ALTERNATIVE APPROACHES TO LARGE-EDDY SIMULATION – IMPLICIT LES*

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1. Introduction

1.1 Relation between SGS-stresses and truncation error

- example: viscous Burgers equation

$$\frac{\partial v}{\partial t} + \frac{\partial F(v)}{\partial x} = \mu \frac{\partial^2 v}{\partial x^2}$$

physical flux function: $F(v) = \frac{v^2}{2}$

- projection onto grid (discretization of the solution, continuous operators):

$$\frac{\partial v_N}{\partial t} + \frac{\partial F(v_N)}{\partial x} = \mu \frac{\partial^2 v_N}{\partial x^2} + \mathcal{G}_{SGS}$$

SGS error: $\mathcal{G}_{SGS} = \frac{1}{2} \frac{\partial (v_N^2 - v^2)}{\partial x}$

- numerical approximation of the Burgers equation (discretization of operators):

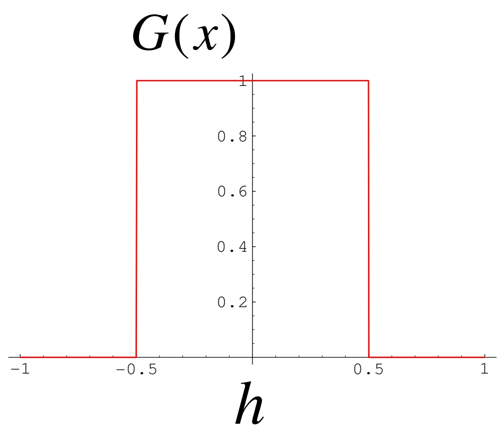
$$\frac{\partial \bar{u}_N}{\partial t} + G * \frac{\partial \tilde{F}_N(\tilde{u}_N)}{\partial x} = \mu \frac{\delta^2 \bar{u}_N}{\delta x^2}$$

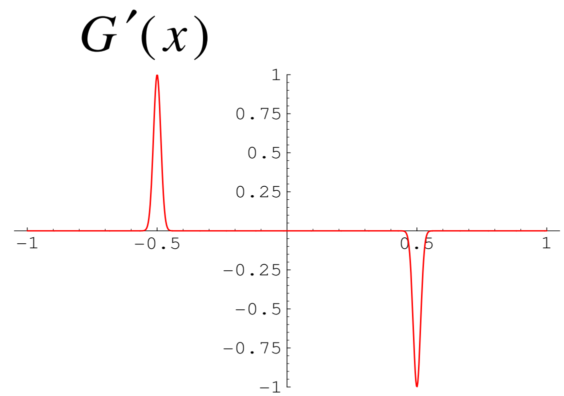
1. Introduction

- most obvious connection between filtering approach and numerical discretization: finite-volume method

- finite-volume tools:

  - volume averaging = top-hat filter





  - reconstruction = approximate deconvolution : $\tilde{u}_N \doteq u_N$

  - consistent numerical flux function: $\tilde{F}_N$

1. Introduction

- re-write discretized Burgers equation (modified differential equation):

$$\frac{\partial \bar{u}_N}{\partial t} + G * \frac{\partial F(u_N)}{\partial x} = \mu \frac{\delta^2 \bar{u}_N}{\delta x^2} + \mathcal{G}_N$$

- truncation error:

$$\mathcal{G}_N = G * \frac{\partial F(u_N)}{\partial x} - G * \frac{\partial \tilde{F}_N(\tilde{u}_N)}{\partial x}$$

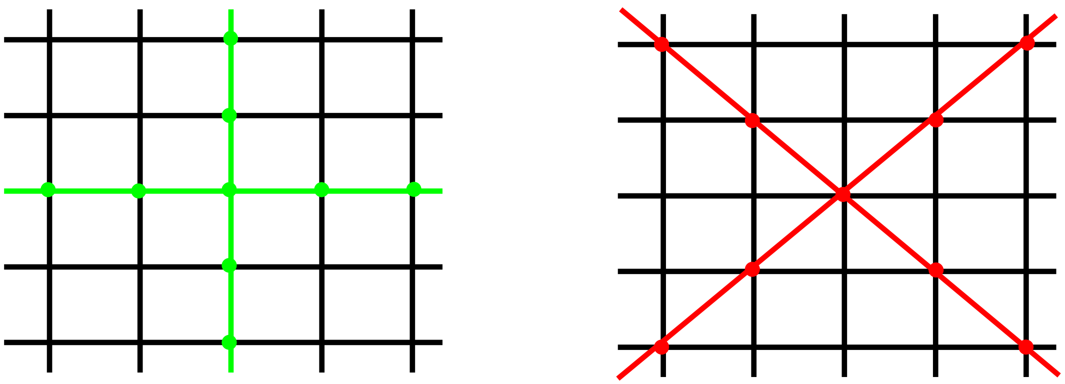
- if $\mathcal{G}_N$ approximates $\bar{\mathcal{G}}_{SGS}$ *in some sense* for finite h the truncation error constitutes an implicit SGS model
- if $\mathcal{G}_N$ does not approximate $\bar{\mathcal{G}}_{SGS}$ it will interfere with an explicit model if not h is made small enough (spectral or high-order methods or explicit filtering)

1.2 Intermediate conclusion:

- LES is the extension of numerical approximation theory to finite h, where the asymptotic convergence range has not been reached
- instead of making the truncation error vanish, now the issue is to design the truncation error such that a physically relevant coarse-grained solution is obtained
- note the relation to entropy regularizations for shock-capturing schemes (e.g. vanishing viscosity concept):
  in order to obtain a proper weak solution the truncation error has to cause a positive entropy contribution

1.3 Current competing approaches

- multidirectional upwinding (Kawamura & Kuwahara 1984)



$$\frac{\delta u_N}{\delta x_i} = \frac{2}{3}\frac{\delta^{upwind} u_N}{\delta x_i} + \frac{1}{3}\frac{\delta^{upwind} u_N}{\delta x_i}$$

1. Introduction

- Flux-Corrected Transport (Boris & Grinstein 1992)

$$\tilde{u}_N = \tilde{u}_N^{ho} - \left(1 - \Gamma(\overline{u}_N)\right)\left(\tilde{u}_N^{ho} - \tilde{u}_N^{lo}\right)$$

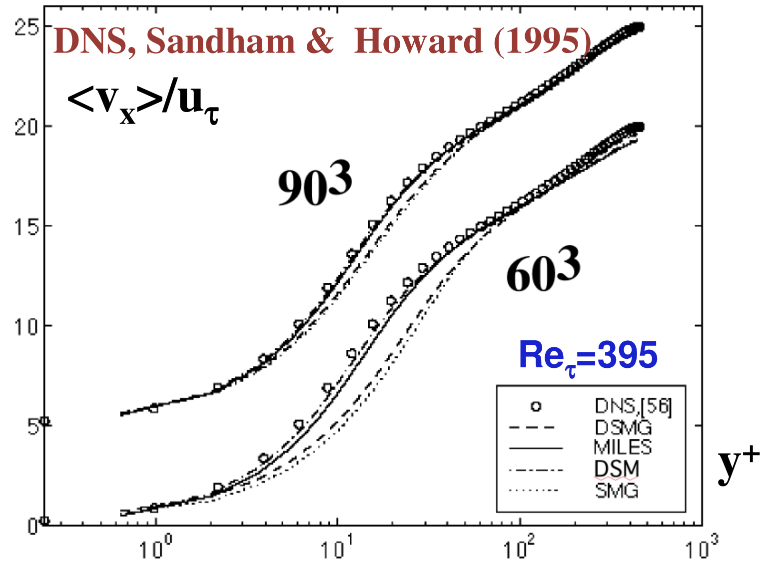
$$0 \leq \min\left(\left|\Gamma(r)\right|, \left|\Gamma(r)/r\right|\right) \leq 2$$

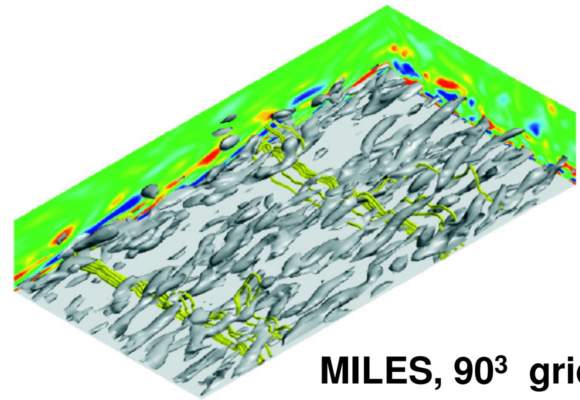
r some measure of density gradients

- Riemann solvers (Porter & Woodward 1998)
- MPDATA (Margolin & Smolarkiewicz 1998)
- Spectral vanishing viscosity (Tadmor 1990)

