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Computational multiscale methods for turbulent single- and two-phase flows

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Micro Abstract
Variational multiscale methods for LES of turbulent single- and two-phase flows are presented. To recover the subgrid-scale velocity, multifractal scale similarity in the enstrophy field of turbulent flow is exploited. The extended finite element method allows for sharply representing discontinuities at the interface of two-phase flow on a fixed grid. Various numerical examples, ranging from turbulent flow past a backward-facing step to turbulent bubbly channel flow, illustrate the methods.

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Introduction

Turbulent flows are omnipresent in the natural environment and the technical field of engineering. For instance, turbulent boundary layers control the drag acting on aircraft, the turbulent mixing of fuel and oxidizer enables efficient combustion engines, and the understanding of turbulent atmospheric flows leads to accurate weather forecasting. In the following, novel computational multiscale methods for turbulent single- and two-phase flows are briefly presented. The reader is referred to [4–9] for full methodical details, more elaborate discussions of the approaches and a thorough presentation of various numerical examples. Motivated by the application to Large-Eddy Simulation (LES) of turbulent flow, all numerical methods build on the framework of the Variational Multiscale Method (VMM). First, the Algebraic Variational Multiscale-Multigrid-Multifractal Method (AVM^4) for LES of turbulent single-phase flow is derived. Then, the AVM^4 is further enhanced to LES of turbulent two-phase by incorporating it into a face-oriented stabilized Nitsche-type eXtendend Finite Element Method (XFEM), leading to the eXtended AVM^4 (XAVM^4).

1 AVM^4 for LES of turbulent single-phase flow

LES of turbulent flow aims at resolving only the larger flow scales, while the influence of the smaller scales on the larger ones is modeled. The fundamental step of LES is thus the separation of the larger, resolved scales and smaller, unresolved (or subgrid) scales which is accomplished here by means of the VMM. Apart from terms depending on the resolved-scale quantities only, the variational multiscale formulation of the incompressible Navier-Stokes equations exhibits further terms, in particular the cross- and subgrid-scale Reynolds-stress terms, which include the unknown subgrid-scale velocity.

To determine the subgrid-scale velocity, multifractal scale similarity in gradient-magnitude fields of turbulent flows, such as the enstrophy field, is exploited. In the multifractal subgrid-scale modeling approach, as originally proposed in [2], the subgrid-scale velocity field is calculated from the subgrid-scale vorticity field via the law of Biot-Savart. The reconstruction of the subgrid-scale vorticity $\hat{\boldsymbol{\omega}}$, decomposed into its magnitude $\|\hat{\boldsymbol{\omega}}\|$ and orientation vector $\hat{\mathbf{e}}_{\boldsymbol{\omega}}$ of unit length, consists of two steps. First, the magnitude of the subgrid-scale vorticity field is derived by a multiplicative cascade distributing the subgrid-scale enstrophy $\|\hat{\boldsymbol{\omega}}\|^2$ within each element:

$$\|\hat{\boldsymbol{\omega}}\|(\mathbf{x},t) = \left[\left(1-\alpha^{-\frac{4}{3}}\right)^{-1}\left(2^{\frac{4\mathcal{N}}{3}}-1\right)\left(2^{\mathcal{N}}\right)^3 \prod_{n=1}^{\mathcal{N}} \mathcal{M}_n(\mathbf{x},t)\right]^{\frac{1}{2}} \|\delta\boldsymbol{\omega}^h\|, \tag{1}$$

where $\delta(\cdot)^h$ denotes smaller resolved scales (i.e., scales between the element length h and a larger scale αh), $\mathcal{N}$ the number of cascade steps and $\mathcal{M}_n$ the multipliers determining the multifractal distribution of the subgrid-scale enstrophy. In a second step, the orientation of the subgrid-scale vorticity field is determined using an additive decorrelation cascade:

$$\hat{\mathbf{e}}_{\boldsymbol{\omega}}(\mathbf{x},t) = \mathcal{I}\delta\mathbf{e}^h_{\boldsymbol{\omega}}(\mathbf{x},t) + (1-\mathcal{I})\sum_{n=1}^{\mathcal{N}} \boldsymbol{\delta}^*_n, \tag{2}$$

where $\mathcal{I}$ denotes the intermittency factor, defined from a correlation between $\hat{\boldsymbol{\omega}}$ and $\delta\boldsymbol{\omega}^h$, and $\boldsymbol{\delta}^*_n$ the decorrelation increments. Finally, the subgrid-scale velocity $\hat{\mathbf{u}}$ is obtained from $\hat{\boldsymbol{\omega}}$ via the law of Biot-Savart as

$$\hat{\mathbf{u}}(\mathbf{x},t) = B\delta\mathbf{u}^h(\mathbf{x},t), \tag{3}$$

where

$$B \sim \left(1-\alpha^{-\frac{4}{3}}\right)^{-\frac{1}{2}} 2^{-\frac{2\mathcal{N}}{3}} \left(2^{\frac{4\mathcal{N}}{3}}-1\right)^{\frac{1}{2}}. \tag{4}$$

