

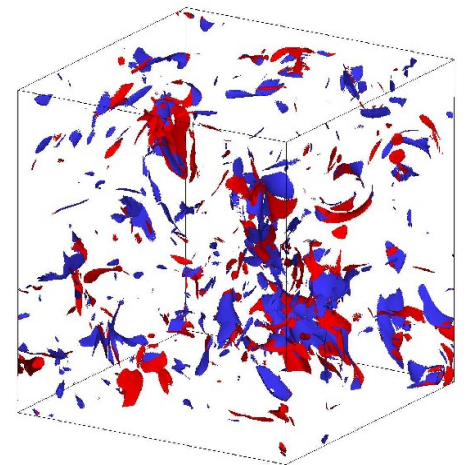
Numerical modeling of MHD turbulence

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de la CÔTE d'AZUR



Les Houches, 26.02.2013

Outline

- Why MHD turbulence?
- Why numerical modeling?
- How to model numerically?
- Applications

Why MHD turbulence?

Simplest macroscopic description of a conducting flow

- fluid description (not kinetic)
- one fluid – quasi neutral
- non relativistic

Magnetohydrodynamic field equations

$$\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{v} = -\nabla P + \mathbf{j} \times \mathbf{B} + \nu \Delta \mathbf{v} + \mathbf{F}_v \quad \text{Momentum equation}$$

$$\frac{\partial \mathbf{B}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{B} = \mathbf{B} \cdot \nabla \mathbf{v} + \eta \Delta \mathbf{B} + \mathbf{F}_B \quad \text{Induction equation}$$

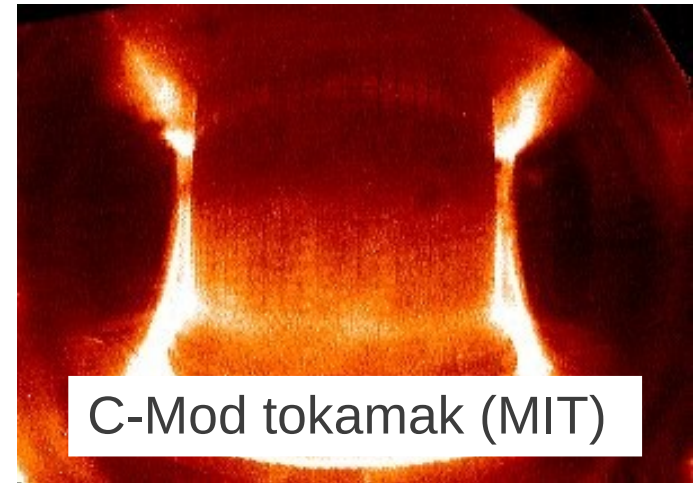
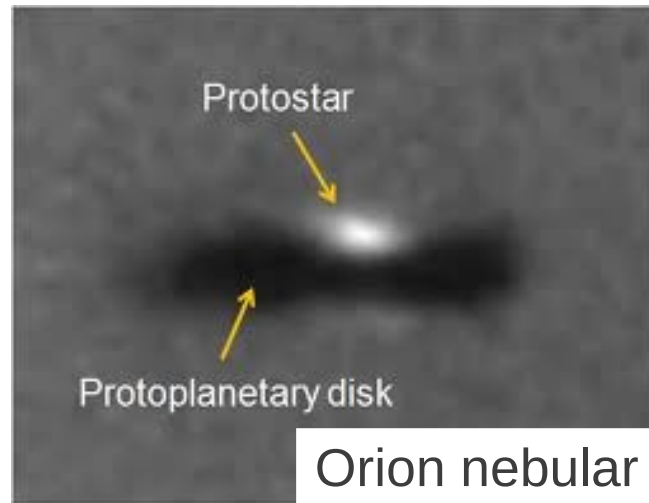
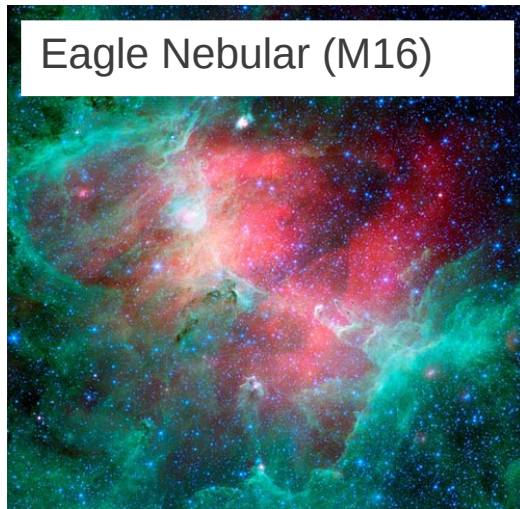
$$\nabla \cdot \mathbf{B} = \nabla \cdot \mathbf{v} = 0 \quad \text{Incompressible flow}$$

\mathbf{F}_v and \mathbf{F}_B : forcing terms

+ boundary conditions!!!

Why MHD turbulence?

- **Fundamental questions:** universality, scaling laws, isotropy, ...
- **Applications :** Heliosphere, Solar wind, Dynamos, Interstellar medium, Fusion experiments, ...

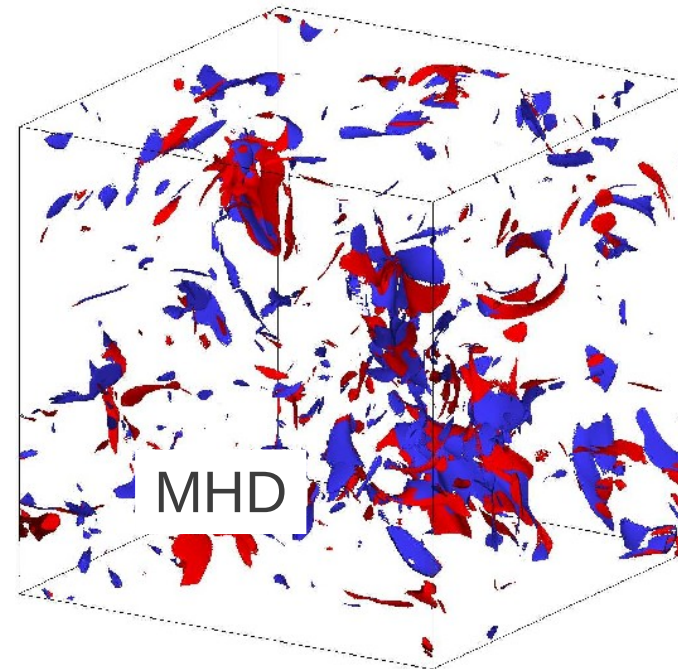
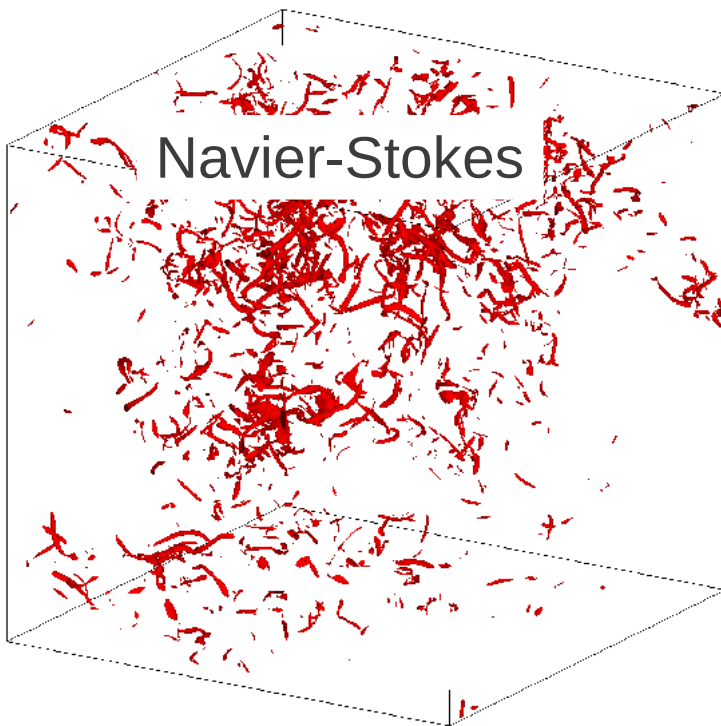


Caution: MHD turbulence is a very complicated state

- non-linear
- high $Re \rightarrow$ many degrees of freedom $\sim Re^{9/4}$
- Proving uniqueness and existence of solution to Navier-Stokes equations \rightarrow 1 million Dollar

Why numerical modeling?

- Access to detailed data
- Focus on idealized situation
- Understanding nature by simplified models
- Supercomputer provide remote laboratory
- might be much cheaper than experiments
- free (peer-reviewed) access to European resources



How to model numerically

- Numerical derivatives
- Fast Fourier Transforms
- Resolution issues: inertial and dissipation range
- Floating point precision
- Parallelization
- What can be done with a supercomputer?