Channel Flow Simulations

Fureby & Grinstein, JCP (September 2002)





MILES, 90^3 grid

typical computational cost:
SMG=1, DSMG=1.2, DSM=1.60, MILES=0.90

MILES : FCT-based
DSM : Differential Stress Model
SMG : Smagorinsky Model
DSMG : Dynamic Smagorinsky Model

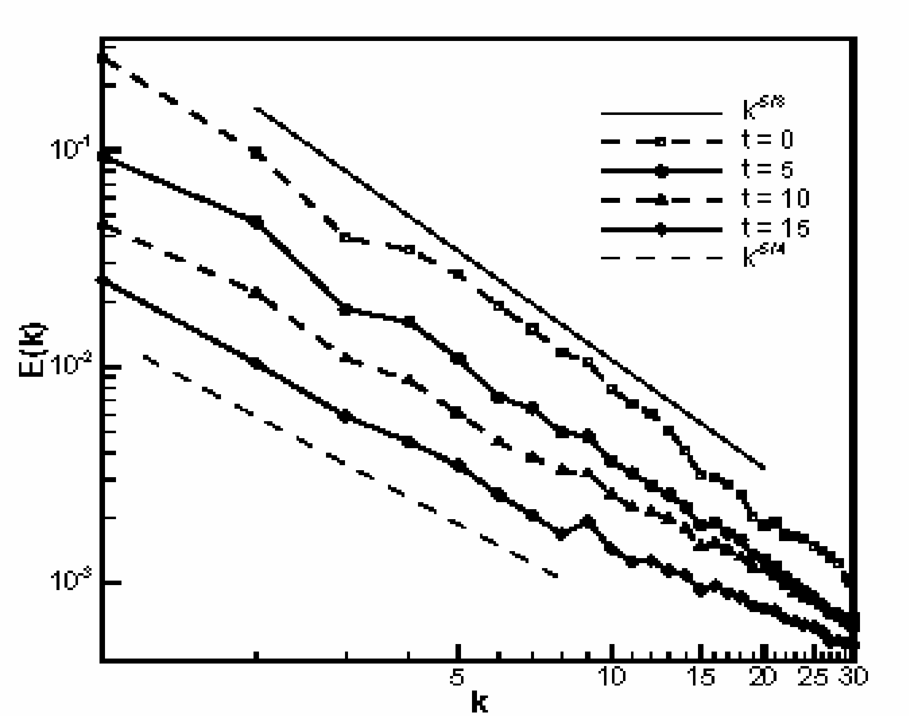
MILES reproduces first & second order moments of the velocity field

- almost as accurately as significantly more-complex SGS models
- better than isotropic eddy viscosity models

1. Introduction

- prediction of MPDATA (Smolarkiewicz, Margolin, 1998), results of Domaradzki, Radakrishnan, 2004

3D energy spectrum



2. ALDM – an enviromnent for implicit SGS model design

2.1 ALDM based on high-order finitve-volume methods

- consider 1D – adaptive local deconvolution method (ALDM), A., Hickel, Franz, JCP 2004

$$\frac{\partial u}{\partial t} + \frac{\partial F(u)}{\partial x} = 0 \qquad \frac{\partial \bar{u}_N}{\partial t} + \frac{\tilde{F}_N(\tilde{u}_N)\big|_{h/2} - \tilde{F}_N(\tilde{u}_N)\big|_{-h/2}}{h} = 0$$

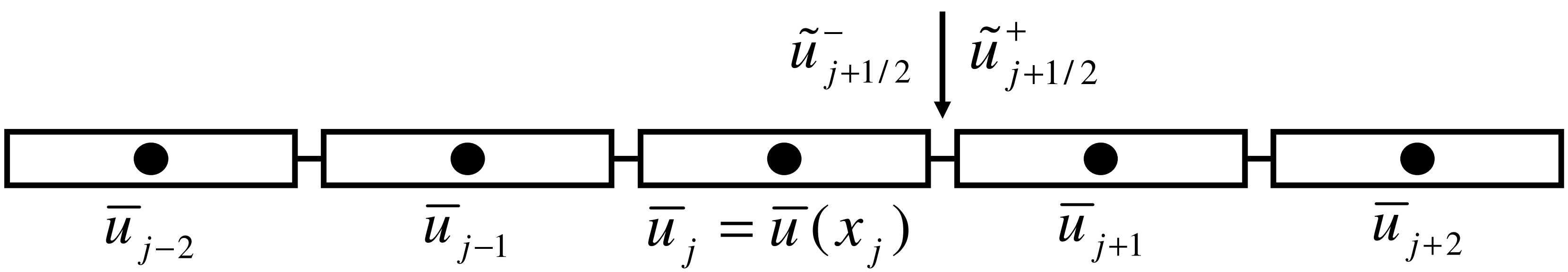
finite volume discretisation

- approximation of the unfiltered solution $\tilde{u}_{j+1/2}$ from $\left\{\bar{u}_{j+\mu}\right\}_{\mu=-\mu_l}^{\mu_r}$
- reconstruction on space of local interpolation polynomials of order at most k $\Leftrightarrow$ local deconvolution (Harten, 1987)

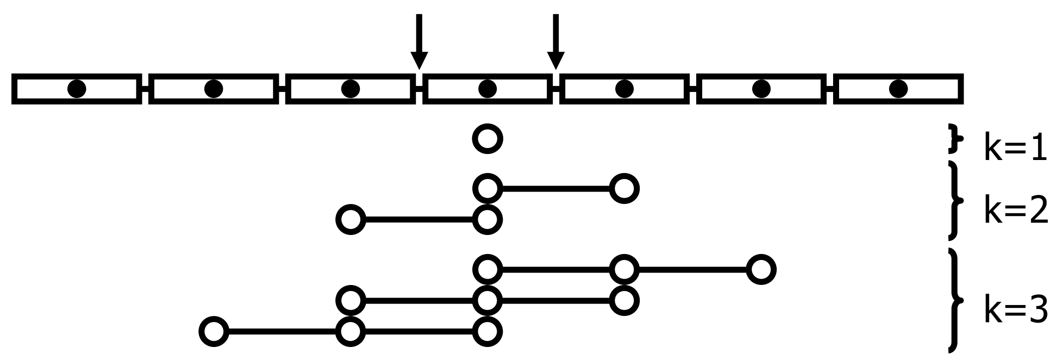
2. ALDM – an enviromnent for implicit SGS model design

- consistent numerical flux-function

$$\tilde{F}(x_{j+1/2}) = F\left(\frac{\tilde{u}^{+}_{j+1/2} + \tilde{u}^{-}_{j+1/2}}{2}\right) - \sigma_{j+1/2}\left(\tilde{u}^{+}_{j+1/2} - \tilde{u}^{-}_{j+1/2}\right)$$



- admissible interpolation polynomials for deconvolution



2. ALDM – an enviromnent for implicit SGS model design

- approximation polynomials

$$p^{\pm}_{k,r}(x_{j\mp 1/2}) = \sum_{l=0}^{k-1} c^{\pm}_{k,r,l}(x_j) \quad \bar{u}_{j-r+l}$$

- adaptive local interpolation

$$\tilde{u}^{\pm}(x_{j\mp 1/2}) = \sum_{k=1}^{K} \sum_{r=0}^{k} \omega^{\pm}_{\mathrm{k,r}}(x_j) p^{\pm}_{\mathrm{k,r}}(x_{j\mp 1/2})$$

- weight factors $\omega^{\pm}_{\mathrm{k,r}}$ contain

  - smoothness measure $\beta = \sum_{\mu=-r}^{k-r-2} \left| \bar{u}_{j+\mu+1} - \bar{u}_{j+\mu} \right|$

  - model parameter $\gamma^{\pm}_{k,r}$, $\sigma_{j+1/2}$

2.2 Example: Burgers equation

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} = \nu \frac{\partial^2 u}{\partial x^2}$$

- modified differential equation analysis (MDEA) provides :
  - identification of the implicit SGS model
  - determination of the model parameters

2. ALDM – an enviromnent for implicit SGS model design

- explicit Smagorinsky model $\overline{\mathcal{G}}_{SGS} = 2C_S h^2 \left|\frac{\partial \overline{u}}{\partial x}\right| \frac{\partial^2 \overline{u}}{\partial x^2}$

