VMS 2008 Workshop on Variational Multiscale Methods

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An Algebraic Variational Multiscale-Multigrid Method for Large Eddy Simulation of Turbulent Flow

Volker Gravemeier

Emmy Noether Research Group
Technical University of Munich

Martin Kronbichler

Scientific Computing
University of Uppsala

Michael W. Gee, Wolfgang A. Wall

Chair for Computational Mechanics
Technical University of Munich

Outline

- Three-Scale Variational Multiscale LES
- Algebraic Multigrid Scale Separation
- Fourier Analysis
- Numerical Examples

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Three Different Approaches to LES

Traditional LES (introduced 1960s, e.g., books by Geurts, John, Sagaut)

- resolved + unresolved scales, scale separation via (implicit) filtering
- various models, one widely-used option: (dynamic) subgrid-viscosity model

Three-Scale VMLES (introduced Hughes et al. (2000) + various authors)

- coarse + fine resolved +unres. scales, scale separation via variat. projection
- dominating model option so far: (dynamic) subgrid-viscosity model

Residual-Based VMLES (introduced Calo (2004) + e.g., Bazilevs (2007))

- resolved + unresolved scales, scale separation via variational projection
- modeling: approximate analytical representation -> stabilized methods

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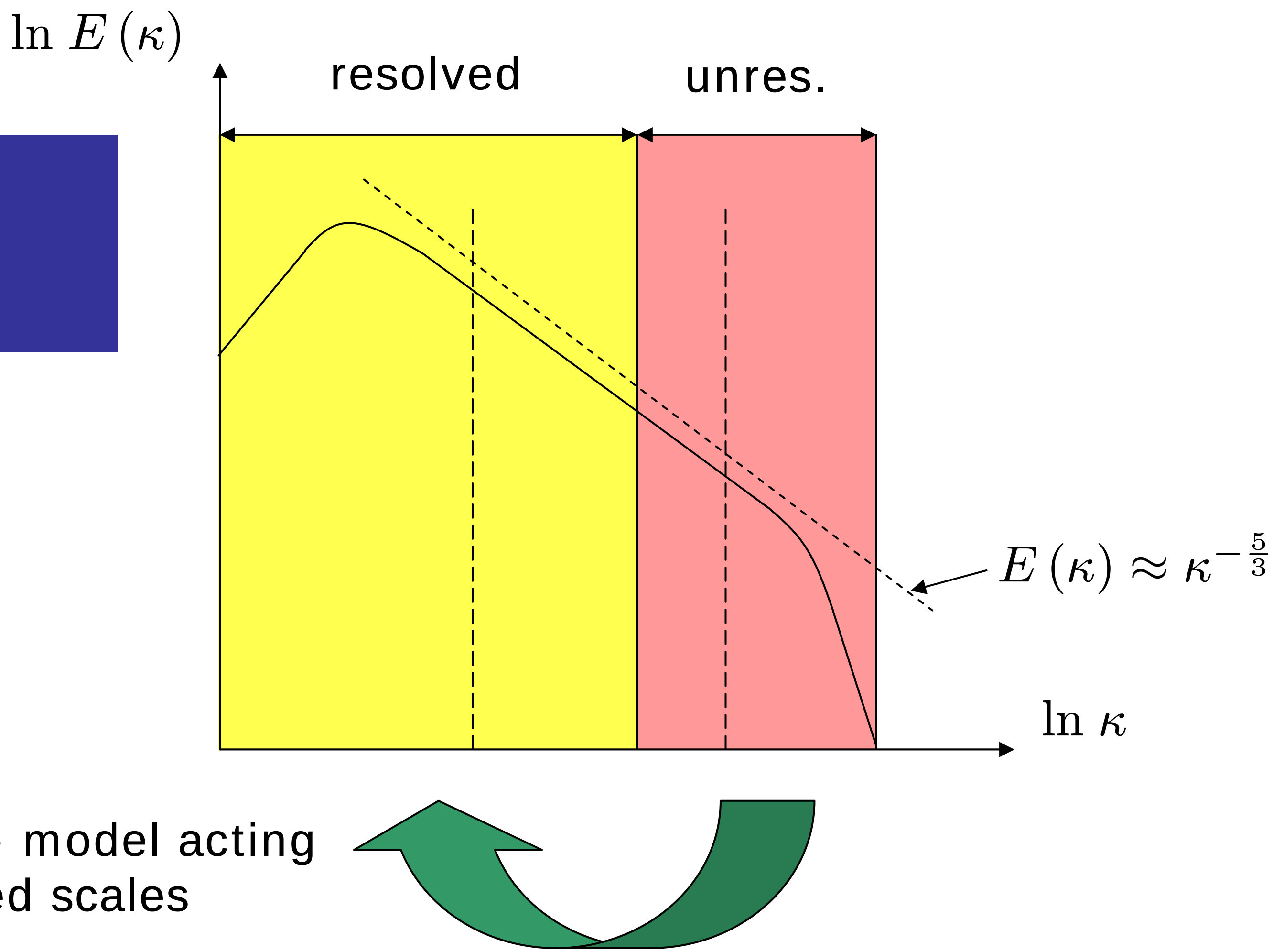
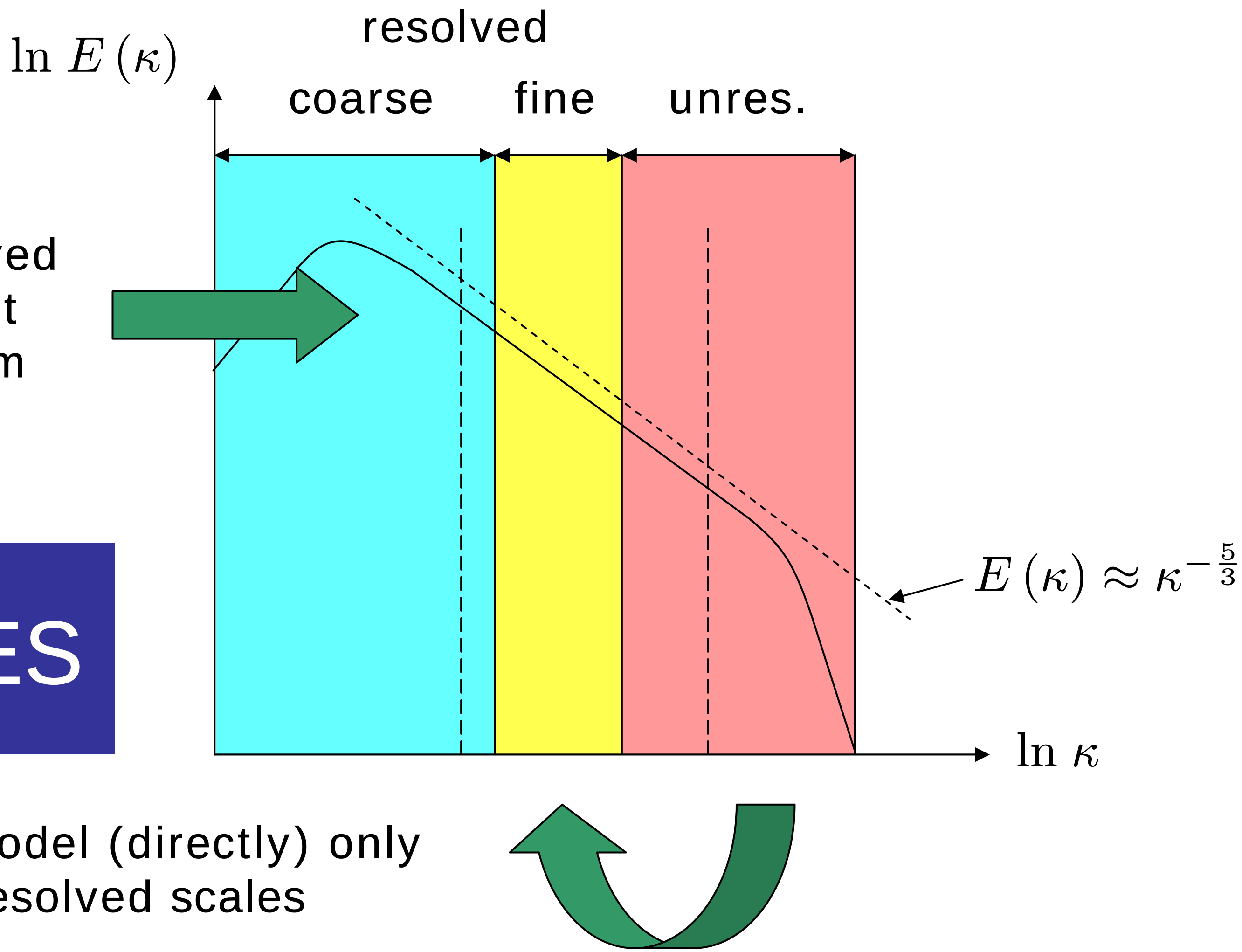
Kolmogorov Energy Spectrum: Traditional LES