The multifractal approximation of the subgrid-scale velocity $\hat{\mathbf{u}}$ depends on the velocity $\delta\mathbf{u}^h$ at the smaller resolved scales. The necessary further separation of the resolved scales into larger and smaller ones is realized via level-transfer operators from plain aggregation **A**lgebraic **M**ultigrid methods. The **M**ultifractal approximation of the subgrid-scale velocity is then inserted into the cross- and subgrid-scale Reynolds-stress terms of the variational multiscale formulation. The present **VMM** is completed by accompanying residual-based multiscale terms to provide a stable numerical method. The final modeled formulation is thus referred to as the AVM^4. Further details of the derivation of the AVM^4 may be found in [7]. Extensions of the AVM^4 to passive scalar transport in turbulent flow and to turbulent variable-density flow at low Mach number are shown in [5, 6].

Figure 1 displays the mean streamwise velocity of turbulent channel flow at friction Reynolds number $\mathrm{Re}_\tau = 395$. The velocity is normalized by the friction velocity and plotted in wall units as usual. Three different grids with 32^3, 64^3 and 128^3 elements are considered. For comparison, results obtained with an SUPG/PSPG/Grad-div Stabilized Method (SPGSM), a (complete) Residual-Based VMM (RBVMM) including the residual-based multiscale forms of the remaining cross- and subgrid-scale Reynolds-stress term in addition to the SUPG, PSPG and grad-div term, and a form of the Dynamic Smagorinsky Model (DSM) are shown. Moreover, Direct Numerical Simulation (DNS) data taken from [3] and marked by "DNS MKM99" are depicted. The AVM^4 provides by far the best results. In particular, the results obtained with the AVM^4 are already for the medium discretization very close to the DNS data such that the improvement owing to the finer discretization is only of small amount.

2 XAVM^4 for LES of turbulent two-phase flow

Next, two contiguous bulk fluids separated by a deformable interface are considered. The fluid flows on both sides of the interface may be turbulent, and the turbulent structures may also interact with the interface. The computational grid captures the larger scales in both fluid flows such that the same modeling situation as for LES of turbulent single-phase flow is encountered in the bulk flows. The interface is assumed to be resolved in a DNS-like manner, and additional subgrid-scale modeling with respect to underresolved interfaces is not taken into account.

The interface Γ_{int} is considered infinitely thin and, therefore, appears as a discontinuity in the flow field. At the interface, a localized surface-tension force acts, and density as well as viscosity change discontinuously, leading to strong and/or weak discontinuities in the pressure field p and the velocity field $\mathbf{u}$. These discontinuities are expressed in terms of two jump conditions:

$$[\![\mathbf{u}]\!] = 0 \qquad \text{on } \Gamma_{\text{int}}, \tag{5}$$

$$[\![-p\mathbf{I} + 2\mu\boldsymbol{\varepsilon}(\mathbf{u})]\!] \cdot \mathbf{n}_{\text{int}} = -\gamma\kappa\mathbf{n}_{\text{int}} \quad \text{on } \Gamma_{\text{int}}, \tag{6}$$

where the jump operator is defined as $[\![\cdot]\!] := (\cdot)_- - (\cdot)_+$. Interface conditions (5) and (6) couple the fluid flows in both subdomains, each governed by the incompressible Navier-Stokes equations. Variables corresponding to the first and the second fluid are marked by $(\cdot)_+$ and $(\cdot)_-$, respectively. Furthermore, μ denotes the dynamic viscosity, γ the surface-tension coefficient, which is assumed constant, $\kappa = -\nabla \cdot \mathbf{n}_{\text{int}}$ the curvature of the interface and $\mathbf{n}_{\text{int}}$ the unit normal vector on the interface.

To describe the evolution of the interface, the level-set method is applied. The level-set method captures the interface implicitly on a fixed grid via the zero iso-contour of a signed distance function and constitutes a convenient way to represent interfaces that are subject to large and complex deformations as encountered in turbulent flow. However, representing the interface implicitly leads to elements that are cut by the interface. As a result, the aforementioned discontinuities occur within the element. The XFEM allows for reproducing arbitrary discontinuities inside elements by enriching the function spaces with appropriate discontinuous functions. To represent jumps and/or kinks in the pressure and velocity field, jump enrichments based on a symmetric Heaviside function

$$\Psi(\mathbf{x}, t) = \begin{cases} -1 & \text{in fluid “-”}, \\ +1 & \text{in fluid “+”} \end{cases} \tag{7}$$

are applied. As the velocity field merely exhibits a kink, but not a jump, Nitsche's method is used to weakly couple the two individual fluid flows, i.e., to impose the velocity interface condition (5). To ensure numerical stability for arbitrary interface locations, face-oriented ghost-penalty stabilization terms (see, e.g., [1]) are included for intersected elements. Further face-oriented fluid stabilization terms in the interface region enhance the method to high-Reynolds-number flows governed by the Navier-Stokes equations. Residual-based multiscale terms in the interior of the fluid subdomains complete the Nitsche-type XFEM. For further details and depiction of the complete formulation, the reader is referred to [9].