- implicit representation by suitable choice of parameters

$$\mathcal{G}_N = 2C_S \left|\frac{\partial \overline{u}}{\partial x}\right| \frac{\partial^2 \overline{u}}{\partial x^2} h^2 - \frac{1}{6} C_S \left|\frac{\partial \overline{u}}{\partial x}\right| \frac{\partial^4 \overline{u}}{\partial x^4} h^4 + O(h^6)$$

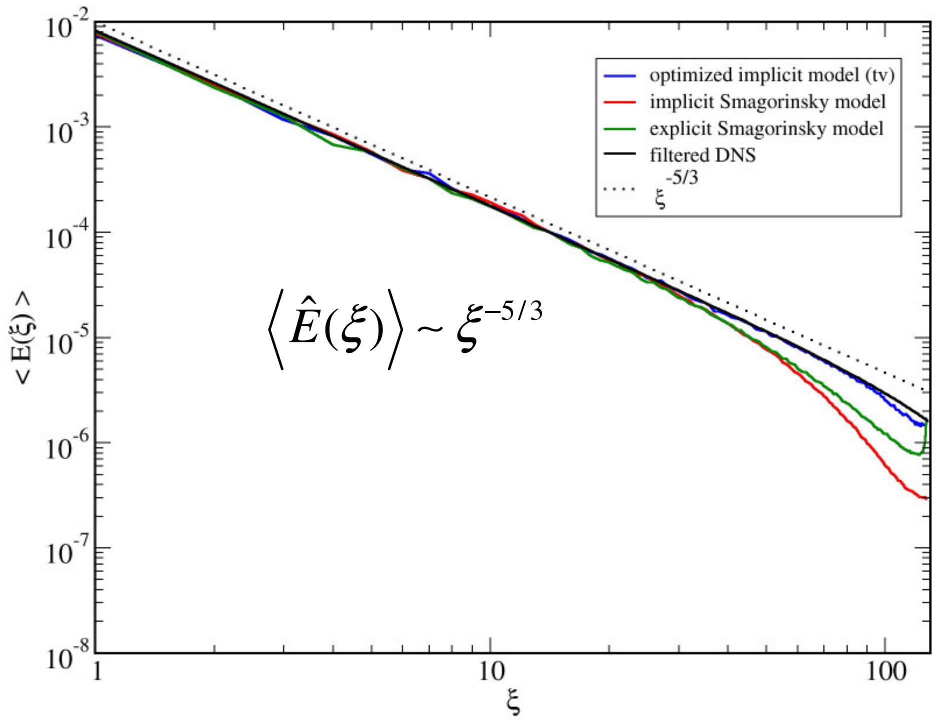
- parameters determined by evolutionary optimization

$$\varepsilon_N = \left(-0.111 \left(\frac{\partial \overline{u}}{\partial x} \frac{\partial^2 \overline{u}}{\partial x^2} + \overline{u} \frac{\partial^3 \overline{u}}{\partial x^3} \right) + 0.667 \left| \frac{\partial \overline{u}}{\partial x} \right| \frac{\partial^2 \overline{u}}{\partial x^2} \right) h^2 + O(h^4)$$

- Burgers equation with broad-band forcing (Cheklov, Yakhot, 1995)

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} = \nu \frac{\partial^2 u}{\partial x^2} + f(x,t)$$

$$\hat{f}(\xi,t) = 0.04 \frac{1}{\sqrt{|\xi|\tau}} \mathrm{e}^{i\varphi}$$



3. ALDM for 3D Navier-Stokes Equations

3.1 Extension of ALDM framework to 3D

- several approximations for deconvolution in the transverse directions
- isotropy of resulting scheme results in 5 independent model parameters
- one-dimensional model for Burgers equation cannot be used
- for details refer to Hickel, Adams, Domaradzki, "An adaptive local deconvolution method for implicit LES", JCP 2005, to appear

3.2 3D Model development

- physical-space modified-differential-equation analysis infeasible
- truncation error can be expressed as spectral numerical viscosity
- MDEA for 3D energy spectrum

3. ALDM for 3D Navier-Stokes Equations

- model parameters determined by evolutionary optimization
- optimization target is minimum deviation from spectral eddy viscosity for isotropic turbulence
- prediction by E.D.Q.N.M. (Chollet, 1984)

$$\nu(\xi / \xi_C) = 0.441 C_K^{-3/2} \sqrt{\frac{E(\xi_C)}{\xi_C}} \left(34.47\, e^{3.03 \xi_C / \xi}\right)$$

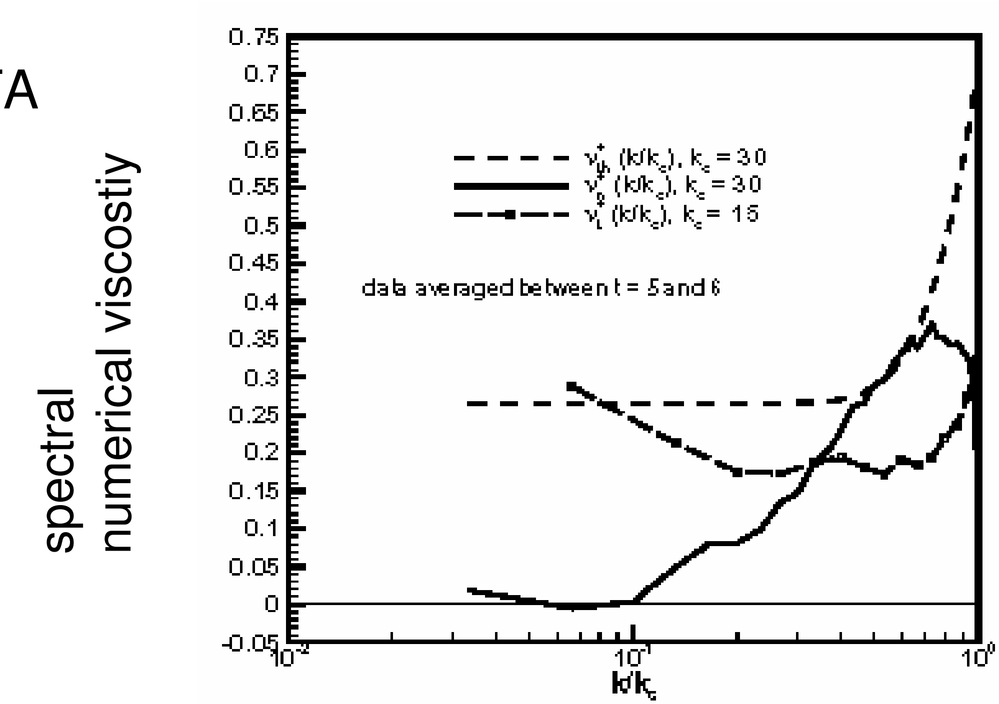
- modified-differential-equation for 3D energy spectrum

$$\frac{\partial E(\xi)}{\partial t} - T(\xi) + 2\nu\xi^2 E(\xi) = \hat{G}^{-1}(\xi) \int_{|\underline{\xi}|=\xi} \underline{\hat{u}}_N^*(\underline{\xi}) \cdot \underline{\mathcal{G}}_N(\underline{\xi})\, d\underline{\xi}$$

- spectral numerical viscosity

$$2\nu_{num}(\xi)\,\xi^2\,E(\xi) = \hat{G}^{-1}(\xi)\int_{|\underline{\xi}|=\xi} \underline{\hat{u}}_N^*(\underline{\xi})\cdot\underline{\mathcal{G}}_N(\underline{\xi})\,d\underline{\xi}$$