Introduction

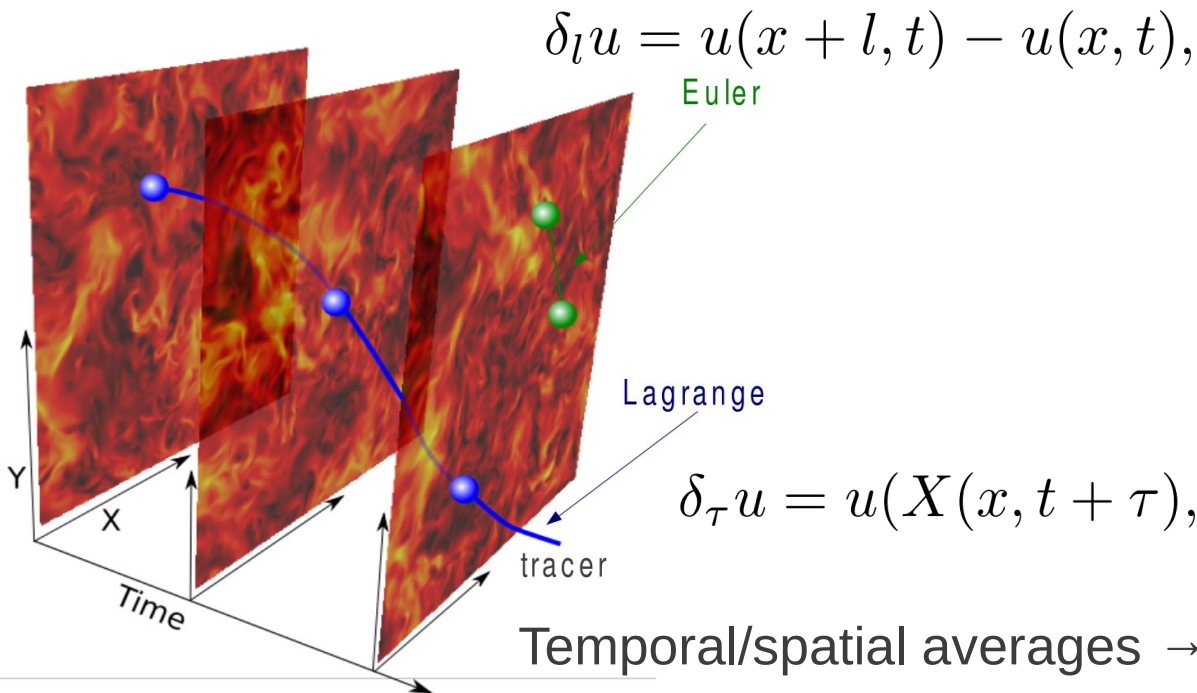
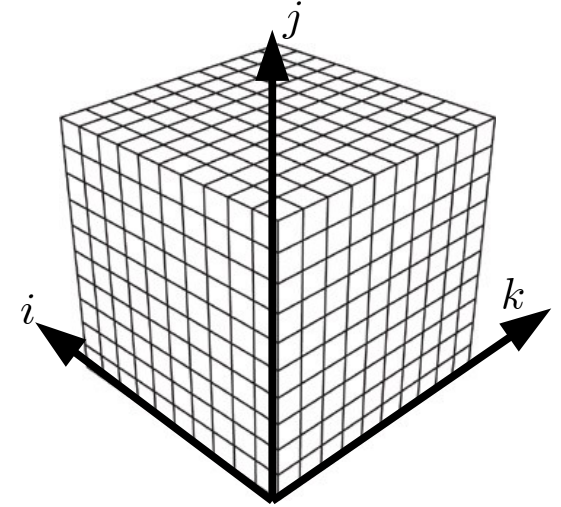
Discretization: $v(x, t) \rightarrow v_{ijk}^n \equiv v(x_i, x_j, x_k, t_n)$

Time integration: $v_{ijk}^{n+1} = F(v_{ijk}^n)$

- Runge-Kutta
- Adams-Bashforth
- Leap-Frog
- ...

Solve accurately the MHD equations!

Here only **uniform** grids:



$$\delta_l u = u(x + l, t) - u(x, t),$$

Euler

Lagrange

$$\delta_\tau u = u(X(x, t + \tau), t + \tau) - u(x, t),$$

Temporal/spatial averages \rightarrow statistical data: $S_p(l) = \langle (\delta_l u)^p \rangle$

Tracer (fluid element) trajectories

$$\frac{d\mathbf{X}(\mathbf{x}, t)}{dt} = \mathbf{v}(\mathbf{X}(\mathbf{x}, t))$$

\mathbf{v} solution of the MHD equations

Numerical derivatives

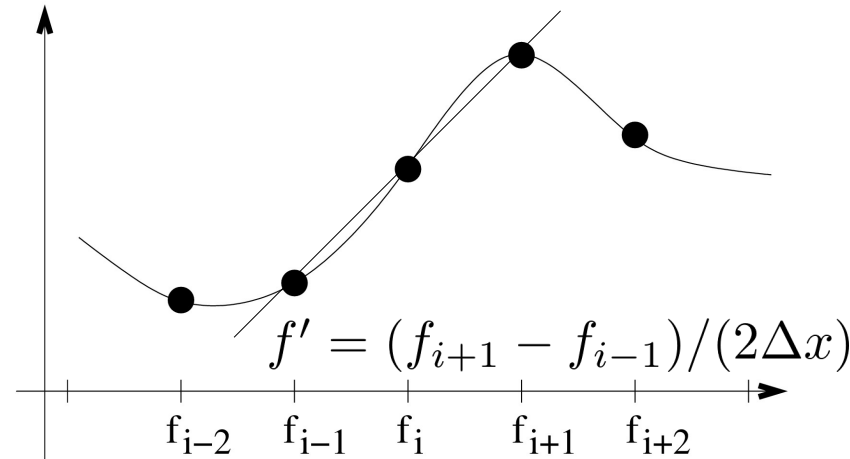
How to approximate a derivative: $f' \equiv \partial_x v$

Finite differences: $f'_i = \sum_{j=-N}^N g_j f_j$

advantages: explicit (high speed)

flexibility: (boundary conditions)

drawbacks: order $p \rightarrow$ stencil has $p+m(-1)$ points
high order \rightarrow high communication



Compact schemes: $\sum_{j=-m}^m h_j f'_j = \sum_{j=-n}^n g_j f_j$

advantages: balance of left and right hand side terms \rightarrow smaller stencil

drawback: implicit \rightarrow more complicated to solve : $m=1 \rightarrow$ tridiagonal matrix

Spectral scheme: $f_K(x) = \sum_{k=-K}^K \widehat{f}_k e^{ikx}$ $f' = \widehat{ik f_K}$

advantages: exponential accuracy: for a periodic $f(x) \in C^m$

$$\|f - f_K\|_{L^p_{(0,2\pi)}} \leq CK^{-m} \|f^{(m)}\|_{L^p_{(0,2\pi)}}.$$

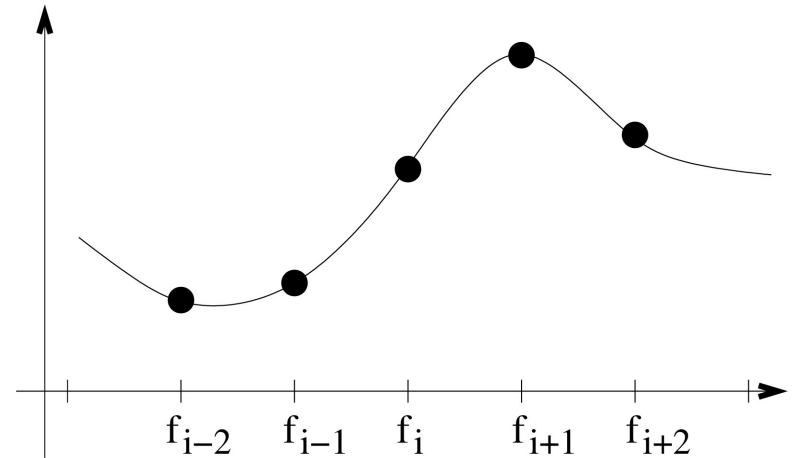
drawbacks: convolutions (N^2 operations) for non-linearities \rightarrow pseudo-spectral with FFTs
problems for discontinues functions
computation of modes $\widehat{f}_K =$ global operation

Fast Fourier Transforms

Quadratic term $f(x) = a(x) \cdot b(x) \hat{=} (v \cdot \nabla v)$

$$\begin{aligned} (\widehat{f(x)})_k &= \int a(x)b(x)e^{ikx} dx \\ &= \int \hat{a}(k - k_1)\hat{b}(k_1)dk_1 \end{aligned}$$

→ N^2 operations → numerically expensive



Speudo-spectral: Derivatives in Fourier-Space, Products in real space
Transformations with Fast Fourier Transformations (FFT)

Idea: Discrete Fourier Transform = sum of 2 transforms of half length

$$\begin{aligned} \hat{f}_k &= \sum_{j=0}^{N/2-1} e^{2\pi ik(2j)/N} f_{2j} + \sum_{j=0}^{N/2-1} e^{2\pi ik(2j+1)/N} f_{2j+1} \\ &= \sum_{j=0}^{N/2-1} e^{2\pi ikj/(N/2)} f_{2j} + W^k \sum_{j=0}^{N/2-1} e^{2\pi ikj/(N/2)} f_{2j+1} = \hat{f}_k^{even} + W^k \hat{f}_k^{odd} \end{aligned}$$

Fast Fourier Transforms (2)

Iterate this decomposition $\log_2 N$ times in even and odd transforms ...

$$\text{Second level: } \hat{f}_k = \hat{f}_k^{ee} + W^k \hat{f}_k^{eo} + W^k \hat{f}_k^{oe} + (W^k)^2 \hat{f}_k^{oo}$$

Number of operations of a FFT: $N \log_2 N$

Why?

- $\log_2 N$ levels
- N operations per level s : $0 \leq k \leq N/2^s - 1$ (period halving)
for the computation of 2^s functions

