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INTRODUCTION

We address the basic equation in Large Eddy Simulation (LES) of turbulent flow: the filtered Navier-Stokes equation. The focus will be on the subgrid stress and on the relation between the filtered fields and the best possible approximation of the underlying non-filtered fields. The best approximated fields, found via deconvolution (Geurts 1997; Domaradzki and Loh 1999), will be used to formulate the filtered Navier-Stokes equation such that its model variables are best approximations of the velocity- and pressure-fields and simultaneously the tendencies in the equation are best approximations of the measurable forces. LES does not prescribe a specific filter, even though the conclusions that are drawn from LES depend on the choice of the filter. The reconstructed Navier-Stokes equation will be seen to make a unification of all low-pass filtered Navier-Stokes equations. We will show which wave-wave interactions contribute to the remaining subgrid stress term. The reconstructed Navier-Stokes equation will be related to the classic subfilter formulation of the filtered Navier-Stokes equation, which is shown to introduce aliasing effects. The expectation values of the subgrid stresses in both new and classic formulation term will be related to Reynolds-decompositions of the flow. Data from a field-experiment on atmospheric boundary layer flow will be used to illustrate the theory.

1. LES BASICS

In Large Eddy Simulation (LES) one reduces the number of nodes required for a simulation in full detail ($\sim \text{Re}^{9/4}$) to a number of nodes that fits into a computer by low-pass filtering (symbol $\bar{}$) the equation of motion (NS):

$$\text{NS}(u_i, p) \longrightarrow \overline{\text{NS}}(u_i, p) \quad (1)$$

In classic LES one rearranges terms and addresses the following equation, with the appearance of the original Navier-Stokes equation, but now expressed in filtered fields (sum over double indices):

$$\overline{\text{NS}}(u_i, p) \longrightarrow \text{NS}(\bar{u}_i, \bar{p}) + \text{corrections} \quad (2a)$$

$$\frac{\partial \bar{u}_i}{\partial t} + \frac{\partial}{\partial x_j} (\bar{u}_i \bar{u}_j) = -\frac{\partial}{\partial x_i} \bar{p}_{\text{mod}} + \nu \nabla^2 \bar{u}_i - \frac{\partial}{\partial x_j} \text{Deviat}(\tau_{ij}) \quad (2b)$$

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where p_{mod} is a modified pressure, τ_{ij} a subgrid-stress, which has to be modelled:

$$\bar{p}_{\text{mod}} \equiv \frac{\bar{p}}{\rho} + \text{Trace}(\bar{\tau}) \quad (2c)$$

$$\tau_{ij} \equiv \bar{u}_i \bar{u}_j - (\bar{u}_i)(\bar{u}_j) \quad (2d)$$

$$\text{Deviat}(\tau_{ij}) \equiv \tau_{ij} - \frac{1}{3} \text{Trace}(\tau) \delta_{ij} \quad (2e)$$

According to functional analysis the best resolved approximation q^r of measurable quantity is an orthogonal projection of the non-filtered field q onto the available functional space in LES. It is constructed from filtered field \bar{q} by a conditional deconvolution over a range $[-k_r, k_r]$, which comprizes all resolved scales that have not been suppressed to insignificance (we use threshold value 0.05 for the suppression) by low-pass filter G (symbol $\hat{}$ is a Fourier transform):

$$\begin{aligned} q^r(\mathbf{x}) &\equiv \int_{-k_r}^{k_r} \frac{\hat{q}(\mathbf{k})}{\hat{G}(\mathbf{k})} e^{i\mathbf{k}\cdot\mathbf{x}} d\mathbf{k} = \int_{-k_r}^{k_r} \frac{\hat{G}(\mathbf{k})\hat{q}(\mathbf{k})}{\hat{G}(\mathbf{k})} e^{i\mathbf{k}\cdot\mathbf{x}} d\mathbf{k} \\ &= \int_{-k_r}^{k_r} \hat{q}(\mathbf{k}) e^{i\mathbf{k}\cdot\mathbf{x}} d\mathbf{k} = \bar{q}_{\text{cutoff}}(\mathbf{x}) \quad \text{reconstructed quantity} \end{aligned} \quad (3)$$

