ANALYSIS OF SUBGRID SCALES AND SUBGRID SCALE MODELING FOR SHOCK-BOUNDARY-LAYER INTERACTION

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ABSTRACT

An alternative approach to large-eddy simulation based on approximate deconvolution (ADM) is compared with standard subgrid scale models by *a priori* tests for supersonic compression ramp flow. With ADM an approximation of the non-filtered field is obtained by truncated series expansion of the inverse filter operator. Scale-similarity model and ADM give the best correlation of subgrid scale terms with filtered DNS data. Lower correlations are obtained with the dynamic mixed model, the dynamic Smagorinsky model, and the standard Smagorinsky model. It is also found that explicit compressible subgrid scale contributions cannot be neglected and require modeling.

1. INTRODUCTION

Large-eddy simulation (LES) has matured to be a tool for studying simple turbulent flows at flow parameters which render direct numerical simulation (DNS) unfeasible. For physically and geometrically complex flows, however, LES still suffers from fundamental modeling problems. In this contribution we address the LES of supersonic compression corner flow, which exhibits considerable physical complexity due to the interaction of shock, separation, and turbulence in an ambient inhomogeneous shear flow. An obvious requirement for a reliable subgrid-scale (SGS) model is that it reproduces filtered DNS data with acceptable accuracy. We focus on *a priori* analysis of several standard SGS models and compare them with a new approximate deconvolution model developed by Stolz and Adams (1999). DNS data for supersonic compression ramp flow (Adams, 1998) are used for this purpose. Of particular concern are SGS terms in the energy equation, since compressibility effects can be expected to be significant for this type of flow.

Frequently one uses variable-density extensions of incompressible subgrid scale models for compressible flows. In this case the trace of the subgrid scale stress tensor is modeled explicitly (Yoshizawa, 1986) or is incorporated into the filtered pressure (Vreman, 1995). For the subgrid scale heat flux an eddy-diffusivity ansatz is used whereas other subgrid scale terms in the energy equation are commonly neglected. Most eddy-diffusivity models share the problem of predicting compressibility effects properly with their counterparts in standard turbulence modeling for the Reynolds-averaged Navier-Stokes equations. Since scale-similarity model (SSM) and approximate deconvolution model (ADM) reconstruct subgrid scale information directly from the resolved scales, they readily give approximations to all subgrid scale terms.

2. FUNDAMENTAL EQUATIONS

The flow is governed by the conservative Navier-Stokes equations in curvi-linear coordinates. Filtering can be applied to the equations in two different ways (Jordan, 1999). The first possibilty is to filter the Navier-Stokes equations in physical space and to transform the filtered equations subsequently into computional space. This procedure generally results in an inhomogenous filter kernel with varying filter width. Since an inhomogenous filter operator does not commute with the derivative operators a commutation error arises (Ghosal and Moin, 1995). The second possibility is to first transform the equations into computional space and subsequently apply the filter in this space. In this case homogenous filter kernels with a constant filter width can be used within the domain execept for the boundaries. The filter width in real space is an integer multiple of the mesh size. We now obtain, however a commutation error from the fact that transformation and filter operation do not commute. Results depend only weakly on which procedure is chosen but the second approach is computionally more efficient (Jordan, 1999). The commutation error can be explicitly derived and we give expressions fort the error terms below.

We define a filter operation in computational space $\underline{\xi}$ by

$$\overline{u}(\underline{\xi}) = G(\underline{\xi} - \underline{\xi}') \otimes u(\underline{\xi}') = \int_{\Omega} G(\underline{\xi} - \underline{\xi}')\; u(\underline{\xi}')\; d\underline{\xi}' \quad (1)$$

where G is a filter function with characteristic filter width Δ and Ω is the computational domain. We apply the filter to the Navier-Stokes equations in computional space and obtain the fundamental equations for the resolved conservative variables $\{\overline{\rho},\ \overline{\rho}\tilde{u}_i,\ \check{E}\}$. Favre-filtered quantities are denoted by "$\tilde{\bullet}$". They are computed from a mass-weighted filtering operation

$$\tilde{\phi} = \frac{\overline{\rho\phi}}{\overline{\rho}}$$

"$\check{\bullet}$" indicates that the respective quantities are computed with filtered variables. The equations include formally an $\mathcal{O}(\Delta^2)$ commutation error as has been mentioned previously. They are derived following Vreman (1995) except that here filtering is done in computational space. In three dimensions the filter operation is applied by a tensor-product of the one-dimensional operators eq. (1). For the nomenclature of the following equations we refer to Vreman (1995) and Adams (1998).

