On the modelling of sub-grid scale physics in under-resolved gyrokinetic simulations

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GYROKINETICS FOR ITER

Why under-resolved simulations? (I)

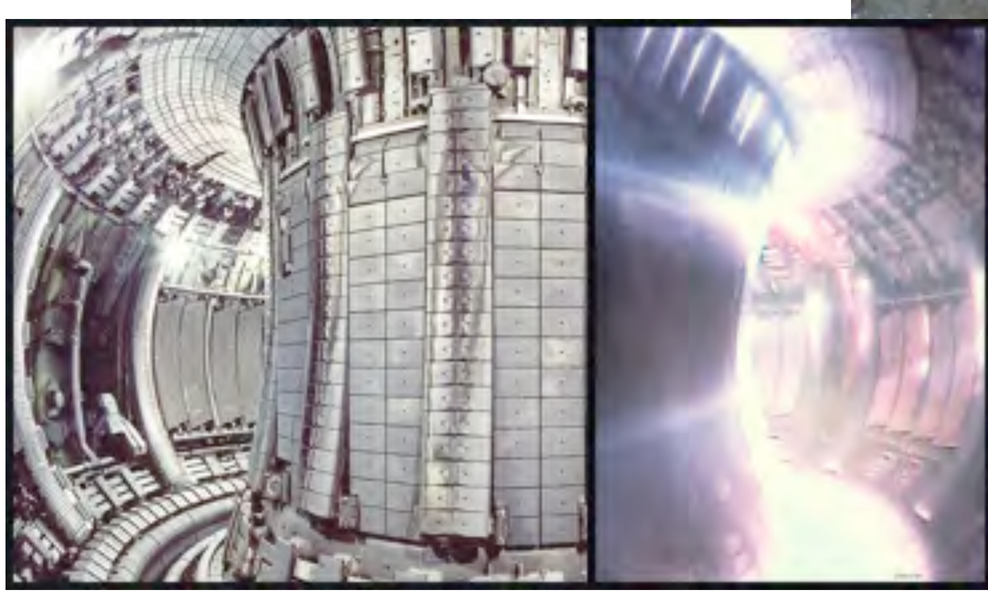
In many complex systems, simulating the entire dynamics is definitively out of reach of today's computers...

- Geophysics: dynamics of the atmosphere and of the oceans.

- Astrophysics: evolution of stars, galaxies...

- Aeronautics: airplane...

- Tokamak physics.



Why under-resolved simulations? (II)

Various options are possible instead of solving the full set of first-principle equations for the complete problem:

- simulate a simplified model (transport code);

- simulate simpler problems (slab geometry, collisionless limit, ...);

- simulate only a sub-domain (core plasma simulations without plasma-wall interaction, ...).

The examples are taken from tokamak physics, but similar approaches have been developed in the simulation of geophysical, astrophysical, biological, industrial,... problems.

Another option has also been considered, mainly in the simulation of turbulence in fluids:

- under-resolved simulations of the first-principle equation, i.e. solve the real problem on a coarse grid.

In fluid turbulence, this approach is usually referred to as **Large-Eddy Simulation (LES)**

LES for fluid turbulence (I)

The Navier-Stokes equation is a first principle equation (Newton law expressed for continuous media), that describes the conservation of momentum:

$$\partial_t u_i + u_j \partial_j u_i = -\partial_i (p/\rho) + \nu \partial_j \partial_j u_i$$

The Reynolds number is defined by: $$R_e = \frac{U\,L}{\nu}$$

U and L are respectively a characteristic velocity and a characteristic length of the flow and ν is the viscosity of the fluid.

Simulating the complete dynamics of a turbulent flows requires huge grids and very long simulations (number of grid points ~ $R_e^{9/4}$, number of time steps ~ $R_e^{3/4}$).

This has prompted the development of LES for which the direct numerical computation is limited to the largest scales of turbulence (*under-resolved simulations*) while a model is added to account for the effects of the small-scale motions.

