Παντα ρει (everything flows)

Theoretical Computational Fluid Mechanics

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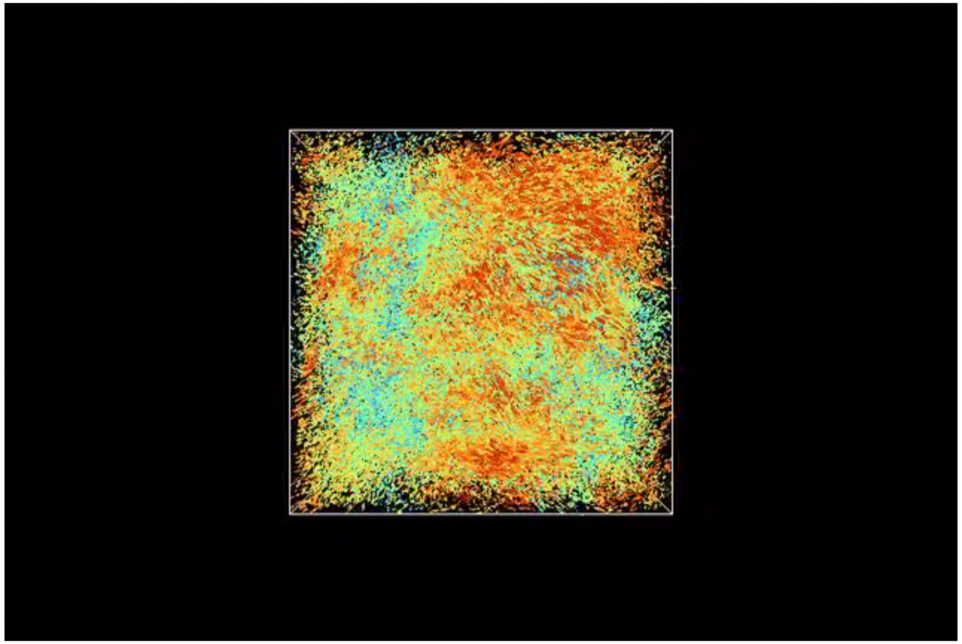
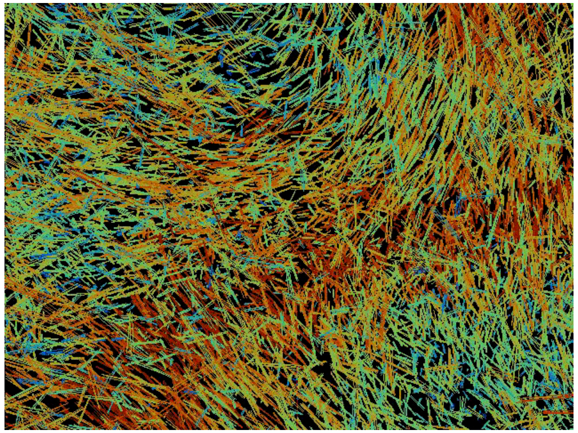
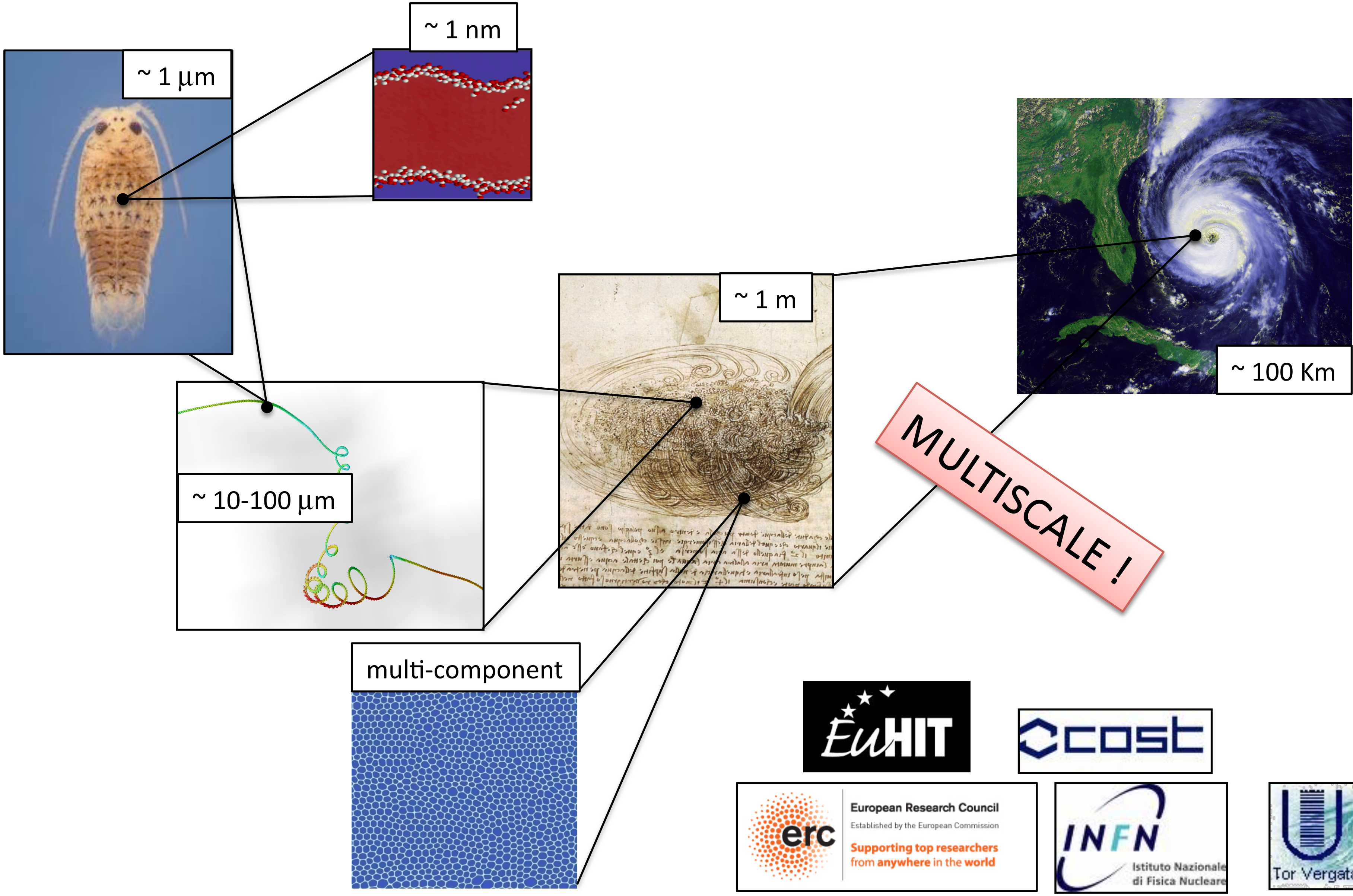
Alghero, Maggio 2015





Παντα ρει (everything flows)

a guided (dangerous) ride inside turbulence



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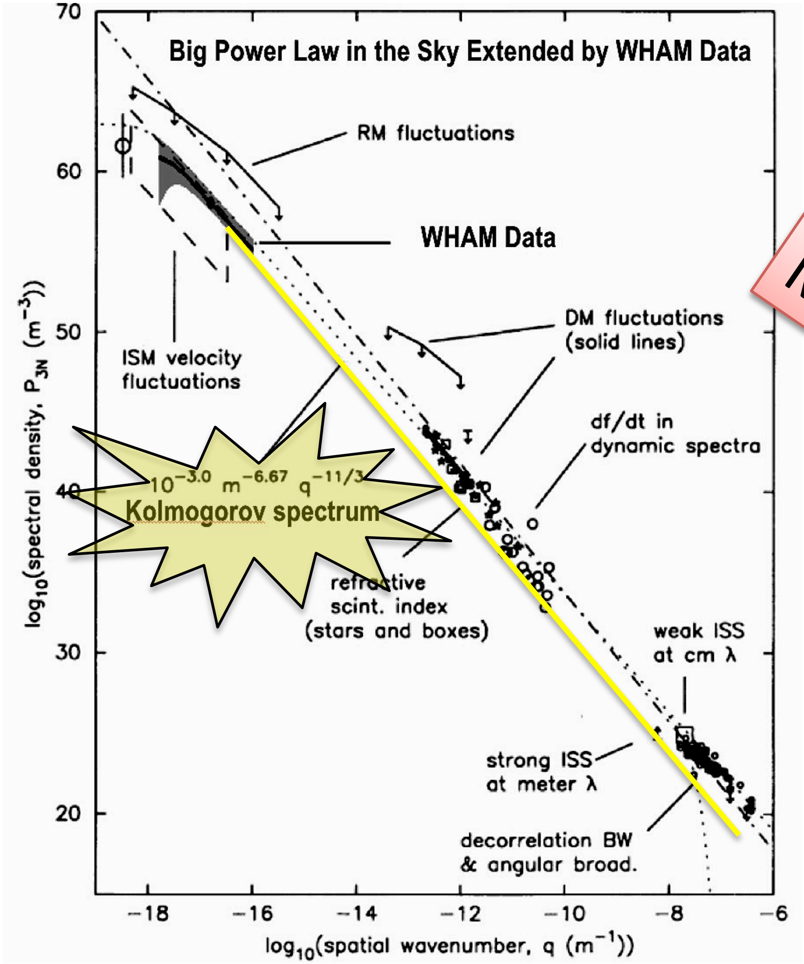
Tor Vergata

$\Pi\alpha\nu\tau\alpha$ $\rho\varepsilon\iota$ (everything flows)

a guided (dangerous) ride inside turbulence



MULTISCALE !

The "Big Power Law in the Sky" compiled originally by Armstrong, Rickett, & Spangler, with the Wisconsin Hα Mapper (WHAM)

ON THE SHOULDERS OF GIANTS...

Leonardo da Vinci (~ 1500): "doue la turbolenza de si genera **[injected]**; doue la turbolenza dell aqua si mantiene **[advected]** plugho; doue la turbolenza dell acqua si posa **[dissipated]**"

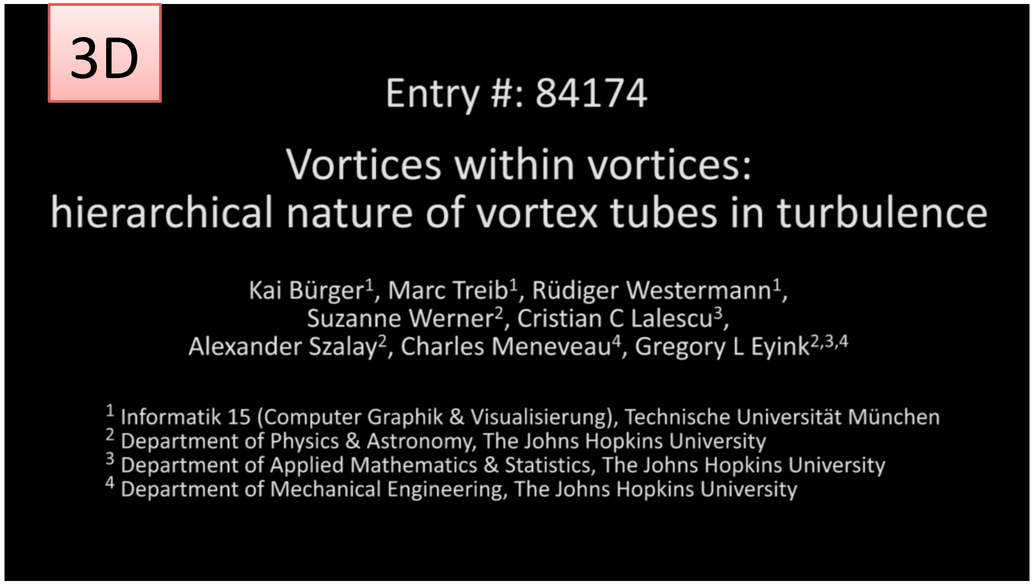
Sir H. Lamb (1932): "I am an old man now, and when I die and go to Heaven there are two matters on which I hope enlightenment. One is quantum electrodynamics (QED) and the other is turbulence of fluids. About the former, I am really rather optimistic."

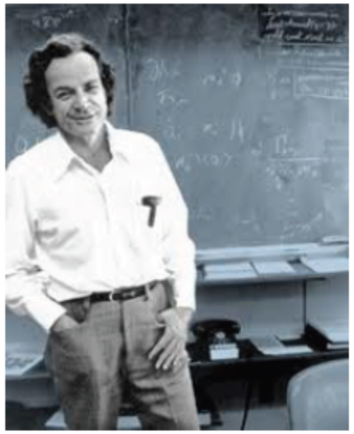
J. Von Neumann (1949) "[…] The entire experience with the subject indicates that the purely analytical approach is beset with difficulties, which at the moment are prohibitive. […] Under these conditions there may be some hope to "break the deadlock" by extensive, but well-planned computational efforts.

R.P. Feynman (1970): "Certainly. I've spent years trying to solve some difficult problems without success. The theory of turbulence is one. In fact, it is still unsolved."

NAVIER-STOKES 3D-2D

(NASA/Goddard Space Flight Center Scientific Visualization Studio)



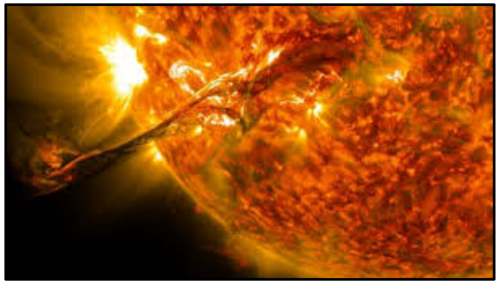


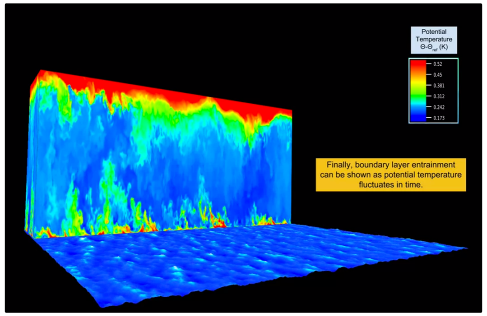
"With turbulence, it's not just a case of physical theory being able to handle only simple cases—we can't do any. We have no good fundamental theory at all." (Feynman, 1979, Omni Magazine, Vol. 1, No.8).

WHERE IS THE PROBLEM?

$$\begin{cases} \partial_t \mathbf{v} + (\mathbf{v} \cdot \partial)\mathbf{v} = -\partial P + \nu \Delta \mathbf{v} + \mathbf{F} \\ \partial \cdot \mathbf{v} = 0 \\ + \ Boundary\ Conditions \end{cases}$$

- Too many turbulences?
- Can we disentangle universal from non-universal properties?
- Can we understand universal properties?
- Does it ‘computing’ mean ‘understanding’? (Computo ergo sum?)





SIMPLE FLUID & COMPLEX FLOWS

$$\partial_t v + v\partial v = -\partial p + \nu \Delta v \quad +F(B,B) \quad +g\theta \quad +\sum_i c_0(u_i, v)\delta(r - r_i) \quad +f$$

$$\partial_t \theta + v \cdot \partial \theta = \chi \partial^2 \theta$$

$$\partial_t B + v \cdot \partial B = B \cdot \partial v + \chi \partial^2 B$$

$$\partial \cdot v = 0$$

+ boundary conditions

$$\frac{du_i(r_i,t)}{dt} = -\rho_f |u_i - v|(u_i - v)$$

$$+\rho_f\left(\frac{Dv}{Dt} - \frac{Du_i}{Dt}\right) + (u_i - v) \times \omega$$

control parameter:

$$Re = \frac{l_0 v_0}{\nu}$$

$$\begin{cases} Re \rightarrow \infty \\ \nu \rightarrow 0 \end{cases}$$

SIMPLE FLUID & COMPLEX FLOWS

$$\begin{cases} \partial_t v + v\partial v = -\partial p + \nu \Delta v \quad + F(B,B) \quad + g\theta \quad + \sum_i c_0(u_i, v)\delta(r - r_i) \quad + f \\ \partial_t \theta + v \cdot \partial \theta = \chi \partial^2 \theta \\ \partial_t B + v \cdot \partial B = B \cdot \partial v + \chi \partial^2 B \\ \partial \cdot v = 0 \end{cases}$$

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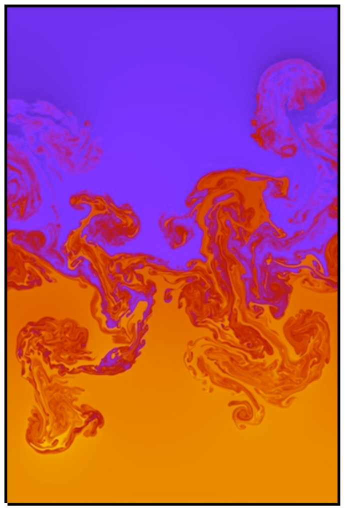
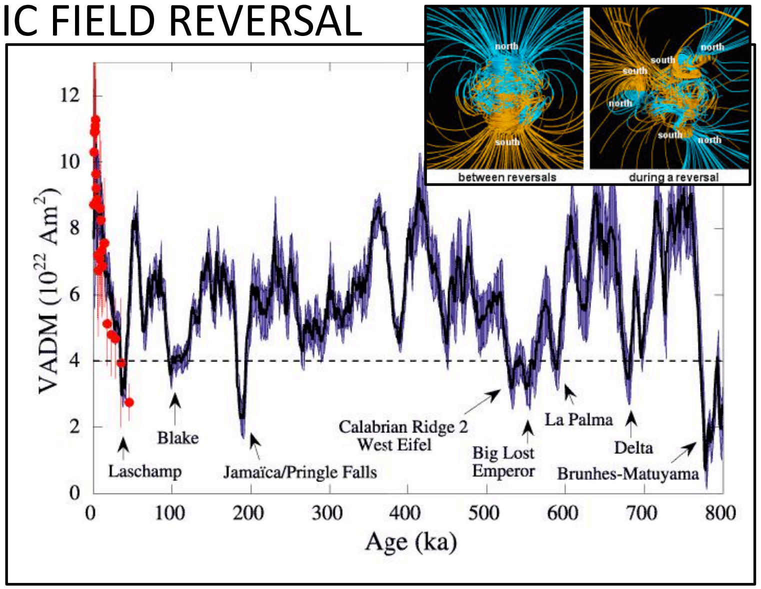
θ_{up} COLD



θ_{down} WARM

CONVECTION

MAGNETIC FIELD REVERSAL



SIMPLE FLUID & COMPLEX FLOWS

$$\begin{cases} \partial_t v + v\partial v = -\partial p + \nu \Delta v \quad + F(\mathbf{B},\mathbf{B}) \quad + g\theta \quad + \sum_i c_0(u_i, v)\delta(r - r_i) \quad + f \\ \partial_t \theta + \mathbf{v}\cdot\boldsymbol{\partial}\theta = \chi \partial^2 \theta \\ \partial_t \mathbf{B} + \mathbf{v}\cdot\boldsymbol{\partial}\mathbf{B} = \mathbf{B}\cdot\boldsymbol{\partial}\mathbf{v} + \chi\partial^2 \mathbf{B} \\ \partial \cdot v = 0 \\ \text{+ boundary conditions} \end{cases}$$

$$\begin{cases} \frac{du_i(r_i,t)}{dt} = -\rho_f |u_i - v|(u_i - v) \\ +\rho_f\left(\frac{Dv}{Dt} - \frac{Du_i}{Dt}\right) + (u_i - v)\times\omega \end{cases}$$

