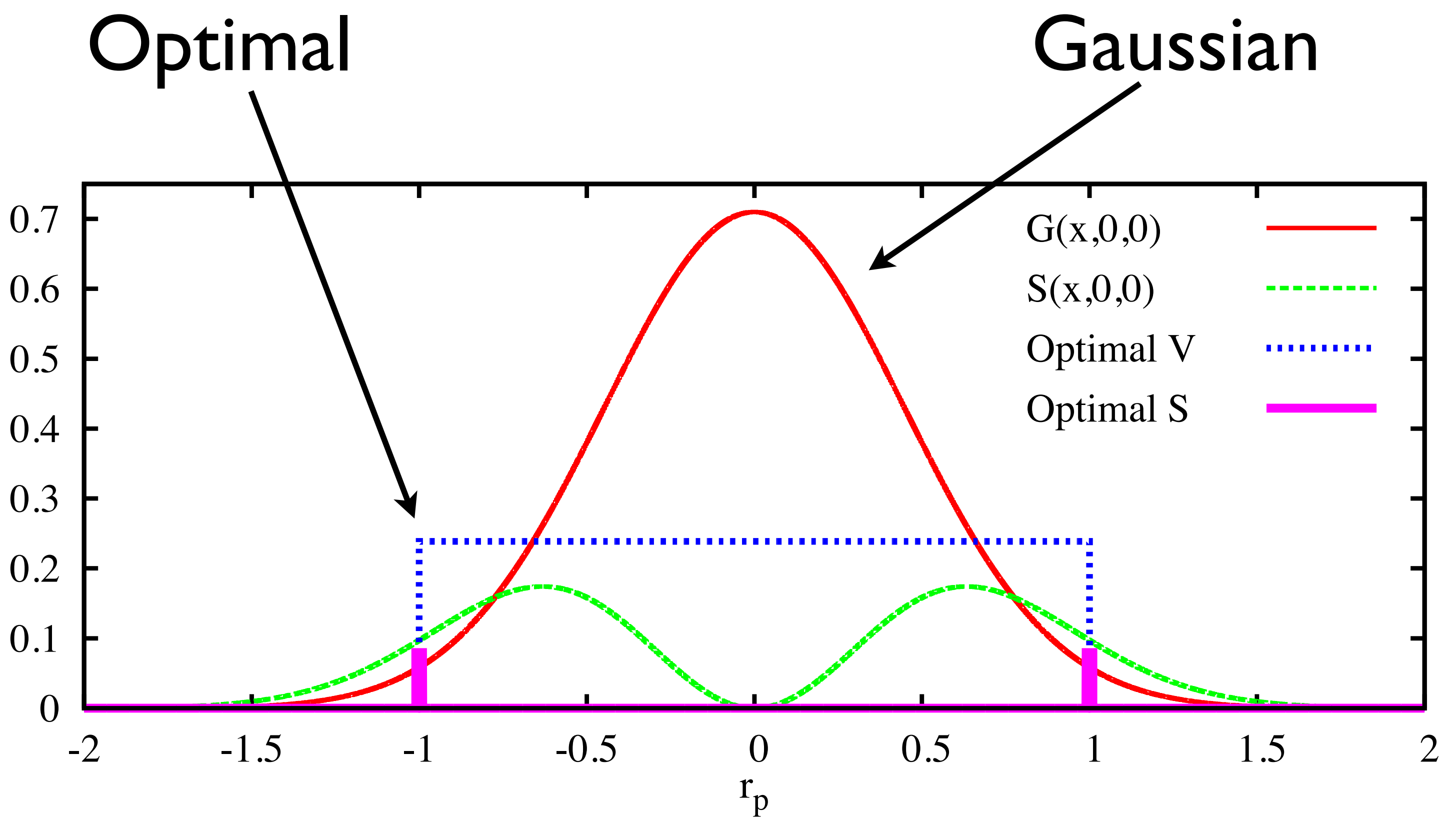


Figure 1: Real space one-dimensional projection, on the direction (x,0,0), of filter functions. The volume gaussian filter is $G(\mathbf{x}) = (1/(\sqrt{2\pi}\sigma))^3 \exp(-\mathbf{x}^2/(2\sigma^2))$, while the surface convolution kernel turns out to be $S(\mathbf{x}) = (\mathbf{x}^2/(2\sigma^2))G(\mathbf{x})$. The optimal shape of volume and surface filter functions are also shown.

History force

$$
\begin{aligned}
\frac{d\mathbf{v}}{dt} &= \beta\left[\frac{D\mathbf{u}}{Dt}\right]_V + \frac{3\nu\beta}{{r_p}^2}\left([\mathbf{u}]_S - \mathbf{v}\right) \\
&+ \frac{3\beta}{r_p}\int_{t-t_h}^{t}\left(\frac{\nu}{\pi(t-\tau)}\right)^{\frac{1}{2}}\frac{d}{d\tau}\left([\mathbf{u}]_S - \mathbf{v}\right)d\tau \\
&+ c_{Re_p}\frac{3\nu\beta}{{r_p}^2}\left([\mathbf{u}]_S - \mathbf{v}\right) + \left(1 - \frac{3\,\rho_f}{\rho_f + 2\,\rho_p}\right)\mathbf{g}
\end{aligned}
$$

History force based on the Basset-Boussinesq diffusive kernel, ~ $(t - \tau)^{-1/2}$, while t_h the time over which the memory effect is significant

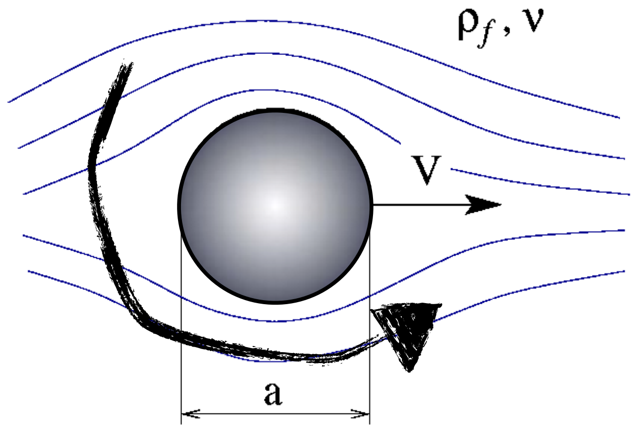
History force

$$
\begin{aligned}
\frac{d\mathbf{v}}{dt} &= \beta\left[\frac{D\mathbf{u}}{Dt}\right]_V + \frac{3\nu\beta}{{r_p}^2}\left([\mathbf{u}]_S - \mathbf{v}\right) \\
&+ \frac{3\beta}{r_p}\int_{t-t_h}^{t}\left(\frac{\nu}{\pi(t-\tau)}\right)^{\frac{1}{2}}\frac{d}{d\tau}\left([\mathbf{u}]_S - \mathbf{v}\right)d\tau \\
&+ c_{Re_p}\frac{3\nu\beta}{{r_p}^2}\left([\mathbf{u}]_S - \mathbf{v}\right) + \left(1 - \frac{3\ \rho_f}{\rho_f + 2\ \rho_p}\right)\ \mathbf{g}
\end{aligned}
$$

Schiller-Naumann (SN) parametrization

$$c_{Re_p} = 0.15 \cdot Re_p^{0.687} \qquad Re_p < 1000$$

Particle may also rotate: Torque ?

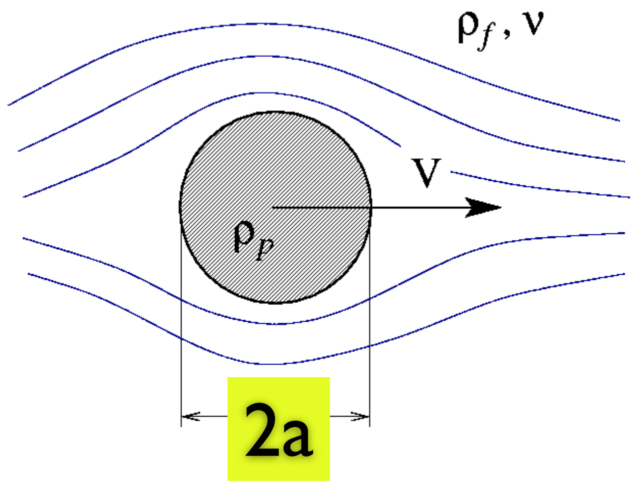


$$\frac{d\omega}{dt} = \frac{\rho_f}{\rho_p} \left(\left[\frac{D\mathbf{\Omega}}{Dt} \right]_V + \frac{15\nu}{a^2} \left([\mathbf{\Omega}]_S - \omega \right) \right)$$

Step back: Simplified particle's equation of motion

$a << \eta$

$Re_a = a v_a / \nu << 1$



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

$$\frac{d\mathbf{v}}{dt} = \beta \frac{D}{Dt}\mathbf{u}(\mathbf{x}(t), t) - \frac{1}{\tau_p}(\mathbf{v} - \mathbf{u}(\mathbf{x}(t), t))$$

$$\beta = \frac{3\rho_f}{\rho_f + 2\rho_p} \qquad \tau_p = \frac{1}{3\beta}\frac{a^2}{\nu} \qquad St \equiv \frac{\tau_p}{\tau_\eta} = \frac{1}{3\beta}\frac{a^2}{\eta^2}$$

iCFDdatabase: LIGHT

(essentially: Maxey & Riley Phys. Fluids 1983, T.R.Auton et al. JFM 1988)

Another step back

$$\frac{d\boldsymbol{x}}{dt} = \boldsymbol{v}$$

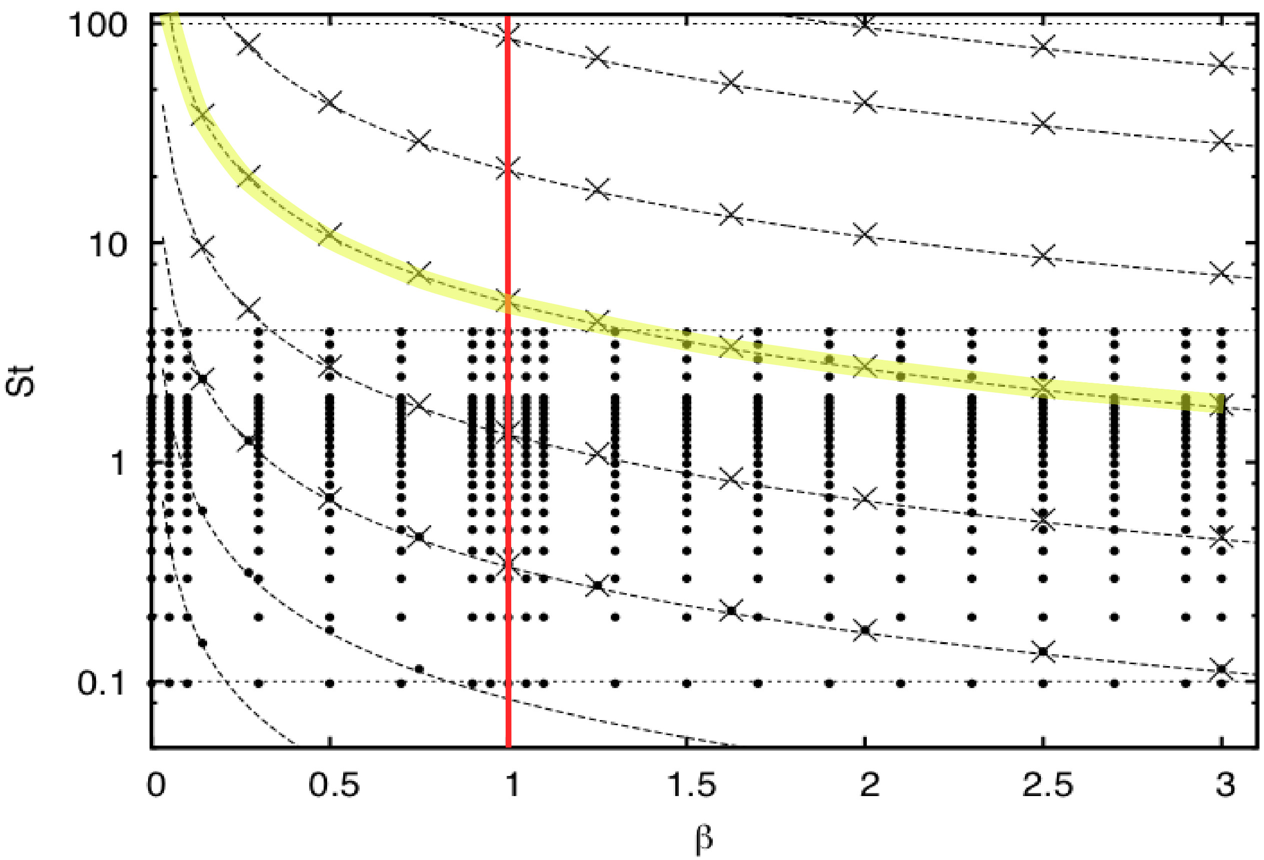
$$\frac{d\boldsymbol{v}}{dt} = -\frac{1}{\tau_p}\left(\boldsymbol{v} - \boldsymbol{u}(\boldsymbol{x}(t), t)\right)$$

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

iCFDdatabase: HEAVY

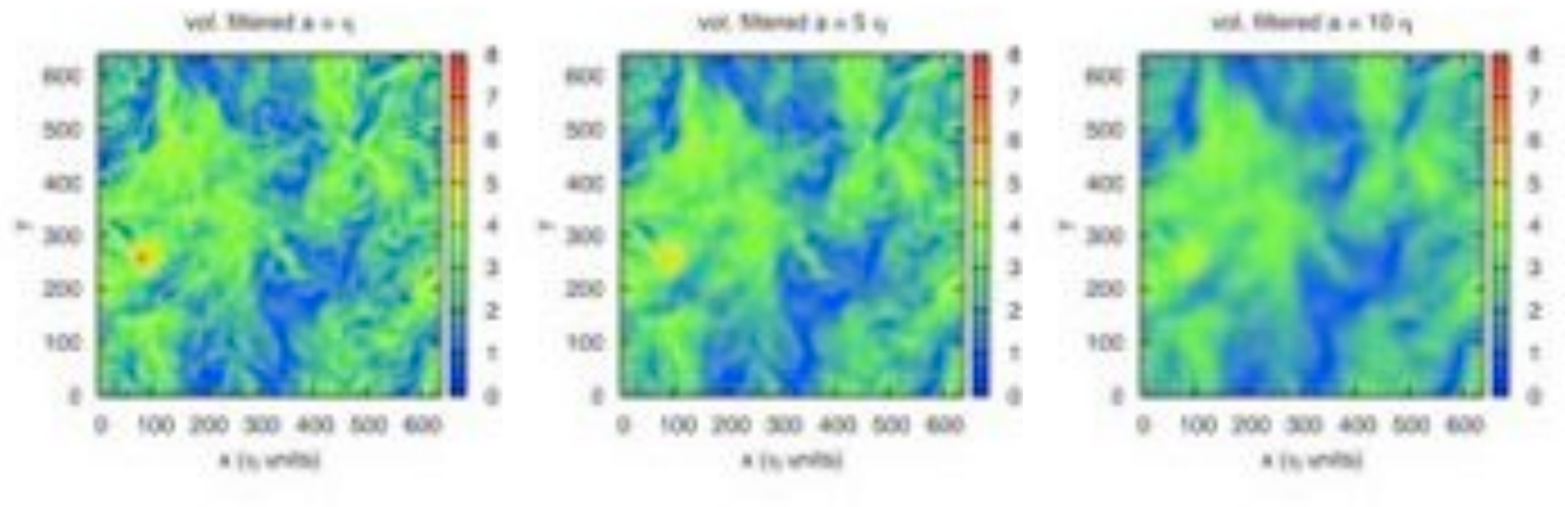
Radius

$$\tau_p = \frac{r_p^2}{3\beta\nu} \qquad \beta \equiv \frac{3\ \rho_f}{(\rho_f + 2\ \rho_p)}$$



$\longleftarrow r_p = \mathrm{const}$

Particles in LES vs. finite size



Finite size particles ⟷ Particle in LES velocity field

Duality between the problem of finite size particles and point-wise particles in a LES velocity field

Tracers: DNS vs. Experiments

Tracers

TOC

- *Perfect testcase to compare against experiments* (no modeling uncertainties) ! Will expose all issues due to numerics and experiments...

- Reynolds number issues
- Structure functions of velocity differences
- acceleration
- effect of vortex filaments
- pair and shape evolution

Toschi and Bodenschatz. Lagrangian Properties of Particles in Turbulence.
ANNUAL REVIEW OF FLUID MECHANICS (2009) vol. 41 pp. 375-404

Multifractal framework

The "standard model"

$$S_p(r) = \langle [\boldsymbol{v}(\boldsymbol{x}+\boldsymbol{r}) - \boldsymbol{v}(\boldsymbol{x})]^p \rangle$$

$$S_p(r) = \langle (\delta_r v)^p \rangle \sim \langle v_0^p \rangle \int_I dh \left(\frac{r}{L_0} \right)^{hp+3-D(h)}$$

$$S_p(r) \sim \left(\frac{r}{L_0} \right)^{\zeta_p}$$

Multi-fractal model
Parisi-Frisch 1995

$$\eta \ll r \ll L_0$$

$$\zeta_p = \inf_h (hp + 3 - D(h))$$

$$D(h)$$

See lecture of L. Biferale

Lagrangian velocity statistics

$$S_p(r) \equiv \langle (u(x+r) - u(x))^p \rangle \sim r^{\zeta_E(p)}$$

$$S_p(\tau) \equiv \langle (v(t+\tau) - v(\tau))^p \rangle \sim \tau^{\zeta_L(p)}$$

$$S_2(\tau) = c_0 \varepsilon \cdot \tau$$

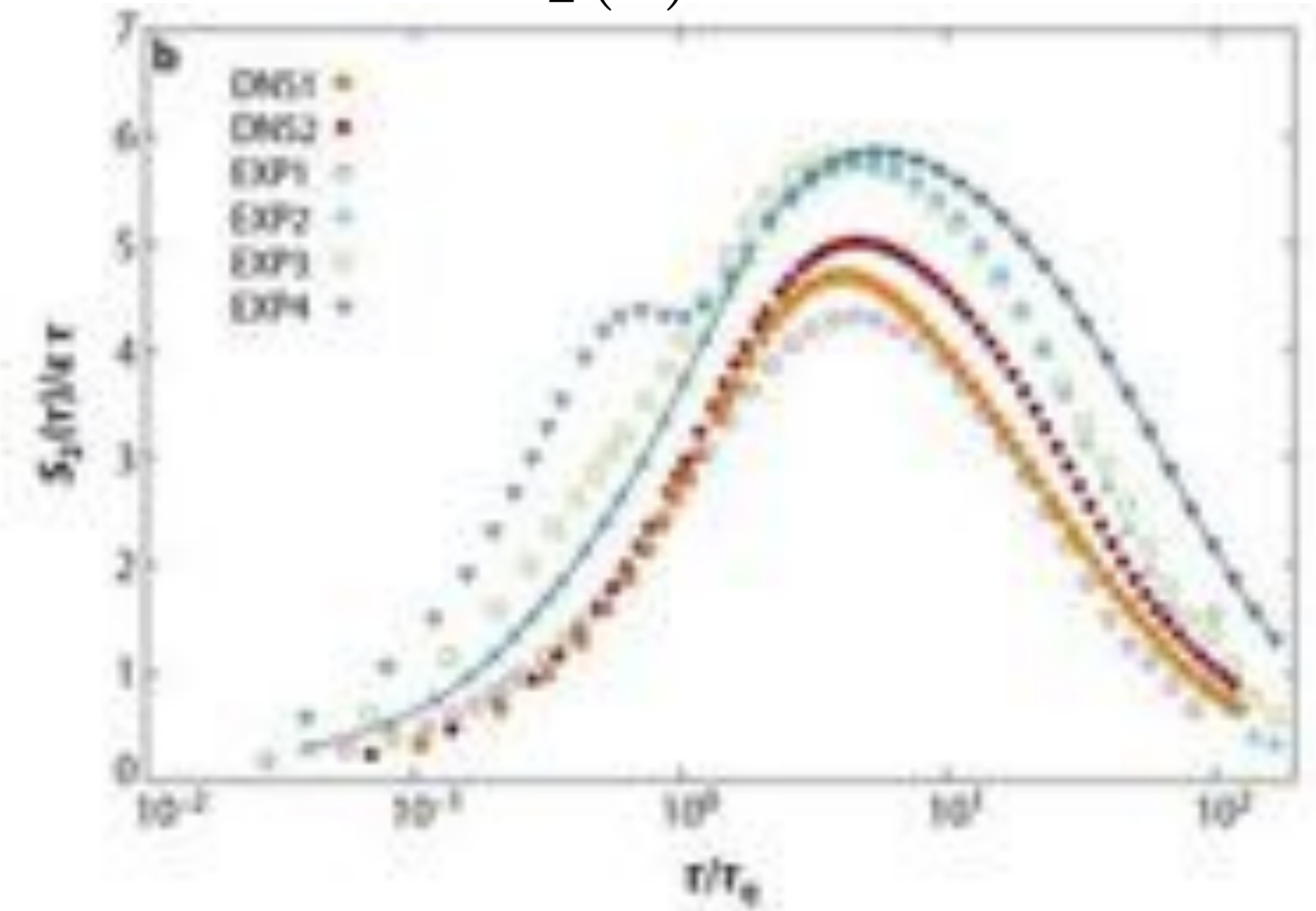
$$\tau_\eta \ll \tau \ll T_L$$

Does it exist and how to estimate $\zeta_L(p)$?

In Eulerian turbulence we have $\zeta_E(p) = \inf_h (hp + 3 - D(h))$

S_2: where we stand

$$S_2(\tau) \propto \varepsilon\tau$$



Biferale et al. Lagrangian structure functions in turbulence: A quantitative comparison between experiment and direct numerical simulation, Phys Fluids 20 (6):065103 (2008)

MF: Lagrangian velocity statistics

We assume that τ and r are linked by the typical eddy turn over time at the given spatial scale

$$\tau_r \sim r/\delta_r u$$

Bridge between eulerian and lagrangian description:

$$\delta_\tau v \sim \delta_r u \qquad \tau \sim \frac{L_0^h}{v_0} r^{1-h}$$

Lagrangian structure functions

MF: Lagrangian structure functions

Multifractal prediction for the Lagrangian structure functions

$$S_p(\tau) \sim \langle v_0^p \rangle \int_{h \in I} \mathrm{d}h \left(\frac{\tau}{T_L} \right)^{\frac{hp+3-D(h)}{1-h}}$$

Same D(h) that for the Eulerian field !!

where

$$\zeta_L(p) = \inf_h \left(\frac{hp + 3 - D(h)}{1-h} \right)$$

This allow us to actually predict the following value:

$$\frac{\zeta_L(4)}{\zeta_L(2)} = 1.71 \qquad \frac{\zeta_L(6)}{\zeta_L(2)} = 2.16 \qquad \frac{\zeta_L(8)}{\zeta_L(2)} = 2.72$$

Velocity structure functions (tracers)

Eulerian (space) -> Lagrangian (time)

$$\delta_r v = v_0 \cdot \left(\frac{r}{L_0}\right)^h$$

$$\delta_\tau v \sim \left(\frac{\tau}{T_L}\right)^{\frac{h}{1-h}}$$

$$\delta_\tau v = v_0 \cdot \left(\frac{\tau}{T_L}\right) \cdot \left[\left(\frac{\tau}{T_L}\right)^\beta + \left(\frac{\tau_\eta}{T_L}\right)^\beta\right]^{\frac{2h-1}{\beta(1-h)}}$$

$$\delta_\tau v \sim \left(\frac{\tau}{T_L}\right)^{\frac{h}{1-h}}$$

$$\delta_r v \propto \tau$$

Start from Eulerian

$$D(h)$$

$$\beta = 4$$

Magnifying glass: Local Scaling Exponents

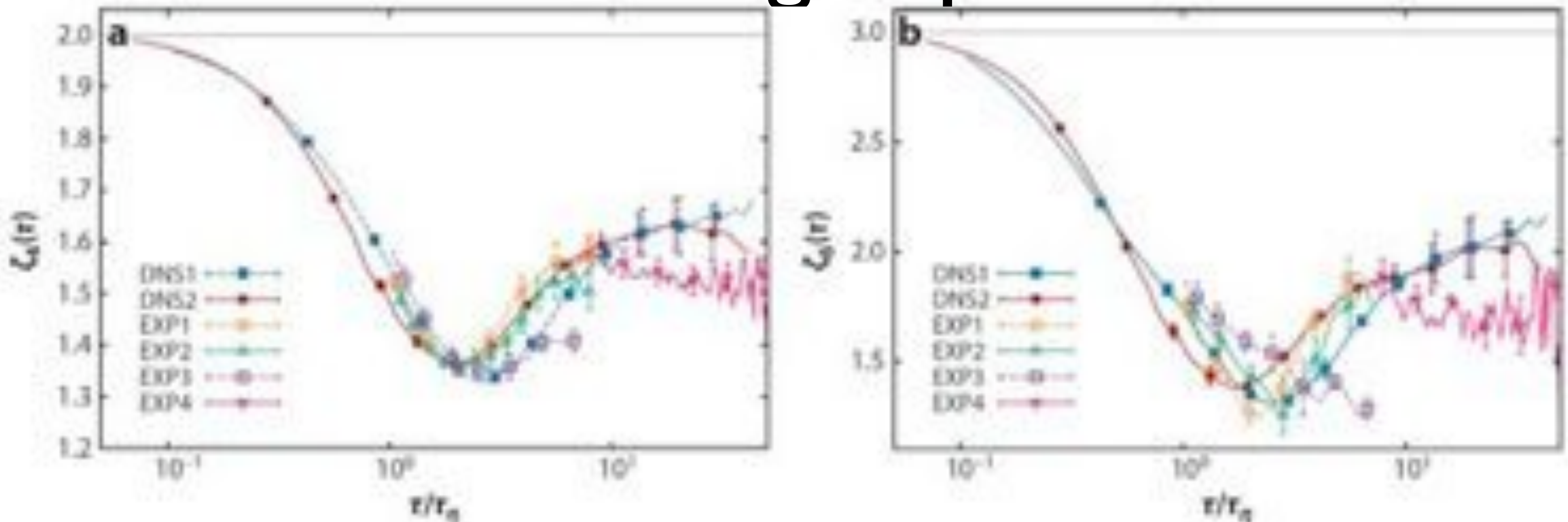
$$\zeta_p(\tau) = \frac{\mathrm{d}\log(S_p(\tau))}{\mathrm{d}\log(S_2(\tau))}$$