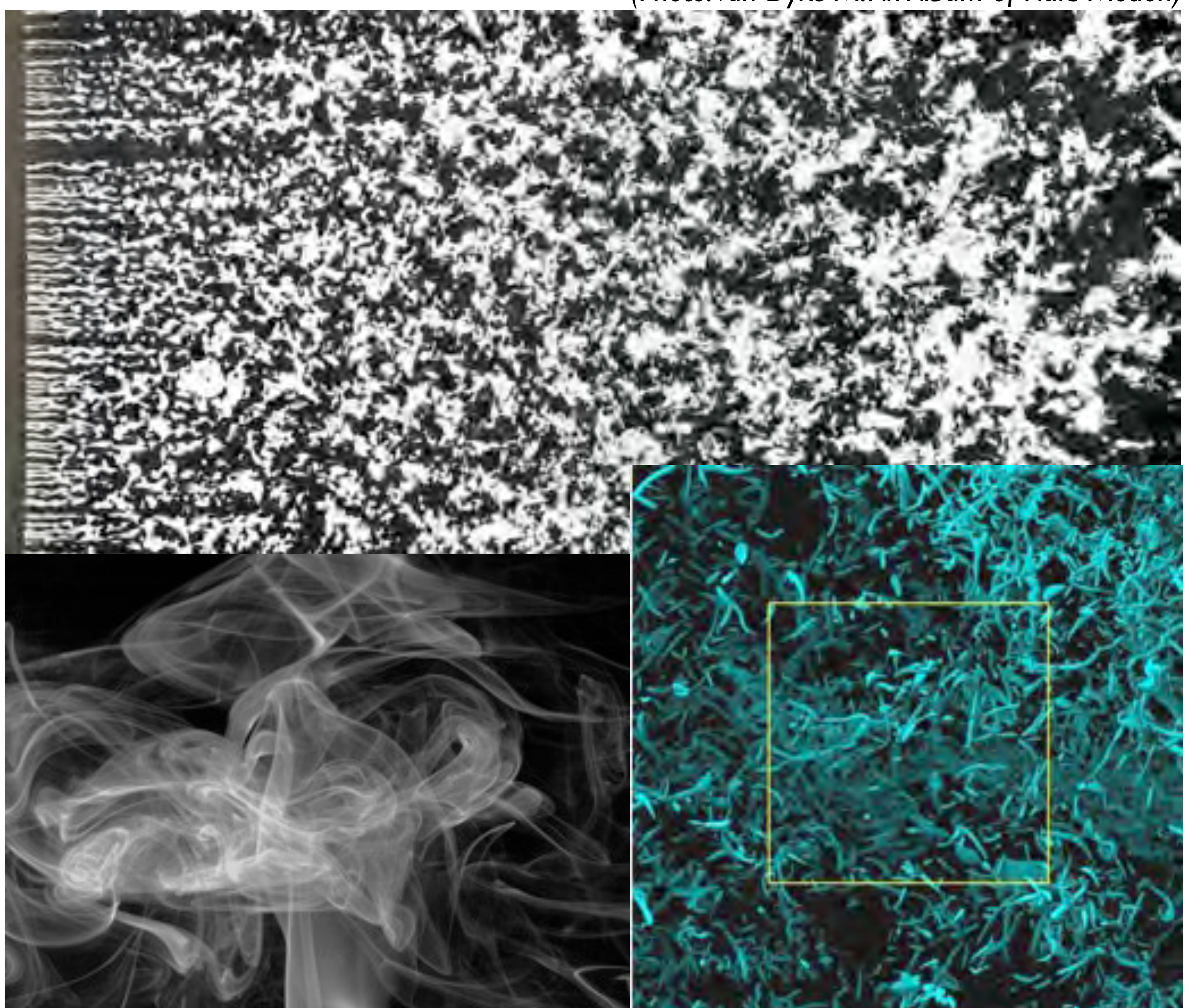
U. Frisch. *Turbulence: The Legacy of A. N. Kolmogorov*. Cambridge University Press, 1995

LES for fluid turbulence (II)

The development of LES is ***not*** justified by the existence of a scale separation between "large eddies" and "small scales structures".