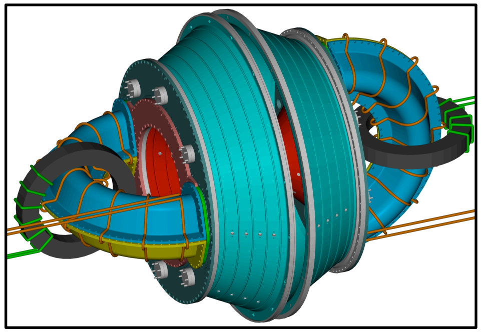
control parameter:

$$Re = \frac{l_0 v_0}{\nu}$$

$$\begin{cases} Re \to \infty \\ \nu \to 0 \end{cases}$$

ROTATING CONVECTION

WIND FARMS



MAGNETIC DYNAMO

SIMPLE FLUID & COMPLEX FLOWS

$$
\begin{cases}
\partial_t v + v \cdot \partial v = -\partial P + \nu \partial^2 v \ + F(\boldsymbol{B},\boldsymbol{B}) \ + \boldsymbol{g}\theta \ + \sum_i c_0(\boldsymbol{u}_i, \boldsymbol{v})\delta(\boldsymbol{r} - \boldsymbol{r}_i) \ + f \\
\partial_t \theta + \boldsymbol{v} \cdot \boldsymbol{\partial} \theta = \chi \partial^2 \theta \\
\partial_t \boldsymbol{B} + \boldsymbol{v} \cdot \boldsymbol{\partial} \boldsymbol{B} = \boldsymbol{B} \cdot \boldsymbol{\partial} \boldsymbol{v} + \chi \partial^2 \boldsymbol{B} \\
\partial \cdot v = 0 \\
\text{+ boundary conditions}
\end{cases}
$$

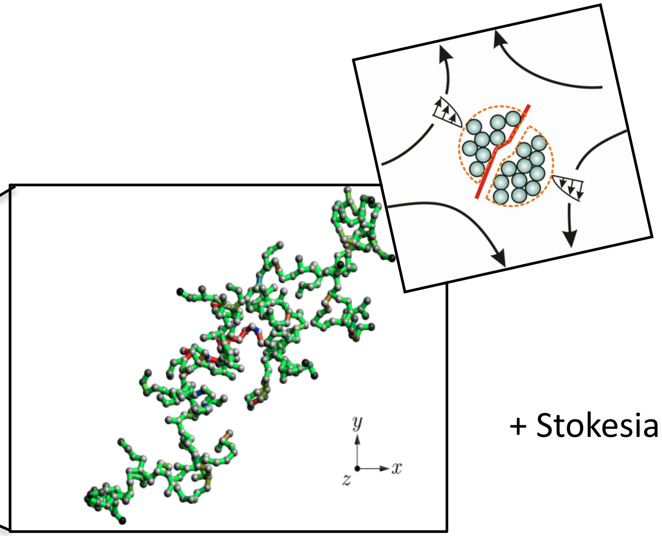
temperature

magnetic field

$$
\begin{cases}
\dfrac{d\boldsymbol{u}_i(\boldsymbol{r}_i, t)}{dt} = -\rho_f |\boldsymbol{u}_i - \boldsymbol{v}|(\boldsymbol{u}_i - \boldsymbol{v}) \\
+\rho_f \left(\dfrac{D\mathbf{v}}{Dt} - \dfrac{D\boldsymbol{u}_i}{Dt}\right) + (\boldsymbol{u}_i - \boldsymbol{v}) \times \boldsymbol{\omega}
\end{cases}
$$

small particles/colloidal aggregates:
Stokes drag, added mass, lift force, etc...

DISPERSION OF TWO DIFFERENT SPECIES OF SMALL PARTICLES/AGGREGATES IN A TURBULENT FLOW



+ Stokesian dynamics

COAGULATION/FRAGMENTATION OF COLLOIDAL AGGREGATES IN TURBULENT FLOWS

SIMPLE FLUID & COMPLEX FLOWS

$$\partial_t v + v\partial v = -\partial p + \nu\Delta v \quad +F(B,B) \quad +g\theta \quad +\sum_i c_0(u_i,v)\delta(r-r_i) \quad +f$$

$$\partial_t\theta + v\cdot\partial\theta = \chi\partial^2\theta$$

$$\partial_t B + v\cdot\partial B = B\cdot\partial v + \chi\partial^2 B$$

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control parameter:

$$Re = \frac{l_0 v_0}{\nu}$$

$$\begin{cases} Re \to \infty \\ \nu \to 0 \end{cases}$$

- Homogeneous & Isotropic Turbulence
- Fully periodic 3D domain
- Gaussian delta-correlated forcing
- Incompressible

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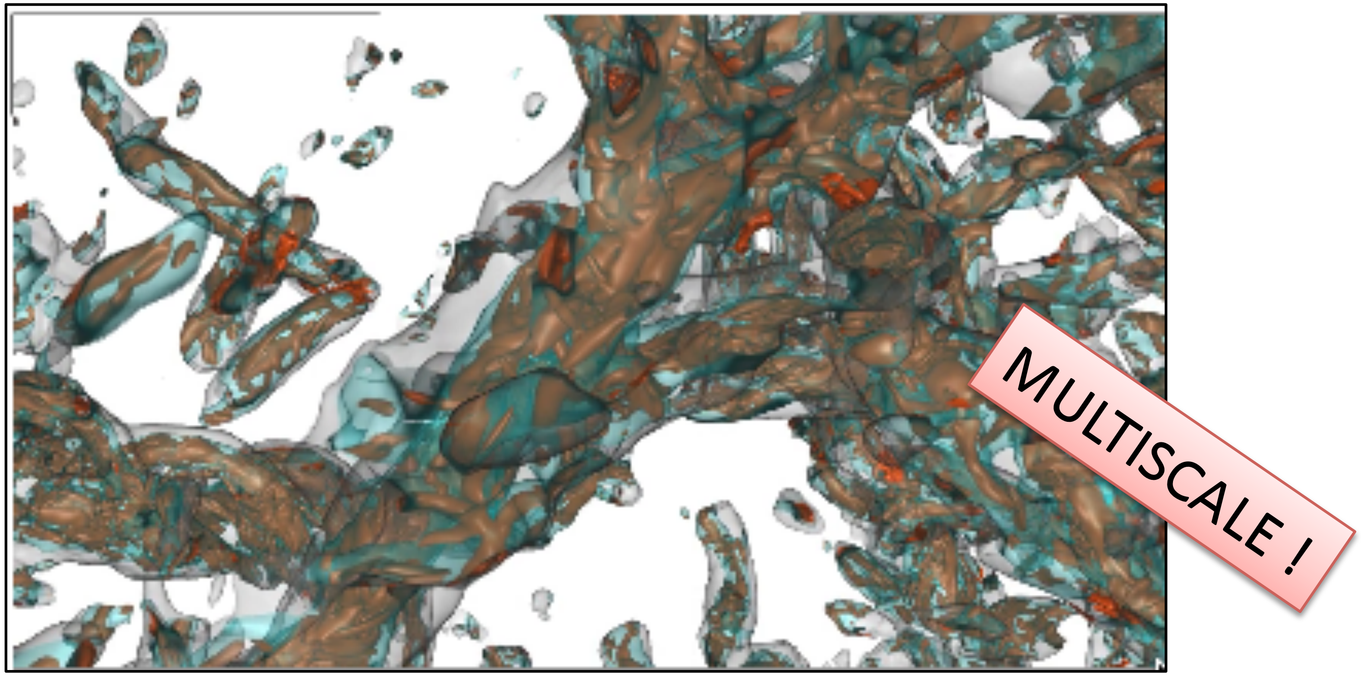
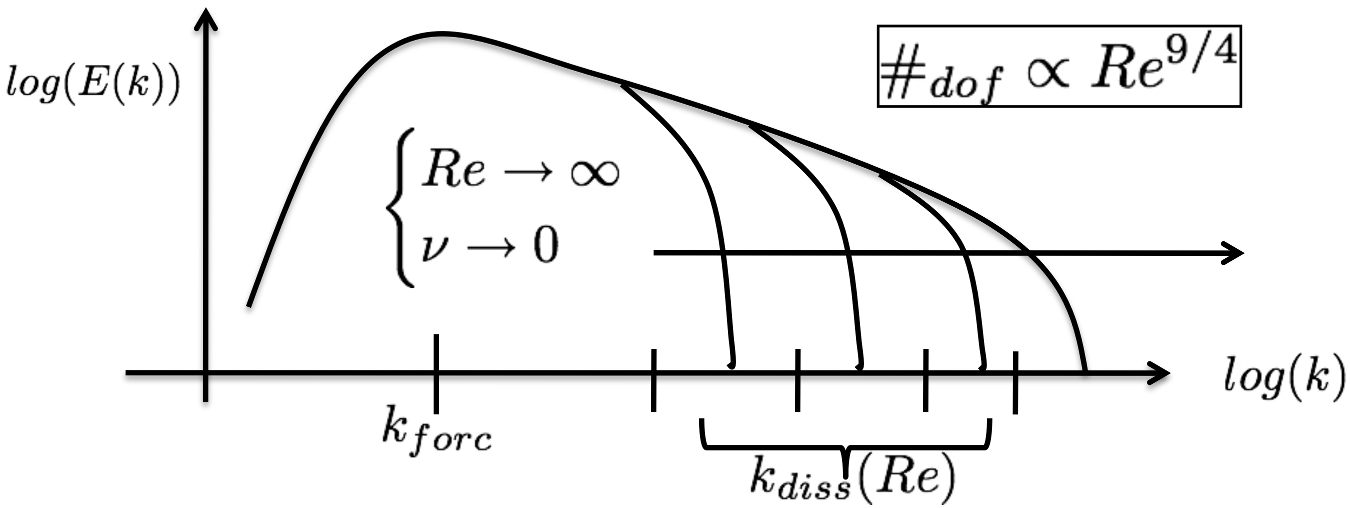
Navier–Stokes Equation

This is the equation which governs the flow of fluids such as water and air. However, there is no proof for the most basic questions one can ask: do solutions exist, and are they unique? Why ask for a proof? Because a proof gives not only certitude, but also understanding.

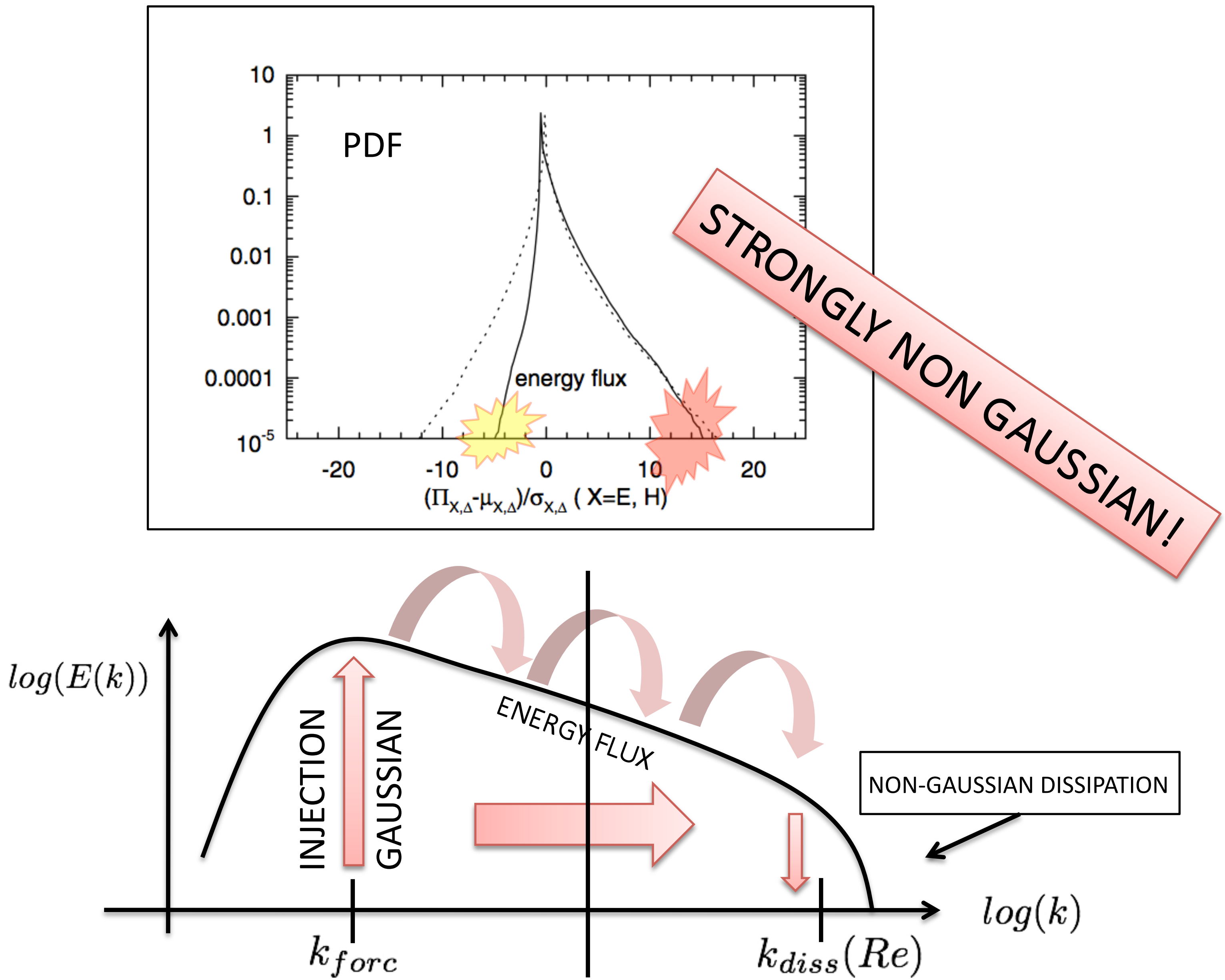
1. NAVIER-STOKES 3D

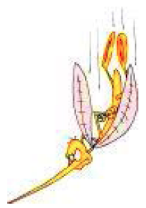




$$\#_{dof} \propto Re^{9/4}$$

2. NAVIER-STOKES 3D

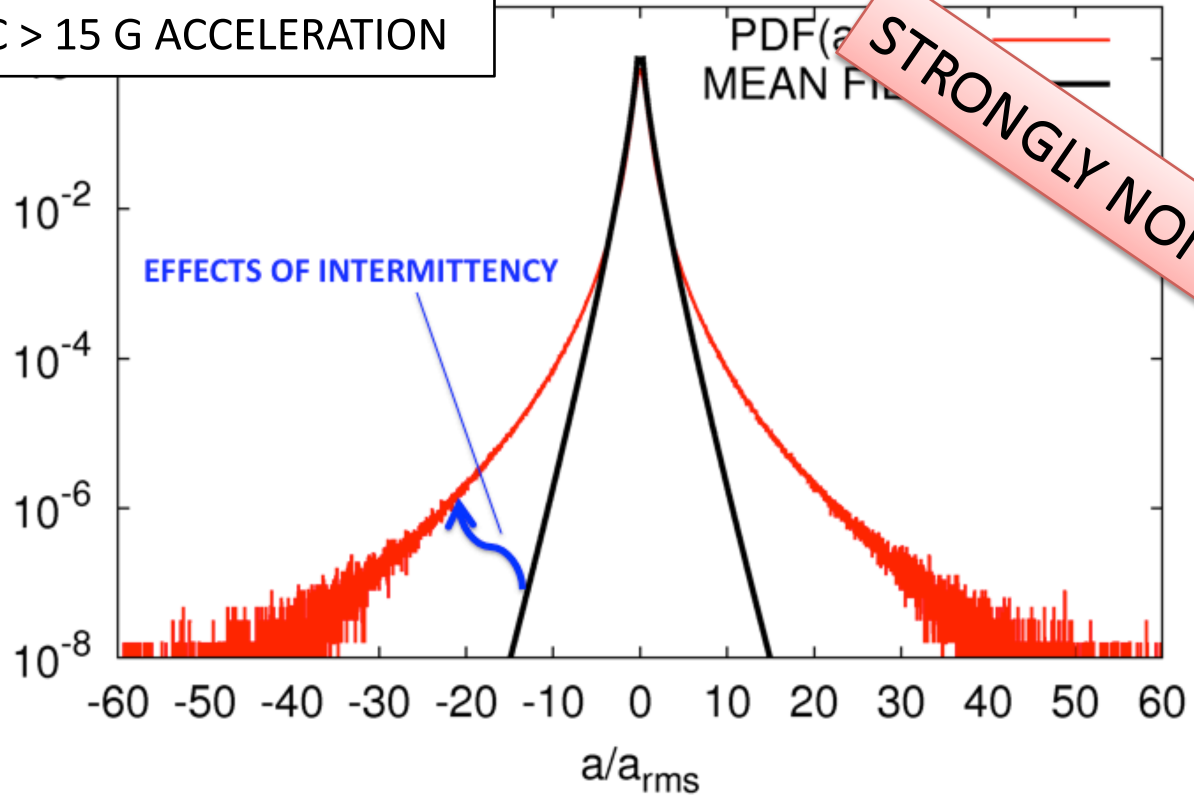




- wind speed 18km/h (5m/sec)
- height above ground 1m
- roughness height 0.05m (farmland with few trees in summer time)

⇓ τ_η = 5 msec and η = 0.5 mm

EVERY 15 SEC > 15 G ACCELERATION



STRONGLY NON GAUSSIAN!

ACCELERATION PROBABILITY DISTRIBUTION FUNCTION (PDF) AT RE ~ 10^5 [Bi04]
COMPARED WITH THE PREDICTION FROM MEAN FIELD (KOLMOGOROV THEORY)

IF YOU WANT TO PREDICT/CONTROL EXTREME EVENTS YUO **CANNOT** NEGLECT INTERMITTENCY

L. B., G. Boffetta, A. Celani, B. Devenish, A. Lanotte and F. Toschi *Phys. Rev. Lett.* **93**, 064502, 2004.

Turbulent luminance in impassioned van Gogh paintings

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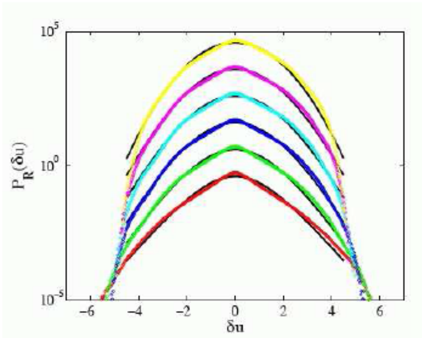


FIG. 2: Semilog plot of the probability density $P_R(\delta u)$ of luminance changes δu for pixel separations $R = 60, 240, 400, 600, 800, 1200$ (from bottom to top). Curves have been vertically shifted for better visibility. Data points were fitted, according to Ref. [13], and the results are shown in full lines; parameter values are $\lambda = 0.2, 0.15, 0.12, 0.11, 0.09, 0.0009$ (from bottom to top).

