Incompact3d User Group Meeting

High-order numerical dissipation: Why and how?

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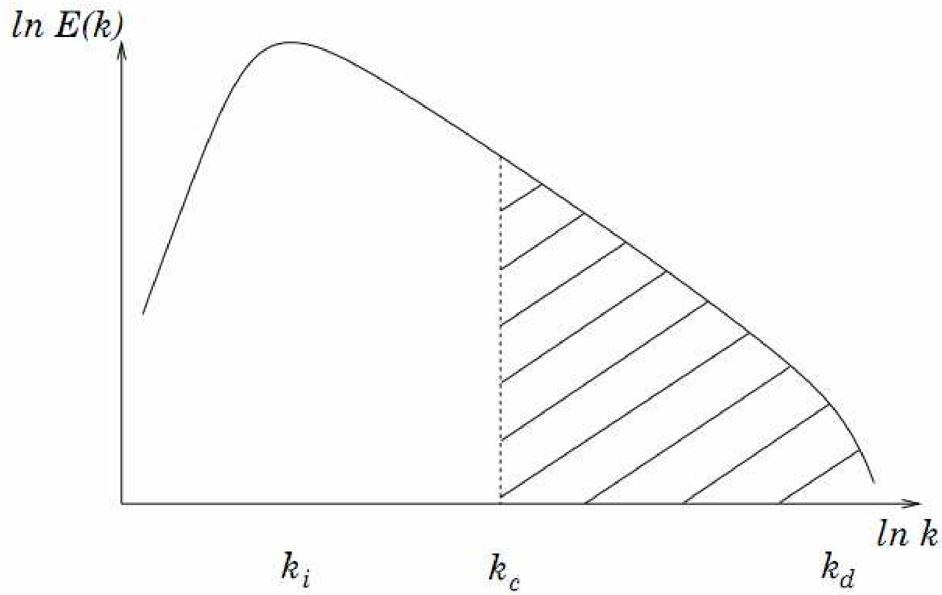
Introduction

- Basics of LES
- Implicit LES (numerical dissipation)
- High-order numerical dissipation via the viscous term (Incompact3d schemes)
- Calibration of numerical dissipation for subgrid scale modelling
- Applications
  - LES of turbulent channel flow
  - LES of impinging and free jets
  - LES of 3D Taylor-Green flow

Basics of LES

- Principle



- General filter

$$\bar{f}(\vec{x}) = \int G(\vec{x}, \vec{x}')f(\vec{x}')d\vec{x}'$$

- Basic assumption

$$\varepsilon_r = \overline{\frac{\partial f}{\partial x_i}} - \frac{\partial \bar{f}}{\partial x_i}$$

Basics of LES

- Filtered momentum equations

$$\frac{\partial \bar{u}_i}{\partial t} + \frac{\partial}{\partial x_j}(\bar{u}_i \bar{u}_j) = -\frac{1}{\rho}\frac{\partial \bar{p}}{\partial x_i} + \frac{\partial}{\partial x_j}\left\{\nu\left(\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i}\right) - \tau_{ij}\right\}$$

only valid if ε_r=0

- Subgrid-scale tensor

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

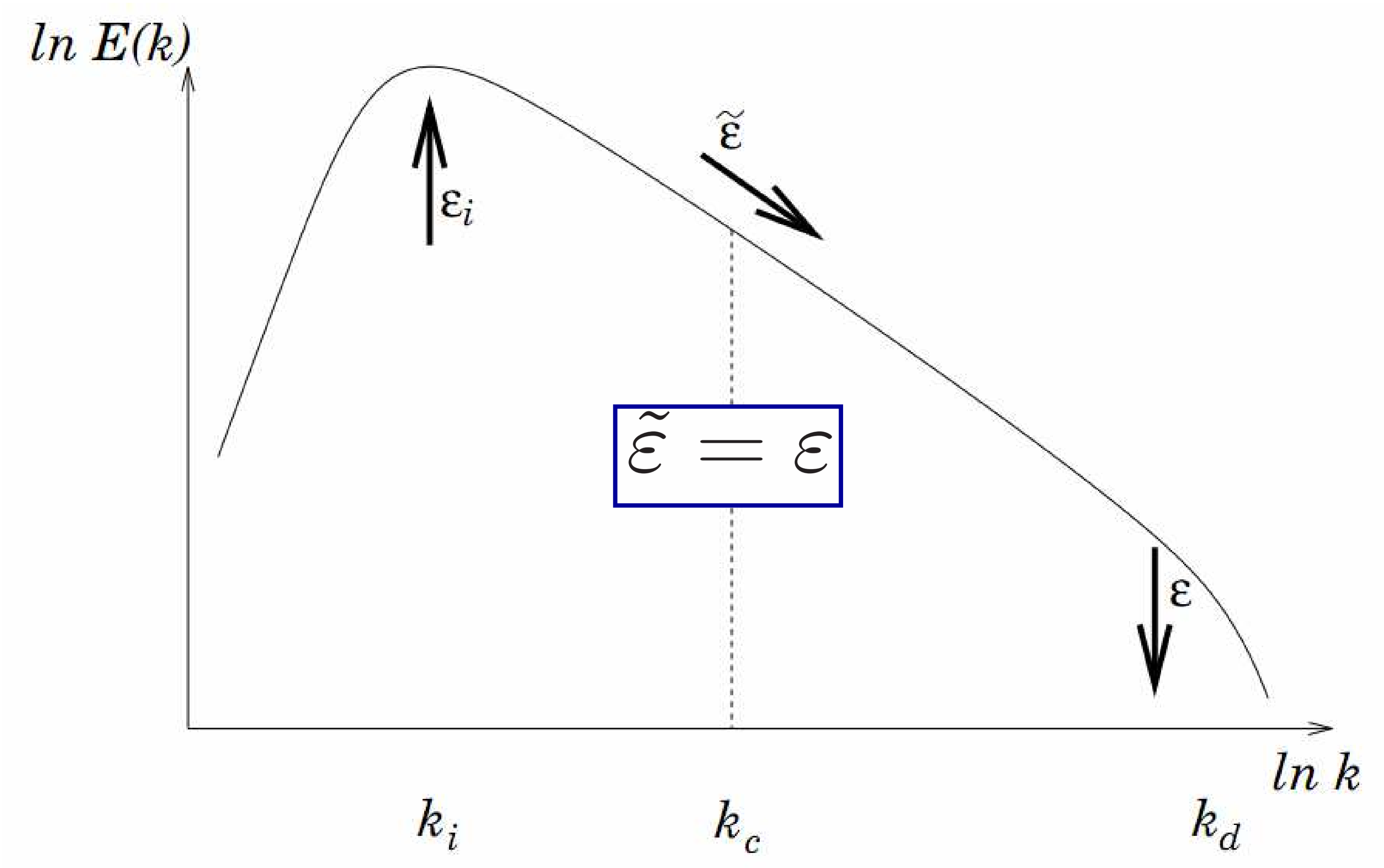
- Filtered kinetic energy equation

$$\begin{aligned}\frac{\partial K}{\partial t} + \bar{u}_j \frac{\partial K}{\partial x_j} &= -\frac{1}{\rho}\frac{\partial(\bar{u}_i \bar{p})}{\partial x_i} + \nu \frac{\partial^2 K}{\partial x_j x_j} - \nu \frac{\partial \bar{u}_i}{\partial x_j}\frac{\partial \bar{u}_i}{\partial x_j} \\ &\quad - \frac{\partial(\tau_{ij}\bar{u}_i)}{\partial x_j} + \underbrace{\tau_{ij}\frac{\partial \bar{u}_i}{\partial x_j}}_{-\tilde{\varepsilon}}\end{aligned}$$

$$\boxed{\tilde{\varepsilon} = -\tau_{ij}\bar{S}_{ij}}$$

Basics of LES

- Model calibration guidelines



Basics of LES

- Boussinesq hypothesis

$$\tau_{ij} - \frac{1}{3}\tau_{kk}\delta_{ij} = -2\nu_t \bar{S}_{ij} \quad \rightarrow \quad \boxed{\tilde{\varepsilon} = 2\nu_t \bar{S}_{ij}\bar{S}_{ij}}$$

- Model filtered equations

$$\frac{\partial \bar{u}_i}{\partial t} + \frac{\partial}{\partial x_j}(\bar{u}_i \bar{u}_j) = -\frac{1}{\rho}\frac{\partial \bar{P}}{\partial x_i} + \frac{\partial}{\partial x_j}\left\{(\nu + \nu_t)\left(\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i}\right)\right\}$$

- Smagorinsky model

$$\nu_t = (C_s \Delta_c)^2 \sqrt{2\bar{S}_{ij}\bar{S}_{ij}}$$

- Dynamic model : self-calibration of C_s

- Scale similarity model, deconvolution model, etc.

Basic assumptions

1. "Commutation error ε_r is negligible compared with subgrid stresses": **X** (distorted filter/mesh)
2. "Discretization errors are negligible compared with subgrid stresses": **X** ($\Delta_c = \Delta x$)
3. "Aliasing errors are negligible compared with subgrid stresses": **X** ($\Delta_c = \Delta x$)
4. "Subgrid modelling is weakly sensitive to numerical errors": **X** ($\Delta_c = \Delta x$)
5. "LES is successful because viscous dissipation scales on large-scale motions": √

→ General underestimation of the importance of numerical errors

→ Weakness of the LES formalism

Especially for Incompact3d!

Alternative: Implicit LES

"For LES, a lack of formalism could be better than a weak (fake?) formalism"

- **<u>Principle:</u>** large-scale dynamics is left free from modelling whereas small-scale dynamics (subjected to strong numerical errors) is damped **(regularization)**.

  - With the "help" of numerical errors
    → MILES approach (dissipative upwind schemes)
    → Explicit filtering (artificial dissipation)
    <u>Drawbacks:</u> uncontrolled artificial dissipation, loss of time consistency for explicit filtering
  - With an extra dissipative operator
    → Hyperviscosity (spectral methods)
    → Spectral Vanishing Viscosity (spectral methods)
    <u>Drawbacks:</u> restricted to academic geometry, calibration

Implicit LES using Incompact3d

- **Principle:** introduction of **targeted regularization** using a specific property of compact schemes

- **Advantages:**
  - Numerical dissipation can be controlled
  - No extra operator (via the viscous term)
  - Numerical errors are the source of numerical dissipation (no extra error due to discretization)
  - Preserves high-order accuracy
  - Compatible with DNS and LES

Compact schemes for the second derivative

- Second derivative

$$\alpha f''_{i-1} + f''_i + \alpha f''_{i+1} = a\,\frac{f_{i+1} - 2f_i + f_{i-1}}{\Delta x^2} + b\,\frac{f_{i+2} - 2f_i + f_{i-2}}{4\Delta x^2} + c\,\frac{f_{i+3} - 2f_i + f_{i-3}}{9\Delta x^2}$$

- Modified square wave number

f=exp(ikx) → f"=-k" exp(ikx)
≠-k² exp(ikx)

$$k''\Delta x^2 = \frac{2a\left[1-\cos(k\Delta x)\right] + \frac{b}{2}\left[1-\cos(2k\Delta x)\right] + \frac{2c}{9}\left[1-\cos(3k\Delta x)\right]}{1 + 2\alpha\cos(k\Delta x)}$$