This operation should always be carried out on LES-fields before conclusions are made. Otherwise one will get a filtered, distorted view of the flow. We see that, independent from the choice of the filter type, the reconstructed fields are equivalent to cut-off filtered fields. This is good news: the seemingly arbitrary choice of the filter has no consequences for the conclusions that will be drawn from LES. By placing this cut-off at the Nyquist-point of the numerical grid ($k_{\text{Nyq}} = \pi/\Delta$), one maximizes the correspondence between 'true' (measurable) and simulated fields.

One could have conditionally de-filtered the equation of motion *a priori* and express as many terms as possible in reconstructed fields:

$$\begin{aligned} \overline{\text{NS}}(u_i, p) &\longrightarrow (\text{NS}(u_i, p))^r \\ &\longrightarrow (\text{NS}(u_i^r, p^r))^r + \text{correction terms} \end{aligned} \quad (4a)$$

Written out this gives the (Galilean invariant) reconstructed Navier-Stokes equation:

$$\frac{\partial u_i^r}{\partial t} + \frac{\partial}{\partial x_j} (u_i^r u_j^r) = -\frac{\partial}{\partial x_i} p_{\text{mod}}^r + \nu \nabla^2 u_i^r - \frac{\partial}{\partial x_j} \text{Deviat}(\alpha_{ij}) \quad (4b)$$

where we use:

$$p_{\text{mod}}^r \equiv \frac{p^r}{\rho} + \text{Trace}(\bar{\alpha}) \quad (4c)$$

$$\alpha_{ij} \equiv (u_i u_j)^r - (u_i^r u_j^r) \quad (4d)$$

To prevent aliasing one has to use a doubly dense grid to store the intermediate products before the final reconstruction operation is done.

2. COMPARISON OF RECONSTRUCTED AND CLASSIC FORMULATIONS

Tensor α_{ij} is the great unknown in LES and has to be parameterized. To get better insight into the influence of either τ_{ij} from the classic LES-formulation, or α_{ij} in the proposed *a priori* reconstructed LES-formulation, we make Fourier-decompositions of $\partial_j \alpha_{ij}$ and $\partial_j \tau_{ij}$:

$$\frac{\partial}{\partial x_i} \widehat{\{\alpha_{ij} \text{ or } \tau_{ij}\}}(\mathbf{k}) = \int_{-\infty}^{\infty} i F_j(\mathbf{k}', \mathbf{k}'') \left(\hat{u}_i(\mathbf{k}') \hat{u}_j^*(\mathbf{k}'') \right) d\mathbf{k}' \quad (5a)$$

with $\mathbf{k}'' \equiv \mathbf{k}' - \mathbf{k}$ and

$$F_{j,\alpha}(\mathbf{k}', \mathbf{k}'') \equiv \hat{G}_{\text{cutoff},k_r}(\mathbf{k}' - \mathbf{k}'') \cdot \left(1 - \hat{G}_{\text{cutoff},k_r}(\mathbf{k}') \hat{G}_{\text{cutoff},k_r}(\mathbf{k}'') \right) (k'_j - k''_j) \quad (5b)$$

$$F_{j,\tau}(\mathbf{k}', \mathbf{k}'') \equiv \left(\hat{G}(\mathbf{k}' - \mathbf{k}'') - \hat{G}(\mathbf{k}') \hat{G}(\mathbf{k}'') \right) (k'_j - k''_j) \quad (5c)$$

Functions \mathbf{F}_α and \mathbf{F}_τ express the proportionality of non-linear eddy interactions $\hat{u}_i(\mathbf{k}') \hat{u}_j^*(\mathbf{k}'')$ between eddies of wavevector \mathbf{k}' and \mathbf{k}'' in the respective subgrid-stress terms. One-dimensional analogues of \mathbf{F} are drawn in figure 1: \mathbf{F}_α is shown on the left, \mathbf{F}_τ for cut-off filtering is shown in the centre and its equivalent for Gauss-filtering on the right.

