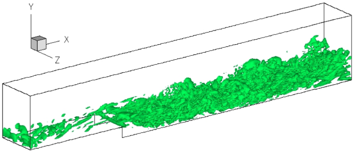
Variational multiscale modeling of turbulent incompressible flows

Gert H. Lube



Institute for Numerical and Applied Mathematics
Georg-August-University of Göttingen
D-37083 Göttingen, Germany

Lecture III in DK-Seminar
"Numerical Simulations in Technical Sciences"
TU Graz, March 10-12, 2009

Outline

Joint work with:

T. Knopp (DLR Göttingen), X. Zhang (Singapore), L. Röhe, J, Löwe, T. Heister

Outline

Incompressible Navier-Stokes model

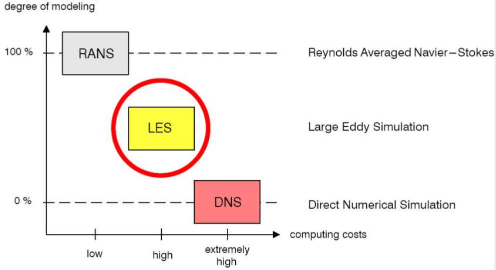
Fluid motion (Navier-Stokes + continuity equations)

Find velocity u and pressure p in $(0,T) \times \Omega$:

$$\partial_t u - \nabla \cdot (\nu \underbrace{(\nabla u + \nabla u^T)}_{=: \, 2D(u)}) + (u \cdot \nabla) u + \nabla p = f$$

$$\nabla \cdot u = 0$$

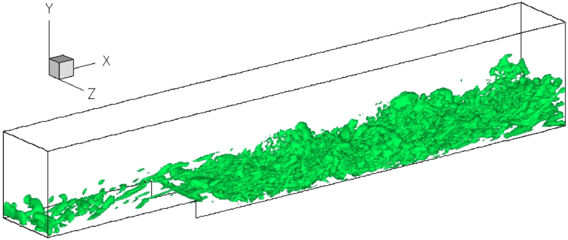
Numerical simulation of turbulent flows:



Example of turbulent incompressible flows

Isothermal flow over backward facing step

- Numerical simulation of X. Zhang with FVM-TAU-code
- **D**etached-**e**ddy **s**imulation (Large-eddy simulation + wall-functions)



Backward facing step at $Re_h = 5.100$: Isosurface of Q-invariant

Remark: Some results for this example are shown in next three slides.

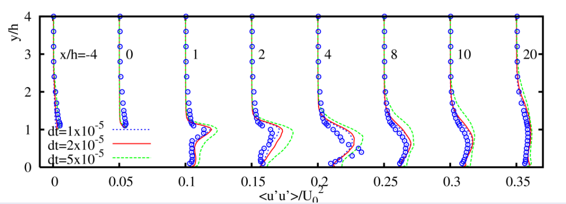
Some basic problems I:

(1) High requirements w.r.t. stability

- A-priori estimates for kinetic energy:

$$\|u(t)\|^2_{L^2(\Omega)} \quad \leq \quad e^{-C_F\sqrt{\nu}t}\|u(0)\|^2_{L^2(\Omega)} + \frac{1}{C_F\sqrt{\nu}}\int_0^t e^{C_F\sqrt{\nu}(\tau-t)}\|f(\tau)\|^2_{L^2(\Omega)}\,d\tau$$

- Very weak dissipativity: $\rightsquigarrow$ sensitivity w.r.t. data errors etc.
- Stiff-stable, accurate time semi-discretization required: e.g. BDF(2)



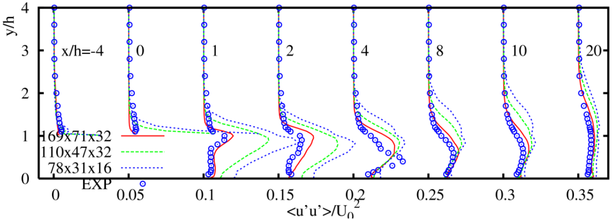
Some basic problems II:

(2) High requirements w.r.t. accuracy

$\leadsto$ Extremely fine meshes in all directions and in time required,

Example: LES of flow over backward-facing step $Re_\tau = 37500$

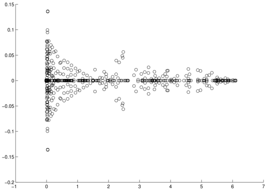
- Proper resolution of mean velocity profile requires mesh with time step $\delta t = 10^{-5}$ and fine mesh in all (!) spatial directions