Resolution issues: inertial range

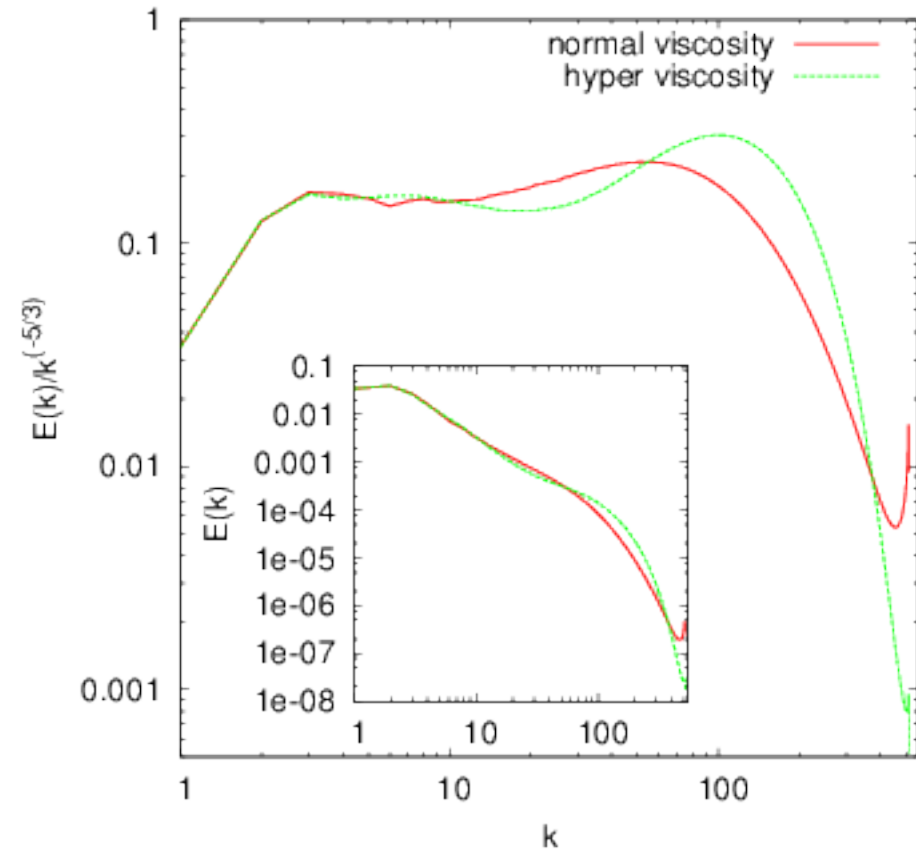
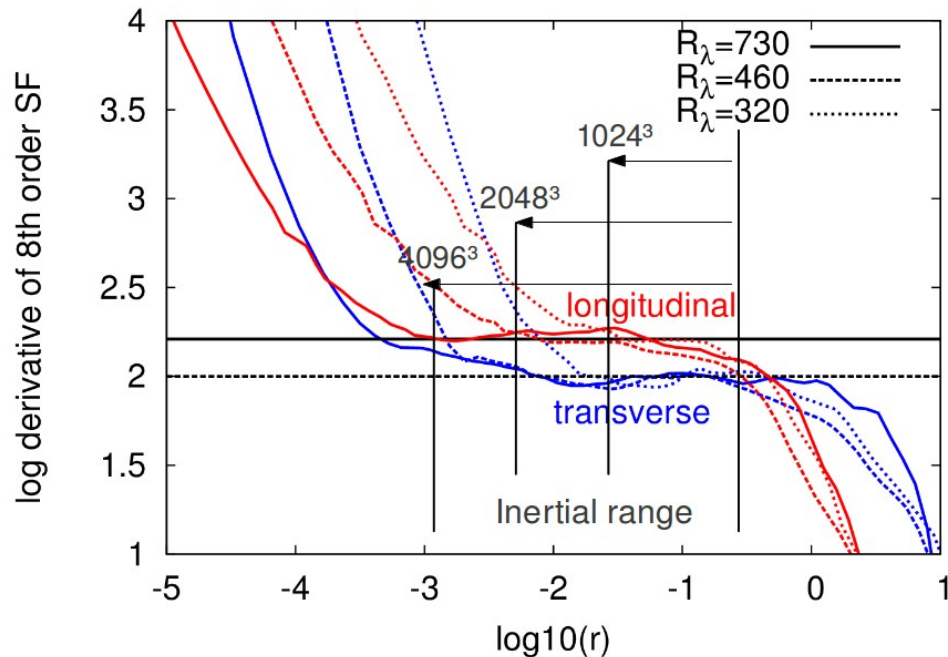
Which resolution of the turbulent flow? A) inertial range statistics

Forcing at large scales fixes L . Variation of ν determines $Re = \frac{L u_{rms}}{\nu}$

Respect $k_{max}\eta \geq 1.5$

Small differences in the scaling behavior of two different types of structure functions

large $Re \rightarrow$ inertial range broadens

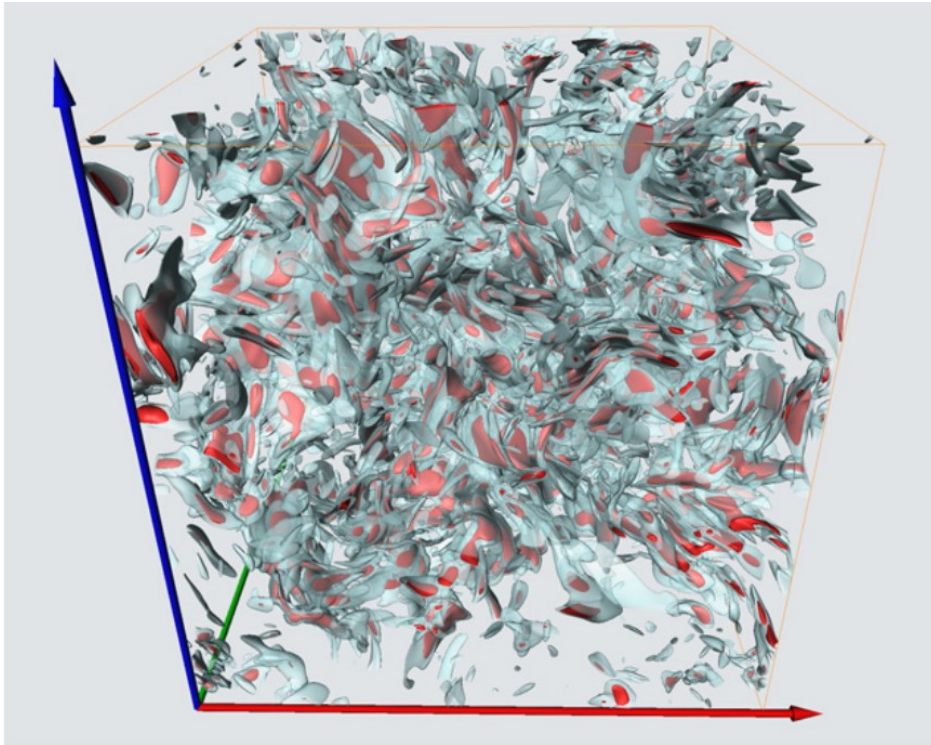


Hyper viscosity: $\Delta u \rightarrow \Delta^2 u$

Resolution issues: dissipation range

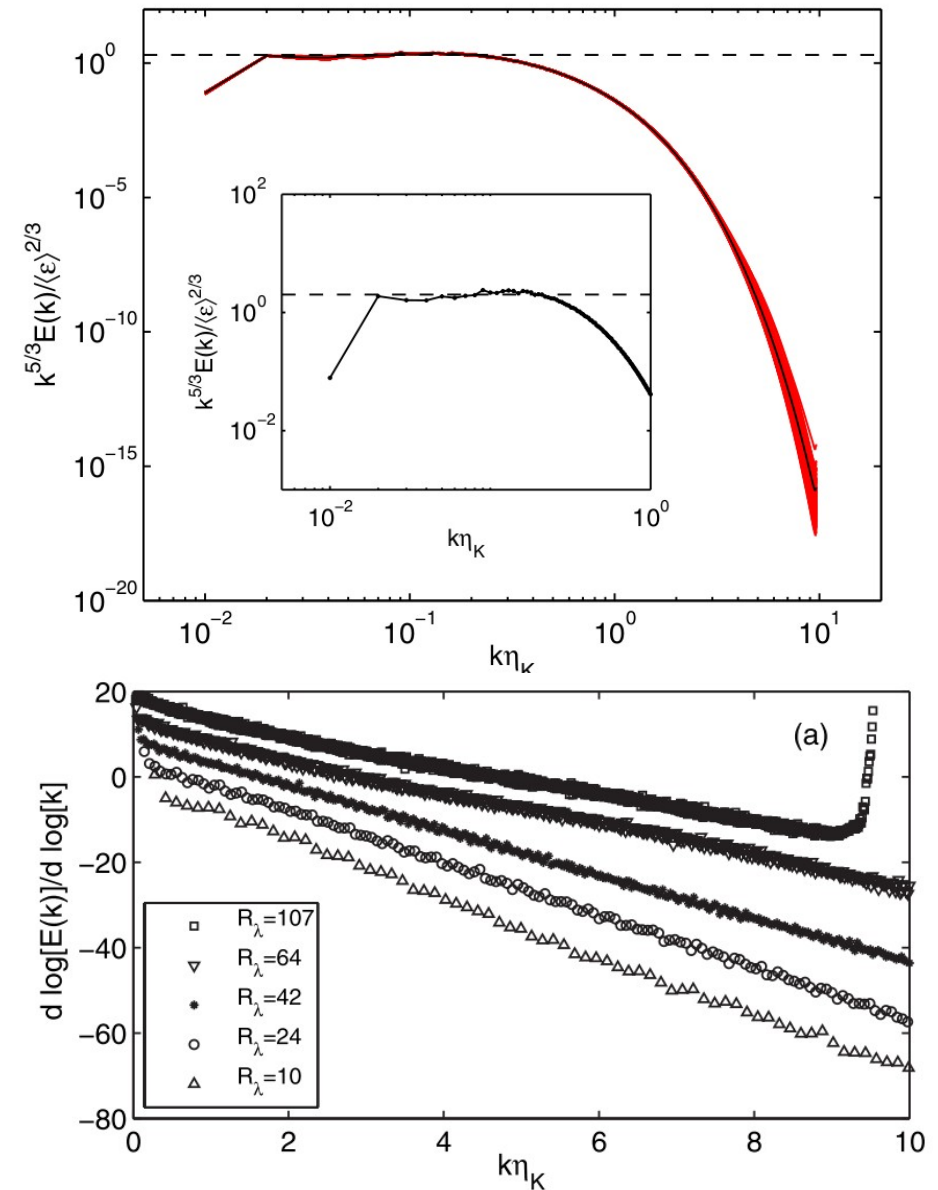
Which resolution of the turbulent flow?

B) dissipation range statistics



$$k_{max}\eta = 10 - 34$$

Schumacher (2007) EPL



Floating point precision

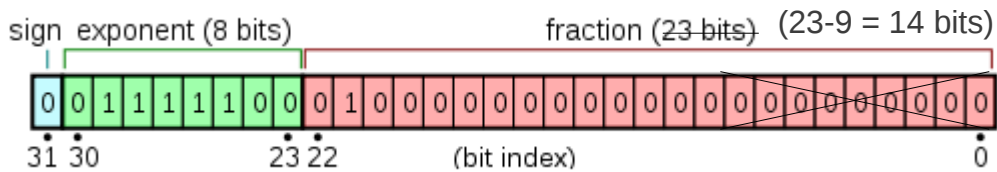
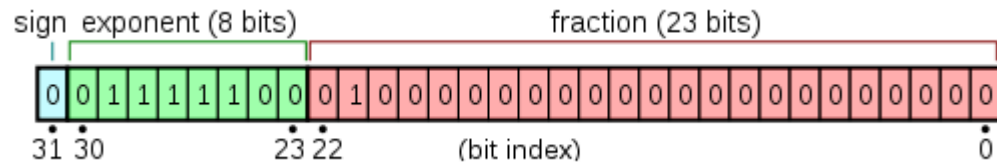
Which floating point precision is needed?