Starry night

Road with Cypress and Star

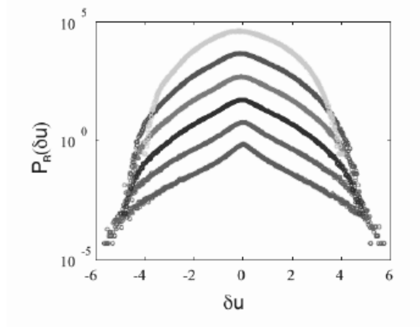
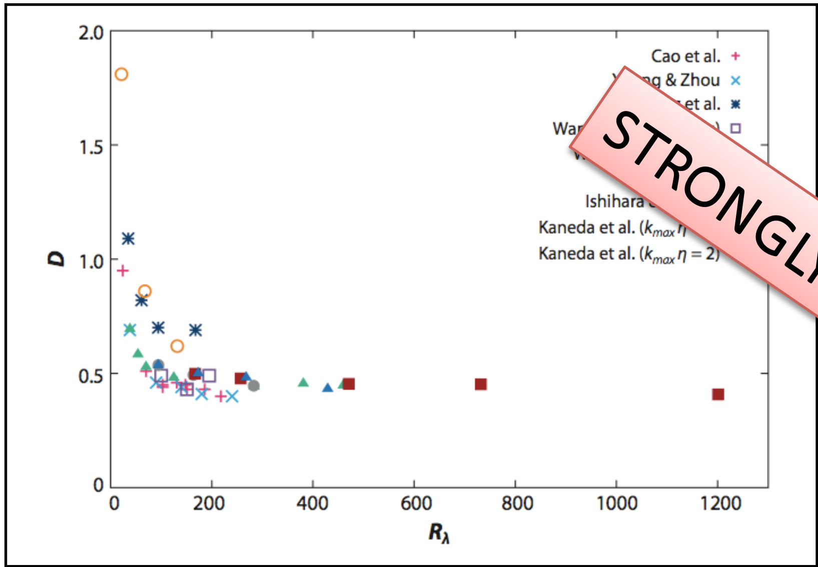


FIG. 5: Left: *Road with Cypress and Star* (Rijksmuseum Kröller-Müller, Otterlo). Right: PDF for pixel separations $R = 2, 5, 15, 20, 30, 60$ (from bottom to top). The studied image was taken from the WebMuseum-Paris, webpage.

3. NAVIER-STOKES 3D

NO ROOM FOR QUASI-EQUILIBRIUM APPROACHES



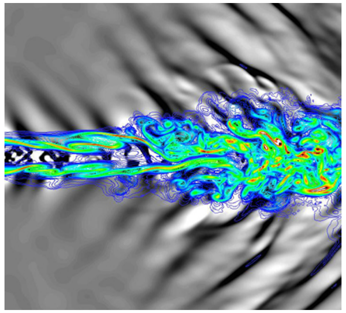
STRONGLY OUT-OF-EQUILIBRIUM!

$$\partial_t v + v\partial v = -\partial p + \nu\Delta v$$

$$\lim_{Re\to\infty} \epsilon = \lim_{\nu\to 0} \nu\langle(\partial v)^2\rangle \to const.$$

DISSIPATIVE ANOMALY

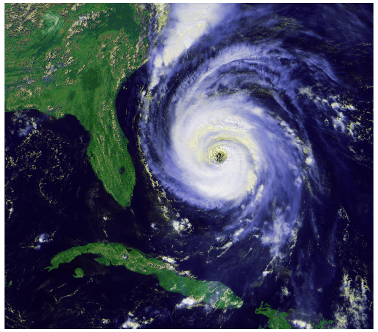
$$\#_{dof} = (\frac{k_{diss}}{k_{forc}})^3 \sim Re^{9/4}$$



laboratory flow

$$Re \sim 10^5 - 10^9$$

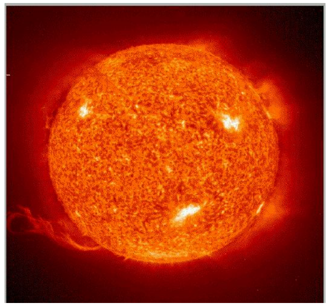
$$\#_{dof} \sim 10^{11} - 10^{20}$$



atmosph. flow

$$Re \sim 10^8 - 10^{12}$$

$$\#_{dof} \sim 10^{18} - 10^{30}$$



astrophys. flow

$$Re > 10^{15}$$

$$\#_{dof} \sim \infty$$

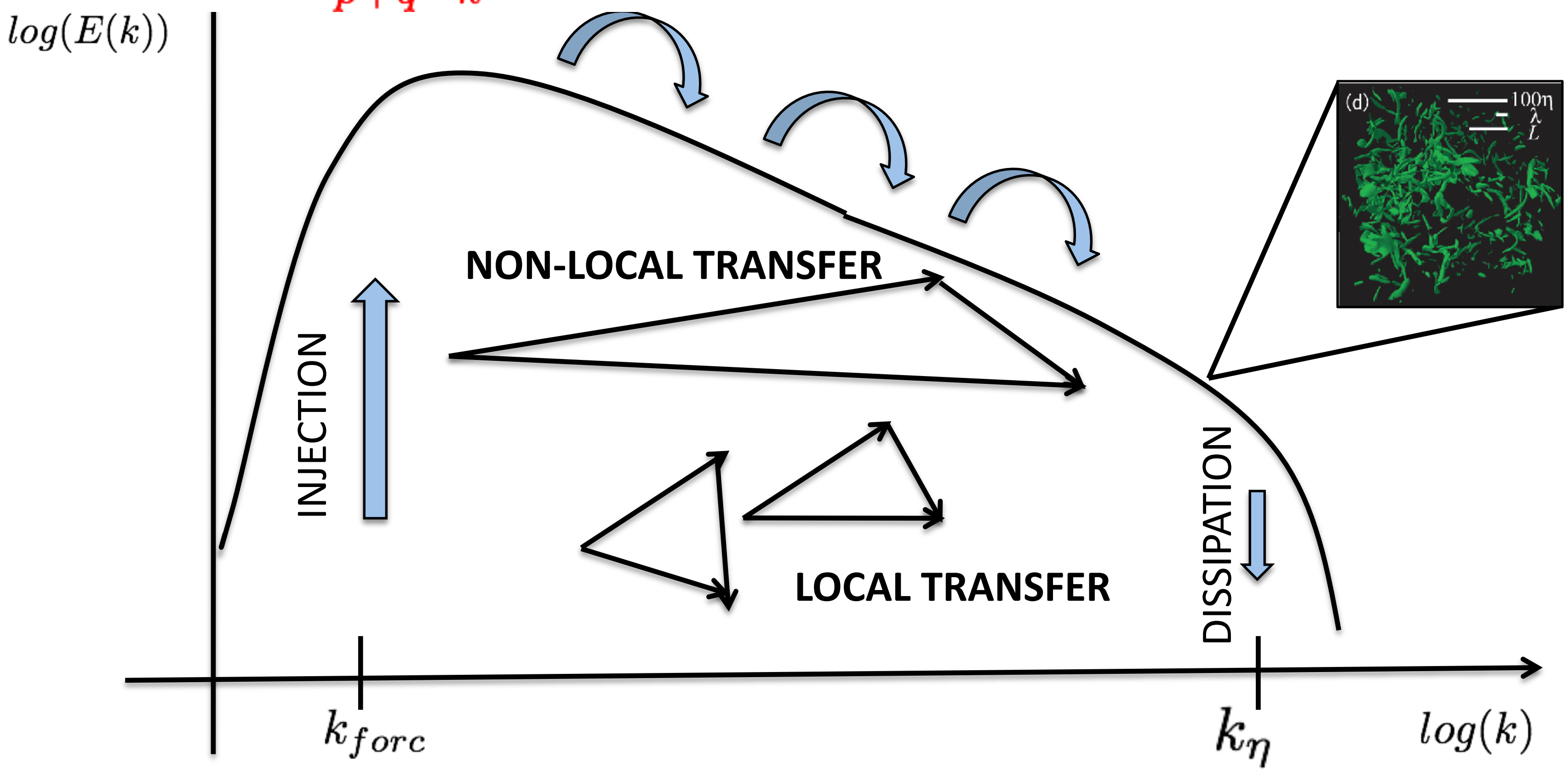
state-of-the-art Direct Numerical Simulation:

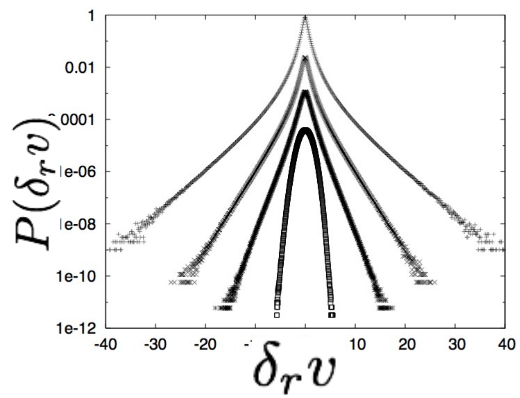
Isotropic, homogeneous Fully Periodic Flows
Pseudo-Spectral Methods.
Resolution 12000^3 (Y. Kaneda, APS 2014)

Reynolds : 10^8,
Storage of 1 velocity configuration (double precision): 40 Tbyte
RAM requirements for time marching ~ 160 Tbyte

Moral: brute force Direct Numerical Simulations able to saturate any computing power (present and/or future): Computo ergo sum?

$$\partial_t u(k) = ik \sum_{p+q=k} u(p)u(q) + -ikP(k) + \nu k^2 u(k) + f(k)$$





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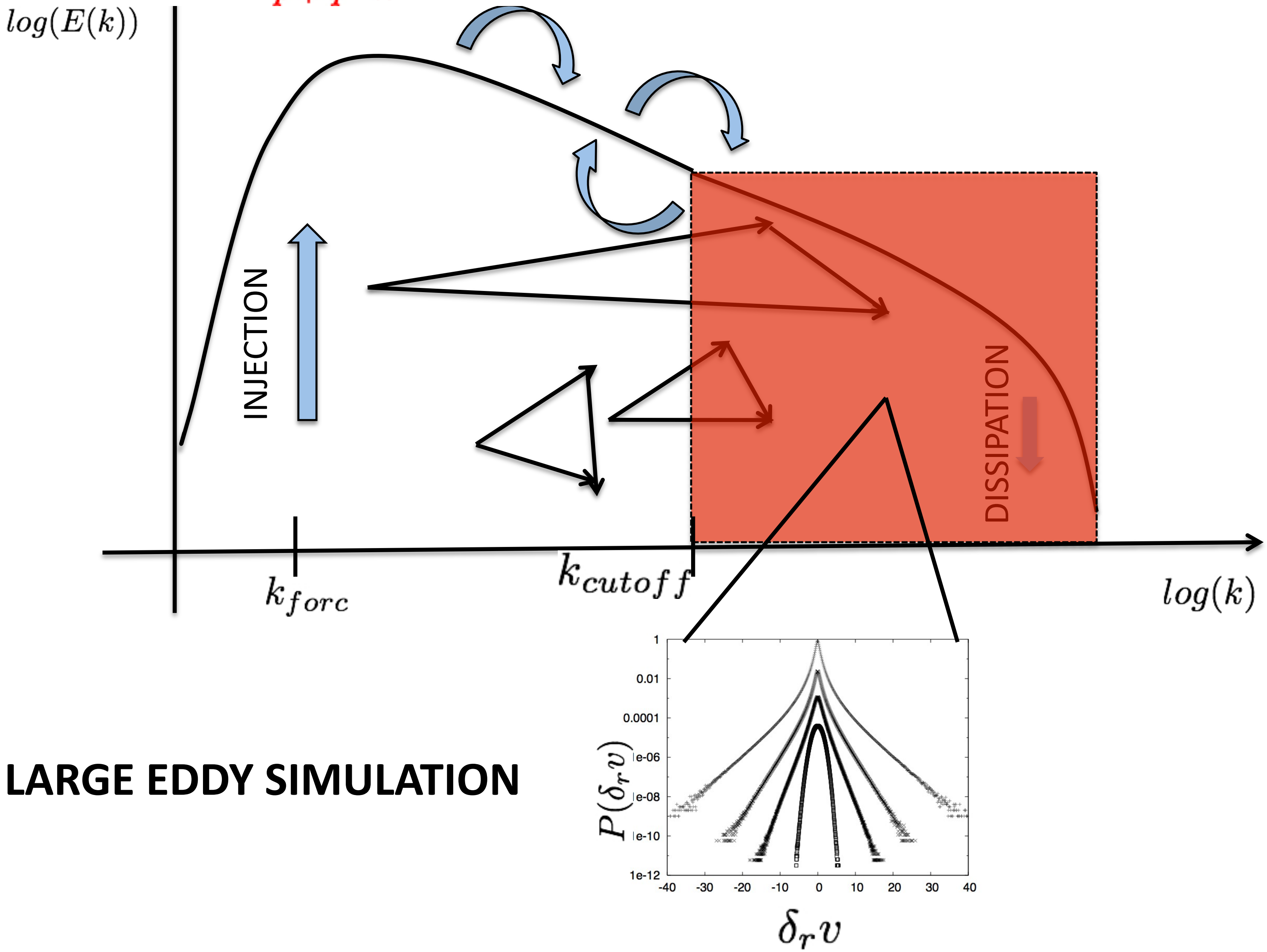
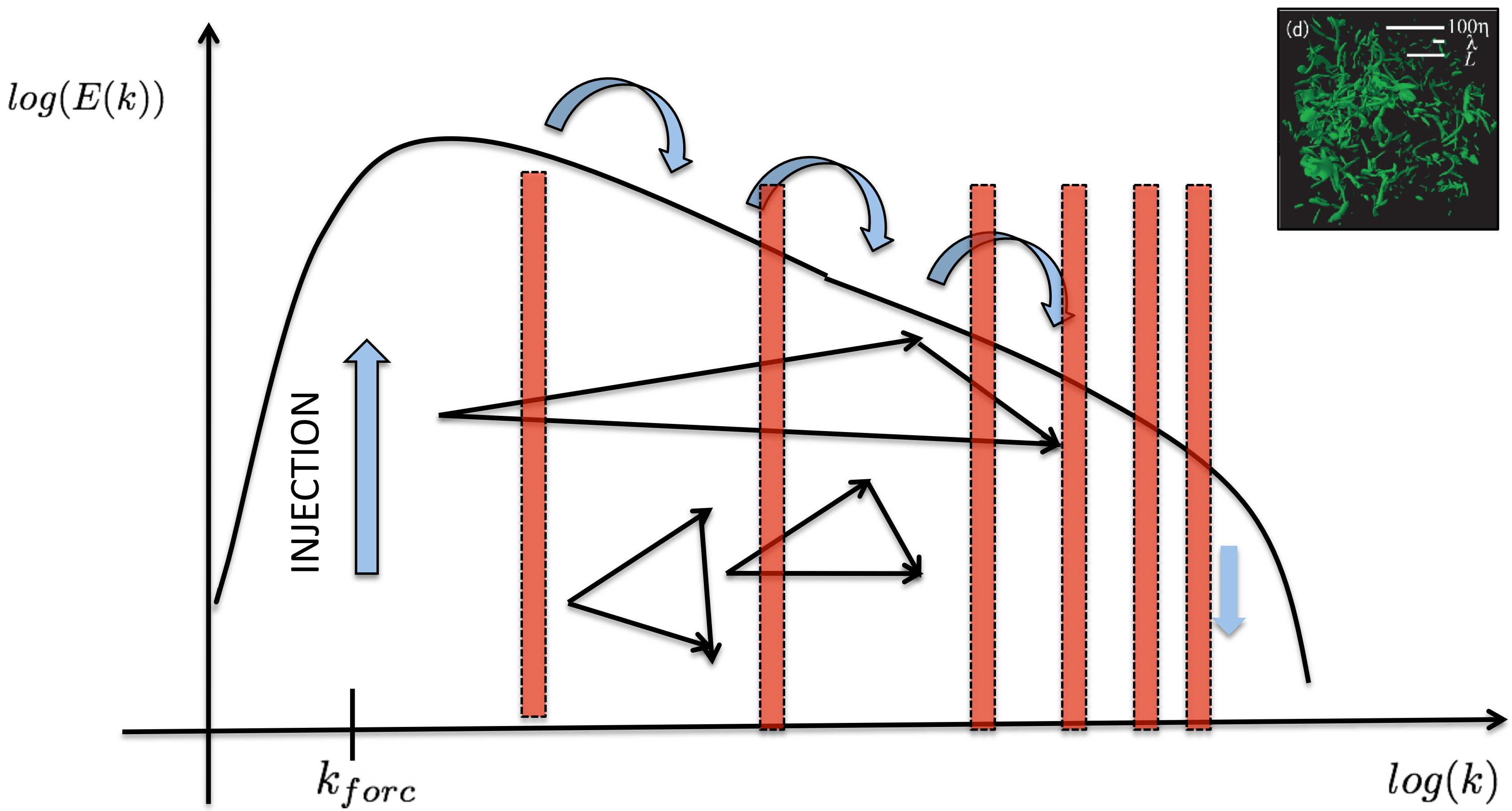


LARGE EDDY SIMULATION



$$\mathbf{v}^D(\mathbf{x},t) = \mathcal{P}^D \mathbf{v}(\mathbf{x},t) = \sum_{\mathbf{k}\in\mathcal{Z}^3} e^{i\mathbf{k}\cdot\mathbf{x}}\, \gamma_{\mathbf{k}} \mathbf{u}(\mathbf{k},t)\,.$$

DECIMATED WITH PROBABILITY ~ $1 - k^{D_F - 3}$

HOMOGENEOUS & ISOTROPIC & SELF-SIMILAR (NO EXTERNAL SCALES)