- prediction by MPDATA



- model parameters – optimization results

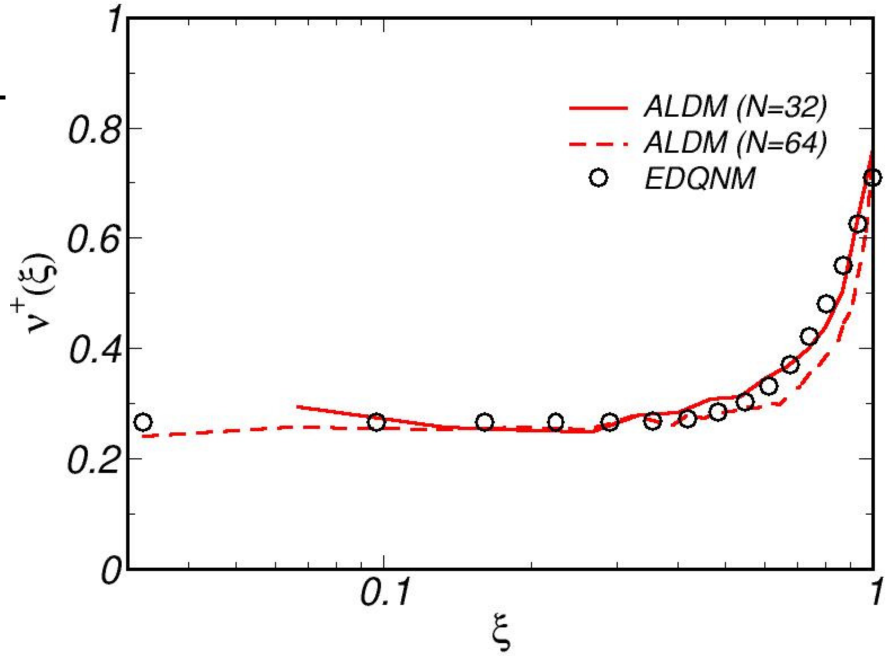
Best.

fitness	0.0054850
γ_{31}^{o}	0.0500300
γ_{21}^{+}	1.0000000
γ_{31}^{+}	0.0855000
γ_{32}^{+}	0.0190200
σ_A	0.0689100

Average of upper 50.

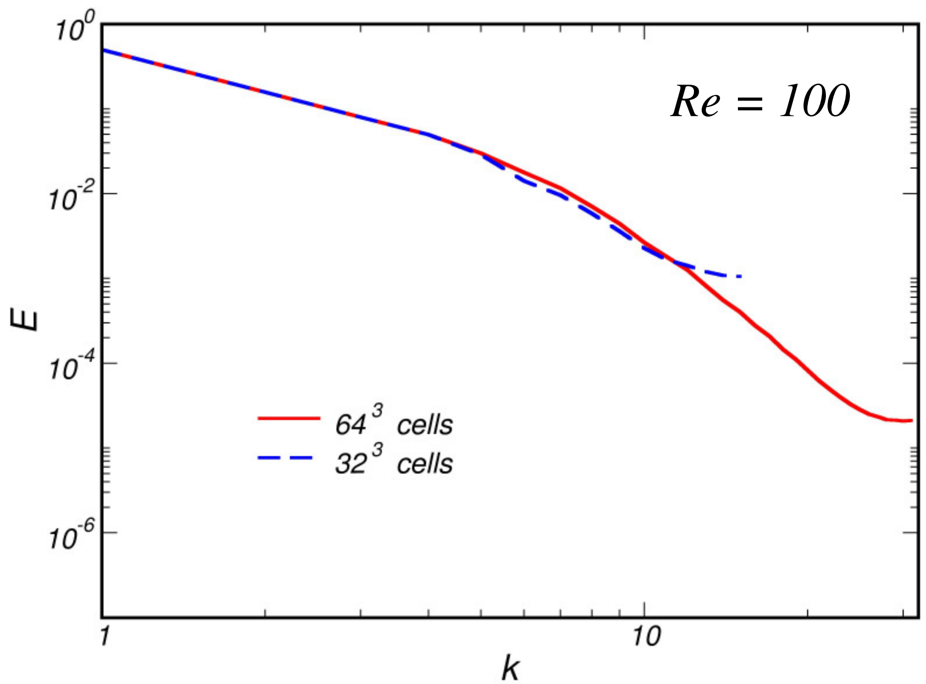
fitness	0.0054860 $\pm$0.0000004	($\pm$0.0 %)
γ_{31}^{o}	0.0501310 $\pm$0.0001948	($\pm$0.4 %)
γ_{21}^{+}	1.0000000 $\pm$0.0000000	($\pm$0.0 %)
γ_{31}^{+}	0.0845990 $\pm$0.0001628	($\pm$0.2 %)
γ_{32}^{+}	0.0189470 $\pm$0.0001435	($\pm$0.8 %)
σ_A	0.0689194 $\pm$0.0000965	($\pm$0.1 %)

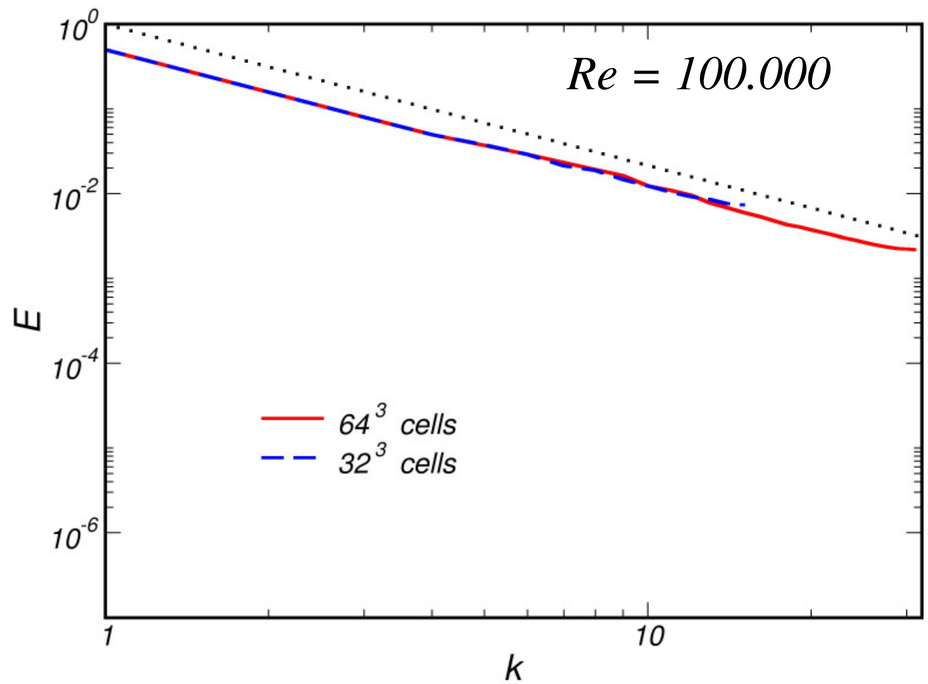
- model parameters – optimization results