LES



Subgrid-scale model acting
on **all** resolved scales

Kol. Energy Spectrum: Three-Scale VMLES



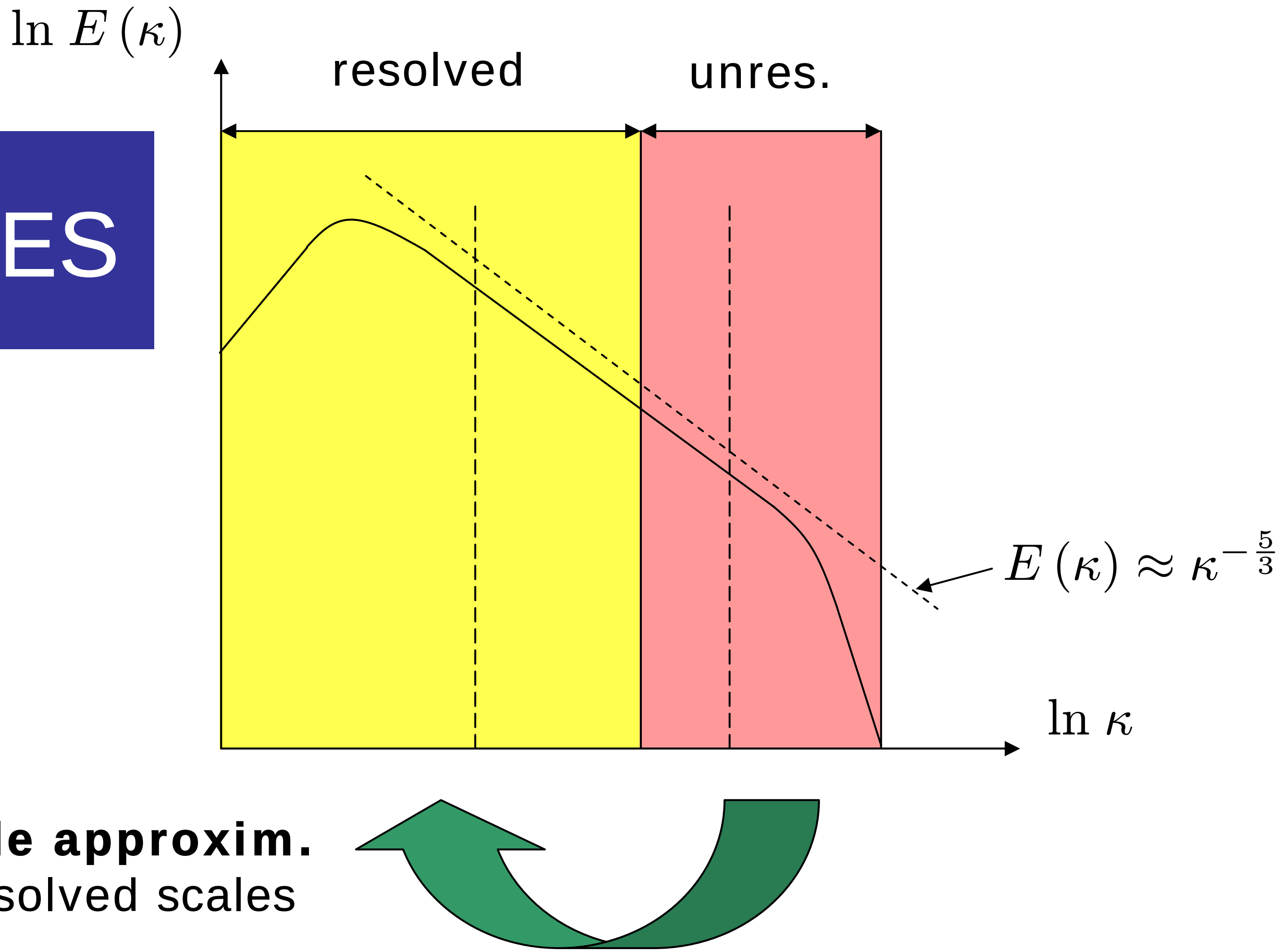
Coarse resolved scales without modeling term

3VMLES

Subgrid-scale model (directly) only acting on **fine** resolved scales

Kol. Energy Spectrum: Residual-Based VMLES

RBVMLES



Unresolv.-scale approxim.
acting on **all** resolved scales

Strong and Weak Formulation of Navier-Stokes

$$\frac{\partial \mathbf{u}}{\partial t} + \nabla \cdot (\mathbf{u} \otimes \mathbf{u}) - 2\nu \nabla \cdot \varepsilon(\mathbf{u}) + \nabla p = \mathbf{f} \quad \text{in } \Omega \times]0,T]$$ (momentum equ.)

$$\nabla \cdot \mathbf{u} = 0 \quad \text{in } \Omega \times]0,T]$$ (continuity equ.)

$$\mathbf{u} = \mathbf{g} \quad \text{on } \Gamma_g \times]0,T]$$ (Dirichlet b.c.)

$$\sigma \cdot \mathbf{n} = \mathbf{h} \quad \text{on } \Gamma_h \times]0,T]$$ (Neumann b.c.)

$$\mathbf{u} = \mathbf{u}_0 \quad \text{in } \Omega \times \{0\}$$ (initial condition)

$$B_{\mathrm{NS}}(\mathbf{v}, q; \mathbf{u}, p) = \boxed{B_{\mathrm{M}}(\mathbf{v}; \mathbf{u}, p) + B_{\mathrm{C}}(q; \mathbf{u})} = (\mathbf{v}, \mathbf{f})_\Omega$$ where

$$B_{\mathrm{M}}(\mathbf{v}; \mathbf{u}, p) = \left(\mathbf{v}, \frac{\partial \mathbf{u}}{\partial t}\right)_\Omega + (\mathbf{v}, \nabla \cdot (\mathbf{u} \otimes \mathbf{u}))_\Omega + (\varepsilon(\mathbf{v}), 2\nu\varepsilon(\mathbf{u}))_\Omega - (\nabla \cdot \mathbf{v}, p)_\Omega$$

$$B_{\mathrm{C}}(q; \mathbf{u}) = (q, \nabla \cdot \mathbf{u})_\Omega$$

3-Scale Velocity Separation

[Hughes et al. (2000), Collis (2001), Gravemeier (2003), ...]

3-scale separation of velocity weighting/solution functions + funct. spaces:

$\mathcal{V} = \overline{\mathcal{V}}^h \oplus \mathcal{V}'^h \oplus \hat{\mathcal{V}}$	$\mathcal{S} = \overline{\mathcal{S}}^h \oplus \mathcal{S}'^h \oplus \hat{\mathcal{S}}$	$\mathbf{v} = \overline{\mathbf{v}}^h + \mathbf{v}'^h + \hat{\mathbf{v}}$	$\mathbf{u} = \overline{\mathbf{u}}^h + \mathbf{u}'^h + \hat{\mathbf{u}}$

coarse resolved + fine resolved + unresolved scales

3 subproblems:

$$B_{\mathrm{M}}\left(\overline{\mathbf{v}}^h; \overline{\mathbf{u}}^h + \mathbf{u}'^h + \hat{\mathbf{u}}, p^h + \hat{p}\right) = \left(\overline{\mathbf{v}}^h, \mathbf{f}\right)_\Omega$$

→ coarse-scale eq.

$$B_{\mathrm{M}}\left(\mathbf{v}'^h; \overline{\mathbf{u}}^h + \mathbf{u}'^h + \hat{\mathbf{u}}, p^h + \hat{p}\right) = \left(\mathbf{v}'^h, \mathbf{f}\right)_\Omega$$

→ fine-scale eq.

$$B_{\mathrm{M}}\left(\hat{\mathbf{v}}; \overline{\mathbf{u}}^h + \mathbf{u}'^h + \hat{\mathbf{u}}, p^h + \hat{p}\right) = \left(\hat{\mathbf{v}}, \mathbf{f}\right)_\Omega$$

→ unres.-scale eq.

model dissipative effect on **fine** resolved scales ← not solved for

3-Scale Velocity Separation

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coarse resolved + fine resolved + unresolved scales

3 subproblems:

$$B_{\mathrm{M}}\left(\overline{\mathbf{v}}^h; \overline{\mathbf{u}}^h + \mathbf{u}'^h, p^h\right) = \left(\overline{\mathbf{v}}^h, \mathbf{f}\right)_\Omega$$

→ model. c.-s. eq.

$$B_{\mathrm{M}}\left(\mathbf{v}'^h; \overline{\mathbf{u}}^h + \mathbf{u}'^h, p^h\right) + \left(\varepsilon(\mathbf{v}'^h), 2\nu'_{\mathrm{T}}\varepsilon(\mathbf{u}'^h)\right) = \left(\mathbf{v}'^h, \mathbf{f}\right)_\Omega$$

→ model. f.-s. eq.

Standard Smagorinsky model

$$\nu'_{\mathrm{T}} = (C_{\mathrm{S}} h)^2 \left|\varepsilon(\mathbf{u}'^h)\right|$$

model dissipative effect on **fine** resolved scales ← not solved for

Add PSPG Term: Circumventing LBB

[Hughes et al. (1986)]

Modeled coarse- and fine-scale momentum equation:

$$B_{\mathrm{M}}\left(\overline{\mathbf{v}}^h;\overline{\mathbf{u}}^h+\mathbf{u}'^h,p^h\right)=\left(\overline{\mathbf{v}}^h,\mathbf{f}\right)_\Omega$$

$$B_{\mathrm{M}}\left(\mathbf{v}'^h;\overline{\mathbf{u}}^h+\mathbf{u}'^h,p^h\right)+\left(\varepsilon(\mathbf{v}'^h),2\nu'_{\mathrm{T}}\varepsilon(\mathbf{u}'^h)\right)=\left(\mathbf{v}'^h,\mathbf{f}\right)_\Omega$$

Modeled continuity equation:

$$B_{\mathrm{C}}\left(q^h;\mathbf{u}^h\right)+\left(\nabla q^h,\tau\mathcal{R}_{\mathrm{M}}\left(\mathbf{u}^h,p^h\right)\right)=0$$

Two modeling terms: fine-scale subgrid-viscosity term and PSPG term

Practical Solution Strategies: Overview

	Explicit approach	Monolithic approach	
		p-type scale separation	h-type scale separation
FEM	Two-level FEM (RFB on small-scale level)	Hierarchical FEM (continuous/disc.) L_2-projection	**Multigrid scale separation (project. and non-project. scale separation possible)**
FVM			
FDM			Discrete smooth filters (non-projective) Sampling + interpolation (applied in dynamic model)
SM		Spectral or sharp cutoff filter Discrete smooth filters (non-projective)	

Source: V. Gravemeier, The variational multiscale method for laminar and turbulent flow, *Archives of Computational Methods in Engineering - State of the Art Reviews* 13 (2006) 249-324

Multigrid Approaches to (VM)LES

- Early geometric multigrid approaches to traditional LES, e.g., by Voke (1989) and Terracol *et al.* (2001) (also Sagaut *et al.* (2006))
- Volume-agglomeration method within finite volume / finite element formulation for scale separation in three-scale VMLES by Koobus and Farhat (2004)
  - ➢ challenging grid-based macro-cell agglomeration procedure via dual grid (Lallemand *et al.* (1992))
- Geometric multigrid method within finite volume formulation for scale separation in three-scale VMLES by Gravemeier (2006)
  - ➢ generation and maintenance of an additional grid required
- Related method by John & Kaya (2005), John *et al.* (2006): L_2-projection using two grids

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Multigrid Ingredients

5 items are required:

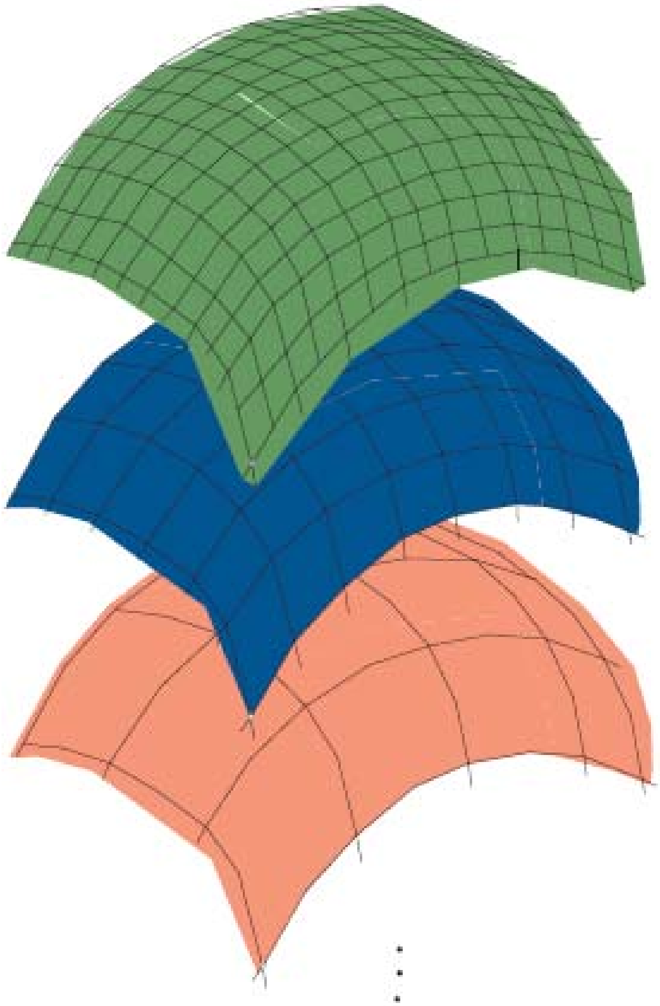
1) A couple of grids or levels

2) A system of equations on each grid/level

3) Some approximate solution technique on each grid/level (relaxation)

4) A way to get from one grid/level to another (restriction / prolongation)

5) An algorithm or preconditioner

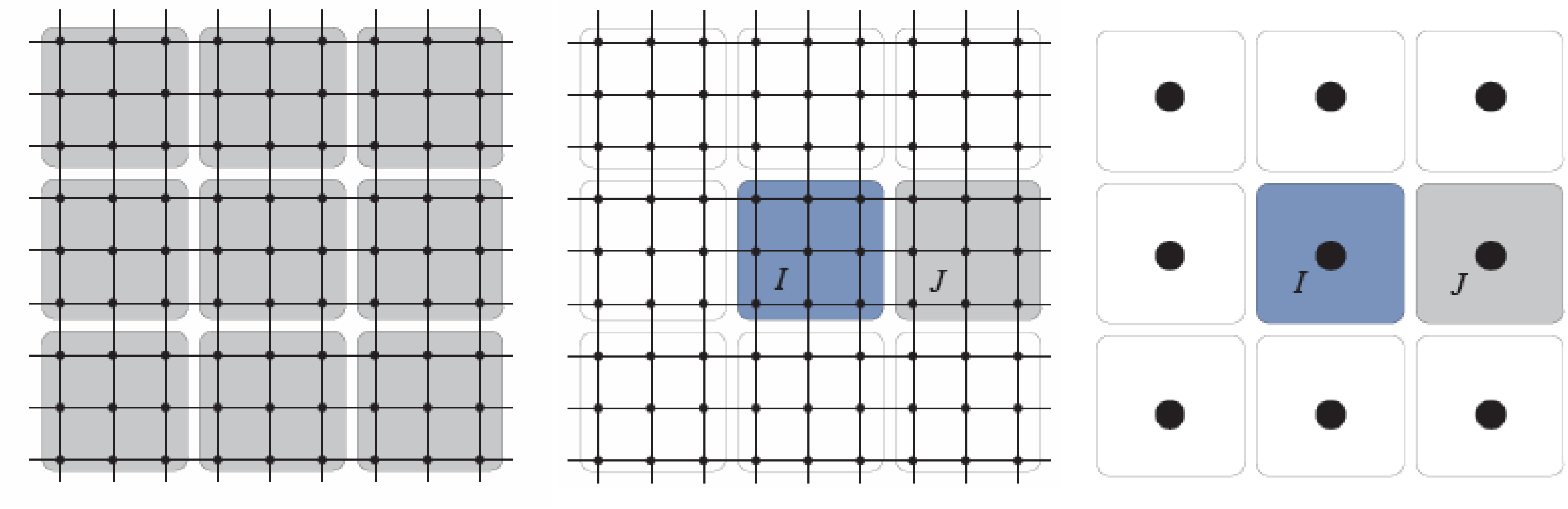


Variants of Algebraic Multigrid (AMG) Methods

- Classical AMG ("Ruge-Stüben-AMG") <-> Aggregation-based AMG
- Smoothed Aggregation AMG (SA-AMG) introduced by Vanek et al. (1996), optimal method for solution of elliptic problems, but inadequate for hyperbolic problems
- Plain Aggregation AMG (PA-AMG) better suited for hyperbolic problems, but sub-optimal when elliptic parts play a considerable role (e.g., in diffusion-dominated regions)
- Recent approach in form of a Petrov-Galerkin SA-AMG by Sala and Tuminaro (2008) for solving non-symmetric linear equation systems

Plain and Smoothed Aggregation AMG

Aggregations due to connectivity/strength of connections of matrix entries:



(Tentative) prolongation operator matrix: $\hat{\mathbf{P}}$

$\hat{\mathrm{P}}_{iI} = 1$ if *i*-th entry in *I*-th aggregate, else $\hat{\mathrm{P}}_{iI} = 0$

Potential smoothing: $\mathbf{P} = \mathbf{S}\hat{\mathbf{P}}$ with smoother $\mathbf{S}$

Restriction:

$\mathbf{R} = \mathbf{P}^{\mathrm{T}}$

Reminder: Scale-Separated N-S Equations

Modeled coarse- and fine-scale momentum equation:

$$B_{\mathrm{M}}\left(\overline{\mathbf{v}}^h;\overline{\mathbf{u}}^h+\mathbf{u}'^h,p^h\right)=\left(\overline{\mathbf{v}}^h,\mathbf{f}\right)_\Omega$$

$$B_{\mathrm{M}}\left(\mathbf{v}'^h;\overline{\mathbf{u}}^h+\mathbf{u}'^h,p^h\right)+\left(\varepsilon(\mathbf{v}'^h),2\nu'_{\mathrm{T}}\varepsilon(\mathbf{u}'^h)\right)=\left(\mathbf{v}'^h,\mathbf{f}\right)_\Omega$$

Modeled continuity equation:

$$B_{\mathrm{C}}\left(q^h;\mathbf{u}^h\right)+\left(\nabla q^h,\tau\mathcal{R}_{\mathrm{M}}\left(\mathbf{u}^h,p^h\right)\right)=0$$

Two modeling terms: fine-scale subgrid-viscosity term and PSPG term

Multigrid Scale-Separated N-S Equations

Multigrid scale separation:
[Harten (1996)]

$$\mathbf{v} = \mathbf{v}^{3h} + \mathbf{v}^{\delta h} + \hat{\mathbf{v}} \qquad \mathbf{u} = \underbrace{\mathbf{u}^{3h} + \mathbf{u}^{\delta h}}_{\mathbf{u}^h} + \hat{\mathbf{u}}$$

Modeled coarse- and fine-scale momentum equation:

$$B_{\mathrm{M}}\left(\mathbf{v}^{3h}; \mathbf{u}^{3h} + \mathbf{u}^{\delta h}, p^h\right) = \left(\mathbf{v}^{3h}, \mathbf{f}\right)_\Omega$$

$$B_{\mathrm{M}}\left(\mathbf{v}^{\delta h}; \mathbf{u}^{3h} + \mathbf{u}^{\delta h}, p^h\right) + \left(\varepsilon(\mathbf{v}^{\delta h}), 2\nu_{\mathrm{T}}^{\delta h}\varepsilon(\mathbf{u}^{\delta h})\right) = \left(\mathbf{v}^{\delta h}, \mathbf{f}\right)_\Omega$$

Modeled continuity equation:

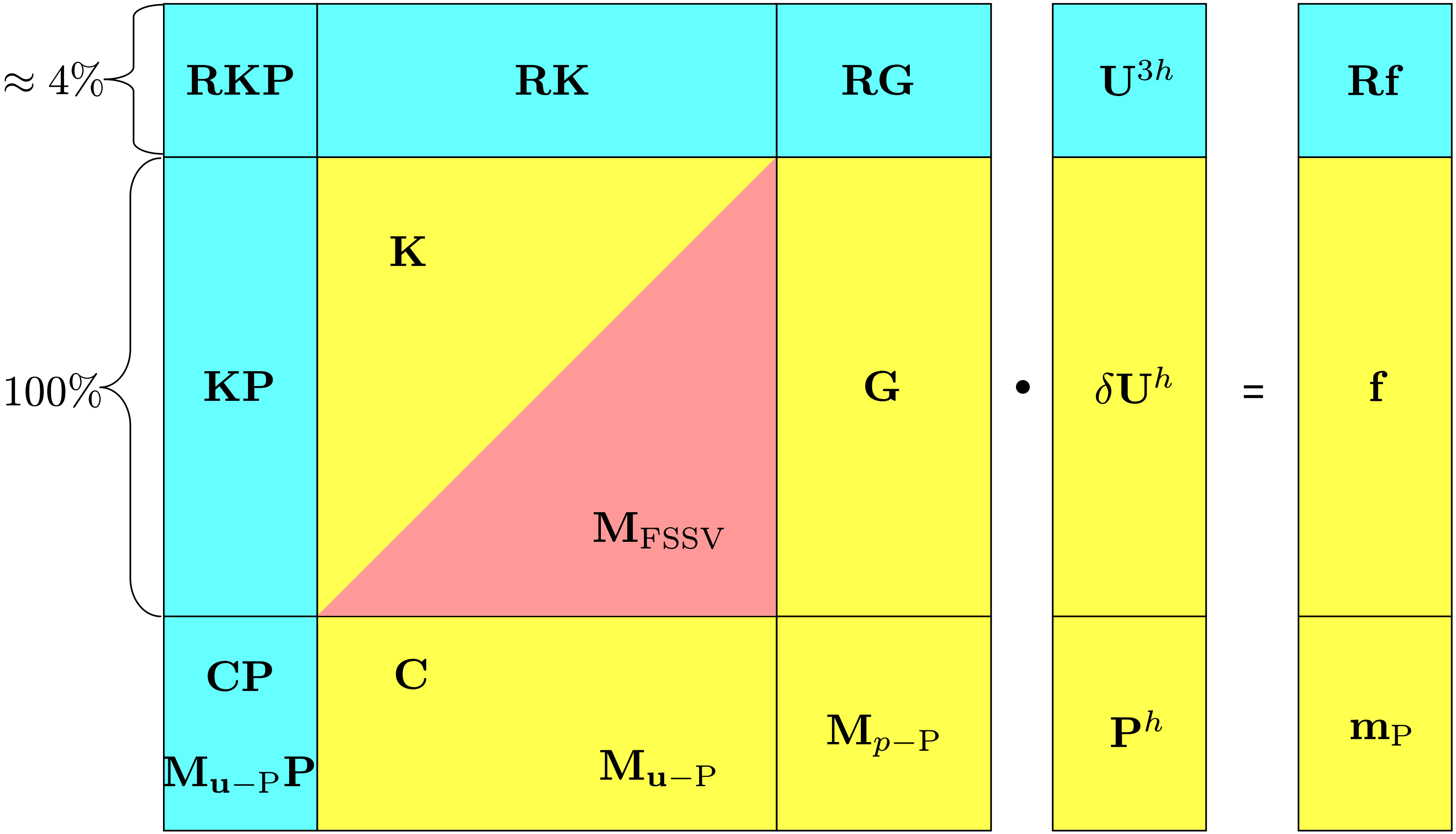
$$\nu_{\mathrm{T}}^{\delta h} = \left(C_{\mathrm{S}} h\right)^2 \left|\varepsilon(\mathbf{u}^{\delta h})\right|$$