Navier-Stokes simulation with 256^3 grid-points

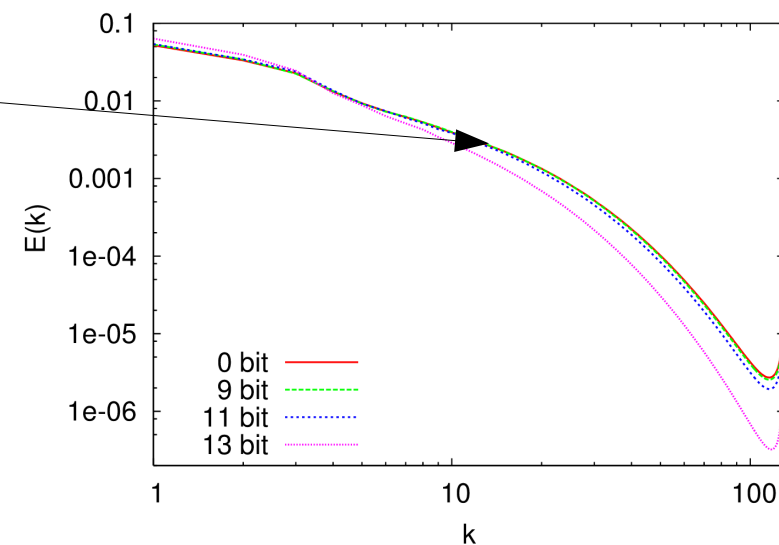
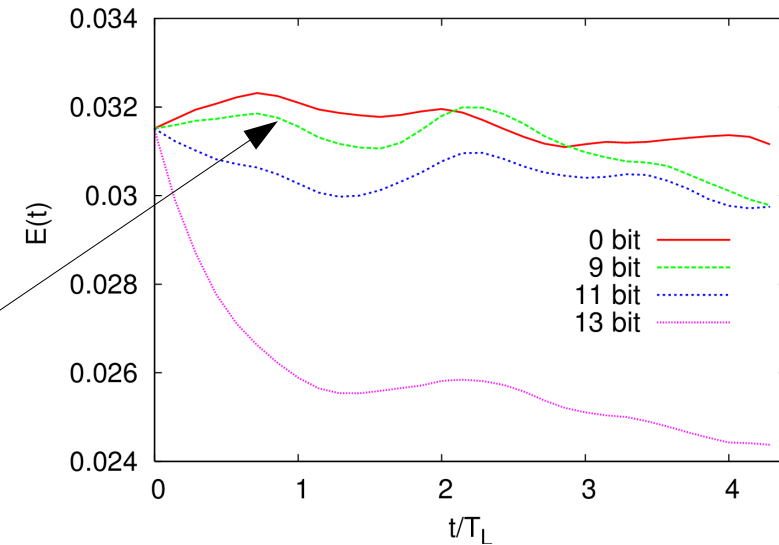
single-precision

$$k_{max}\eta = 1.5$$

artificial noise on n bits



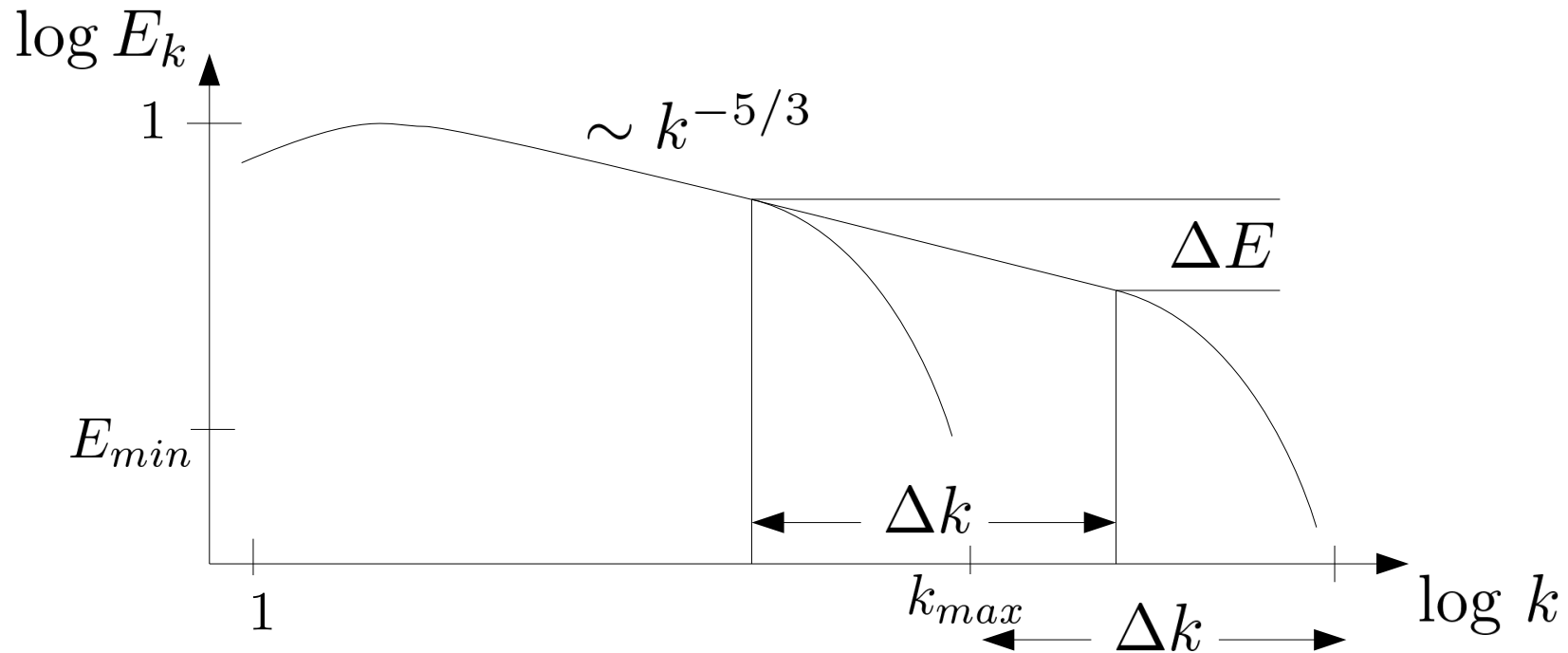
14 bits in fraction are sufficient for 256^3 simulation



Floating point precision (2)

What maximal resolution can be run in single precision?

- 9 bits more → 512 times larger number
- Assume Kolmogorov spectrum $E_k \sim k^{-5/3}$

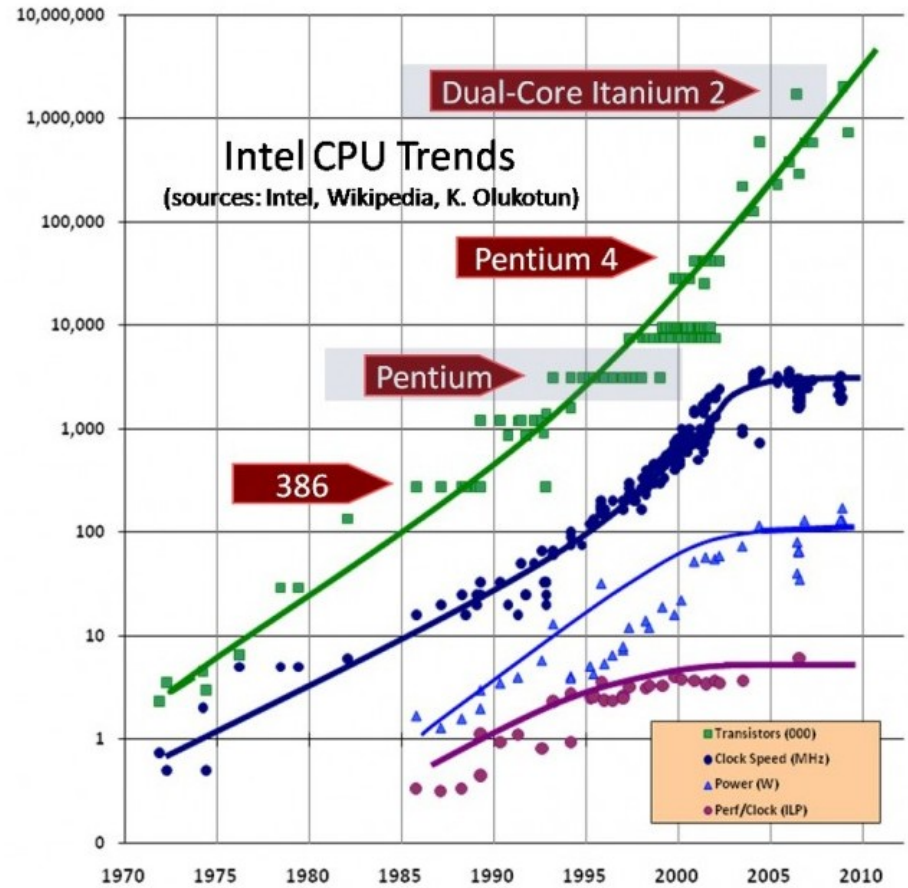
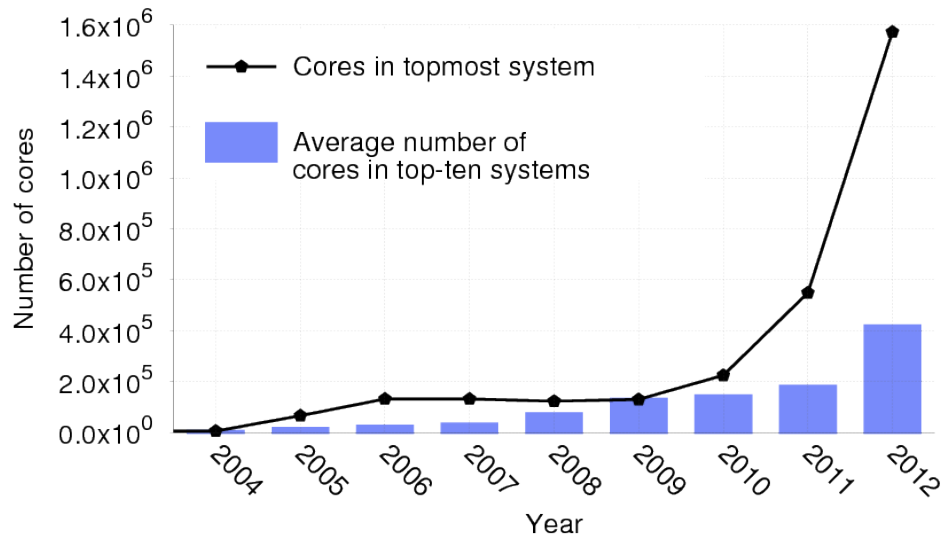
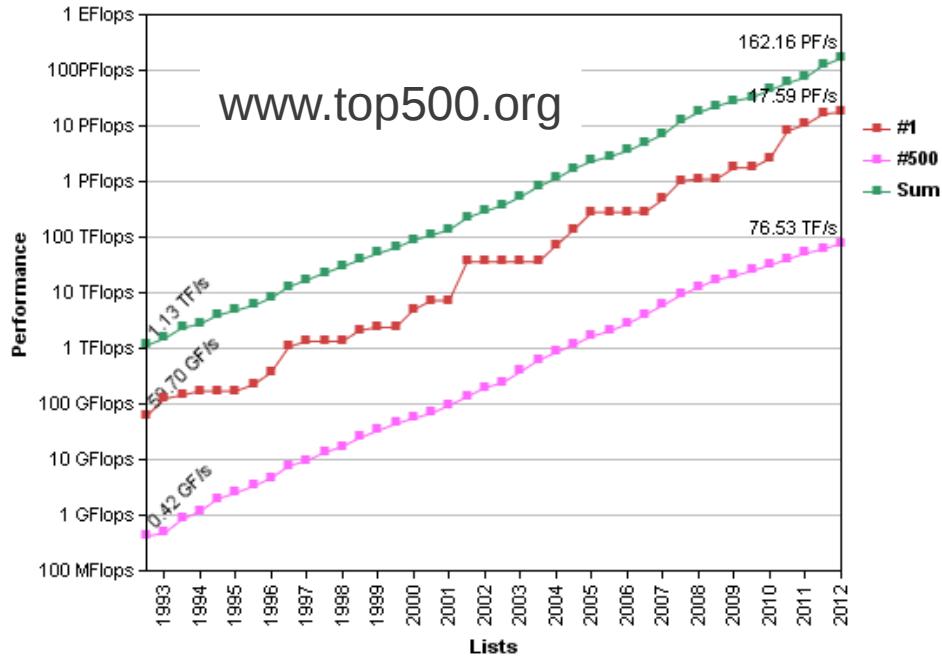