4.1 Forced isotropic turbulence

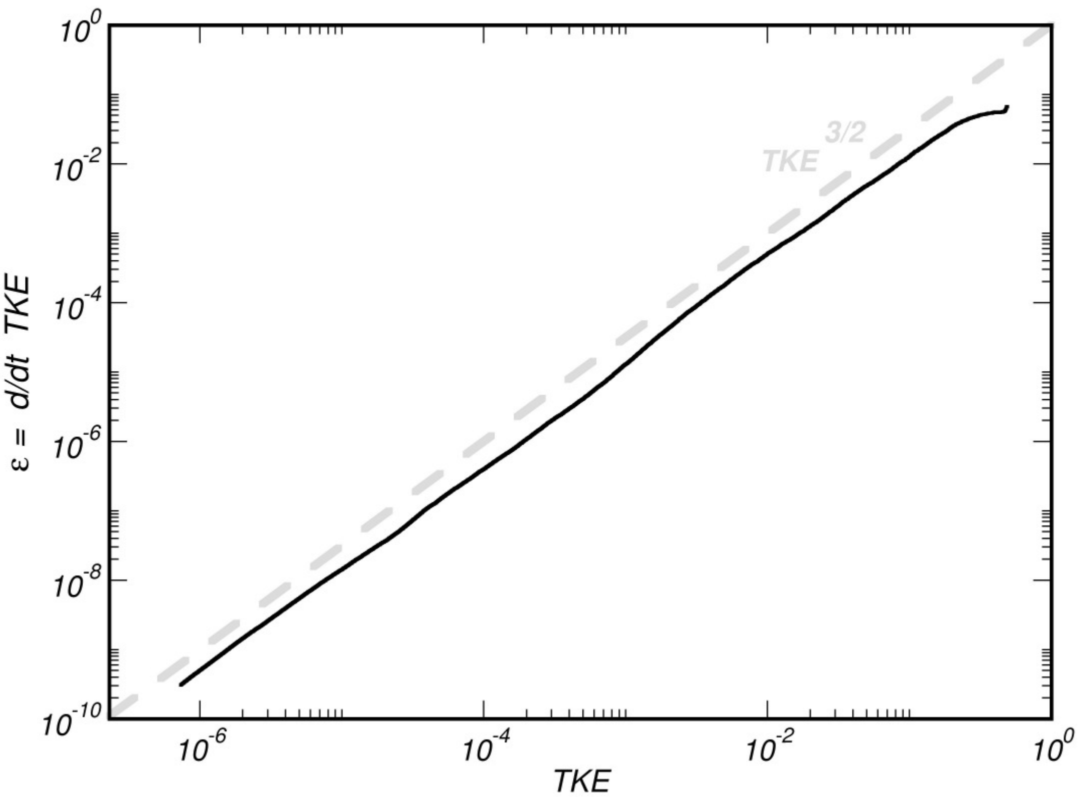
- 3D energy spectra





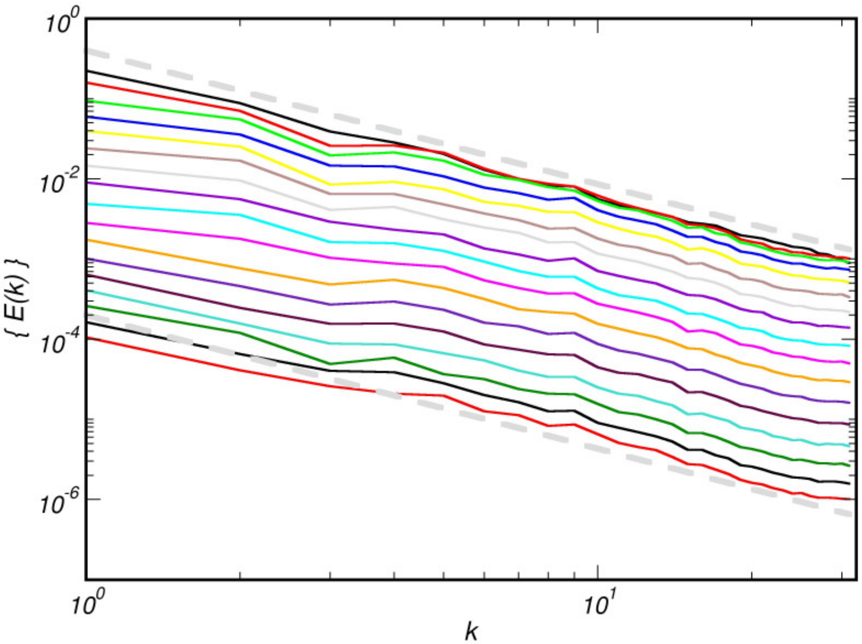
4.2 Decaying isotropic turbulence in the limit of vanishing viscosity

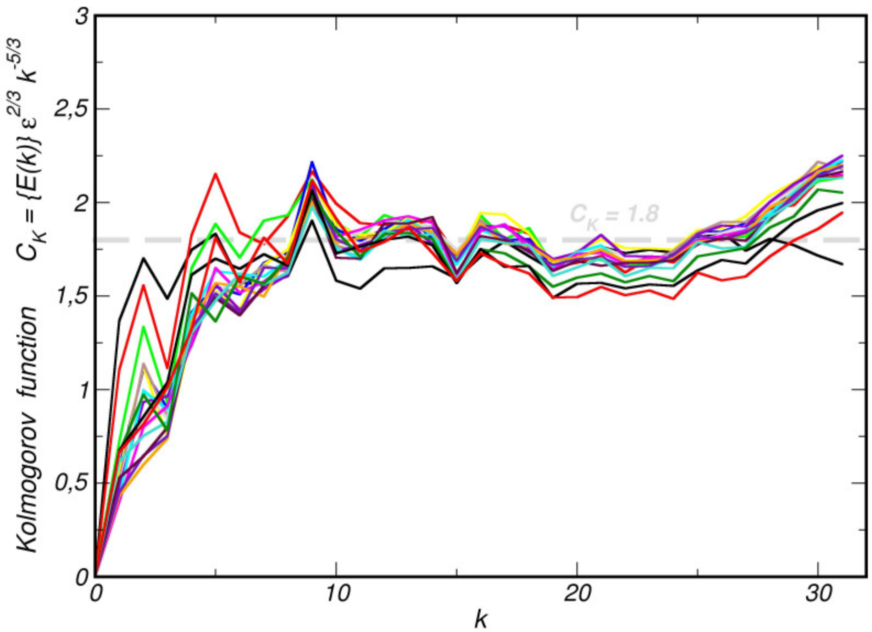
- dissipation rate vs. turbulent kinetic energy



4. ALDM Validation

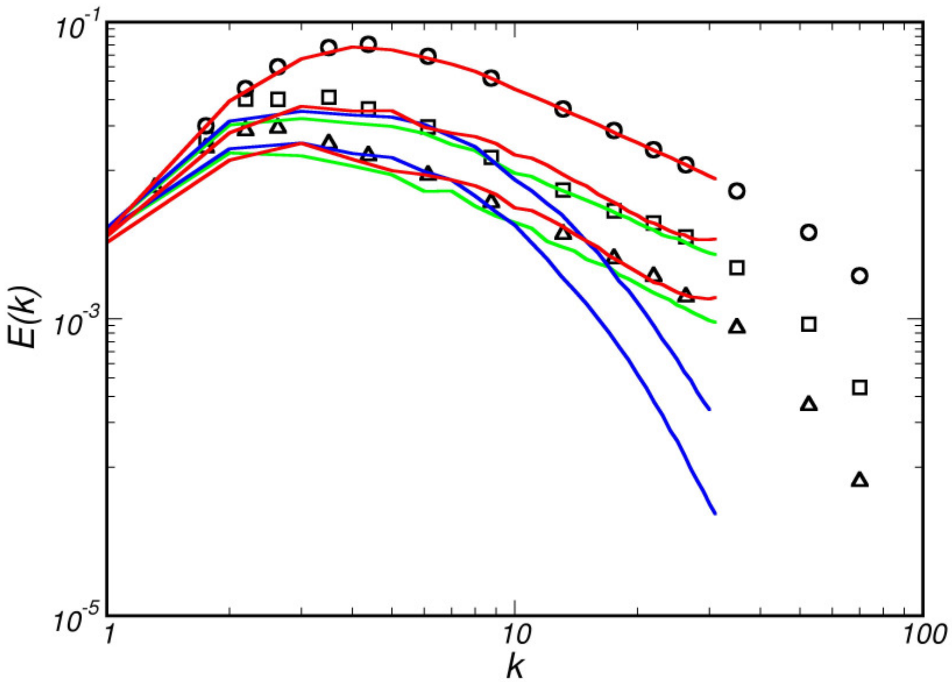
- 3D energy spectra, temporal evolution
- compensated spectra, temporal evolution





4.3 Decaying isotropic turbulence at finite Reynolds number

- case of Comte-Bellot, Corrsin (1971)
- resolution 64^3
- Reynolds number $Re_\lambda = 72 \cdots 50$



3-d energy spectra at three positions or times, respectively (tU_0/M = 42, 98 and 171).

symbols: measurements

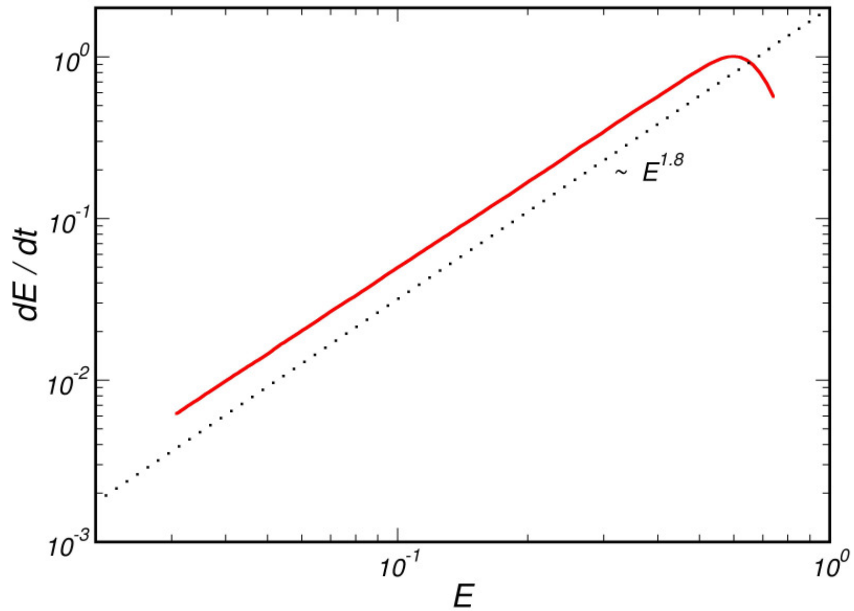
Smagorinsky model (C_S=0.10)