The main difference between our proposed reconstructed formulation of the LES-equation and the classic formulation is the presence in the central and right plot in figure 1 of interactions of two eddies which are both resolved ($|\mathbf{k}'|, |\mathbf{k}''| \leq k_r$). These interactions can in principle be calculated from the resolved velocity field via filter-inversion and can therefore be taken into account, as is shown in the plot on the left for the new formulation. Not taking into account these resolved-resolved interactions is a serious omission, as can be seen from e.g. the central plot. The purpose of filtering was to eliminate the small scales, but the contribution to the tendency of the resolved velocity fields, induced by these resolved-resolved interactions, has a wave-vector $\mathbf{k} = \mathbf{k}' - \mathbf{k}''$. This can give a subgrid wave, e.g. along the negative diagonals in figure 1, where $\mathbf{k} = 2\mathbf{k}'$. In practice this would mean that the grid has to be doubly refined every timestep, or one would have to allow these waves to alias onto resolved waves. The reconstructed formulation of the filtered Navier-Stokes equation does not have this aliasing problem.

One can try to improve the classic LES-formulation by extracting the resolved-resolved interactions from the subgrid stress (Biringen and Reynolds 1981):

$$\frac{\partial \bar{u}_i}{\partial t} + \frac{\partial}{\partial x_j} \overline{u_i^r u_j^r} = -\frac{\partial}{\partial x_j} \bar{p}_{\text{mod}} + \nu \nabla^2 \bar{u}_i - \frac{\partial}{\partial x_j} \text{Deviat}(\beta_{ij}) \quad (6a)$$

where $\bar{\beta}$ is a subgrid stress (and \bar{p}_{mod} the corresponding modified pressure) defined by:

$$\beta_{ij} \equiv \overline{u_i u_j} - \overline{u_i^r u_j^r} \quad (6b)$$

This formulation is only Galilean invariant for filters including a spectral cut-off at the Nyquist-point of the grid. Moreover we see that the advective term requires estimation of the reconstructed velocity. Therefore a further pursuit of non-reconstructed formulation (6a), i.e. postponing the reconstruction of the velocity field until completion of the simulation, will not give any numerical advantage above *a priori* reconstruction of the filtered equation: for every timestep the field is reconstructed anyhow and renaming this intermediate quantity to be the model variable of the simulation instead of the filtered field makes the two formulations equivalent for filters including the just mentioned cut-off. We conclude that the reconstructed formulation of the LES-equation is superior to the filtered and 'improved' filtered formulations.

3. EXPECTATION VALUE OF THE SUBGRID STRESS

As an onset to subgrid stress modelling we will now show the impact of Reynolds-averaging for those cases where an expectation value for the mean flow profile is known. We decompose the velocity into its local expectation value (indicated with symbol \mathcal{E}) and a turbulent fluctuating part (indicated with a tilde) with use of the following relation:

$$u_i = \mathcal{E}(u_i) + \tilde{u}_i \quad \text{with} \quad \mathcal{E}(\tilde{u}_i) = 0 \quad (7)$$

With this decomposition we can show that the expectation-value of the subgrid-stress term is:

$$\mathcal{E}\left(\frac{\partial}{\partial x_j} \alpha_{ij}\right) = \frac{\partial}{\partial x_j} \left\{ \left\{ \mathcal{E}(u_i) \mathcal{E}(u_j) \right\}^r - \left\{ \mathcal{E}(u_i) \right\}^r \left\{ \mathcal{E}(u_j) \right\}^r \right\} \quad (8)$$

This term *does not depend on the statistics of turbulent quantities!* Only mean flow characteristics are required. This relation also implies that assumptions like "in ensemble sense the subgrid velocity field obeys the inertial sub-range spectrum" do *not* lead to insight into the expectation value of the subgrid stress, because "nothing more can be expected". Such assumptions will only help with the modelling of the fluctuating part of the subgrid stress. Knowledge of e.g. a log-law for the velocity-profile will give a good hint for the mean value of the subgrid stress. Instantaneous slab-averages may even help to tune the instantaneous stresses.