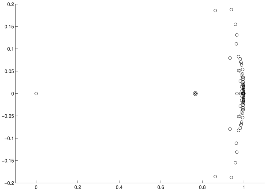


Some basic problems III:

(3) Robust and efficient algorithms required

- CHORIN-type splitting of velocity/ pressure with fast solvers for pressure-Poisson problem *or*
- Fully-coupled parallel approach to preconditioned saddle-point problems





Ph.D. project of T. Heister (2008 - ...):

- Fast algebraic solvers for incompressible flow problems
- Robust preconditioners (w.r.t. viscosity ν, mesh size h and time step δt)

Outline

Weak form of incompressible Navier-Stokes flow

$$
\begin{aligned}
\partial_t u - \nabla \cdot (2\nu D(u)) + (u \cdot \nabla) u + \nabla p &= f \quad \text{in } \Omega_T = (0,T) \times \Omega \\
\nabla \cdot u &= 0 \quad \text{in } \Omega_T \\
u(0) &= u_0 \quad \text{in } \{0\} \times \Omega
\end{aligned}
$$

$$
\mathcal{V} := H^1(0,T;\mathbf{V}) \times L^2(0,T;\mathbf{Q}), \quad \mathcal{W} := L^2(0,T;\mathbf{V} \times \mathbf{Q}), \quad \mathbf{V} \times \mathbf{Q} := [H_0^1(\Omega)]^d \times L_0^2(\Omega)
$$

Weak form:

$$
\begin{aligned}
&\text{Find } U = (u,p) \in \mathcal{V} \quad s.t. \quad u(0) = u_0 \quad \text{and} \\
&B(U,V) := A(U,V) + r(u,v) \quad = \quad (f,v) \qquad \forall V = (v,q) \in \mathcal{W}
\end{aligned}
$$

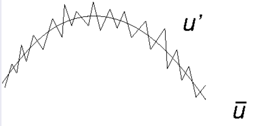
$$
\begin{aligned}
A(U,V) &:= (\partial_t u, v)_{\Omega_T} + (2\nu D(u), D(v))_{\Omega_T} - (p, \nabla \cdot v)_{\Omega_T} + (q, \nabla \cdot u)_{\Omega_T} \\
r(u,v) &:= ((u \cdot \nabla) u, v)_{\Omega_T}
\end{aligned}
$$

VMS-decomposition Hughes (2000 - ...), Collis (2003)

Decomposition of trial and test spaces:

large (resolved) scales + fine (resolved) scales + fine (unresolved) scales

$$\mathcal{V} = \overline{\mathcal{V}} \oplus \tilde{\mathcal{V}} \oplus \hat{\mathcal{V}} \qquad U = \overline{U} + \tilde{U} + \hat{U}$$
$$\mathcal{W} = \overline{\mathcal{W}} \oplus \tilde{\mathcal{W}} \oplus \hat{\mathcal{W}} \qquad V = \overline{V} + \tilde{V} + \hat{V}$$



Decomposition of weak form:

$$
\begin{aligned}
B(\overline{U} + \tilde{U} + \hat{U}, \overline{V}) &= (f, \bar{v}) \qquad \forall \overline{V} \in \overline{\mathcal{W}} \\
B(\overline{U} + \tilde{U} + \hat{U}, \tilde{V}) &= (f, \tilde{v}) \qquad \forall \tilde{V} \in \tilde{\mathcal{W}} \\
B(\overline{U} + \tilde{U} + \hat{U}, \hat{V}) &= (f, \hat{v}) \qquad \forall \hat{V} \in \hat{\mathcal{W}}
\end{aligned}
$$

Reformulation of VMS-decomposition

Reformulation of decomposed problem:

- Linearized Navier-Stokes operator: $B'(W,U,V) := A(U,V) + c(w,u,v)$
- with $c(w,u,v) := ((w\cdot\nabla u + u\cdot\nabla w, v)_{\Omega_T}$

$$
\begin{aligned}
B(\overline{U},\overline{V}) + B'(\overline{U},\tilde{U},\overline{V}) + r(\tilde{u},\overline{v}) &= (f,\overline{v}) \\
&\quad -[B'(\overline{U},\hat{U},\overline{V}) + r(\hat{u},\overline{v}) + c(\tilde{u},\hat{u},\overline{v})] \\
B'(\overline{U},\tilde{U},\tilde{V}) + r(\tilde{u},\tilde{v}) &= (f,\tilde{v}) - B(\overline{U},\tilde{V}) \\
&\quad -[B'(\overline{U},\hat{U},\tilde{V}) + r(\hat{u},\tilde{v}) + c(\hat{u},\hat{u},\tilde{v})] \\
B(\overline{U}+\hat{U},\hat{V}) + B'(\overline{U}+\tilde{U},\hat{U},\hat{V}) &= (f,\hat{v}) + r(\hat{u},\hat{v})
\end{aligned}
$$

Goal: Simplification of "blue" and "red" terms

VMS modelling assumptions and model simplification

VMS assumptions:

(A.1) Scale separation: No direct influence of $\hat{U}$ on $\overline{U}$

$$B'(\overline{U}, \hat{U}, \overline{V}) + r(\hat{u}, \overline{v}) + c(\tilde{u}, \hat{u}, \overline{v}) = 0 \;\; \forall \overline{V} \in \overline{\mathcal{W}}$$

(A.2) Unresolved scales dissipate energy from small resolved scales

$$B'(\overline{U}, \hat{U}, \tilde{V}) + r(\hat{u}, \tilde{v}) + c(\hat{u}, \hat{u}, \tilde{v}) \;\approx\; S(\tilde{U}, \tilde{V})$$

with **subgrid viscosity model** $S : \; (\overline{\mathcal{V}} \oplus \tilde{\mathcal{V}}) \cup (\overline{\mathcal{W}} \oplus \tilde{\mathcal{W}})$

Model simplification I: (A1) $\rightsquigarrow$ Skip third equation.

$$\begin{aligned} B(\overline{U}, \overline{V}) + B'(\overline{U}, \tilde{U}, \overline{V}) + r(\tilde{u}, \overline{v}) &= (f, \overline{v}) && \forall \overline{V} \in \overline{\mathcal{W}} \\ B(\overline{U}, \tilde{V}) + B'(\overline{U}, \tilde{U}, \tilde{V}) + r(\tilde{u}, \tilde{v}) + S(\tilde{U}, \tilde{V}) &= (f, \tilde{v}) && \forall \tilde{V} \in \tilde{\mathcal{W}} \end{aligned}$$

Model reduction

Simplification I:

$$\begin{aligned} B(\overline{U},\overline{V}) + B'(\overline{U},\tilde{U},\overline{V}) + r(\tilde{u},\overline{v}) &= (f,\overline{v}) \qquad \forall \overline{V} \in \overline{\mathcal{W}} \\ B(\overline{U},\tilde{V}) + B'(\overline{U},\tilde{U},\tilde{V}) + r(\tilde{u},\tilde{v}) + S(\tilde{U},\tilde{V}) &= (f,\tilde{v}) \qquad \forall \tilde{V} \in \tilde{\mathcal{W}} \end{aligned}$$

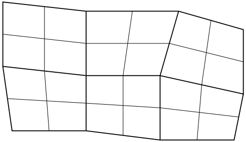
$\rightsquigarrow$ (after some calculation)

Simplification II:

$$\begin{aligned} B(\overline{U}+\tilde{U},\overline{V}) &= (f,\overline{v}) \qquad \forall \overline{V} \in \overline{\mathcal{W}} \\ B(\overline{U}+\tilde{U},\tilde{V}) + S(\tilde{U},\tilde{V}) &= (f,\tilde{v}) \qquad \forall \tilde{V} \in \tilde{\mathcal{W}} \end{aligned}$$

Result: VMS-decomposition of incompressible Navier-Stokes problem with subgrid viscosity model (still to be fixed)

Discrete VMS-version on FEM-level



Two-level setting with FE spaces:

$\mathcal{V}_H \subseteq \mathcal{V}_h \subset \mathcal{V}, \quad \mathcal{W}_H \subseteq \mathcal{W}_h \subset \mathcal{W}$

$$
\begin{array}{lll}
\mathcal{V}_h := \overline{\mathcal{V}} \oplus \tilde{\mathcal{V}}, & \overline{\mathcal{V}} := \mathcal{V}_H & \tilde{\mathcal{V}} = \tilde{\mathcal{V}}_h := (Id - \Pi)\mathcal{V}_h \\
\mathcal{W}_h := \overline{\mathcal{W}} \oplus \tilde{\mathcal{W}}, & \overline{\mathcal{W}} := \mathcal{W}_H & \tilde{\mathcal{W}} = \tilde{\mathcal{W}}_h := (Id - \Pi)\mathcal{W}_h
\end{array}
$$