The local exponents $\zeta_p(\tau)$ act as **magnifying glass**, probing locally the value of the scaling exponents. By comparing with $S_2(\tau)$ we also take advantage of the Extended Self Similarity (ESS)

Power law scaling →

→ plateaux for local scaling exponents

Local scaling exponents



$$S_p(\tau) \equiv \langle (v(t+\tau) - v(t))^p \rangle \sim \tau^{\zeta_L(p)}$$

$$\zeta_p(\tau) = \frac{\mathrm{d}\log\left(S_p(\tau)\right)}{\mathrm{d}\log\left(S_2(\tau)\right)}$$

Biferale et al. Lagrangian structure functions in turbulence: A quantitative comparison between experiment and direct numerical simulation, Phys Fluids 20 (6):065103 (2008)

No.	R_λ	v'_{rms}	ε	ν	η	L	T_L	τ_η	T	Δx	N^3	N_p
DNS1	183	1.5	0.886	0.00205	0.01	3.14	2.1	0.048	5	0.012	512^3	0.96×10^6
DNS2	284	1.7	0.81	0.00088	0.005	3.14	1.8	0.033	4.4	0.006	1024^3	1.92×10^6

No.	R_λ	v'_{rms} (m/s)	ε ($\mathrm{m^2/s^3}$)	η (μm)	τ_η (ms)	T_L (s)	N_f (f/τ_η)	meas. vol. in (L^3)	Δx (μm/pix)	N_R	N_{tr}
EXP1	350	0.11	2.0×10^{-2}	84	7.0	0.63	35	$0.4\times0.4\times0.4$	50	500	9.3×10^5
EXP2	690	0.42	1.2	30	0.90	0.16	24	$0.3\times0.3\times0.3$	80	480	9.6×10^5
EXP3	815	0.59	3.0	23	0.54	0.11	15	$0.3\times0.3\times0.3$	80	500	1.7×10^6
EXP4	690	0.42	1.2	30	0.90	0.16	24	$0.7\times0.7\times0.7$	200	1200	6.0×10^6

Experiments trajectories

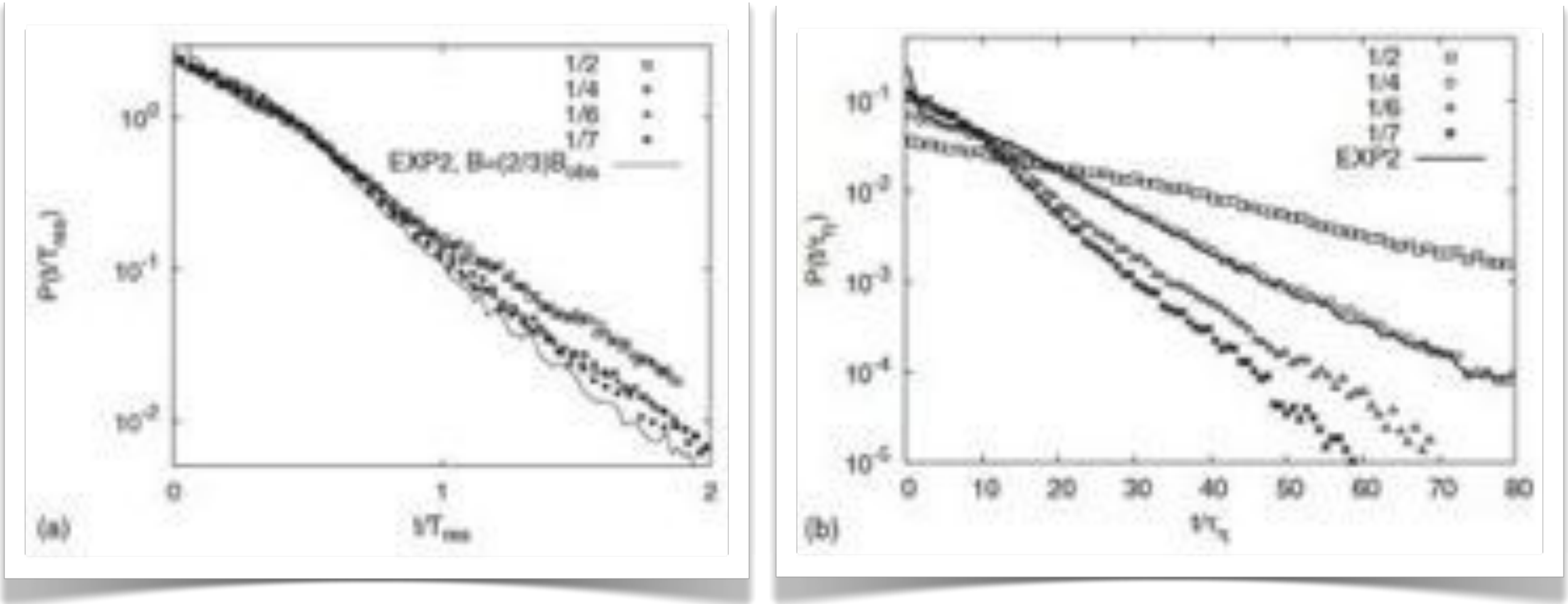


FIG. 6. (a) Comparison of the probability $\mathcal{P}(t/T_{res})$ that a trajectory lasts a time t vs t/T_{res} for the experiment EXP2 and for DNS2 trajectories measured in different numerical measurement domains $\mathcal{L}/\mathcal{B}=\frac{1}{2},\frac{1}{4},\frac{1}{6},\frac{1}{7}$, where T_{res} is the residence time and $\mathcal{L}=2\pi$ is the computational box. For DNS trajectories, T_{res} is determined from the size of the subdomain as $T_{res}=L/v'_{rms}$. For experimental trajectories, $T_{res}=(\frac{2}{3})B_{obs}/v'_{rms}$, where B_{obs} is the size of the measurement volume, as given in Table I. Data for $t/T_{res}>2$, for DNS at $\mathcal{L}/\mathcal{B}=\frac{1}{4},\frac{1}{6},\frac{1}{7}$ and for the experiment, have been cut out. (b) Comparison of the probability $\mathcal{P}(t/\tau_\eta)$ that a trajectory lasts a time t vs t/τ_η for the same data as before.

Biferale et al. Lagrangian structure functions in turbulence: A quantitative comparison between experiment and direct numerical simulation. Phys Fluids (2008) vol. 20 (6) pp. 065103

Finite trajectory length

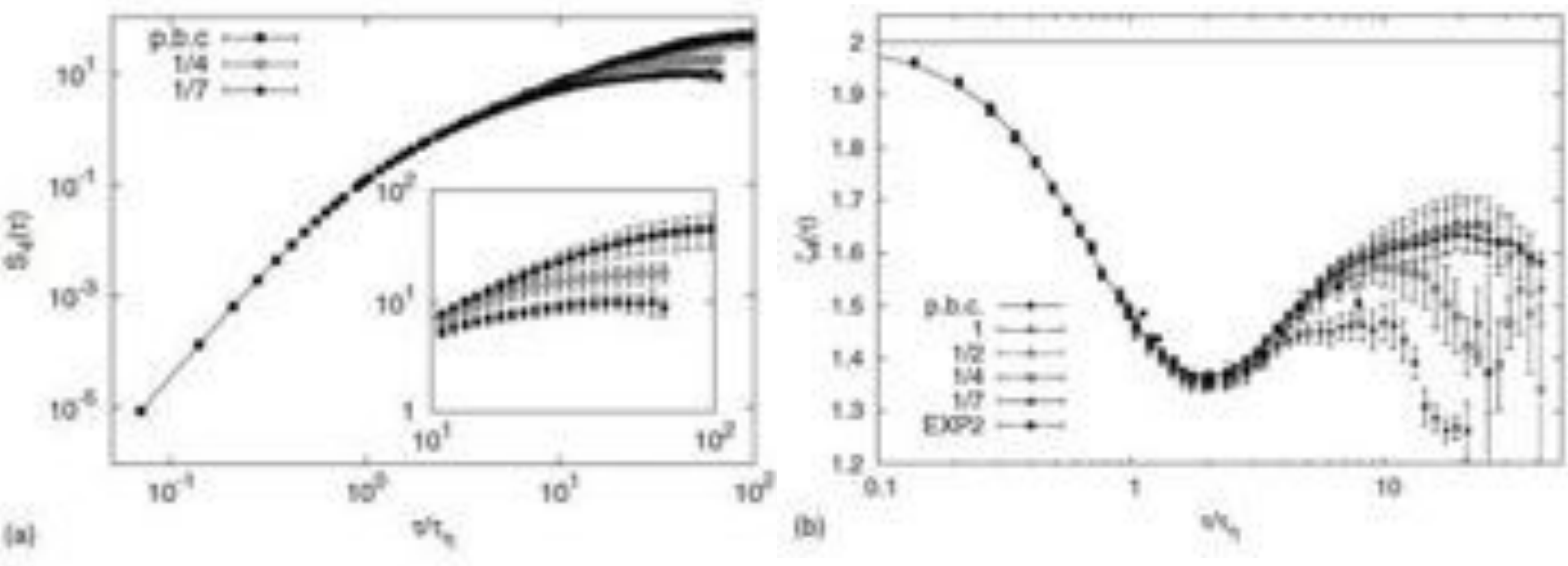
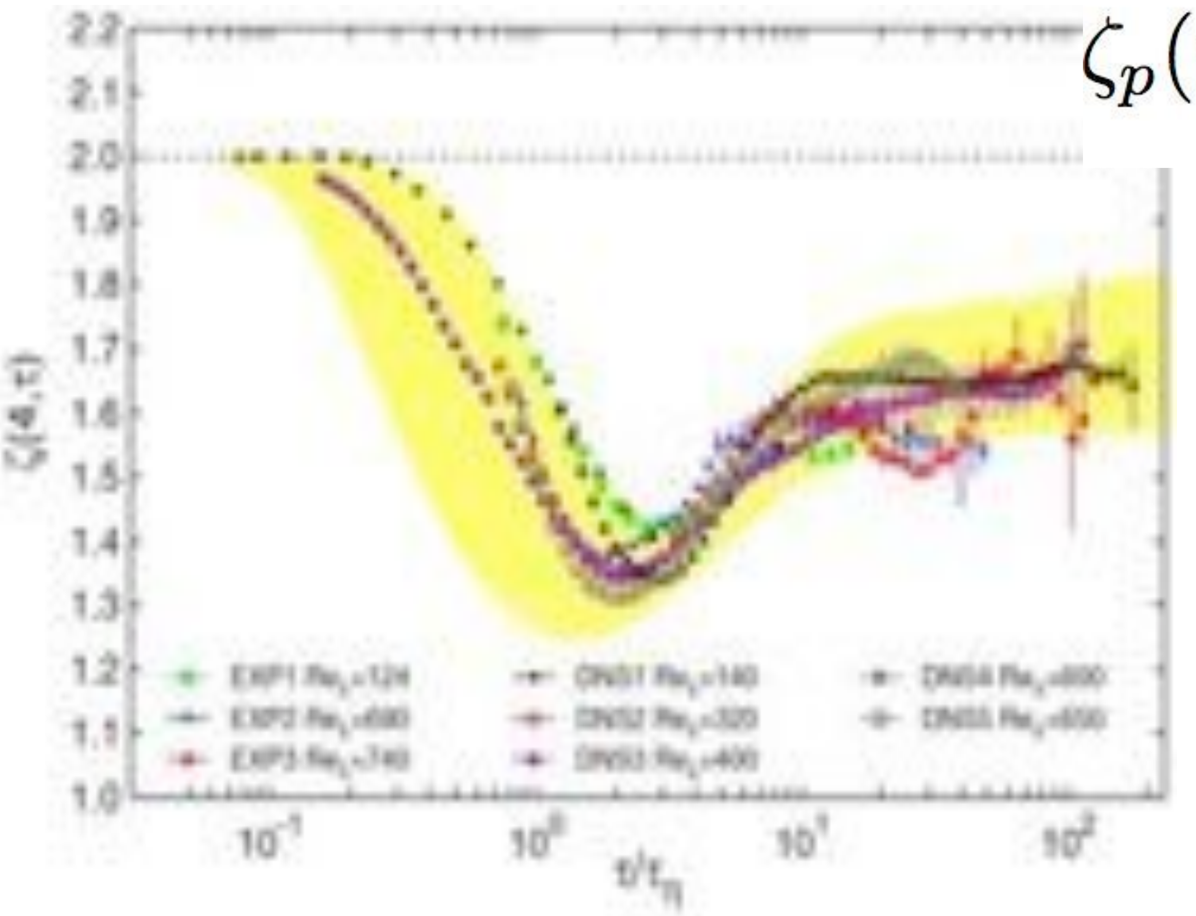


FIG. 7. (a) The fourth-order structure function $S_4(\tau)$ vs τ/τ_η measured from DNS2 trajectories for both full length trajectories (and with periodic boundary conditions) and for trajectories in smaller measurement volumes $L/B = \frac{1}{4}, \frac{1}{7}$. (b) The logarithmic local slope $\zeta_4(\tau)$ measured from DNS2 trajectories for both the full length trajectories (periodic boundary conditions) and for trajectories in smaller measurement volumes $L/B = 1, \frac{1}{2}, \frac{1}{4}, \frac{1}{7}$. Note the tendency toward a less developed plateau, at smaller and smaller values, as the measurement volume decreases. In the same plot, we also compare the local slope of EXP2, whose trajectory length distribution is well reproduced by DNS2 data in the subvolume $\mathcal{L}/B = \frac{1}{4}$.

Biferale et al. Lagrangian structure functions in turbulence: A quantitative comparison between experiment and direct numerical simulation. Phys Fluids (2008) vol. 20 (6) pp. 065103

Universality of Lagrangian Turbulence

$$\zeta_p(\tau) = \frac{\mathrm{d}\log\left(S_p(\tau)\right)}{\mathrm{d}\log\left(S_2(\tau)\right)}$$



A. Arneodo, R. Benzi, J. Berg, L. Biferale, E. Bodenschatz, A. Busse, E. Calzavarini, B. Castaing, M. Cencini, L. Chevillard, R. T. Fisher, R. Grauer, H. Homann, D. Lamb, A. S. Lanotte, E. Leveque, B. Luthi, J. Mann, N. Mordant, W. C. Muller, S. Ott, N. T. Ouellette, J. F. Pinton, S. B. Pope, S. G. Roux, F. Toschi, H. Xu, and P.K. Yeung
Universal intermittent properties of particle trajectories in highly turbulent flows.
Physical Review Letters, 100(25):254504–5, 2008.

Effect of vortex on SF bottleneck

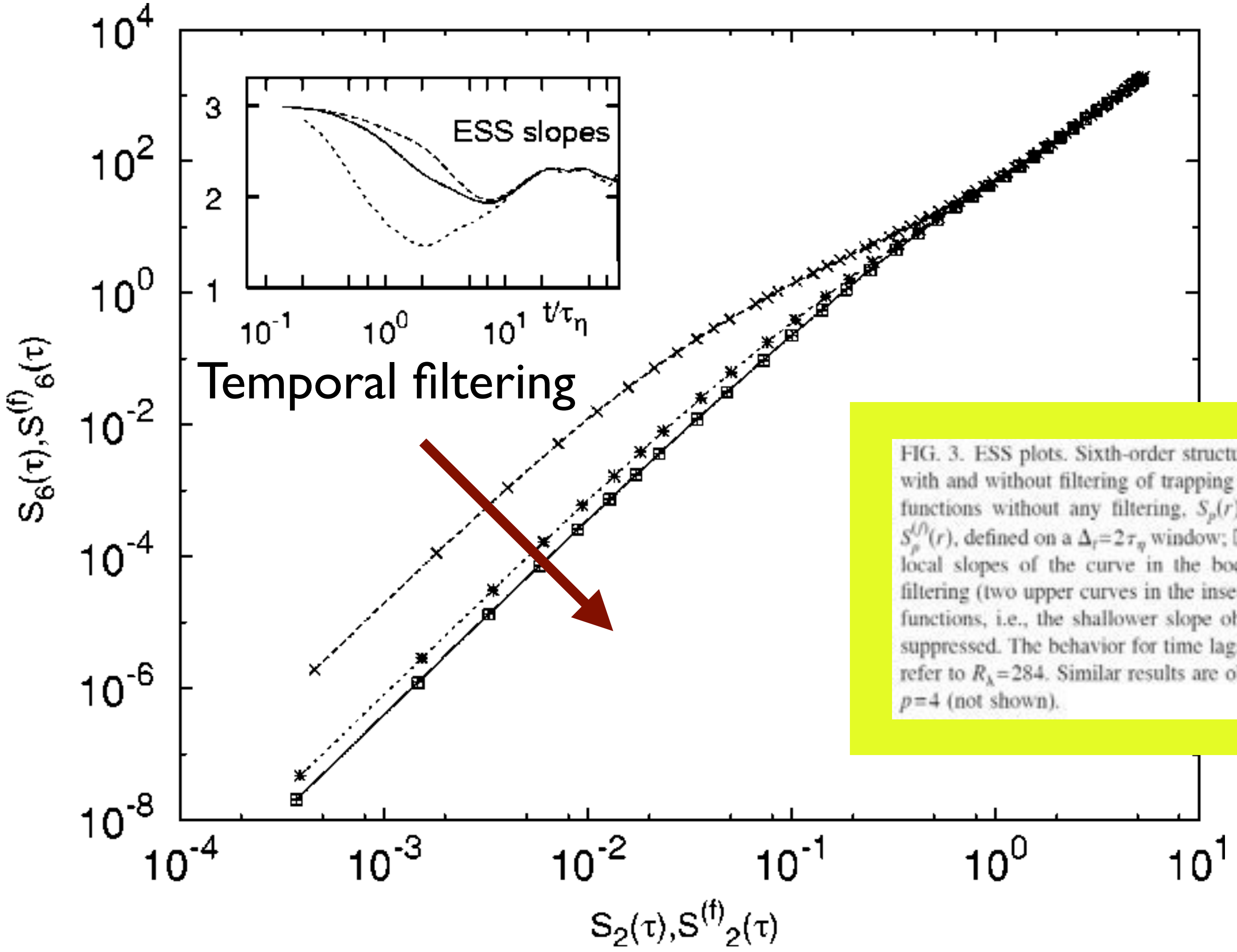


FIG. 3. ESS plots. Sixth-order structure functions vs the second-order one, with and without filtering of trapping events. Symbols refer to: × structure functions without any filtering, $S_p(r)$; * structure function with filtering, $S_p^{(f)}(r)$, defined on a $\Delta_t=2\tau_\eta$ window; □ with filtering on $\Delta_t=4\tau_\eta$. Inset: ESS local slopes of the curve in the body of the figure vs $\log(\tau/\tau_\eta)$. Upon filtering (two upper curves in the inset), the "bottleneck" effect on structure functions, i.e., the shallower slope observed in the neighborhood of τ_η, is suppressed. The behavior for time lags longer than $10\tau_\eta$ is unchanged. Data refer to $R_\lambda=284$. Similar results are obtained for structure function of order $p=4$ (not shown).

L. Biferale, G. Boffetta, A. Celani, A. Lanotte and F. Toschi Particle trapping in three-dimensional fully developed turbulence
Physics of Fluids 17 2 (2005) 021701.

Lagrangian Structure function

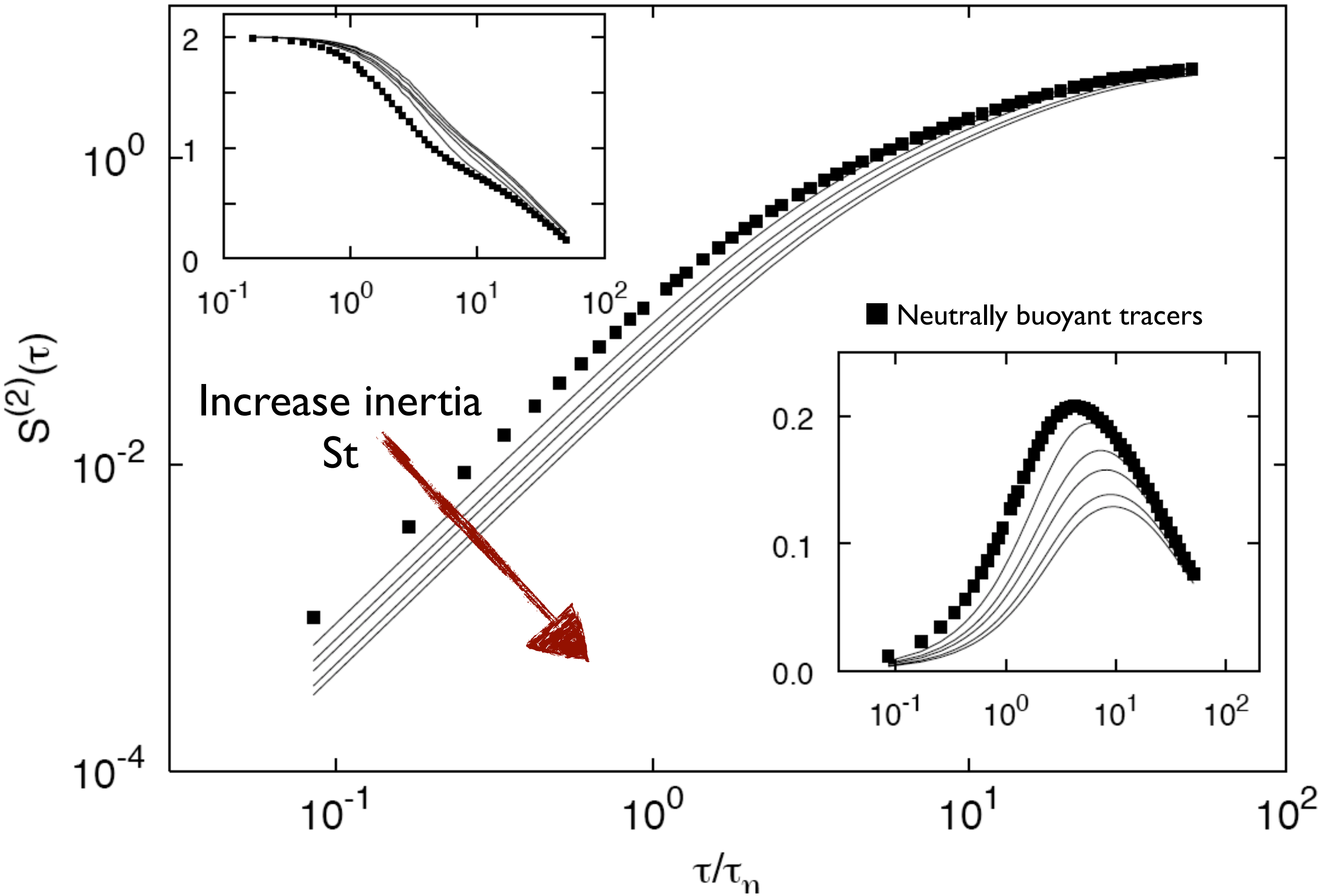


Figure from: Bec et al. Effects of vortex filaments on the velocity of tracers and heavy particles in turbulence.
Phys Fluids (2006) vol. 18 (8) pp. 081702

Local slopes (order 4 vs. 2)