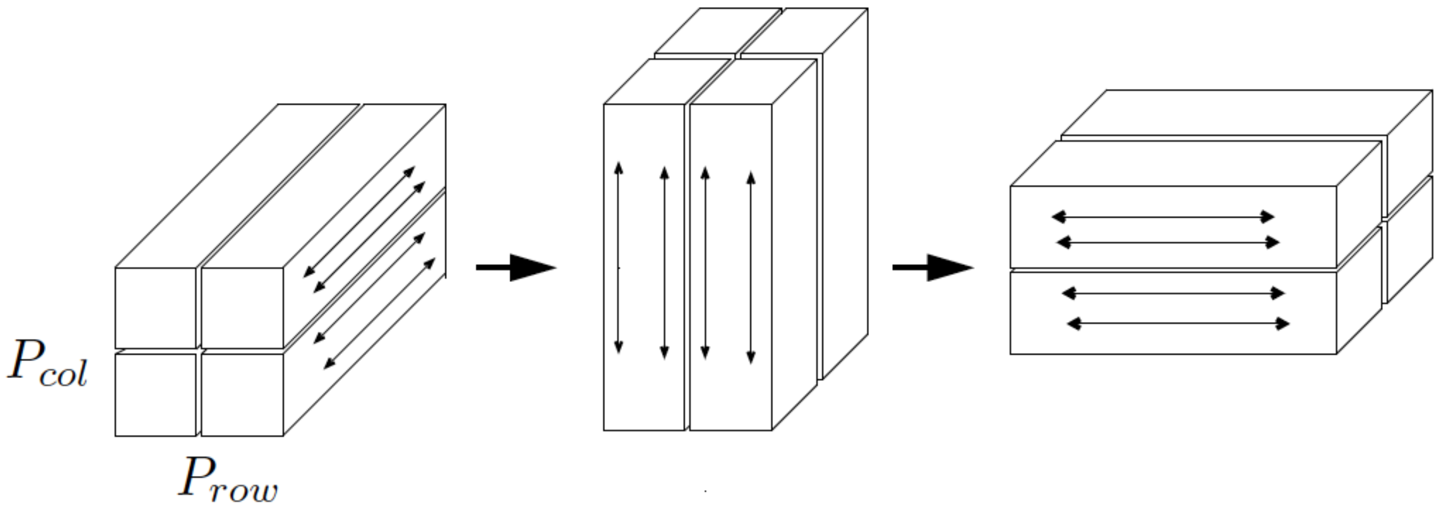
$$\begin{cases} \partial_t v_i(x) = -(v_j(x)\partial_j)v_i(x) - \partial_i P + \nu\partial^2 v_i(x) + f_i(x) \\ \partial_i v_i = 0 \quad \partial^2 P = \partial_i \partial_j v_i v_j \end{cases}$$

$$\begin{cases} \partial_t u(k) = ik \sum_{p+q=k} u(p)u(q) + -ikP(k) + \nu k^2 u(k) + f(k) \\ k \cdot u(k) = 0 \end{cases}$$

$$\sum_{p+q=k} u(p)u(q) = IFFT[FFT[u]\partial_i FFT[u]]$$

Introduction

$$N^3 \ \text{grid}, \quad P_{row} \times P_{col} = P \ \ \text{(number of MPI processes)}$$



- 3D FFT: FFT(X)→ transpose→ FFT(Z) →transpose→ FFT(Y)
- Optimal performance: $P_{row} \ll P_{col}$ for given P (*Pekurovsky SIAM J. Sci. comp.'12*)

$$\boxed{P/(N/2) \leq P_{col} \leq N, \quad P/N \leq P_{row} \leq N/2}$$

MPI+OpenMP Hybrid algorithm

- Coarse grained MPI decomposition - can make P_{row} smaller !
- Decrease load imbalance by cylindrical truncation in Fourier space
- Can overlap computation with communication using *MPI_THREAD_SERIALIZED* approach
- All threads make MPI calls in *serialized* fashion

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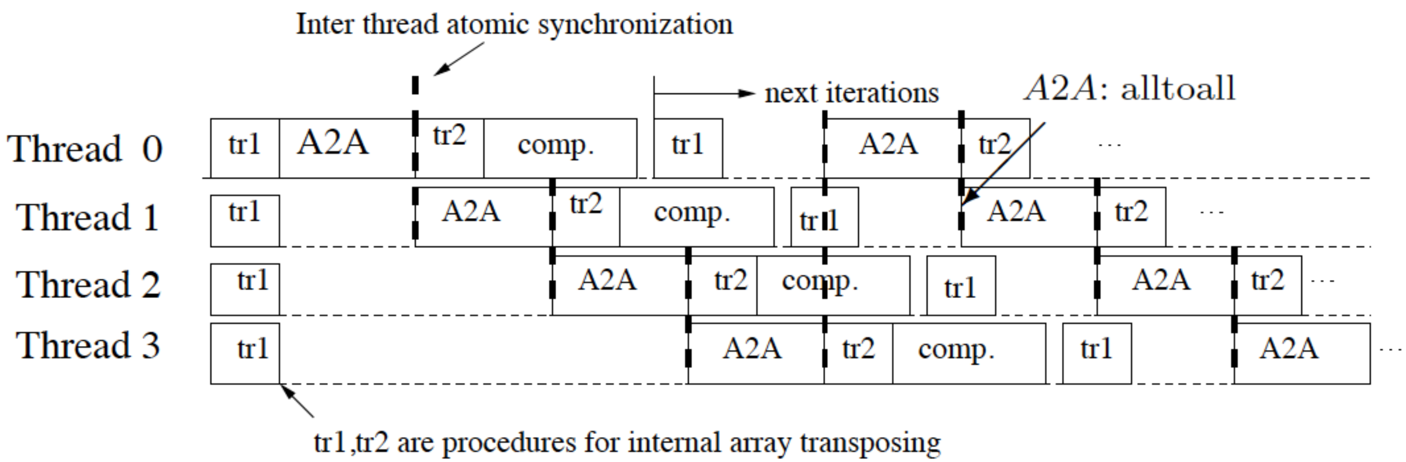


Memory locality matters!

Goal - less thread synchronization, longer pipeline!

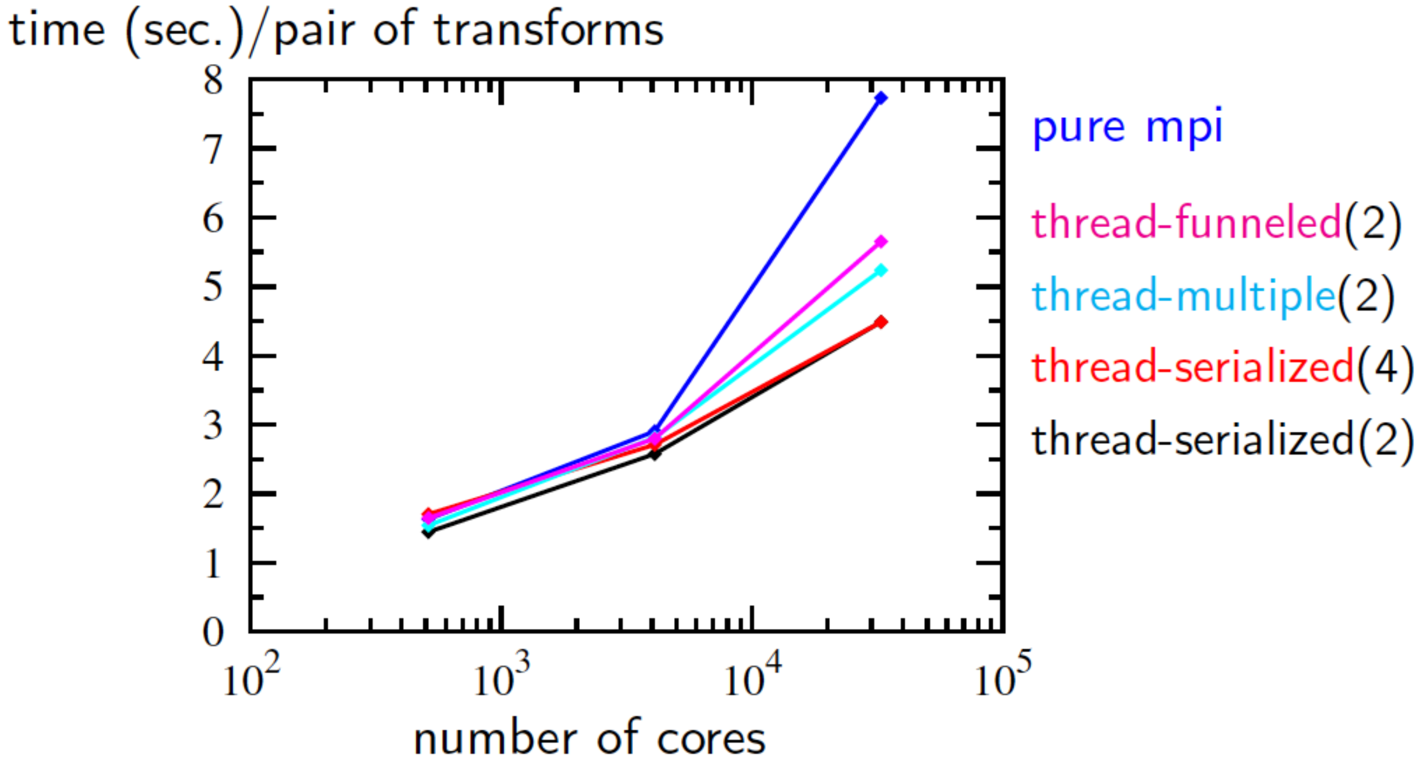
- Consider scenario of 5 field variables u, v, w, ϕ_1, ϕ_2 using 2 threads:
  - Thread 0 gets u, v, w
  - Thread 1 gets ϕ_1, ϕ_2

Golden Rule for Non-Uniform Memory Access (**ccNUMA**): First touch

- First Touch: memory page mapped into local memory of processor that first touches it!
- "touch" means "write", not "allocate"

Weak scaling - 3D FFT

- Weak scaling results on Blue Waters (XE6, periodic 3D torus topology)



Summary on hybrid 3D FFT algorithm

- At small problem sizes, pure MPI for 3D FFT is efficient However, at large problem sizes ($32k$ cores and beyond), scaling of pure MPI based 3D FFT deteriorates
- A hybrid approach makes the MPI decomposition more coarse grained, decreases latency and avoids intra-node communication
- Overlap between communication and computation possible, although may be network dependent
- DNS code based on hybrid MPI, openMP has been developed. Performance results similar to 3D FFT trends. However, not better than Coarray Fortran based global transposes

SIMPLE FLUID & COMPLEX FLOWS

$$
\begin{cases}
\partial_t v + v \cdot \partial v = -\partial P + \nu \partial^2 v \; + F(B,B) \; + \boldsymbol{g}\theta \; + \sum_i c_0(\boldsymbol{u}_i, \boldsymbol{v}) \delta(\boldsymbol{r} - \boldsymbol{r}_i) \; + f \\
\partial_t \theta + \boldsymbol{v} \cdot \boldsymbol{\partial} \theta = \chi \partial^2 \theta \\
\partial_t \boldsymbol{B} + \boldsymbol{v} \cdot \boldsymbol{\partial B} = \boldsymbol{B} \cdot \boldsymbol{\partial v} + \chi \partial^2 \boldsymbol{B} \\
\partial \cdot v = 0
\end{cases}
$$

+ boundary conditions

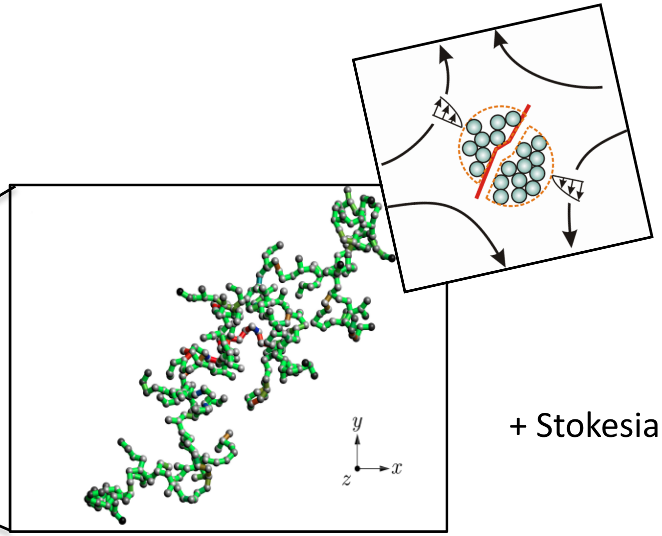
temperature

magnetic field

$$
\begin{cases}
\dfrac{d\boldsymbol{u}_i(\boldsymbol{r}_i, t)}{dt} = -\rho_f |\boldsymbol{u}_i - \boldsymbol{v}| (\boldsymbol{u}_i - \boldsymbol{v}) \\
+\rho_f (\dfrac{D\mathbf{v}}{Dt} - \dfrac{D\boldsymbol{u}_i}{Dt}) + (\boldsymbol{u}_i - \boldsymbol{v}) \times \boldsymbol{\omega}
\end{cases}
$$

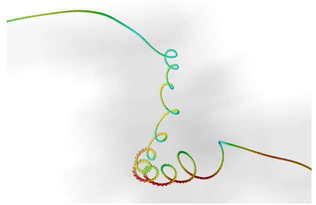
small particles/colloidal aggregates:
Stokes drag, added mass, lift force, etc...

DISPERSION OF TWO DIFFERENT SPECIES OF SMALL PARTICLES/AGGREGATES IN A TURBULENT FLOW



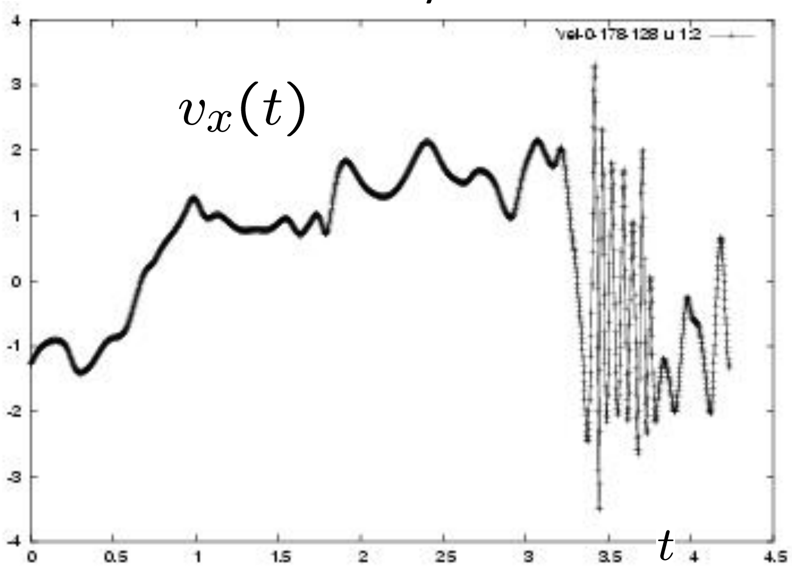
+ Stokesian dynamics

COAGULATION/FRAGMENTATION OF COLLOIDAL AGGREGATES IN TURBULENT FLOWS

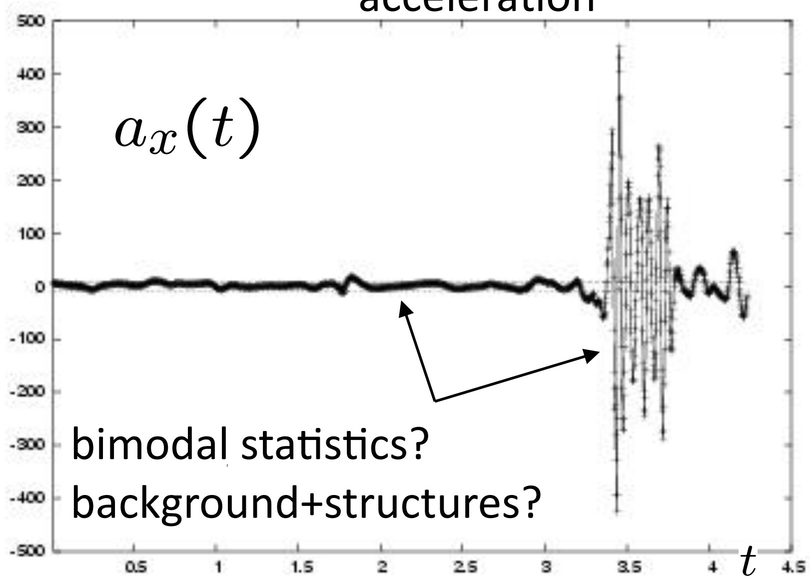


TRAPPING INTO VORTEX FILAMENTS

velocity



acceleration



Particle trapping in three-dimensional fully developed turbulence

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Dipartimento di Fisica and INFN, Università degli Studi di Roma "Tor Vergata," Via della Ricerca Scientifica 1, 00133 Roma, Italy

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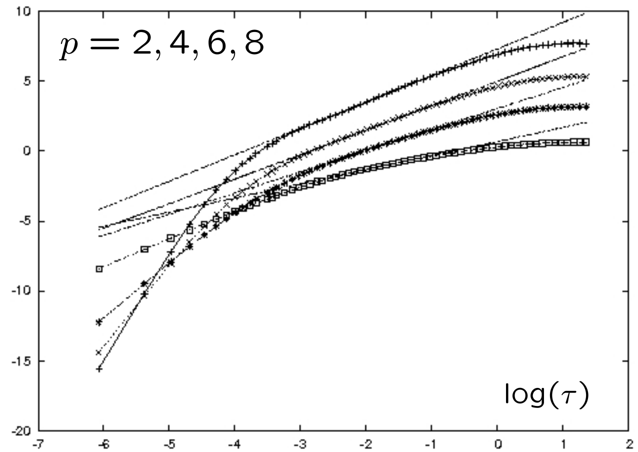
Istituto per le Applicazioni del Calcolo, CNR, Viale del Policlinico 137, 00161 Roma, Italy

[see also La Porta et al Nature 2001)]



Numerical simulation

$$\partial_t \mathbf{u} + (\mathbf{u} \cdot \nabla)\,\mathbf{u} = -\frac{1}{\rho}\nabla p + \nu \nabla^2 \mathbf{u} + \mathbf{F}$$