$$B_{\mathrm{C}}\left(q^h; \mathbf{u}^h\right) + \left(\nabla q^h, \tau \mathcal{R}_{\mathrm{M}}\left(\mathbf{u}^h, p^h\right)\right) = 0$$

PSPG-Stabilized N-S Matrix Formulation

$$\begin{bmatrix} \mathbf{K} & \mathbf{G} \\ \mathbf{C} \quad \mathbf{M}_{\mathbf{u}-\mathrm{P}} & \mathbf{M}_{p-\mathrm{P}} \end{bmatrix} \bullet \begin{bmatrix} \mathbf{U}^h \\ \mathbf{P}^h \end{bmatrix} = \begin{bmatrix} \mathbf{f} \\ \mathbf{m}_{\mathrm{P}} \end{bmatrix}$$

Extended AVM^3 Formulation

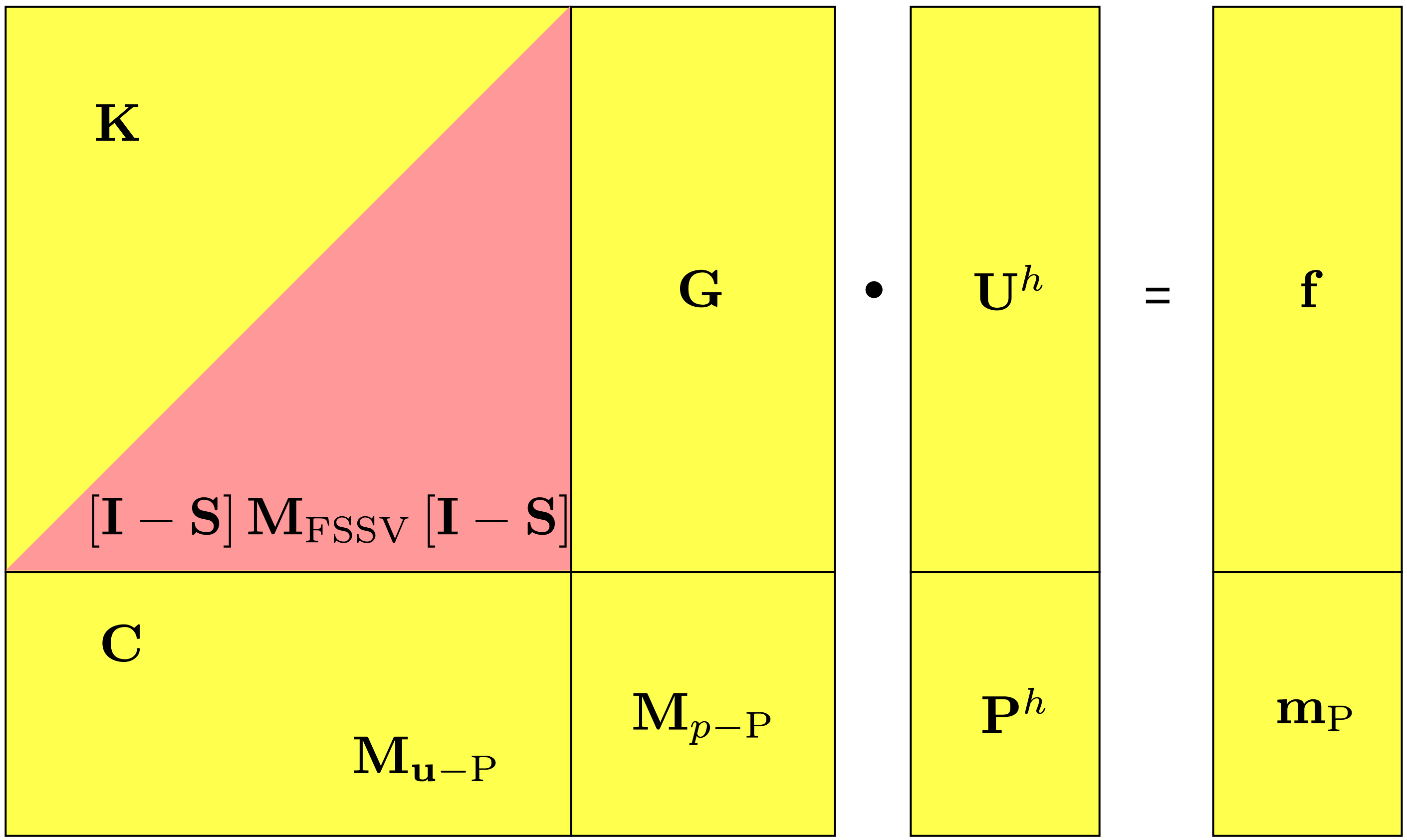


Remarks

- Extended AVM^3 formulation based on plain aggregation AMG: projective scale separation into coarse and fine (velocity) scales purely algebraically without need for an additional discretization
- Restriction of subgrid-viscosity matrix to fine scales by simply omitting it in level-transfer process
- Based on “ML” multigrid software package by Sandia NL, development of routine for generation of level-transfer operator matrices
- Multigrid solvers may beneficially exploit *a priori* separation of linear equation system into blocks containing different scales
  - Future work!
- Here: development and use of analogous re-condensed system, solving linear equation system using “standard” AMG solver

Re-Condensed AVM^3 Formulation

Generate scale-separating matrix: $\mathbf{S} = \mathbf{P}\mathbf{R}$



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Analyis of Scale Separation: 1D Model Problem

- Understand properties of scale separation from model equation (here already in variational FE formulation):

$$(v^h, \partial_t u^h)_\Omega + (\partial_x \delta v^h, \partial_x \delta u^h)_\Omega = 0$$

- Uniform discretization, periodic boundary conditions
- Linear finite elements
- Represents linearized, constant-coefficient model

ODE system

- 1D model gives discrete ODE system:

$$\frac{d}{dt}\mathbf{M}\mathbf{U}^h = [\mathbf{I} - \mathbf{S}]\,\mathbf{K}_{\text{diff}}\,[\mathbf{I} - \mathbf{S}]\,\mathbf{U}^h$$

- Also investigated: “one-sided” projection (computational efficiency)

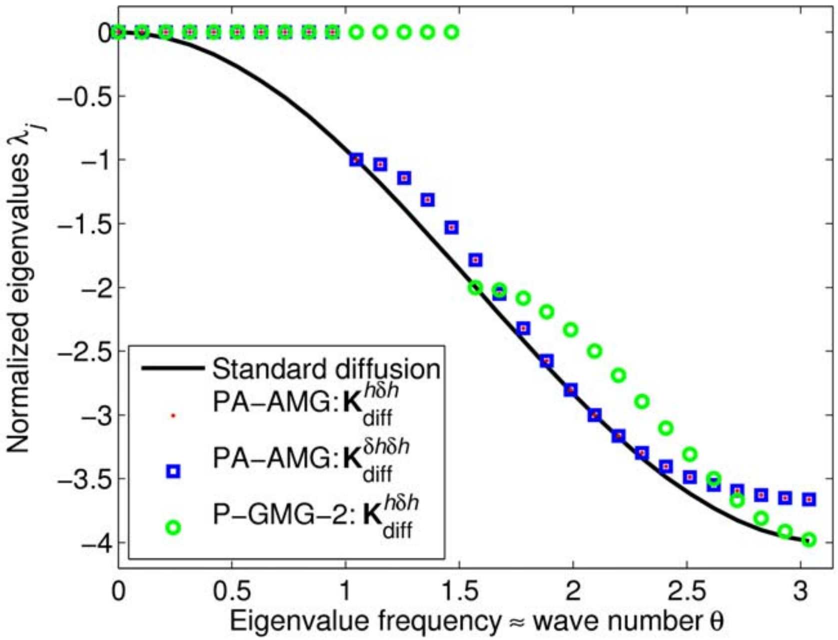
$$\frac{d}{dt}\mathbf{M}\mathbf{U}^h = \mathbf{K}_{\text{diff}}\,[\mathbf{I} - \mathbf{S}]\,\mathbf{U}^h$$

- Compare operators for $\mathbf{K}_{\text{diff}}$ for various scale separations:
  - PA—AMG
  - SA—AMG
  - projective/smoothed geometric multigrid (P/S-GMG-2)