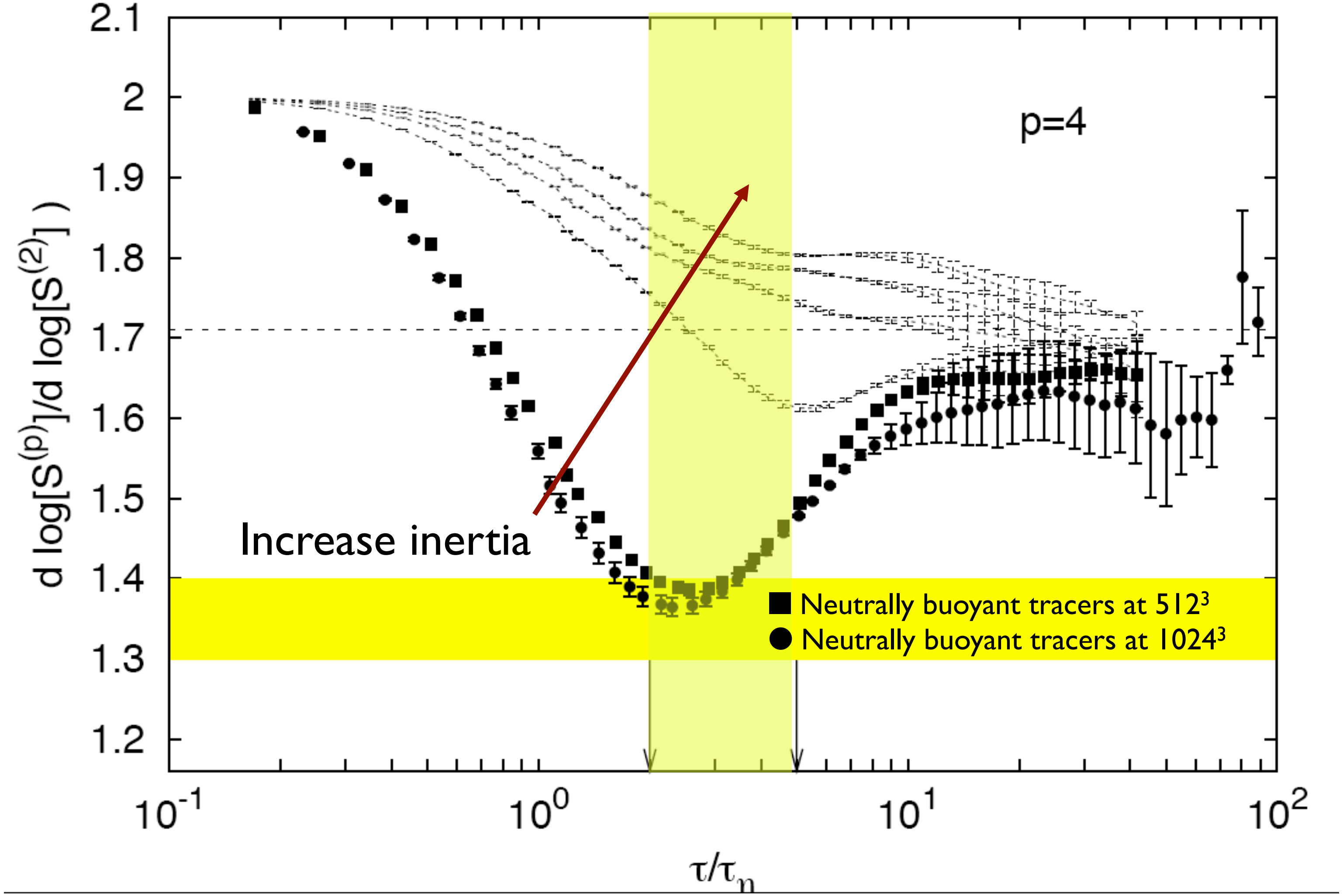


Figure from: Bec et al. Effects of vortex filaments on the velocity of tracers and heavy particles in turbulence. Phys Fluids (2006) vol. 18 (8) pp. 081702

Acceleration statistics

$$a \equiv \frac{\delta v(\tau_\eta)}{\tau_\eta}$$

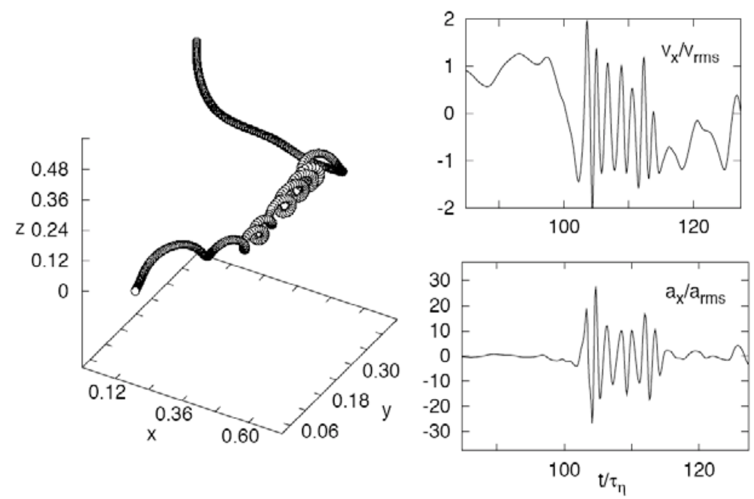


FIG. 1: Trajectory and time series. Left panel: 3D trajectory of a trapping event in vortex filament. Acceleration and velocity fluctuations here reach about 30 and 2 r.m.s. values, respectively (right panels).

Multifractal Statistics of Lagrangian Velocity and Acceleration in Turbulence L. Biferale, G. Boffetta , A. Celani, B. J. Devenish, A. Lanotte and F. Toschi 93 PRL 2004

Biferale et al. Particle trapping in three-dimensional fully developed turbulence. Phys Fluids (2005) vol. 17 (2) pp. 021701

Who contributes to acceleration?

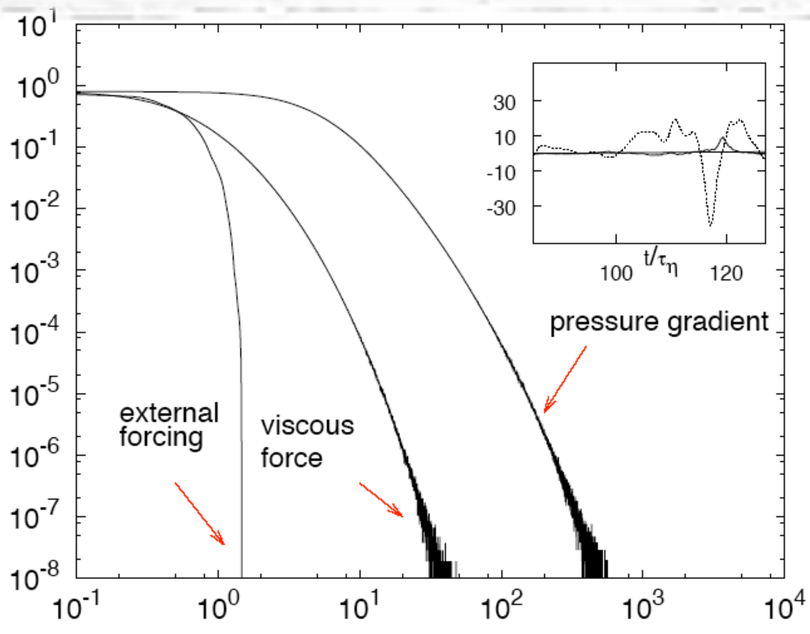


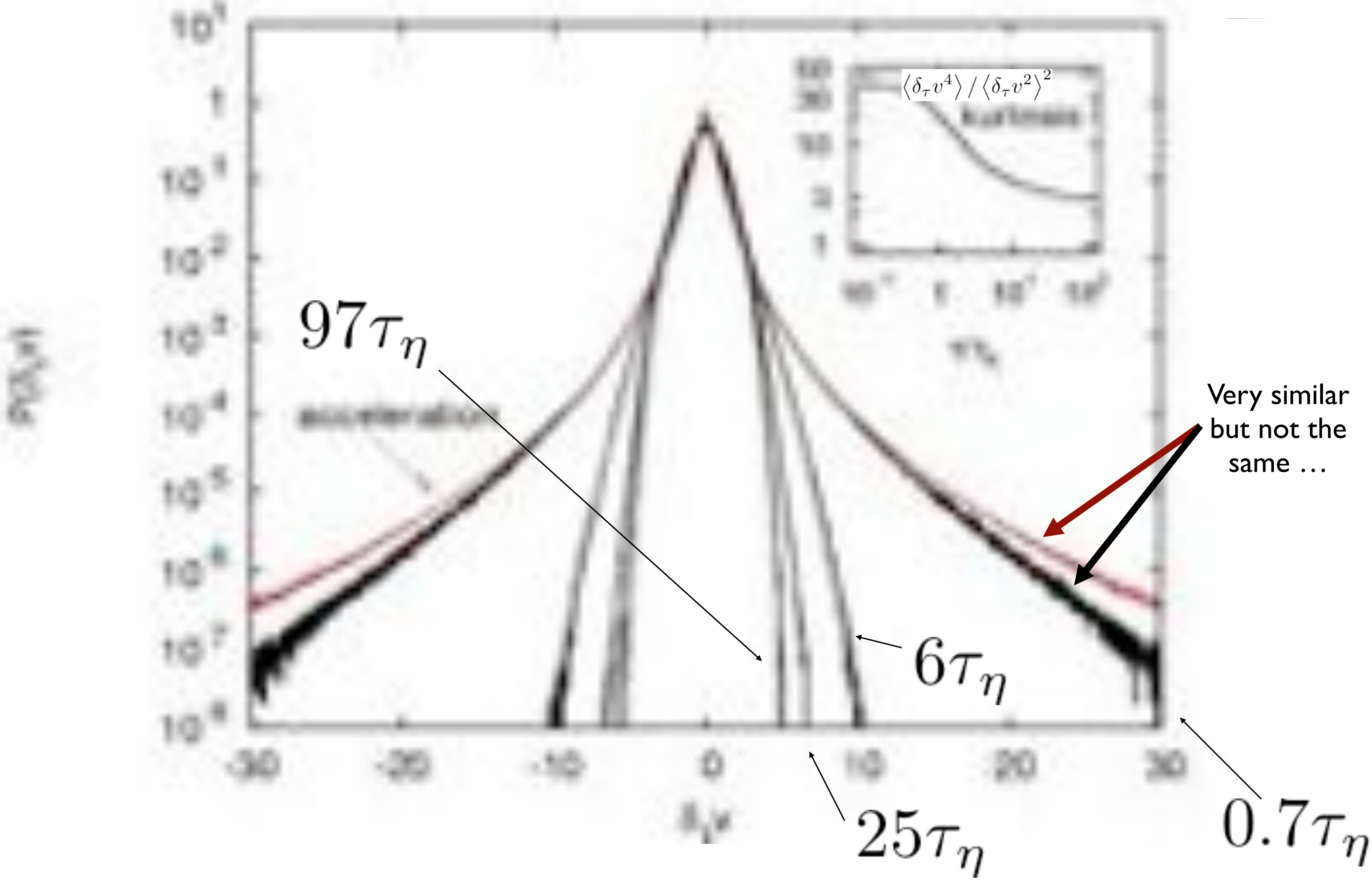
FIG. 5: Log-log plot of PDFs for $-\partial_x p$, $\nu \Delta u_x$, F_x. The external forcing is virtually negligible, and the main contribution to large accelerations is made by pressure gradients. Inset: a typical evolution of the three terms along a particular trajectory. The strongest signal is $\partial_x p$ (dashed line), while the viscous force is activated only as a subleading response to pressure gradients (solid line). The force contribution is indistinguishable from zero.

Who is contributing
to passive particle acceleration?

$$a_L(t) = -\nabla p + \nu \delta^2 v + f_{ext}$$

Almost all contribution
from pressure gradients

Velocity increments vs. acceleration



Biferale et al. Lagrangian statistics in fully developed turbulence. J Turbul (2006) vol. 7 (6) pp. 1-12

Acceleration multifractal's view

$$a \equiv \frac{\delta_{\tau_\eta} v}{\tau_\eta}$$

The small scale fluctuates !!!

$$\eta(h, v_0) \sim \left(\nu L_0^h / v_0\right)^{1/(1+h)}$$

$$a(h, v_0) \sim \nu^{\frac{2h-1}{1+h}} v_0^{\frac{3}{1+h}} L_0^{-\frac{3h}{1+h}}$$

with probability

$$(\tau_\eta(h, v_0)/T_L(v_0))^{(3-D(h))/(1-h)}$$

and for the large scale:

The large scale fluctuates !!!

$$\mathcal{P}(v_0) = \exp(-v_0^2/2\sigma_v^2)/\sqrt{2\pi\sigma_v^2}$$

Acceleration multifractal's view

From standard multifractal arguments:

$$\mathcal{P}(a) \sim \int_{h\in I} \mathrm{d}h\, a^{\frac{h-5+D(h)}{3}} \nu^{\frac{7-2h-2D(h)}{3}} L_0^{D(h)+h-3} \sigma_v^{-1} \times \quad \exp\left(-\frac{a^{\frac{2(1+h)}{3}} \nu^{\frac{2(1-2h)}{3}} L_0^{2h}}{2\sigma_v^2}\right)$$

Supposing without intermittency (K41 case)

$$\mathcal{P}^{K41}(\tilde{a}) \sim \tilde{a}^{-5/9} R_\lambda^{-1/2} \exp\left(-\tilde{a}^{8/9}/2\right)$$

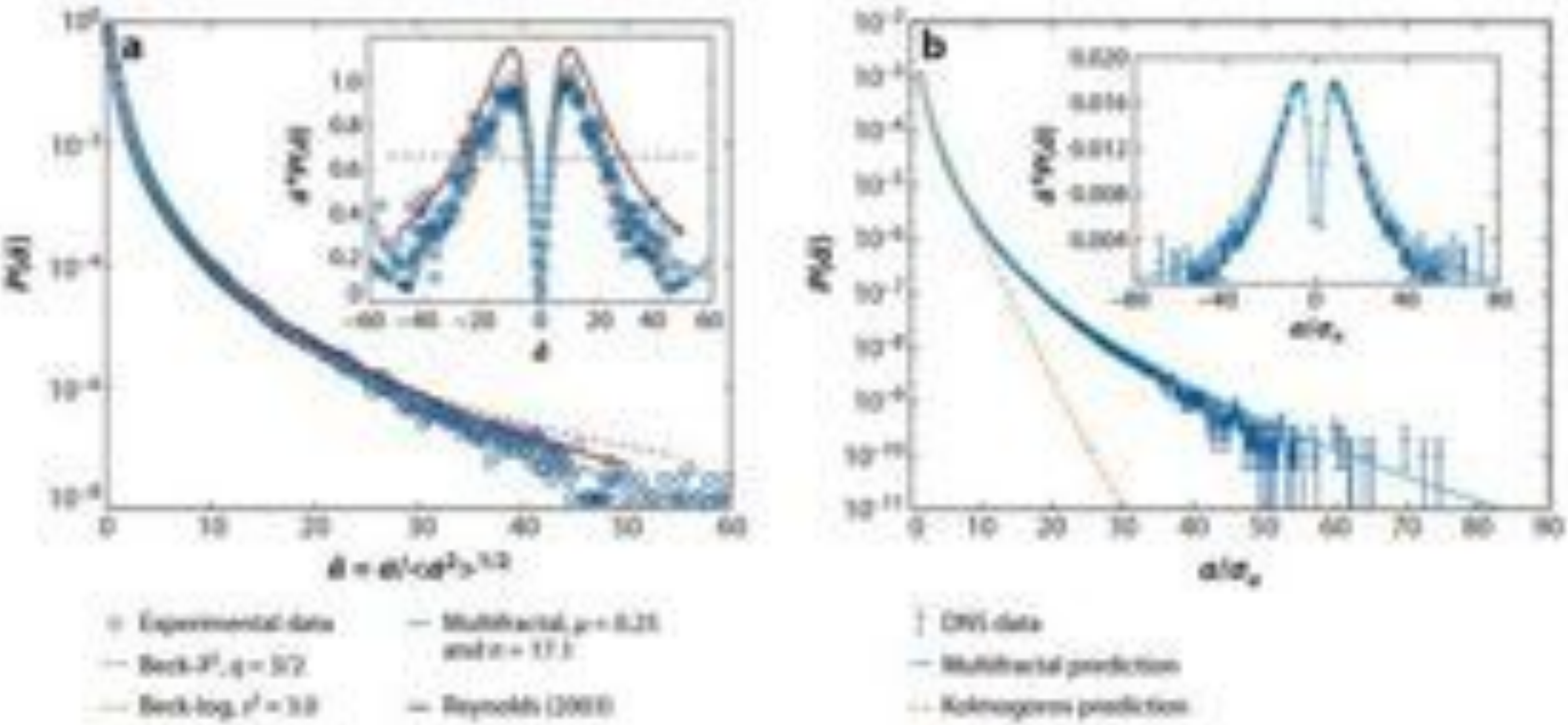
…with h=1/3

Also able to make other predictions,
i.e. acceleration variance conditioned to velocity value:

$$\langle a^2 | v_0 \rangle \sim \int_{h\in I} \mathrm{d}h\, \nu^{\frac{1+4h-D(h)}{1+h}} v_0^{\frac{3+D(h)}{1+h}} L_0^{\frac{D(h)-6h-3}{1+h}}$$

L. Biferale, G. Boffetta, A. Celani, B. Devenish, A. Lanotte, and F. Toschi. Multifractal statistics of lagrangian velocity and acceleration in turbulence. *Physical Review Letters*, 93:064502, 2004.

Forces on tracers (pressure gradient)



Pdf were not put one on top of the other as corresponds to different Re numbers

Toschi and Bodenschatz.
Lagrangian properties of particles in Turbulence.
Ann. Rev. Fluid Mech. (2009) vol. 41 pp. 375-404

High acceleration vs. small scale vorticity

Small scale bottleneck and vortex filaments

Centripetal and longitudinal acceleration

Centripetal $\boldsymbol{a}_c = \boldsymbol{a} \times \hat{\boldsymbol{v}}$

Longitudinal $\boldsymbol{a}_l = (\boldsymbol{a} \cdot \hat{\boldsymbol{v}})\hat{v}$

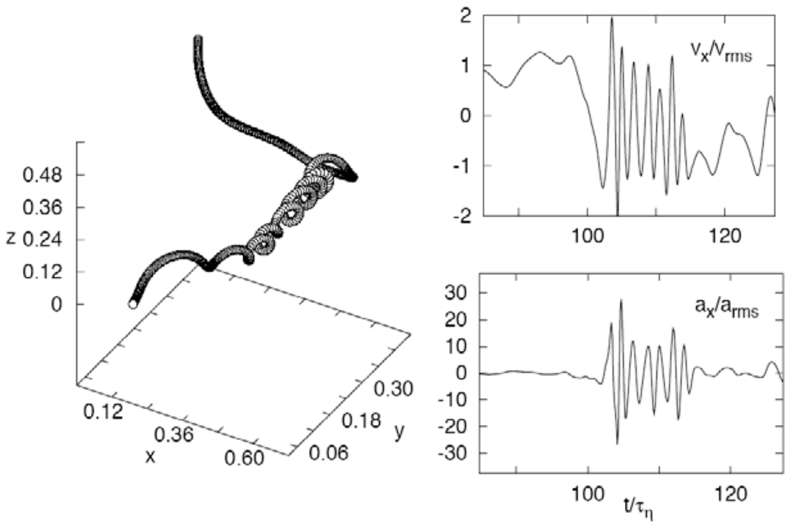
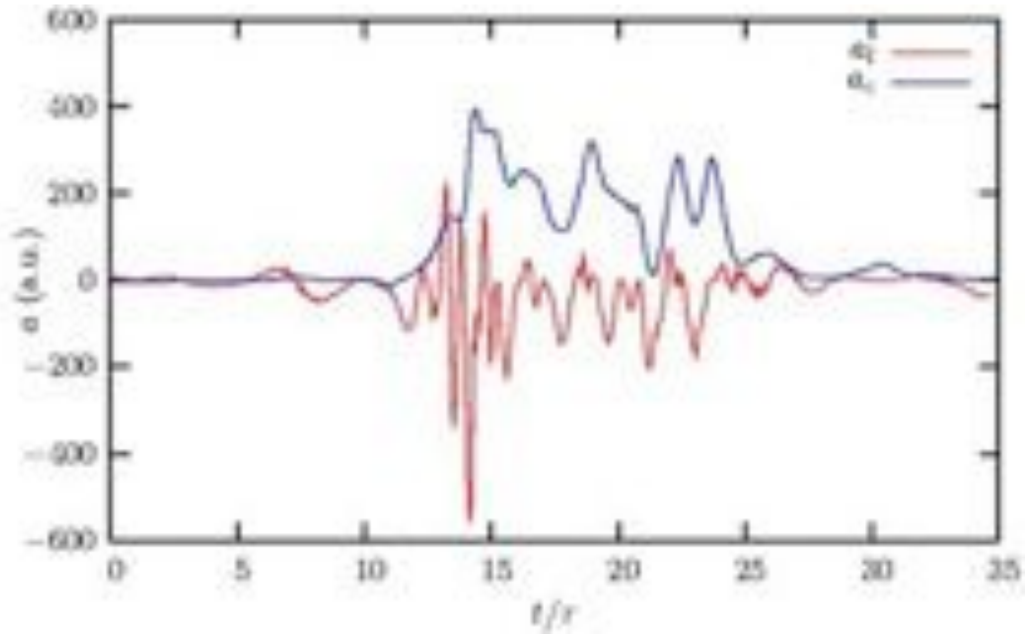


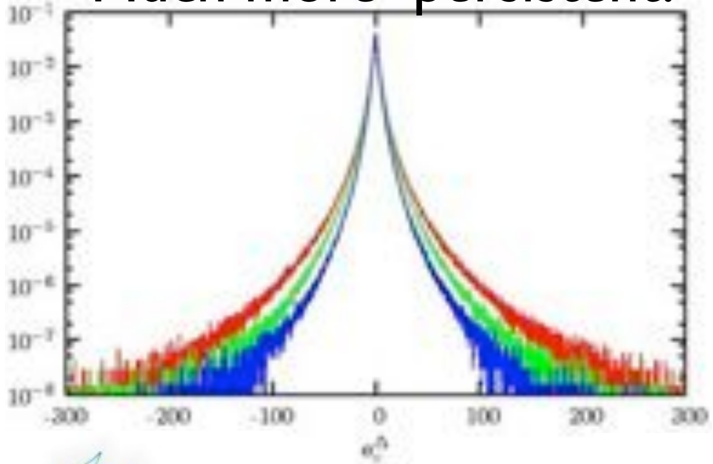
FIG. 1: Trajectory and time series. Left panel: 3D trajectory of a trapping event in vortex filament. Acceleration and velocity fluctuations here reach about 30 and 2 r.m.s. values, respectively (right panels).

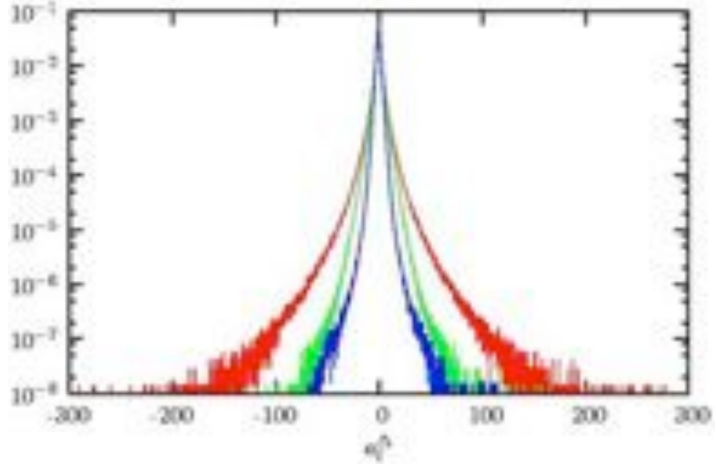


Pdf of acceleration and trapping events

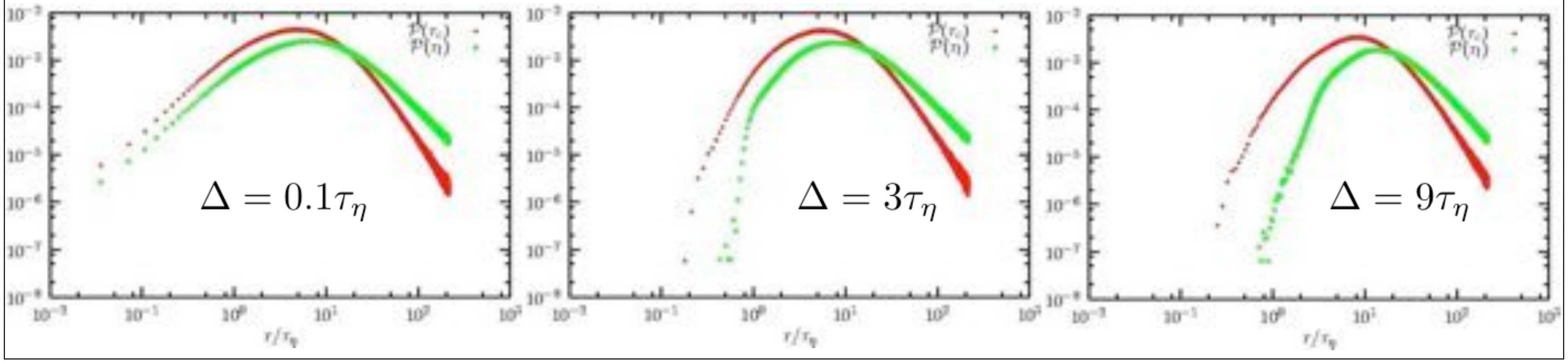
Pdfs of a_c and a_l coarse grained over window of different size, Δ.

Much more persistent!