→ singularity at α=1/2 for k=k_c

Compact schemes for the second derivative

- 4 parameters: a,b,c,α
- 4 order conditions

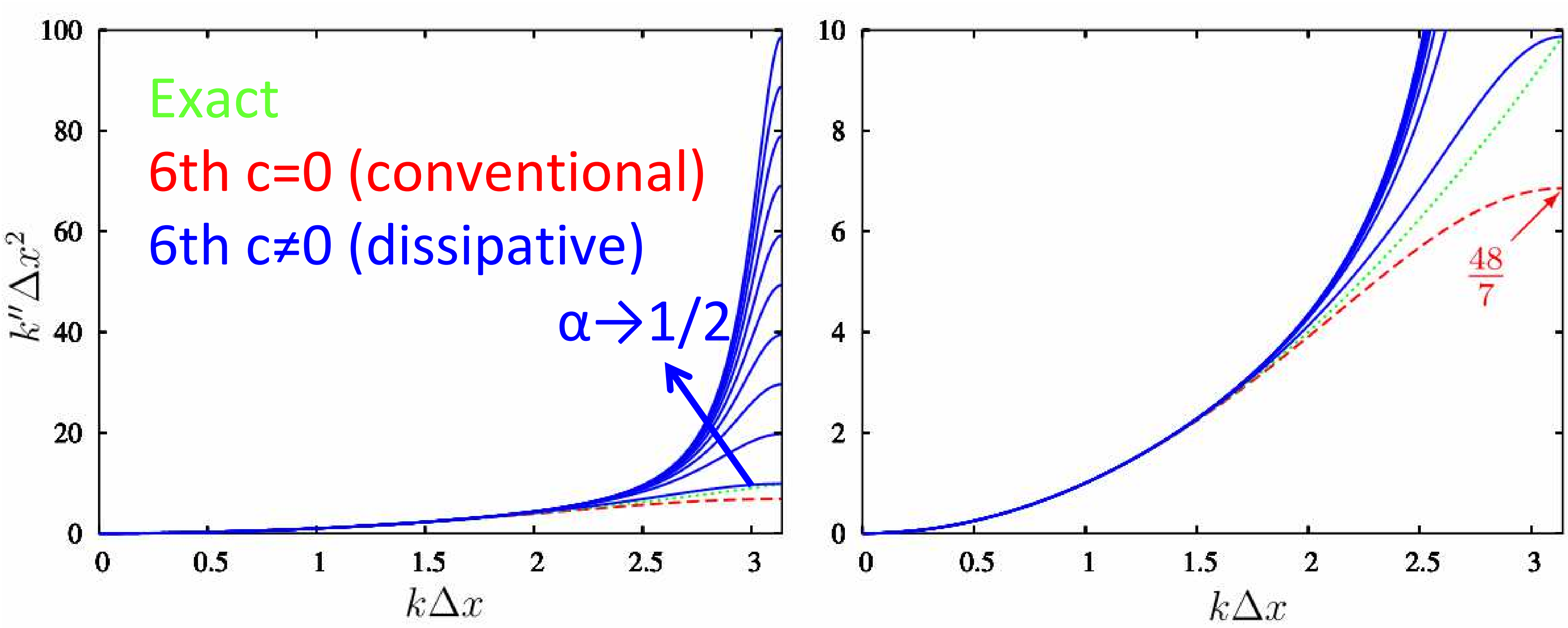
$a+b+c=1+2\alpha$	(Δx^2 condition)
$a+4b+9c=12\alpha$	(Δx^4 condition)
$a+16b+81c=30\alpha$	(Δx^6 condition)
$a+64b+729c=56\alpha$	(Δx^8 condition)

→ **If Δx^8 condition is sacrificed, α can be chosen freely while preserving the 6th order accuracy**

→ **If Δx^6 condition is sacrificed, α and another coefficient can be chosen freely while preserving the 4th order accuracy**

→ **The choice $\alpha \to 1/2$ leads to $k'' \to \infty$ at $k \approx k_c$**

Modified square wave number



- The exact differentiation is given by **k"=k²**
- For conventional schemes, **k"<k²** near the cutoff
  → sub-dissipative behaviour
- For present scheme, **k"≈k²** except for $k \approx k_c$ where **k">>k²**
  → over-dissipative behaviour

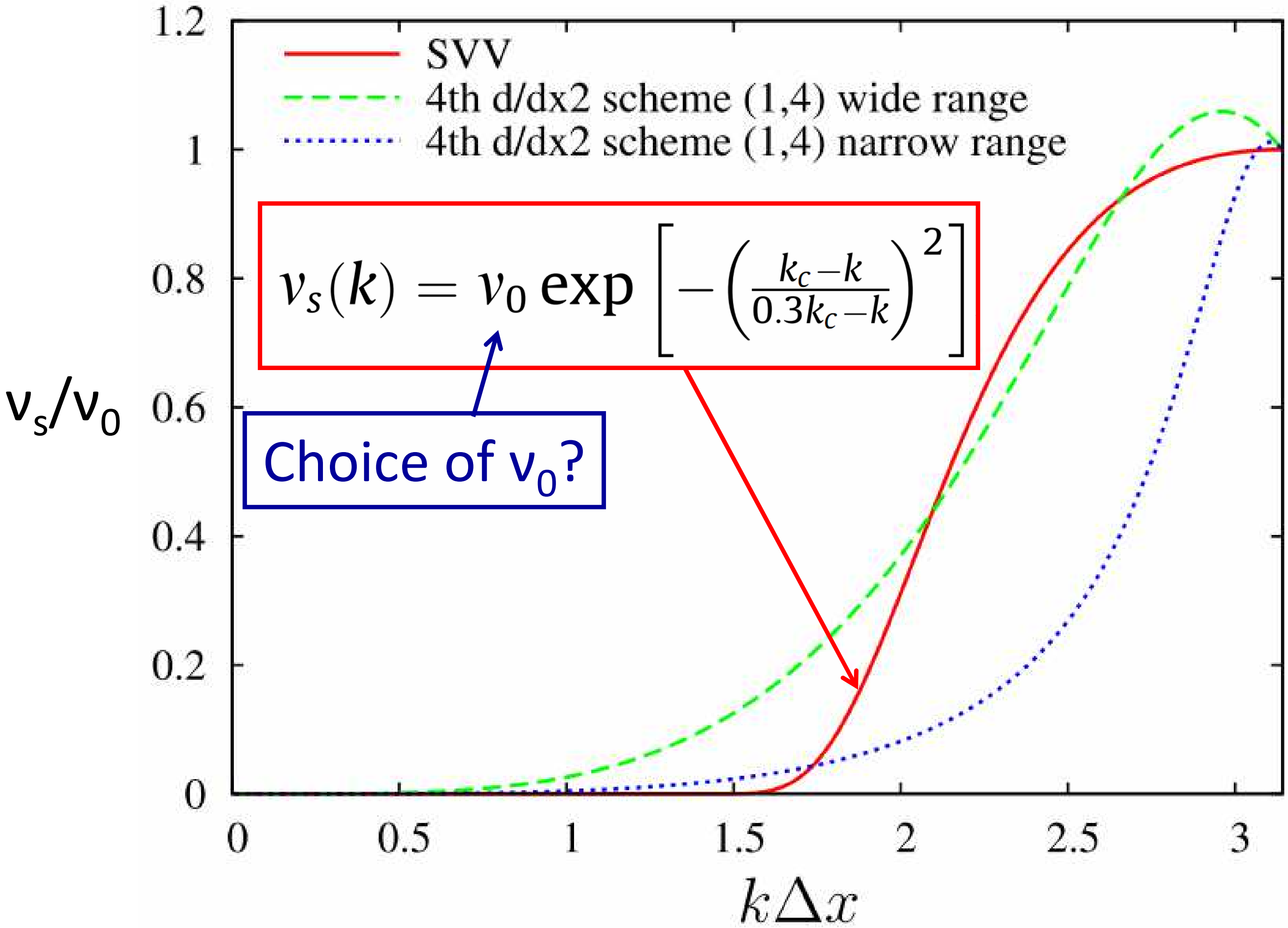
Equivalence with spectral viscosity

- The over-estimation of k^2 introduces a spectral viscosity with

$$\nu_s'' = \nu(k'' - k^2)/k^2$$

- Can be used to mimic subgrid scale dissipation
  - Hyperviscosity: $\nu_s = \nu_0 \; k^{2n-2}$
  - Spectral Vanishing Viscosity: $\nu_s(k) = \nu_0 \exp\left[-\left(\frac{k_c - k}{0.3k_c - k}\right)^2\right]$