$$\Delta E = 512 = (\Delta k)^{5/3} \quad k_{max} = 256 \Delta k = 256 \cdot 512^{3/5} = 10752$$

8192³ simulations are possible in single precision

Parallelization

Performance Development



At the end ... huge number of standard computing cores connected with a very fast network with an essentially distributed memory

Parallelization (2)

Message Passing Interface (MPI): Data transfer between cores with different ram

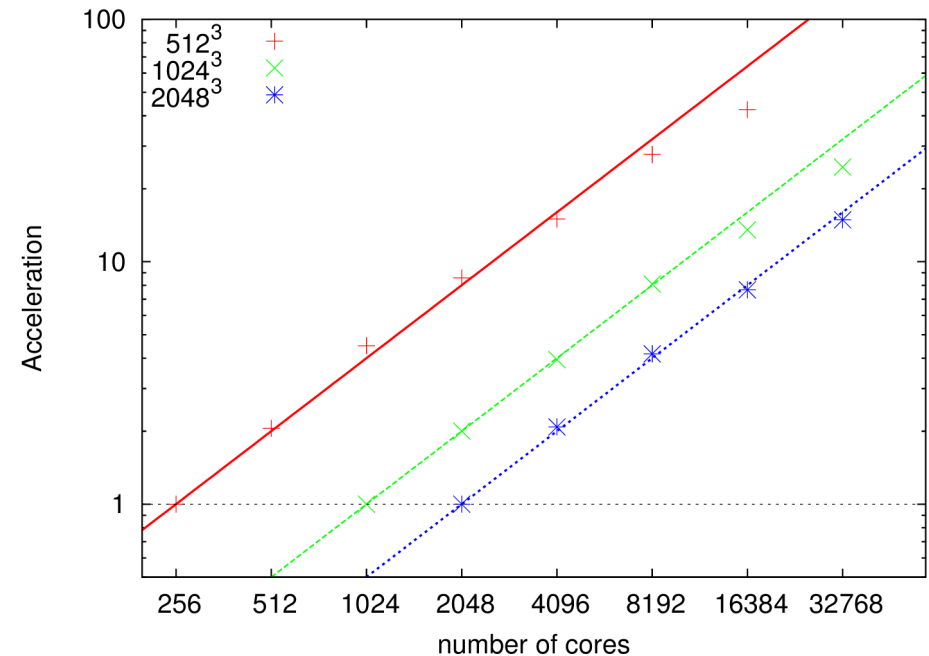
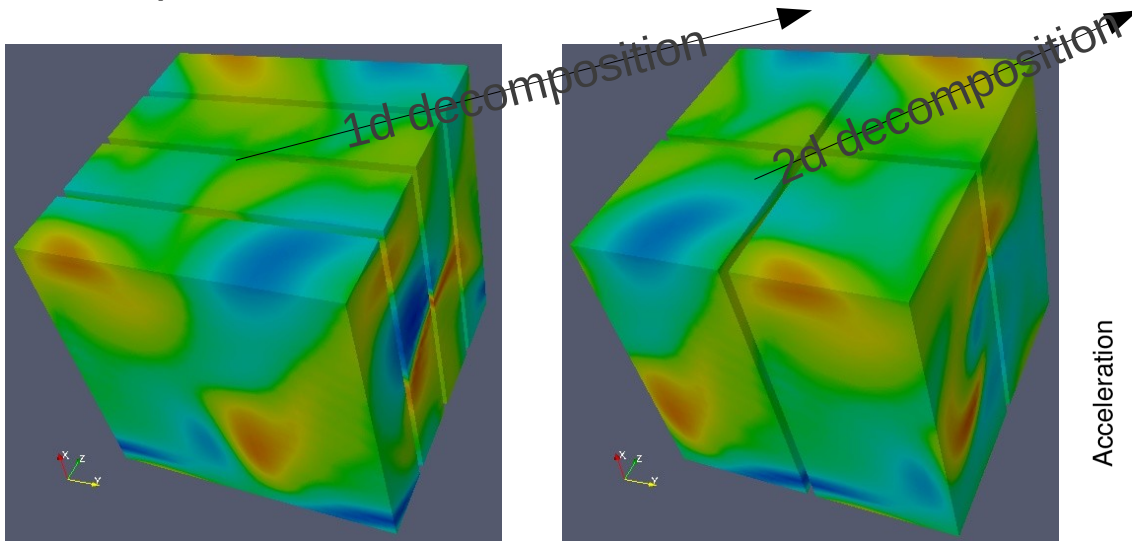
Library with functions:

```
int MPI_Send(void *buf, int count, MPI_Datatype datatype, int dest, int tag, MPI_Comm comm)
int MPI_Recv(void *buf, int count, MPI_Datatype datatype, int source, int tag, MPI_Comm comm, MPI_Status *status)
```

+ the same in non-blocking + global communications such as

```
int MPI_Alltoall(void *sendbuf, int sendcount, MPI_Datatype sendtype, void *recvbuf, int recvcount, MPI_Datatype recvtype,
                MPI_Comm comm)
```

Free parallel FFT libraries such as FFTW and P3DFFT



MPI + OpenMP/Threads (on shared memory)

What is possible

TURING (IDRIS, 31st of TOP500):

BlueGene/Q: 0.84 Pflop, 65 Tbyte RAM, 400 kW energy consumption

Simulation:

4096³ grid-points ($Re \simeq 40000$)

Approx. 8TByte RAM

10 LET = 40 Days = 60 Million CPU h

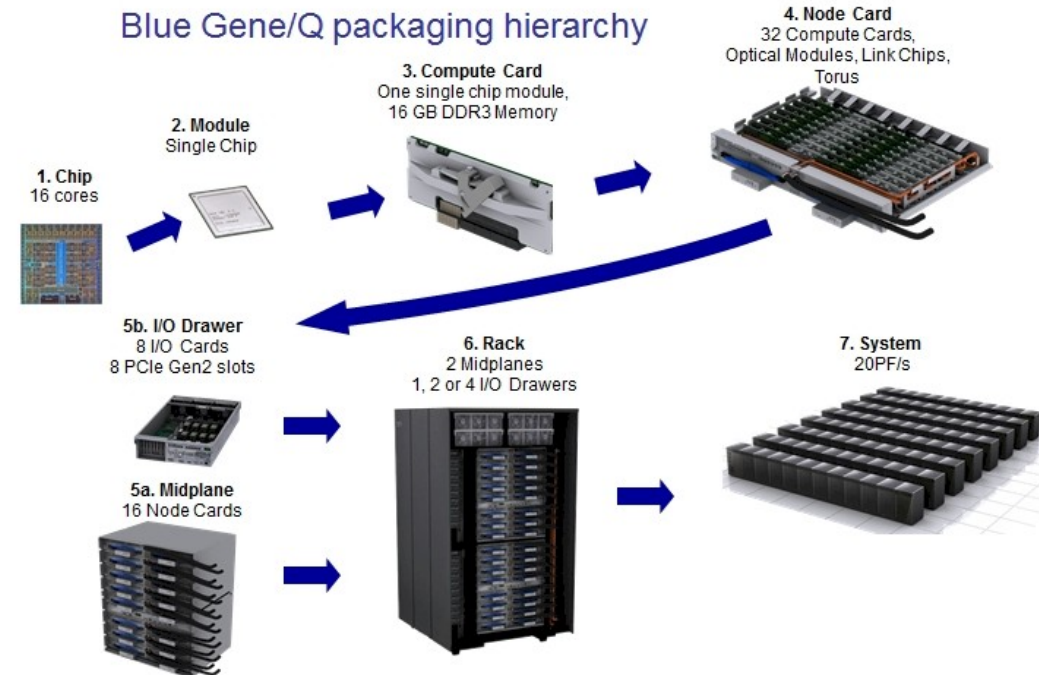
PRACE (Partnership for advanced computing in Europe)

Electricity: 400000 kWh = 45 k euros (if 1kWh = 0.11 cents as in France, else ...)