The coexistence of structures with various characteristic lengths is indeed ubiquitous in fluid turbulence.

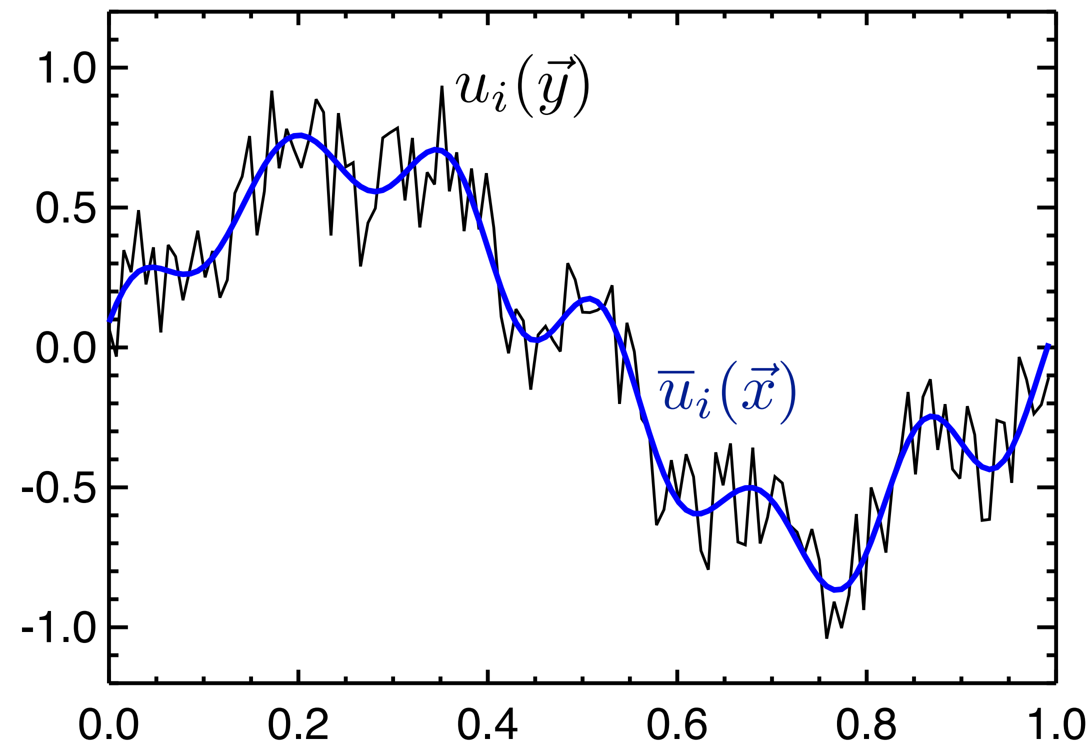
(Photo: Van Dyke M. An Album of Fluid Motion)



Y. Kaneda, University of Nagoya

LES are rather based on an artificial scale separation mainly driven by computer limitations.

The scale separation is introduced by a filtering operator that smoothes out all the scales smaller than a given $\overline{\Delta}$.



$$\overline{u}_i(\vec{x}) = \int d\vec{y}\; G(\vec{x}-\vec{y};\overline{\Delta})\, u_i(\vec{y})$$

LES for fluid turbulence (III)

The LES equation (filtered Navier-Stokes equation) reads:

$$\partial_t \overline{u}_i + \overline{u}_j \partial_j \overline{u}_i = -\partial_i (\overline{p}/\rho) + \nu \partial_j \partial_j \overline{u}_i - \partial_j \tau_{ij}$$

The sub-grid scale stress tensor represents the effect of the under-resolved (small) scales on the resolved (large) scales:

$$\tau_{ij} = \overline{u_i \, u_j} - \overline{u}_i \, \overline{u}_j$$

This sub-grid scale stress tensor is not expressed in terms of the resolved velocity field only and must be modelled!