Spectral Vanishing Viscosity

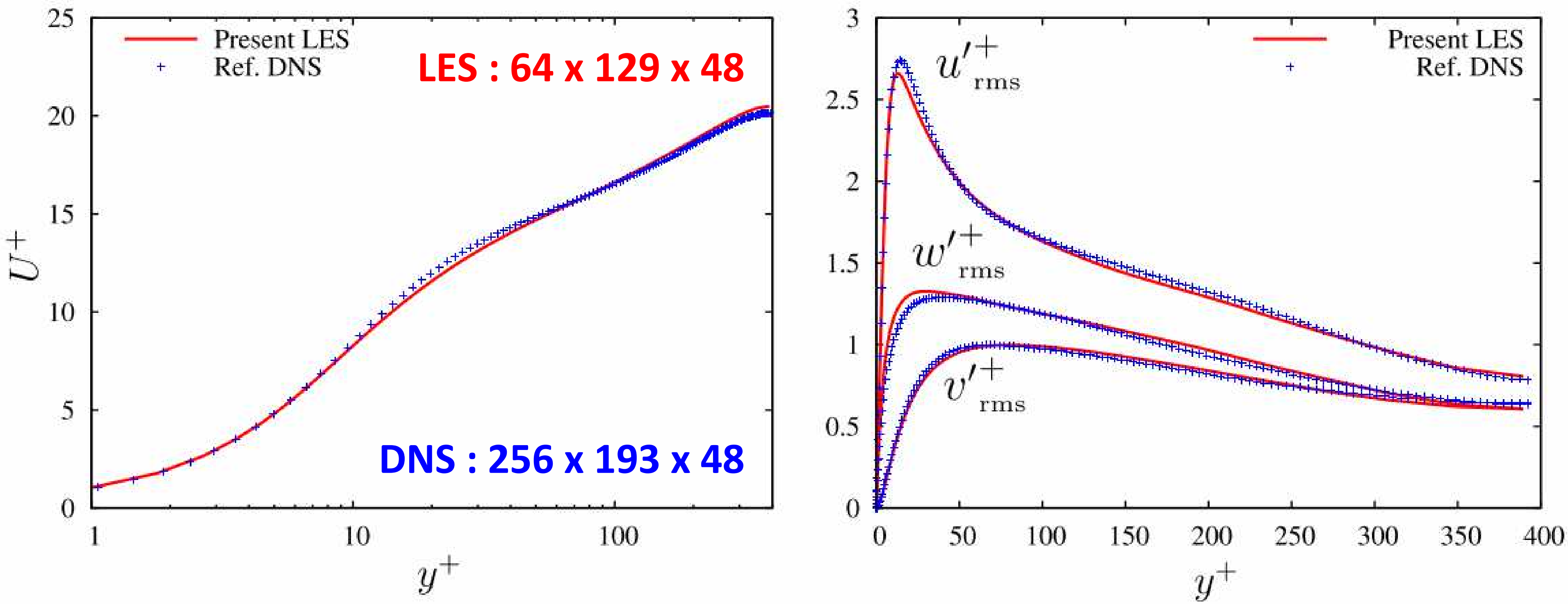


LES using SVV

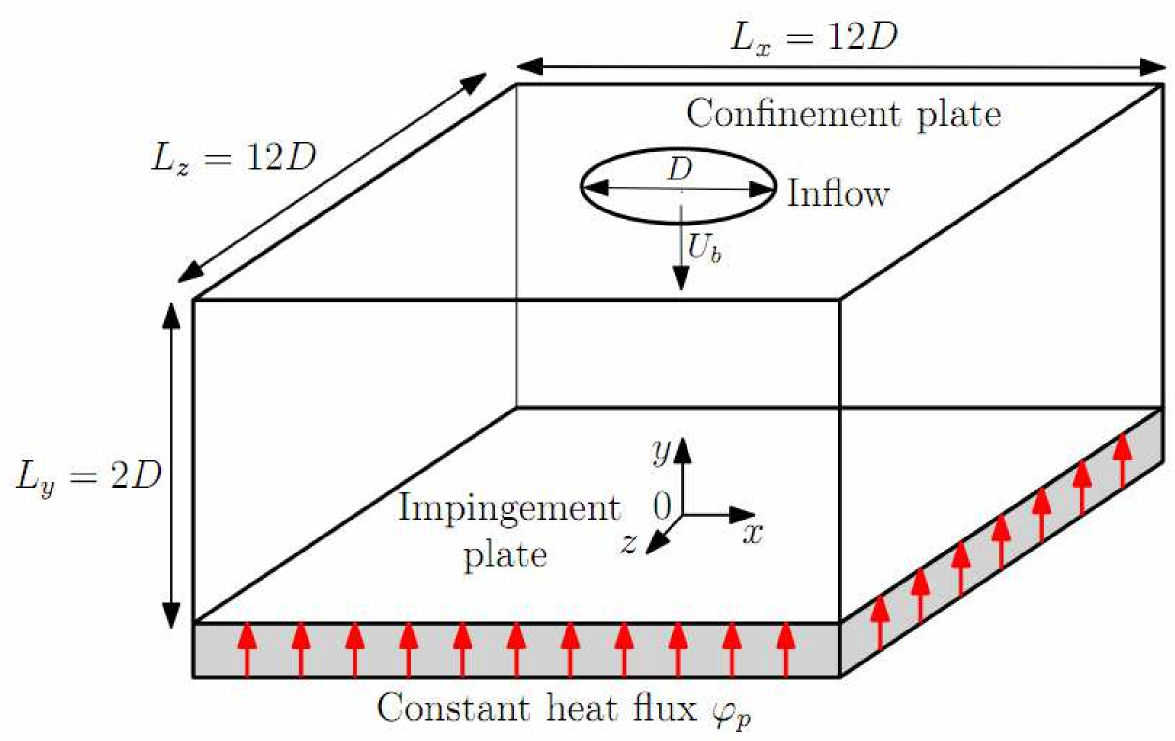
Turbulent channel flow

$$L_x \times L_y \times L_z = 2\pi h \times 2h \times \pi h$$

$\nu_0/\nu=3$



LES of Turbulent Impinging Jet



Cases	$n_x \times n_y \times nz$	Second derivative schemes	Subgrid-scale model
O6DNS	$1541 \times 401 \times 1541$	$O(\Delta x^6)$	no model
O4SVV	$257 \times 401 \times 257$	$O(\Delta x^4)$	SVV (ν_0/ν=19)
O6WALE	$257 \times 401 \times 257$	$O(\Delta x^6)$	WALE
LO6DNS	$257 \times 401 \times 257$	$O(\Delta x^6)$	no model

