Deconvolution of induced spatial discretization filters subgrid modeling in LES: application to two-dimensional turbulence

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Abstract. The paper presents a new approximate deconvolution subgrid model for Large Eddy Simulation in which corrections to implicit filtering due to spatial discretization are integrated explicitly. The top-hat filter implied by second-order central finite differencing is a key example, which is discretised using the discrete Fourier transform involving all the mesh points in the computational domain. This discrete filter kernel is inverted by inverse Wiener filtering. The inverse filter obtained in this way is used to deconvolve the resolved scales of the implicitly filtered velocity field on the computational grid. Subgrid stresses are subsequently calculated directly from the deconvolved velocity field. The model was applied to study decaying two-dimensional turbulence. Results were compared with predictions based on the Smagorinsky model and the dynamic Germano model. A posteriori testing in which Large Eddy Simulation is compared with filtered Direct Numerical Simulation obtained with a Fourier spectral method is included. The new model presented strictly speaking applies to periodic problems. The idea of recovering a high-order inversion of the numerically induced filter kernel can be extended to more general non-periodic problems, also in three spatial dimensions.

1. Introduction

Two-dimensional flows do not occur in nature nor in the laboratory, nevertheless researching two-dimensional turbulence has many applications in geophysical flows (e.g. atmosphere and oceans), astronomy and plasma physics [1]. During the last decades studies of two-dimensional turbulence have developed significantly and many experiments have been carried out ([1], [2], [3], [4]). It is common to use a Large-eddy simulation (LES) technique for complex turbulent flows, which resolves only large-scale structures and only models small (subgrid) scales. The effects of the subgrid scales on the resolved scales are computed by so called subgrid-scale (SGS) models. Application of LES enables to obtain results which have a good agreement with the direct numerical simulations (DNS) results, while, due to coarser spatial meshes, the computational cost of performing LES is much lower than the cost of performing DNS.

There are different approaches for LES modeling. Smagorinsky model [5], which is based on an artificial eddy-viscosity parametrization and which assumes that the resolved scales carry the most of the energy and that at the subgrid scales production and dissipation are equal. Smagorinsky introduced a Smagorinsky constant $C_s$, which usually equals a number in range of
0.1 to 0.25. Germano proposed a dynamic Smagorinsky model [6] with a Smagorinsky constant which is variable in time and space. The latter model has been applied to many applications ([7], [8], [9]).

Another approach to model subgrid stresses is an inverse filtration of the resolved velocity. Geurts [10] developed an approximate higher-order polynomial inversion for the top-hat filter and proposed a generalized mixed similarity model. The inverse filtering strategy of the explicitly defined filters was extensively tested on the mixing layer LES by Kuerten et al. [11]. Domaradzki and Saiki [12] invented another method to evaluate unresolved velocity field based on kinematic adjustment of the resolved and unresolved fields and a dynamic step coupling the small scales to large scales through nonlinear interactions. Stolz and Adams [13] proposed an alternative method of inversion which they called Approximate Deconvolution Model (ADM) based on repeated filtering according to the concept of Van Cittert [14]. The ADM approach was applied by Aniszewski et al. [15] for modeling of the subgrid surface tension in the LES for two-phase flows. More recently, Wang and Ihme [16] and Wang et al. [17] applied inverse filtration for turbulent combustion modeling. They applied the ADM and the Wiener inverse filtration [18]. Nikolaou and Vervisch [19] applied the ADM approach while Domingo and Vervisch [20] used the differential filter for inversion in turbulent combustion LES modeling. Three deconvolution methods were tested in the context of turbulent combustion modeling by Mehl et al. [21]: the approximate deconvolution method based on Van Cittert iterative deconvolution, a Taylor decomposition-based method, and the regularised deconvolution method based on the minimisation of a quadratic criterion.

This paper presents another Large-eddy simulation model, used in two-dimensional incompressible decaying turbulence. A Wiener deconvolution filter for the second-order central finite difference schemes has been implemented. The results have been compared to Smagorinsky model, dynamic Smagorinsky model, DNS, and filtered DNS data.