4. APPLICATION TO MEASURED DATA

To show the above relations in practice, we collected 24 hours of 20 Hz samples with a sonic anemometer at two heights (4 m and 100 m) above grass in Cabauw. The powerspectrum of 1 hour of samples is presented in figure 2, which shows inertial decay over the last two decades of the spectrum. We adopt an LES-gridspacing of $\Delta = 25$ m, corresponding with 102 samples for the data collected at

4 m. For the filter we take a spectral cut-off at $k_{\text{Nyq}} = [\pi/25] \text{ m}^{-1}$ to avoid the final deconvolution step.

We subtracted the mean velocity and used the time-series to construct a 1D-equivalent of the relations that were presented above and estimated the total filtered longitudinal advection $\overline{\partial_x(u^2)}$ of momentum in mean flow direction and its powerspectrum. This is (the 1D equivalent of) the non-linear term at which LES aims, but which cannot be calculated during LES, since it requires the squared *non-filtered* velocity. The powerspectrum is shown in grey in figures 3 and 5, the physical-space values over an arbitrary segment of the domain are given in grey in figures 4 and 6. For classic LES-equation (2b) we estimated the resolved and subgrid advective terms. These are shown in figures 3 and 4. Equivalents for reconstructed LES-equation (4b) are shown in figures 5 and 6.

We see that all dynamics involved in the reconstructed Navier-Stokes equation is resolvable. In the classic formulation the subgrid term is dominated by non-resolved contributions and the resolved advection and residual subgrid effects show short-range fluctuations. It should be clear that the classic LES-formulation unnecessarily complicates things and that the reconstructed formulation gives a better, aliasing-free approximation of the filtered total advection, leaving less to subgrid modelling. To quantify this we calculated ratios (X_{new} for the reconstructed equation and X_{old} for the classic equation) of the rms-values of the respective subgrid-stress terms to the rms of the total filtered advective term. For the record taken at 4 m we found $X_{\text{new}} = 0.38$ and $X_{\text{old}} = 0.70$. For the 100 m records the ratios were found in the ranges $X_{\text{new}} \in [0.19 - 0.48]$ with a meanvalue of 0.30 and $X_{\text{old}} \in [0.28 - 0.85]$ with a mean value of 0.53. These values show that advection in the classic LES-equation is dominated by 'subgrid' effects. In the reconstruction formulation the majority of advective dynamics is now represented by the resolved term.

5. CONCLUSIONS

We have de-convolved the filtered Navier-Stokes equation over those wavenumbers which are resolved and for which the filter is invertible. Our proposed model variables are the 'reconstructed' velocity- and pressure fields. The resulting 'reconstructed Navier-Stokes equation' (which still allows for *any* filter type) is equivalent to a Navier-Stokes equation, which is spectrally truncated at the Nyquist wavenumber of the LES. The truncation error is incorporated in the model as the subgrid stress term and was shown to be Galilean invariant. We conclude that we have addressed and solved three problems in LES:

- Subjectiveness, connected with the selection of the filter. The reconstructed Navier-Stokes equation allows for any type of low-pass filter but always gives the same solution. In the new formulation the mag-

nitude of the required subgrid dynamics, which still has to be parameterized, is substantially reduced when compared with the classic formulation.