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

$$\dot{\mathbf{x}}(t) = \mathbf{u}(\mathbf{x}(\mathbf{t}), \mathbf{t})$$

$$\frac{d\mathbf{v}}{dt} = \beta \frac{D\mathbf{u}}{Dt} + \frac{1}{\tau}(\mathbf{u} - \mathbf{v})$$

$$\dot{\mathbf{x}}(t) = \mathbf{v}(t)$$

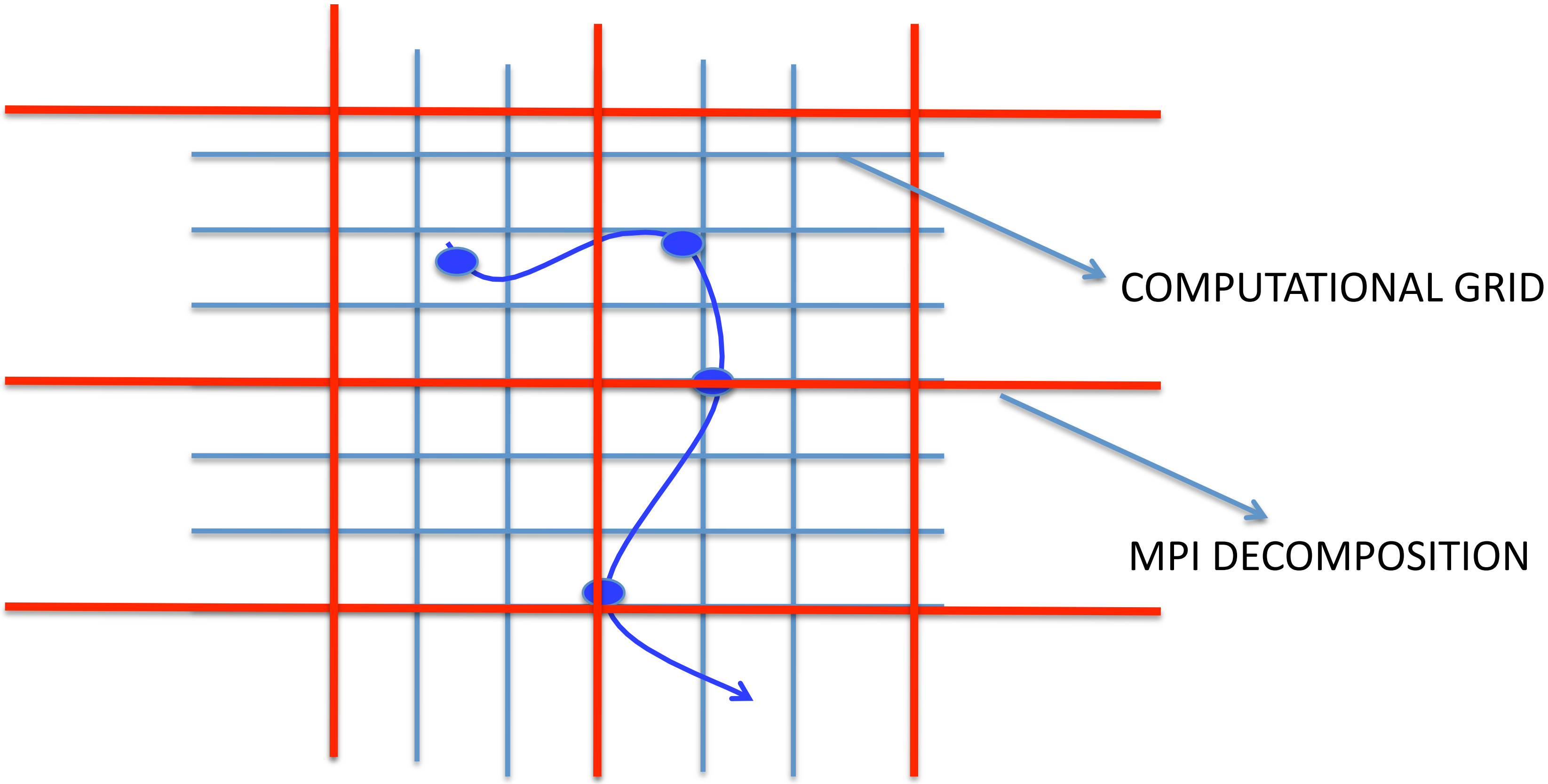
$$St = \frac{\tau}{\tau_\eta}$$

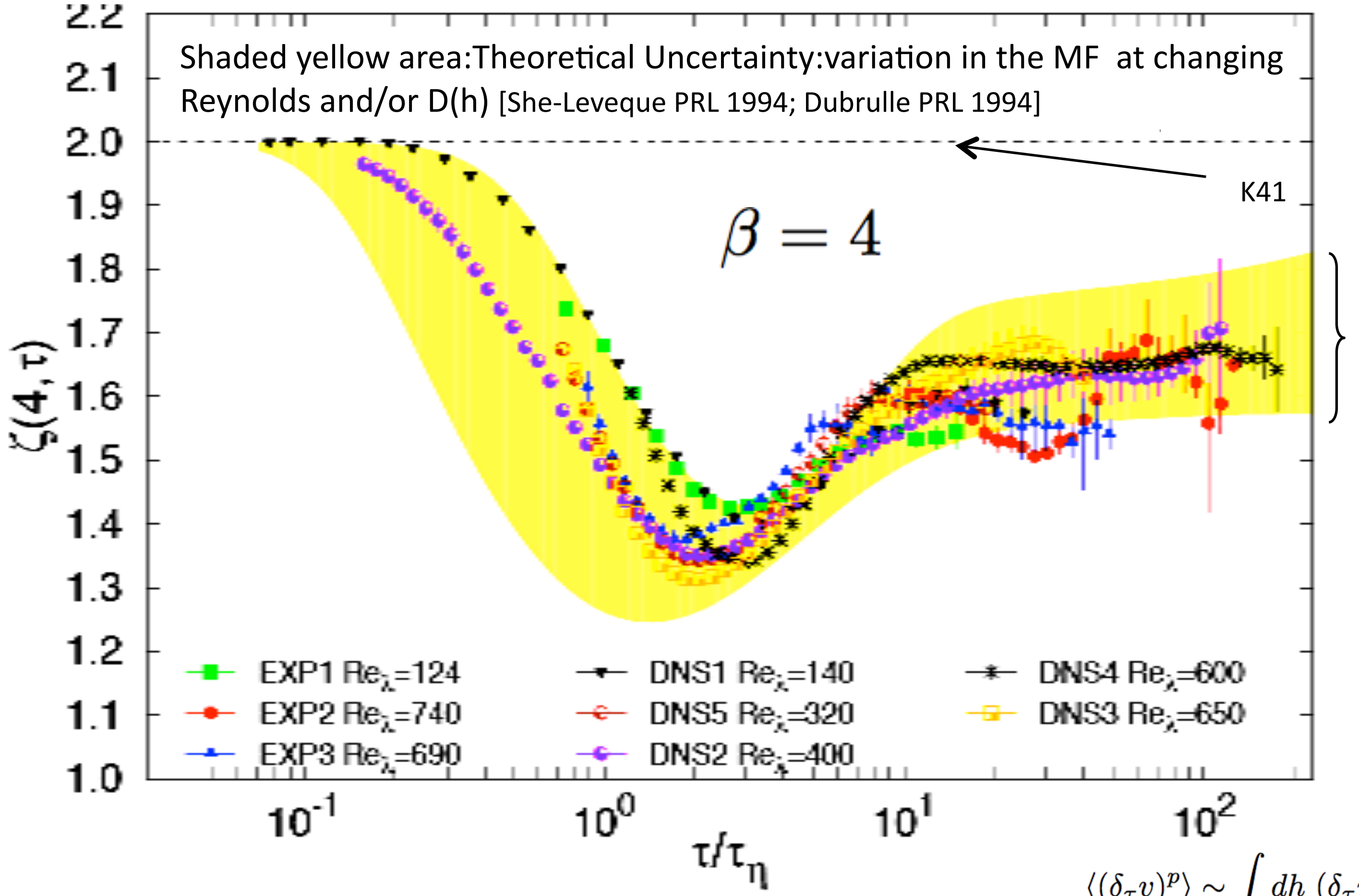
Blu Gene the lab

- 3-D homogeneous isotropic flow at $Re_\lambda \sim 300$
- Regular cubic box (1024^3 grid points) with periodic BC
- 256 sources where anyone emits 2000 tracers every τ_η for 180 emissions
- **4×10^{11} particle pairs with $r(0) < \eta$**

NEED FOR

1) INTERPOLATION (trilinear, b-spline, hermite, etc....)
2) MPI across nodes to keep track of the trajectory





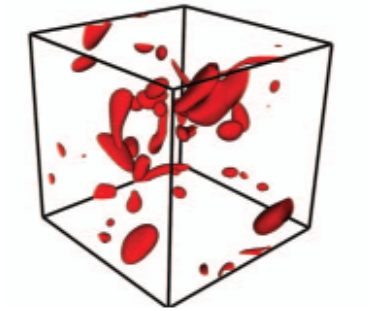
$$\langle(\delta_\tau v)^p\rangle \sim \int dh\ (\delta_\tau v)^p\ \mathcal{P}_h(\frac{\tau}{T_L}, \frac{\tau_\eta}{T_L})$$

International Collaboration for Turbulence Research, A. Arneodo,[1] J. Berg,[2] R. Benzi,[3] L. Biferale,[3] E. Bodenschatz,[4] A. Busse,[5] E. Calzavarini,[6] B. Castaing,[1] M. Cencini,[7] L. Chevillard,[1] R. Fisher,[8] R. Grauer,[9] H. Homann,[9] D. Lamb,[8] A.S. Lanotte,[10] E. Leveque,[1] B. Lüthi,[11] J. Mann,[2] N. Mordant,[12] W.-C. Müller,[5] S. Ott,[2] N. Oullette,[13] J.-F. Pinton,[1] S.B. Pope,[14] S.G. Roux,[1] F. Toschi,[15,16] H. Xu,[4] and P.K. Yeung[17]

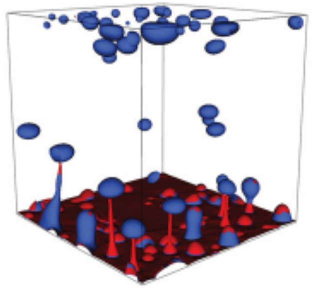
WE LEARN ABOUT:
(i) INTERMITTENCY; (ii) UNIVERSALITY; (iii) ANISOTROPY

Complex Fluid Dynamics: Why & Where ?

$10^{-3} - 10^{0} m$



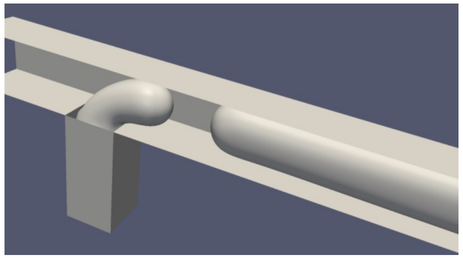
Droplets/Particles in Turbulence



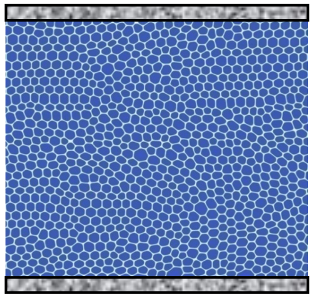
Boiling Fluids

- ✓ How the Heat Transport in a Rayleigh-Bènard Cell is affected by the presence of bubbles ?
- ✓ How Droplets interact with small scales Turbulence ?

$10^{-6} - 10^{-3} m$



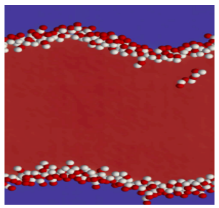
Droplets in Microfluidics



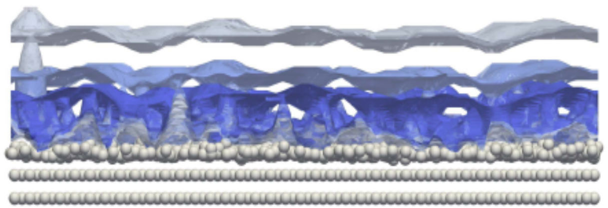
Soft-Glassy Materials

- ✓ Dynamics of Single Droplets: bounded *vs* unbounded geometries ?
- ✓ How The Rheology of a Collection of Droplets is affected by confinement?

$10^{-9} - 10^{-6} m$



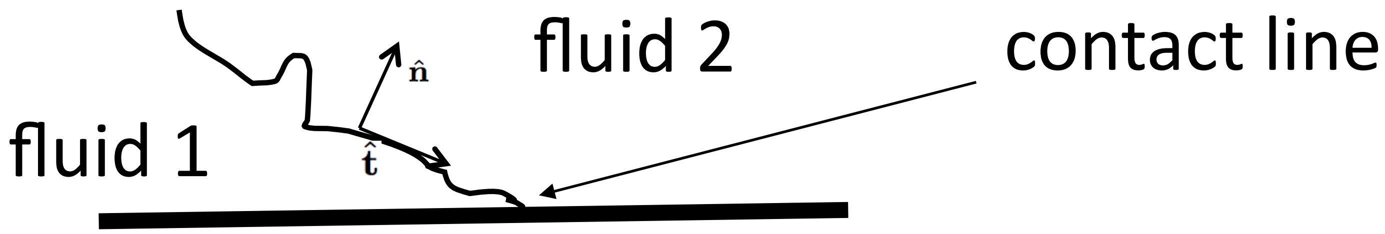
Membranes



Nanofluids

- ✓ How to correcty control surfactant dynamics at the interfaces?
- ✓ How the slip at the liquid-solid interfaces is affected by roughness and wettability ?

Basic Equations



Bulk

$$\partial_t(\rho_i \mathbf{v}_i) + \nabla(\rho_i \mathbf{v}_i \otimes \mathbf{v}_i) = -\nabla P_i + \nabla \tau_i$$

$$\partial \cdot \mathbf{v}_i = 0 \qquad i = 1, 2$$

Interface

$$\begin{cases} \mathbf{v}_1 \cdot \mathbf{n} = \mathbf{v}_2 \cdot \mathbf{n} = \mathbf{v}^i \\ \mathbf{v}_1 \cdot \mathbf{t} = \mathbf{v}_2 \cdot \mathbf{t} \\ (\mathbf{n} \cdot \hat{\tau}_1) \cdot \mathbf{t} = (\mathbf{n} \cdot \hat{\tau}_2) \cdot \mathbf{t} \\ P_2 - P_1 = \dfrac{2\gamma}{R} \end{cases}$$

Ideal discontinuous interface: drawbacks

a) Coalescence of two air bubbles (singular at the merging)

b) Nucleation of a second phase

c) Moving boundary conditions

d) hydrodynamical singularities at the contact line

Van der Waals approach to diffuse interface.

$$F(\rho, T, \partial\rho) = F^0 + \lambda(\partial\rho)^2$$

$$\partial_t \rho + \nabla(\rho \mathbf{v}) = 0$$

$$\partial_t(\rho \mathbf{v}) + \nabla(\rho \mathbf{v} \otimes \mathbf{v}) = -\nabla P^0 + \nabla\tau + \nabla\tau_{\mathbf{Kor}}$$

$$\tau^{ij}_{Kor} = [\rho\partial^2\rho + (\frac{1}{2}\partial\rho)^2]I^{ij} - \partial^i\rho\partial^j\rho$$

Korteweg stress

The 10 orders of magnitude hierarchy


MACROSCOPIC

NAVIER-STOKES

$$\partial_t u + (u \cdot \nabla) u = -\nabla P + \nu \Delta u$$

(continuum description)

⇧ **Chapman-Enskog**

KINETIC

(LATTICE BOLTZMANN)

$$\partial_t f + (v \cdot \nabla f) = -\frac{1}{\tau}(f - f^{eq})$$

(Particles p.d.f.)

⇧

MICROSCOPIC

MOLECULAR DYNAMICS

$$\frac{d^2 \mathbf{r}_i}{dt^2} = -\sum_j \nabla \mathcal{V}_{ij}$$

(particle-particle interactions)

Brief overview of (continuum) kinetic theory

The central quantity in kinetic theory is the *probability density function* whose evolution is described by the Boltzmann Equation → $f = f(\mathbf{x}, \xi, t)$

$$\partial f + \xi \cdot \nabla f + \frac{1}{m}\mathbf{K} \cdot \nabla_\xi f = Q(f, f)$$ → collision operator

$$f^{(eq)}(\mathbf{x}, \mathbf{u}, t) = \frac{\rho(\mathbf{x}, t)}{(2\pi T(\mathbf{x}, t))^{3/2}} exp\left(-\frac{|\xi - \mathbf{u}(\mathbf{x}, t)|^2}{2T(\mathbf{x}, t)}\right)$$

"local" equilibrium ($\in ker(Q)$)

The moments (in the velocities) of the pdf correspond to the hydrodynamic fields:

$$\rho(\mathbf{x}, t) = \int_{R^3} f d^3\xi$$ density

$$\mathbf{u}(\mathbf{x}, t) = \int_{R^3} f\xi d^3\xi$$ velocity

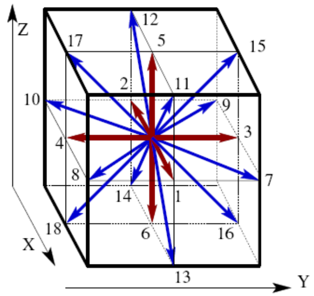
temperature

$$T(\mathbf{x}, t) = \int_{R^3} f|\xi - \mathbf{u}|^2 d^3\xi$$

Lattice BGK Boltzmann Equation

Approximations:

1) Linear collision operator (BGK approximation);
2) Discretization of physical space;
3) Discretization of velocity space (the very strong one!)



$$\xi \longrightarrow \mathbf{c_l}$$

$$f_l(\mathbf{x} + \mathbf{c}_l \Delta t, t + \Delta t) - f_l(\mathbf{x}, t) = -\frac{\Delta t}{\tau}\left(f_l(\mathbf{x}, t) - f_l^{(eq)}(\rho, \mathbf{u}, T)\right)$$

$$Kn \ll 1$$

Chapman-Enskog expansion

$$Kn \sim \frac{\lambda_{mfp}}{L}$$

$$f_l(\boldsymbol{x}, t) = f_l^{(eq)} + Kn f_l^{(1)} + \ldots$$

$$\partial_t \rho + \nabla \cdot (\rho \mathbf{u}) = 0 \quad \rho(\partial_t \mathbf{u} + \mathbf{u} \cdot \nabla \mathbf{u}) = -\nabla P + \nabla \cdot \hat{D}$$

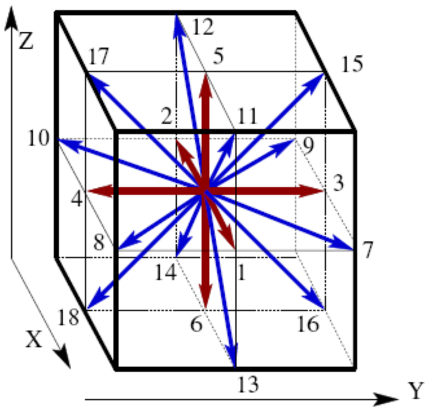
$$\rho(\partial_t T + \mathbf{u} \cdot \nabla T) = -P \nabla \cdot \mathbf{u} + \nabla \cdot (\kappa \nabla T) + \hat{D} : (\nabla \otimes \mathbf{u})$$

$$D_{\alpha\beta} = \eta(\partial_\alpha u_\beta + \partial_\beta u_\alpha) - \frac{2}{3}\eta \delta_{\alpha\beta}(\partial_\gamma u^\gamma)$$

$P = \rho T$ **perfect gas equation of state**

The system is NOT incompressible!

Lattice Boltzmann for multi-phase fluds



$$\partial_t f + (v \cdot \nabla f) = -\frac{1}{\tau}(f - f^{eq}) \quad + F$$

$$F = G_b \sum_I \psi[\rho(x)]\psi[\rho(x + \Delta x)]$$

Intermolecular forces

Pseudo potential

$$\psi(x) = \sqrt{\rho_0}(1 - e^{-\rho/\rho_0})$$

Shan and Chen (1993,1994)

Pressure tensor

$$P_{ij} = \left[c_s^2 \rho + \frac{1}{2} c_s^4 G_b \psi \Delta \psi + \frac{G_b c_s^4}{4} |\nabla \psi|^2\right] \delta_{ij} - \frac{1}{2} c_s^4 G_b \partial_i \psi \partial_j \psi$$

$$P_b = c_s^2 \rho + \frac{1}{2} G_b c_s^2 \psi^2$$

Non ideal gas effects

$$\sigma = -\frac{1}{2} c_s^4 G_b \int |\partial_y \psi|^2 dy$$

Surface tension

Why LB for microflows? LB versus NS

Is it really NS? Yes but….