2. Governing equations and numerical methods
The governing equation is a dimensionless streamfunction-vorticity formulation of the Navier-Stokes equations:

\[
\frac{\partial \omega}{\partial t} + \frac{\partial \psi}{\partial y} \frac{\partial \omega}{\partial x} - \frac{\partial \psi}{\partial x} \frac{\partial \omega}{\partial y} = \frac{1}{Re} \left( \frac{\partial^2 \omega}{\partial x^2} + \frac{\partial^2 \omega}{\partial y^2} \right)
\]

along with Poisson equation:

\[
\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} = -\omega
\]

where \( \omega \) is the vorticity, \( \psi \) is the streamfunction and \( Re \) is the Reynolds number.

The LES filtration operation gives:

\[
\frac{\partial \bar{\omega}}{\partial t} + \frac{\partial \bar{\psi}}{\partial y} \frac{\partial \bar{\omega}}{\partial x} - \frac{\partial \bar{\psi}}{\partial x} \frac{\partial \bar{\omega}}{\partial y} = \frac{1}{Re} \left( \frac{\partial^2 \bar{\omega}}{\partial x^2} + \frac{\partial^2 \bar{\omega}}{\partial y^2} \right) + \Pi
\]

\[
\frac{\partial^2 \bar{\psi}}{\partial x^2} + \frac{\partial^2 \bar{\psi}}{\partial y^2} = -\bar{\omega}
\]

where \( \Pi \) is the subgrid-scale term:

\[
\Pi = \frac{\partial \bar{\psi}}{\partial y} \frac{\partial \bar{\omega}}{\partial x} - \frac{\partial \bar{\psi}}{\partial x} \frac{\partial \bar{\omega}}{\partial y} - \left( \frac{\partial \psi}{\partial y} \frac{\partial \omega}{\partial x} - \frac{\partial \psi}{\partial x} \frac{\partial \omega}{\partial y} \right)
\]

and must be modeled. In the paper we use eddy-viscosity and ADM approaches which are presented in section 3.
The above presented equations are solved using an in-house solver. The time integration is conducted by fourth order Runge-Kutta method [22]. The second-order central difference method [22] was used for spatial discretization in the case of LES calculations while for DNS the Fourier method [23] was employed.

3. Subgrid models

3.1. A new Approximate Deconvolution Model

Numerical discretization introduces a certain implied filtration. It is well known that the filter associated to the second-order central differences is:

\[ \delta_x [u(x_i)] = \frac{1}{2h} (u_{i+1} - u_{i-1}) = \partial_x \left[ \frac{1}{2h} \int_{x_i-h}^{x_i+h} u(\eta) d\eta \right] = \partial_x [L(u)](x_i) \]  

(6)

In Eq. (6) we observe that the numerical derivative may be interpreted as the analytical derivative \( \partial_x \) applied to a filtered signal \( L(u) \) where \( L \) denotes the implied filter, connected uniquely to the adopted discrete derivative. The filter \( L \) can be expressed in a general way as a convolution of the discretised function and the filter kernel:

\[ L(u)(x_i) = \int_{-\infty}^{\infty} G(\eta) u(x_i + \eta) d\eta \]  

(7)

For the second-order finite differences the implied filter kernel reads

\[ G(\eta) = \begin{cases} \frac{1}{2h} & \text{if } -h \leq \eta \leq h \\ 0 & \text{otherwise} \end{cases} \]  

(8)

To apply the implied filter (7) on a numerical mesh, the integral must be approximated using the discretised function \( u \). The simplest choice is the trapezoidal rule for integration leading to the following form of the discrete filter kernel:

\[ G_{D,tr}^{D,tr} = \begin{cases} \frac{1}{4} & \text{if } -h \leq \eta \leq h \\ 0 & \text{otherwise} \end{cases} \]  

(9)

applied in the discrete convolution

\[ L_{D,tr}^{D,tr} (x_i) = \sum_{k=-1}^{1} G_{D,tr}^{D,tr} u_{i+k} \]  

(10)