R.S. Rogallo and P. Moin, *Numerical simulation of turbulent flows*, Annu. Rev. Fluid Mech. (1984)

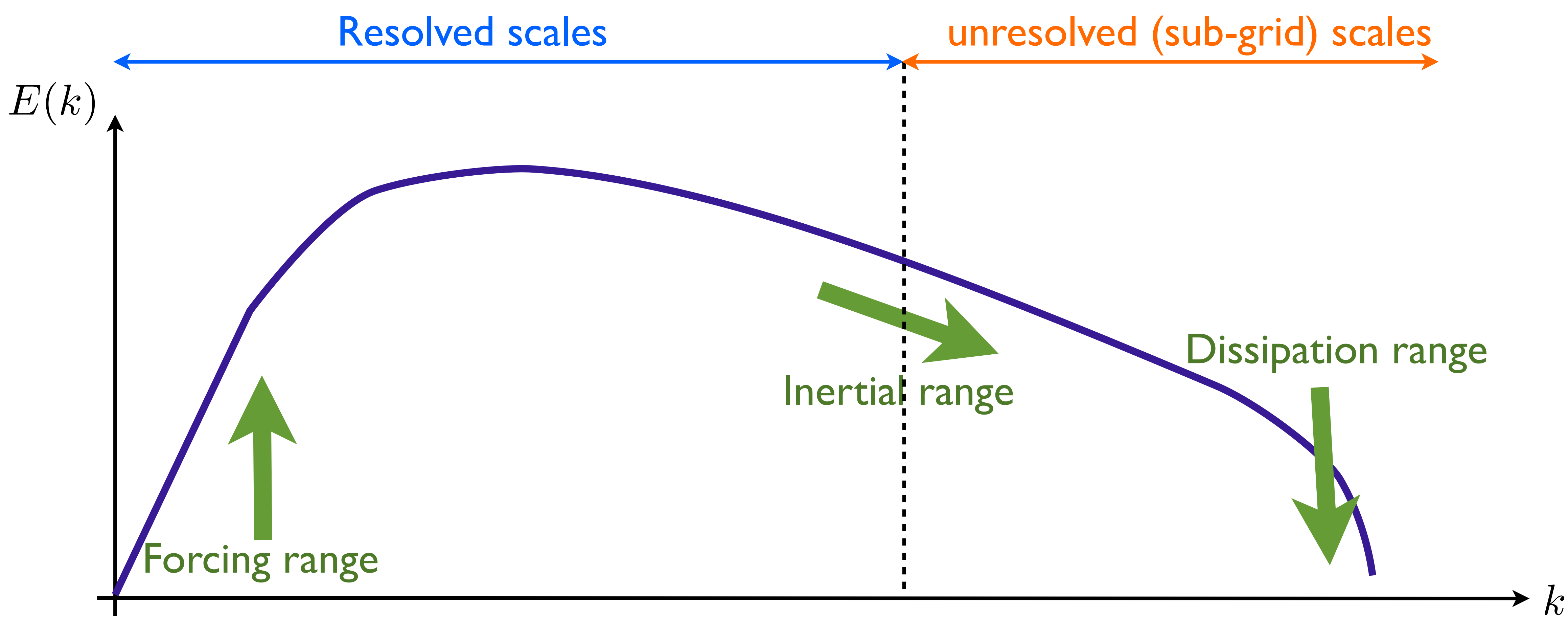
P. Sagaut. *Large Eddy Simulation for Incompressible Flows*. Springer (2001).

...

Subgrid-scale physics? (I)

In fluid turbulence, the kinetic energy in usually injected in the largest scales (mechanical forcing) and dissipated into heat in the smallest scales (viscous effects).

For high Reynolds numbers, the forcing range and the dissipation range are well separated by an inertial range dominated by the nonlinear dynamics.