Velocity statistics

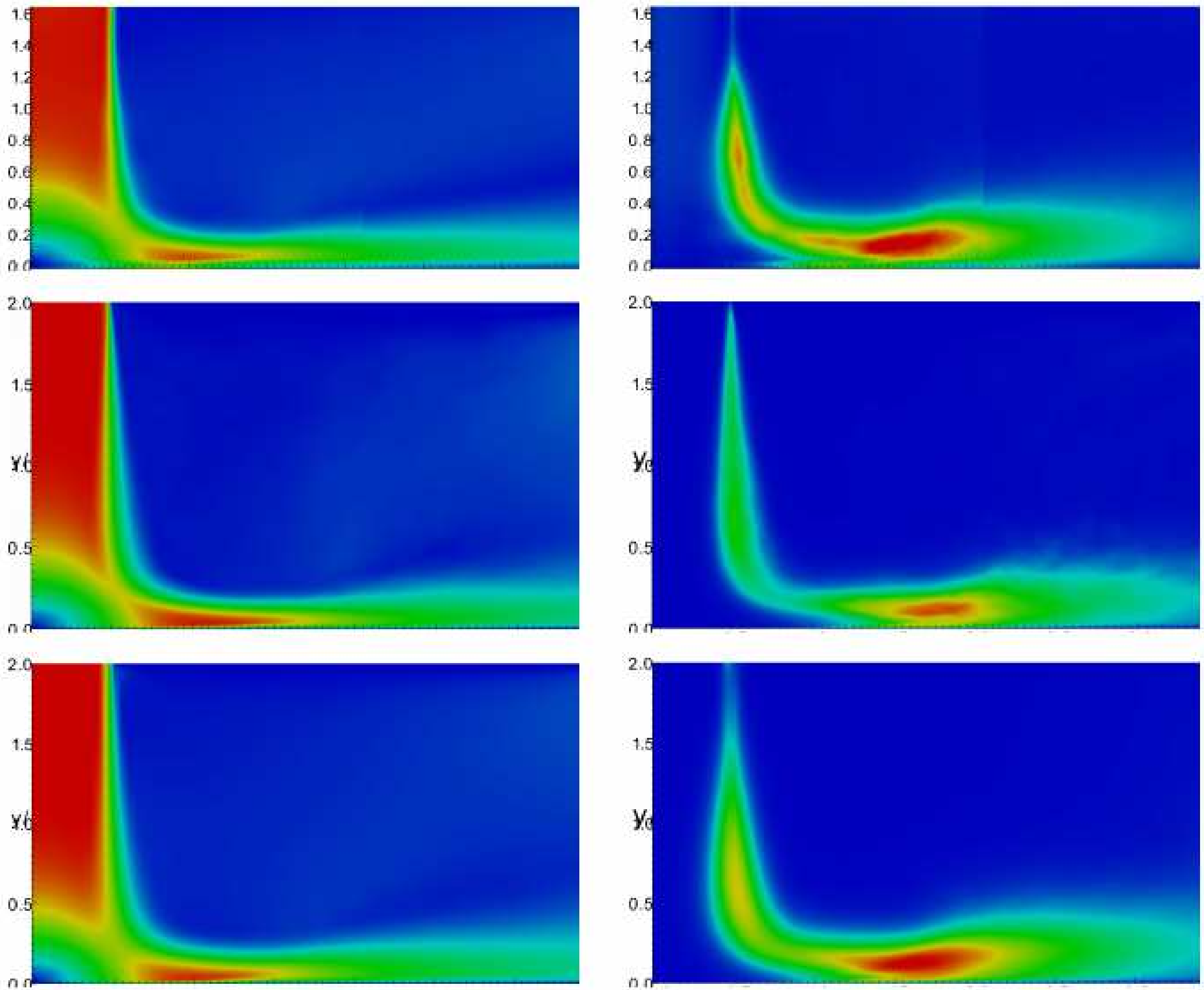
Mean velocity

TKE

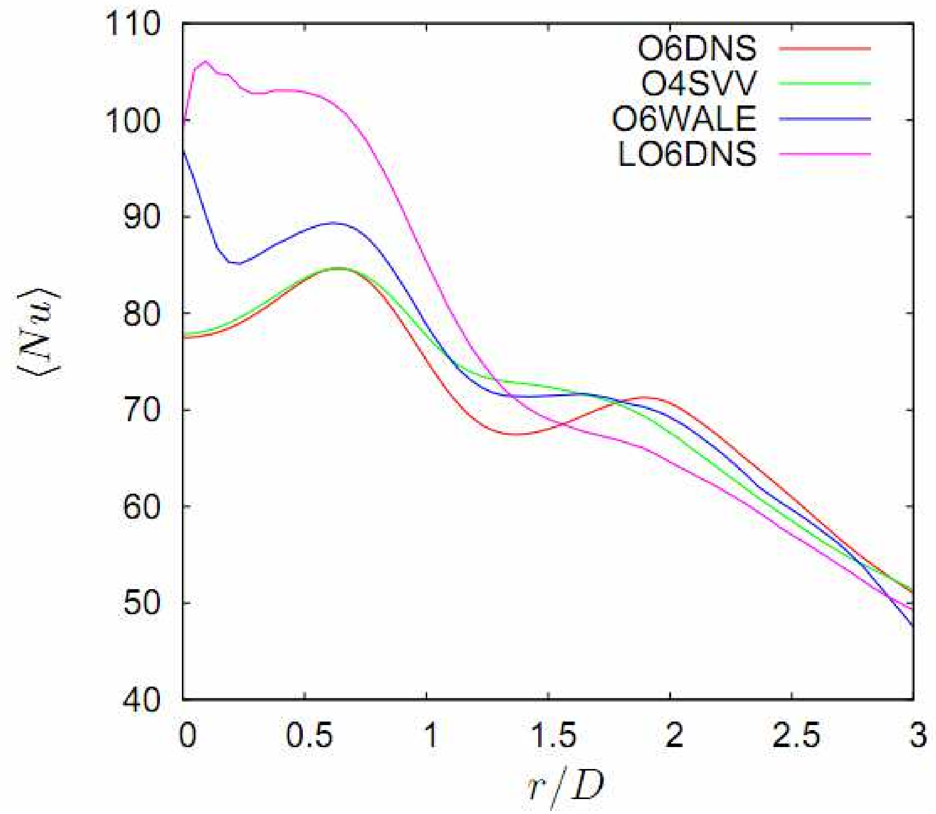
Experiment

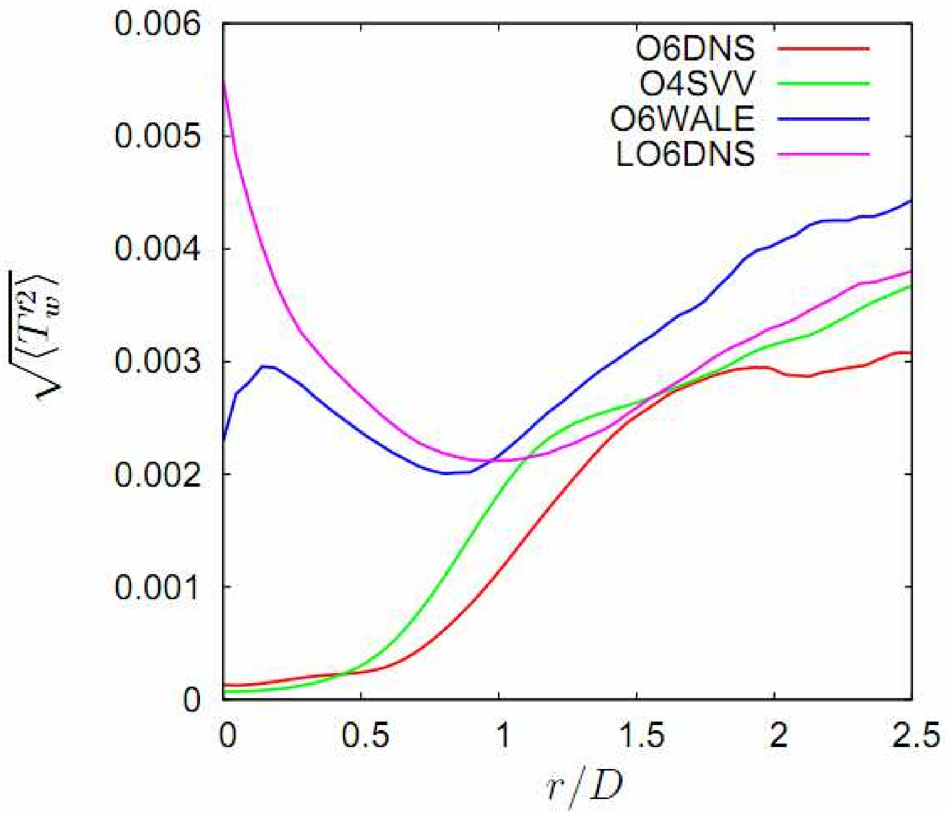
DNS

LES O4-SVV



Wall temperature statistics





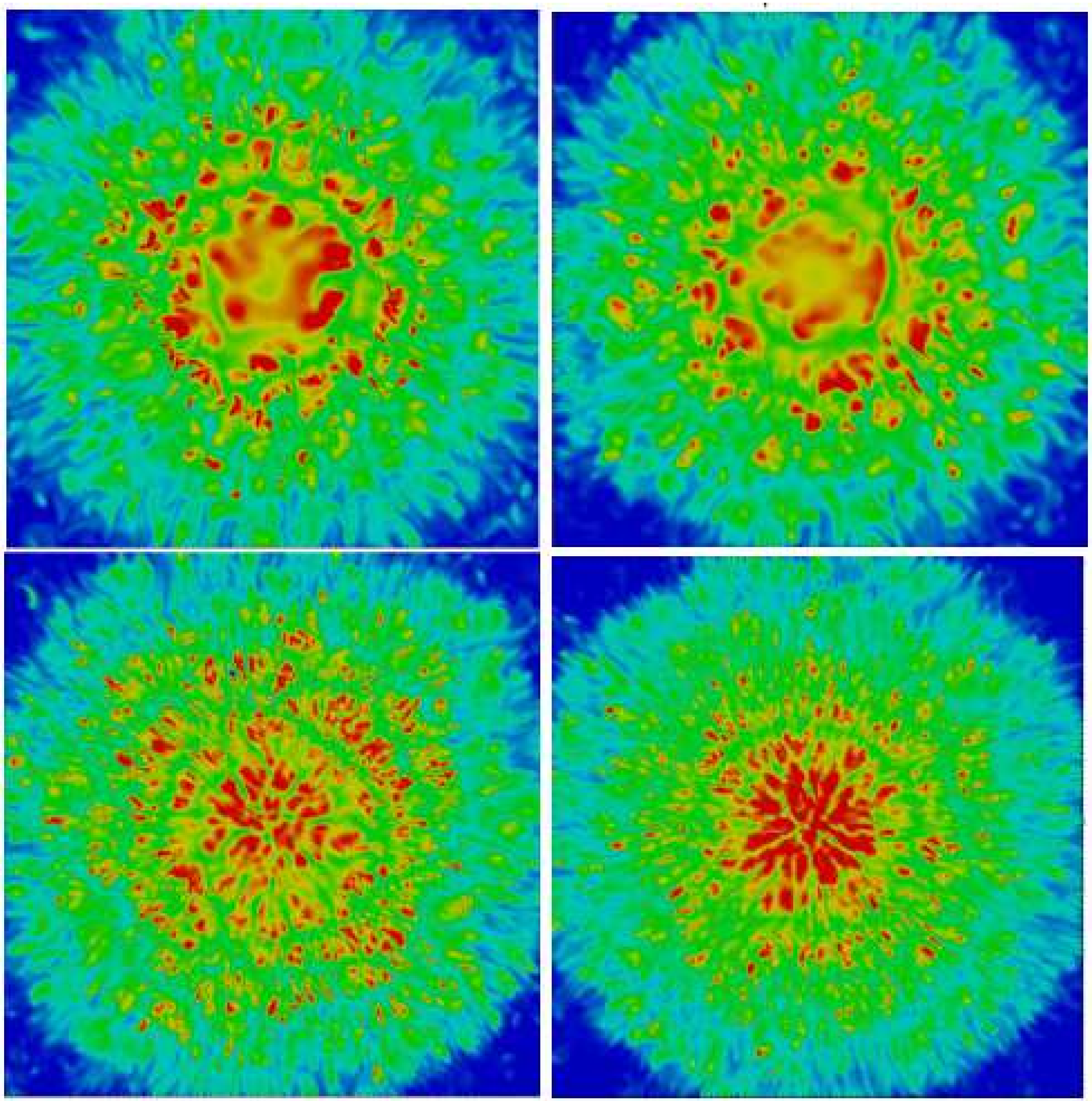
→ Wrong prediction of heat transfer for ν_t subgrid-scale models (Smagorinsky, WALE) as for a low resolution DNS

→ Improvement when targeted numerical dissipation (SVV) is used

Instantaneous Nusselt number

DNS

LES
SVV



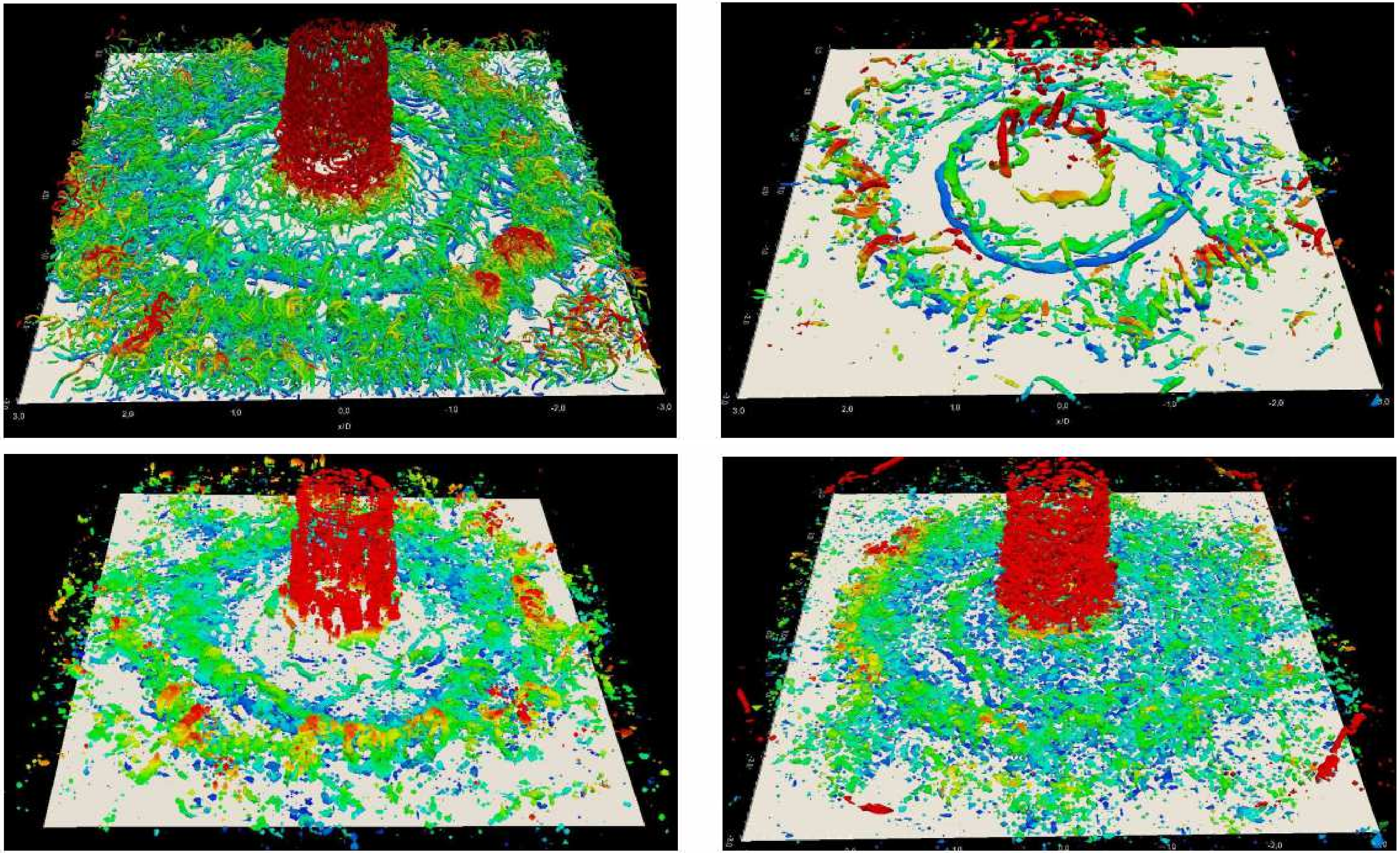
LES
WALE

LES
No model

Instantaneous visualization

DNS

LES SVV



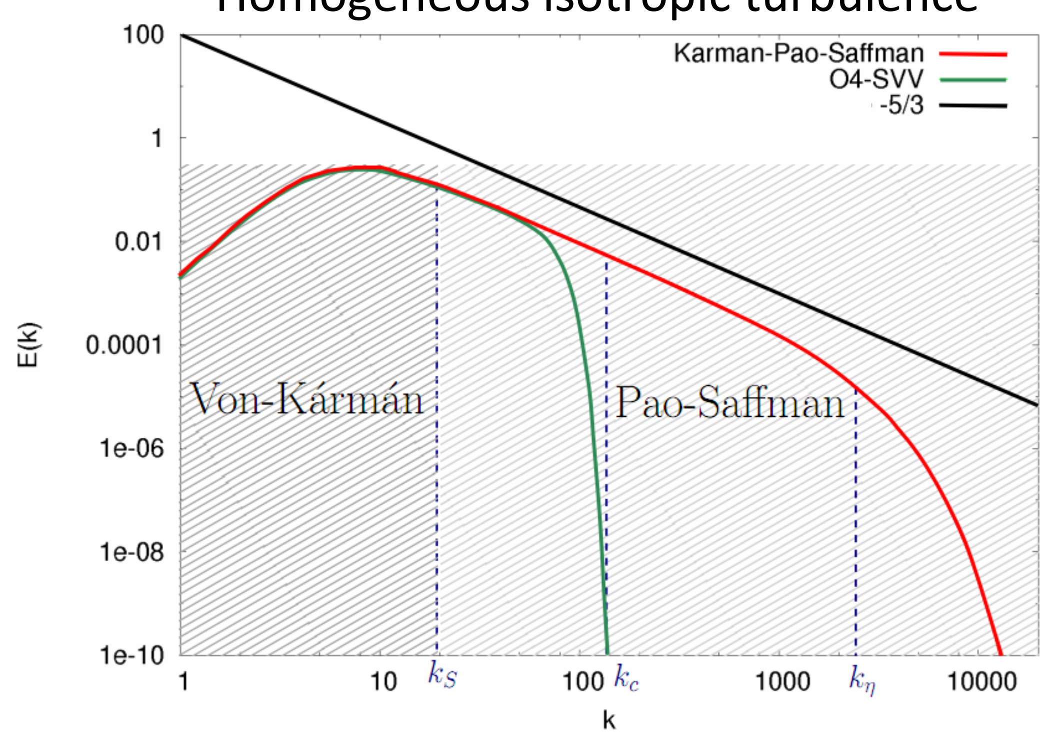
LES WALE

LES No model

Choice of ν_0/ν? Example for free jet flow

- DNS OK at Re=10 000 using 1024^3 grid points
- **Goal:** LES at Re=700 000 using 1024^3 grid points
- **Reference:** DNS at Re=700 000 using $24\,576^3$ grid points

Homogeneous isotropic turbulence



How to choose the spectrum shape?
DNS : $k_s \rightarrow \infty$ / LES : $k_s \rightarrow k_c$

Assumption

$$\int_0^{k_s} E_{DNS}(k)dk = \int_0^{k_s} E_{LES}(k)dk$$

$$\int_0^{k_s} \nu k^2 E_{DNS}(k)dk = \int_0^{k_s} \nu k'' E_{LES}(k)dk$$

DNS/LES dissipation

$$\varepsilon_{DNS} = 2\nu \int_{k_s}^{\infty} k^2 E_{DNS}(k)\ dk$$

$$\varepsilon_{LES} = 2\nu \int_{k_s}^{k_c} k''_{LES} E_{LES}(k)\ dk$$

Principle: find ν_0/ν to obtain

$$\varepsilon_{LES} = \varepsilon_{DNS}$$

Modelling of the spectrum shape

- Lin equation

$$\frac{\partial E(k,t)}{\partial t} = T(k,t) - 2\nu k^2 E(k,t)$$

  - Energy injection at k_i
  - Steady Kolmogorov spectrum for $k>k_i$

Pao equation (1968)

$$\frac{1}{C_K} k^{5/3} E'(k) + \left(\frac{5}{3C_K} k^{2/3} + 2k_\eta^{-4/3} k^2 \right) E(k) = 0$$