-Non linearity is local

-No Poisson solver for the pressure

-On line stress (no space derivatives)

-emergent diffusion

-Emergent complexity

-Complex geometries

-Parallel computing

$$\Delta P = 0$$

$$\Delta t < \Delta x$$

And not

$$\Delta t < \Delta x^2$$

$$F(\rho)\partial_p f$$

Recipes

1) Take a diffuse interface model with a given interface width

2) Develop an algorithm to simulate it

3) If macroscopic: be careful about the multi-scale bottleneck -> $dx < \lambda < \eta << L$

4) If mesoscopic physics-> check the robustness at changing λ

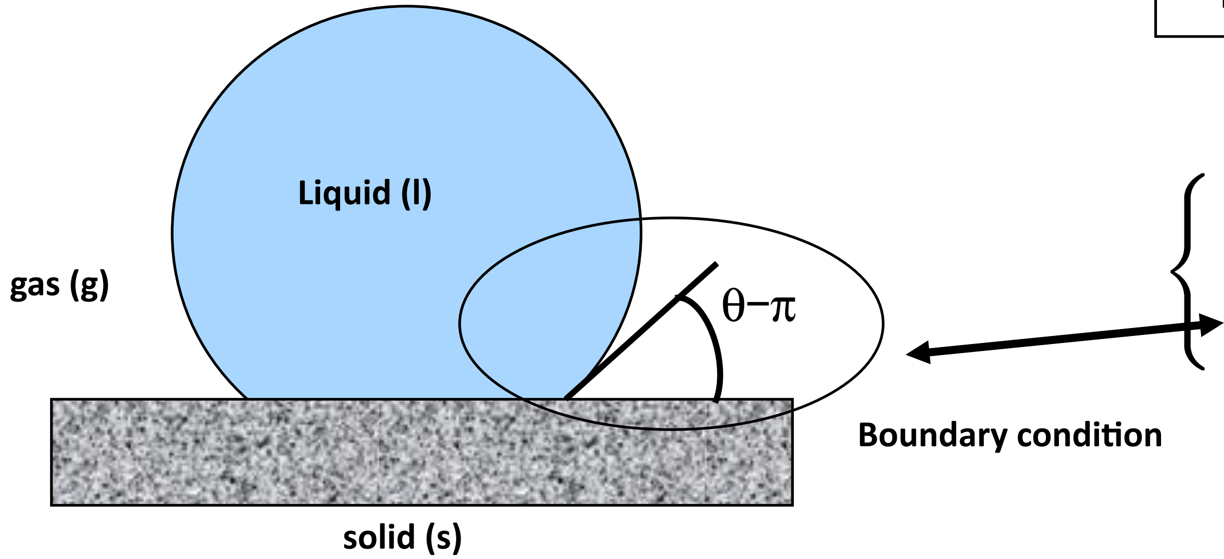
5) If nanoscopic physics-> check the consistency of taking statistical equilibrium

Modelling wetting properties in lattice Boltzmann

Benzi R., Biferale L.,Sbragaglia M., Succi S. and Toschi F Phys. Rev. E 74, 021509 (2006).

Mechanical equilibrium

$$\begin{cases} \partial_j P_{i,j}(\psi, G_b) \\ \boxed{\psi(\boldsymbol{x}_w) = \psi_w} \end{cases}$$



$$cos\theta = \frac{\int_{sg} |\partial_y \psi|^2 dy - \int_{sl} |\partial_y \psi|^2 dy}{\int_{lg} |\partial_y \psi|^2 dy}$$

M. Sbragaglia, R. Benzi, L. Biferale, S. Succi and F. Toschi
Phys. Rev. Lett. 97, 204503 (2006).

Shan-Chen Operation

⇩

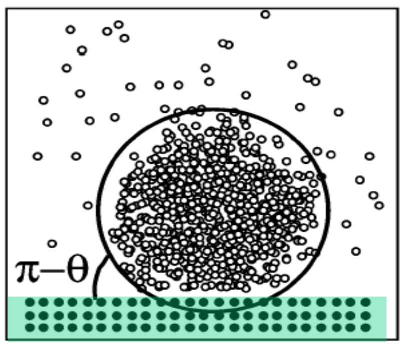
Heuristic mapping

$$V_{ij} = \epsilon \left[\left(\frac{r_0}{r_{ij}} \right)^{12} - c_{ij} \left(\frac{r_0}{r_{ij}} \right)^{6} \right]$$

$$F = G_b \sum_l \psi(x)\psi(x + c_l \Delta t) c_l$$

$$\epsilon / KT \Rightarrow G_b$$

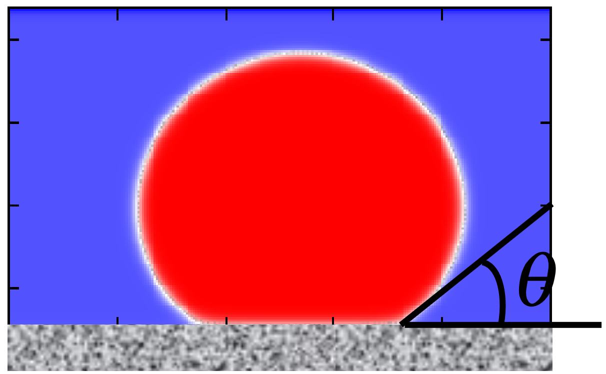
$$c_{fs} / KT \Rightarrow \psi_w$$



Barrat et al. (1993)

$$\theta(G_b, \psi_w)$$

Contact angle



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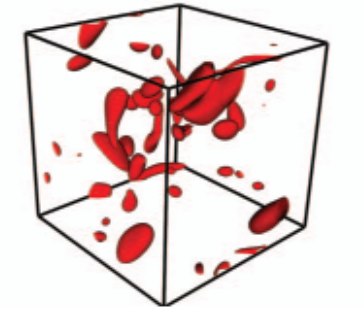
$10^{-3} - 10^{0} m$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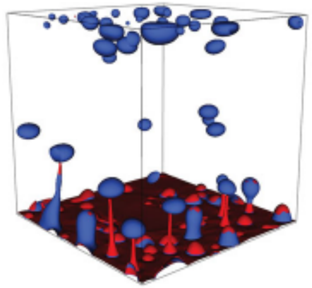
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- ✓ How the Heat Transport in a Rayleigh-Bènard Cell is affected by the presence of **bubbles** ?
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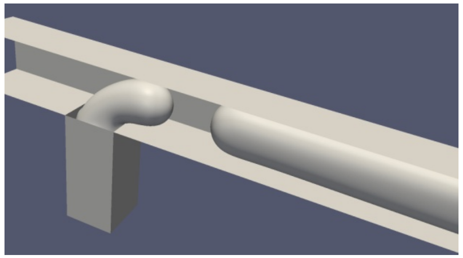
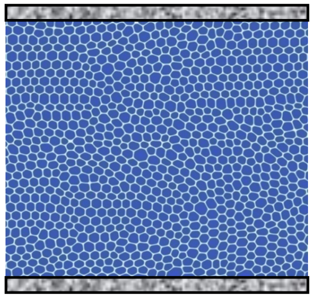

Droplets in Microfluidics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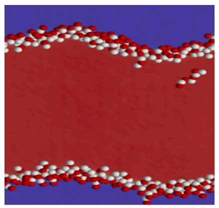
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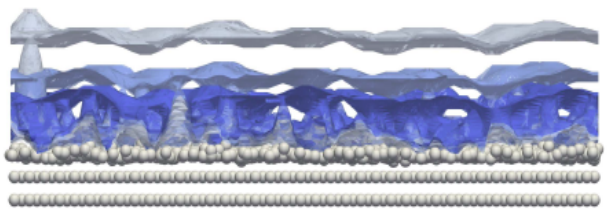

Nanofluids

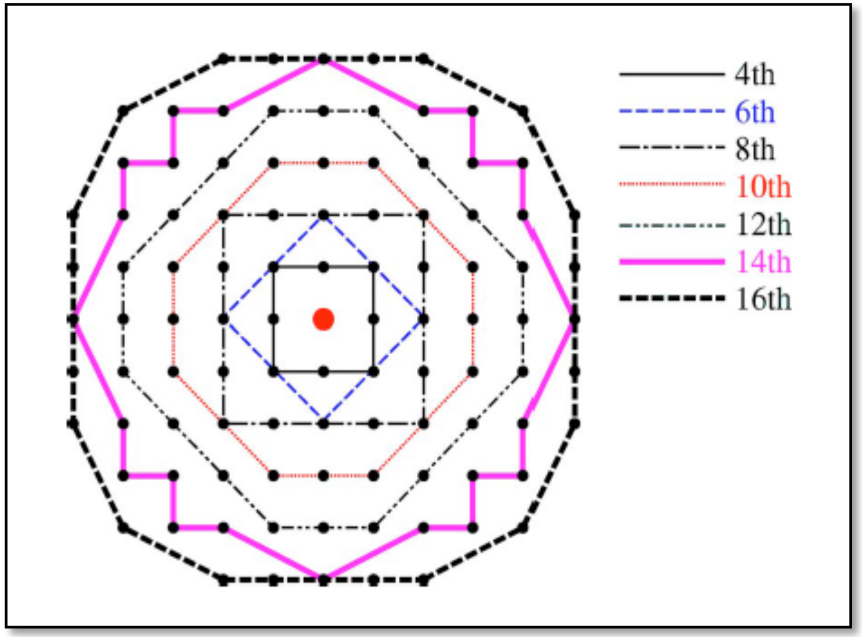
- ✓ How to correcty control surfactant dynamics at the **interfaces**?
- ✓ How the slip at the liquid-solid **interfaces** is affected by roughness and wettability ?

Spurious (velocity) effects at curved interfaces

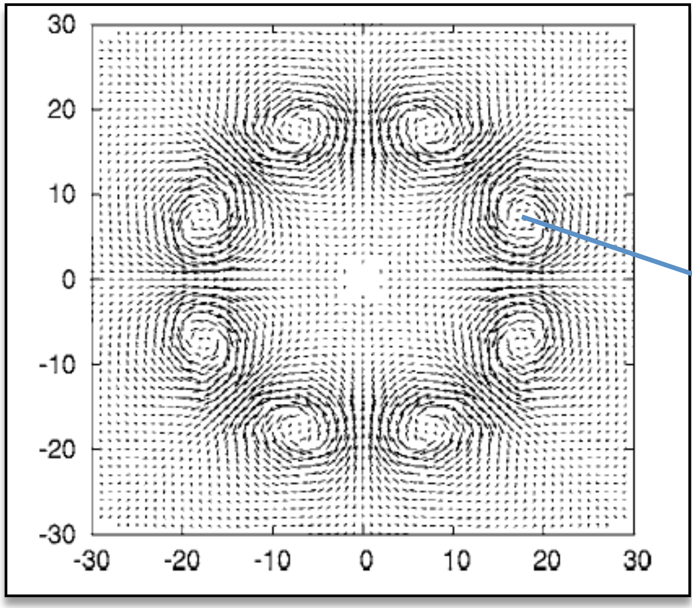
$$\vec{F} = -\mathcal{G}\psi(\vec{r})\sum_i w_i \psi(\vec{r}+\vec{c}_i)\vec{c}_i$$

Playing with Potential Range

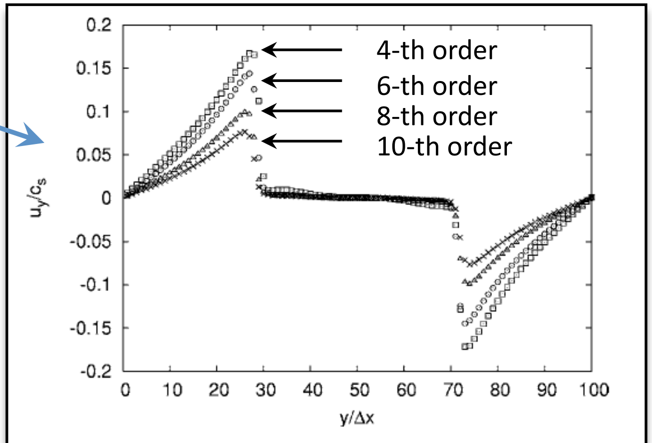
$$\sum_i c_i^{k_1} c_i^{k_2} \ldots c_i^{k_n} w_i \rightarrow \text{Isotropic}$$



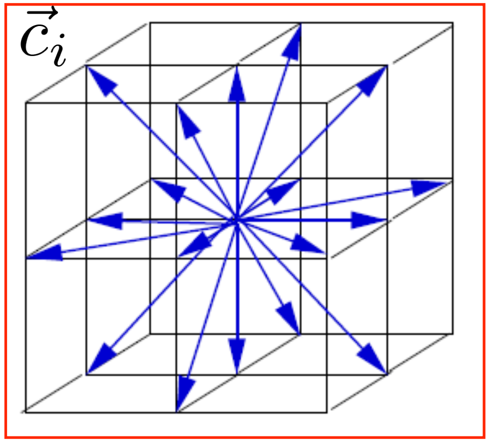
M. Sbragaglia et al., Physical Review E 75, 026702 (2007)

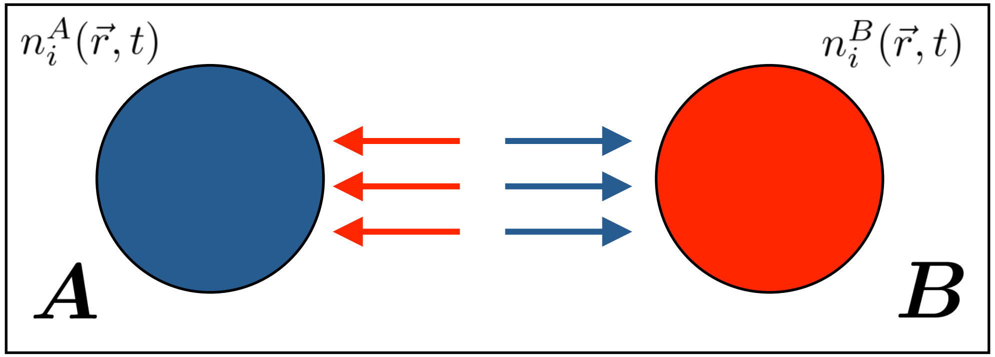


Stationary **(!!! ??? !!!!)** velocity distribution at curved interfaces



Increasing Complexity: Multicomponent LBM





$$\vec{F}^{(A)}(\vec{r}) = g_{AB}\rho_A(\vec{r})\sum_i w_i \rho_B(\vec{r}+\vec{c}_i)\vec{c}_i$$

$$\vec{F}^{(B)}(\vec{r}) = g_{AB}\rho_B(\vec{r})\sum_i w_i \rho_A(\vec{r}+\vec{c}_i)\vec{c}_i$$

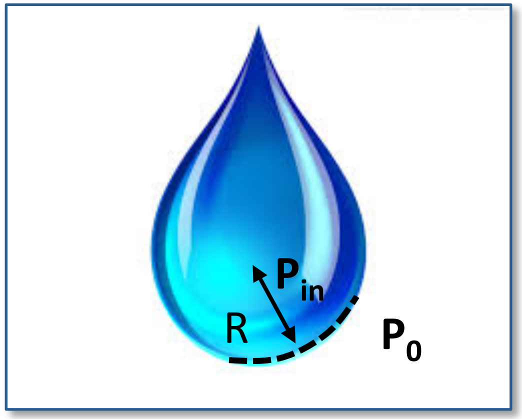
A Few Reference Works:

X. Shan & H. Chen, Physical Review E 47, 1815 (1993)
X. Shan & H. Chen, Physical Review E 49, 2941 (1994)
X. Shan, Physical Review E 77, 066702 (2008)
M. Sbragaglia & X. Shan, Physical Review E 84, 036703 (2011)

Highlight 1:

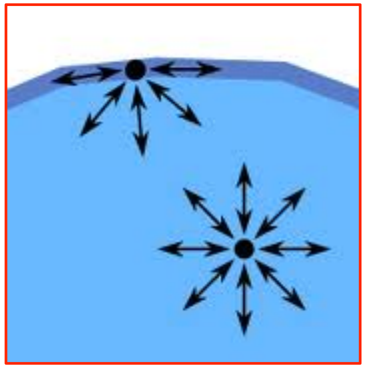
Modelling Wetting Problems with LBM

Basics of Capillarity/Wettability



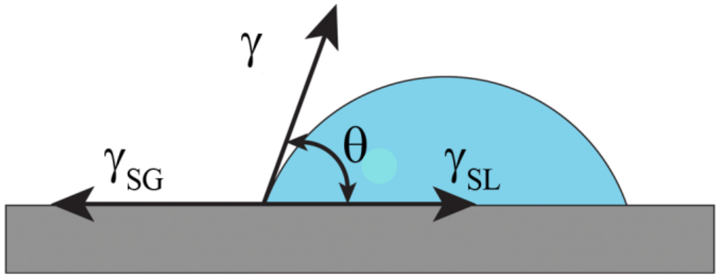
$$\Delta P = P_{in} - P_0 = \gamma \left(\frac{1}{R_1} + \frac{1}{R_2} \right)$$

Laplace Law (Surface Tension)

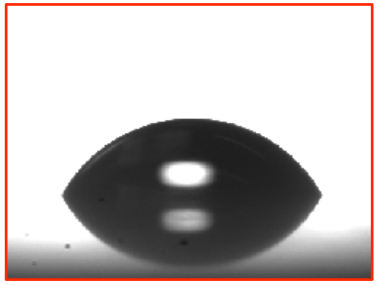


Cohesive forces between liquid molecules responsible for the Surface Tension (Minimization of Free Surface)

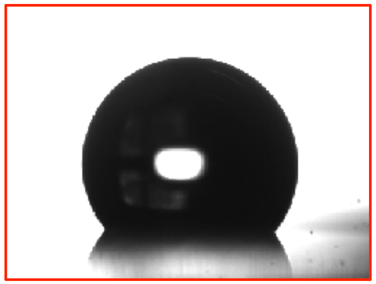
Wetting



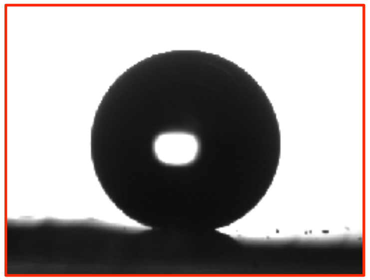
$$\cos\theta = \frac{\gamma_{SG} - \gamma_{SL}}{\gamma}$$