- Incomparability. In classic LES it was not clear how the (numerical) model variables should best be compared with or translated into physical values from measurements or outcomes from different LES-studies. Tendencies and model variables in the reconstructed Navier-Stokes equation were shown to give the best estimates.
- An aliasing problem, which has been shown to have serious consequences for the simulation of the convective atmospheric boundary layer in classic LES, but which is absent in the new formulation.

The solution of these problems is equivalent to a combination of the following classic techniques: adoption of a spectral cut-off filter and anti-aliasing of the advective term by truncation of its spectrum at the Nyquist wavenumber of the LES. The expectation value of the (both classic and reformulated) subgrid term is solely determined by the mean velocity profile. It does not depend on the turbulent spectrum, which only induces fluctuations in subgrid dynamics. The present analysis assumes a spectral LES. When finite differences are used to estimate differential operators, then a second filter will enter the filtered Navier-Stokes equation (Ghosal 1996; Carati et al. 2001). Future study will have to make clear if the influence of this second filter on the outcomes of non-spectral LES can be optimized by the selection of one specific type of filter.

Acknowledgment

Jan Slager is acknowledged for performing the measurements. The investigations were supported by the EU, contract EVK2-CT-1999-00051 EUROCS (European Project on Cloud Systems in Climate Models).

6. REFERENCES

- Biringen, S. and W. Reynolds, 1981: Large-eddy simulation of the shear-free turbulent boundary layer. *J.Fluid Mech.*, **103**, 53–63.
- Carati, D., G. Winckelmans, and H. Jeanmart, 2001: On the modelling of the subgrid-scale and filtered-scale stress tensors in large-eddy simulation. *J.Fluid Mech.*, **441**, 119–138.
- Domaradzki, J. and K.-C. Loh, 1999: The subgrid-scale estimation model in physical space representation. *Phys.Fluids*, **11(8)**, 2330–2342.
- Geurts, B., 1997: Inverse modeling for large-eddy simulation. *Phys.Fluids*, **9(12)**, 3585–3587.
- Ghosal, S., 1996: An analysis of numerical errors in large-eddy simulations of turbulence. *J.Comput.Phys.*, **125**, 187–206.

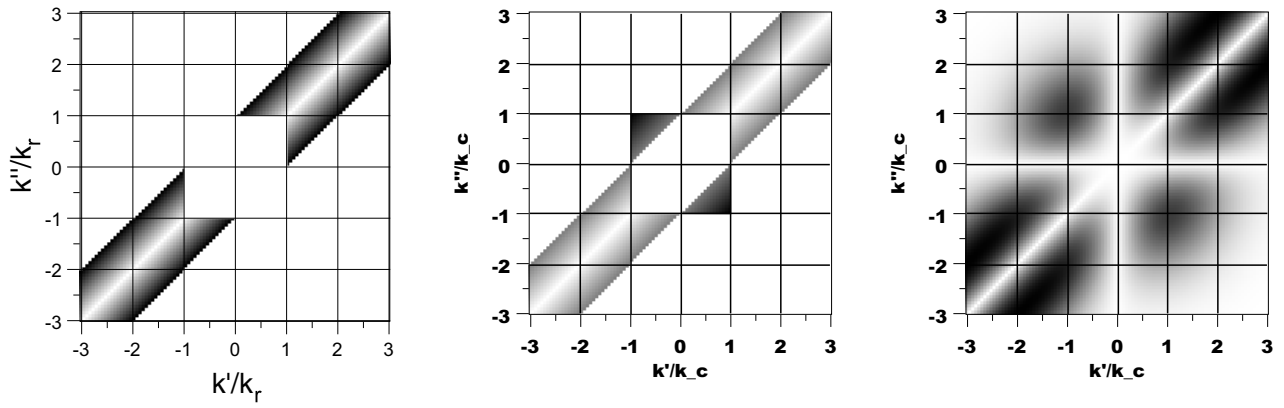


Figure 1: Interaction selection functions F (absolute value) for subfilter stresses. White represents zero, the darkest colour represents the maximum value. Left: F_α for the reconstructed equation; centre: F_τ for the classic subgrid stress using a cut-off filter; right: F_τ for a Gauss filter. k_c is the point where the filter has a value of 0.05, the strongest suppression which we consider to be invertible.