BlueGene/Q is the most efficient Supercomputer: 2GFlop/W (Green500)



TURING (IDRIS) 65536 cores



Discontinuities

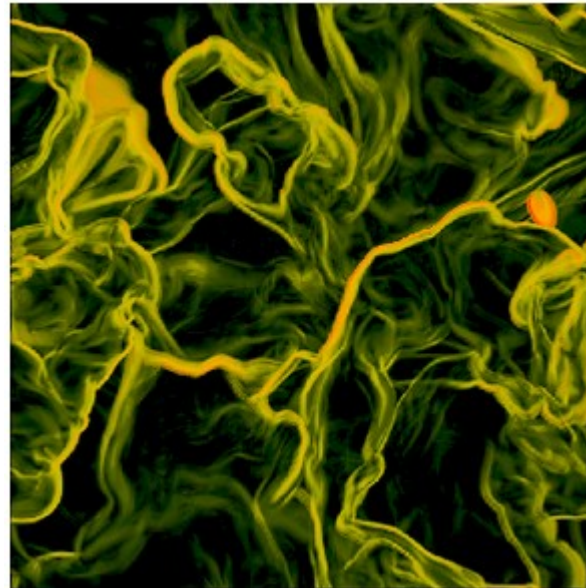
Incompressible Navier-Stokes: $\Delta \mathbf{v} \rightarrow$ smooth solution

Highly compressible Flows \rightarrow shocks = discontinuities \rightarrow Gibbs oscillations

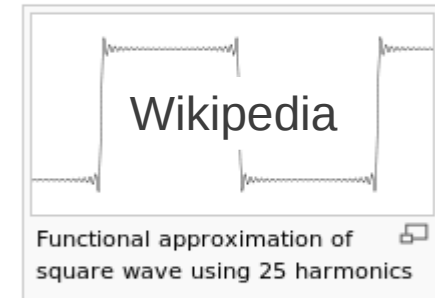
Finite volume scheme

Central Weighted Essentially
Non-Oscillatory scheme

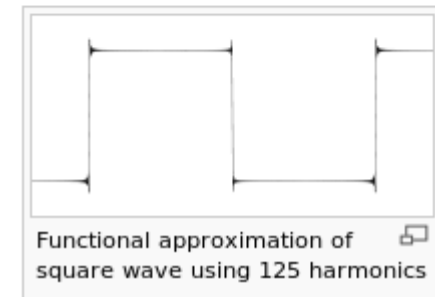
Beetz, Schwarz et al. (2008) Phys. Lett. A



Functional approximation of square wave using 5 harmonics



Functional approximation of square wave using 25 harmonics

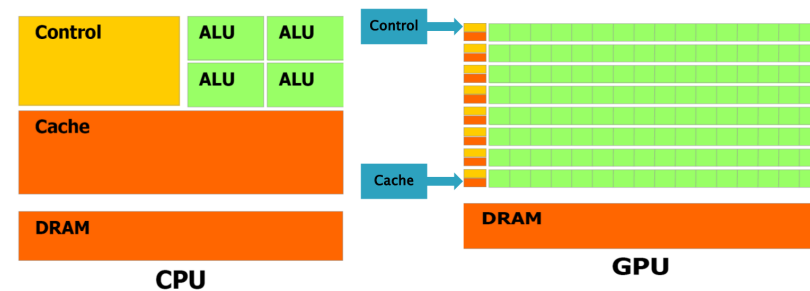


Functional approximation of square wave using 125 harmonics

New trends: Graphic cards (CUDA, OpenCL)

- 2688 simple cores arranged in multiprocessors
- small cache per multiprocessor
- big (6TByte) global memory

very fast multiprocessors slow memory bandwidth



APPLICATIONS

- Universality
- Planet formation
- Turbulent dynamo
- Transport of tracers and Impurities

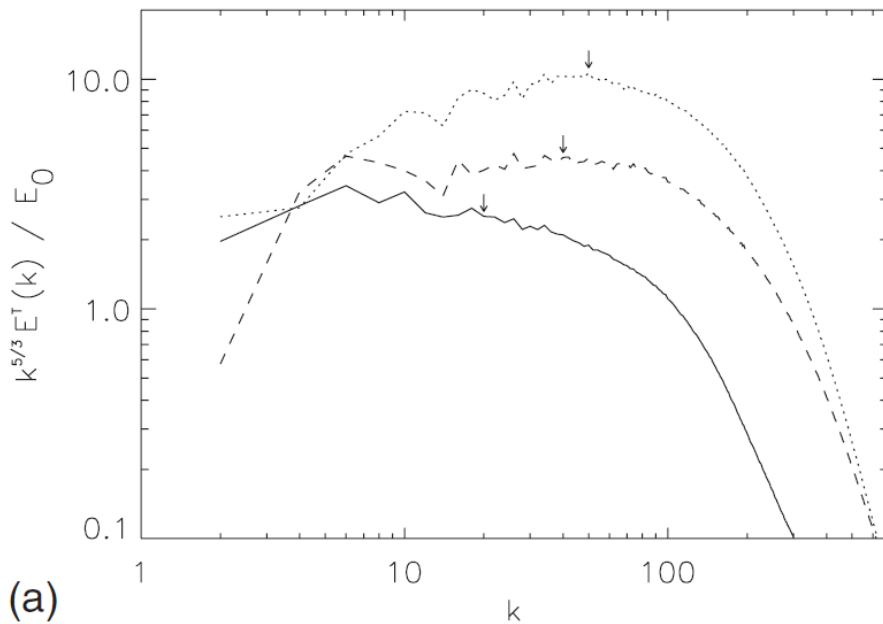
Universality

Problem: Are scaling laws universal ?

Spseudo-spectral simulations of decaying MHD turbulence

Different initial conditions

Energy spectra:

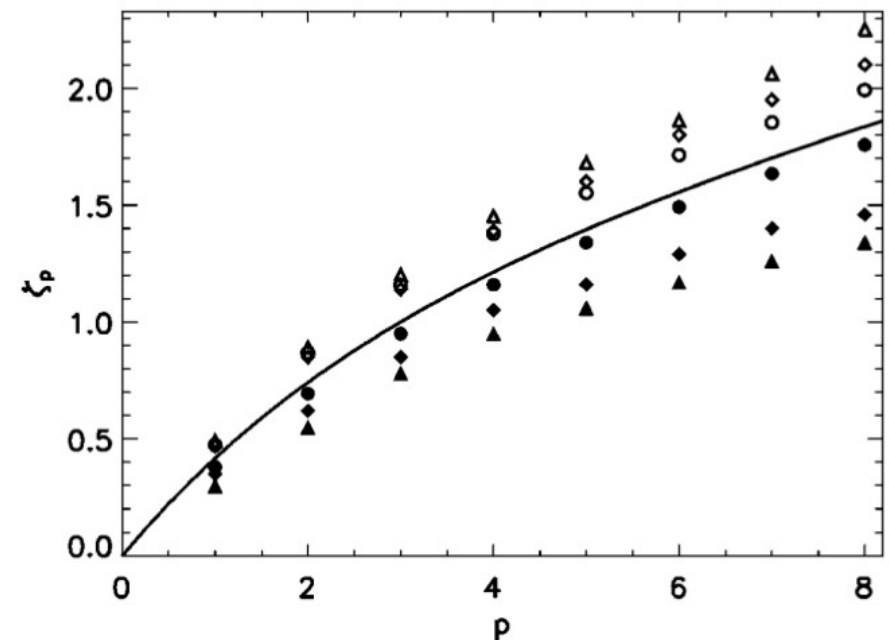


Lee, Brachet et al. (2012) PRE

Different mean magnetic fields

$$S_p(l) = \langle (\delta z_l)^p \rangle \sim l^{\zeta_p}$$

$$z^\pm = v \pm B$$

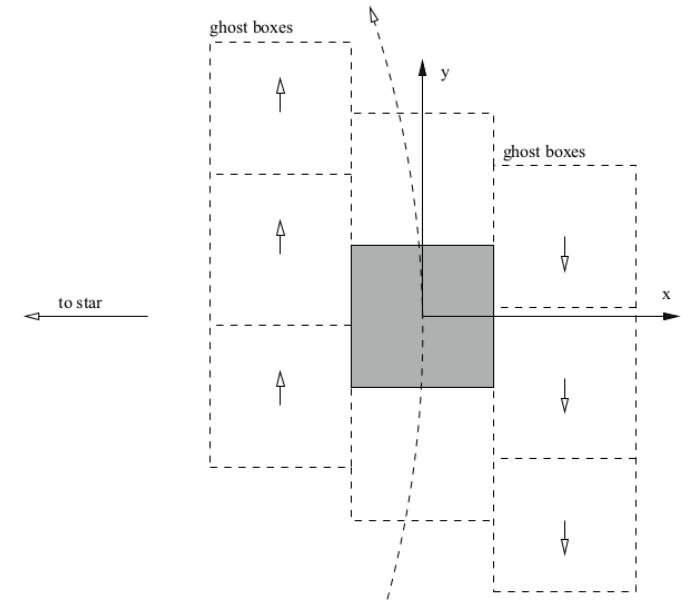


Müller, Biskamp et al. (2003) Phy. Rev. E

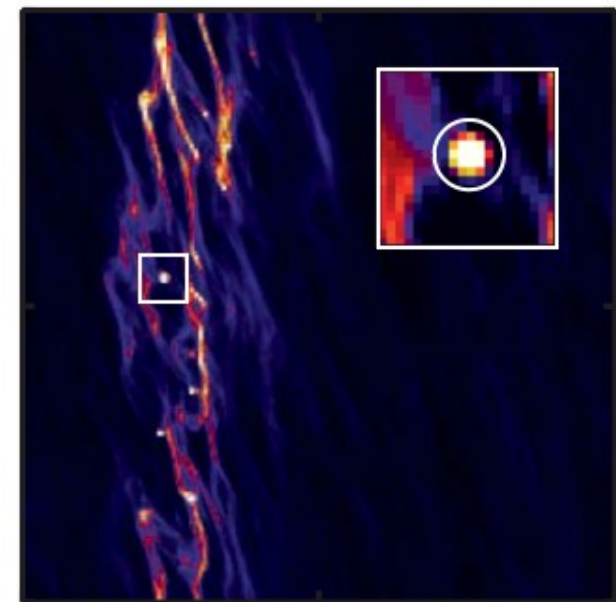
Planet formation

Problem: How to grow m-size boulders to km-size planetisimals?