Having known the discrete form of the implied filter kernel its approximate inverse can be found. First, the Wiener type inverse filtering will be applied, limiting the attention to periodic problems in the domain \( 0 < x < 1 \). Taking Fourier series of the discrete filter kernel over the computational domain

\[ \hat{G}_{D,tr}^{D,tr} = \frac{1}{N} \sum_{i=1}^{N} G_{D,tr}^{D,tr} \exp(-2\pi i k x_i), \quad k = -K, \ldots, K \]  

(11)

where \( i = \sqrt{-1} \) and \( N = 2K + 1 \) is odd number of mesh points. The inverse filter kernel in Fourier space is defined as

\[ \hat{Q}_{D,tr}^{D,tr} = \frac{1}{G_{D,tr}^{D,tr} N^2} \]  

(12)

and the inverse filter kernel in the physical space is found by the inverse Fourier transform.
\[ Q_i^{D,tr} = \sum_{k=-K}^{K} \hat{Q}_k^{D,tr} \exp^{2\pi i k x_i} \quad i = 1, \ldots, N \] (13)

However, one can expect that the accuracy of the discretised filtration depends on the form of the discrete kernel. Taking an advantage of the periodic boundary conditions in the current problem, the discretised function can be approximated by the Fourier series as

\[ L^{D,Fo}(u)(x_i) = \frac{1}{2h} \int_{-h}^{h} u(\eta) \, d\eta \approx \frac{1}{2h} \int_{-h}^{h} \left( \hat{u}_k e^{2\pi i k \eta} + \hat{u}_0 \right) \, d\eta = \] (14)

\[ \frac{1}{2h} \left[ \sum_{k=-K}^{K} \hat{u}_k e^{2\pi i k \eta} \left( e^{2\pi i k h} - e^{-2\pi i k h} \right) \frac{2\pi i k}{2\pi i k} + 2\hat{u}_0 h \right] = \]

\[ \frac{1}{2h} \left[ \sum_{k=-K}^{K} \hat{u}_k e^{2\pi i k \eta} \sin(2\pi kh) \frac{2\pi i k}{\pi k} + 2\hat{u}_0 h \right] \] (15)

Introducing the inverse Fourier transform into the last equation leads to

\[ L^{D,Fo}(u)(x_i) = \frac{1}{2h} \left[ \sum_{k=-K}^{K} e^{2\pi i k h} \sin(2\pi kh) \frac{2\pi i k}{\pi k} \times \right. \]

\[ \times \left. \sum_{q=-K}^{K} u_{i+q} e^{-2\pi i k(i+q)h} + 2h \frac{1}{N} \sum_{q=-K}^{K} u_{i+q} \right] = \] (16)

\[ \sum_{q=-K}^{K} u_{i+q} \left[ \sum_{k=-K}^{K} e^{-2\pi i kqh} \sin(2\pi kh) \frac{2\pi i k}{2\pi k} + \frac{1}{N} \right] = \]

\[ \sum_{q=-K}^{K} u_{i+q} \left[ \sum_{k=1}^{K} \cos(-2\pi kqh) \sin(2\pi kh) \frac{2\pi i k}{\pi k} + \frac{1}{N} \right] \]
Finally, the discrete filter kernel in the case of Fourier approximation for the second-order central differences reads
\[
G_{D,Fo}^q = \sum_{k=1}^{K} \frac{\cos(-2\pi kqh) \sin(2\pi kh)}{\pi k} + \frac{1}{N} \quad (17)
\]
and the filter kernel of its inverse counterpart is established from Eqs (12) and (13). In the ADM approach the discrete filter and its inverse are used to determine the subgrid-scale term (5) directly.

3.2. The Smagorinsky model and the dynamic Smagorinsky model
The Smagorinsky model [5] is the pioneer and one of the most popular subgrid-scale models used in LES. The Smagorinsky model is based on an eddy viscosity assumption in which the subgrid-scale term is defined as:
\[
\Pi = \nu_t \left( \frac{\partial^2 \omega}{\partial x^2} + \frac{\partial^2 \omega}{\partial y^2} \right) \quad (18)
\]
where \( \nu_t \) is turbulent viscosity and in the case of the Smagorinsky model is established as:
\[
\nu_t = (C_s \Delta)^2 \left( \bar{S}_{ij} \bar{S}_{ij} \right)^{1/2} \quad (19)
\]
where \( C_s \) is the Smagorinsky constant, \( \Delta \) is the filter width and \( S \) is the strain rate tensor.