$\theta < 90°$
hydrophilic



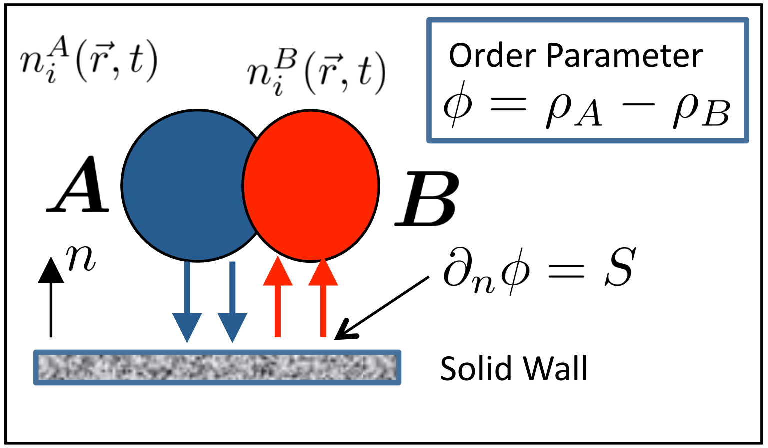
$\theta > 90°$
hydrophobic

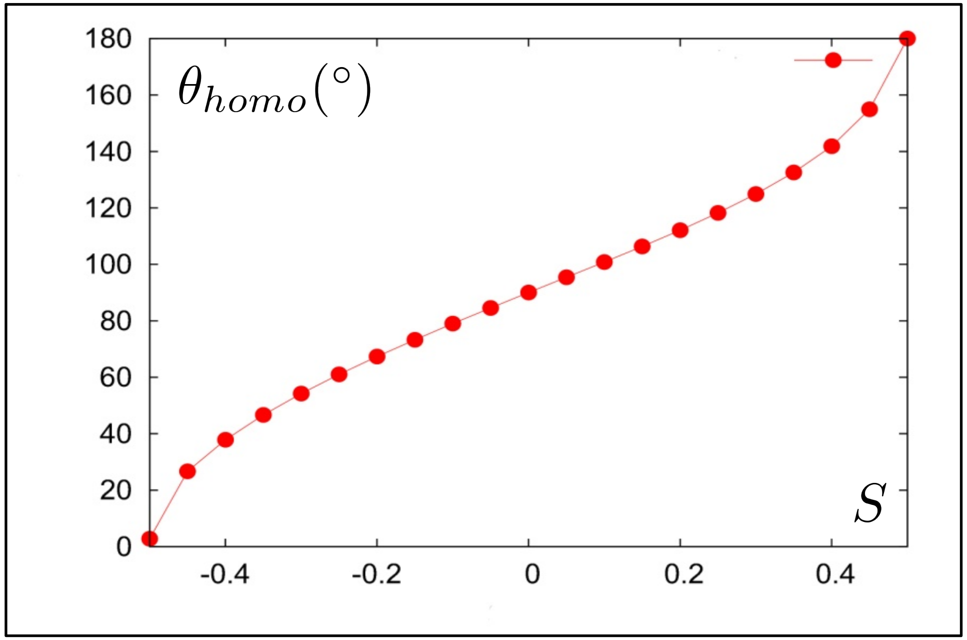


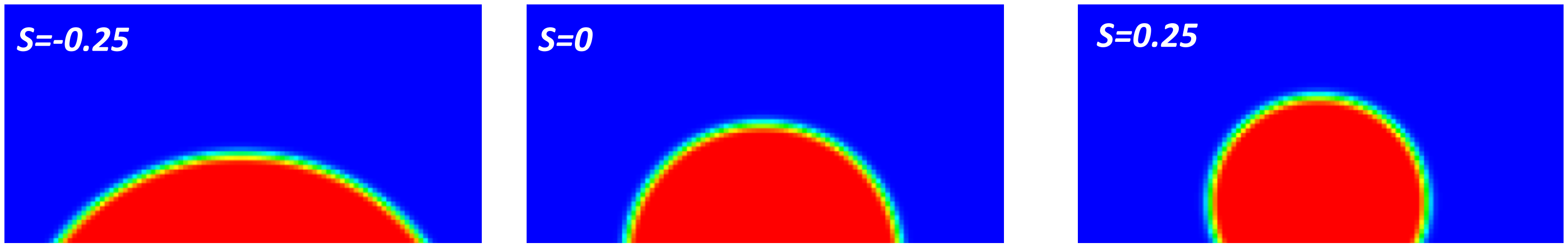
$\theta \geq 150°$
super-hydrophobic

Non Ideal Forces: Modelling Wettability

Non-Ideal Fluid-Solid Interactions!

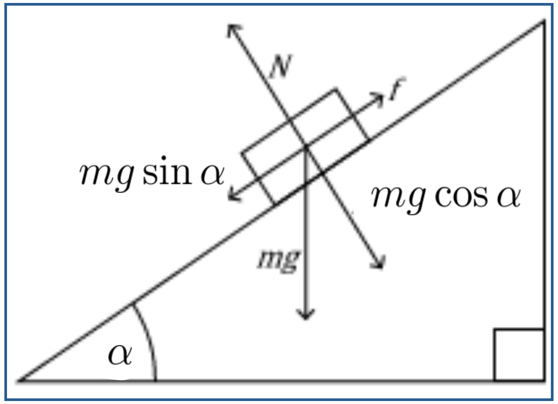






Hydrophilic **Neutral Wetting** **Hydrophobic**

Droplets on Inclined Planes (Sliding & Pearling)

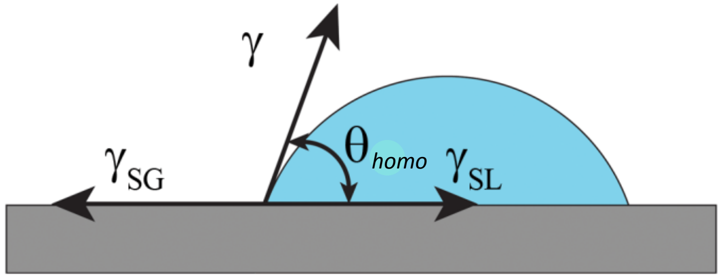


$$Ca = \eta U/\gamma$$

Capillary number (viscous/surface)

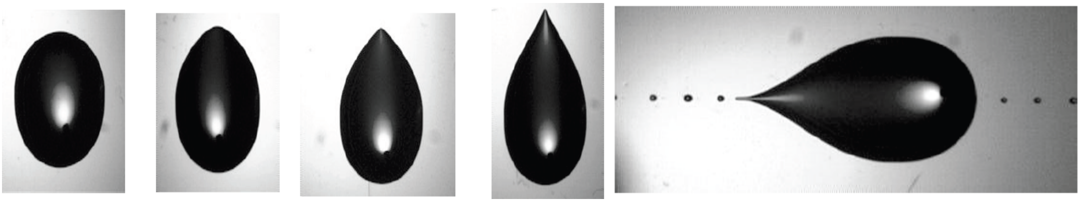
$$Bo = V^{2/3}\rho g \sin\alpha/\gamma$$

Bond number (gravity/surface)



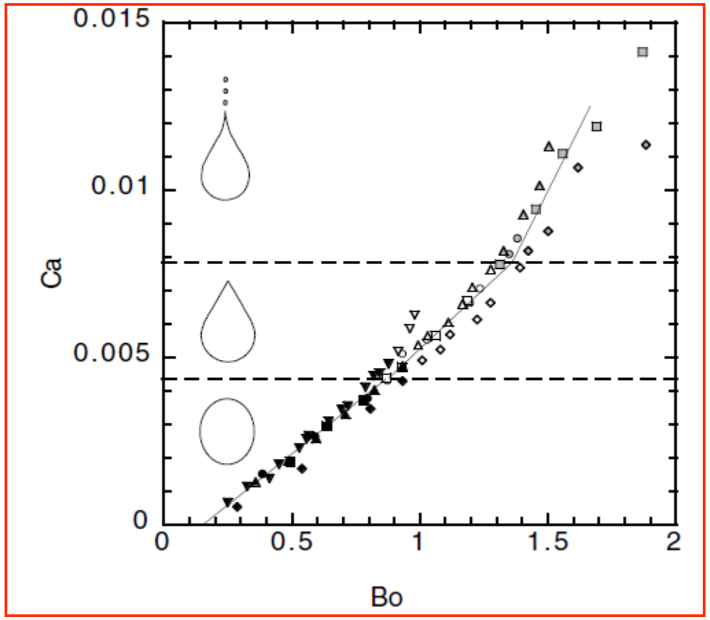
$$\cos\theta_{homo} = \frac{\gamma_{SG} - \gamma_{SL}}{\gamma}$$

Increasing Capillary Number.....

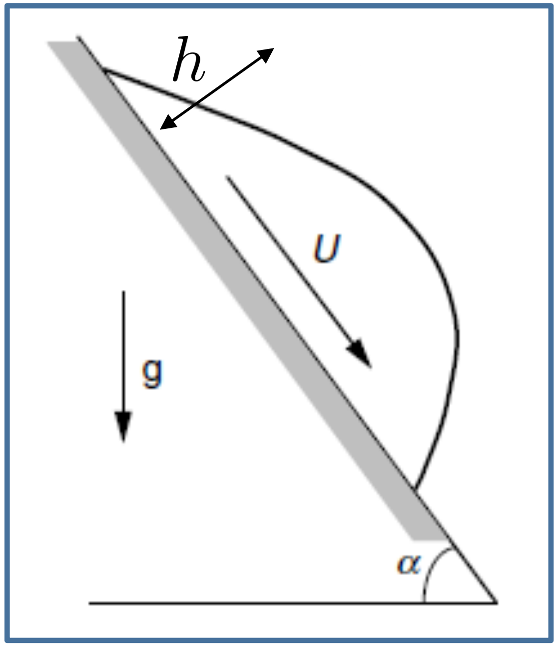


rounded | corner | cusp | pearling

Podgorsky et al., Phys. Rev. Lett . (**2001**)



Sliding Droplets on Homogeneous Substrates



$$\frac{\Phi_b}{\Phi_w} \sim \frac{R_b}{h c(\theta)} \ll 1$$

Viscous Dissipation at the contact line is dominating !

$$\Phi_w \sim c(\theta)\eta L U^2$$

Dissipation in the perimeter $L = 2\pi R_b$ liquid wedge

$$\Phi_b \sim \eta V_b \frac{U^2}{h^2}$$

Dissipation in the bulk $V_b \sim A_b h = \pi R_b^2 h$

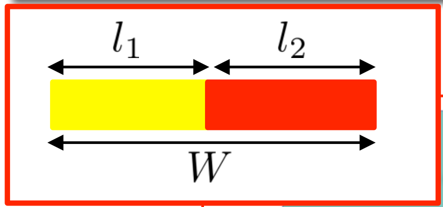
$Ca = \eta U/\gamma$ Capillary number (viscosity/surface)

$Bo = V^{2/3}\rho g/\gamma$ Bond number (gravity/surface)

$$Ca \sim Bo/c(\theta)$$

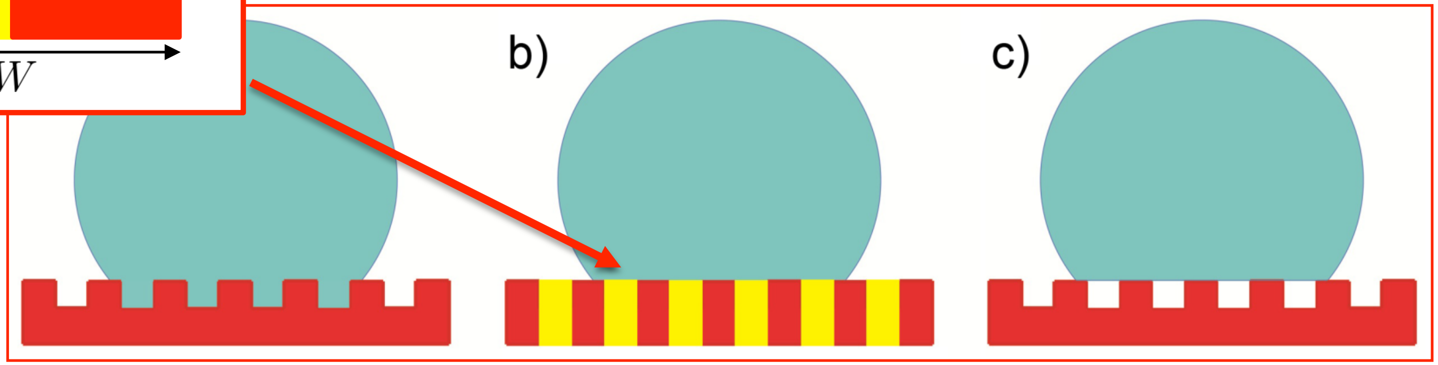
$$\Phi_w + \Phi_b \approx c(\theta) L \eta U^2 = \rho V_b g U \sin\alpha$$

Sliding on heterogeneous surfaces

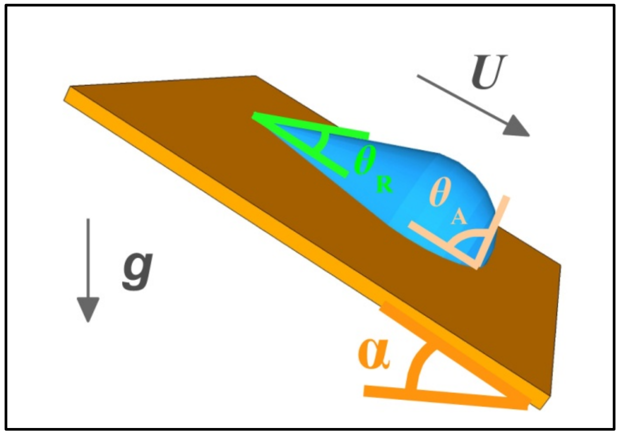


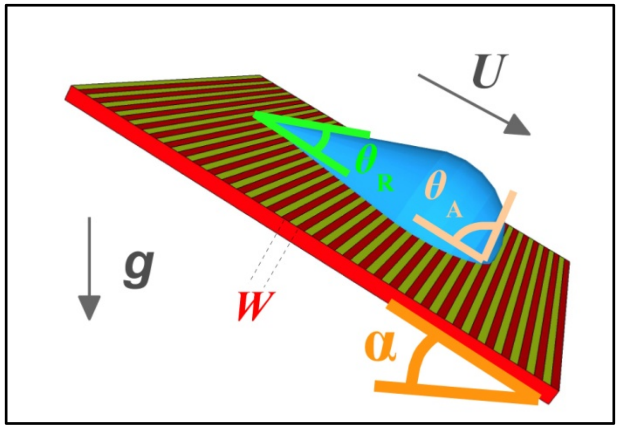
$f_1 = l_1/W$
$f_2 = l_2/W$

Real Surfaces: Heterogeneity & Roughness



$$\cos\theta_{hete} = f_1 \cos\theta_1 + f_2 \cos\theta_2$$ (Cassie Equation)



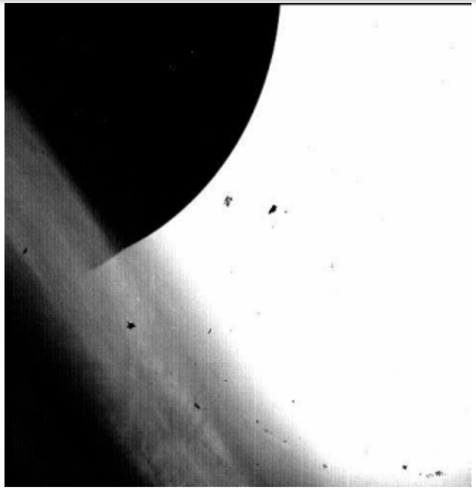


$$\theta_{hete} = \theta_{homo}$$

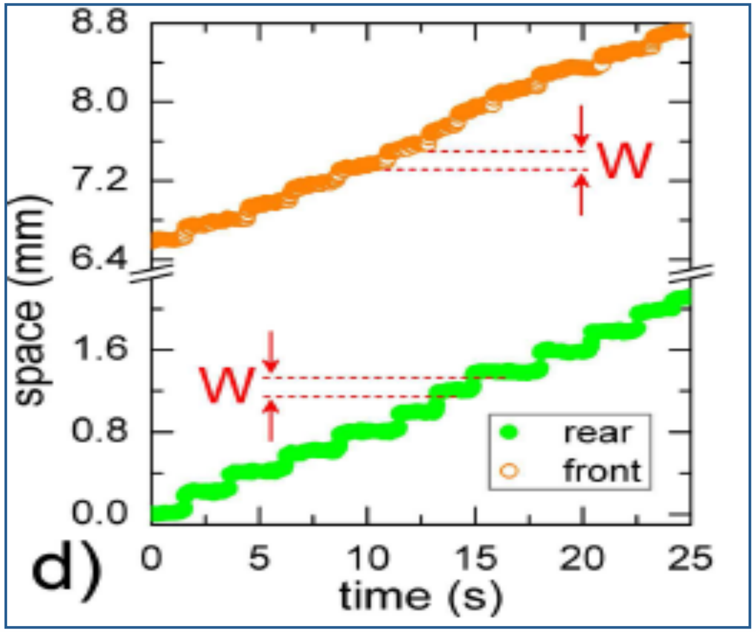
Same statics….what about the dynamics ?!?