- DNS of MHD shearing box
- Heavy particles
- 2-way coupling
- High order finite differences
(pencil code, <http://www.nordita.org/pencil-code/>)



- Particles concentrate in high-pressure regions
- Acceleration of gravitational collapse
- Accelerated boulder growth



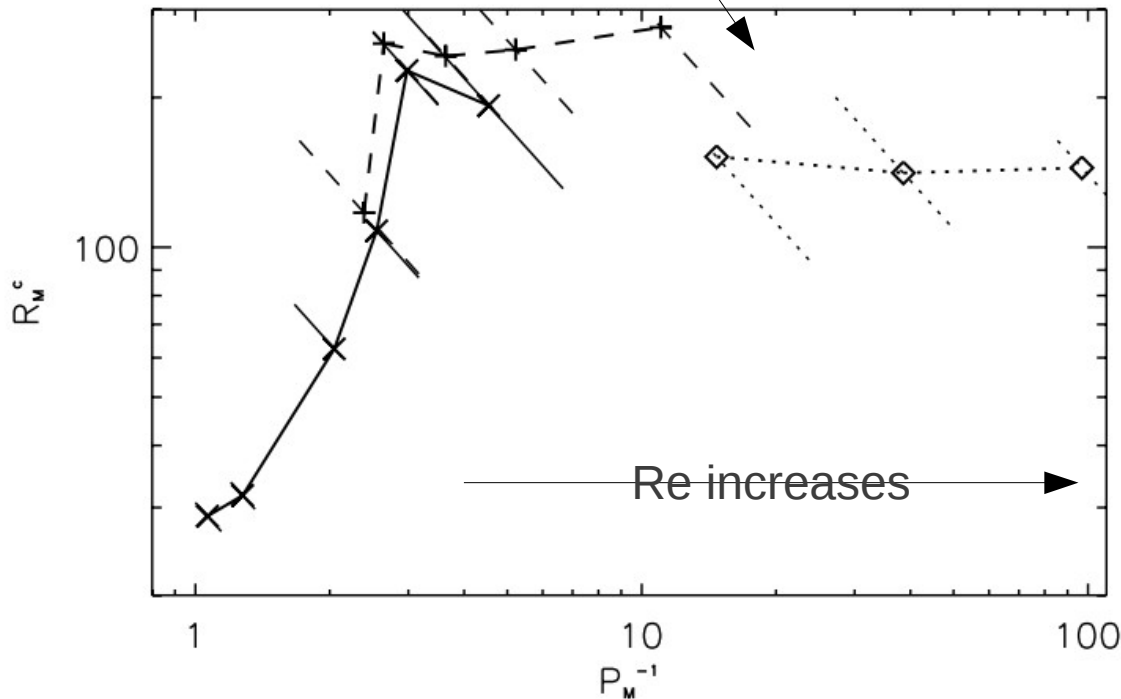
Johansen, Oishi et al. (2007) Nature
Johansen, Klahr et al. (2011) A&A

Turbulent dynamo

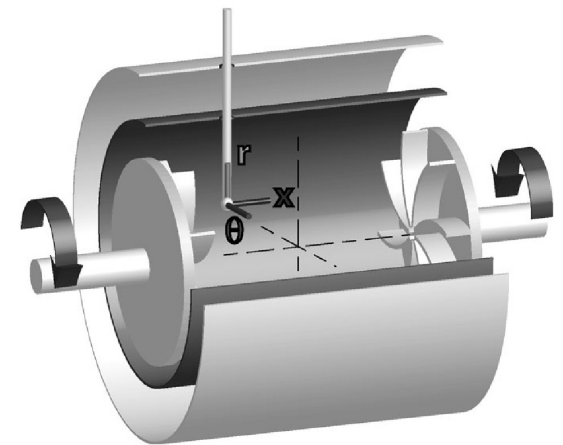
Problem: How does the dynamo onset scale with the Reynolds number?

- DNS of MHD flow in periodic box with Taylor Green forcing
- First, onset increases with Re
- Later, onset saturates

$$\mathbf{F} = F_0 \begin{pmatrix} \sin(k_0 x) \cos(k_0 y) \cos(k_0 z) \\ -\cos(k_0 x) \sin(k_0 y) \cos(k_0 z) \\ 0 \end{pmatrix}$$



VKS experiment

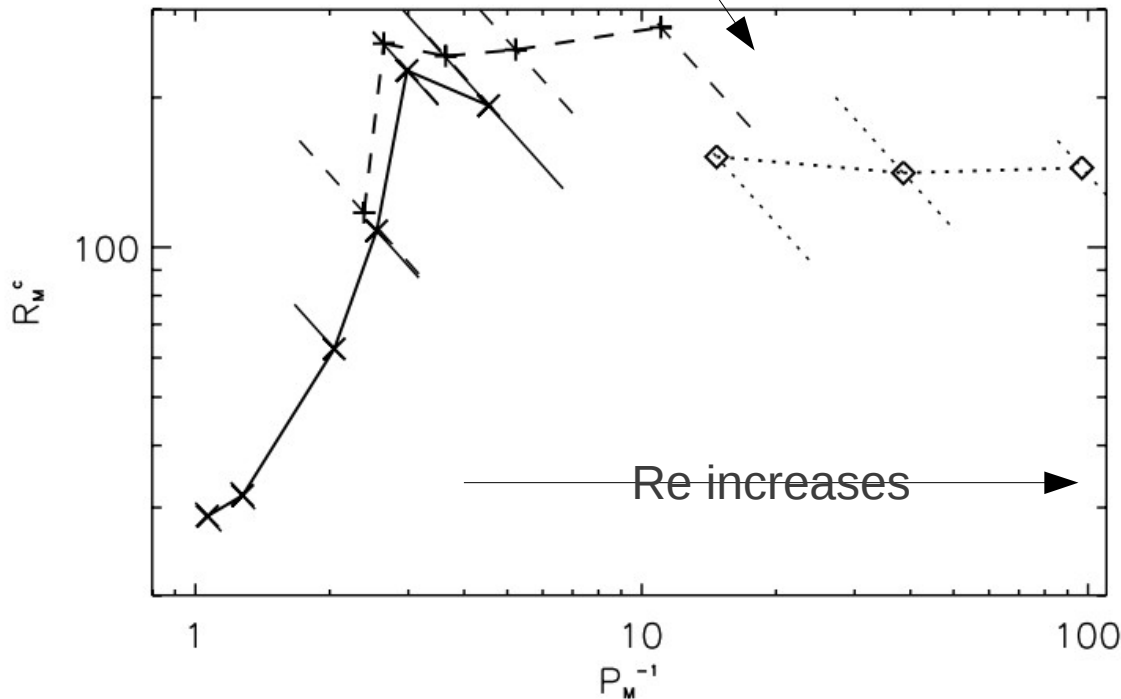


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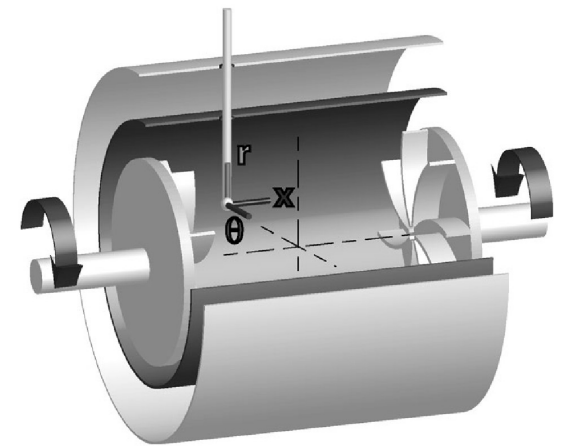
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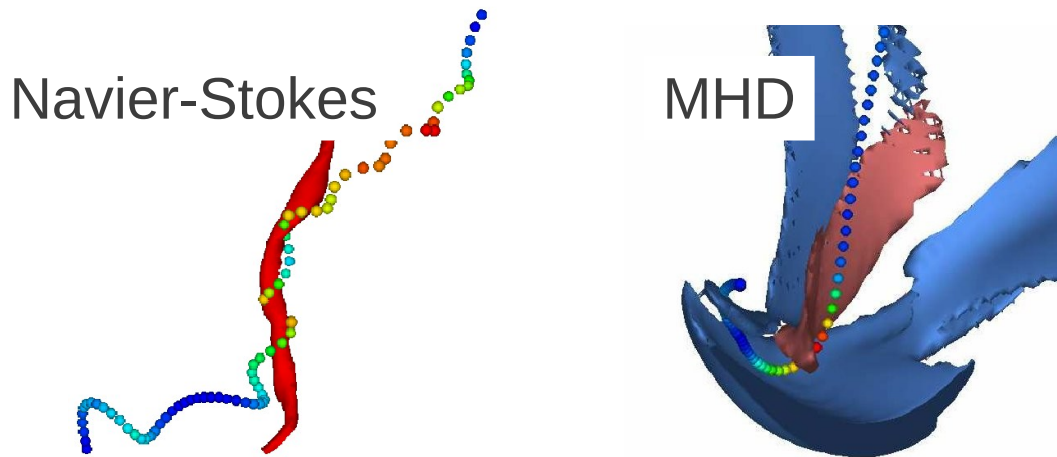