The filtered continuity equation is

$$\frac{1}{J}\frac{\partial\overline{\rho}}{\partial t} + \frac{\partial}{\partial\xi_i}\left(\frac{\overline{\rho}\tilde{u}_j}{J}\frac{\partial\xi_i}{\partial x_j}\right) = \gamma_{C1} + \gamma_{C2} \quad (2)$$

where

$$\gamma_{C1} = \frac{\partial}{\partial\xi_k}\left(\frac{\overline{\rho u_j}}{J}\frac{\partial\xi_k}{\partial x_j}\right) - \frac{\partial}{\partial\xi_k}\left(\overline{\frac{\rho u_j}{J}\frac{\partial\xi_k}{\partial x_j}}\right) \quad (3a)$$

$$\gamma_{C2} = \frac{\partial}{\partial\xi_k}\left(\frac{\overline{\rho u_j}}{J}\frac{\partial\xi_k}{\partial x_j}\right) - \overline{\frac{\partial}{\partial\xi_k}\left(\frac{\rho u_j}{J}\frac{\partial\xi_k}{\partial x_j}\right)} \quad (3b)$$

γ_{C1} is an $\mathcal{O}(\Delta^2)$ error term, which results from the non-identity mapping between computational space ξ_i and physical space x_i (commutation error). γ_{C2} is an error due to variable filter width. In our case the filter G is not an explicit function of ξ_i and γ_{C2} vanishes.

The filtered momentum equations are

$$\begin{aligned}\frac{1}{J}\frac{\partial\overline{\rho}\tilde{u}_i}{\partial t} + \frac{\partial}{\partial\xi_k}\left(\frac{\overline{\rho}\tilde{u}_i\tilde{u}_j}{J}\frac{\partial\xi_k}{\partial x_j} + \frac{\overline{p}}{J}\delta_{ij}\frac{\partial\xi_i}{\partial x_j}\right) - \frac{\partial}{\partial\xi_k}\left(\frac{\check{\sigma}_{ij}}{J}\frac{\partial\xi_k}{\partial x_j}\right) &= \\ = -\frac{\partial}{\partial\xi_k}\left(\frac{\overline{\rho}\tau_{ij}}{J}\frac{\partial\xi_k}{\partial x_j}\right) + \beta_i + \gamma_{I1i} + \gamma_{I2i}\end{aligned} \quad (4)$$

where

$$\gamma_{I1i} = \frac{\partial}{\partial\xi_k}\left(\frac{\overline{\rho u_i u_j + p\delta_{ij} - \sigma_{ij}}}{J}\frac{\partial\xi_k}{\partial x_j}\right) - \frac{\partial}{\partial\xi_k}\left(\overline{\frac{\rho u_i u_j + p\delta_{ij} - \sigma_{ij}}{J}\frac{\partial\xi_k}{\partial x_j}}\right) \quad (5a)$$

$$\gamma_{I12} = \frac{\partial}{\partial\xi_k}\left(\frac{\overline{\rho u_i u_j + p\delta_{ij} - \sigma_{ij}}}{J}\frac{\partial\xi_k}{\partial x_j}\right) - \overline{\frac{\partial}{\partial\xi_k}\left(\frac{\rho u_i u_j + p\delta_{ij} - \sigma_{ij}}{J}\frac{\partial\xi_k}{\partial x_j}\right)} \quad (5b)$$

with the abbreviations

$$\overline{\rho}\tau_{ij} = \overline{\rho}(\widetilde{u_i u_j} - \tilde{u}_i\tilde{u}_j) \qquad \sigma_{ij} = \frac{\mu}{Re}S_{ij}$$

$$S_{ij} = \frac{\partial\xi_k}{\partial x_j}\frac{\partial u_i}{\partial\xi_k} + \frac{\partial\xi_k}{\partial x_i}\frac{\partial u_j}{\partial\xi_k} - \frac{2}{3}\frac{\partial\xi_k}{\partial x_l}\frac{\partial u_l}{\partial\xi_k}\delta_{ij} \qquad \beta_i = \frac{\partial}{\partial\xi_k}\left(\frac{\overline{\sigma}_{ij} - \check{\sigma}_{ij}}{J}\frac{\partial\xi_k}{\partial x_j}\right)$$

The term β_i arises from the non-linearity of the viscous stresses. γ_{I1} and γ_{I2} are error terms analogous to γ_{C1} and γ_{C2}.