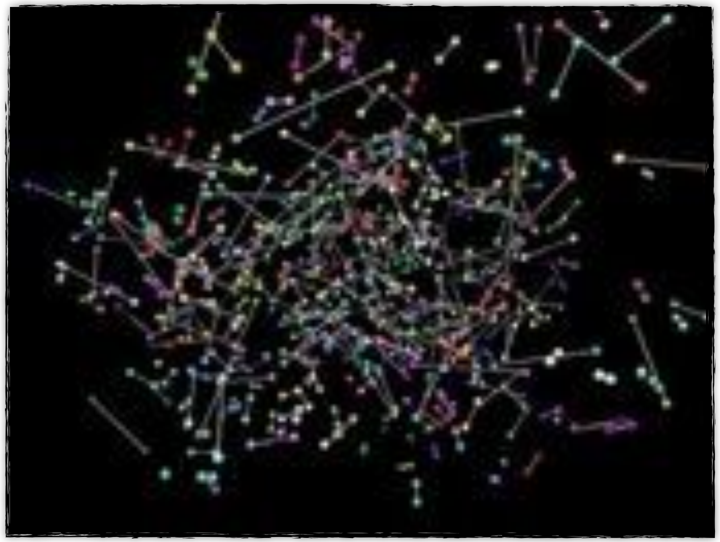


$$\tau_{\{c,l\}} \equiv \frac{\langle |\boldsymbol{v}| \rangle_\Delta}{\langle a_{\{c,l\}} \rangle_\Delta}$$



Evolution of Sizes and Shapes

Multi-particle Lagrangian statistics in fully developed turbulence

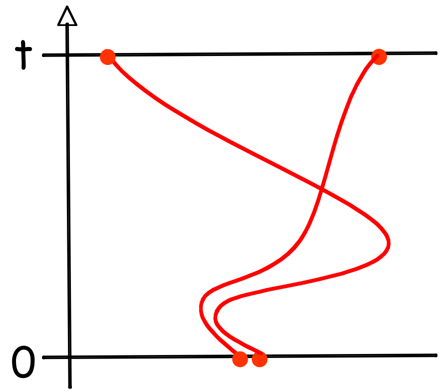


Sizes (two particle statistics)
- Richardson model for relative dispersion
- exit time statistics

Shapes (multi particle statistics)
- shape evolution
- stationary distribution of shapes

Two-particle, single time statistics

Classical problem introduced by L.F. Richardson in 1926 to describe diffusion in the atmosphere.
First empirical evidence of Kolmogorov scaling in turbulence (actually 15 years before K41...)



The basic quantity of interest is the relative separation between the trajectories of two particles

$$R(t) = x_1(t) - x_2(t)$$

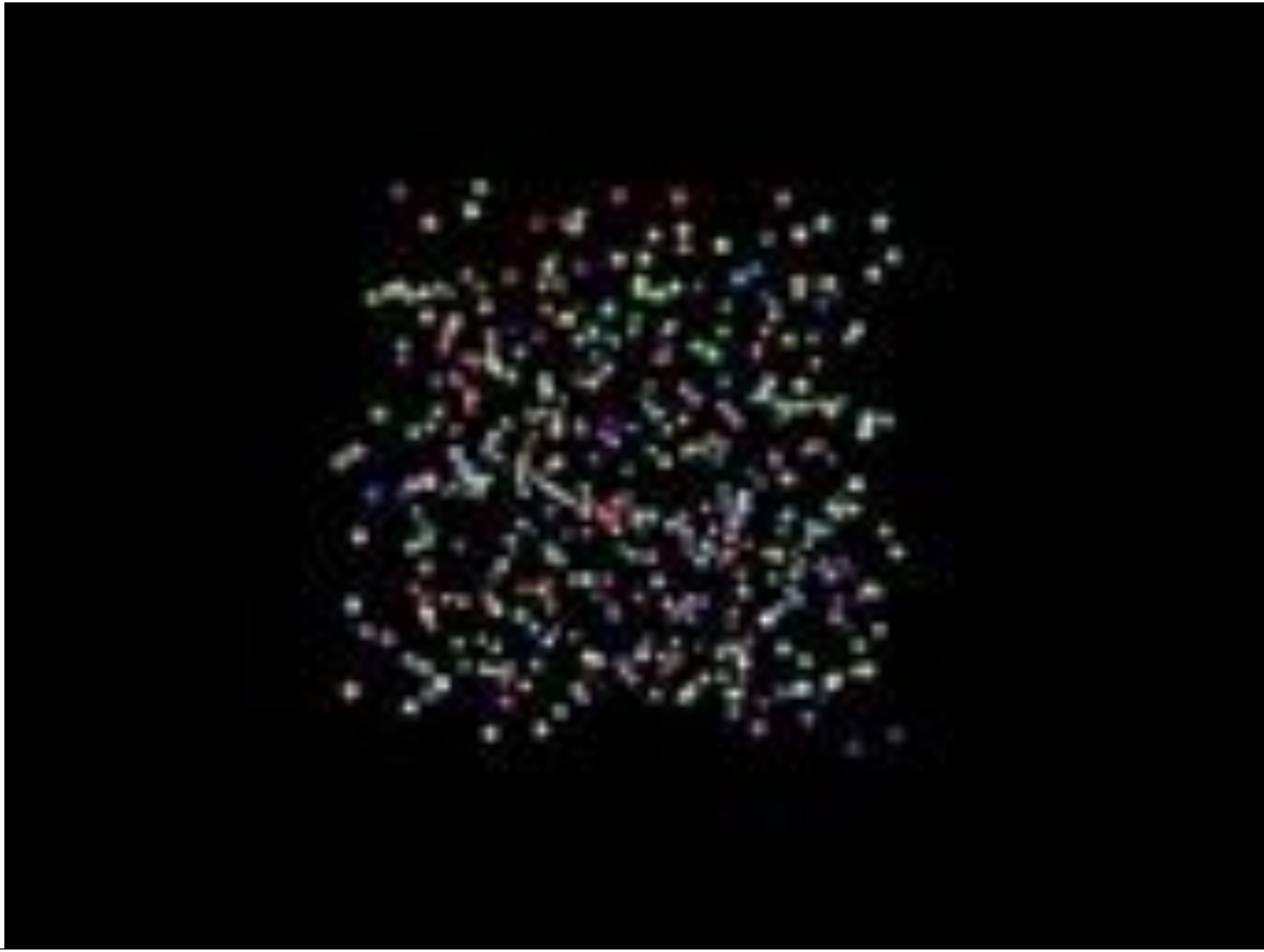
The evolution of separation is governed by the velocity differences:

$$\frac{dR}{dt}(t) = \delta u(R(t), t)$$

The R(t) growth do depends on the spatial scaling of velocity differences

Numerical relative dispersion

evolution of $5x10^5$ particle pairs starting from $R(0)\approx\eta$



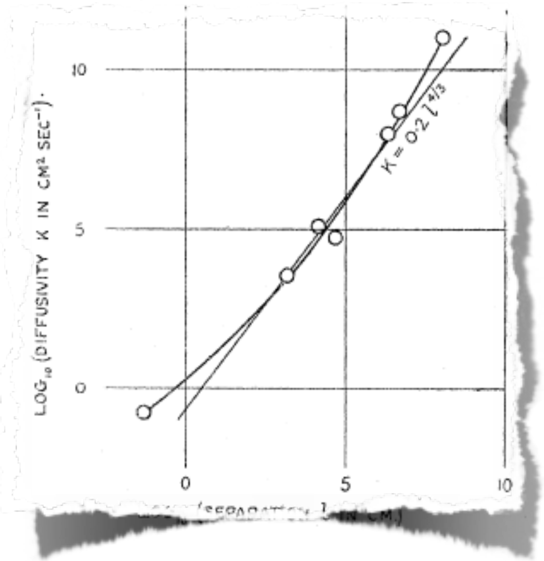
Richardson diffusion

Diffusion equation for distance-neighbor function q(R,t) with scale-dependent diffusivity K(R)

$$\frac{\partial q(R,t)}{\partial t} = \frac{\partial}{\partial R_i}\left[K(R)\frac{\partial q(R,t)}{\partial R_i}\right]$$

From experimental data

$$K(R) = \alpha\varepsilon^{1/3}R^{4/3}$$



- separation pdf is not Gaussian:

$$q(R,t) = C(t)\exp\left(-\frac{9R^{2/3}}{4\alpha\varepsilon^{1/3}t}\right)$$

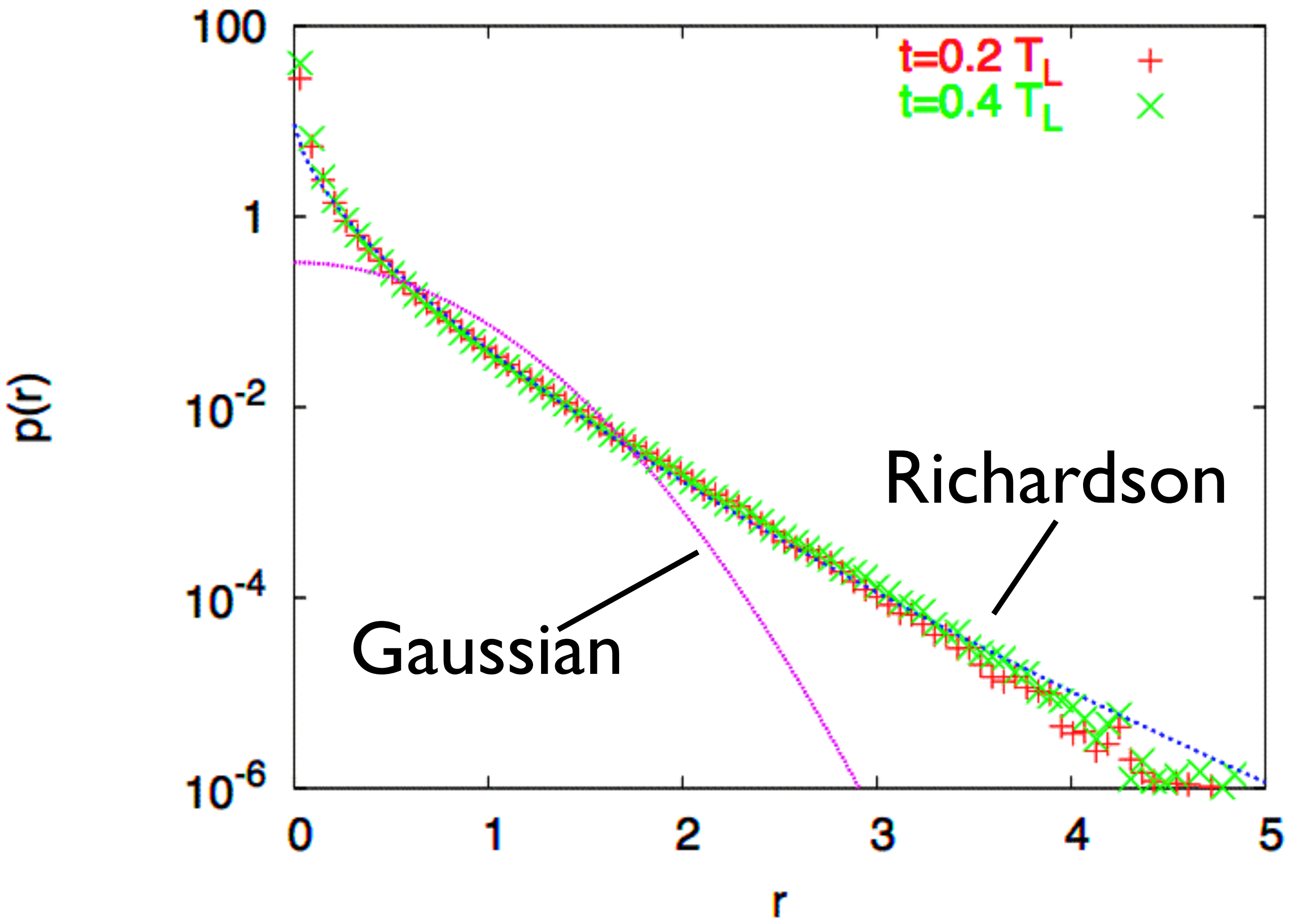
- explosive separation (faster than ballistic)

$$\langle R^2(t)\rangle = g\varepsilon t^3$$

g: Richardson (universal) constant

L.F. Richardson, Atmospheric diffusion shown on a distance-neighbour graph, The proceedings of the Royal Society A - **756** (1926)

Pdf of relative separation and Richardson



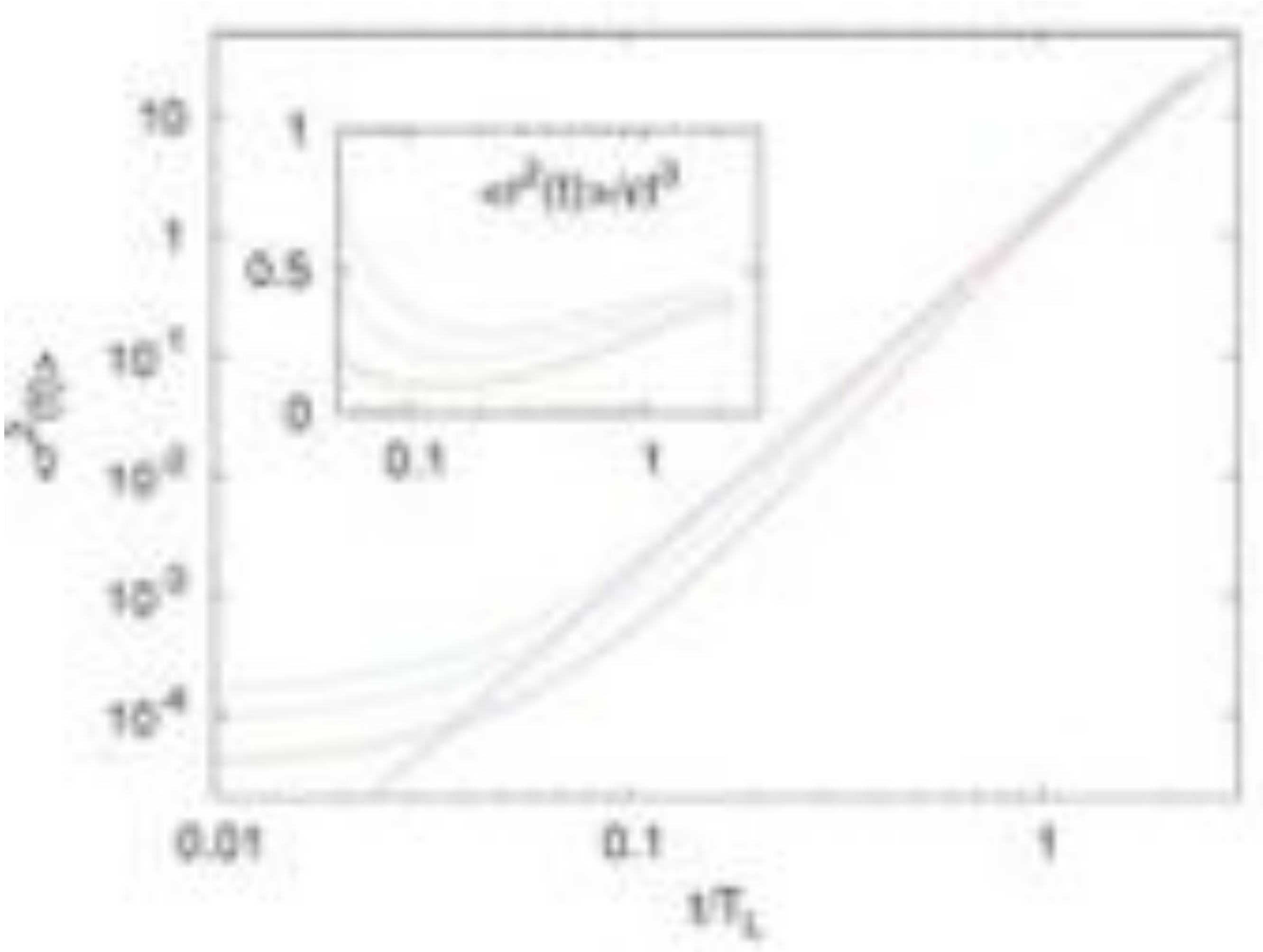
Richardson PDF

$$p(r,t) = C(t)\exp\left(-\frac{9r^{2/3}}{4\alpha t}\right)$$

Biferale et al. Lagrangian statistics in fully developed turbulence. J Turbul (2006) vol. 7 (6) pp. 1-12

Test of Richardson separation

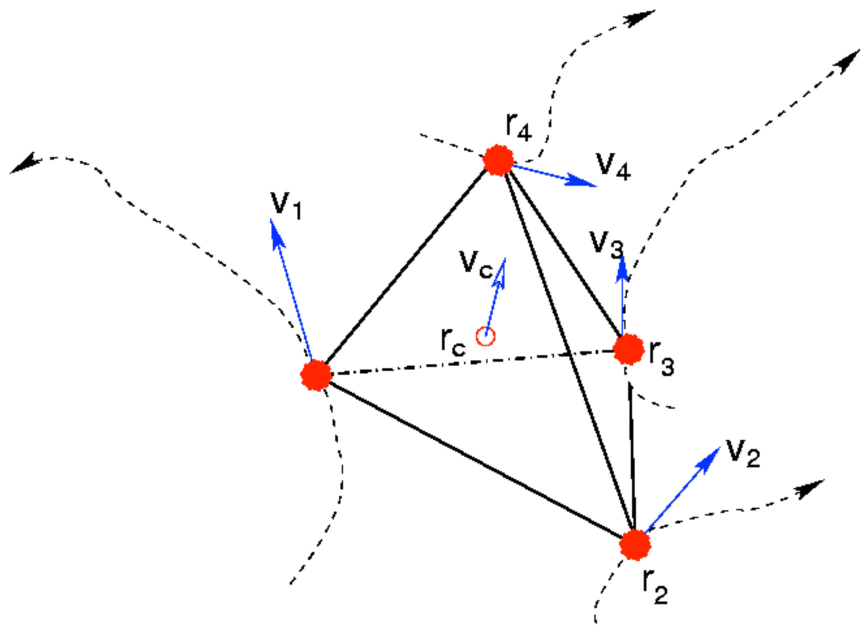
Variance of separation close to Richardson law $<r^2(t)> \approx t^3$ but large deviations !



precise determination of Richardson constant $g = <r^2>/\varepsilon t^3$ is not possible.

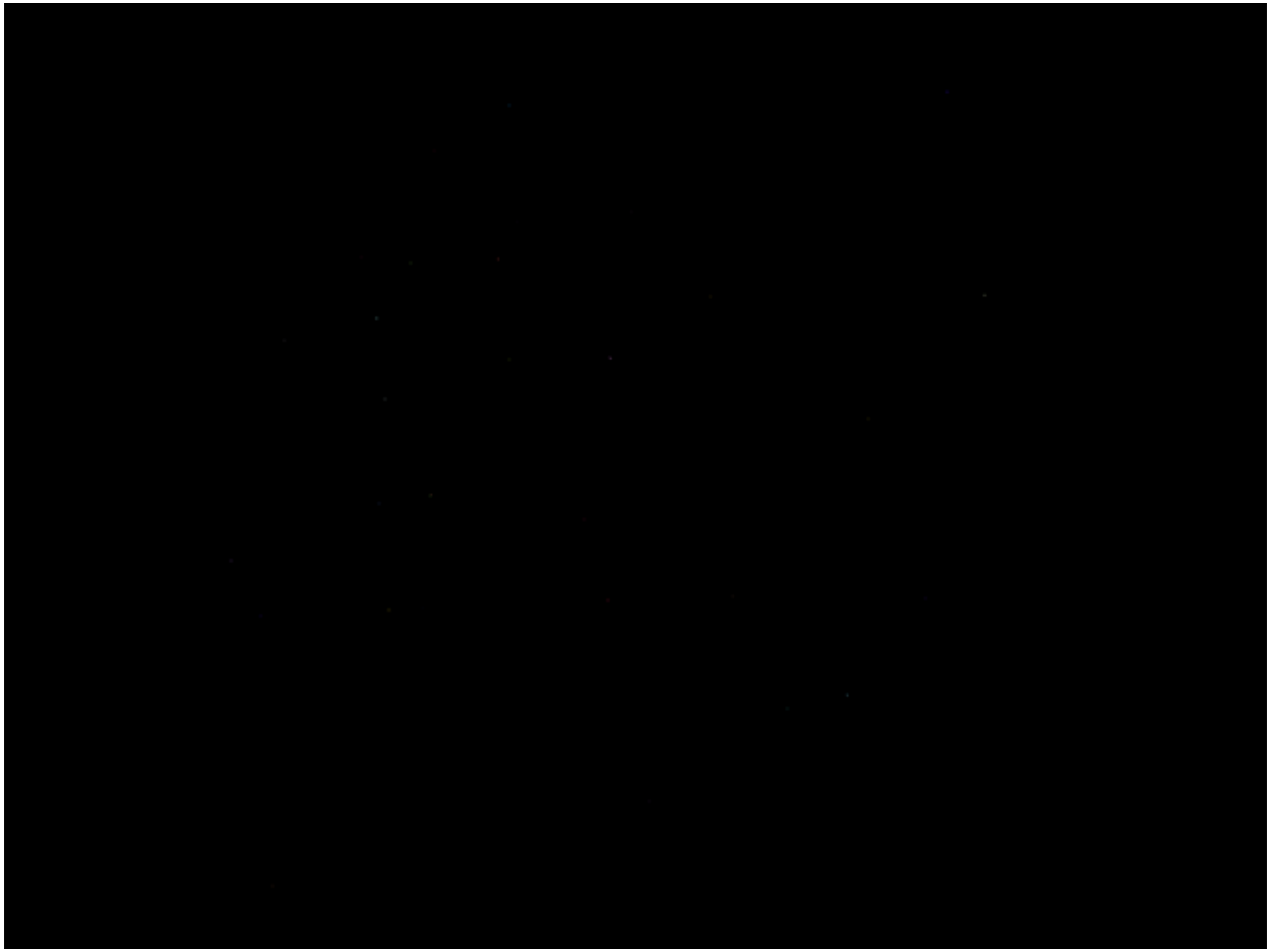
Biferale et al. Lagrangian statistics of particle pairs in homogeneous isotropic turbulence. Phys Fluids (2005) vol. 17 (11) pp. 115101

Multi-particle statistics: shape evolution



Evolution of shapes in turbulence

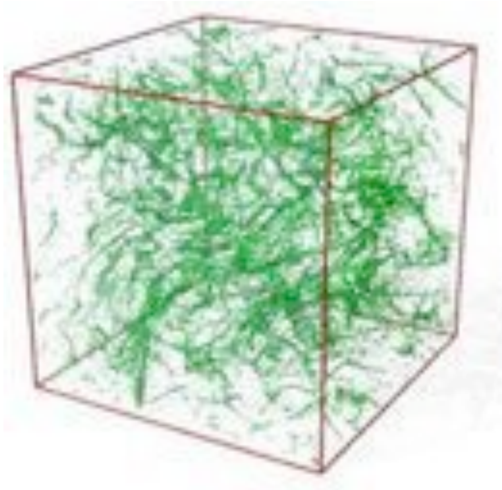
Evolution of ~10^5 tetrahedra starting from the Kolmogorov scale with regular shape



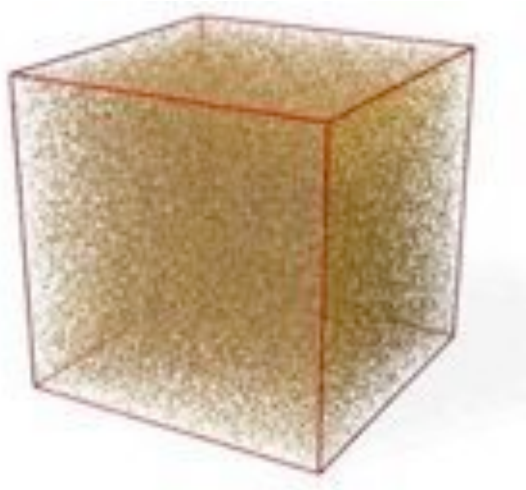
Multiparticle dispersion in fully developed turbulence
L. Biferale, G. Boffetta, A. Celani, B. J. Devenish A. Lanotte F. Toschi,
PHYSICS OF FLUIDS 17, (2005) 111701

Particles with inertia

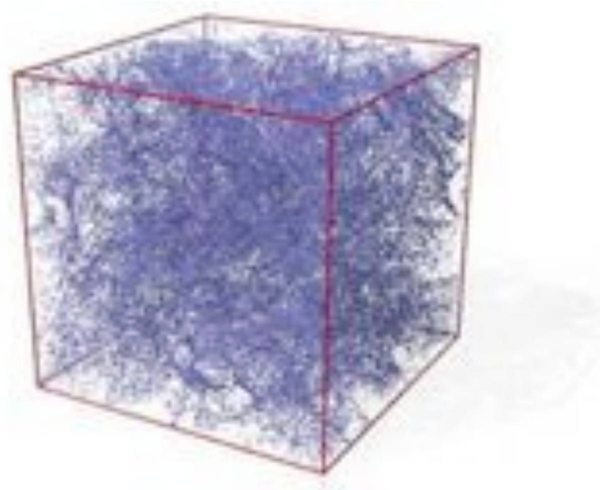
Space distribution



Light



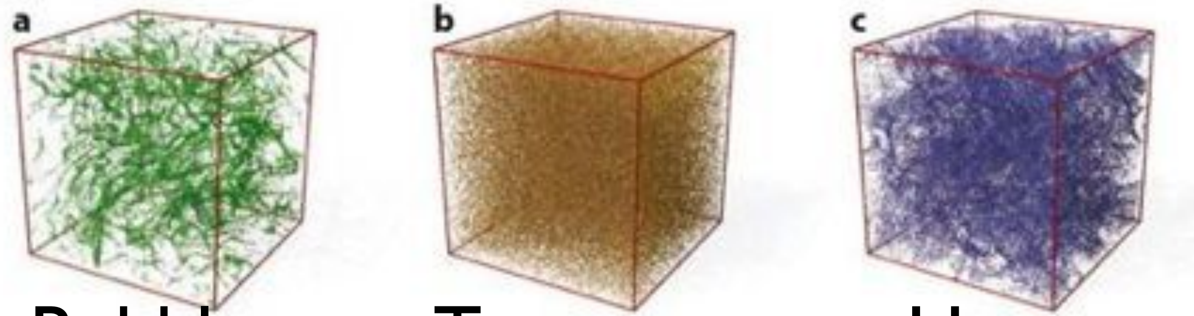
Neutral



Heavy

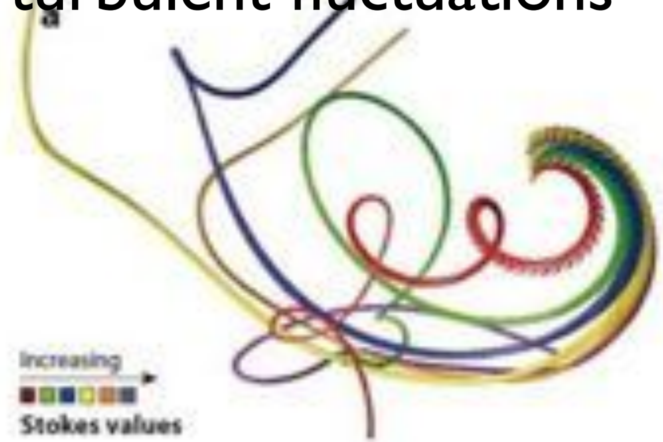
All effects of inertia, in a slide...