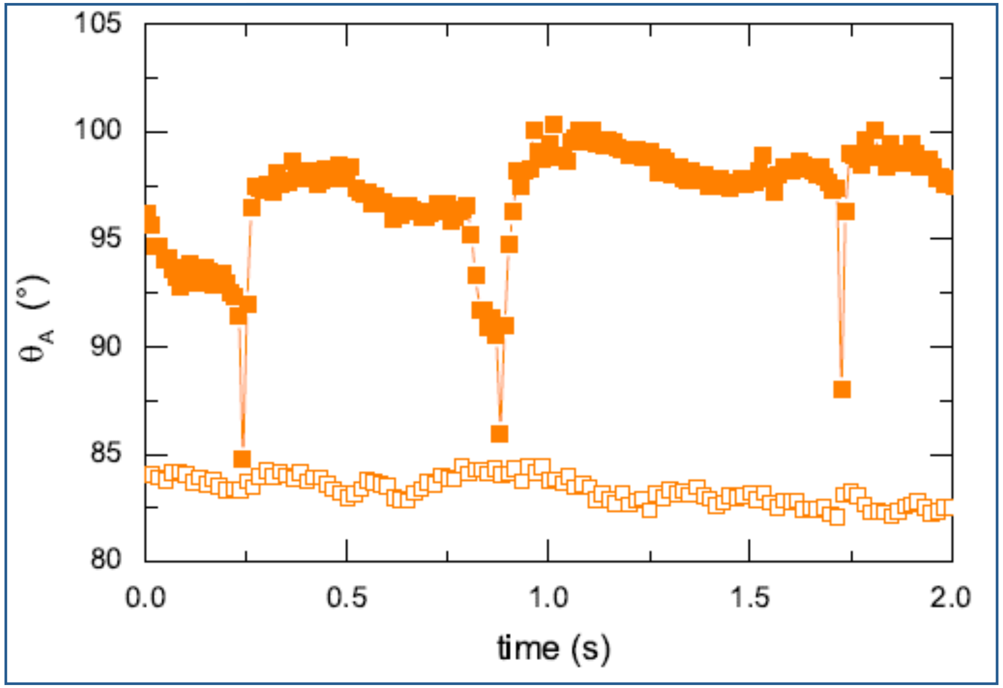
Sliding Droplets on Heterogeneous Surfaces

Varagnolo *et al.* , Phys. Rev. Lett. **111**, 066101 (2013)

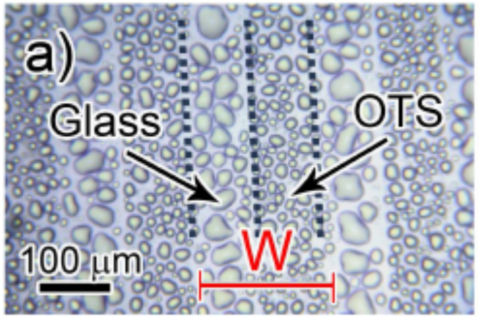


Advancing contact line: **Stick & Slip** Dynamics

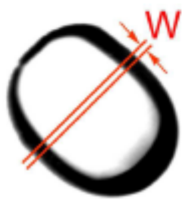




Same statics....order of magnitude slower!!



droplet on heteogeneous Surfaces



$30\ \mu l$ droplet

$W = 200\ \mu m$

Insight From Equations of Motion

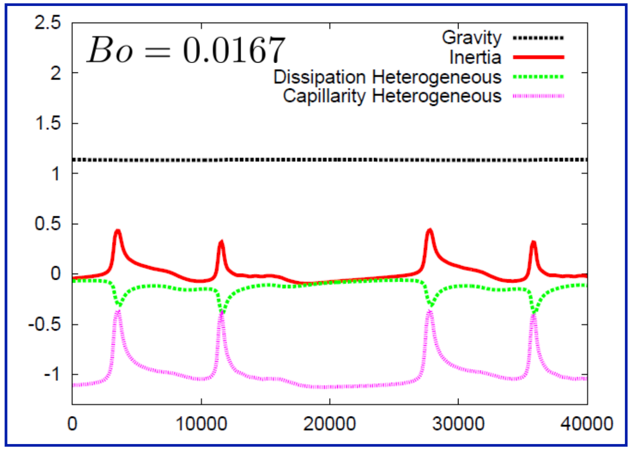
$$\begin{cases} \partial_t \rho + \partial_\alpha(\rho u_\alpha) = 0 \\ \rho\left[\partial_t u_x + u_\alpha \partial_\alpha u_x\right] = -\partial_\beta P_{x\beta} + \partial_\beta \sigma_{x\beta} + \rho g \sin\alpha\, \delta_{ix} \end{cases}$$

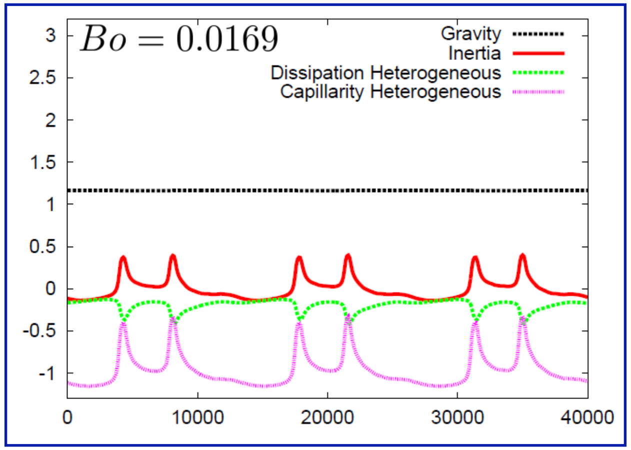
Continuity Equation

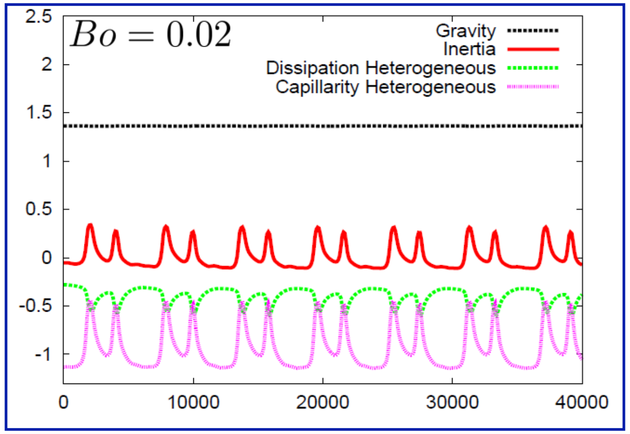
NS Equation

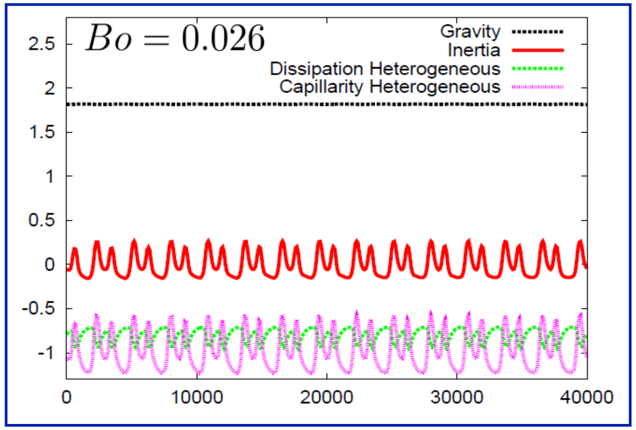
$$Ma(t) = F_{cap}(t) + D(t) + F_g$$

Global Balance Equation
(Integrated over the Droplet Volume)









Insight From Equations of Motion

$$\begin{cases} \partial_t \rho + \partial_\alpha(\rho u_\alpha) = 0 \\ \rho\left[\partial_t u_x + u_\alpha \partial_\alpha u_x\right] = -\partial_\beta P_{x\beta} + \partial_\beta \sigma_{x\beta} + \rho g \sin\alpha \delta_{ix} \end{cases}$$

Continuity Equation

NS Equation

$$Ma(t) = F_{cap}(t) + D(t) + F_g$$

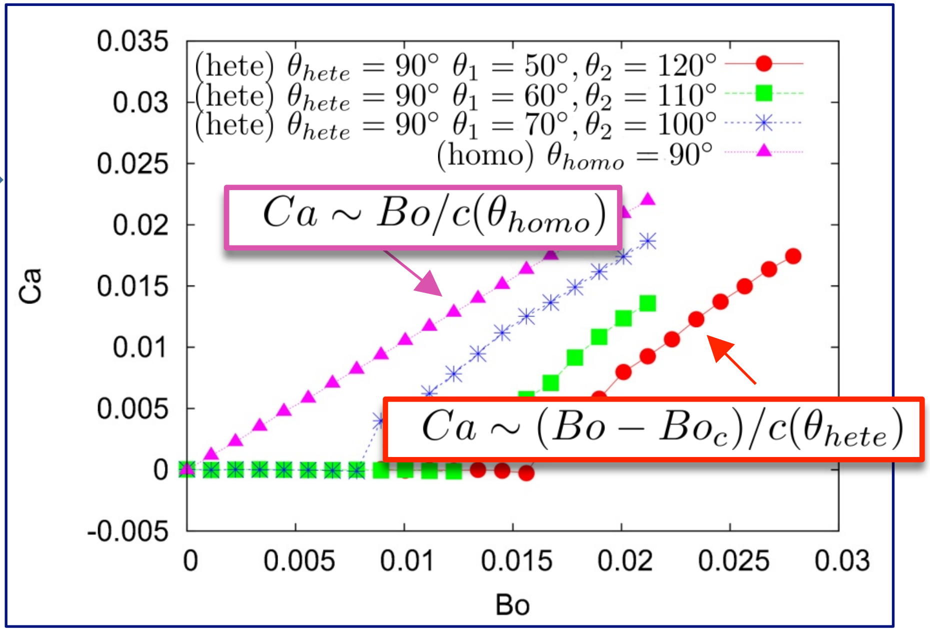
Global Balance Equation
(Integrated over the Droplet Volume)

Simulations performed for the same Static Morphology

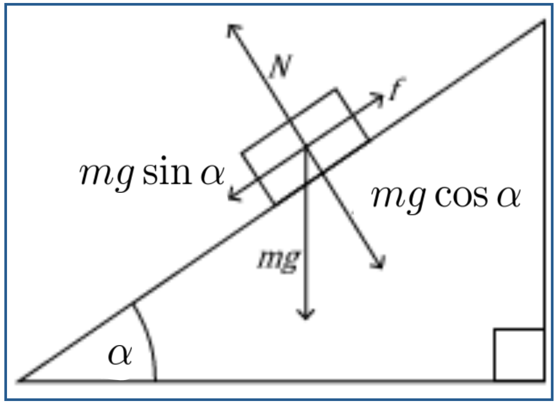
$$\theta_{hete} = \theta_{homo} = 90^\circ$$

Slope parametrized by Cassie Angle ?

$$\cos\theta_{hete} = f_1 \cos\theta_1 + f_2 \cos\theta_2$$



Droplets on Inclined Planes (Sliding & Pearling)



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Capillary number (viscous/surface)

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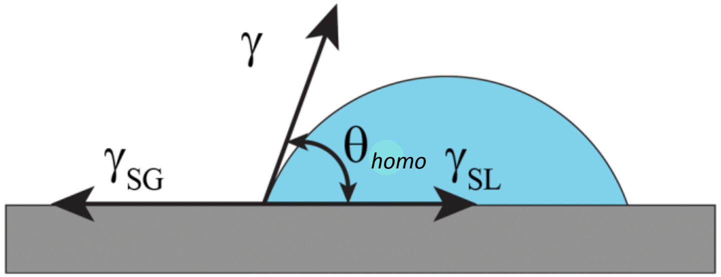
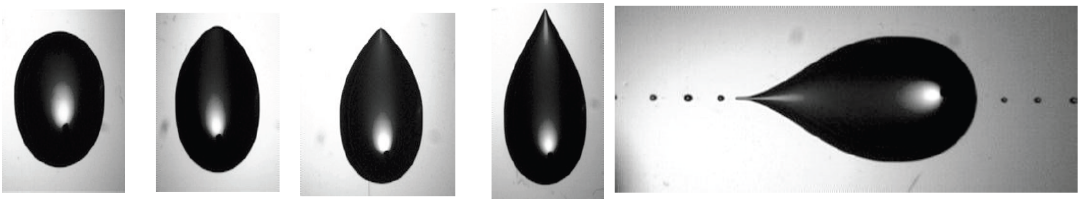
Bond number (gravity/surface)



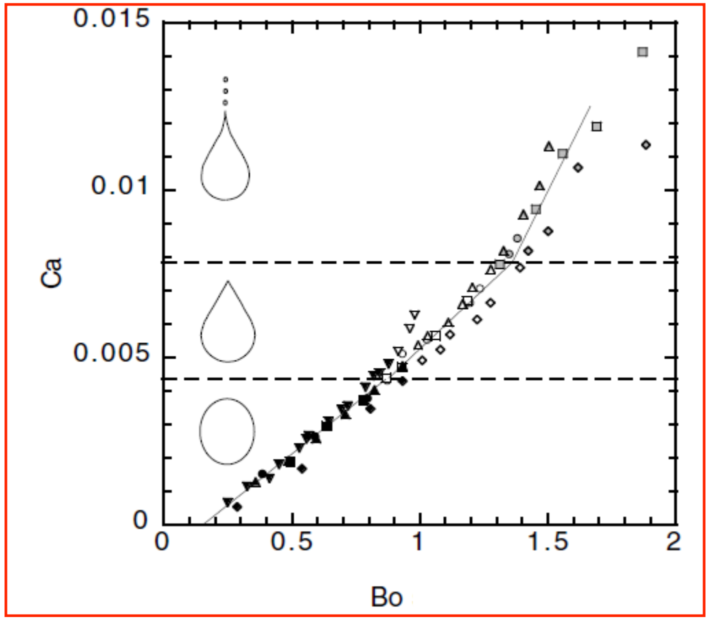
$$\cos\theta_{homo} = \frac{\gamma_{SG}-\gamma_{SL}}{\gamma}$$

Podgorsky et al., Phys. Rev. Lett . (**2001**)

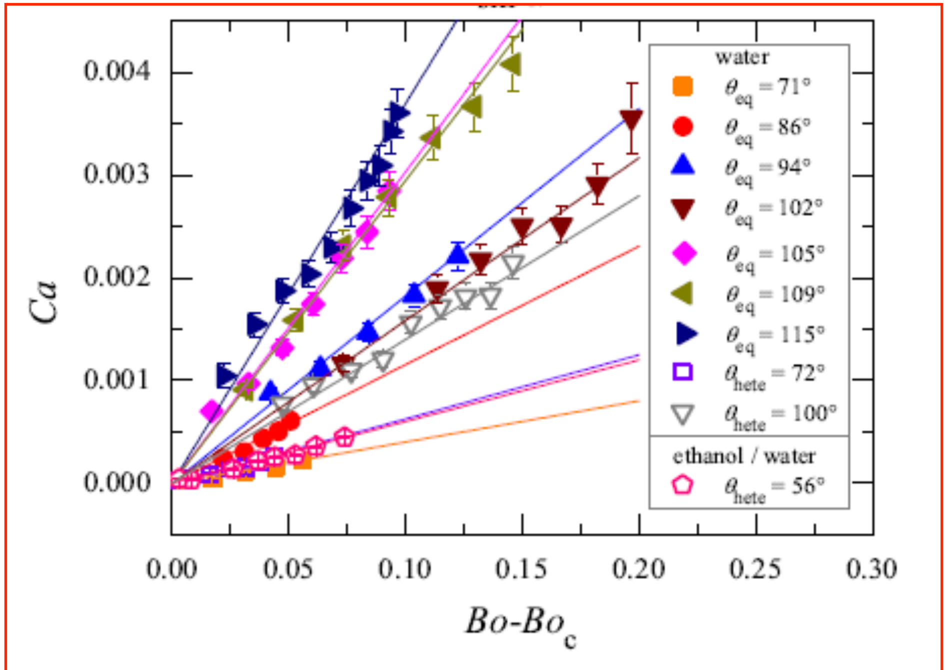
Increasing Capillary Number…..

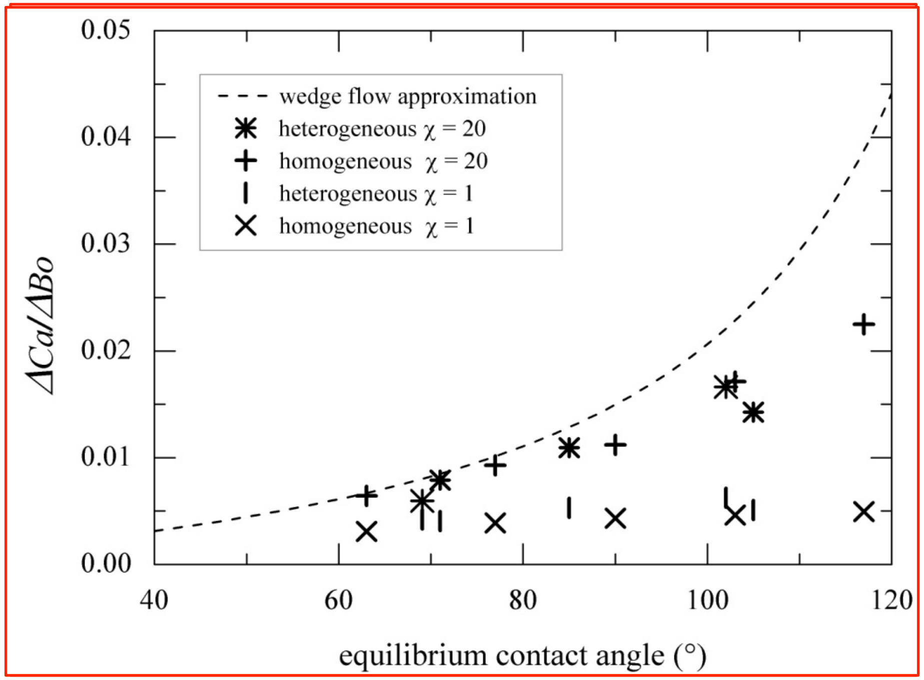


rounded corner cusp pearling



Effective Dissipation: Homogeneous *vs.* Heterogeneous

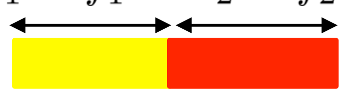


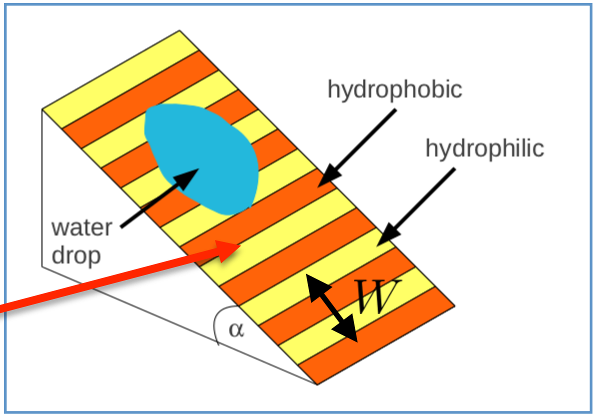


"Effective" Angle for the motion on patterned surfaces

$$\gamma W \cos\theta_{eff} = f_1 W \gamma \cos\theta_1 + f_2 W \gamma \cos\theta_2$$

$$l_1 = f_1 W \quad l_2 = f_2 W$$





$$\cos\theta_{hete} = \cos\theta_{eff} = f_1 \cos\theta_1 + f_2 \cos\theta_2$$

J. von NEUMANN (1949)

These considerations justify the view that a considerable mathematical effort towards a detailed understanding of the mechanism of turbulence is called for. The entire experience with the subject indicates that the purely analytical approach is beset with difficulties, which at this moment are still prohibitive. The reason for this is probably as was indicated above: That our intuitive relationship to the subject is still too loose — not having succeeded at anything like deep mathematical penetration in any part of the subject, we are still quite disoriented as to the relevant factors, and as to the proper analytical machinery to be used.

Under these conditions there might be some hope to 'break the deadlock' by extensive, but well-planned, computational efforts. It must be admitted that the problems in question are too vast to be solved by a direct computational attack, that is, by an outright calculation of a representative family of special cases. There are, however, strong indications that one could name certain strategic points in this complex, where relevant information must be obtained by direct calculations. If this is properly done, and the operation is then repeated on the basis of broader information then becoming available, etc., there is a reasonable chance of effecting real penetrations in this complex of problems and gradually developing a useful, intuitive relationship to it. This should, in the end, make an attack with analytical methods, that is truly more mathematical, possible.[1]