The equation for the resolved-energy $\check{E} = \bar{p}/(\gamma - 1) + \bar{\rho}\tilde{u}_i\tilde{u}_i/2$ is obtained by filtering the enthalpy equation and by adding the filtered momentum equation, multiplied by $\tilde{u}_i$. We prefer the formulation using the resolved energy, although this give rise to a pressure-dilatation term α_3 in eq (6.), since $\check{E}$ does not explicitly contain subgrid scale contributions. This is different when the filtered energy $\bar{E} = \bar{p}/(\gamma-1)+\bar{\rho}\tilde{u}_i\tilde{u}_i/2+\tau_{ii}/2$ is used, where τ_{ii} is the trace of the subgrid scale stress tensor (Domaradzki *et al.*, 1998). This formulation is blurred by the explicit presence of a modeled term in a resolved quantity.

The resolved energy equation is

$$\frac{1}{J}\frac{\partial \check{E}}{\partial t} + \frac{\partial}{\partial \xi_k}\left(\frac{\check{E}+\bar{p}}{J}\tilde{u}_j\frac{\partial \xi_k}{\partial x_j}\right) - \frac{\partial}{\partial \xi_k}\left(\frac{\check{\sigma}_{ij}\tilde{u}_i}{J}\frac{\partial \xi_k}{\partial x_j}\right) + \frac{\partial}{\partial \xi_k}\left(\frac{\check{q}_j}{J}\frac{\partial \xi_k}{\partial x_j}\right) = \\ = -\alpha_1 - \alpha_2 - \alpha_3 + \alpha_4 + \alpha_5 - \alpha_6 + \gamma_{E1} + \gamma_{E2} \tag{6}$$

where

$$\gamma_{H1} = \frac{\partial}{\partial \xi_k}\left[\left(\overline{\frac{pu_j}{\gamma-1} + q_j}\right)\frac{1}{J}\frac{\partial \xi_k}{\partial x_j}\right] - \frac{\partial}{\partial \xi_k}\left[\overline{\left(\frac{pu_j}{\gamma-1} + q_j\right)\frac{1}{J}\frac{\partial \xi_k}{\partial x_j}}\right] + \frac{1}{J}\overline{p\frac{\partial u_j}{\partial \xi_k}}\frac{\partial \xi_k}{\partial x_j} - \\ - \overline{\frac{p}{J}\frac{\partial u_j}{\partial \xi_k}\frac{\partial \xi_k}{\partial x_j}} + \overline{\frac{\sigma_{ij}}{J}\frac{\partial u_i}{\partial \xi_k}\frac{\partial \xi_k}{\partial x_j}} - \frac{1}{J}\overline{\sigma_{ij}\frac{\partial u_i}{\partial \xi_k}}\frac{\partial \xi_k}{\partial x_j} \tag{7a}$$

$$\gamma_{E1} = \tilde{u}_i\gamma_{I1i} + \gamma_{H1}$$

$$\gamma_{H2} = \frac{\partial}{\partial \xi_k}\left[\overline{\left(\frac{pu_j}{\gamma-1} + q_j\right)\frac{1}{J}\frac{\partial \xi_k}{\partial x_j}}\right] - \overline{\frac{\partial}{\partial \xi_k}\left[\left(\frac{pu_j}{\gamma-1} + q_j\right)\frac{1}{J}\frac{\partial \xi_k}{\partial x_j}\right]} \tag{7b}$$

$$\gamma_{E2} = \tilde{u}_i\gamma_{I2i} + \gamma_{H2}$$

with the abbreviations

$$q_j = \frac{\mu}{(\gamma-1)RePrM^2}\frac{\partial \xi_k}{\partial x_j}\frac{\partial T}{\partial \xi_k}$$

$$\alpha_1 = \tilde{u}_i\frac{\partial}{\partial \xi_k}\left(\frac{\bar{\rho}\tau_{ij}}{J}\frac{\partial \xi_k}{\partial x_j}\right) \qquad \alpha_2 = \frac{1}{\gamma-1}\frac{\partial}{\partial \xi_k}\left(\frac{\overline{pu_j}-\bar{p}\tilde{u}_j}{J}\frac{\partial \xi_k}{\partial x_j}\right)$$