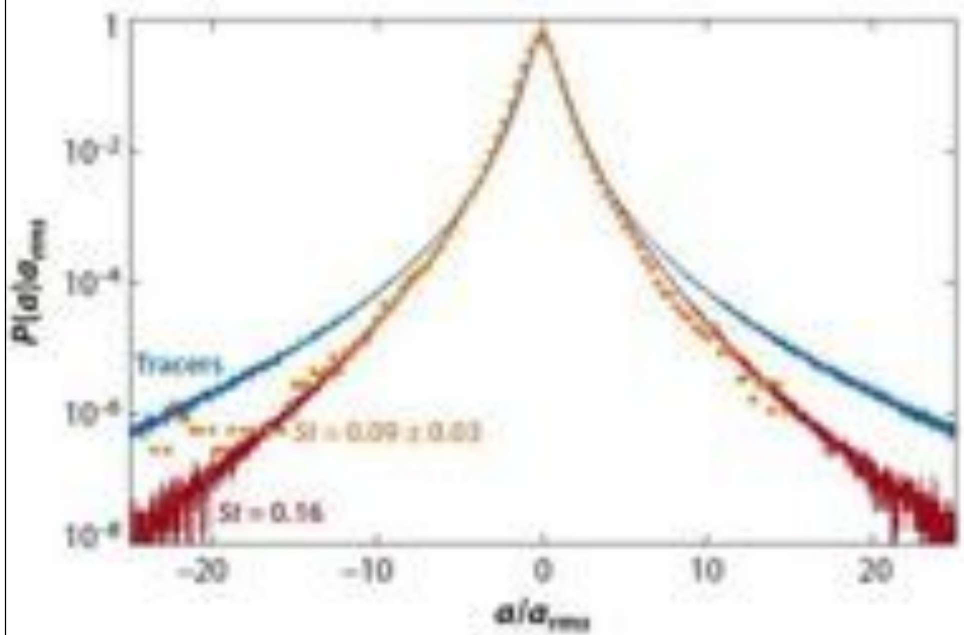
Preferential concentration

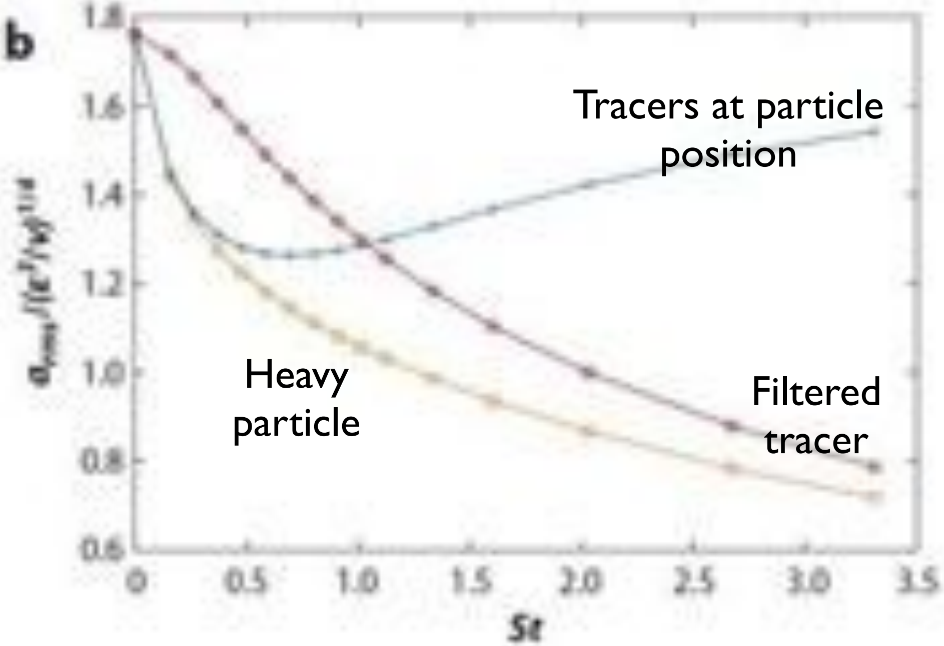


Bubbles Tracers Heavy

Filtering of turbulent fluctuations

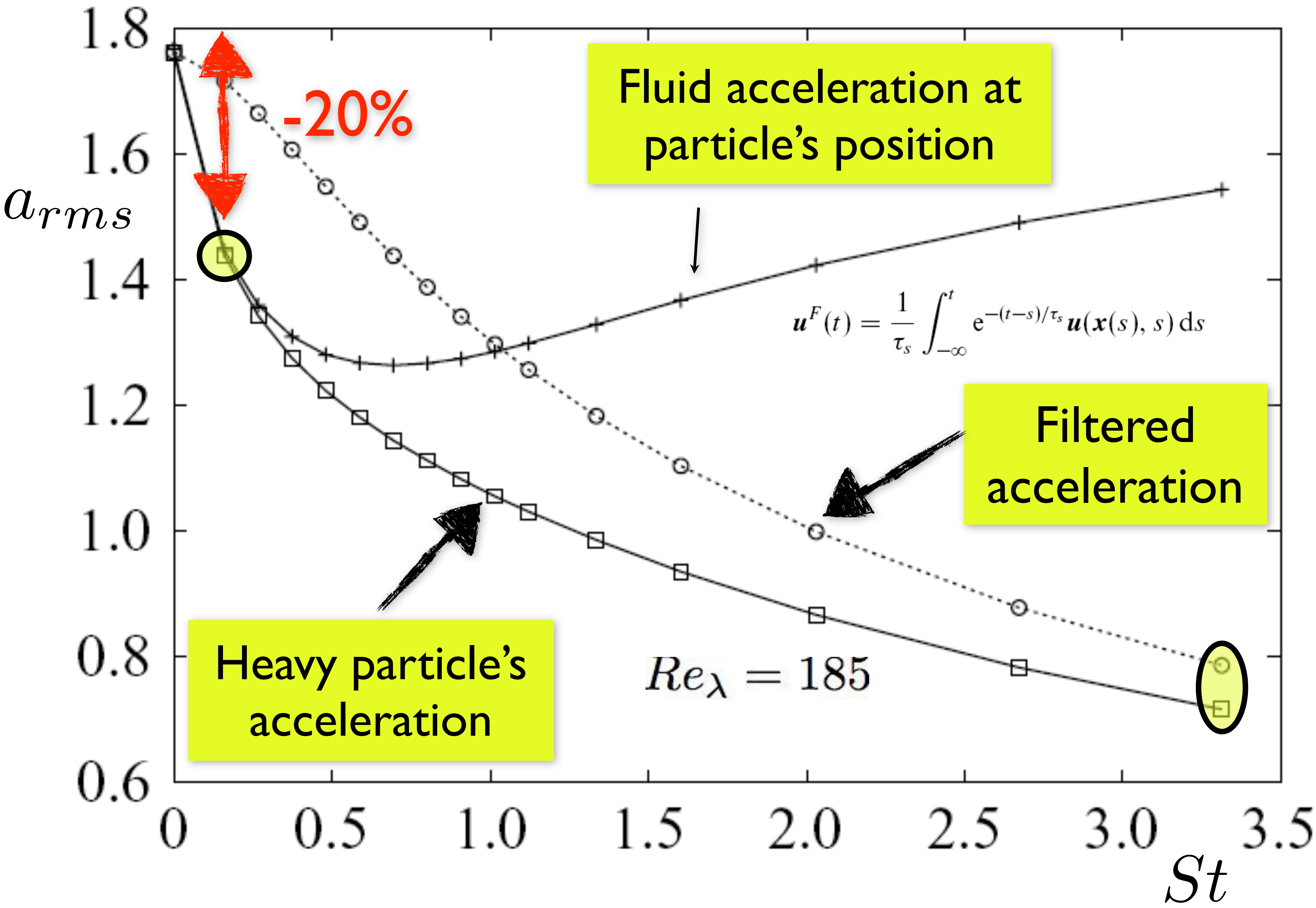




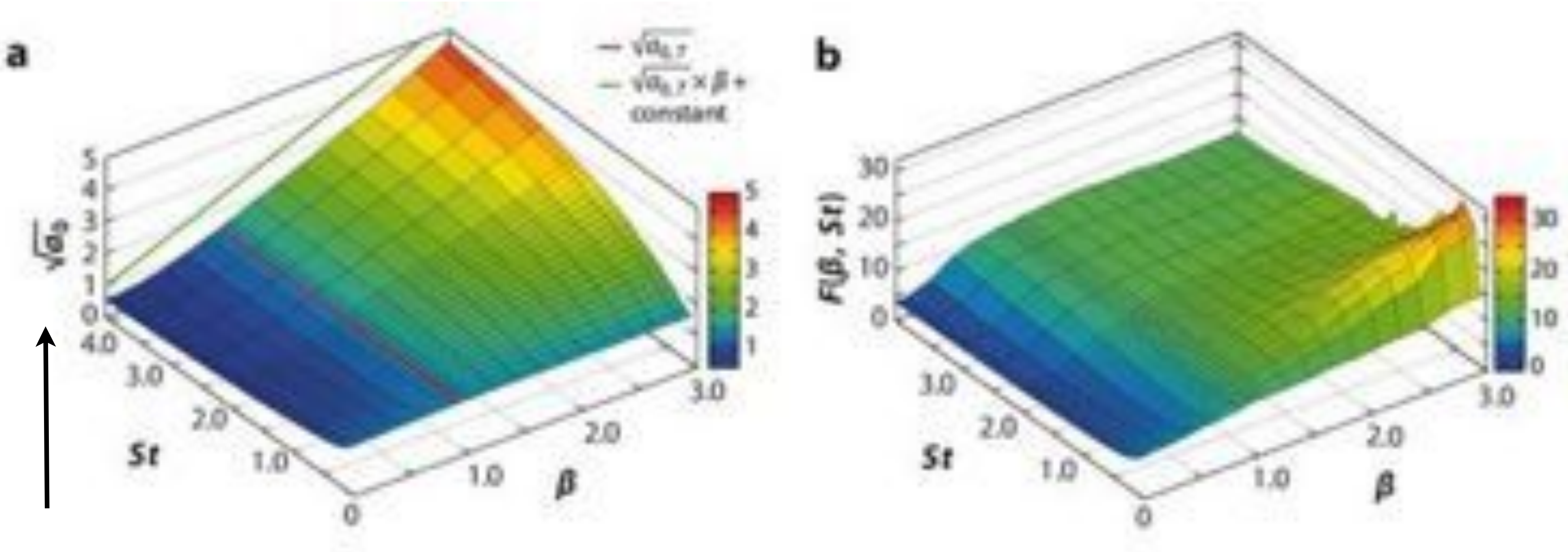


Toschi and Bodenschatz. Lagrangian properties of particles in Turbulence. Ann. Rev. Fluid Mech. (2009) vol. 41 pp. 375-404

Acceleration at varying Stokes no model yet



More general picture of forces



a_{rms}

$$St = \frac{\tau}{\tau_\eta} \qquad \beta = \frac{3\rho_f}{\rho_f + 2\rho_p}$$

$$\frac{d\boldsymbol{v}(t)}{dt} = \beta \frac{D\boldsymbol{u}(\boldsymbol{x},t)}{Dt} - \frac{1}{\tau}\left[\boldsymbol{v}(t) - \boldsymbol{u}(\boldsymbol{x}(t),t)\right]$$

Toschi and Bodenschatz. Lagrangian properties of particles in Turbulence. Ann. Rev. Fluid Mech. (2009) vol. 41 pp. 375-404

Kaplan-Yorke dimension: DKY

Particle equations of motion defines a dissipative dynamical system
Attractor's dimension in the (x,v) space: Kaplan-Yorke dimension D_{KY}

DKY

$$d_L \equiv J - \frac{\lambda_1 + \cdots + \lambda_J}{\lambda_{J+1}}$$

$$\lambda_1 + \cdots + \lambda_J \geq 0$$
$$\lambda_1 + \cdots + \lambda_{J+1} < 0$$

6 Lyapunov exponents
computed by tracking

$$\mathbf{R}(t) \equiv (\delta\mathbf{x}(t), \delta\mathbf{v}(t))$$

$$\frac{d\mathbf{R}}{dt} = \mathcal{M}_t \mathbf{R}$$

$$\lambda_i = \lim_{T\to\infty} \gamma_i(T)$$

stretching rates

Standard orthonormalization
Gram-Schmidt procedure adopted

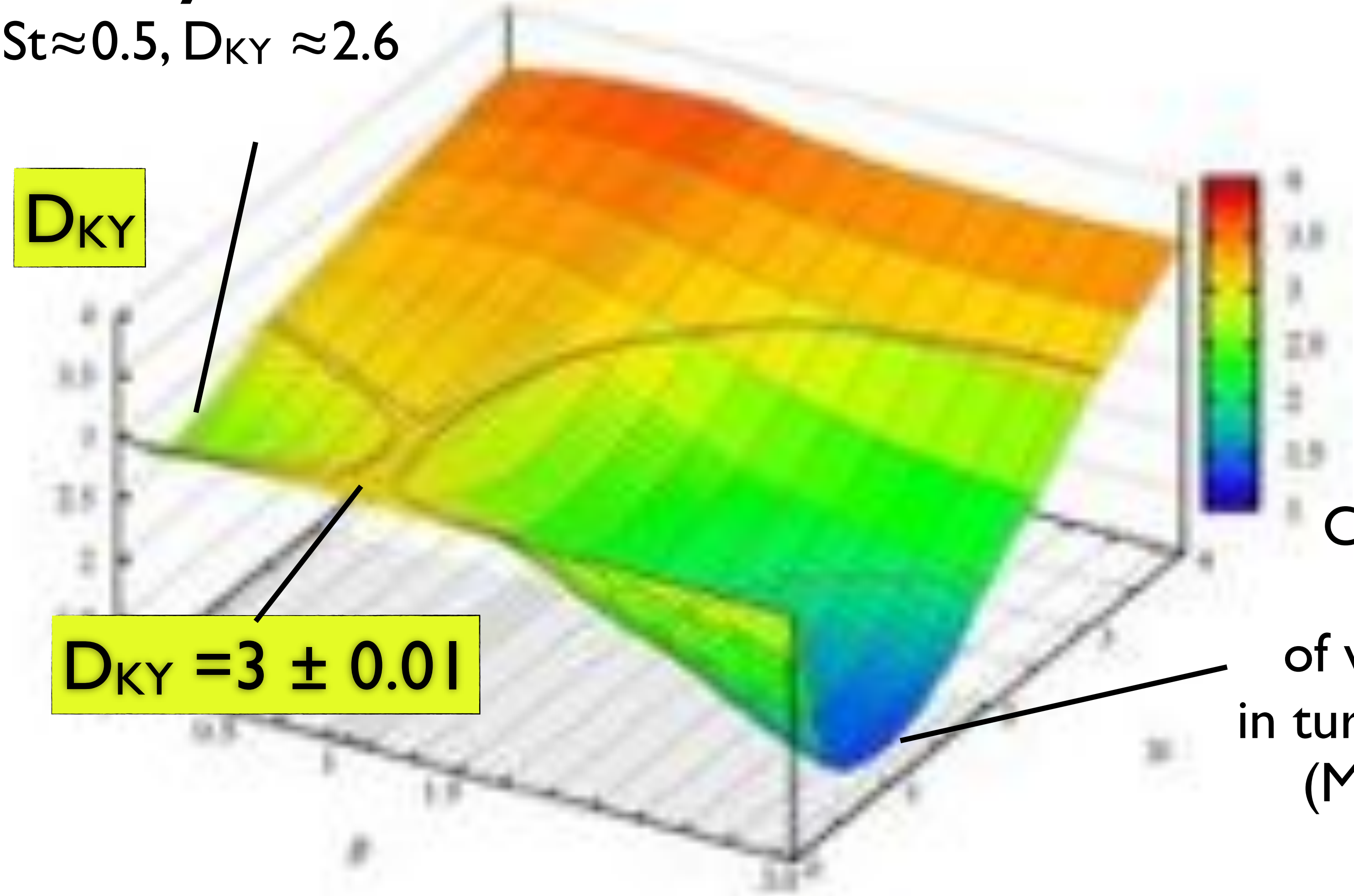
As in Bec Phys. Fluids (2003), Bec JFM (2005), Bec et al. Phys. Fluids (2006)

Kaplan-Yorke dimension

Balance between contraction and expansion

$$D_{KY} \equiv J - \frac{\lambda_1 + \cdots + \lambda_J}{\lambda_{J+1}} \qquad \begin{array}{l} \lambda_1 + \cdots + \lambda_J \geq 0 \\ \lambda_1 + \cdots + \lambda_{J+1} < 0 \end{array}$$

Heavy min. at
St≈0.5, D_{KY} ≈2.6



D_{KY}

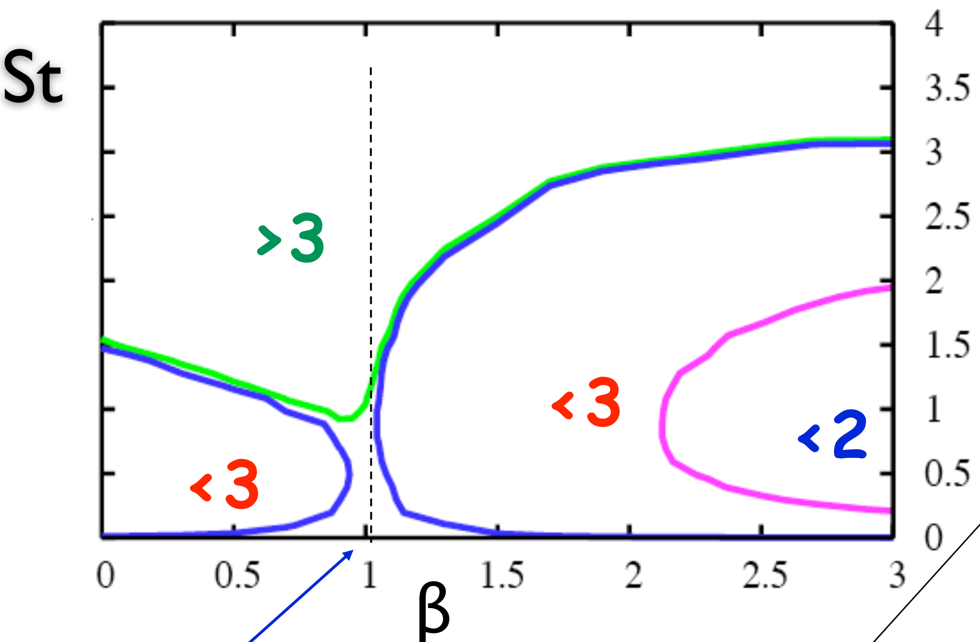
D_{KY} =3 ± 0.01

Light min at
St≈1, D_{KY}≈1.4

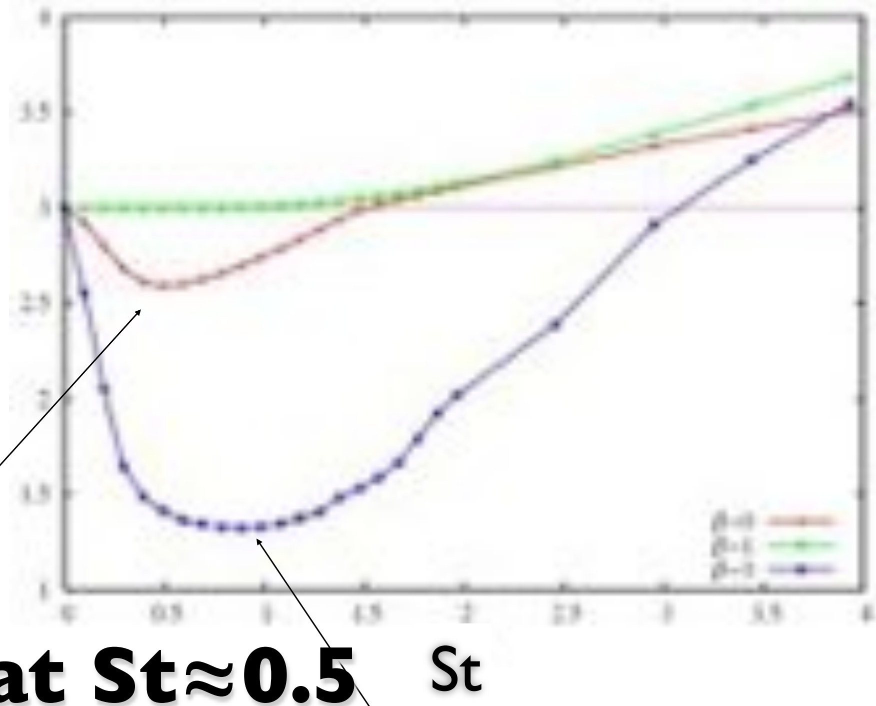
Close to fractal dimension
of vortex filaments
in turbulence? D_ω≈1.1
(Moisy & Jimenez
JFM04)

Projection of D_{KY}

Horizontal projection



Vertical projection



$D_{KY} = 3 \pm 0.01$

Heavy min at St≈0.5

Light min at St≈1

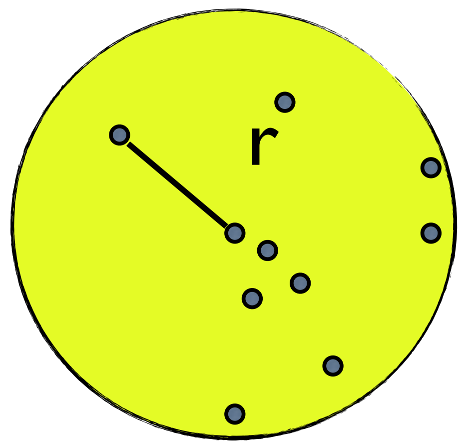
$$D_\omega \to 1.1 \pm 0.1$$

Close to fractal dimension of vortex filaments in turbulence (Moisy & Jimenez JFM 04)

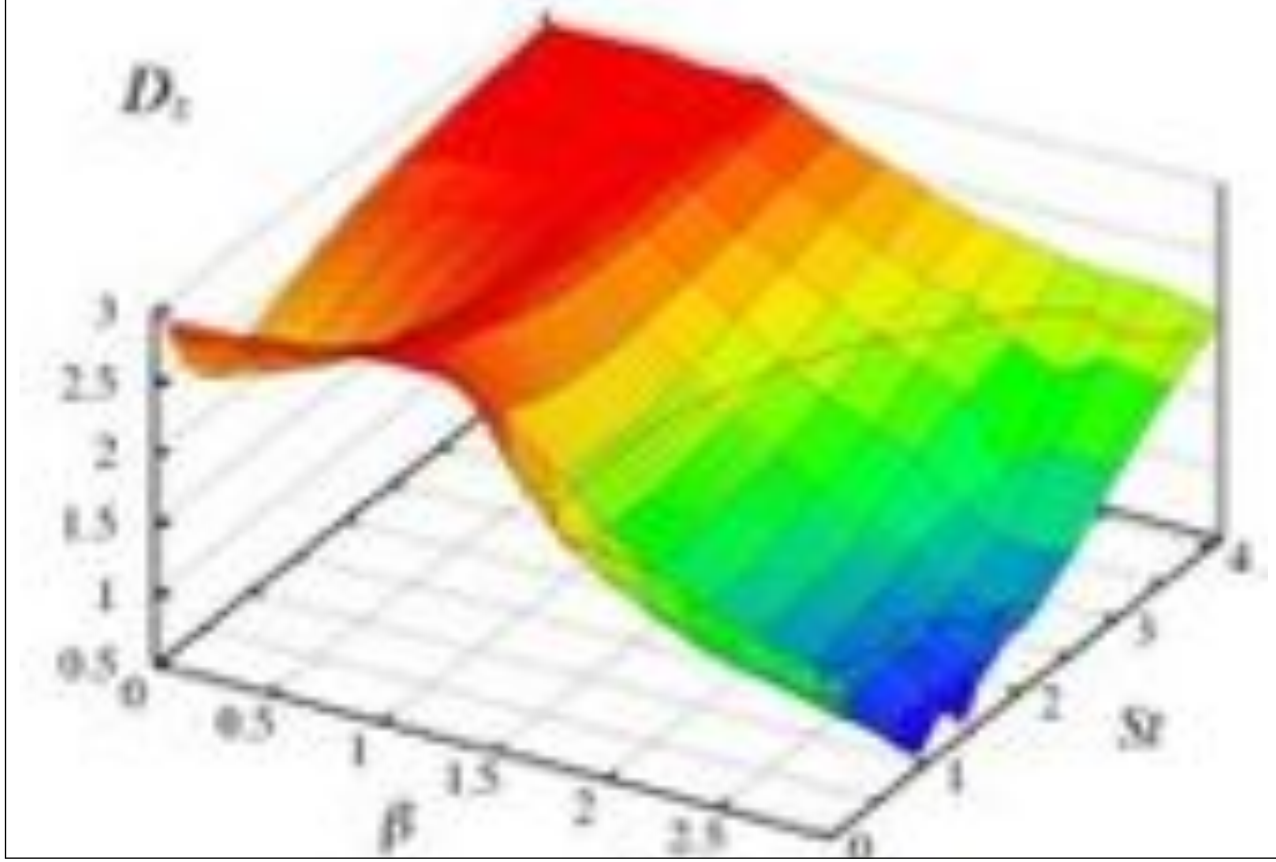
Correlation dimension D_2

$P_2(r)$ Probability to find a couple of particle whose distance is below r.

$$\text{At} \quad r \ll \eta \qquad P_2(r) = A\, r^{D_2}$$



fractal dimension hierarchy: $D_2 \leq D_1 = D_{KY}$



Same features as D_{KY}

Morphological analysis of point clouds

Calzavarini et al. Dimensionality and morphology of particle and bubble clusters in turbulent flow. J Fluid Mech (2008) vol. 607 pp. 13-24

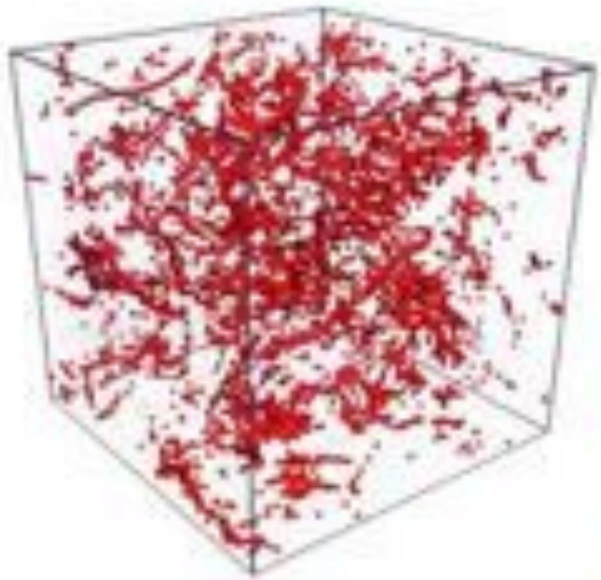
- Put balls $\mathcal{B}_r(\mathbf{x}_i)$ with radius ***r*** around each particle ***i***
- Let r increase
- Measure total **volume**, **surface**, **mean curvature** and **Euler characteristic** of the emerging structure

$$\mathcal{A}_r = \bigcup_{i=0}^{N} \mathcal{B}_r(\mathbf{x}_i)$$

Minkowski functionals provide complete morphological characterization of point cloud!