VKS experiment

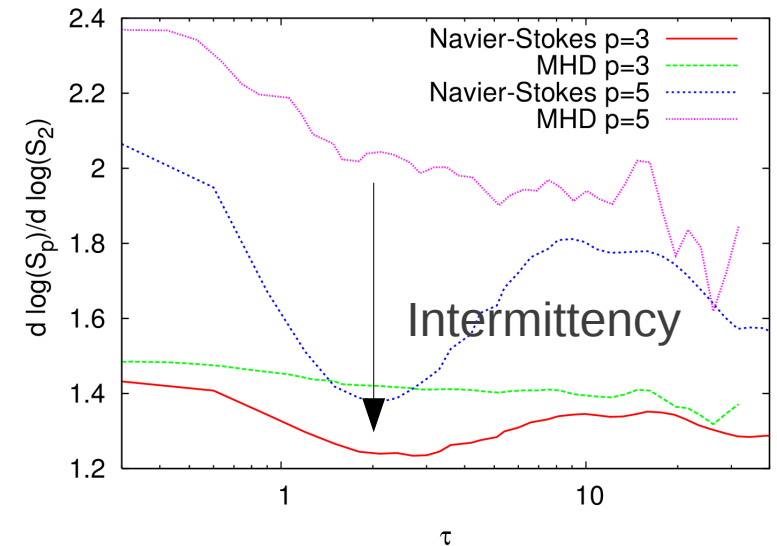


Transport of tracers

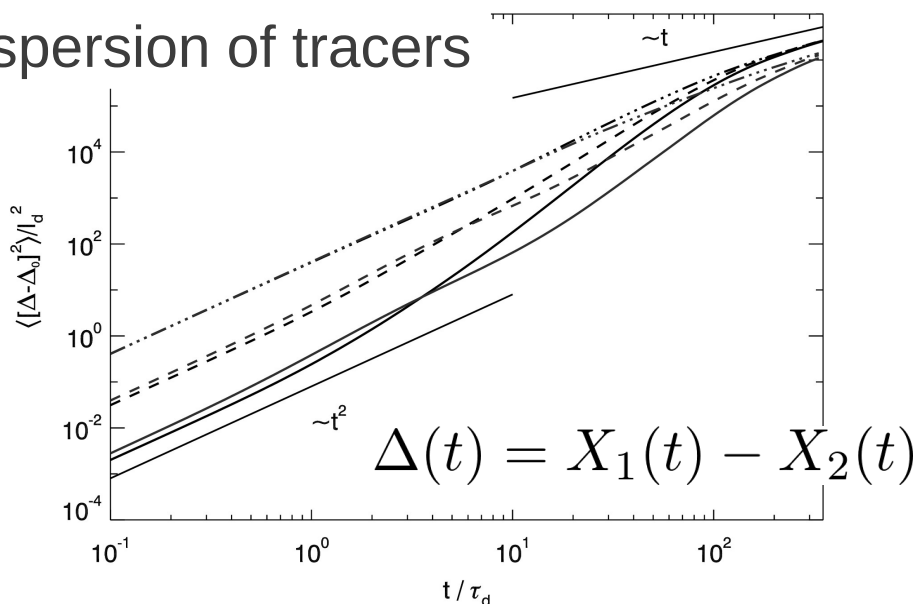
Problem: Statistical properties of fluid element trajectories



$$S_p(\tau) = \langle (\delta_\tau u)^p \rangle$$



Dispersion of tracers



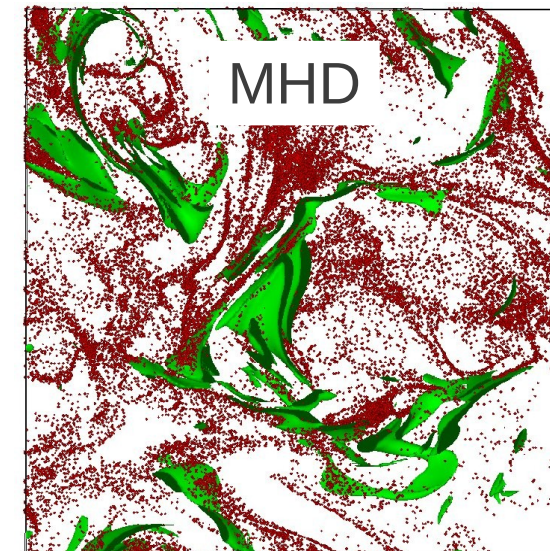
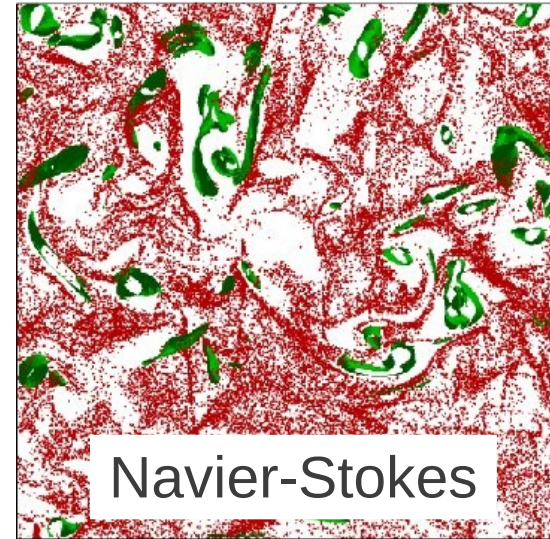
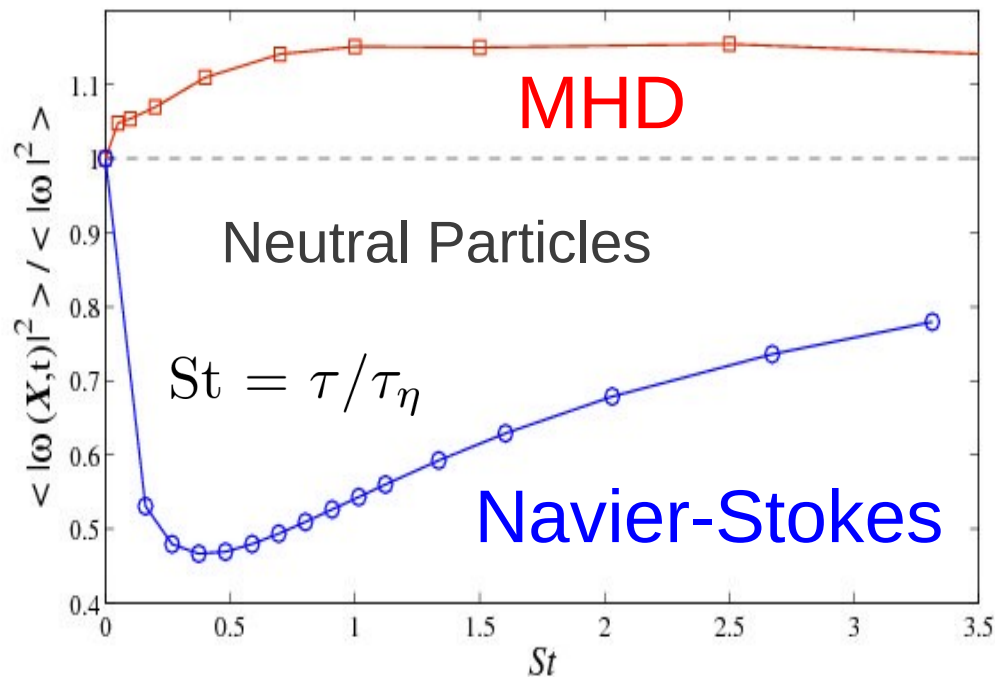
- MHD velocity increments are less intermittent than Navier-Stokes ones
- Accelerated (Richardson) MHD dispersion is delayed due to alignment to mean magnetic field
- B-transverse dispersion is reduced

Transport of impurities

Problem: Where do inertial particles go in MHD turbulence?

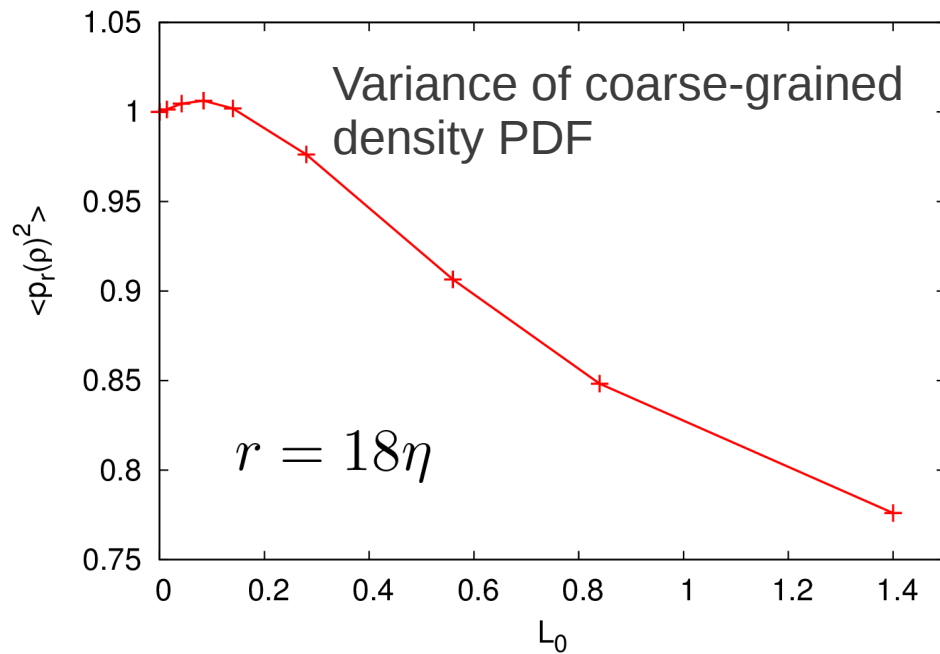
$$\ddot{X} = \underbrace{\frac{1}{\tau} [u(X, t) - \dot{X}]}_{\text{viscous drag}} + \underbrace{\frac{1}{\ell} [E(X, t) + \dot{X} \times B(X, t)]}_{\text{Lorentz force}},$$

$\tau = 2\rho_p a^2 / (9\rho_f \nu)$: particle response time a : radius
 $\ell = \rho_p c / (\rho_c \sqrt{4\pi\rho_f})$: length-scale



Transport of charged impurities

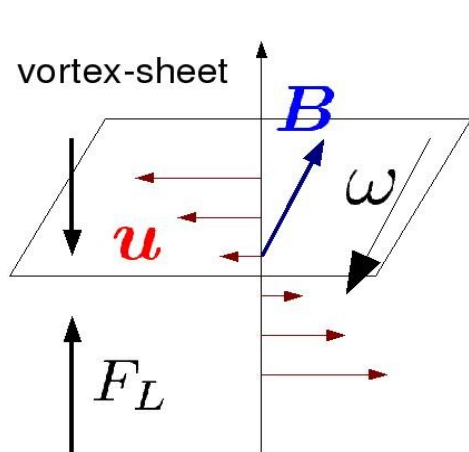
Clustering of charged particles $b > 0$



Lorentz-number

$$Lo = \tau B_{\text{rms}}/\ell$$

Effect of Lorentz-force with respect to inertial drag



Vortex-sheet selection

$\boldsymbol{\omega} \cdot \mathbf{B} < 0$: attractive sheet

$\boldsymbol{\omega} \cdot \mathbf{B} > 0$: repulsive sheet