$$\alpha_3 = \frac{1}{J}\left(\overline{p\frac{\partial u_j}{\partial \xi_k}} - \bar{p}\frac{\partial \tilde{u}_j}{\partial \xi_k}\right)\frac{\partial \xi_k}{\partial x_j} \qquad \alpha_4 = \frac{1}{J}\left(\overline{\sigma_{ij}\frac{\partial u_i}{\partial \xi_k}} - \bar{\sigma}_{ij}\frac{\partial \tilde{u}_i}{\partial \xi_k}\right)\frac{\partial \xi_k}{\partial x_j}$$

$$\alpha_5 = \frac{\partial}{\partial \xi_k}\left(\frac{\tilde{u}_i\bar{\sigma}_{ij} - \tilde{u}_i\check{\sigma}_{ij}}{J}\frac{\partial \xi_k}{\partial x_j}\right) \qquad \alpha_6 = \frac{\partial}{\partial \xi_k}\left(\frac{\bar{q}_j - \check{q}_j}{J}\frac{\partial \xi_k}{\partial x_j}\right)$$

Note that the filtered Jacobian $\overline{\partial \xi_i/\partial x_j}$ has been replaced by the unfiltered Jacobian $\partial \xi_i/\partial x_j$. This contributes another error of order $\mathcal{O}(\Delta^2)$. Whereas subgrid-scale stresses formally are analogous to the incompressible case, additional terms appear in eq. (2), (4) and (6) due to the dilatation of the velocity field and due to variable viscosity.

3. SUBGRID SCALE MODELS

We consider Smagorinsky model with Yoshizawa's (1986) extension SYM, the dynamic mixed model DMM (Moin *et al.*, 1991; Zang *et al.*, 1993; Vreman, 1995), the scale-similarity model SSM (Bardina *et al.*, 1983), the 'resolved turbulent stress-model' RTSM with a ratio of filter widths $\hat{\Delta}/\Delta = 2$ (Pruett, 1997), and the approximate deconvolution model, ADM.

In the ADM approach, we replace the unfiltered quantities in the subgrid-scale terms by an approximate deconvolution of the corresponding filtered (resolved) quantities. If $u^\star$ denotes the approximate deconvolution of $\overline{u}$, the SGS terms σ can be approximated by a generalized scale-similarity form

$$\sigma = F(\overline{u}) - \overline{F(u)} \approx F(\overline{u^\star}) - \overline{F(u^\star)} \tag{8}$$

If the filter G has an inverse it can be expanded as an infinite series. We truncate the series after $N+1$ terms and obtain Q_N as an approximation of G^{-1},

$$Q_N = \sum_{\nu=0}^{N}(I-G)^\nu \tag{9}$$

where I is the identity operator. The series on the right-hand side converges uniformly for $N \to \infty$ if $||I-G|| < 1$. The approximate deconvolution of u is then given by

TABLE 1. CORRELATION COEFFICIENT C AND RATIO A OF THE L_2-NORMS FOR DIFFERENT SGS-MODELS.

model		τ_{xx}	τ_{xy}	τ_{xz}	τ_{yy}	τ_{yz}	τ_{zz}	α_1
L_2 - norms $\cdot 10^3$		10.297	3.124	2.363	5.955	1.613	4.637	4497
Smagorinsky/	C	0.813	0.514	-0.227	0.721	-0.092	0.660	0.215
Yoshizawa	A	2.113	7.430	2.470	1.160	4.328	1.289	2.116
dynamic	C	0.947	0.850	0.696	0.849	0.578	0.695	0.592
mixed-model	A	1.481	1.364	1.055	2.186	1.542	1.827	0.934
scale-simi-	C	0.967	0.918	0.862	0.949	0.846	0.945	0.854
larity model	A	1.554	1.906	1.628	2.943	2.509	2.902	2.875
resolved tur-	C	0.914	0.784	0.632	0.907	0.694	0.904	0.670
bulent stress	A	2.872	4.731	3.326	6.509	6.775	5.961	9.515
approximate	C	0.998	0.995	0.991	0.996	0.985	0.994	0.962
deconvolution	A	1.057	1.046	1.058	1.148	1.090	1.178	1.299

$$u^\star = Q_N * \bar{u} \tag{10}$$

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The approximation (9) has first been suggested for image reconstruction (van Cittert, 1931) and was applied recently to LES by Stolz and Adams (1999). Truncated iteration, which corresponds to the truncated series (9), is a well-known procedure in regularizing ill-posed problems. Note that all convolution and deconvolution operations are defined in real space and no reference to Fourier space needs to be made. For the results shown in section 4 we used $N = 7$. ($N = 3$ already gives acceptable results.)