Visualization of A_r

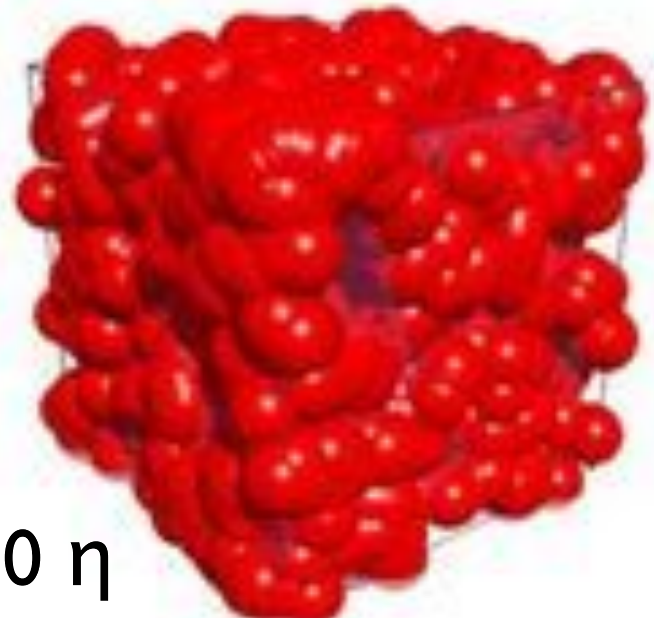
$2 \cdot 10^4$ particles with $\beta=3$ and St=1



radius = 0.5 η

radius = 3 η

r



radius = 10 η

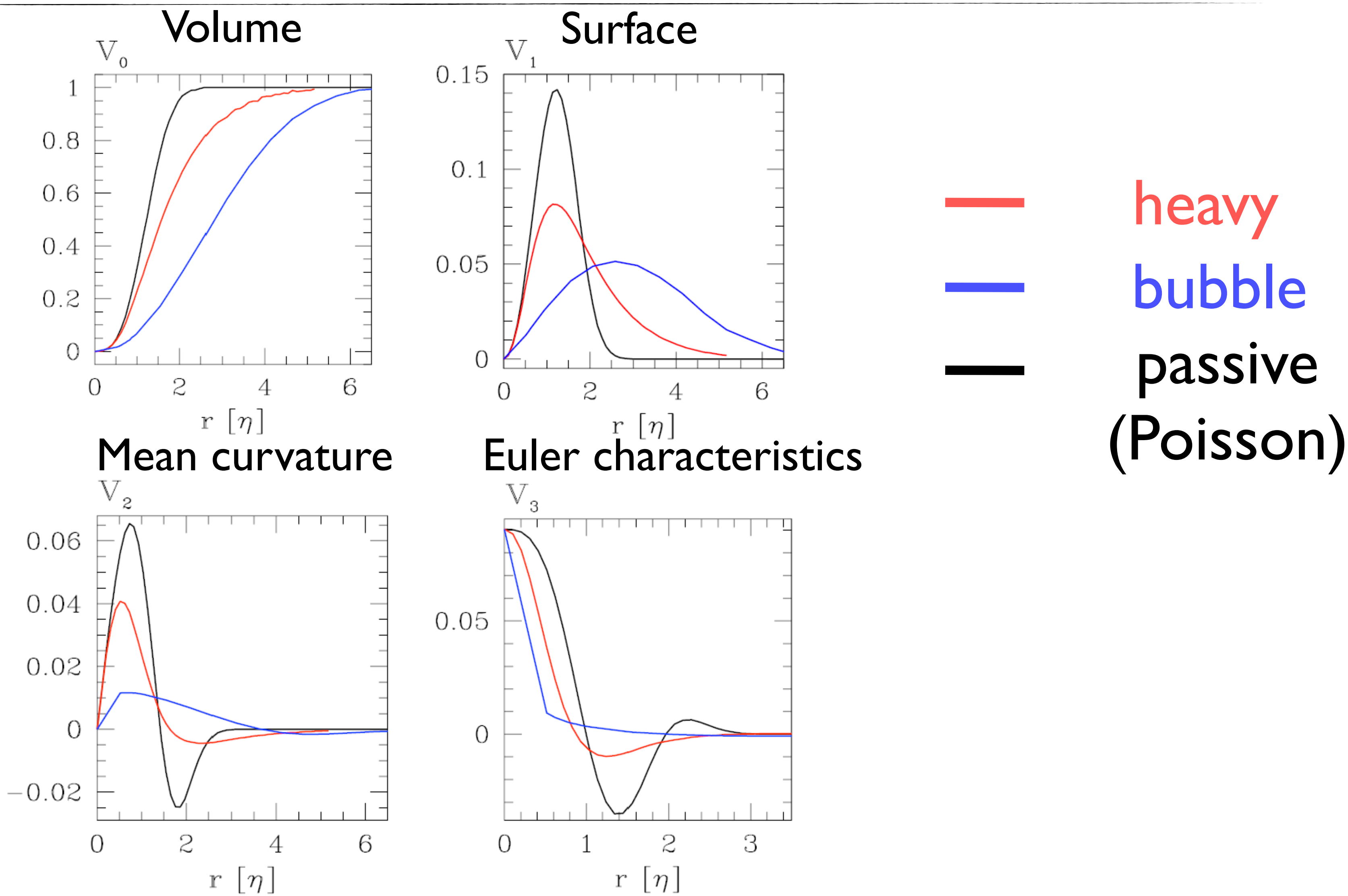
Minkowski functionals $V_\mu(r)$ in 3D

μ	$V_\mu(r)$	geometric quantity
0	V	V Volume
1	A/6	A Surface
2	H/(3 π)	H Mean curvature
3	χ	χ Euler characteristic

χ = vertices (corners) - edges + faces

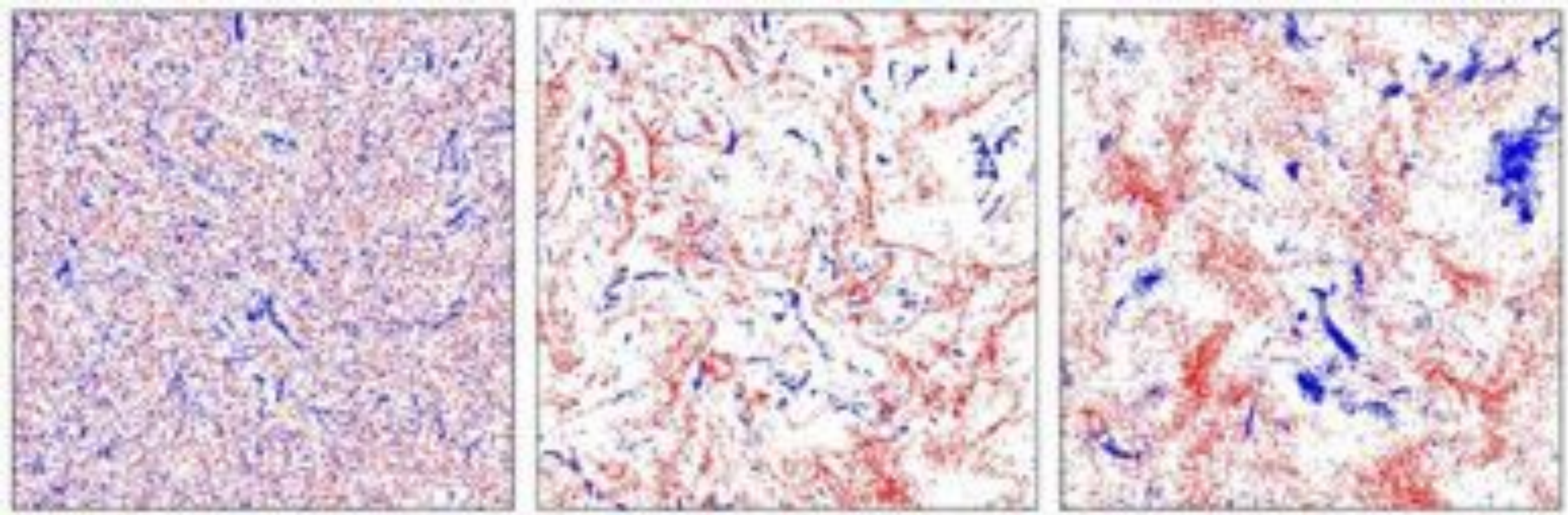
see: Mecke, K.R., Buchert, T. and Wagner, H. (1994). Robust morphological measures for large scale structure in the universe. Astron. Astrophys., 288, 697-704.

Minkowski functionals



Calzavarini et al.
Dimensionality and morphology of particle and bubble clusters in turbulent flow.
J Fluid Mech (2008) vol. 607 pp. 13-24

Turbulence induced segregation



Slice $320\eta \times 320\eta \times 8\eta$ of heavy β=0 (red) and light β=3 (blue) particle positions. From left to right $St = 0.1, 1, 4.1$. Data refer to the simulation at $\mathrm{Re}_\lambda = 180$.

- Particles evolved in the same velocity field
- Snapshot taken at the same time

Calzavarini et al. Quantifying turbulence-induced segregation of inertial particles. Phys Rev Lett (2008) vol. 101 (8) pp. 084504

Segregation observable

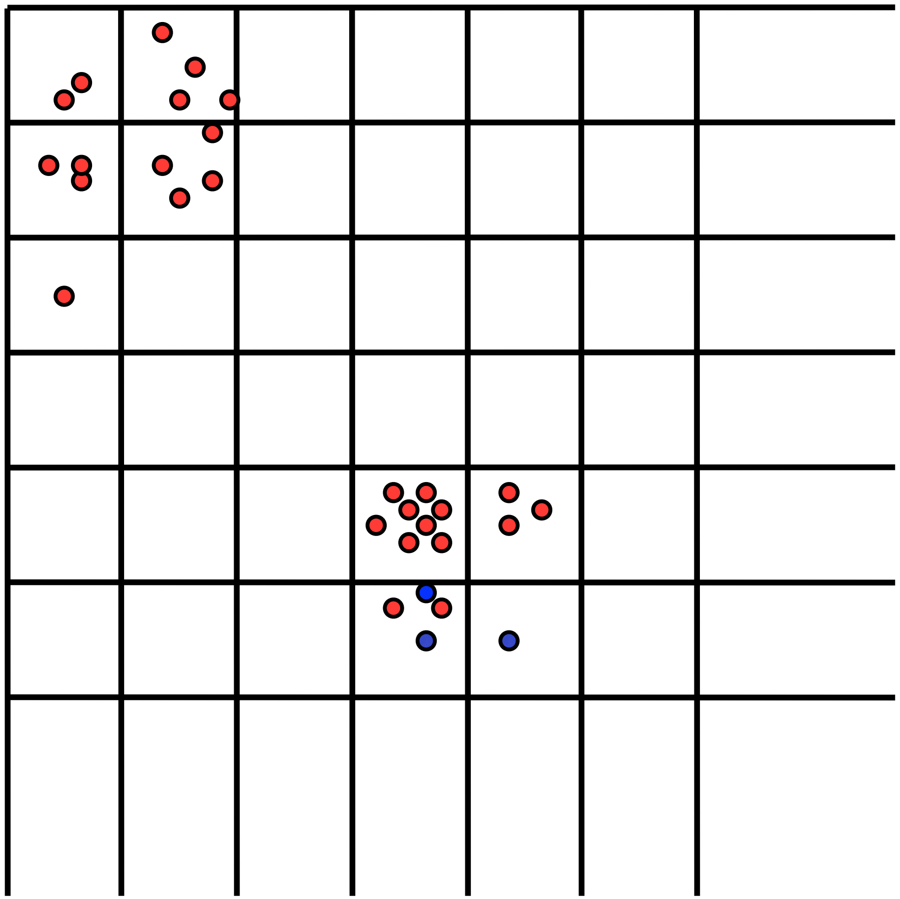
- Segregation is **scale dependent**

$$\mathcal{M}(r) = \left(\frac{L}{r}\right)^3$$

$$S_{\alpha_1,\alpha_2}(r) = \frac{1}{N_{\alpha_1} + N_{\alpha_2}} \sum_{i=1}^{\mathcal{M}(r)} |n_i^{\alpha_1} - n_i^{\alpha_2}|$$

- Idea: measure segregation as a function of the scale to define a **segregation length**

Possible segregation observable



If not overlapping

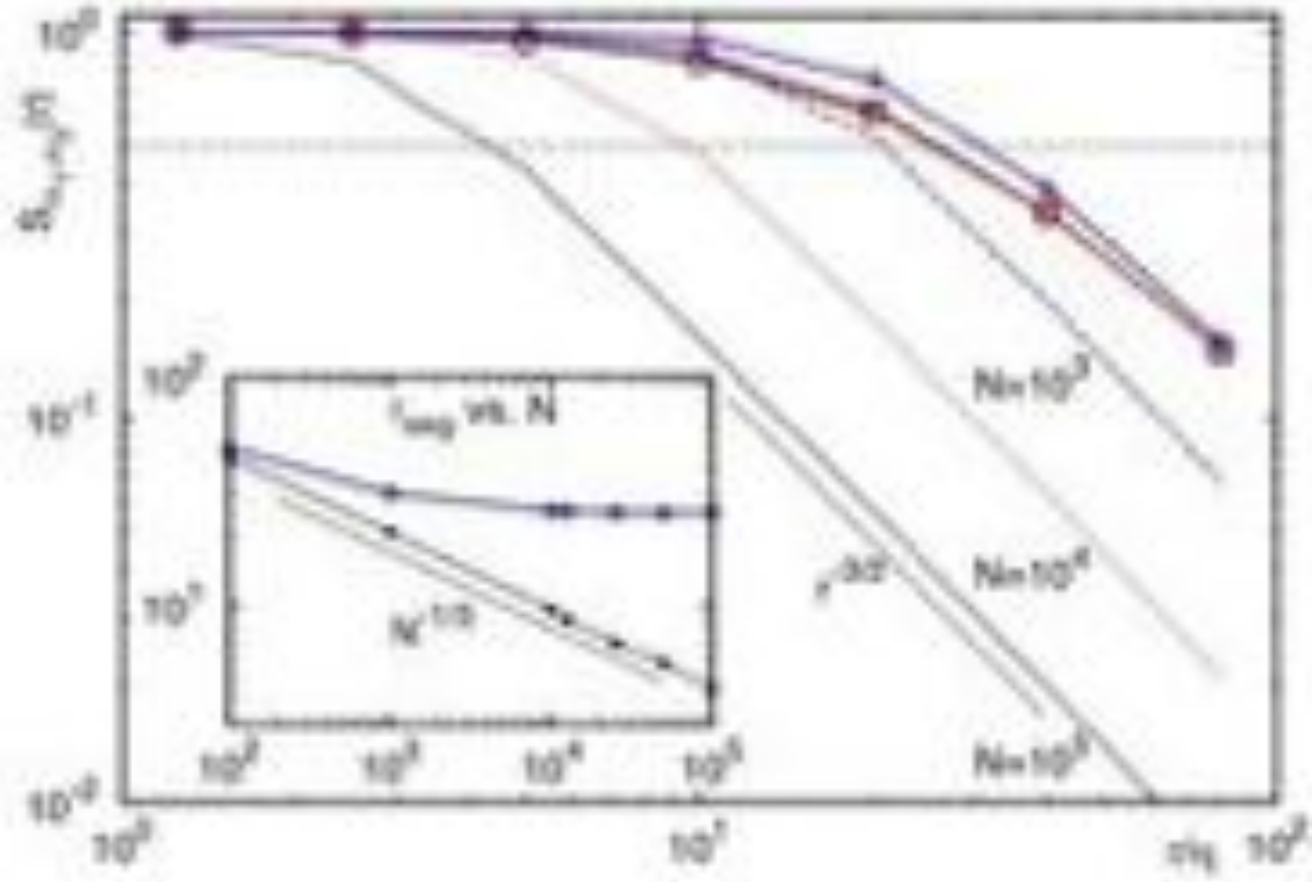
$$S_{\alpha_1,\alpha_2}(r) = 1$$

If perfectly overlapping

$$S_{\alpha_1,\alpha_2}(r) = 0$$

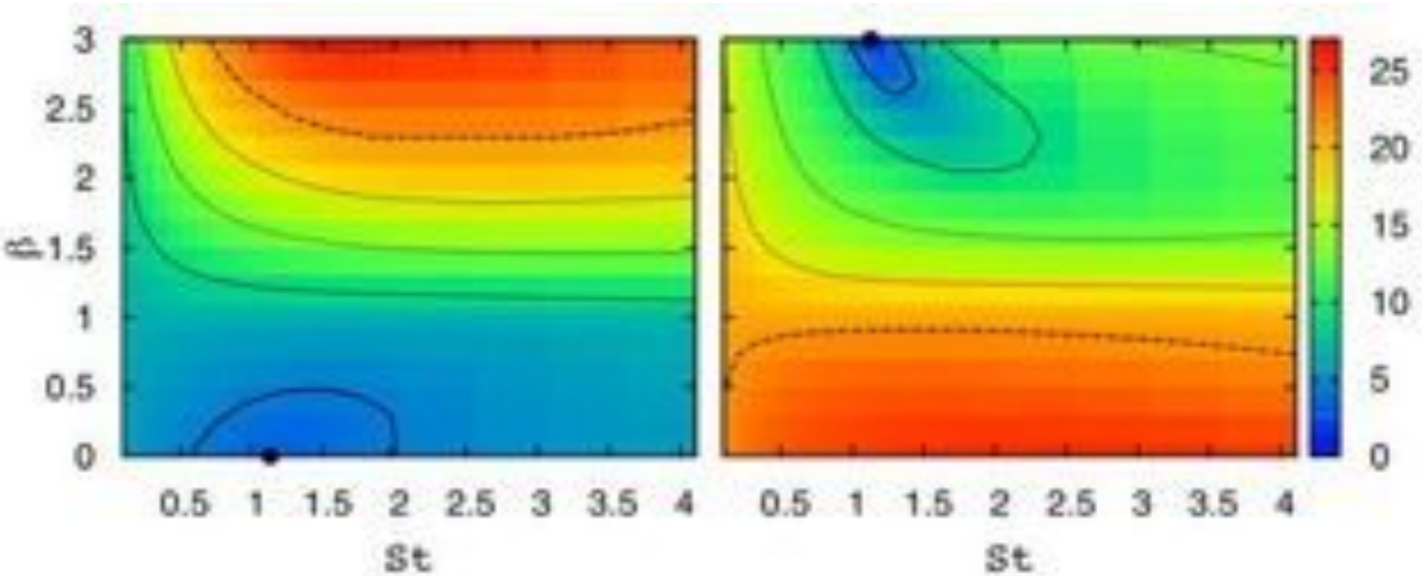
$$S_{\alpha_1,\alpha_2}(r) = \frac{1}{N_{\alpha_1} + N_{\alpha_2}} \sum_{i=1}^{\mathcal{M}(r)} |n_i^{\alpha_1} - n_i^{\alpha_2}|$$

Robustness



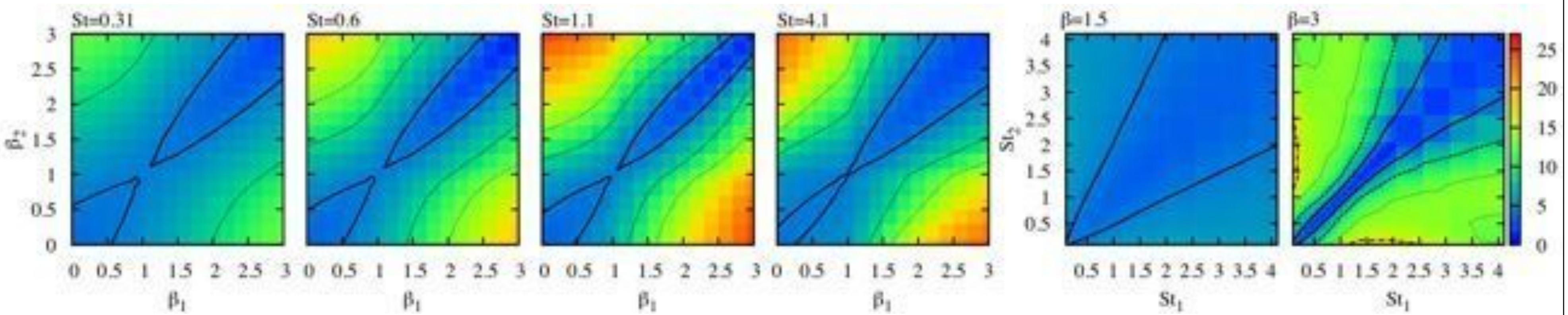
$S_{\alpha_1,\alpha_2}(r)$ vs r for $\alpha_1 = (\beta_1 = 0, St_1 = 1.1)$ (heavy type) and $\alpha_2 = (\beta_2 = 3, St_2 = 1.1)$ (light type) at varying the particle number $N = N_{\alpha_1} = N_{\alpha_2}$. Dashed and dotted lines show the same observable for uniformly distributed particles samples of various size N. The segregation length defined by $S_{\alpha_1,\alpha_2}(r_{seg}) = 1/2$ is shown in the inset, for both heavy vs light particles and for the Poissonian samples, as a function of the particle number N. For the latter the expected scaling behaviors, i.e. $S \propto r^{-3/2}$ and $r_{seg,h} \propto N^{-1/3}$, are also indicated.

Results for r_{seg}



r_{seg} measured between particle distributions with $\beta = 0$, $St = 1.1$ (left) and $\beta=3$, $St=1.1$ (right) vs distributions with generic β, St. The solid contour line, traced at $r_{seg} = r_{seg,h} \equiv L/N^{1/3}$, sets the sensitivity level to distinguish between segregated and unsegregated particle distributions. The dashed and dotted lines are drawn at $r_{seg} = n \cdot r_{seg,h}$, with $n = 2, \ldots, 6$. The color scale codes the value of r_{seg} in units of the Kolmogorov scale, η.