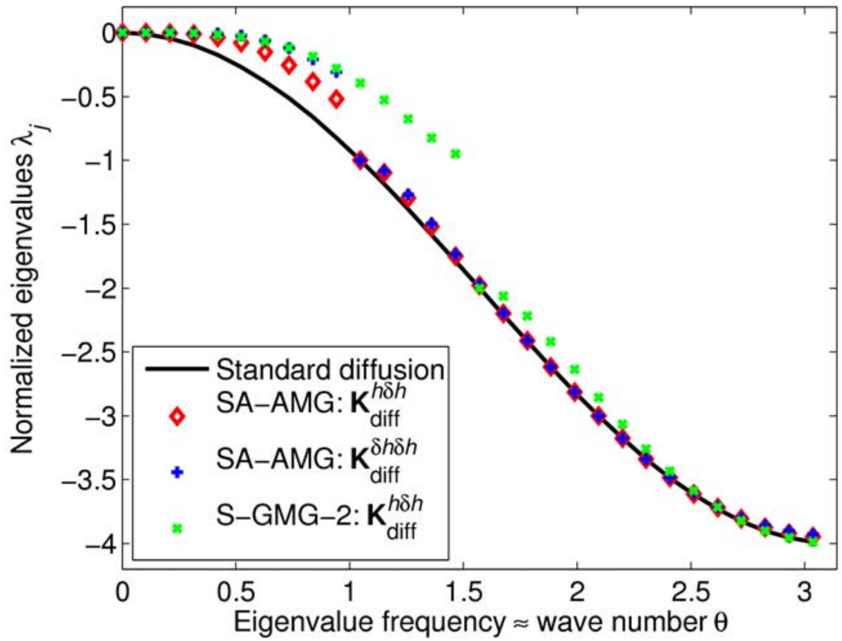
- Include comparison to standard (all-scale) subgrid-viscosity term

Eigenvalues (h=1/60)

Eigenvalues govern temporal evolution of model:



projective scale separation



smoothed scale separation

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The Competitors

(1) Traditional LES with dynamic Smagorinsky model (DSM) + PSPG

(2) Residual-Based Variational Multiscale Method (RBVMM)

Besides PSPG term, the following stabilization terms are included:

a) SUPG term

b) grad-div term (bulk viscosity term, LSIC,...)

c) cross-stress term

d) Reynolds-stress term

(according to Bazilevs *et al.* (2007), transient + viscous stab. terms omitted)

Parameter Definitions

[Deardorff (1970), Franca and Valentin (2000), Barrenechea and Valentin (2002)]

Smagorinsky model parameter: $C_\mathrm{S} = 0.1$

SUPG, PSPG, cross-stress, and Reynolds-stress terms:

$$\tau_\mathrm{M} = \frac{1}{\frac{1}{c_\mathrm{T}\Delta t}\cdot\max(\xi_1,1)+\frac{4\nu}{m_\mathrm{k}h^2}\cdot\max(\xi_2,1)} \qquad \xi_1 = \frac{4\nu c_\mathrm{T}\Delta t}{m_\mathrm{k}h^2} \qquad \xi_2 = \frac{m_\mathrm{k}\|u^h\|h}{2\nu}$$

grad-div term:

$$\tau_\mathrm{C} = \frac{\|u^h\|h}{2}\cdot\min\left(\xi_2,1\right) \qquad \xi_2 = \frac{m_\mathrm{k}\|u^h\|h}{2\nu}$$

Overview: Turbulent Flow Problems

[Sagaut (2006)]

Homogeneous turbulent flows (0 directions of inhomogeneity)

Turbulent flows featuring 1 spatial direction of inhomogeneity

Turbulent flows featuring 2 spatial directions of inhomogeneity

Turbulent flows being completely inhomogeneous

Overview: Turbulent Flow Problems

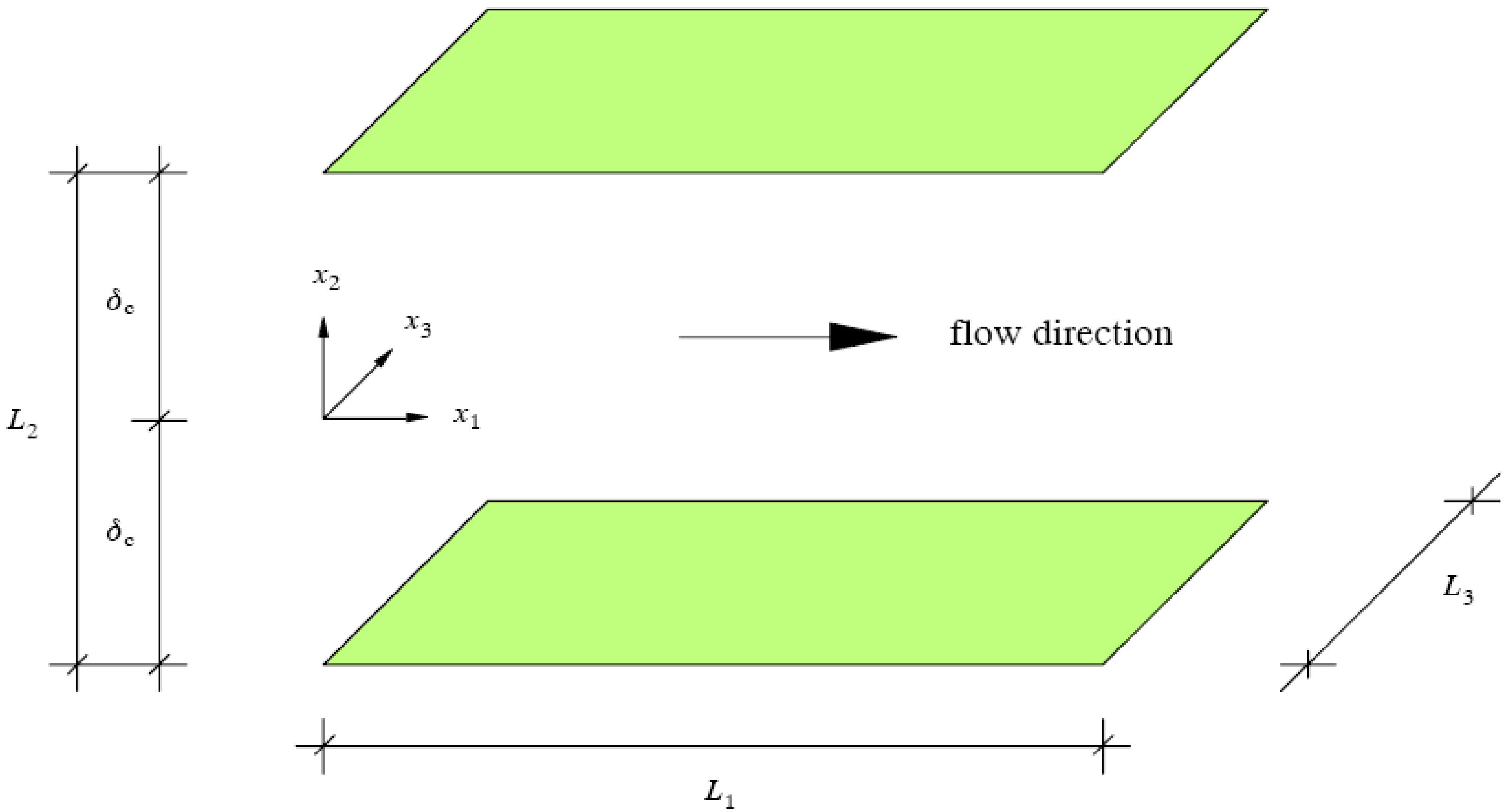
Homogeneous turbulent flows (0 directions of inhomogeneity)