4. A PRIORI ANALYSIS OF SGS MODELS

For an assessment of the various SGS models we perform an *a priori* analysis using a DNS data base for turbulent supersonic compression ramp flow (Adams, 1998). The filter eq. (1) is discretized by a second-order Padé filter (Lele, 1992). For the grid filter a cut-off wavenumber of $k_c = \pi/4 \cdot h$ is used and for the test filter (where required) $k_c' = \pi/8 \cdot h$.

By inspection of the L_2-norms of the SGS terms in table 1 and table 2, the subgrid-scale stresses τ_{ij} and the terms α_1 to α_4 are identified to be significant subgrid scale contributions to the equations (2), (4) and (6). α_1 is the SGS dissipation, α_2 the pressure-velocity correlation describing the SGS heat flux, α_3 the pressure-dilatation correlation and α_4 the SGS molecular dissipation. For the L_2-norms integration is performed over a domain which roughly corresponds to the section shown in figures 1 and 2.

In order to evaluate the performance of the models, both the correlation coefficient C between filtered DNS (E) and model data (M) and the ratio A of the L_2-norms of the filtered DNS data to the respective model data are computed:

$$C(E, M) = \frac{\langle E(\mathbf{x})M(\mathbf{x})\rangle - \langle E(\mathbf{x})\rangle\langle M(\mathbf{x})\rangle}{\sqrt{\langle (E(\mathbf{x}))^2\rangle}\sqrt{\langle (M(\mathbf{x}))^2\rangle}} \tag{11}$$

and

$$A(E, M) = \sqrt{\frac{\langle (E(\mathbf{x}))^2\rangle}{\langle (M(\mathbf{x}))^2\rangle}} \tag{12}$$

A good correlation is achieved by the models for values of C close to unity, a good prediction of the magnitude by values of A close to unity.

The correlation coefficients C and the ratios A show that the Smagorinsky model SYM correlates poorly with the filtered DNS data (see also figure 1f). The correlation of the RTSM is quite good for $\hat{\Delta}/\Delta = 2$, but the magnitudes are considerably underpredicted. For $\hat{\Delta}/\Delta = 1$, where RTSM is equivalent with the SSM, correlations and magnitudes are improved. The DMM performs quite well, but not as well as the SSM. Correlations C between 96% and 99%, and values of A close to unity are obtained with approximate deconvolution ADM (see also figure 1b). It should be noted that the computational cost of ADM is comparable to SSM and is much less than for the dynamic models.

Four different models have been tested for the most significant SGS-terms α_i of the energy equation. Figure 2d and table 2 show that the full dynamic mixed model FDMM (Vreman, 1995) and an adaptation of the RTSM do not perform well. The SSM and in particular ADM give a significantly improved prediction of the SGS terms (figures 2b and 2c). Both models also provide reasonable predictions for all other SGS terms. Compared with SMM, ADM in addition shows an improved prediction of the magnitudes.

TABLE 2. CORRELATION COEFFICIENT C AND RATIO A OF THE L_2-NORMS FOR DIFFERENT SGS-TERMS OF THE ENERY EQUATION.

model		α_2	α_3	α_4	α_5	α_6
L_2 - norms		3.329	2.254	0.717	0.092	0.181
dynamic	C	0.510		0.137	—	—
mixed model	A	0.762		0.628	—	—
scale-simi-	C	0.838	0.781	0.944	0.805	0.573
larity-model	A	3.001	2.926	5.127	2.981	0.932
resolved tur-	C	0.330	0.552	—	—	—
bulen stress	A	5.759	10.754	—	—	—
approximate	C	0.977	0.959	0.988	0.984	0.879
deconvolution	A	1.144	1.312	1.459	1.208	0.946

5. CONCLUDING REMARKS

We have analyzed a new approach to subgrid-scale modeling based on approximate deconvolution ADM. By *a priori* tests using DNS data of a supersonic compression ramp flow, we have demonstrated that ADM shows significantly better agreement with filtered DNS data than conventional SGS models with the added benefit that ADM gives approximations to all subgrid scale terms. The computational overhead of the ADM is comparable to that of the SSM, which is much less than that required dynamic models. Recent applications of ADM to LES of homogeneous isotropic compressible turbulence (Stolz and Adams, 1999) and incompressible turbulent channel flow (Stolz *et al.*, 1999) show excellent results.