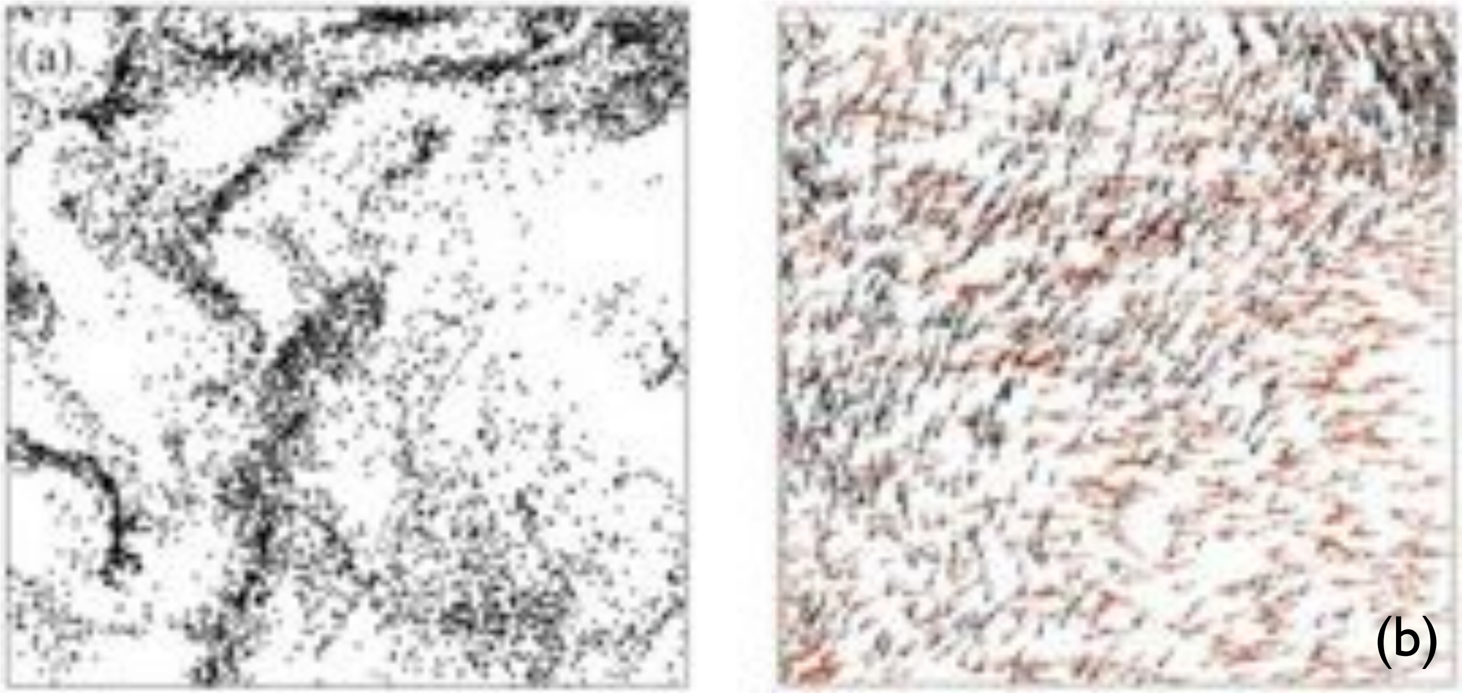
From left to right, segregation length between distribution of particles with $St = (0.31, 0.6, 1.1, 4.1)$ vs the densities β_1, β_2 and (last two panels) for particle couples having the same densities $\beta_1 = \beta_2 = 1.5$ and 3 and different St.



Particle diffusion

- Caustics
- Particles diffusion

Caustics and "particle velocity field"



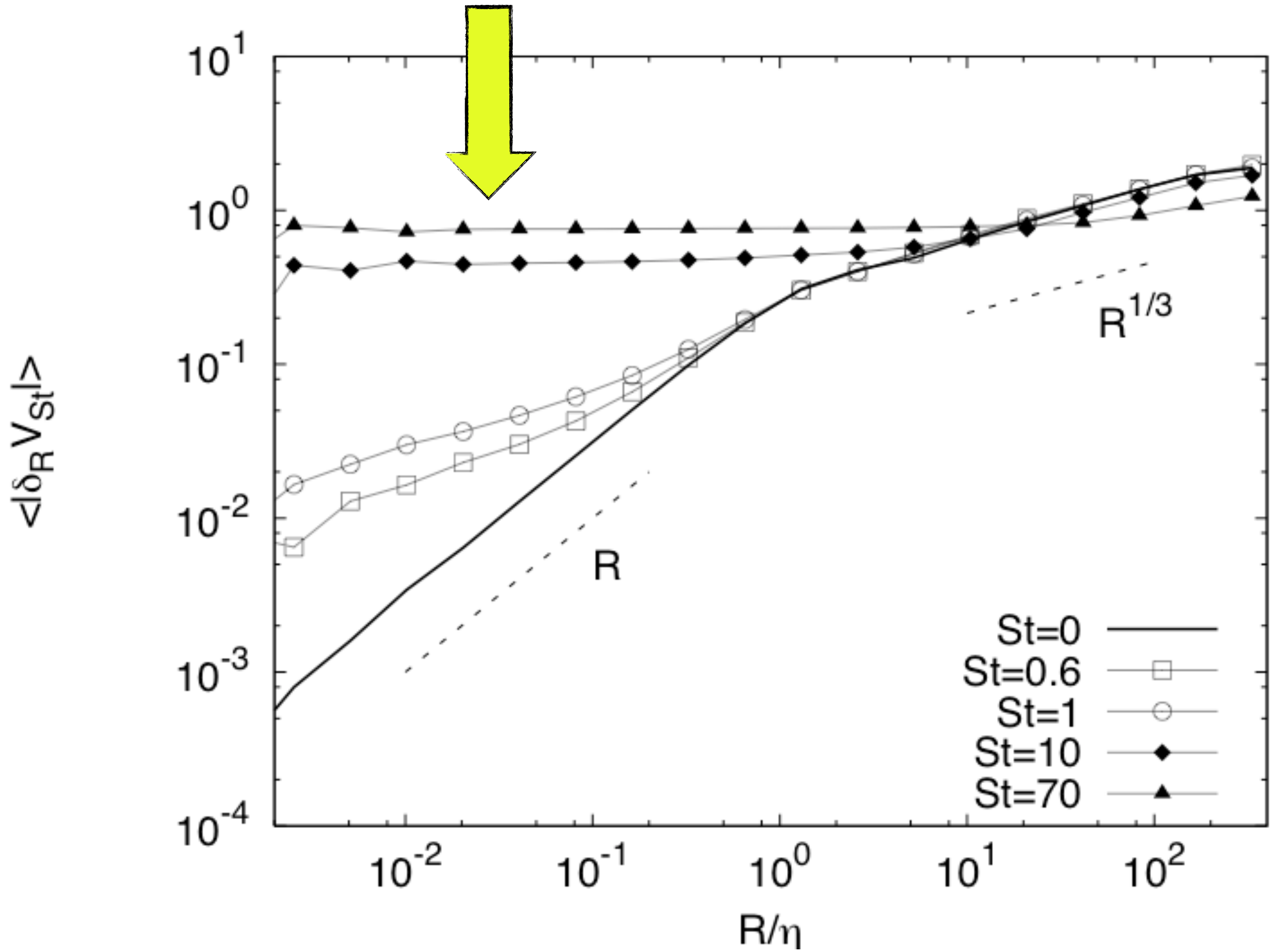
St = 2 St = 20

(a) Snapshot of the position of particles for St = 2 in a slice of size 5η x 100 η x 100 η for $Re_\lambda \approx 400$.

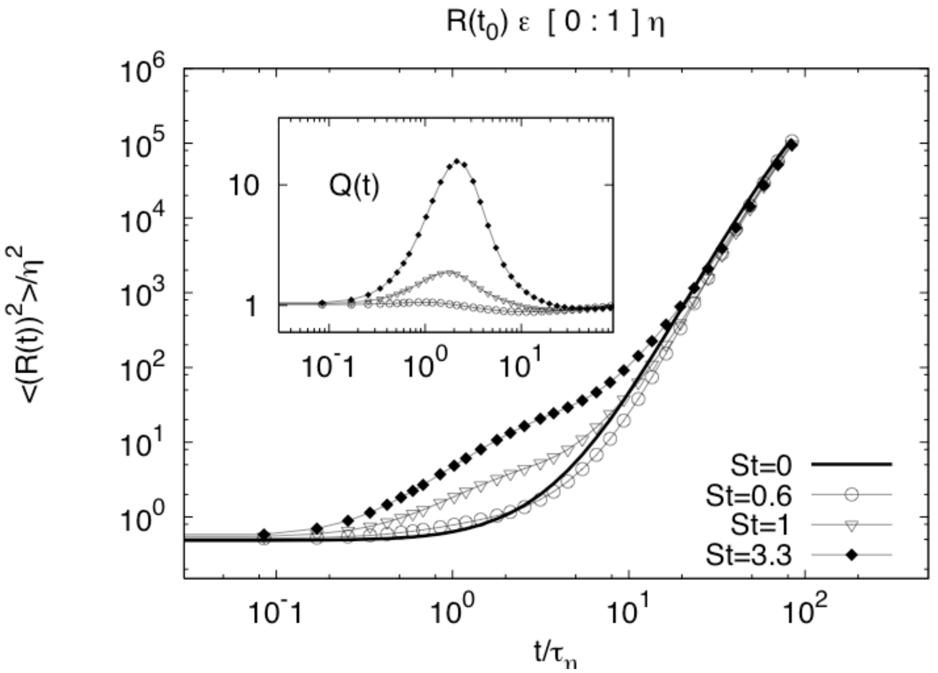
(b) Particle velocity field in the same slice for a larger Stokes, St = 20, showing the existence of regions where particles have different velocities (highlighted by gray and black arrows, respectively).

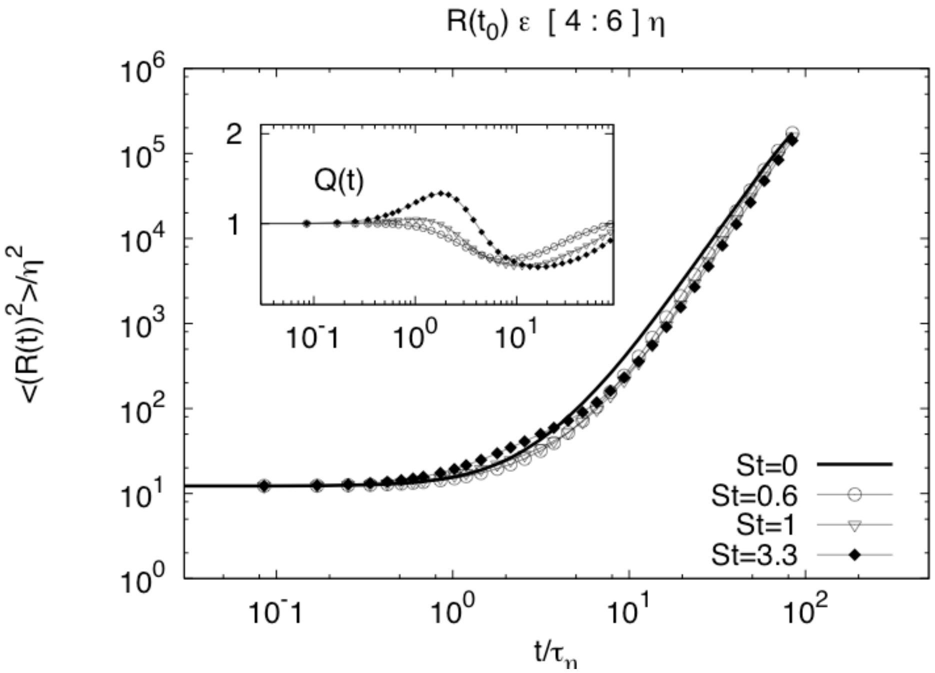
Particles velocity structure functions

The role of caustics



Dispersion & inertia: smaller St





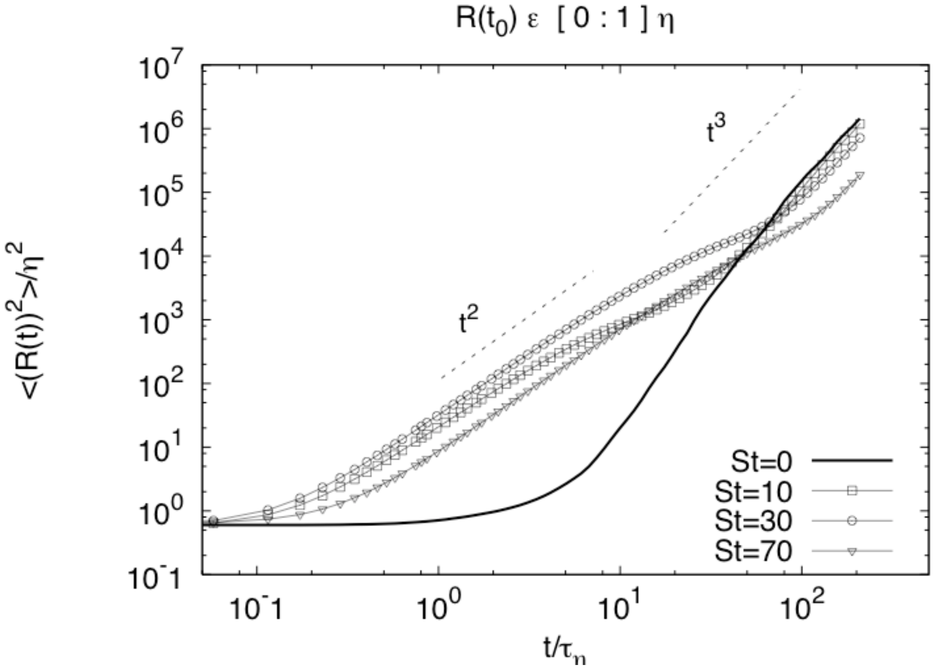
Batchelor 1952

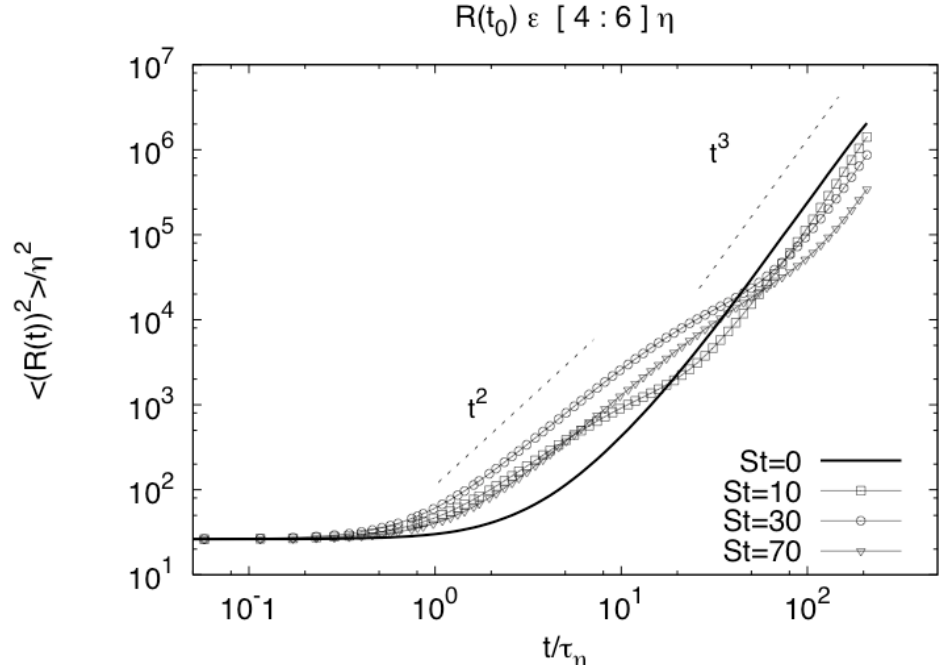
$$Q(t) = \frac{\langle (R(t))^2 \rangle_{St}}{\langle (R(t))^2 \rangle_{St=0}}$$

$$\langle (R(t))^2 | R_0, t_0 \rangle_{(St=0)} \sim g\, t^3 \qquad \tau_\eta \ll (t - t_0) \ll t_B$$

$$\langle (R(t))^2 | R_0, t_0 \rangle_{St=0} \simeq R_0^2 + C(\varepsilon R_0)^{2/3}\, t^2 \qquad t_B \ll (t - t_0) \ll T_L$$

Dispersion & inertia: larger St





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$$\langle (R(t))^2 | R_0, t_0 \rangle_{St=0} \simeq R_0^2 + C(\varepsilon R_0)^{2/3}\, t^2 \qquad t_B \ll (t - t_0) \ll T_L$$

“Large” particles

Particles that are large with respect to turbulent scales do have an effective inertia even when neutrally buoyant (e.g. Plankton)

What is the relations between size-induced and density-induced inertia ?

How to model these effect computationally ?

How to validate the computational model ?

Effect of particle size

$$\mathbf{f}_A = \frac{4}{3}\pi a^3 \rho_f \left(\langle \frac{D\mathbf{u}}{Dt} \rangle_{V_a} + \frac{1}{2}\left(\langle \frac{d\mathbf{u}}{dt} \rangle_{V_a} - \frac{d\boldsymbol{v}}{dt} \right) \right)$$

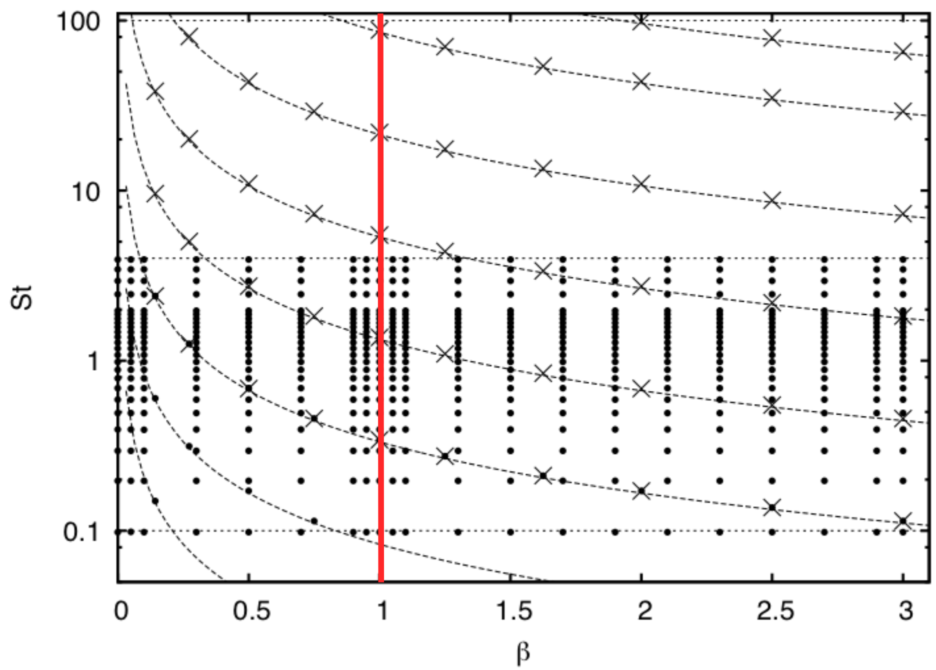
$$\mathbf{f}_D = 6\pi\nu\rho_f a \left(\frac{1}{4\pi a^2} \int_{S_a} \mathbf{u}(\mathbf{x})\ d\mathbf{S} - \boldsymbol{v} \right) = 6\pi\nu\rho_f a \left(\langle \mathbf{u} \rangle_{S_a} - \boldsymbol{v} \right)$$

$$\frac{d\boldsymbol{v}}{dt} = \frac{3\ \rho_f}{\rho_f + 2\ \rho_p} \left(\langle \frac{D\mathbf{u}}{dt} \rangle_{V_a} + \frac{3\nu}{a^2} \left(\langle \mathbf{u} \rangle_{S_a} - \boldsymbol{v} \right) \right)$$

$$(4/3)\pi a^3 \rho_p\ d\boldsymbol{v}/dt = \mathbf{f}_D + \mathbf{f}_A$$

Point particle (PP) model ●

Finite particle (FC) model ×



PP vs. FC models

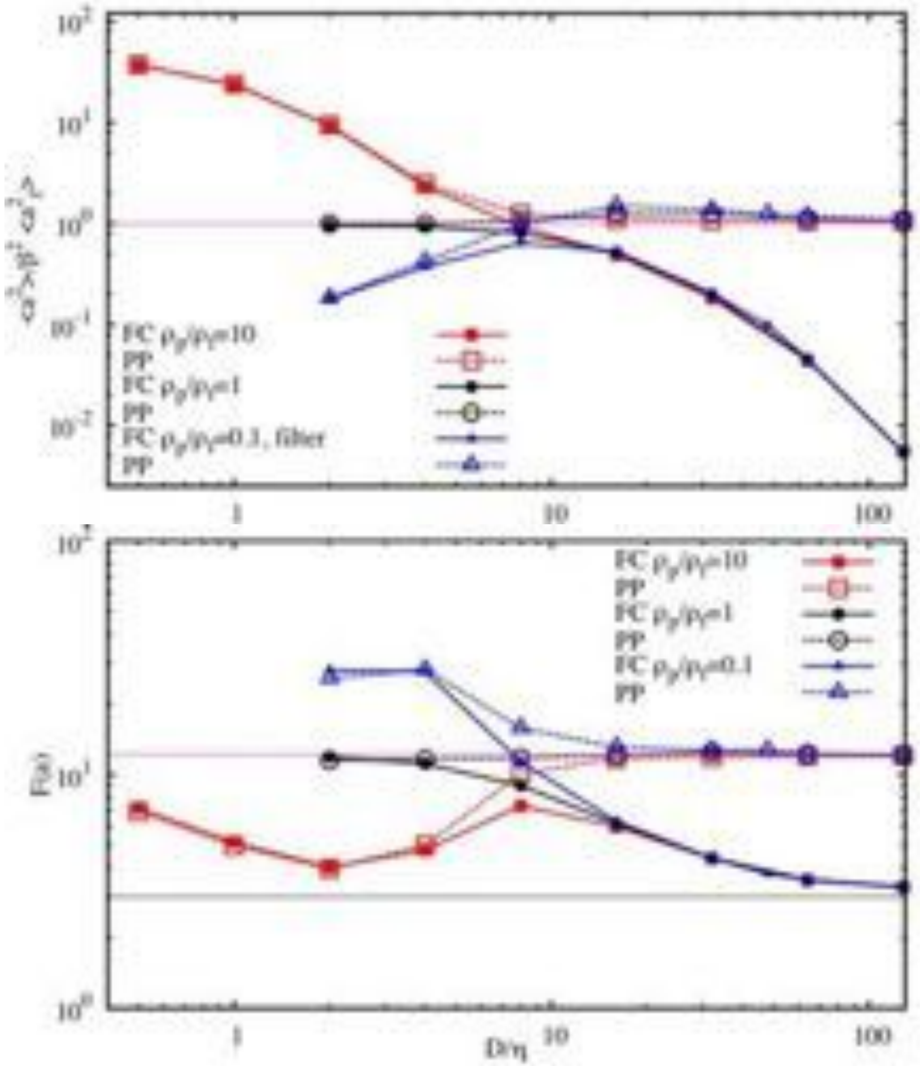
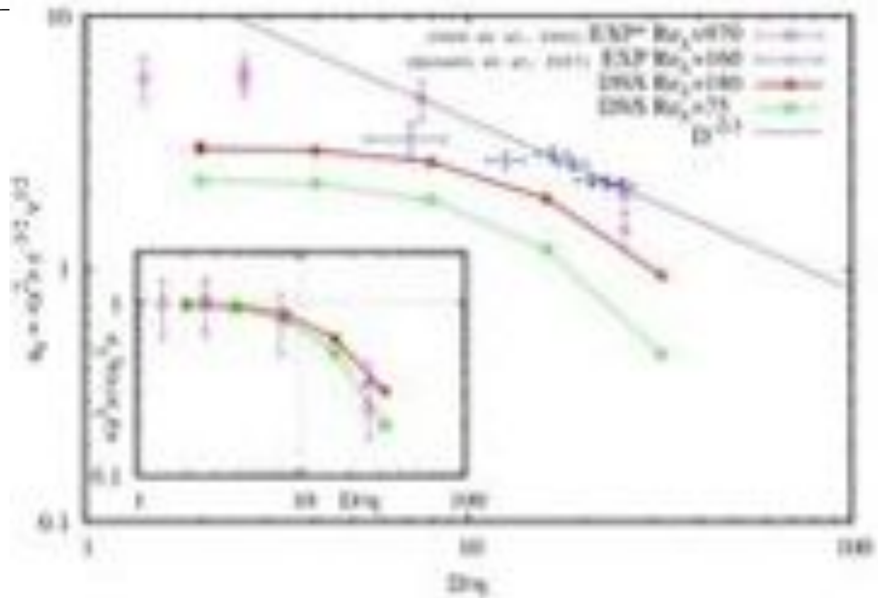
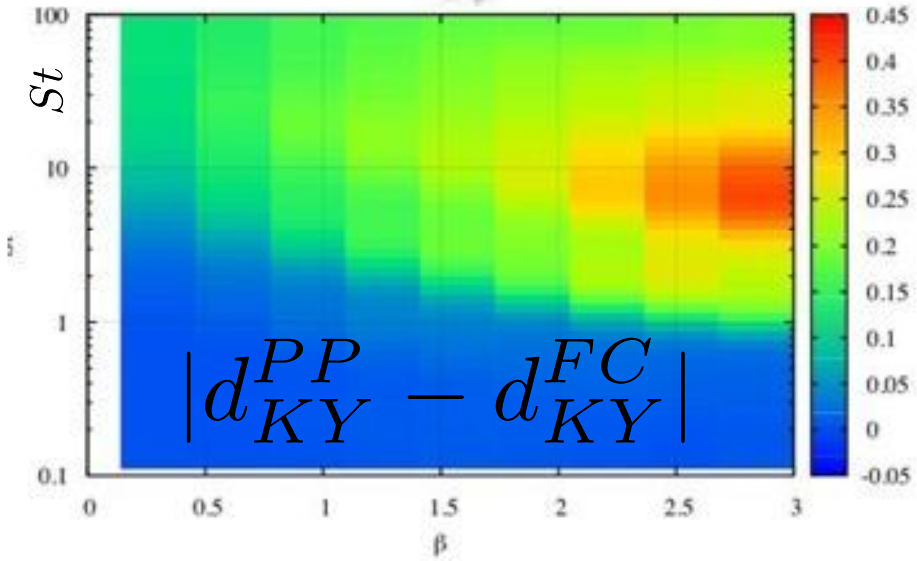


FIGURE 1. (*a*) The acceleration variance $\overline{a^2}$ normalized by $\beta^2\overline{a_f^2}$ versus the particle diameter as derived from the FC model (solid lines/symbols) and from PP the model system (dashed lines/empty symbols). Density ratios shown are $\rho_p/\rho_f = 0.1, 1, 10$, i.e. heavy (□), neutral (○) and light (△) particles. (*b*) Same as above for the acceleration flatness $F(a) = \overline{a^4}/(\overline{a^2})^2$. Horizontal lines shows the flatness of the fluid acceleration $F(a_f)$ and the flatness value for Gaussian distribution $F(a) = 3$. Data from simulations at $Re_\lambda = 75$.