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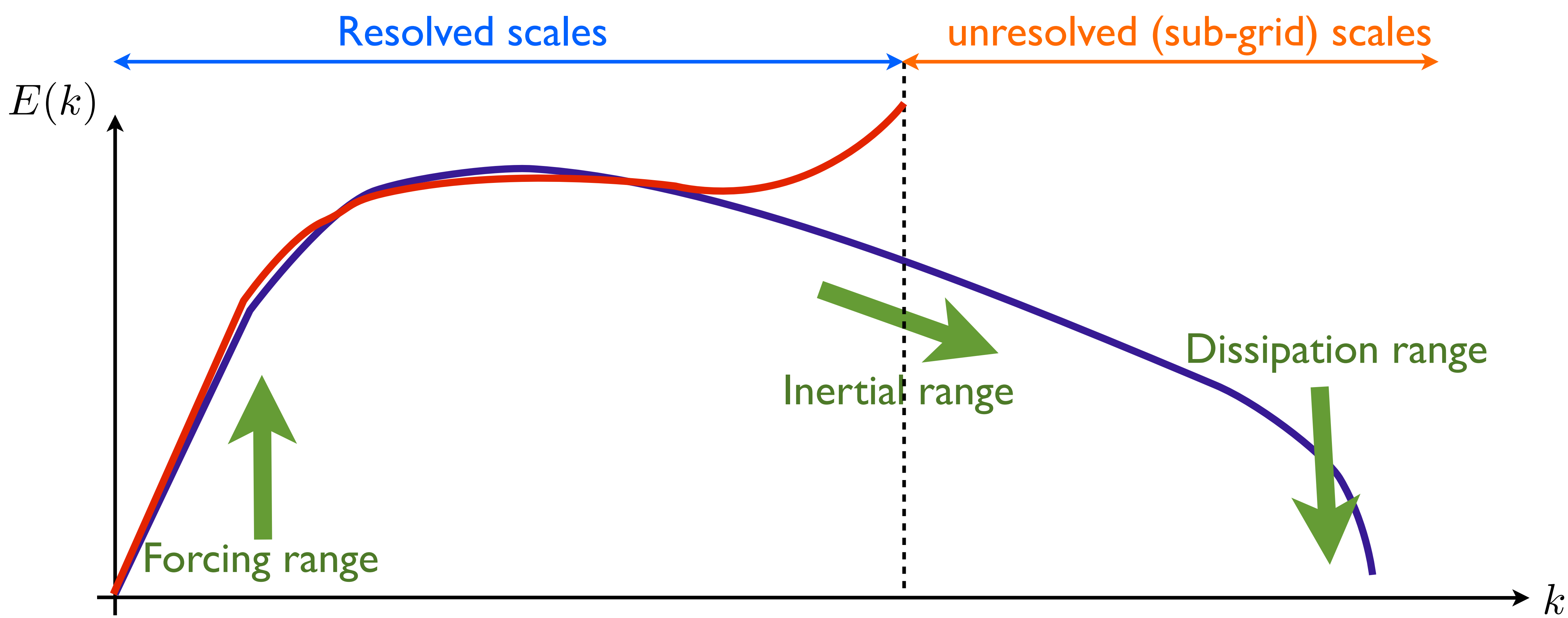