Combing the face-oriented stabilized Nitsche-type **X**FEM, briefly described above, with the **AVM**^{4} results in a comprehensive approach to LES of turbulent two-phase flow, which is referred to as the XAVM^4; see [8]. Its application to turbulent channel flow carrying a bubble of the size of the channel half-width is shown in Figure 2. A visualization of the instantaneous bubble shape together with vortical structures identified via the Q-criterion and colored by the velocity magnitude (red color indicates high velocity and blue color low velocity) is depicted.

Conclusions

The AVM^4 for LES of turbulent single-phase flow as well as its extension XAVM^4 for LES of turbulent two-phase flow, which is obtained by combining the AVM^4 with a face-oriented stabilized Nitsche-type XFEM, have been presented. Selected numerical results have illustrated the performance of the proposed methods.

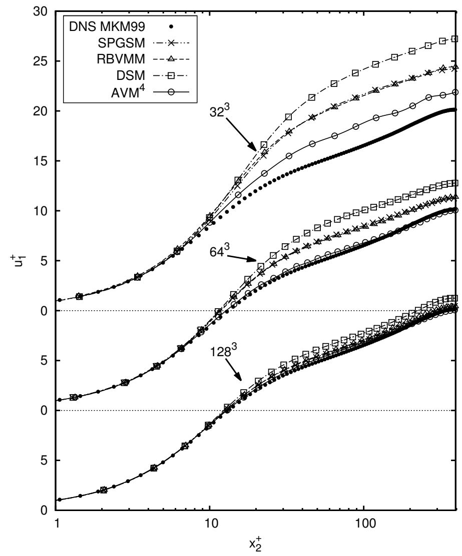

Figure 1. Mean streamwise velocity of turbulent channel flow at $\mathrm{Re}_\tau = 395$.

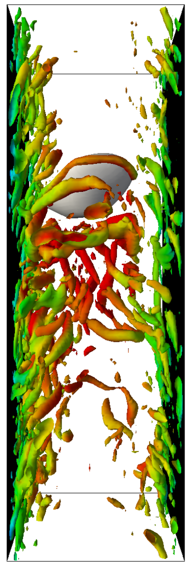

Figure 2. Instantaneous bubble shape and vortical structures of turbulent bubbly channel flow.

References

[1] E. Burman and P. Hansbo. Fictitious domain finite element methods using cut elements: II. A stabilized Nitsche method. *Applied Numerical Mathematics*, 62:328–341, 2012.

[2] G. C. Burton and W. J. A. Dahm. Multifractal subgrid-scale modeling for large-eddy simulation. I. Model development and a priori testing. *Physics of Fluids*, 17:075111, 2005.

[3] R. D. Moser, J. Kim, and N. N. Mansour. Direct numerical simulation of turbulent channel flow up to $\mathrm{Re}_\tau = 590$. *Physics of Fluids*, 11:943–945, 1999.

[4] U. Rasthofer. *Computational multiscale methods for turbulent single and two-phase flows*. Dissertation, Technische Universität München, 2015.

[5] U. Rasthofer, G. C. Burton, W. A. Wall, and V. Gravemeier. An algebraic variational multiscale-multigrid-multifractal method (AVM^4) for large-eddy simulation of turbulent variable-density flow at low Mach number. *International Journal for Numerical Methods in Fluids*, 76:416–449, 2014.

[6] U. Rasthofer, G. C. Burton, W. A. Wall, and V. Gravemeier. Multifractal subgrid-scale modeling within a variational multiscale method for large-eddy simulation of passive-scalar mixing in turbulent flow at low and high Schmidt numbers. *Physics of Fluids*, 26:055108, 2014.

[7] U. Rasthofer and V. Gravemeier. Multifractal subgrid-scale modeling within a variational multiscale method for large-eddy simulation of turbulent flow. *Journal of Computational Physics*, 234:79–107, 2013.

[8] U. Rasthofer, W. A. Wall, and V. Gravemeier. An extended algebraic variational multiscale-multigrid-multifractal method (XAVM^4) for large-eddy simulation of turbulent two-phase flow. *submitted for publication in Journal of Computational Physics*, 2017.

[9] B. Schott, U. Rasthofer, V. Gravemeier, and W. A. Wall. A face-oriented stabilized Nitsche-type extended variational multiscale method for incompressible two-phase flow. *International Journal for Numerical Methods in Engineering*, 104:721–748, 2015.