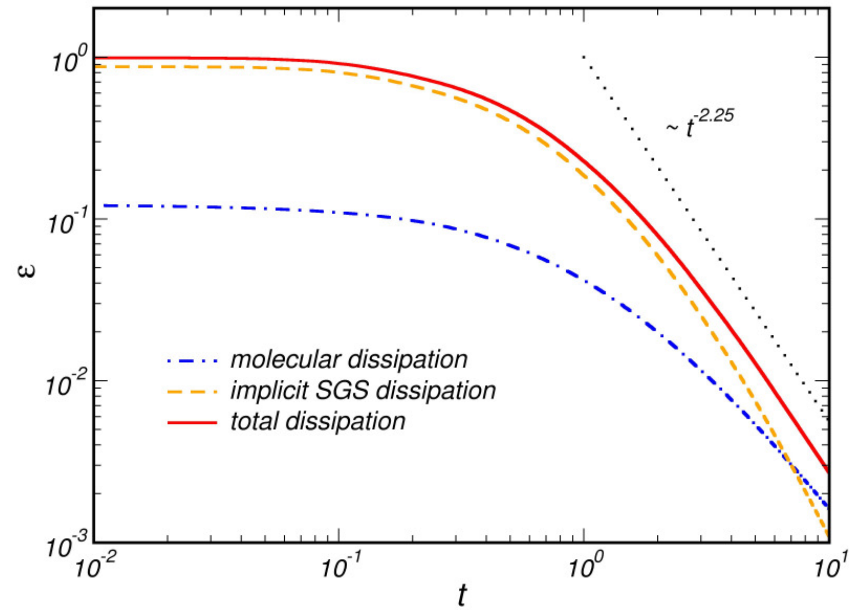
dynamic Smagorinsky model

ALDM

4. ALDM Validation

- dissipation rate vs. turbulent kinetic energy
- contributions to the dissipation rate

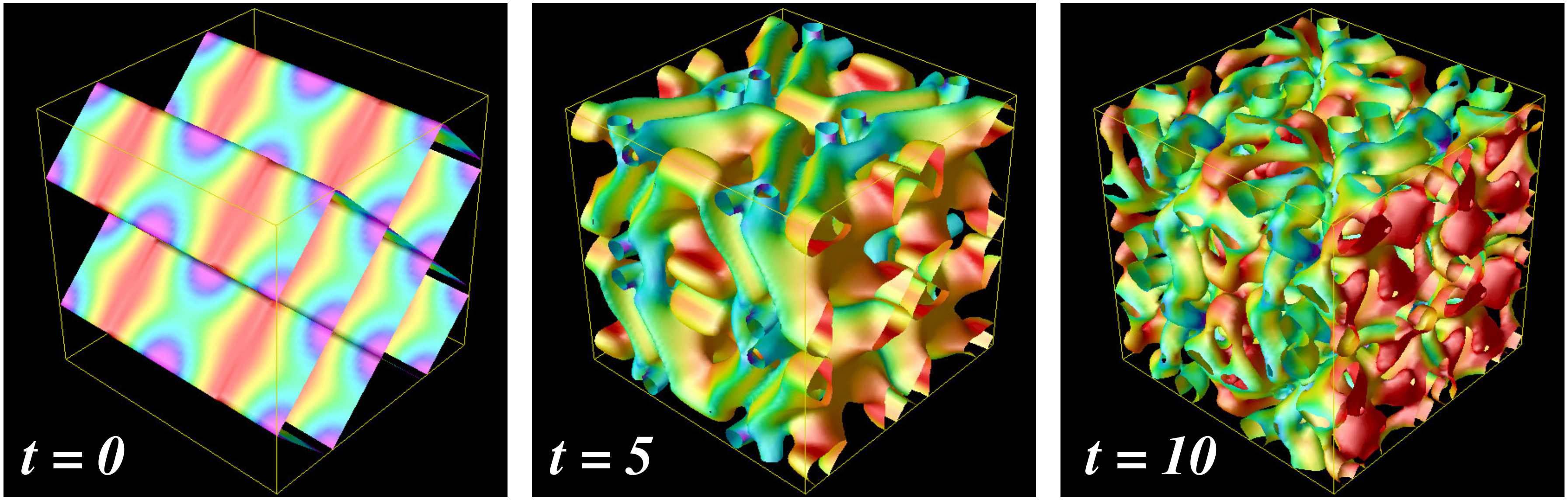




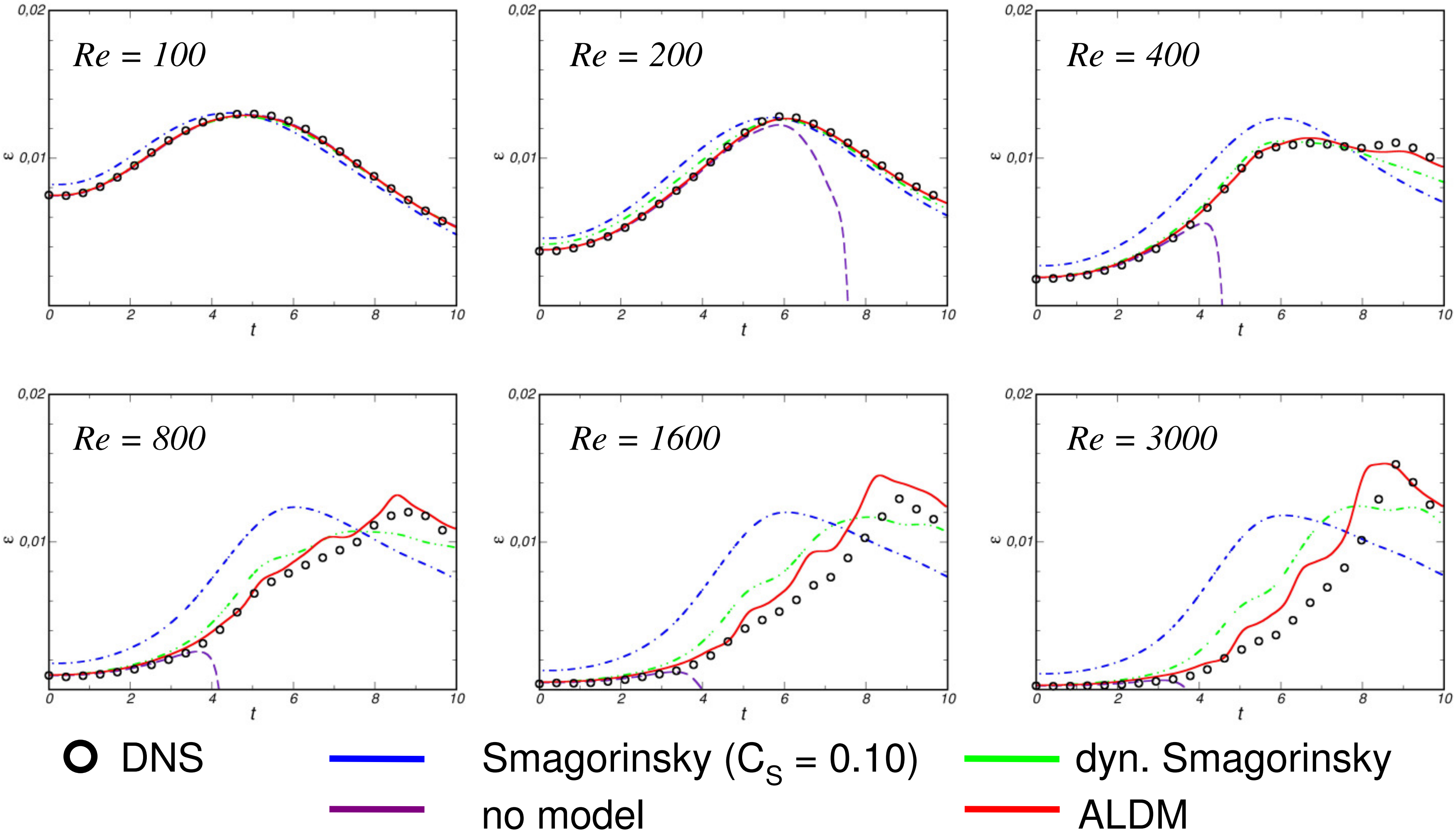
- found $\varepsilon \sim E^{1.8}$ equivalent to $E \sim t^{1.25}$ and $\varepsilon \sim t^{2.25}$
- reasonable agreement with experimentally obtained power laws $E \sim t^{1.21}$ to $E \sim t^{1.25}$