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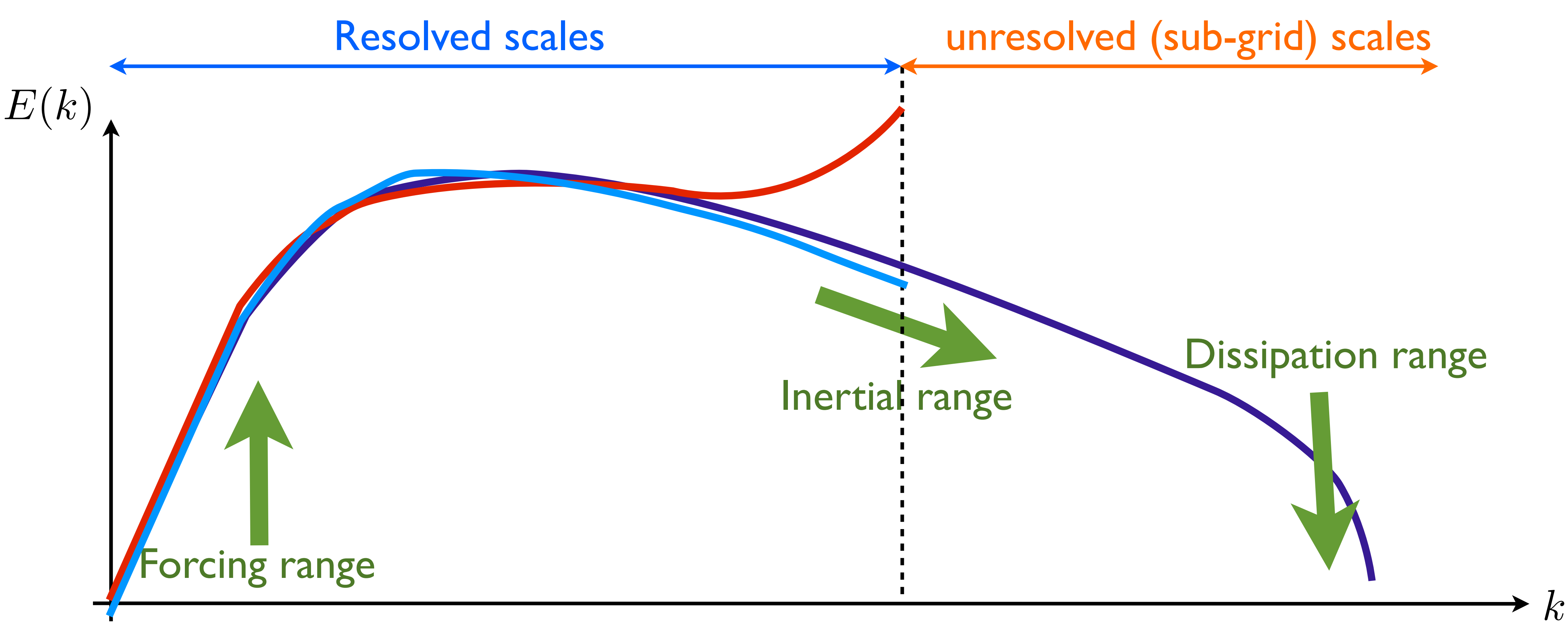
Models for the small scales are expected to drain energy from the large scales in order to mimic the effects of the dissipation range.



Subgrid-scale physics? (II)

In Navier-Stokes turbulence, the main effect of the small & unresolved scales in an LES is thus expected to be the dissipation of the kinetic energy stored in the large & resolved scales.

The simplest model that dissipates large scale energy is the eddy viscosity model:

$$\tau_{ij} = -\nu_{\mathrm{eddy}} \left(\partial_i \overline{u}_j + \partial_j \overline{u}_i\right)$$

J. Smagorinsky, Month. Weather Rev. (1963)

In MHD turbulence, the total (kinetic + magnetic) energy cascade has played the same role as kinetic energy for Navier-Stokes problems.

However, in MHD, energy can be dissipated into heat at small scales by Joule effects as well as by viscous effects.