Discrete VMS-version

$$
\begin{array}{rcll}
B(\overline{U}_h + \tilde{U}_h, \overline{V}_h) & = & (f, \bar{v}_h) & \forall \overline{V}_h \in \overline{\mathcal{W}}_h \\
B(\overline{U}_h + \tilde{U}_h, \tilde{V}_h) + S_h(\tilde{U}_h, \tilde{V}_h) & = & (f, \tilde{v}_h) & \forall \tilde{V}_h \in \tilde{\mathcal{W}}_h
\end{array}
$$

VMS method on FEM-level

Assumption: $S_h(\cdot, \overline{V}) = 0 \quad \forall \overline{V} \in \overline{\mathcal{V}} \cup \overline{\mathcal{W}}$

$\rightsquigarrow$

Compact discrete VMS problem:

$$\text{Find } U_h \in \mathcal{V}_h = \overline{\mathcal{V}} \oplus \tilde{\mathcal{V}} : \quad B(U_h, V) + S_h(U_h, V) = (f, v) \qquad \forall V \in \mathcal{W}_h$$

Assumption on subgrid viscosity model:

(i) Coercivity: $S_h(\tilde{U}, \tilde{U}) \geq c\|\nabla \tilde{U}\|^2 \quad \forall \tilde{U} \in \tilde{\mathcal{W}}$

(ii) Symmetry: $S_h(U, V) = S_h(V, U) \quad \forall U, V \in (\overline{\mathcal{V}} \oplus \tilde{\mathcal{V}}) \cup (\overline{\mathcal{W}} \oplus \tilde{\mathcal{W}})$

$\rightsquigarrow$

Abstract identification problem:

Construction of subgrid viscosity $S_h(\cdot, \cdot)$

Parametrization of turbulence subgrid model

Classical Large-Eddy-Simulation (LES):

- **Scale separation:** via filtering (filter width $\Delta \sim H$)
  $\rightsquigarrow$ Parameter identification: $\frac{H}{h} =?$
- **Classical subgrid viscosity model:** Smagorinsky

$$S_h(U,V) = \Big((C_S\,\Delta)^2 \|D(u)\|_F D(u), D(v) \Big)_\Omega$$

Parameter identification: Smagorinsky constant $C_S =?$
Dynamical variant: $C_S(t,x) =?$

Plan:

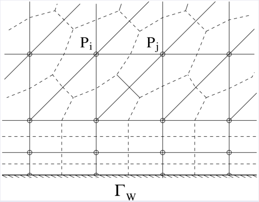
- Some lessons on LES/ DES learned from a finite-volume code
- Some conclusions for LES/ DES with finite element methods

Outline

Experience with low-order finite-volume code

Finite-volume code Theta (DLR Göttingen):

- Vertex-based variant $\sim$ P_1/P_1 or Q_1/Q_1
  $\rightsquigarrow$ pressure stabilization required
- Chorin's decoupling of velocity / pressure



Minimal stabilization:

- Upwind stabilization "dissipates" fluctuations
  $\rightsquigarrow$ Apply Galerkin discretization (as minimal stabilization) !
- Subgrid viscosity model: Smagorinsky model

$$S_h(U,V) = \big((C_S \Delta)^2 \|D(\mathbf{u})\|_F D(\mathbf{u}), D(\mathbf{v}) \big), \qquad C_S = ?$$

- Experiments by X. Zhang (2006–08)

Abstract optimization approach:

- State variable u (here: velocity/pressure) in Hilbert space V
- Parameter vector q (here: model parameter) in control space $Q := \mathbb{R}^{n_p}$
- Abstract state equation (here: Navier-Stokes model)

$$A(u,q) = f \qquad \text{in } V$$

- Linear observation operator $C : V \to Z$ maps $u \mapsto \hat{C}u$ into space of "measurements" $Z := \mathbb{R}^{n_m}$ with $n_m \geq n_p$
- Cost functional $J : V \times Q \to \mathbb{R}$