Germano et al. [6] proposed the dynamic Smagorinsky model in which the Smagorinsky constant is computed dynamically by
\[
C_s^2 \Delta^2 = \frac{LM}{M^2} \quad (20)
\]
where
\[
L = J(\hat{\psi}, \hat{\omega}) - \hat{\omega} \quad (21)
\]
and
\[
M = \kappa^2 |\hat{\bar{S}}| \nabla^2 \hat{\omega} - |\hat{\bar{S}}| \nabla^2 \hat{\omega} \quad (22)
\]
where \( \kappa \) is the ratio between characteristic length scales on the test and basic filters [2]. In this paper the test filter is a trapezoidal filter and \( \kappa = \sqrt{6} \) has been adopted.

3.3. Generation of the initial condition
The initial field has been obtained according to the method proposed by San and Staples [1]. Two-dimensional freely decaying incompressible flow with a square domain of length \( 2\pi \) and with periodic boundary conditions has been taken into consideration. In inviscid flows an inertial range in the energy spectrum is proportional to \( k^{-3} \), where \( k = |k| = \sqrt{k_x^2 + k_y^2} \) is a wavenumber in Fourier space. The initial energy spectrum is assumed to be
\[
E(k) = \frac{a_s}{2} \frac{1}{k_p} \left( \frac{k}{k_p} \right)^{2s+1} \exp\left[-(s + \frac{1}{2})(\frac{k}{k_p})^2\right]
\]
where \( s \) is a shape parameter assumed to be equal 3 and where \( a_s = \frac{(2s+1)^{s+1}}{2^{s+1} s!} \). The maximum value of initial energy spectrum is obtained for \( k_p = 12 \). After introducing a phase function \( \zeta(k) = \xi(k) + \eta(k) \), where \( \xi(k) \) and \( \eta(k) \) are random values from interval \([0, 2\pi]\) chosen independently, we are able to obtain the initial vorticity distribution.
Figure 1: Comparison of the turbulence kinetic energy changing with time for different models. DNS computations were performed with resolution of $1025^2$ and LES computations were performed with resolution of $257^2$.

Figure 2: Comparison of the averaged energy spectra for different models at time $t = 1$. DNS computations were performed with resolution of $1025^2$ and LES computations were performed with resolution of $257^2$.

\[
\tilde{\omega}(k) = \sqrt{\frac{E}{\pi}} e^{i\xi(k)}
\]

Afterwards, using inverse Fourier transform, the initial vorticity in the physical space, the streamfunction, and the velocity field are obtained.
Figure 3: Comparison of the averaged energy spectra for different models at time $t = 5$. DNS computations were performed with resolution of $1025^2$ and LES computations were performed with resolution of $257^2$.

Figure 4: The vorticity field for different models at Re = 1000 and time $t = 1$. (a) Smagorinsky model. (b) dynamic Smagorinsky model. (c) ADM Fo. model. Computations were performed with resolution of $257^2$.

4. Results
In this section results obtained from simulations with different models implemented, including the ADM model from section 3, are presented and compared. The LES results are compared with the DNS computations obtained with the spectral Fourier method and with the DNS results filtered with the filter (17) using the mesh size used for LES. All simulations were performed with a resolution of $1025^2$ for DNS and $257^2$ for LES and for Reynolds numbers $Re = 1000$ and $Re = 4000$. Total non-dimensional time of performace was 10 with a time step $5 \times 10^{-4}$.

Figure 1 shows an evolution of the turbulent kinetic energy obtained with the new ADM model, compared with the results obtained with the Smagorinsky model, the dynamic Smagorinsky model, DNS and the filtered DNS. In the case of $Re = 1000$ the Smagorinsky and the dynamic Smagorinsky models show faster energy decay compared to the filtered DNS
Figure 5: The vorticity field for different models at $Re = 1000$ and time $t = 5$. (a) Smagorinsky model. (b) dynamic Smagorinsky model. (c) ADM Fo. model. Computations were performed with resolution of $257^2$.