Turbulent flow in a channel

Turbulent flows featuring 2 spatial directions of inhomogeneity

Turbulent flows being completely inhomogeneous

Turbulent Flow in a Channel: Geometry

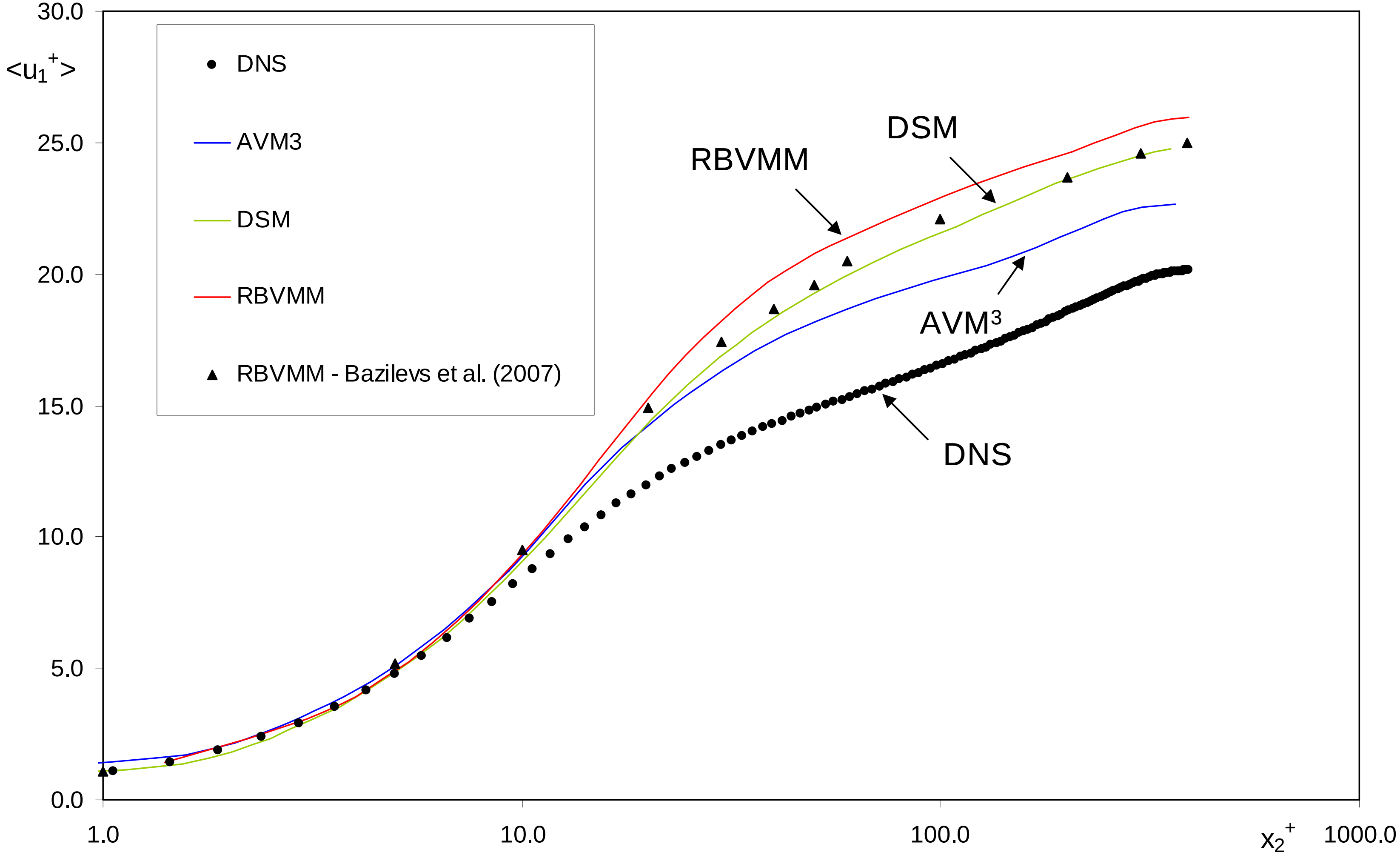


Channel: Numerical Setup

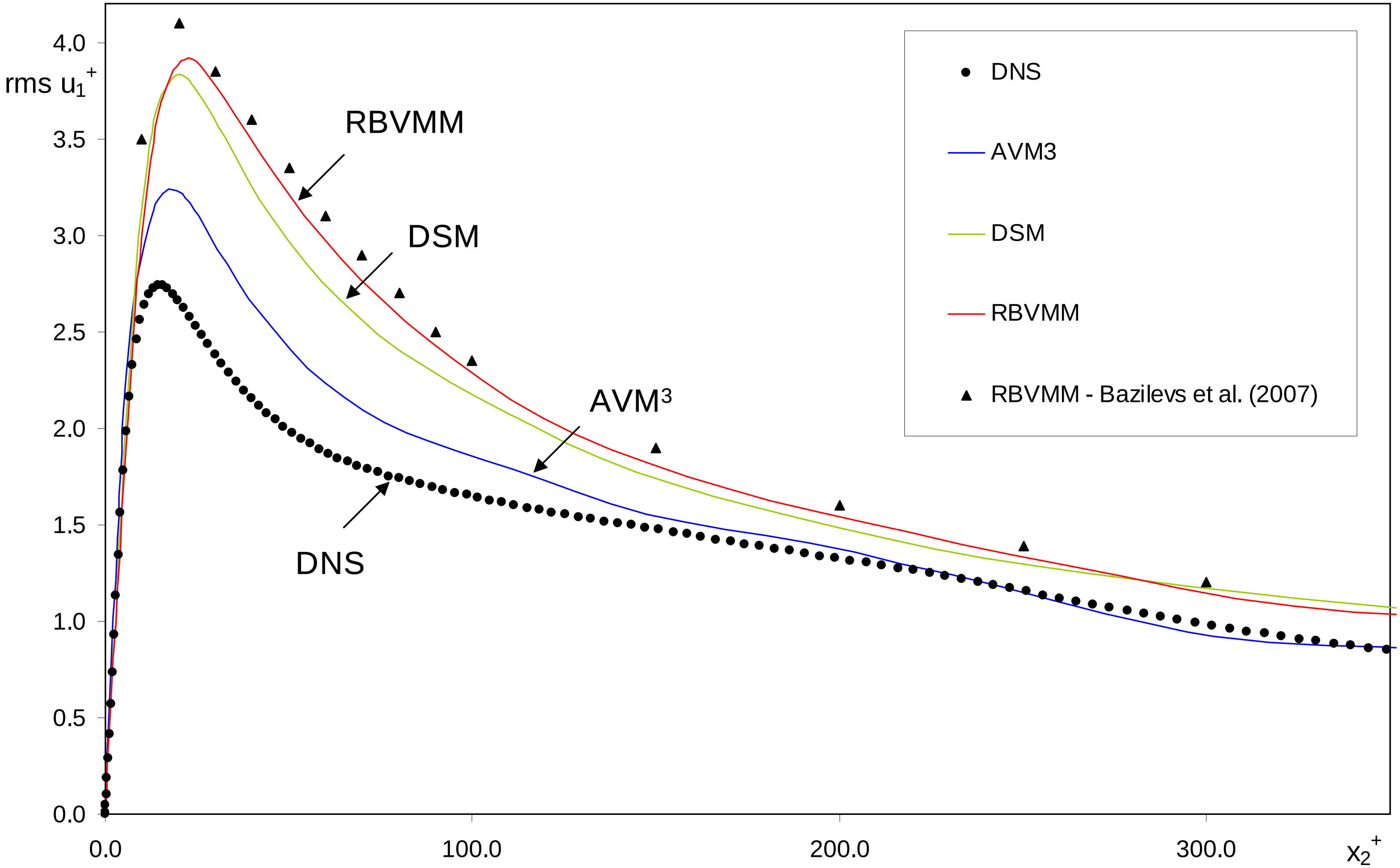
- Reynolds number based on wall-shear velocity: $Re_\tau = \frac{u_\tau \delta_c}{\nu} = 395$
- Channel dimensions: $L_1 \times L_2 \times L_3 = 2\pi\delta_c \times \delta_c \times \frac{2}{3}\pi\delta_c$
- Generalized-α time integration scheme: $\rho_\infty = 0.5,\ \Delta t^+ = \frac{\Delta t u_\tau^2}{\nu} = 0.79$
- 32 linearly interpolated finite elements in each spatial direction
- hyperbolic refinement in wall-normal direction towards walls

$$h_1^+ = 77.56 \qquad h_{2,\mathrm{min}}^+ = 1.32 \qquad h_{2,\mathrm{max}}^+ = 67.78 \qquad h_3^+ = 25.85$$