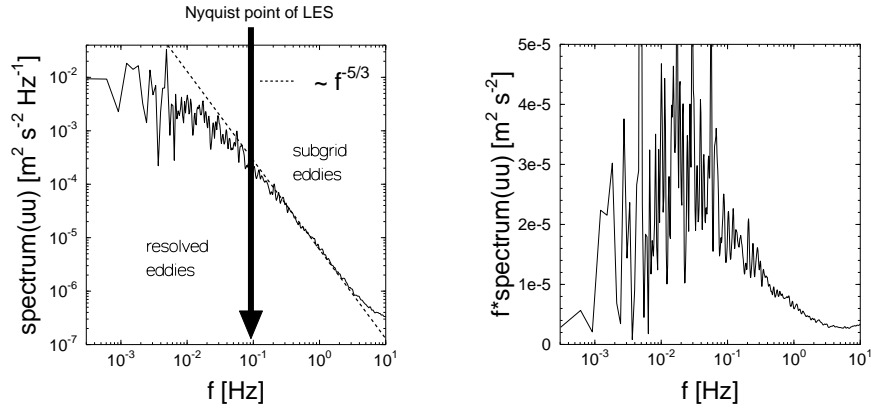


Figure 2: Power-spectrum of streamwise velocity u of the record taken at 4 m. Left: double log-plot including $-5/3$ -law to show inertial range. Right: the y-axis is now linear and multiplied with frequency such that surface areas in the plot are proportional to the power in frequency ranges. The Nyquist-point of the LES will be approximately placed at 0.1 Hz.

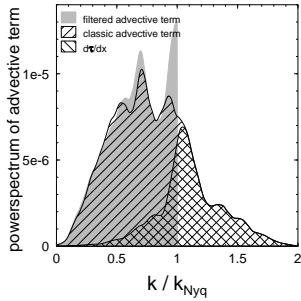


Figure 3: Power-spectra of: grey/white: total filtered advection; ascending lines: resolved advection in (2b); descending lines: residual subgrid stress-term $\partial\tau/\partial x$. Results are based on the cut-off filter.

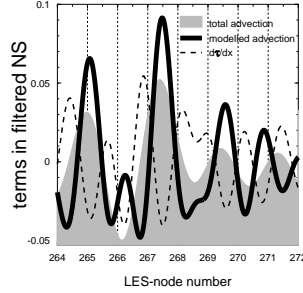


Figure 4: Physical space equivalent of fig. 3: grey/white: total filtered advection; thick line: resolved advective term in (2b); dashed line: subgrid stress-term $\partial\tau/\partial x$.

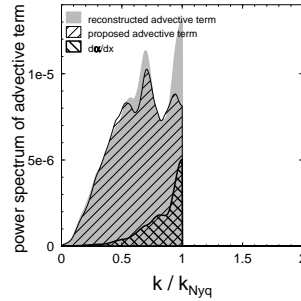


Figure 5: Equivalent of figure 3 for reconstructed Navier-Stokes equation (4b). descending lines: residual subgrid stress-term $\partial\tau/\partial x$

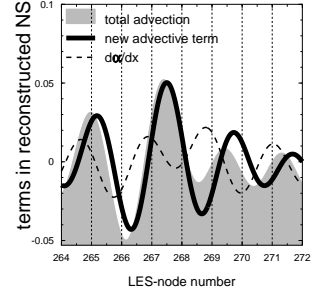


Figure 6: Physical space equivalent of fig. 5: grey/white: total filtered advection; thick line: resolved advective term in (4b); dashed line: subgrid stress-term $\partial\alpha/\partial x$.