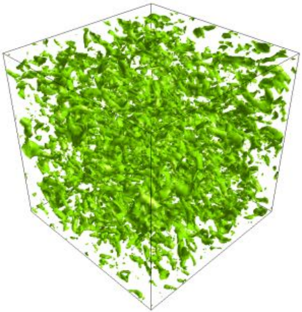
Constrained optimization problem:

$$\text{Minimize } J(u,q) := \frac{1}{2}\|C(u) - \hat{C}\|_Z^2 \quad \text{s.t.} \quad A(u,q) = f$$

Parameter identification in Smagorinsky model I

Basic calibration model: Decaying homogeneous turbulence (DHT)

- **Observation results** $C(u)$**:**
  Results for turbulent kinetic energy $k = \frac{1}{2}\langle (u - \langle u \rangle)^2 \rangle$
  Averaging $\langle \cdot \rangle$ in all homogeneous (here: spatial) directions
- **Measurements** $\hat{C}$**:**
  Careful experimental data for turbulent kinetic energy k (Comte/Bellot)

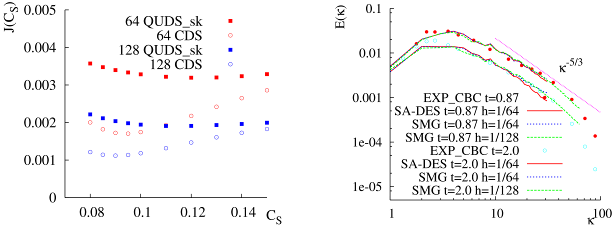


- Turbulent initial value u_0
- Vanishing source $\mathbf{f}$
- Periodic boundary values at opposite sides

Parameter identification in Smagorinsky model II

Results for turbulent kinetic energy $k = \frac{1}{2}\langle(u - \langle u\rangle)^2\rangle$ of DHT

- Fourier space characterization of $k(t)$ via energy spectral density $E(\kappa, t)$
- Cost functional: $J(C_S) = \frac{1}{2}\sum_{j=1}^{2}\sum_{i=1}^{M}\left[E(\kappa_i, C_S, t_j) - E_{\exp}(\kappa_i, t_j)\right]^2$



Calibration of Smagorinsky constant C_S and "optimized" energy spectrum

Very good agreement of:

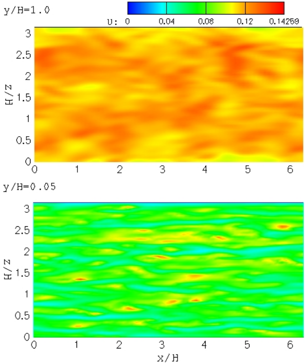
- optimized $C_S = 0.085$ for CDS with $N = 128$ with literature
- spectrum $E(\kappa)$ with Kolmogorov's $\kappa^{-\frac{5}{3}}$-slope in the inertial sub-range

Turbulent channel flow at $Re_\tau = 395$ – I

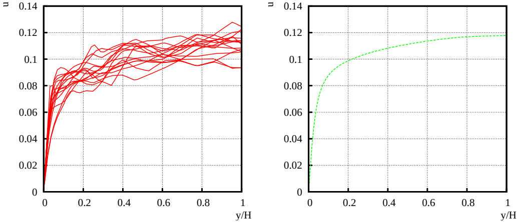
Statistical data averaging $\langle\cdot\rangle$:

$\rightsquigarrow$ in homogeneous directions (in space and time)

Example: Channel flow with homogeneous directions x_1, x_3 and t



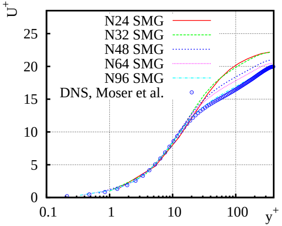
- Instantaneous behaviour of velocity in channel center and at the wall (left)
- Instantaneous and mean profiles of u_1 (below)