4.4 3D Taylor-Green vortex

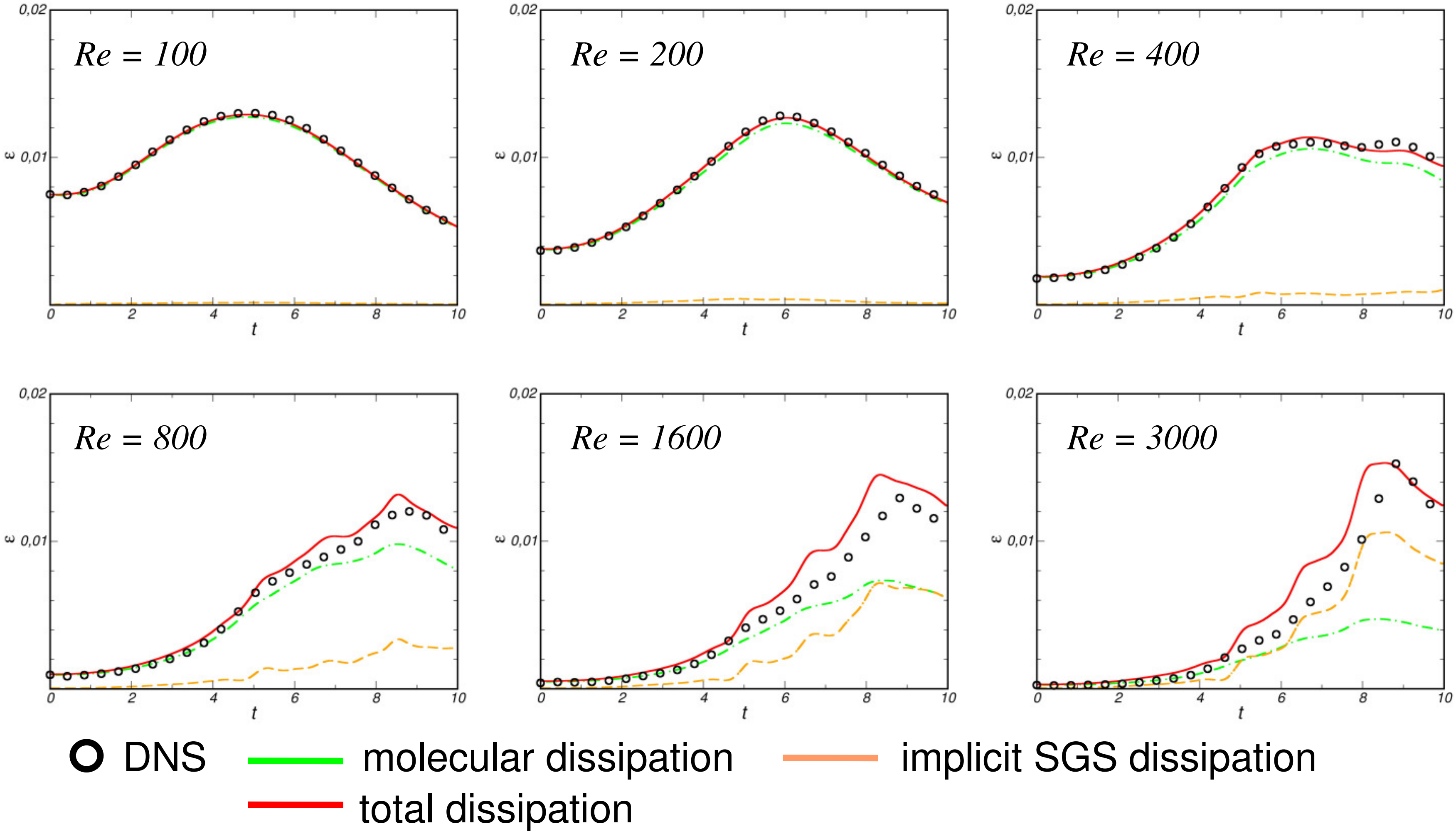
- LES of 8 vortices in a triply periodic box with 64^3 cells.
- Re = 100 , 200 , 400 , 800 , 1600 , 3000.
- visualization of time evolution at Re=400 (second-invariant criterion)



- evolution of the dissipation rate

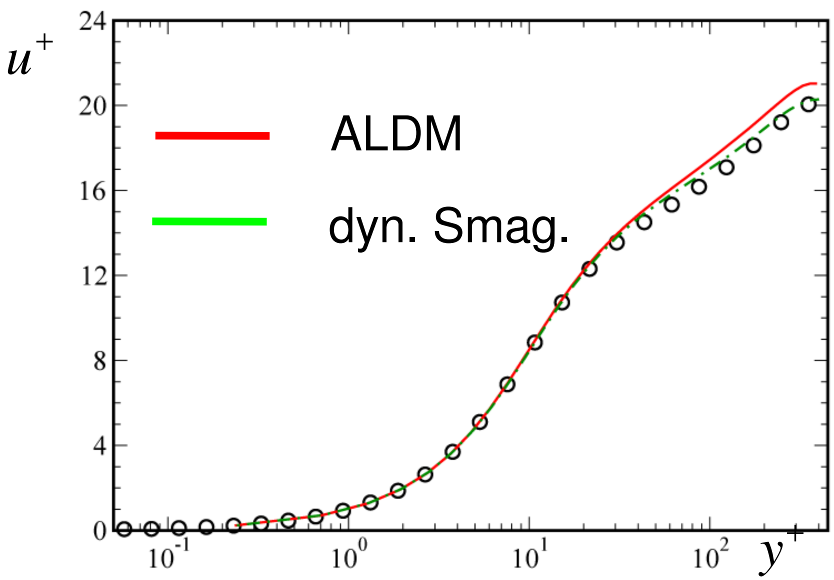


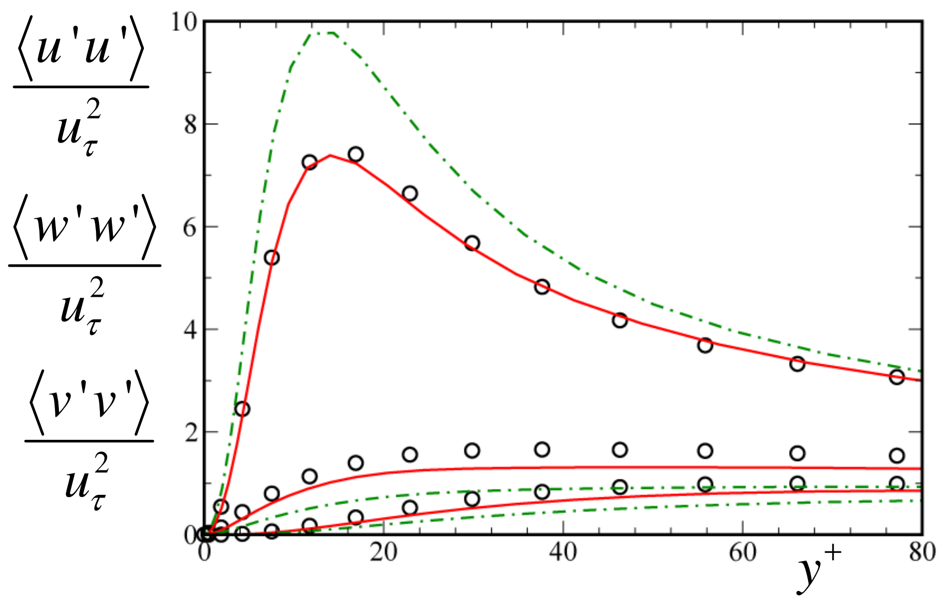
- split of different contributions to the dissipation rate for ALDM



4.5 Turbulent Channel Flow

- resolution 64 x 49 x 48, $Re_\tau = 395$
- low-Reynolds-number modification of numerical-flux parameter
  (power -2/3 in eq. (34) of A.,Hickel, Domaradzki, 2005, instead of -1/3)