→ analytical solution

$$E(k) = C_K \epsilon^{2/3} k^{-5/3} \exp\left(-\frac{3}{2} C_K \left(\frac{k}{k_\eta} \right)^{4/3} \right)$$

DNS $k \in]k_i; +\infty[$

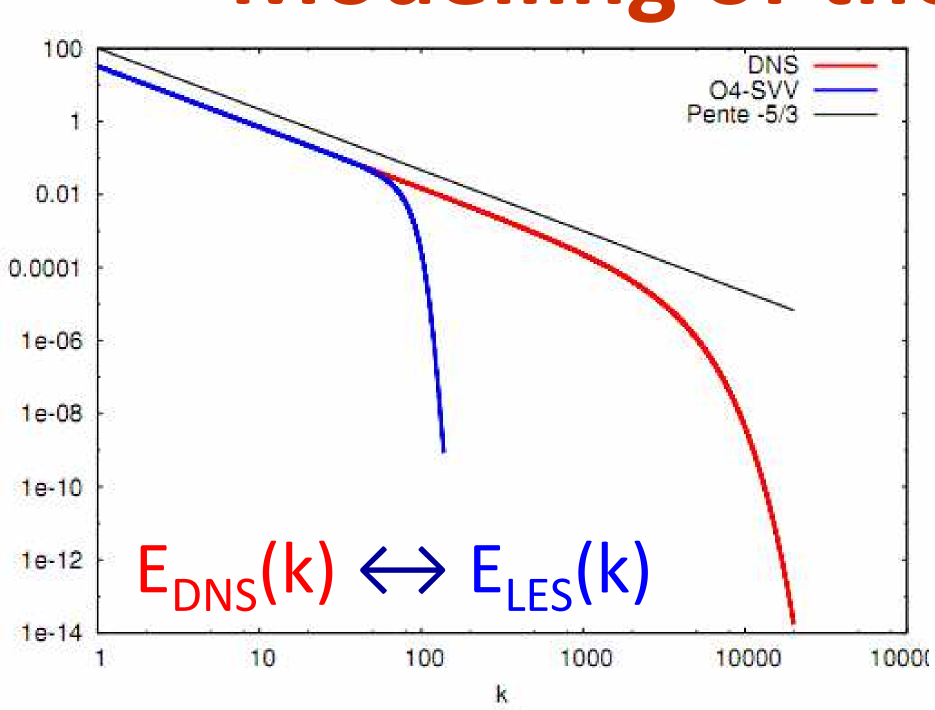
Pao-like equation

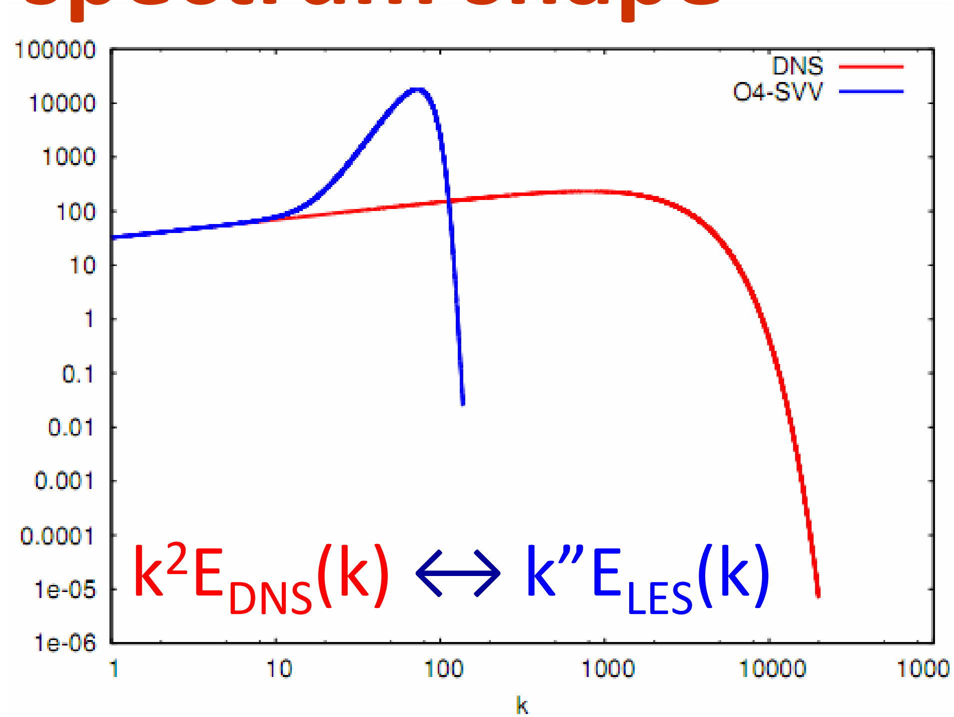
$$\frac{\epsilon^{1/3}}{C_K} k^{5/3} E'(k) + \left(\frac{5\epsilon^{1/3}}{3C_K} k^{2/3} + 2k_\eta^{-4/3} k'' \right) E(k) = 0$$