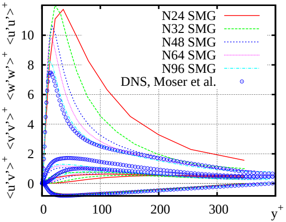


Turbulent channel flow at $Re_\tau = 395$ – II

- Anisotropic resolution of boundary layer region
- First-order statistics: mean streamwise velocity $U = \langle u \rangle e_1$
- Second-order statistics: turbulent kinetic energy $k = \frac{1}{2}\langle (u - \langle u \rangle)^2 \rangle$

  and their normalized variants $U^+ = U/u_\tau, \quad k^+ = k/u_\tau^2$





Grid convergence with N^3 nodes

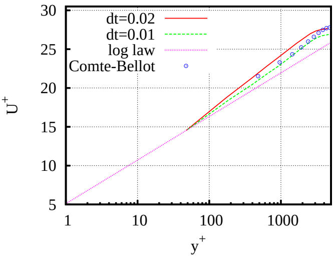
Problem: Wall-resolved LES is almost as expensive as DNS

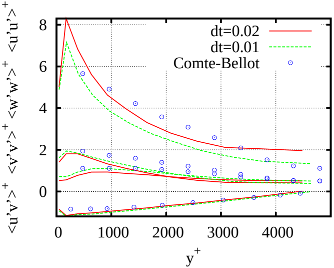
Proper resolution of near-wall region in LES requires $\sim \mathrm{Re}_\tau^2$ nodes (Bagett et al. 1997)

Turbulent channel flow at $Re_\tau = 4.800$

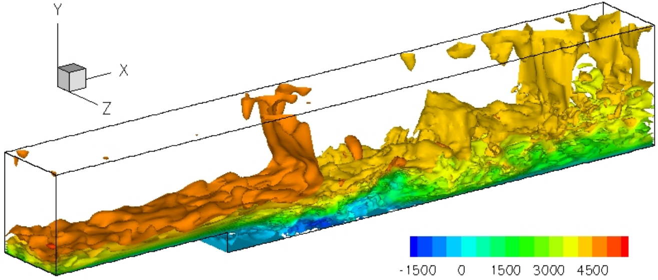
Channel flow at $Re_\tau = 4.800$

- Near-wall modelling with wall-functions replaces anisotropic layer refinement
- First-order statistics: e.g. normalized mean streamwise velocity $U^+ = U/u_\tau, \; U = \langle u \rangle e_1$
- Second-order statistics: e.g. normalized turbulent kinetic energy $k^+ = k/u_\tau^2, \; k = \frac{1}{2}\langle (u - \langle u \rangle)^2 \rangle$





DES for backward facing step at $Re_h = 37.500$

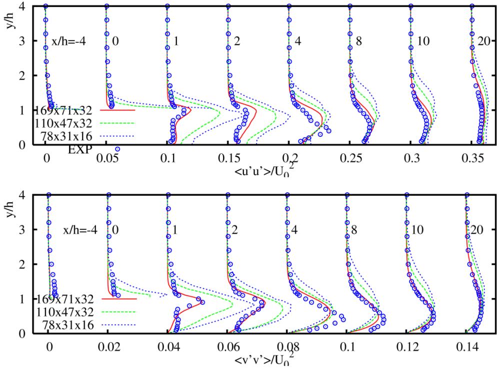


Hybrid approach:

- LES simulation away from boundary layers
- RANS type universal wall-functions used to bridge near-wall region ($y^+ \lesssim 40$)

DES for backward facing step at $Re_h = 37.500$

Hybrid approach allows less fine grids and coarser time steps
$\rightsquigarrow$ model reduction by factor 300



Fluctuations $\langle u_1' u_1' \rangle$ and $\langle u_2' u_2' \rangle$ on different meshes compared to experimental data o

Results by X. Zhang et al. $\rightsquigarrow$ Special issue of CMAME on LES (2009)

Outline

VMS method on FEM-level

Compact discrete VMS problem:

Find $U_h \in \mathcal{V}_h = \mathcal{V}_H \oplus (Id - \Pi_H)\mathcal{V}_h$:

$$B(U_h, V) + S_h(U_h, V) = (f, v) \quad \forall V \in \mathcal{W}_h$$

Problems:

- Definition of $\mathcal{V}_H, \mathcal{V}_h$ and of projector Π_H
- Construction of subgrid viscosity $S_h(\cdot, \cdot)$

Classical Smagorinsky model: $\Pi_H = 0$

$$S_h(U, V) = \left((C_S\Delta)^2 \|D(\mathbf{u})\|_F D(\mathbf{u}), D(\mathbf{v})\right)$$

Major drawback: Scheme has artificial diffusion of $\mathcal{O}(\Delta^{4/3})$

$\rightsquigarrow$ Approach not suitable for higher-order FEM !