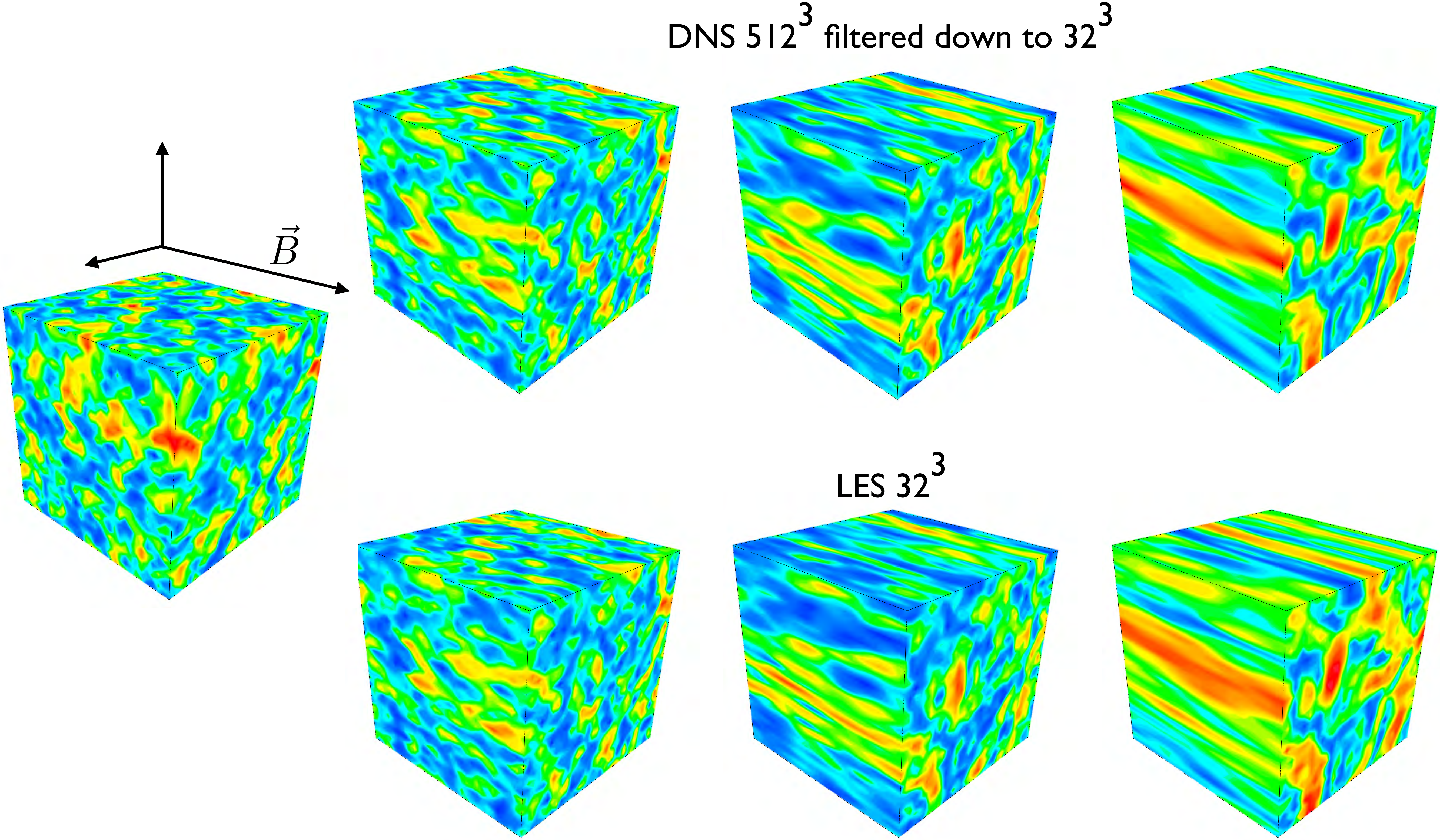
Subgrid-scale models in MHD are thus based on the turbulent viscosity picture as well as turbulent magnetic diffusivity.

Eddy viscosity & eddy magnetic diffusivity models:
A. Yoshizawa (PoF, 1987);
T. Passot, H. Politano, A. Pouquet, & P. L. Sulem (Theor. Comput. Fluid Dyn, 1990);
Y. Zhou & G. Vahala (J. Plasma Phys., 1991);
M. L. Theobald, P. A. Fox & S. Sofia (PoP, 1994)

Dynamic models
O. Agullo, W.-C. Müller, B. Knaepen & D. Carati (PoP, 2001)
W.-C. Müller & D. Carati (PoP, 2002)
B. Knaepen & P. Moin (PoF, 2004)

Alpha models
P. D. Mininni, D.C. Montgomery & A Pouquet (PoF, 2005 - PRE, 2005).
J. Pietarila Graham, P. D. Mininni & A. Pouquet (PRE 2009)

LES for MHD has been shown to perform very well even in presence of a strong magnetic field (anisotropic flows):



B. Knaepen & P. Moin (PoF, 2004)

LES for kinetic turbulence (I)

In the kinetic description of plasmas, the state of the system is characterised by the probability distribution function g which depends on the position, the velocity and time. In the gyrokinetic formalism, this distribution is supposed to be the deviation from a local equilibrium distribution and the general structure of the equation is:

$$\partial_t g = L(g) + N(g,g) + C(g)$$

$L(g)$ is the linear term that depends on the gradient of the equilibrium function