→ numerical solution

LES $k \in]k_i; k_c]$

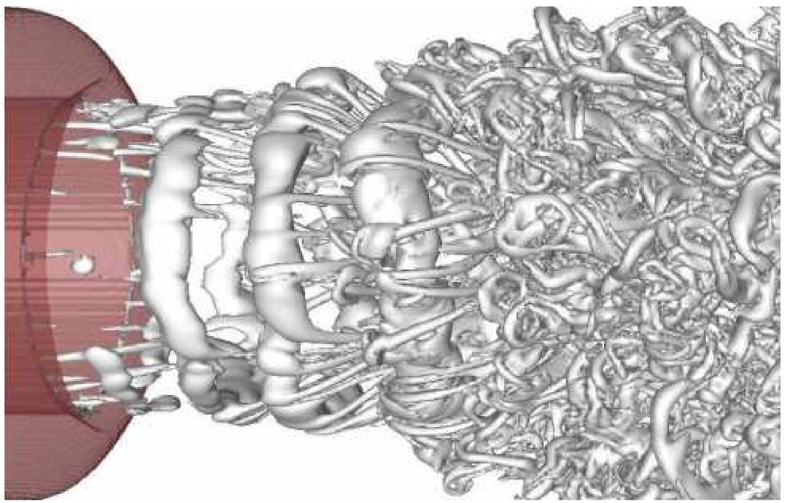
Modelling of the spectrum shape



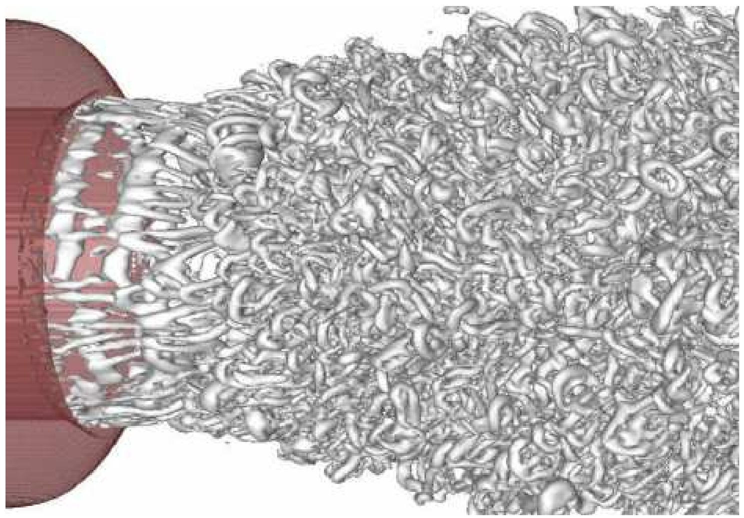


DNS, Re=10 000

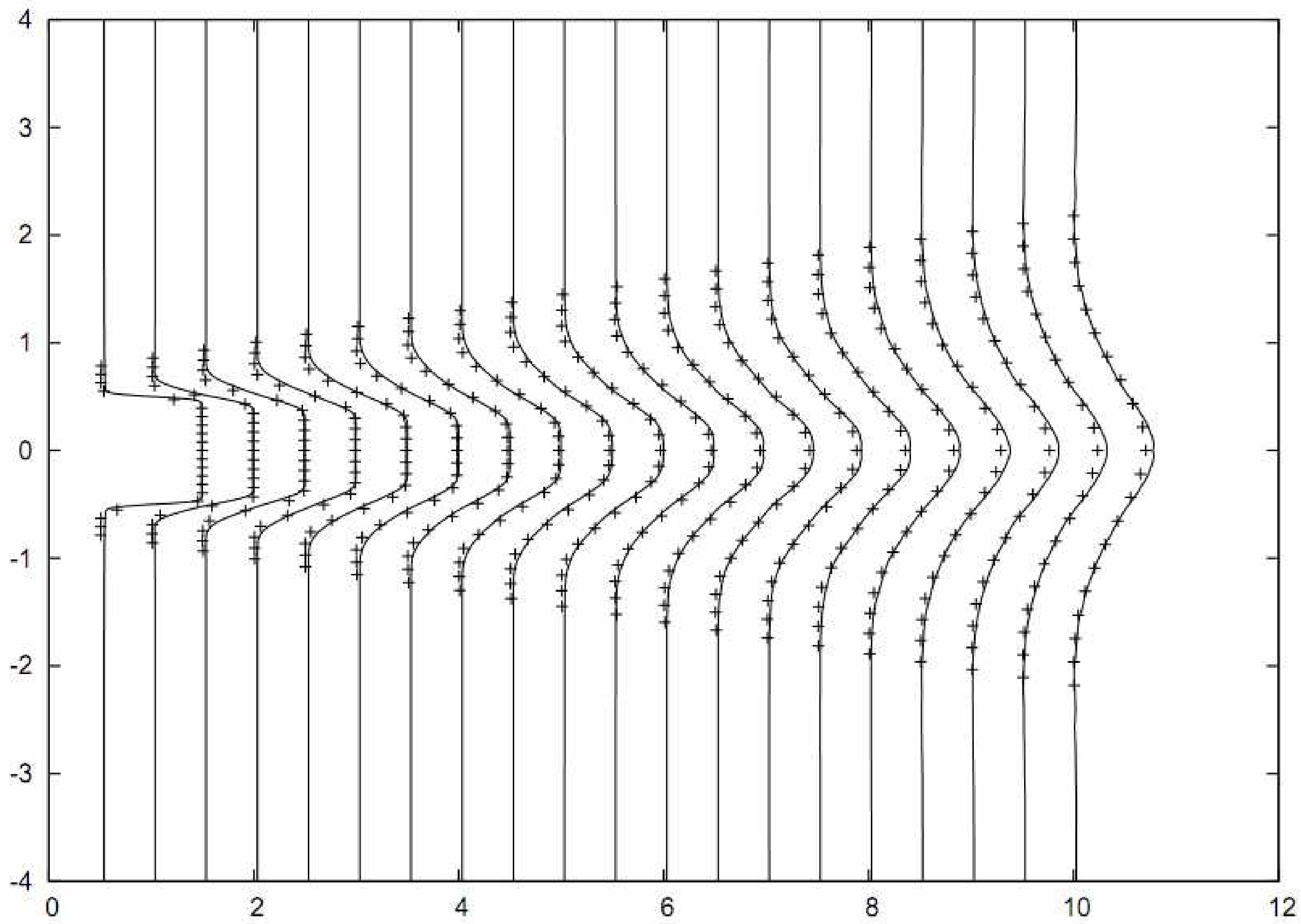
LES, Re=700 000



$\nu_0/\nu=1119 \rightarrow$



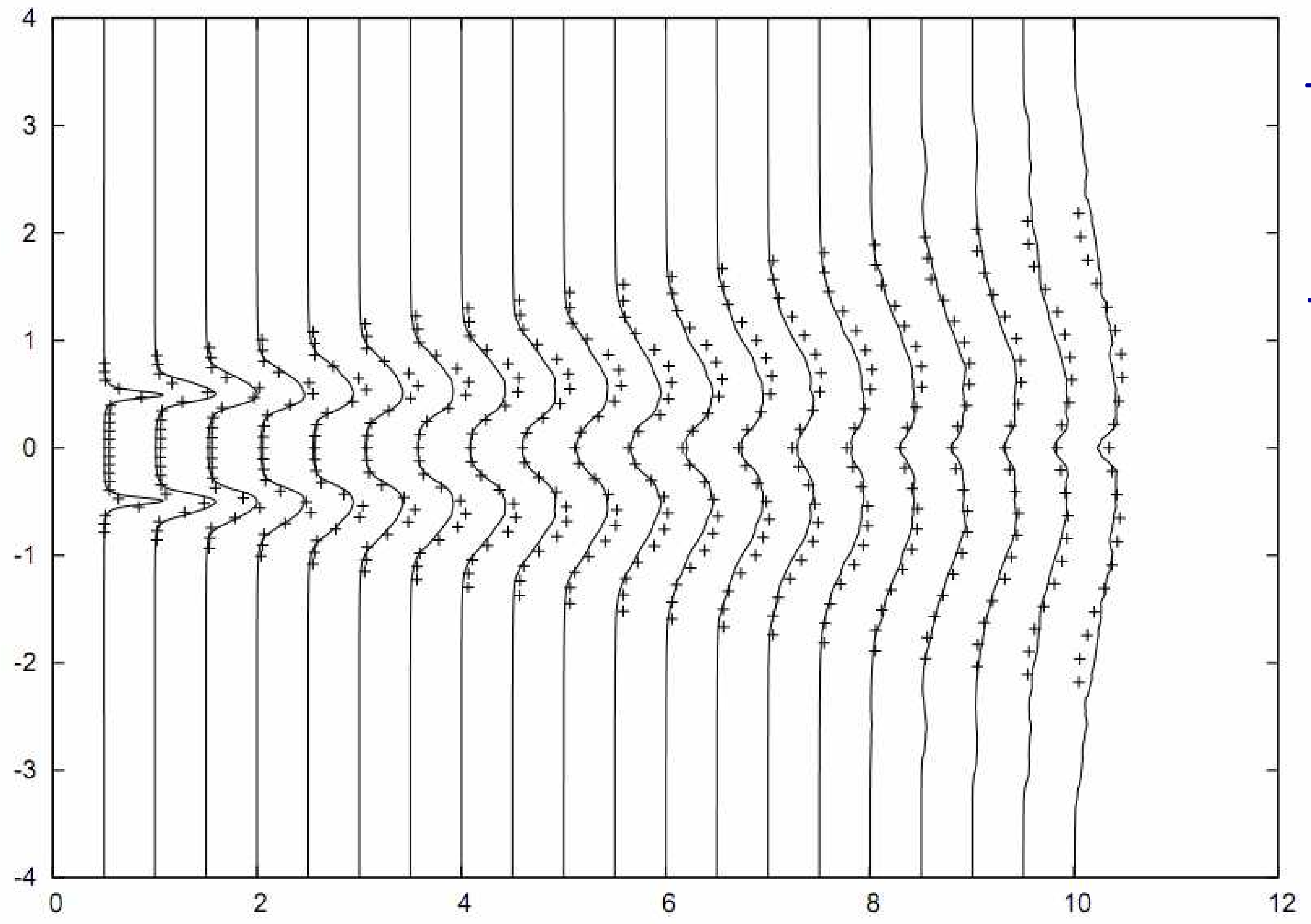
Mean velocity



+ : Exp. P'
Re=700 000

— : LES
Re=700 000

u'rms



+ : Exp. P'
Re=700 000

— : LES
Re=700 000

3D Taylor-Green flow

- Initial conditions

$$\begin{aligned} u_x(x,y,z,t_0) &= V_0 \sin\left(\frac{x}{L}\right)\cos\left(\frac{y}{L}\right)\cos\left(\frac{z}{L}\right) \\ u_y(x,y,z,t_0) &= -V_0 \cos\left(\frac{x}{L}\right)\sin\left(\frac{y}{L}\right)\cos\left(\frac{z}{L}\right) \\ u_z(x,y,z,t_0) &= 0 \end{aligned}$$

- 3D periodic computational domain $\Omega = [-\pi L; \pi L]^3$
- Reynolds number $Re = \dfrac{V_0 L}{\nu}$
- Total kinetic energy – enstrophy – dissipation

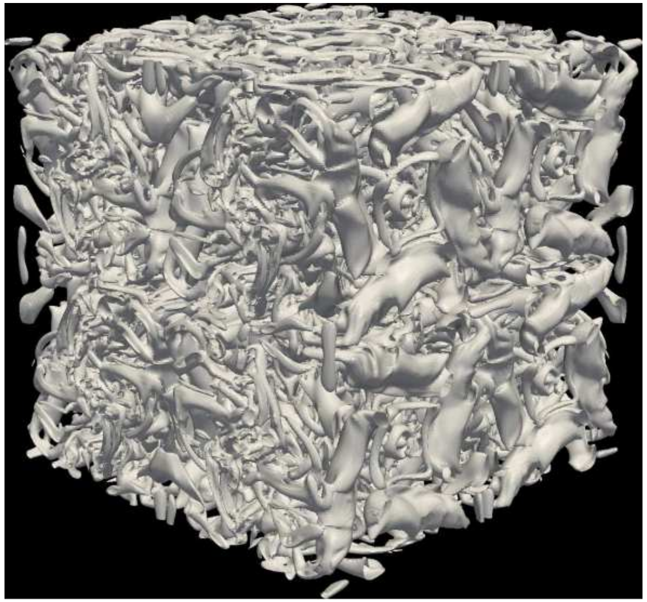
$$E_k = \frac{1}{\Omega}\int_\Omega \frac{\mathbf{u}.\mathbf{u}}{2} d\Omega \quad \xi = \frac{1}{\Omega}\int_\Omega \frac{\omega.\omega}{2} d\Omega \quad \epsilon = 2\mu\xi$$

3D Taylor Green

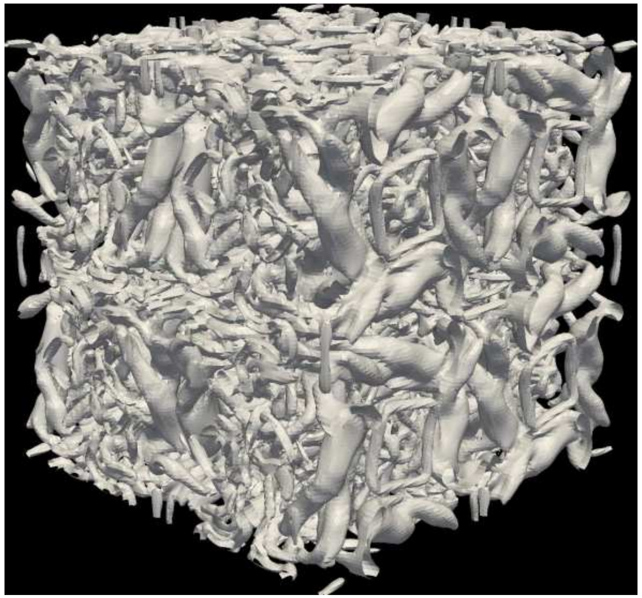
- DNS of reference : Re=1600, $n_x n_y n_z = 256^3$
- OK with results of Van Rees et al. (2011) (fully spectral DNS, $n_x n_y n_z = 512^3$)