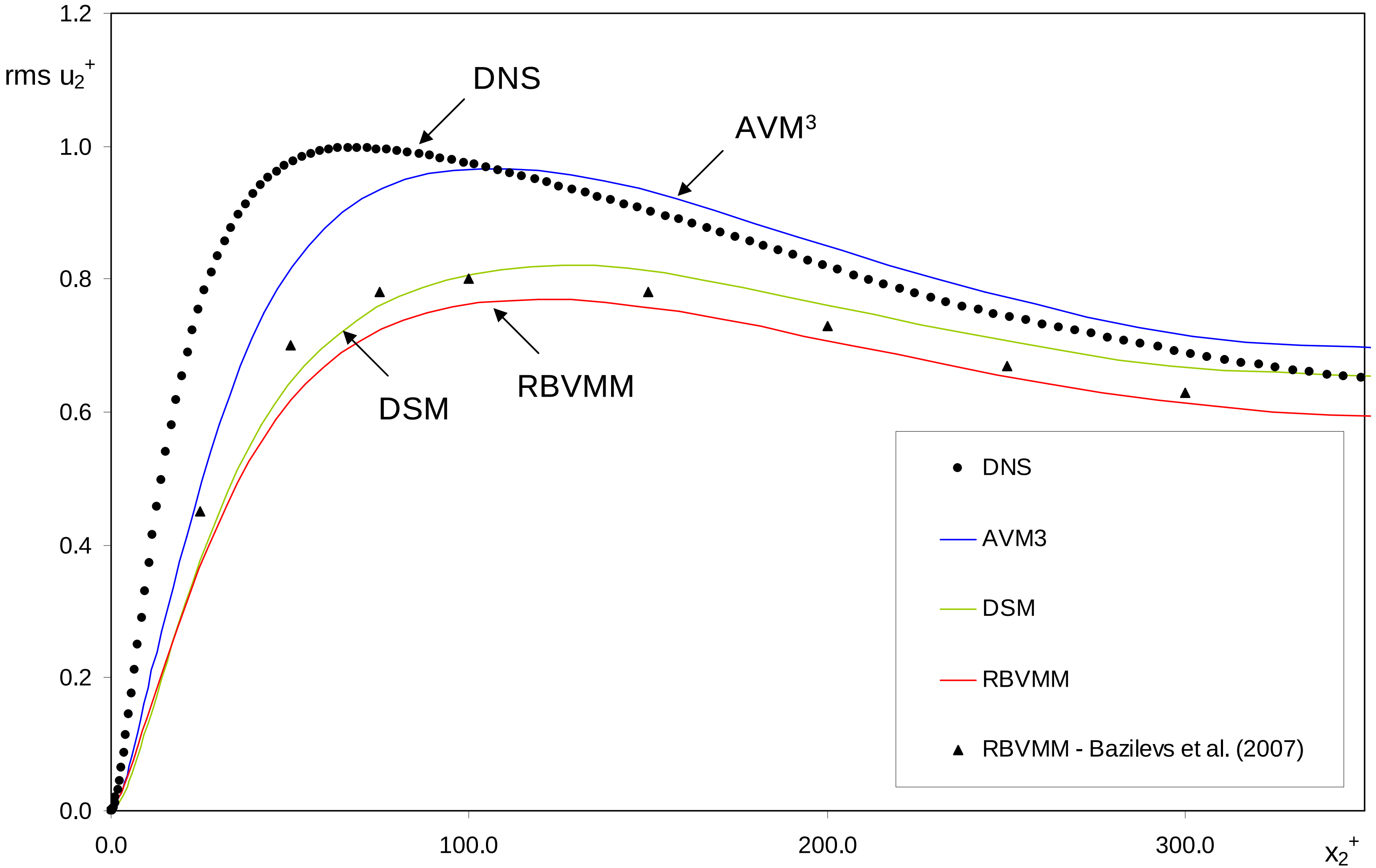
Channel: Mean Streamwise Velocity



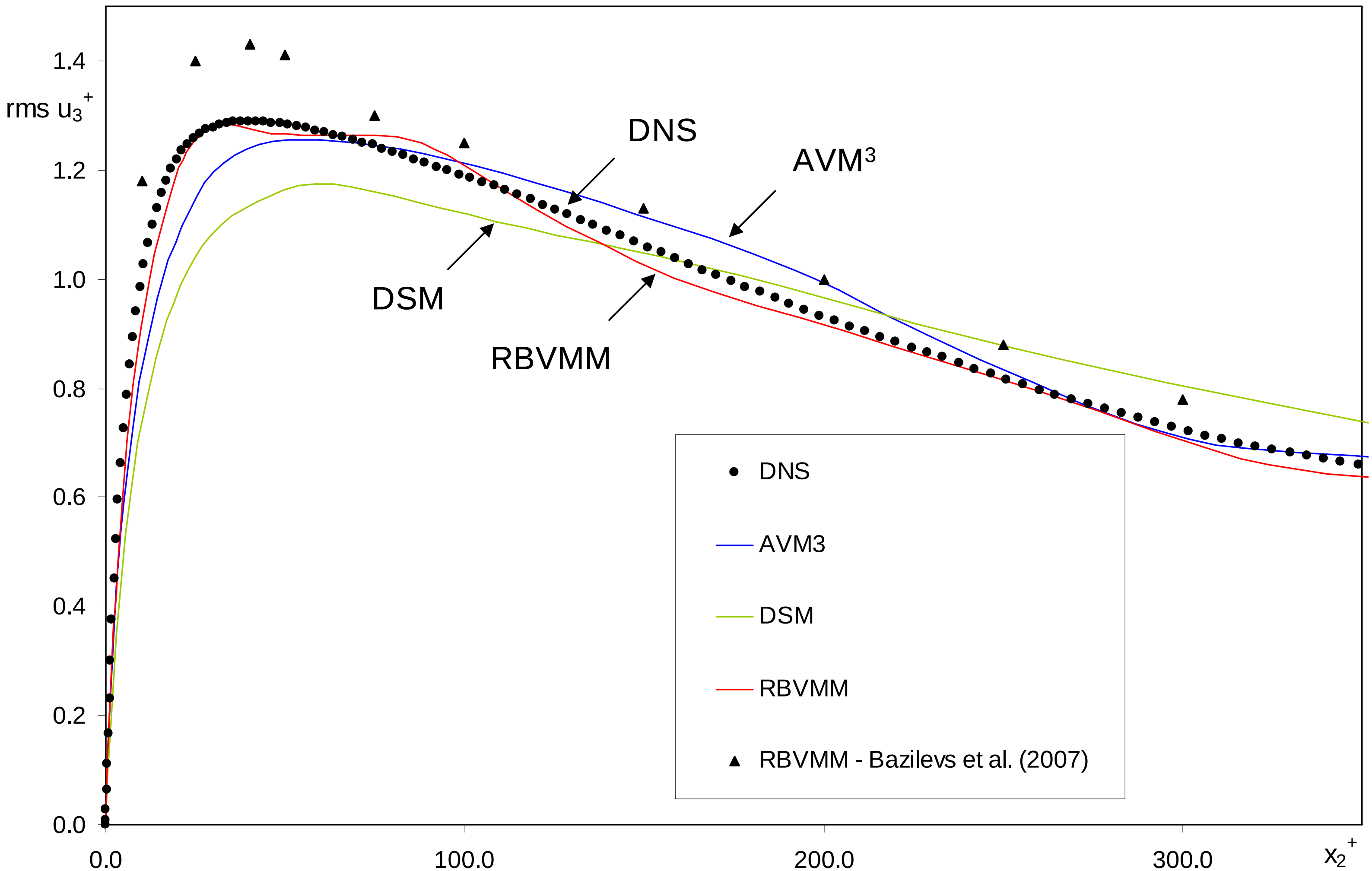
Channel: RMS Streamwise Velocity



Channel: RMS Wall-Normal Velocity



Channel: RMS Spanwise Velocity



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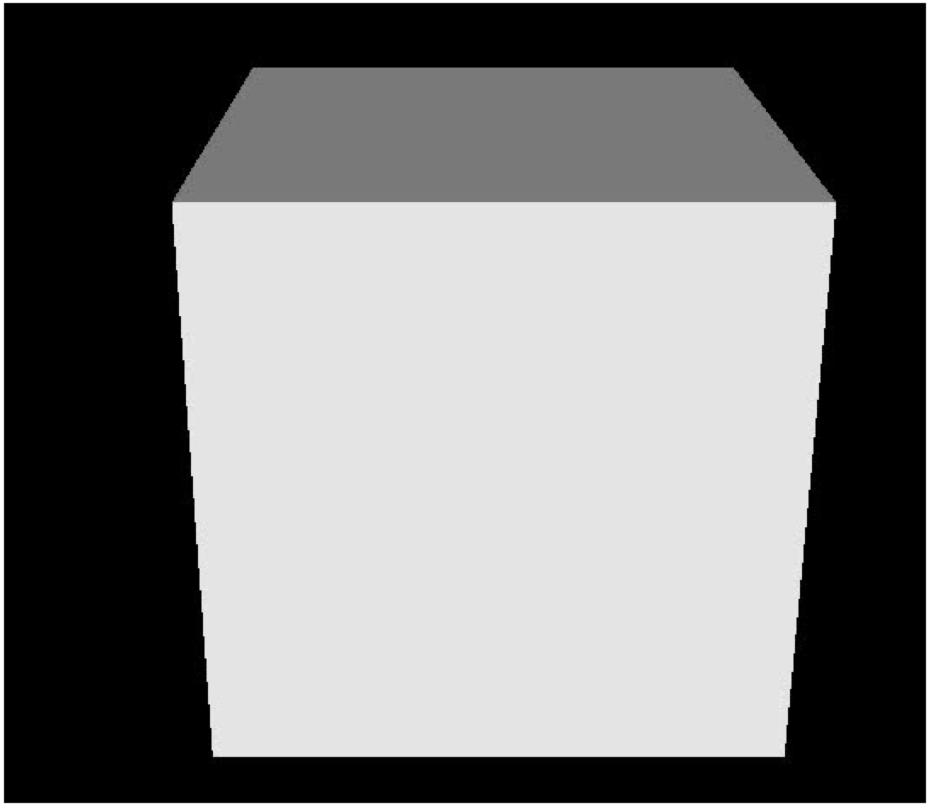
Turbulent flows featuring 2 spatial directions of inhomogeneity

Turbulent recirculating flow in a lid-driven cavity

Turbulent Flow in a Lid-Driven Cavity



Review of this flow problem:

Shankar and Deshpande (2000)

Experimental study:

Prasad and Koseff (1989)

DNS study of Kolmogorov scales:

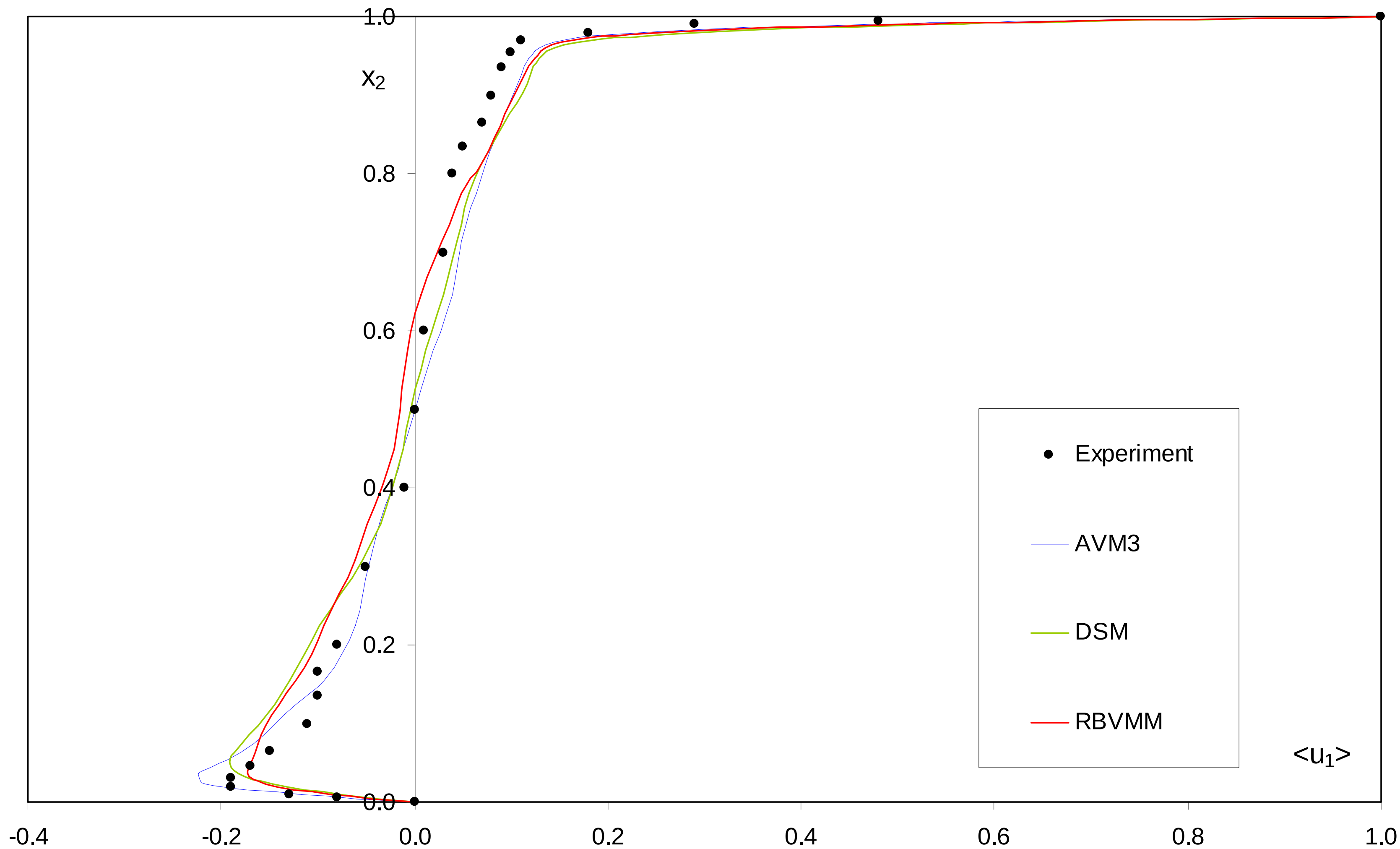
Deshpande and Milton (1998)

Some LES studies: Zang et al. (1993), Bouffanais et al. (2007), ...