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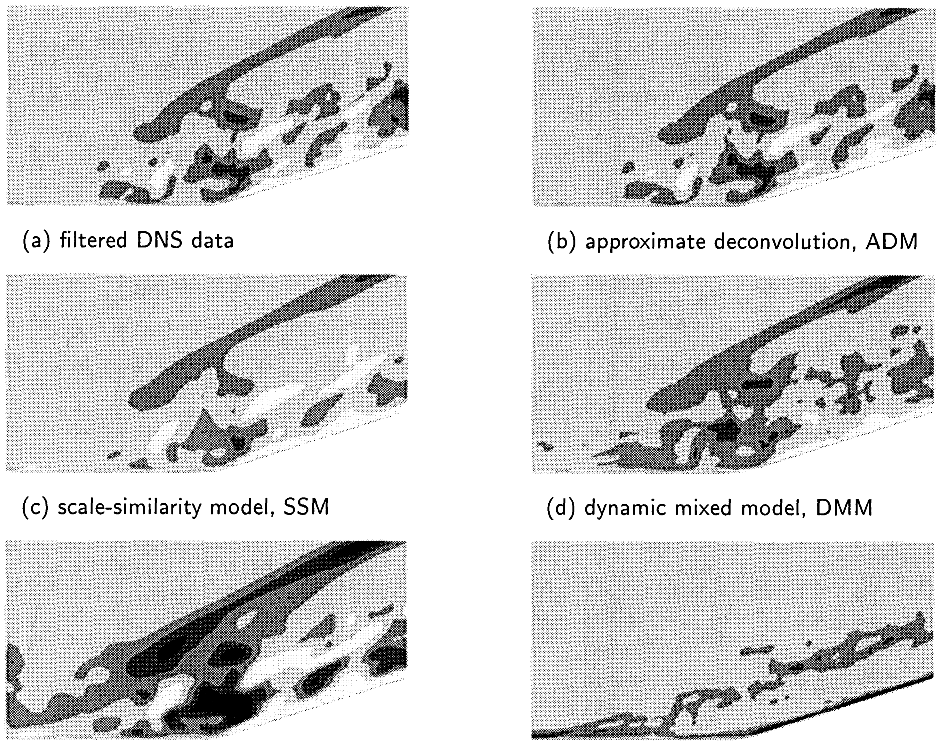


(a) filtered DNS data

(b) approximate deconvolution, ADM

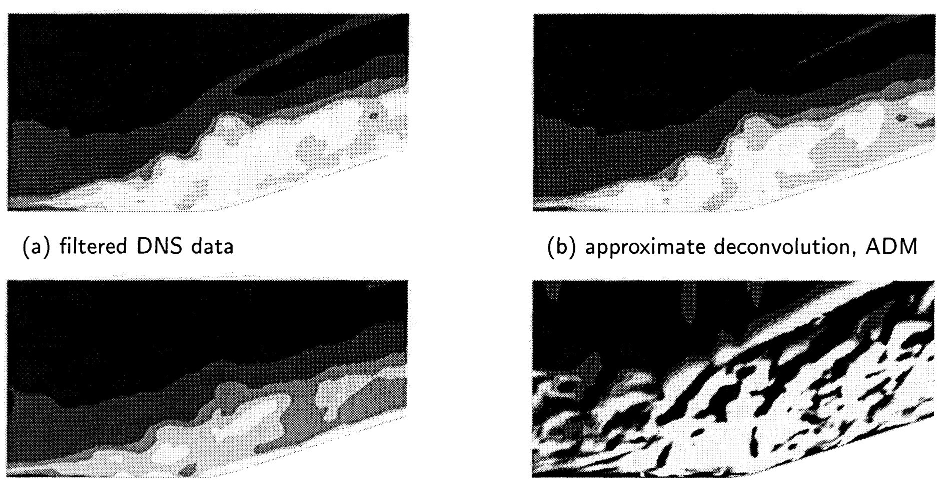
(c) scale-similarity model, SSM

(d) dynamic mixed model, DMM

(e) resolved turb. stress model, RTSM

(f) Smagorinsky / Yoshizawa model

Figure 1. Subgrid-scale stress τ_{xz}. Filtered DNS data and *a priori* SGS model predictions.



(a) filtered DNS data

(b) approximate deconvolution, ADM

(c) scale-similarity model, SSM

(d) full dynamic mixed model, FDMM

Figure 2. Subgrid-scale energy term α_4. Filtered DNS data and *a priori* SGS model predictions.