Animation of Q criterion

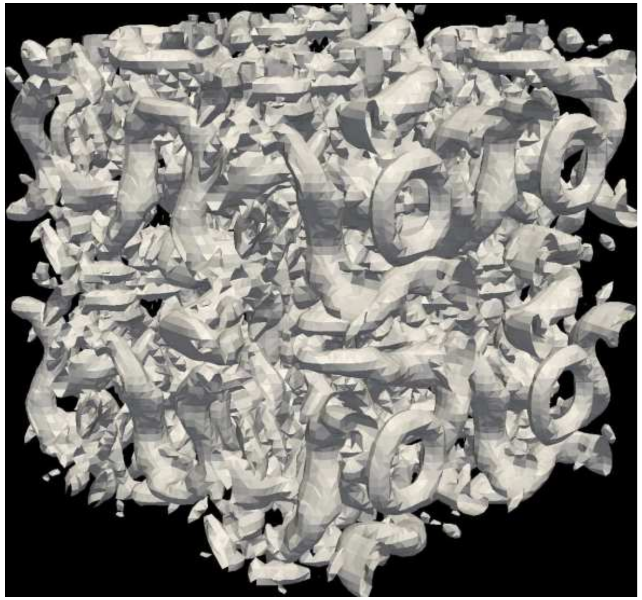
3D Taylor-Green flow



DNS 256^3



LES 128^3
O4 SVV
$\nu_0/\nu=34$

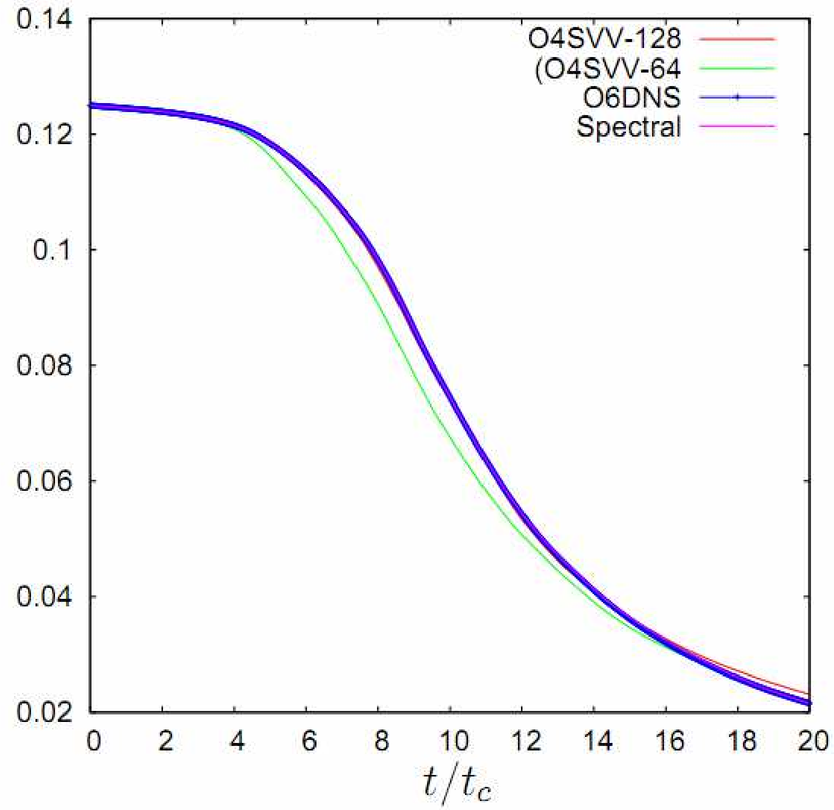


LES 64^3
O4 SVV
$\nu_0/\nu=89$

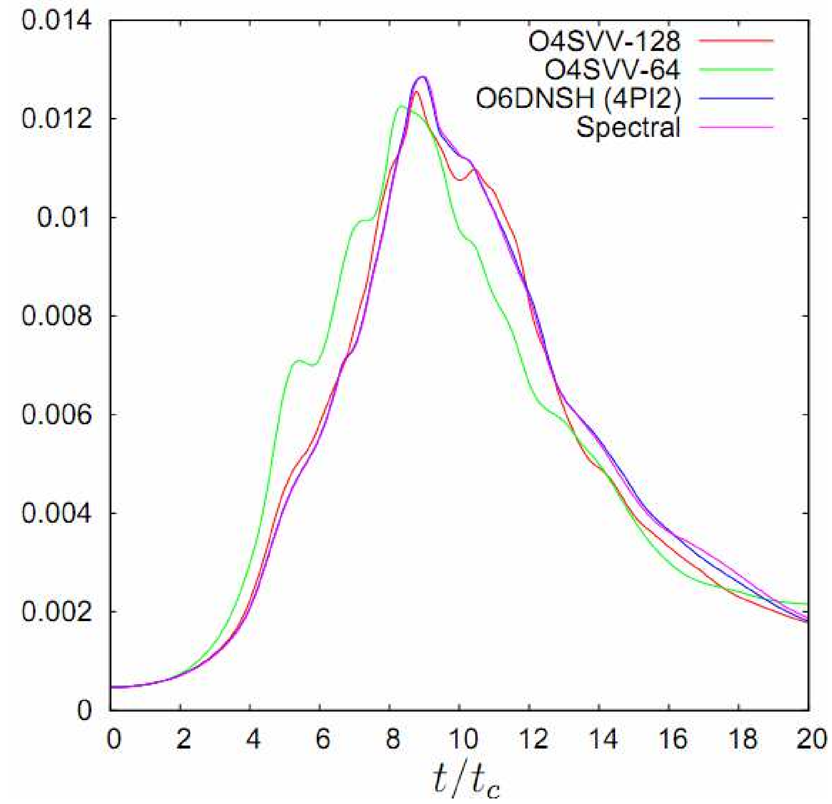
→ no spurious oscillations

3D Taylor-Green flow

$E_k(t)$



$\varepsilon_k(t)$

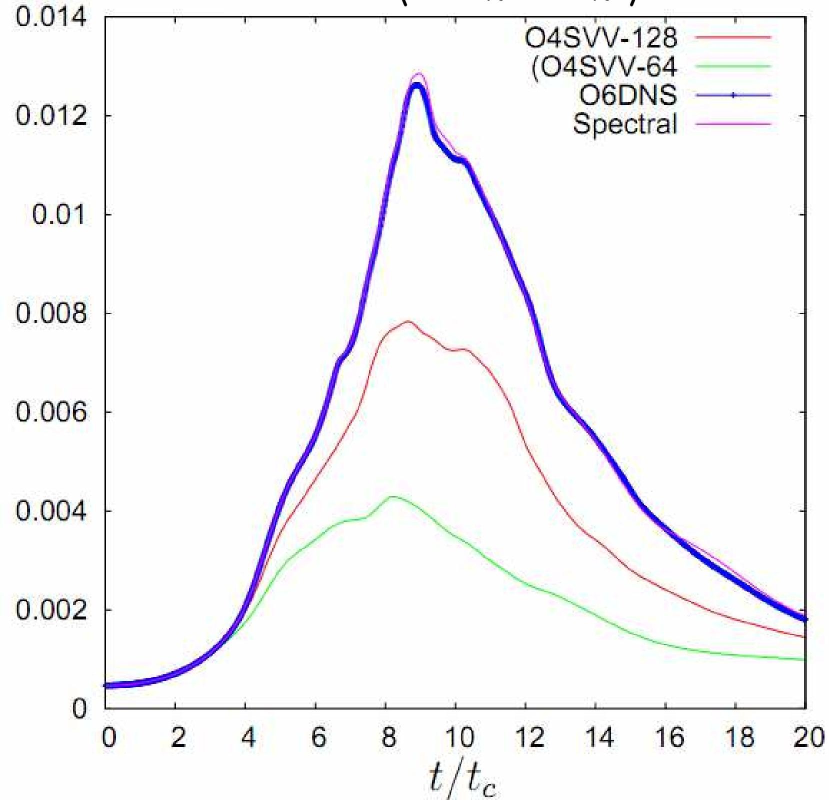


→ good reproduction of 1) the dissipation peak

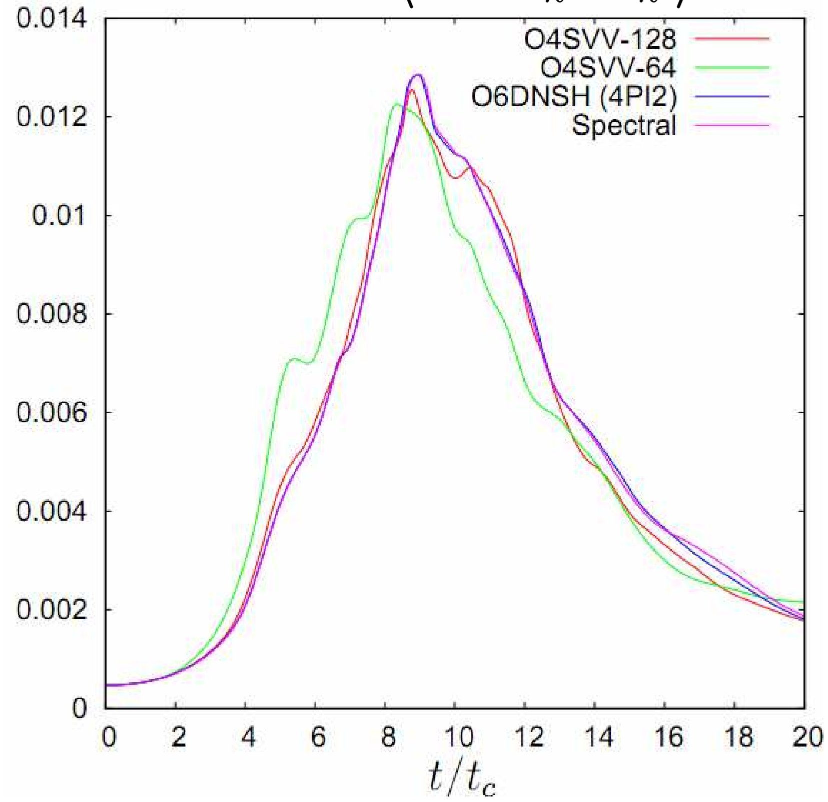
2) the resulting decrease of E_k

3D Taylor-Green flow

$$\varepsilon = \nu \left\langle \frac{\partial u'_i}{\partial x_k} \frac{\partial u'_i}{\partial x_k} \right\rangle$$



$$\varepsilon = -\nu \left\langle u'_i \frac{\partial^2 u'_i}{\partial x_k \partial x_k} \right\rangle$$



→ poor reproduction of the dissipation peak if the conventional definition of ε is used

→ subgrid scale modelling based on first derivatives should be avoided

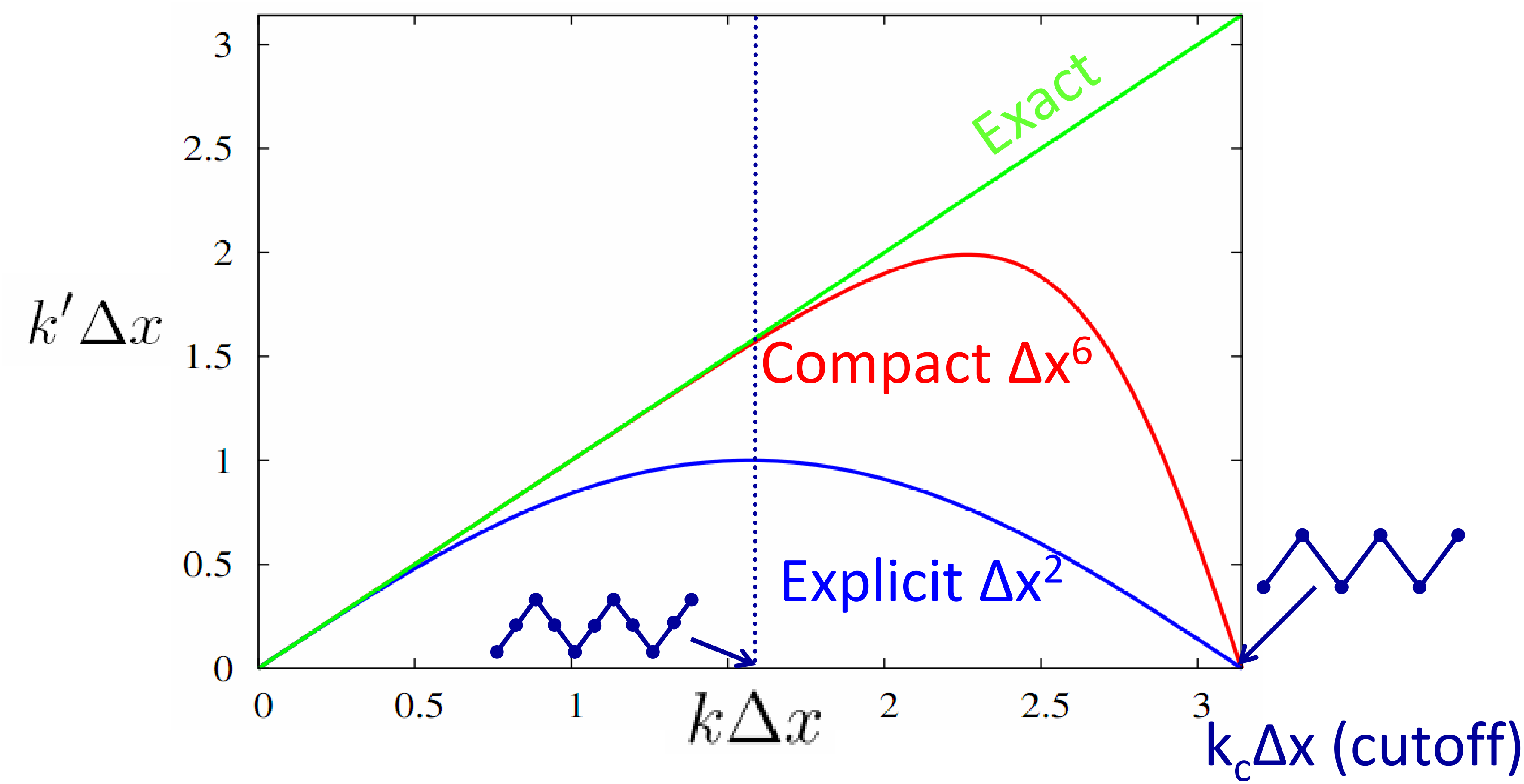
Conclusion
High-order numerical dissipation

- **Why?**
  - To control spurious oscillations (aliasing) in DNS
  - To mimic subgrid-scale model without any extra numerical error in LES
- **How?**
  - Via the viscous term (second derivatives)
  - Using the singularity of the modified wave number at the cutoff for a compact scheme
  - By calibration of the artificial dissipation assuming a Pao-like spectrum (physical subgrid-scale model)

Modified wave number k'

f=exp(ikx) → f'=ik'exp(ikx)

$$k'\Delta x = \frac{a\sin(k\Delta x) + (b/2)\sin(2k\Delta x)}{1 + 2\alpha\cos(k\Delta x)}$$



Resolution properties for a linear convection/diffusion equation

- Model equation

$$\frac{\partial u}{\partial t} = -c\,\frac{\partial u}{\partial x} + \nu \frac{\partial^2 u}{\partial x^2}, \qquad t \geq 0, -\infty < x < +\infty$$