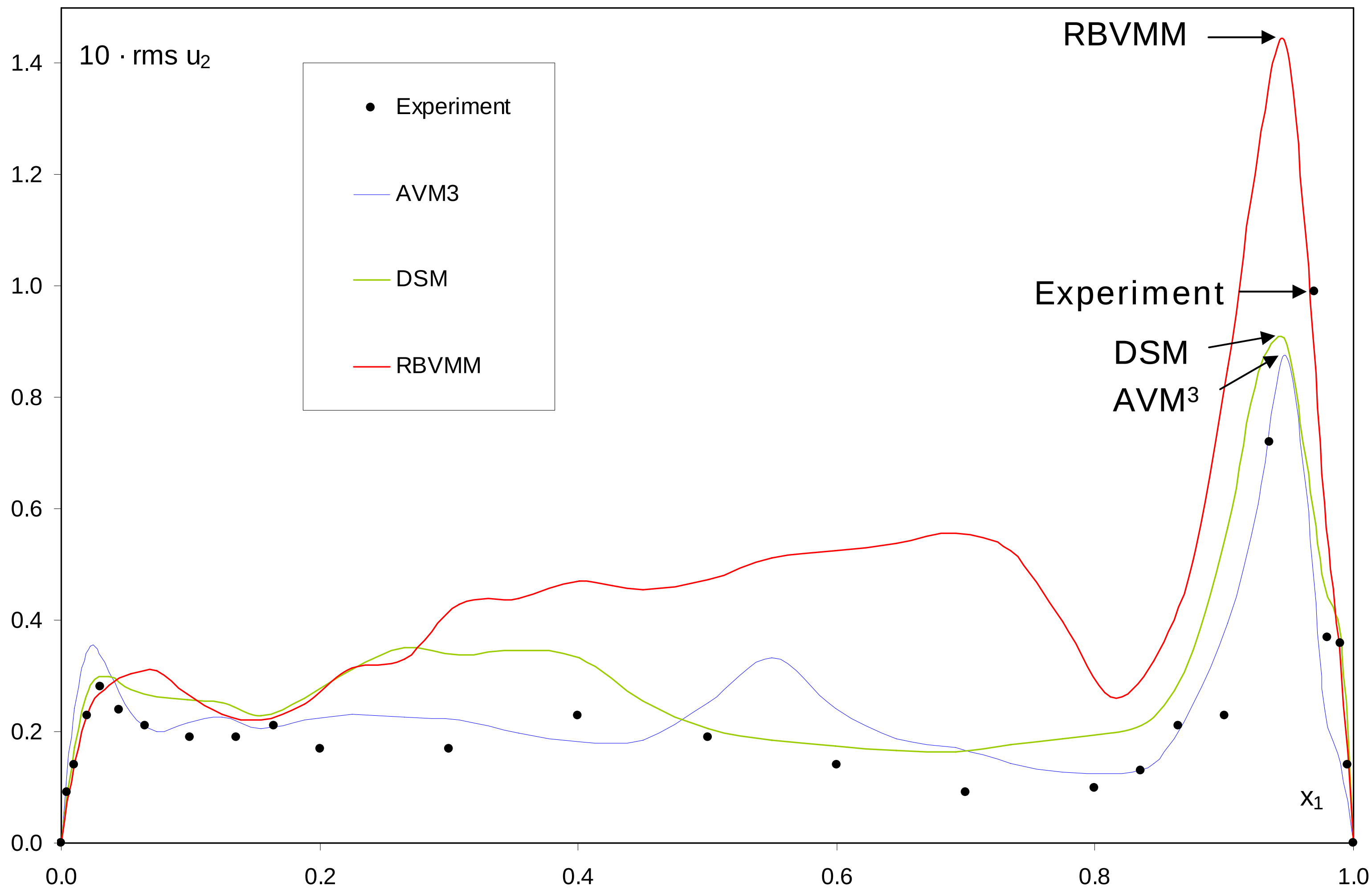
Cavity: Numerical Setup

- Reynolds number based on top-lid velocity: $Re = 10,000$
- Cavity with spanwise aspect ratio (SAR) 1.0: $\Omega = [0,1] \times [0,1] \times [0,1]$
- Crank-Nicolson time integration scheme: $\Delta t = 0.1$
- Initial run time: 5 T_{cav}, statistical evaluation period: 5 T_{cav}
- 32 linearly interpolated finite elements in each spatial direction
- refinement towards walls in x_1- and x_2-direction (min. length: 0.01)
- here: grad-div term added to AVM^3 and DSM for improv. convergence

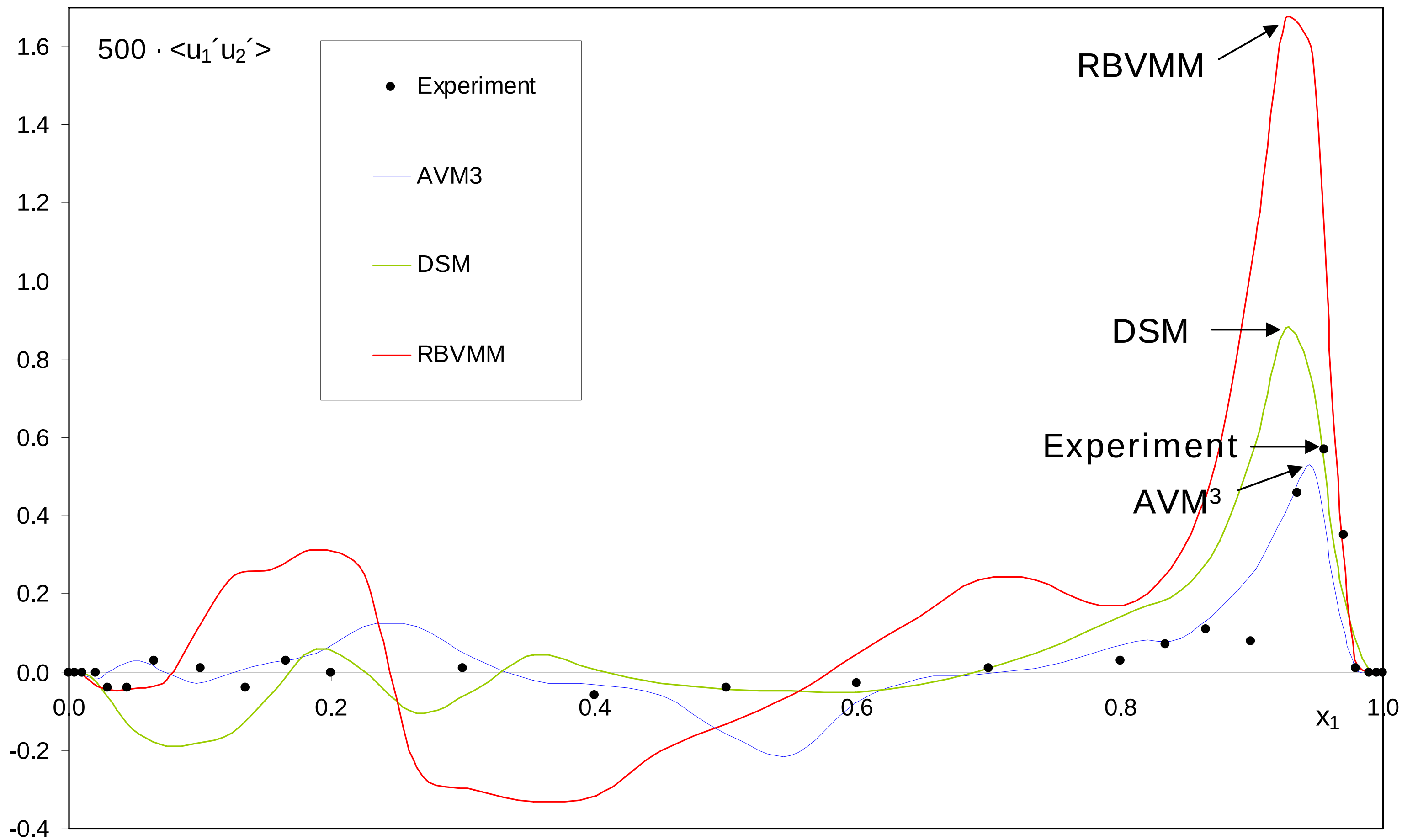
Cavity: Mean Velocity in x_1-direction vs. x_2



Cavity: RMS Velocity in x_2-direction vs. x_1



Cavity: Reynolds-Stress Component 12 vs. x_1



Computing Times

CPU Time	AVM³	RBVMM	DSM
Channel, Re_τ=180, 32^3 elements	1.00	1.06	1.28
Channel, Re_τ=395, 32^3 elements	1.00	1.30	1.16
Channel, Re_τ=590, 64^3 elements	1.00	1.03	1.42
Cavity, Re=3,200, 32^3 elements	1.00	1.60	2.50
Cavity, Re=10,000, 32^3 elements	1.00	1.56	2.53

(normalized by computing time for AVM³)

Conclusions

- **Proposed method:** algebraic variational multiscale-multigrid method (AVM^3) for three-scale VMLES of turbulent flows
- **Crucial features:** projective scale separation in a purely algebraic way using plain aggregation AMG level-transfer operators enables
  - efficient implementation
  - preservation of eigenvectors corresponding to low frequencies (standard models and smoothed scale separation damp low-frequency waves)
- **Computational evaluation:** comparison to residual-based VMLES and traditional dynamic Smagorinsky model for two (three) turbulent flow cases
- **Accuracy:** AVM^3 provides best results for all test cases, from mean flow values to highly sensitive Reynolds-stress components
- **Efficiency:** AVM^3 also computationally most efficient approach for all test cases

Outlook

- Exploitation of “block-separated” extended AVM^3 matrix formulation for efficient solution approach
- Further investigation of potential combinations of residual-based two-scale and three-scale VMLES
- Grad-div term – angel or devil?
- Comprehensive computational evaluation for “turbulent obstacle course”
- Further steps towards LES of turbulent combustion

Outlook: Turbulent Obstacle Course

Homogeneous turbulence is currently not of particular interest to us!

Turbulent flow in a channel

Outlook: Turbulent flow past a square-section cylinder

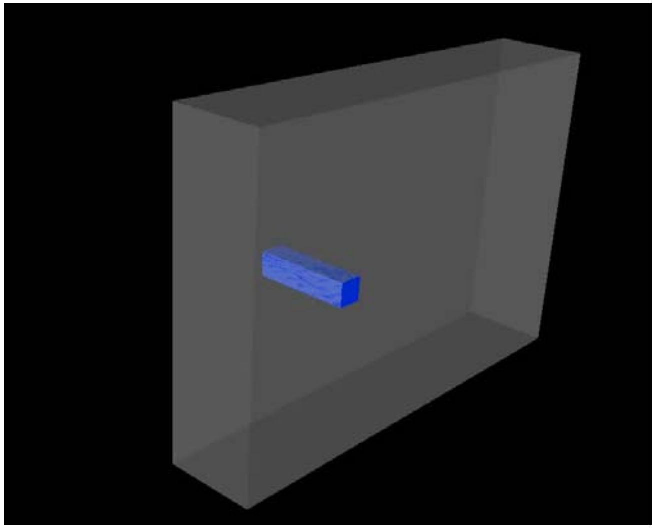
Turbulent recirculating flow in a lid-driven cavity

Outlook: Turbulent Obstacle Course

- Reynolds number: $Re = 22,000$
- Flow domain and boundary conditions:

  Rodi *et al.* (1997): "Status of LES: Results of a Workshop"

- 103,680 elements; C-N: $\Delta t = 0.075$



Outlook: Turbulent flow past a square-section cylinder

→ some early results

Cylinder: Mean Streamwise Velocity