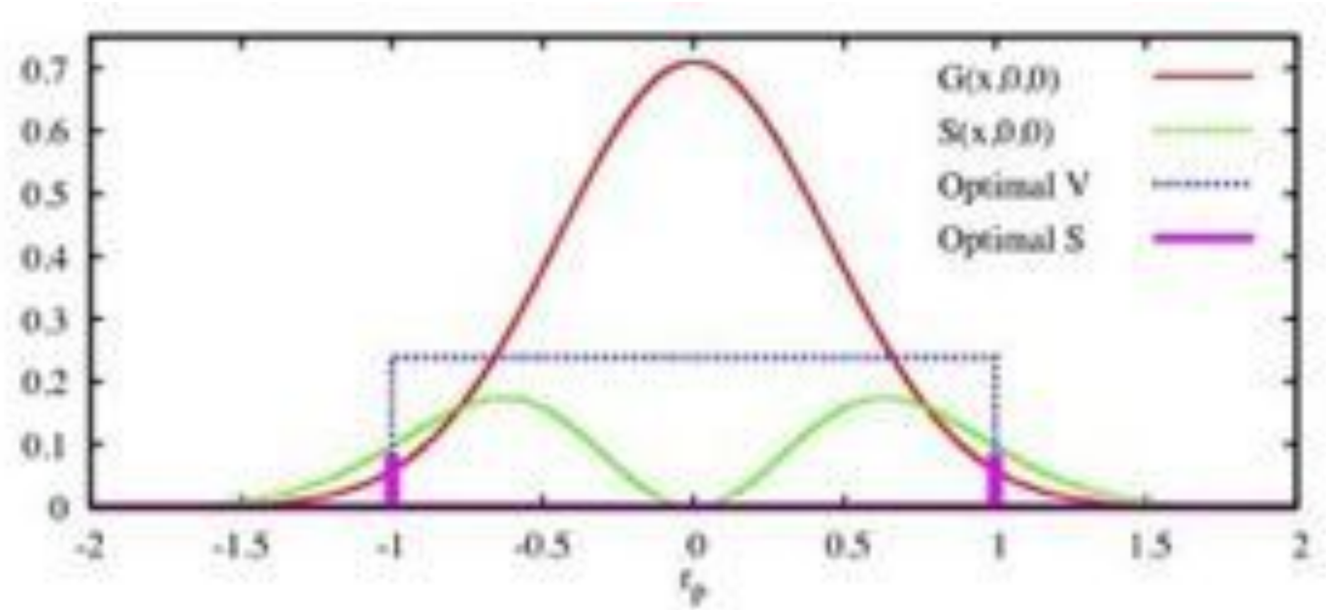
Calzavarini et al. Acceleration statistics of finite-sized particles in turbulent flow: the role of Faxén forces. J Fluid Mech (2009) vol. 630 pp. 179

A more complete model ?

Will consider *only neutrally buoyant* particles

Role of phenomenological terms in eqn for particle ?

+ Finite size Faxen-correction



Impact of trailing wake drag on the statistical properties and dynamics of finite-sized particle in turbulence
Enrico Calzavarini, Romain Volk, Emmanuel Leveque, Jean-Francois Pinton, Federico Toschi
http://lanl.arxiv.org/abs/1008.2888

Equation of motion

$$\frac{d\mathbf{v}}{dt} = \beta\left[\frac{D\mathbf{u}}{Dt}\right]_V + \frac{3\nu\beta}{{r_p}^2}\left([\mathbf{u}]_S - \mathbf{v}\right)$$

$$+ \frac{3\beta}{r_p}\int_{t-t_h}^{t}\left(\frac{\nu}{\pi(t-\tau)}\right)^{\frac{1}{2}}\frac{d}{d\tau}\left([\mathbf{u}]_S - \mathbf{v}\right)d\tau$$

$$+ c_{Re_p}\frac{3\nu\beta}{{r_p}^2}\left([\mathbf{u}]_S - \mathbf{v}\right) + \left(1 - \frac{3\ \rho_f}{\rho_f + 2\ \rho_p}\right)\ \mathbf{g}$$

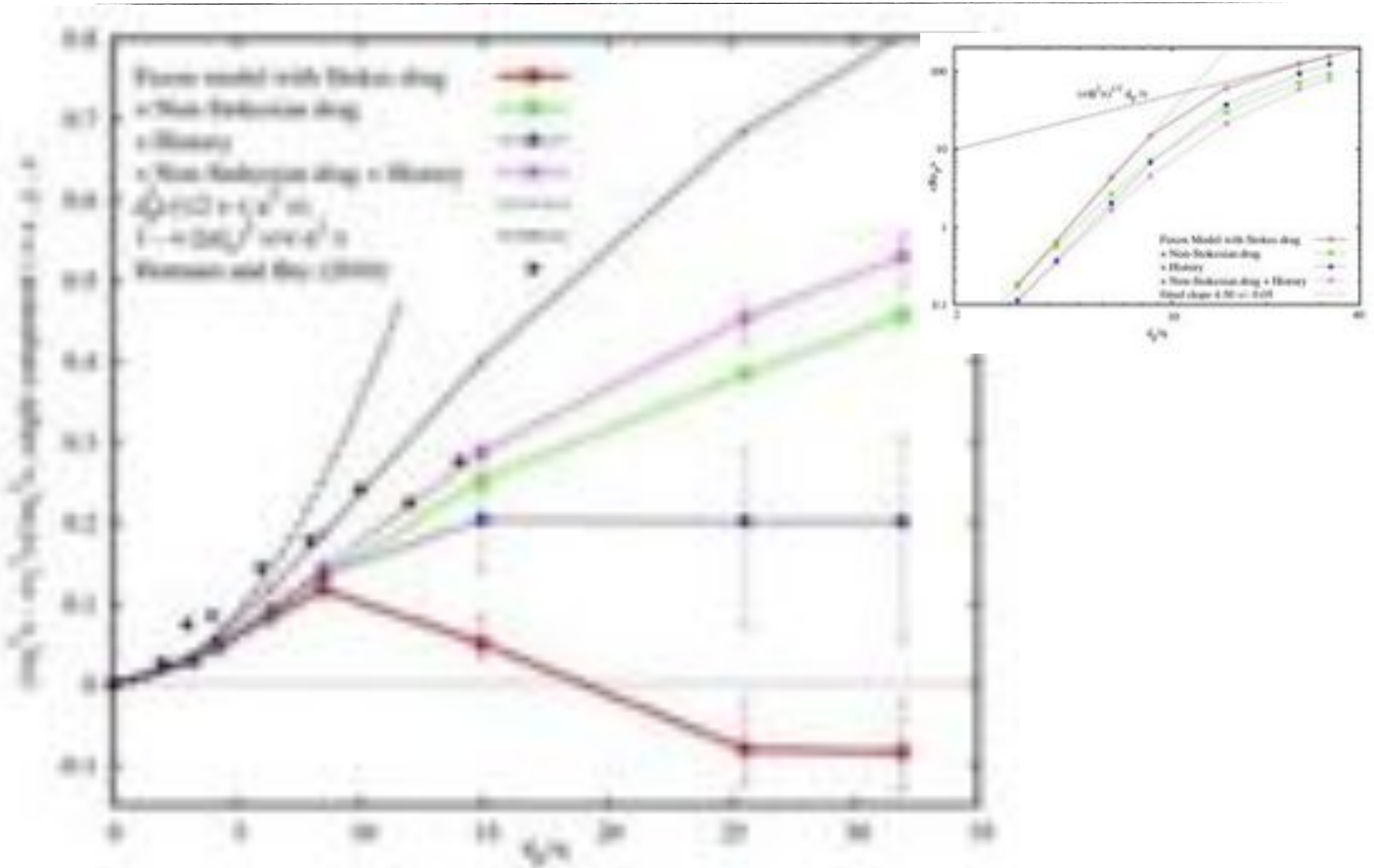
Particle radius r_p

Particle diameter $d_p = 2r_p$

$$Re_p \equiv \left|[\mathbf{u}]_S - \mathbf{v}\right| d_p/\nu$$

$$\beta \equiv \frac{3\ \rho_f}{(\rho_f + 2\ \rho_p)}$$

Large “pointwise” particles: velocity



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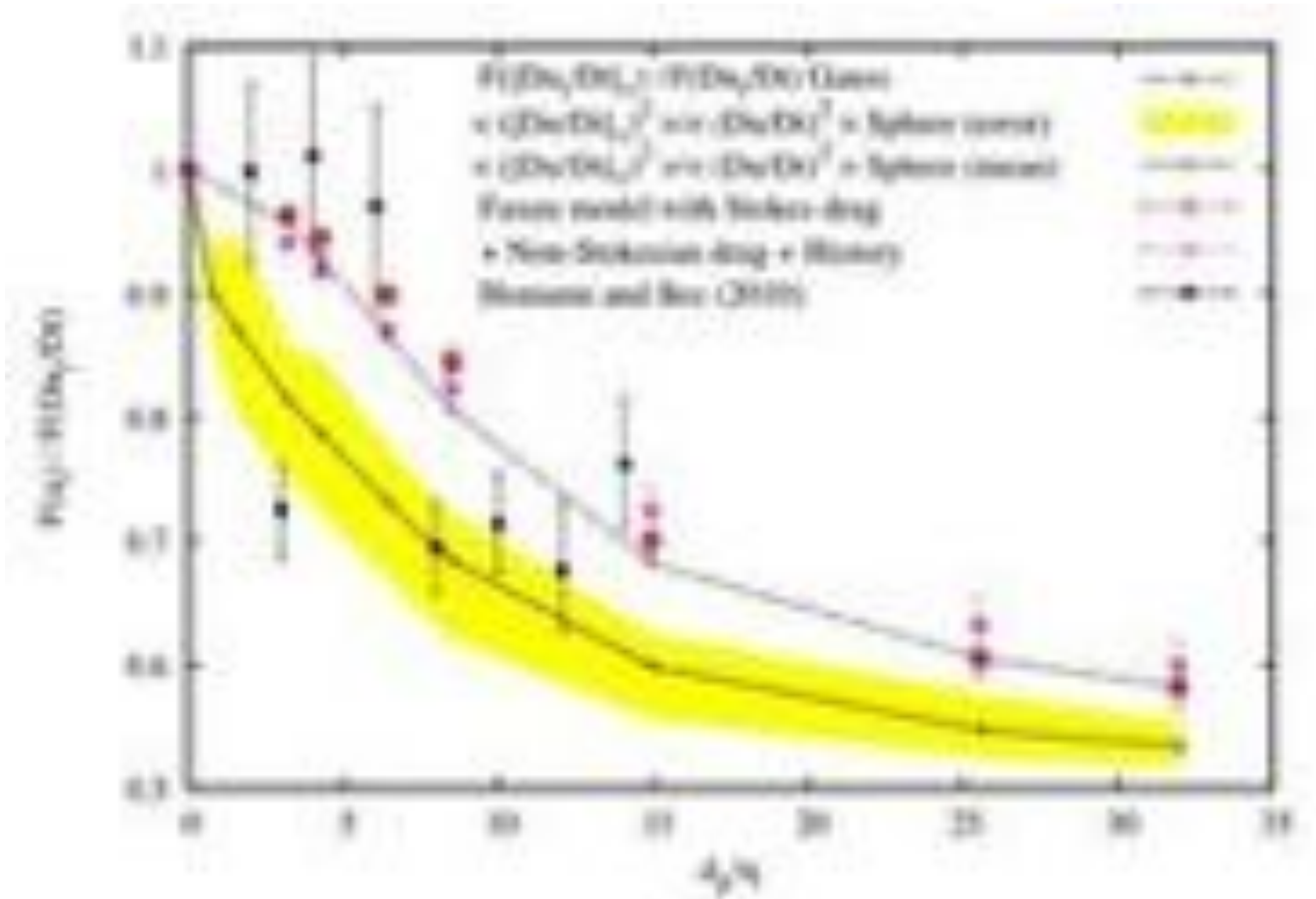
Large “pointwise” particles: flatness of acceleration



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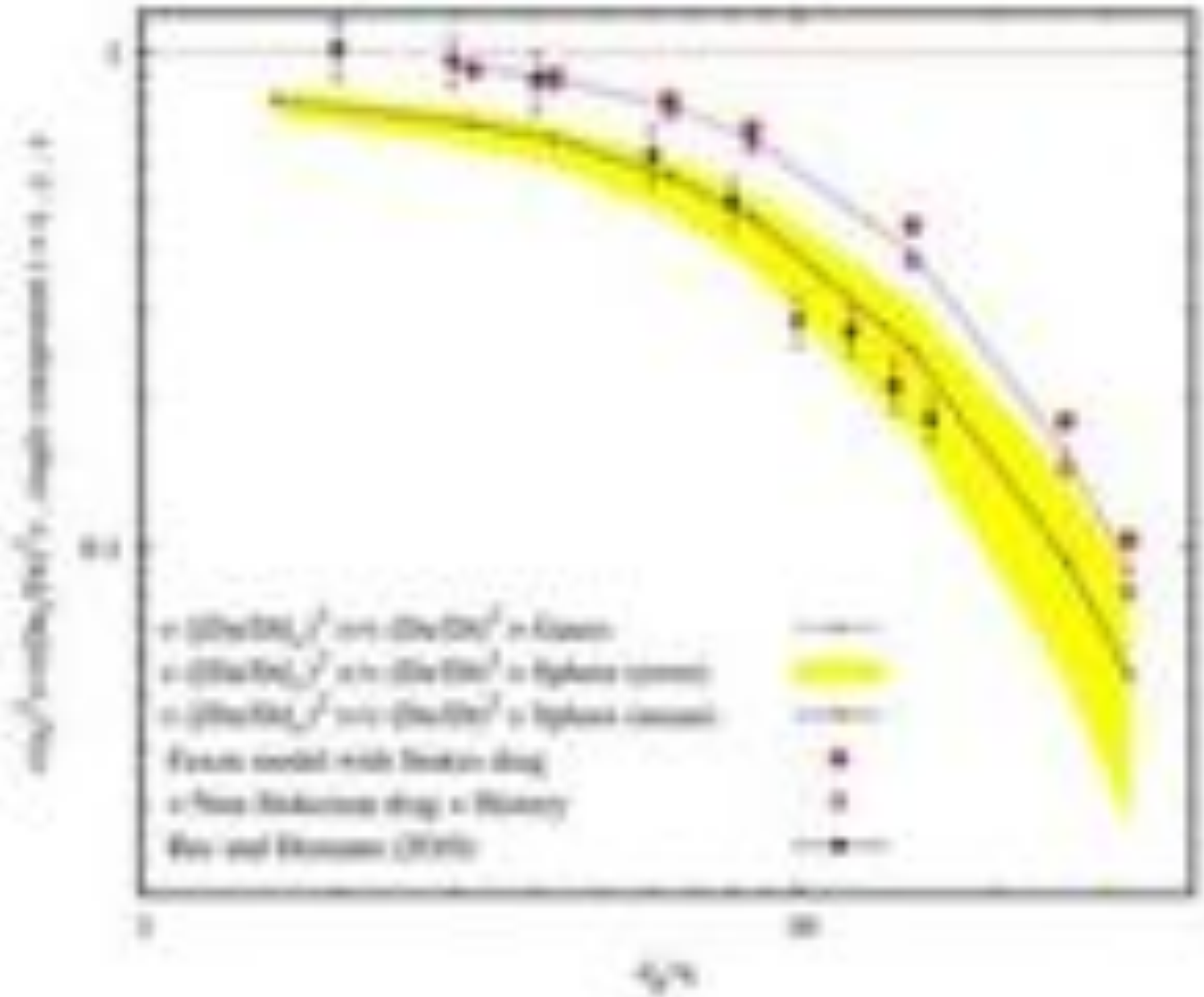

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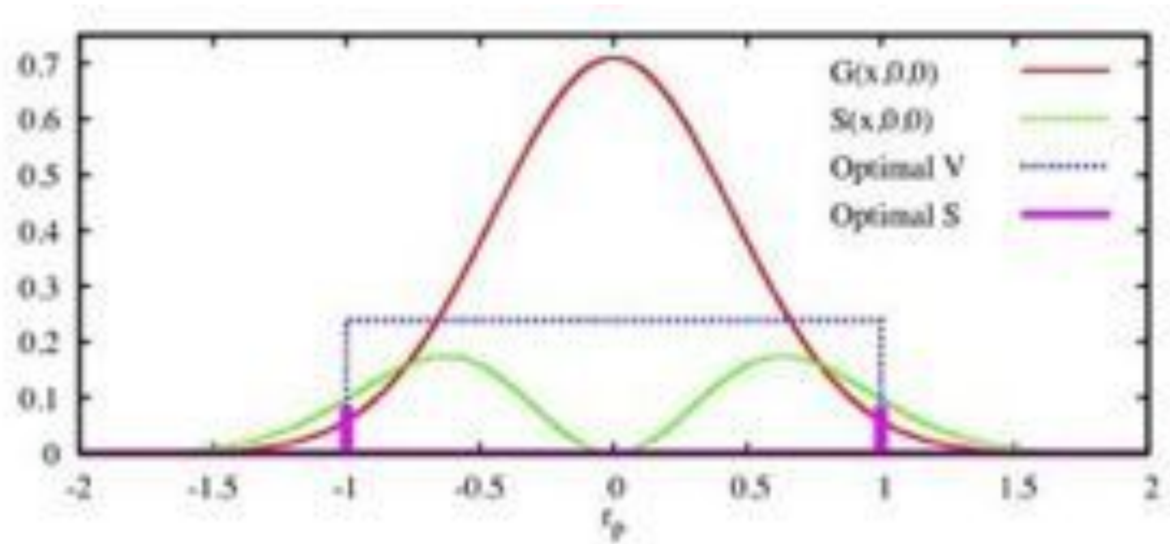
PP model

- Gaussian kernel
  - computationally efficient but biased
  - proper averaging seems promising
  - (from $d_p < 4\eta$ to $d_p \leq 32\eta$!)



A Virtual Laboratory

iCFDdatabase

http://cfd.cineca.it

http://mp0806.cineca.it/icfd.php

30Tbyte

Example of databases

- HEAVY
- LIGHT
- FAT

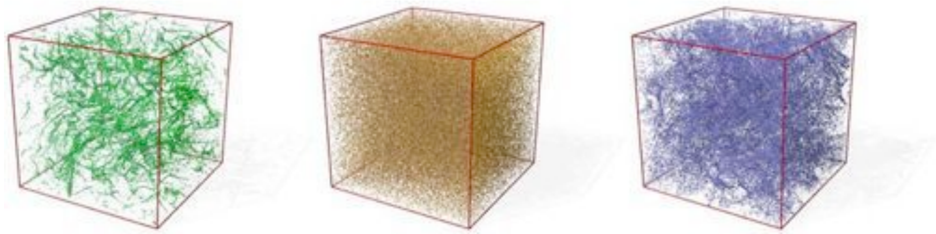
- mp0806.cineca.it/icfd.php

512^3 DNS tracers & heavy & light

N	Re_λ	η	L	T_L	τ_η	T	δx	N_p
512	183	0.01	3.14	2.1	0.048	5	0.012	$1 \cdot 10^8$

Pseudo spectral code - dealiased 2/3 rule - normal viscosity - 100 millions of passive tracers & heavy/light particles- code fully parallelized with MPI+FFTW - Platform IBM SP5 1.9 GHz - 30000 cpu hours - duration of the run: 30 days.

64 different particles classes (ß,St)

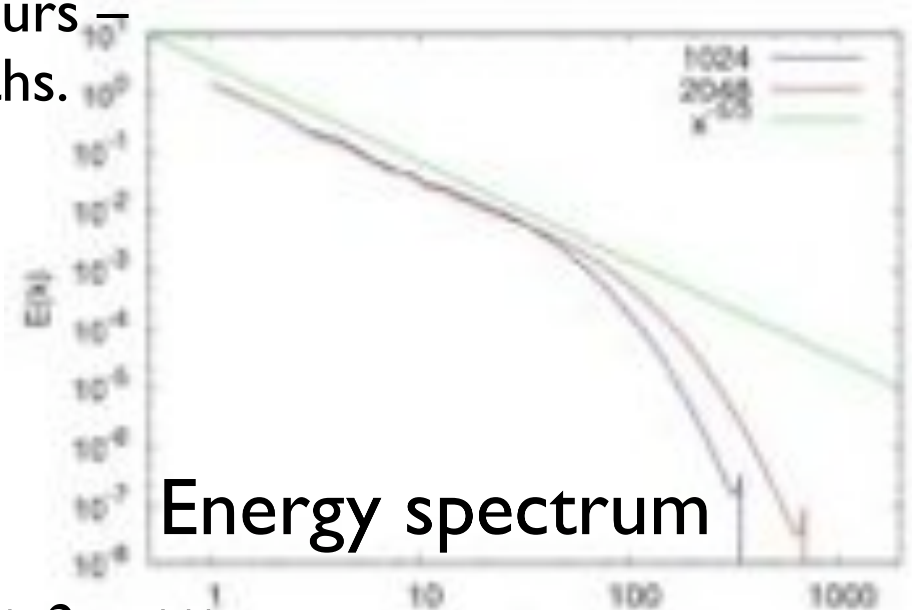


Lagrangian database $(x(t),v(t),u(t),\partial_i u_j\ (t))$ at high resolution

2048^3 DNS with tracers & heavy

N	Re_λ	η	L	T_L	τ_η	T	δx	N_p
2048	400	0.0025	3.14	1.8	0.02	5.9	0.003	$2\cdot 10^9$

Pseudo spectral code - dealiased 2/3 rule - normal viscosity - 2 billions of passive tracers & heavy particles- code fully parallelized with MPI+FFTW - Platform SGI Altix 4700 - 400000 cpu hours – duration of the run: 40 days over 3 months.



Lagrangian database $(x(t), v(t), u(t), \partial_i u_j(t))$ at high resolution

Heavy particles - Lagrangian integration

L^3	256^3	512^3	2048^3
Total particles	32 Mparticles	120 Mparticles	2,1 Gparticles
Stokes/ LyapStokes	16/32	16/32	21
Slow dumps 10 τ_η	2.000.000	7.500.000	101.888.000
Fast dumps 0.1 τ_η	250.000	500.000	203.776
dt	$8\ 10^{-4}$	$4\ 10^{-4}$	$1.1\ 10^{-4}$
Time step ch0+ch1	756 + 1744	900 + 2100	11000+39000
τ_η	0.0746	0.0466	0.02
τ	0.0, 0.0120, 0.0200, 0.0280, 0.0360, 0.0440, 0.0520, 0.0600, 0.0680, 0.0760, 0.0840, 0.1000, 0.1200, 0.152, 0.200, 0.248	0.0, 0.00753454, 0.0125576, 0.0175806, 0.0226036, 0.0276266, 0.0326497, 0.0376727, 0.0426957, 0.0477187, 0.0527418, 0.0627878, 0.0753454, 0.0954375, 0.125576, 0.155714	0, 0, 0, 0.0032, 0.0032, 0.0032, 0.012, 0.012, 0.012, 0.02, 0.02, 0.02, 0.04, 0.06, 0.1, 0.2, 0.4, 0.6, 0.8, 1, 1.4
Disk space used	400 GByte	1 TByte	6.3 Tbytes

HDF5 - trajectory files

```
HDF5 "RM-2006-LIGHT-512.St60.opengl.0.h5" {
GROUP "/" {
  GROUP "DNS" {
    ATTRIBUTE "DNS_DEALIASING" {
      DATATYPE  H5T_IEEE_F32LE
      DATASPACE  SIMPLE { ( 1 ) / ( 1 ) }
      DATA {
      (0): 0.6666
      }
    }
    ATTRIBUTE "DNS_DT" {
      DATATYPE  H5T_IEEE_F32LE
      DATASPACE  SIMPLE { ( 1 ) / ( 1 ) }
      DATA {
      (0): 0.0004
      }
    }
    ATTRIBUTE "DNS_FORCING" {
      DATATYPE  H5T_IEEE_F32LE
      DATASPACE  SIMPLE { ( 1 ) / ( 1 ) }
      DATA {
      (0): 1.2
      }
    }
    ATTRIBUTE "DNS_SIZE" {
```

HDF5 - trajectory files

```
DATASET "BEAM" {
  DATATYPE  H5T_COMPOUND {
    H5T_IEEE_F32LE "x";
    H5T_IEEE_F32LE "y";
    H5T_IEEE_F32LE "z";
    H5T_IEEE_F32LE "ux";
    H5T_IEEE_F32LE "uy";
    H5T_IEEE_F32LE "uz";
    H5T_IEEE_F32LE "vx";
    H5T_IEEE_F32LE "vy";
    H5T_IEEE_F32LE "vz";
    H5T_STD_I32LE "name";
  }
  DATASPACE  SIMPLE { ( 1600, 157 ) / ( H5S_UNLIMITED, H5S_UNLIMITED ) }
  DATA {
  (0,0): {
      114.71,
      230.615,
      405.461,
      -0.739292,
      1.46744,
```

iCFDdatabase

- Would like to do perform analysis on space or time distribution of particles in simple turbulence flows ?

- Do not want to setup state-of-the-art numerical simulations from scratch ?

- Download the appropriate datasets and learn how to read them !

The end.