- Exact solution

$$u(x,t) = \hat{u}_0 e^{\iota k(x-ct)}\, e^{-\nu k^2 t}$$

- Discrete solution using finite difference schemes

$$u(x_i,t) = \hat{u}_0 e^{\iota k\left(x_i - c\frac{k'}{k}t\right)}\, e^{-\nu k'' t}$$

where k’ and k’’ are the **modified wave numbers**

Resolution properties for a linear convection/diffusion equation

- Dispersion error

$$E_{disp} = k'_R/k - 1$$

- Dissipation error

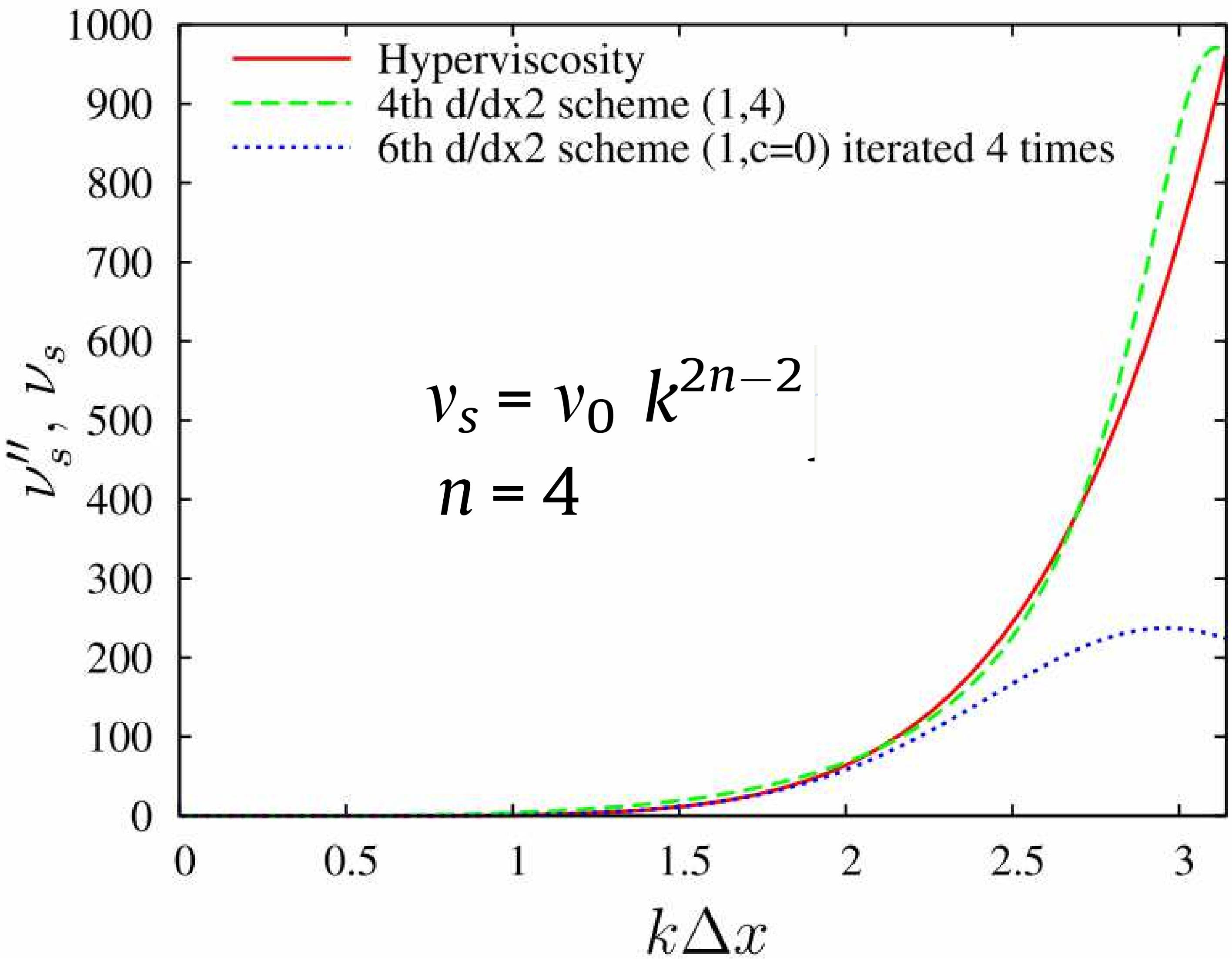
$$E_{diss} = \frac{k'' - k^2}{k^2} - Re_{\Delta x}\frac{k'_I}{k^2\Delta x}$$

where $Re_{\Delta x}$ is the mesh Reynolds number

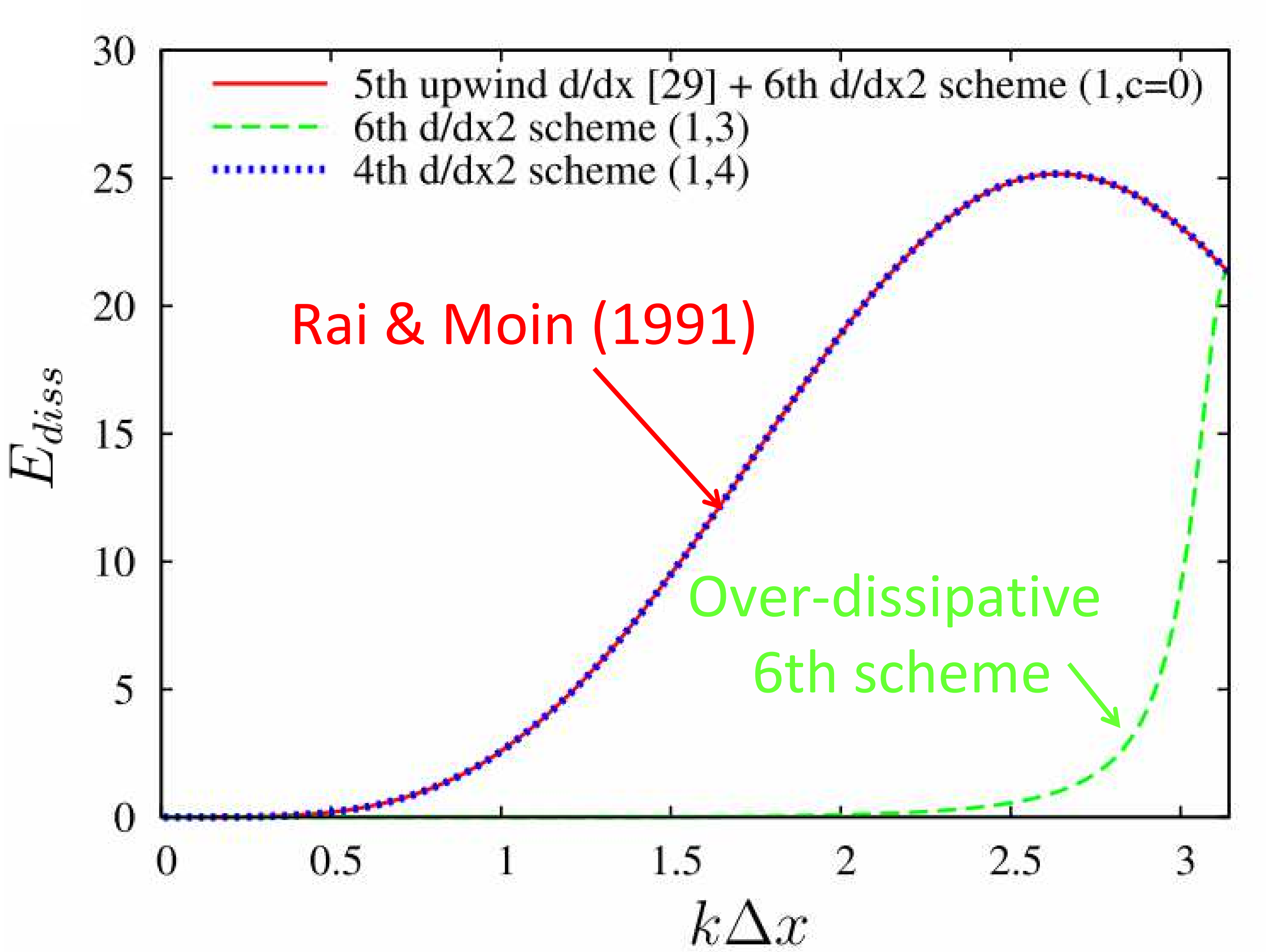
Remark: k' is complex for upwind schemes

$k'=k'_R+ik'_i$

Hyperviscosity

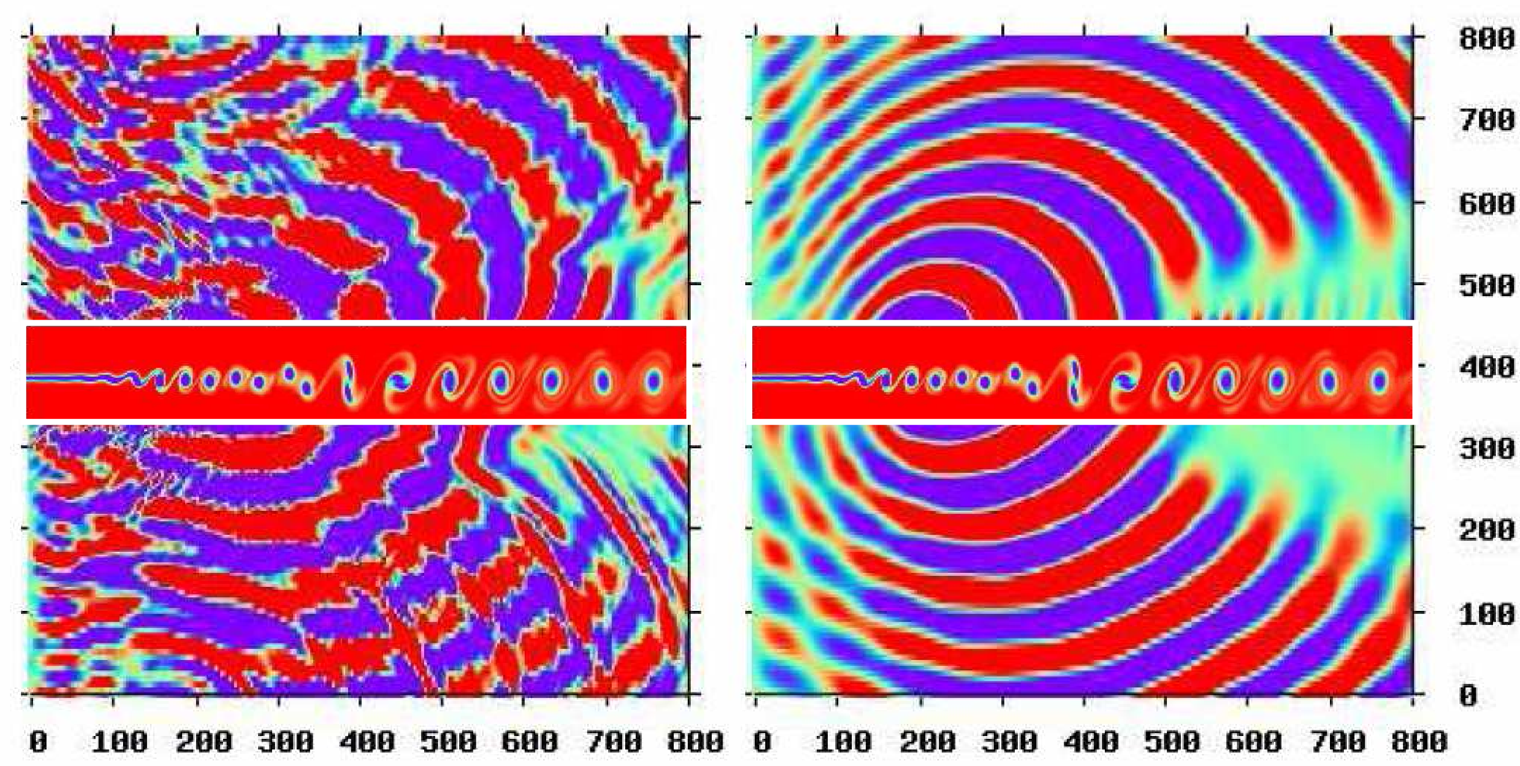


Comparison with an upwind approach



Control of spurious acoustic waves

Direct computation of sound
from a mixing layer using Compact3d



Without
extra-dissipation

With
extra-dissipation (6th)

$$n_x \times n_y = 1035 \times 431$$