Parametrization of subgrid models:

Scale separation: Π_H as L^2-orthogonal projection of $\mathcal{V}_h$ onto $\mathcal{V}_H$

Projection-based VMS-method: V. John et al. *J. Math. Anal. Appl. 2008*

$$S_h(u,v) = \sum_{M\in\mathcal{T}_H} \Big(\tau_M^H(u) D(Id-\Pi_H)(u), D(Id-\Pi_H)(v) \Big)_M$$

- Smagorinsky-type: $\tau_M^H(u) = C_S H^2 \|D(Id-\Pi_H)(u)\|_F$
- Semidiscrete a-priori error estimate for inf-sup stable case

Alternative VMS-method: based on local projection stabilization (LPS)

$$\begin{aligned} S_h(U,V) \quad &= \sum_{M\in\mathcal{T}_H} \Big(\tau_M^H (Id-\Pi_H)D(u), (Id-\Pi_H)D(v) \Big)_M \\ &\quad + \Big(\gamma_M^H (Id-\Pi_H)\nabla\cdot u, (Id-\Pi_H)\nabla\cdot v \Big)_M \end{aligned}$$

First theoretical results of L. Röhe (2008)

Semidiscrete a-priori error estimate of

$$\|(u-u_h)(T)\|_0^2 + \sum_M \int_0^T (2\nu + \nu^*_{T(M)}) \|D(u-u_h)\|_{0,M}^2 dt$$

with artificial viscosity

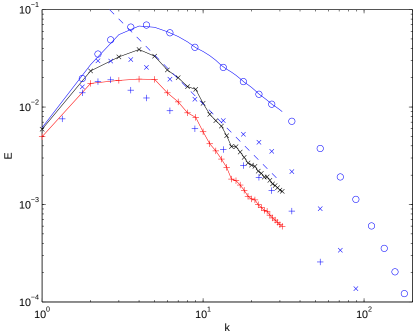
$$\nu^*_{T(M)} := C_S^* \|(Id - \Pi_H) D(u_h)\|_F \left(1 - \frac{\|\Pi_H D(I_h u - u_h)\|_{0,M}^2}{\|D(I_h u - u_h)\|_{0,M}^2} \right) \geq 0$$

- using standard Gronwall technique $\rightsquigarrow$ very large error constants
- no monotonicity of subgrid viscosity term

Goal: Error estimates for first and second order flow statistics !?

First FEM-numerical results for DIHT

FEM-simulation with Q_2/Q_1-elements



Energy spectrum for DIHT with $h = \frac{1}{32}$ (corresponds to $h = \frac{1}{64}$ with FVM)
Results for $t = 0$ (o), $t = 0.87$ (x) and $t = 2.0$ (+)

- So far: Application of $\tau_M^H = (C_S h)^2 \|D(u)\|_F$, $\gamma_M^H = 0$
- Over-diffusive results due to application of all scales in $\|D(u)\|_F$

Outline

Current Ph.D. projects: Extension to FEM simulation

Direct solver via VMS method: based on FE-package `deal.II`

- Higher-order finite elements
- Velocity-pressure approximation with inf-sup compatibility condition
- Stabilization via LPS method

Ph.D. project of L. Röhe:

- Development of solver based on VMS approach (LPS-variant)
- Identification of parameters of subgrid model via optimization tools

Ph.D. project of J. Löwe:

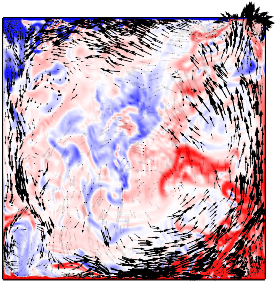
- A-posteriori approach to identification of LPS-parameters
- Extension to (thermally) coupled incompressible flows

Summary

- Variational multiscale approach for (turbulent) incompressible Navier-Stokes problem
- First experience with parameter identification in turbulence models in Ph.D. thesis and postdoc project by X. Zhang (2005 - 2008)
- Extension to FEM within Ph.D. projects (2008 - 2011)

Summary

- Variational multiscale approach for (turbulent) incompressible Navier-Stokes problem
- First experience with parameter identification in turbulence models in Ph.D. thesis and postdoc project by X. Zhang (2005 - 2008)
- Extension to FEM within Ph.D. projects (2008 - 2011)



THANKS FOR YOUR ATTENTION !