$N(g,g)$ is the nonlinear (quadratic) term

$C(g)$ is the collision term

Applying a filter to remove the smallest scales from the distribution function is very simple and leads to same closure problems as in the fluid equations:

$$\partial_t \overline{g} = L(\overline{g}) + N(\overline{g},\overline{g}) + C(\overline{g}) + \mathcal{T}(g)$$

where the new term describing the effects of under-resolved scales on the largest scales is given by:

$$\mathcal{T}(g) = \overline{N(g,g)} - N(\overline{g},\overline{g})$$

LES for kinetic turbulence (II)

The central question is: What is the role of this new term?

Most of the answer can be found in the discussion by Schekochihin *et al*, PPFC (2008).

The conservation of the total (kinetic energy of the particles + electromagnetic energy) does not seem to be a good guide for understanding the effect of the under-resolved scales:

$$\frac{d}{dt}\mathcal{E} = \frac{d}{dt}\,(W + K) \equiv \epsilon = \int \mathbf{E}\cdot\mathbf{J}$$

$$W = \int d^3r\ \frac{|\mathbf{E}|^2 + |\mathbf{B}|^2}{8\pi\epsilon_0} \qquad\qquad K = \int d^3r\ d^3v\ \frac{mv^2}{2}\ g(\mathbf{r},\mathbf{v},t)$$

This conservation law is not very well adapted to design a model for the under-resolved scales for two reasons:

- It represents processes that are <u>reversible</u> (contrary to the energy dissipation into heat by viscous or Joule effects).

- The conserved quantity is a <u>mix of linear and quadratic terms</u> in the distribution function (contrary to kinetic and magnetic energies in fluids).

LES for kinetic turbulence (III)

In kinetic approaches, the free energy has more common features with the kinetic energy in Navier-Stokes:

$$F = \mathcal{E} - TS$$

Schekochihin *et al*, PPFC (2008)

The entropy is defined by in terms of the complete distribution function as:

$$S = -k_b \int d^3r\ d^3v\ f(\mathbf{r}, \mathbf{v}, t)\ \ln f(\mathbf{r}, \mathbf{v}, t)$$

and reduces to $S = -\dfrac{K}{T} - \delta S$ where $\delta S = k_b \displaystyle\int d^3r\ d^3v\ \frac{g^2}{2\, G_0}$

Hence, the kinetic energy of the particles disappears form the free-energy balance:

$$\frac{d}{dt}(W + \delta S) = \epsilon - T\mathcal{K}_c$$

and like the energy in Navier-Stokes and MHD equations, the free energy

- is a quadratic function of the variable;
- its source term is due to external constraints (electromagnetic fields);
- its dissipation is due to irreversible collisional processes.

All the ingredients seem to be present to observe a cascade of free energy in gyrokinetic turbulence...

Adapting LES to gyrokinetic simulations

This collaborative project between Garching and ULB aims at developing LES-like idea for gyrokinetic simulation. It relies on the GENE code (www.ipp.mpg.de/~fsj/gene) which is modified to study the effects of the small scales (diagnostics in post-processing) as well as to account for the under-resolved physics (new model terms in the solver).

Testing the cascade of free energy in well resolved simulations

- analyse the free energy balance in well resolved simulations with the GENE code.

- show that the sub-grid scale term computed from well resolved simulations is indeed a sink for the free energy stored in the large scales.

- compute the free energy transfers between different scales from well resolved simulations.

Analyse the sub-grid scale term

- compute the "exact" sub-grid scale term from well resolved simulations.

- compare this exact term to various models, including the dissipative (regularisation) terms used in today's version of various gyrokinetic codes.

Implement a sub-grid scale model

- test simple hyper-diffusion models that have been proved to dissipate free-energy.

- implement the dynamic procedure, a technique developed in LES of fluid turbulence in order to optimise model parameter in the course of the simulation. Germano, JFM (1992)