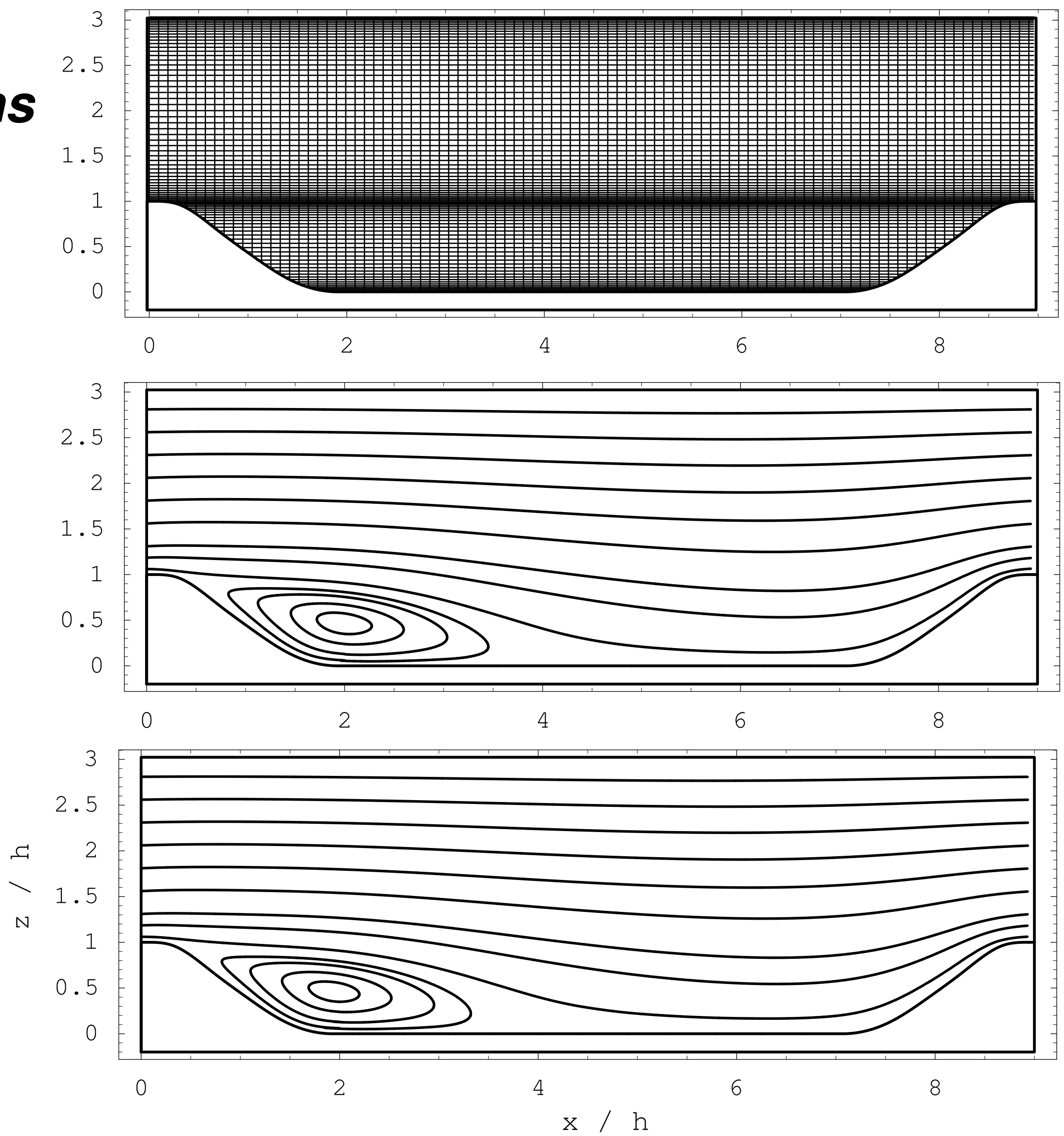




- mass-flux control: $Re_{\bar{U}} = 6862$
- ALDM: $Re_\tau = 375$ dyn. Smag. $Re_\tau = 388$

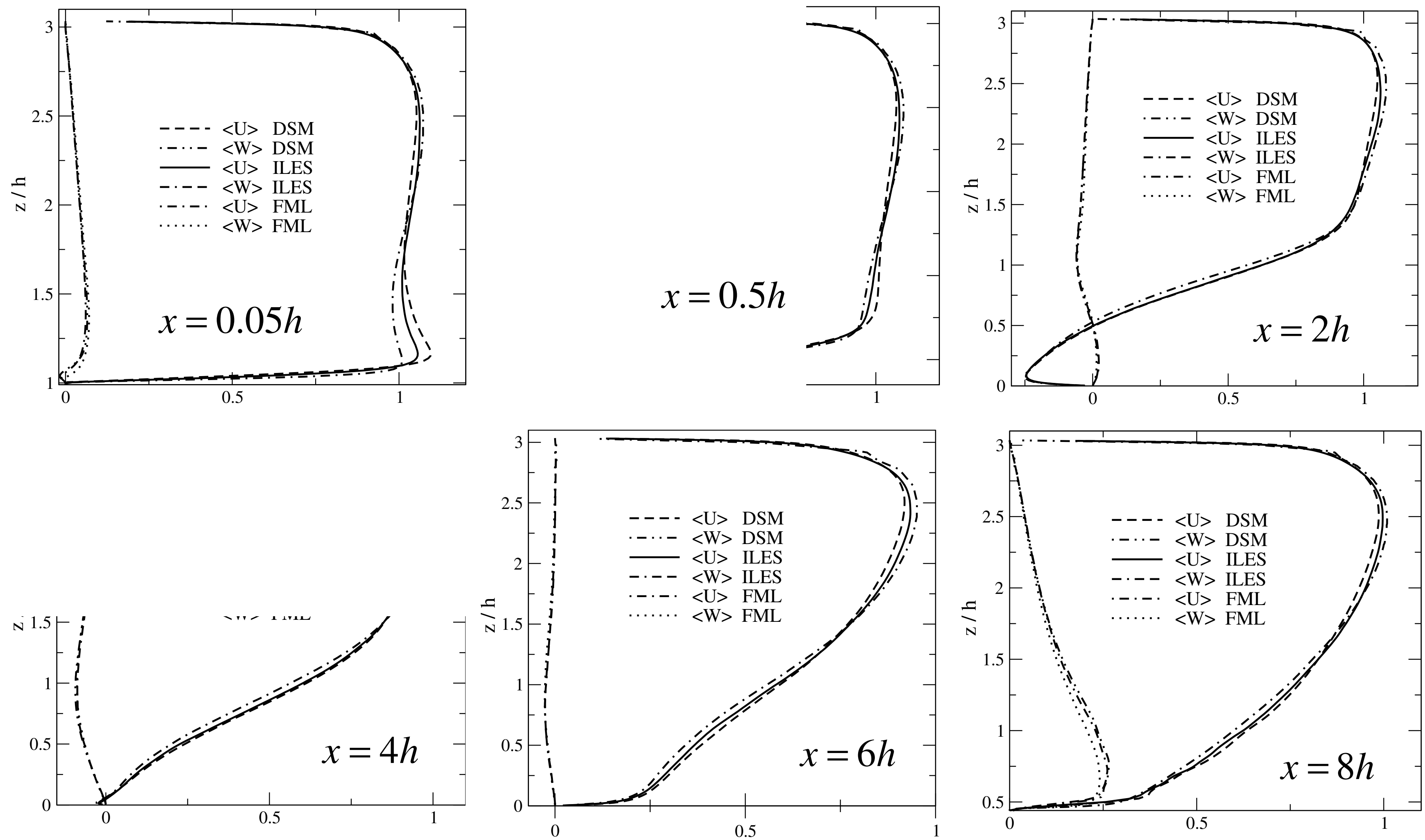
5.1 Periodic Channel with Transversal Constrictions

- Re = 10595
- grid 190 x 170 x 140
- average streamlines with dynamic Smagorinsky model
- average streamlines with ALDM



5. ALDM Application

- mean streamwise velocity profiles (FML: Fröhlich et al., JFM 2005)



6. Conclusions and Outlook

6.1 Accomplishments

- truncation-error structure of finite-volume schemes can be manipulated by
  - reconstruction = approximate deconvolution (local)
  - numerical flux function
- unlike approximation theory, SGS modeling requires truncation error to provide a regularization of the discretization for finite resolution
- by properly designing the truncation error, a numerical scheme can be generated which functions in resolved or non-turbulent flow regions as standard 2nd-order approximation and as including a SGS model in turbulent flow regions
- numerical discretization and SGS modeling can be merged fully

6.2 Further work

- extend ALDM to multi-resolution, adapting the framework of Harten (1998)
- adaptation to geometry-aligned meshes possible, analysis cumbersome
- Cartesian framework preferrable
- add immersed-boundary method based on a combination of ghost-fluid and level-set approaches