Figure 6: The vorticity field for different models at $Re = 4000$ and time $t = 1$. (a) Smagorinsky model. (b) dynamic Smagorinsky model. (c) ADM Fo. model. Computations were performed with resolution of $257^2$.

results. The results obtained with both models are very close to each other, although, the dynamic model is slightly less dissipative. The new ADM model shows the energy decay very close to the filtered DNS results. Initially, the energy decay for the ADM models is slightly faster than the one obtained from filtered DNS. Later for time $t > 5$ the results coincide. In the case of the higher Reynolds number $Re = 4000$ the differences resulting from different subgrid models are much more pronounced. In this case, again, both eddy viscosity models result in the energy decay much faster compared to the ADM model and filtered DNS results. It should be stressed that the ADM model results in the energy decay rate identical to the one obtained from the filtered DNS. Initial energy in the case of the filtered DNS is slightly greater than in the case of the LES but in a long time interval $t < 5$ these lines are nearly parallel. Later, for $t > 5$ the ADM model shows slightly faster energy decay than the filtered DNS. If the initial conditions were identical the results would coincide.

In figures 2 and 3 the averaged energy spectra computed from the velocity fields for various models, in two time instants and two Reynolds numbers, are presented. Again, for both time instants and for both Reynolds numbers, the proposed model turned out to be in a much better agreement with the filtered DNS data, while the Smagorinsky and the dynamic Smagorinsky
models overestimate the filtered energy at fine scales. It seems that the ADM model reproduces much better interaction of the turbulent structures of the scales close to the cut-off wave number, as the energy spectrum coincides with the results of the filtered DNS. The differences in the spectra obtained with ADM model and the eddy viscosity models are more pronounced for higher Reynolds number.

Figures 4, 5, 6, and 7 illustrate the vorticity field obtained for the Smagorinsky model, the dynamic Smagorinsky model, and the proposed model for time $t = 1$ and $t = 5$ and for Reynolds numbers $Re = 1000$ and $Re = 4000$. For $Re = 1000$ at time $t = 1$ all models gave similar results. Visually, the vorticity field characterised by the small scales introduced in the initial condition, after a short time, is predicted by all models in the same manner. However, after a longer time of evolution, for $t = 5$ shown in figure 5, the results with the ADM model are significantly different from the results obtained with the eddy viscosity model. It should be stressed that the results obtained with the Smagorinsky and the dynamic Smagorinsky models are nearly the same. Obviously, all the models predict the process of the small eddies merging and the formation of the larger vortices. However, a different vorticity field resulting from the ADM model indicates that the large scale dynamics predicted with this model is significantly different from those predicted with two eddy viscosity models. A similar situation occurred for the higher Reynolds number, but the differences at time $t = 1$ are slightly more noticeable than for $Re = 1000$. In this case, the vorticity structure obtained with the eddy viscosity models after quite a long time $t = 5$ is almost the same. The ADM model predicts quite a different vorticity field also in the case of the higher Reynolds number.

5. Conclusion
A new ADM model is proposed based on the Wiener inverse filtration and a new form of the discrete filter kernel of the filter implied by the numerical scheme. The model was tested in the case of the 2D decaying turbulence. The results compared with the classical eddy viscosity models and the DNS results show a great potential of the model proposed. The global parameters like the turbulence kinetic energy decay and energy spectral distribution were in significantly better agreement with the DNS result compared with the classical eddy viscosity models. The results presented should be considered as a preliminary analysis of this new ADM model which will be continued with a more advanced analysis of the statistics obtained in 2D and 3D homogeneous turbulence as well as testing in more complicated shear and transitional flows.
Acknowledgements
The research was supported by the Polish National Science Centre, Project No. 2018/29/B/ST8/00262, and by the National Agency for Academic Exchange (NAWA) within the International Academic Partnerships Programme No. PPI/APM/2019/1/00062.

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