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A new modeling approach for large-eddy simulation (LES) is obtained by combining a "regularization principle" with an explicit filter and its inversion. This regularization approach allows a systematic derivation of the implied subgrid model, which resolves the closure problem. The central role of the filter in LES is fully restored, i.e., both the interpretation of LES predictions in terms of direct simulation results as well as the corresponding subgrid closure are specified by the filter. The regularization approach is illustrated with "Leray-smoothing" of the nonlinear convective terms. In turbulent mixing the new, implied subgrid model performs favorably compared to the dynamic eddy-viscosity procedure. The model is robust at arbitrarily high Reynolds numbers and correctly predicts self-similar turbulent flow development. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1529180]

Accurate modeling and simulation of turbulent flow is a topic of intense ongoing research.[1] Modern strategies for turbulent flow are aimed at reducing the dynamical complexity of the underlying system of partial differential equations while reliably predicting the primary flow phenomena. In large-eddy simulation (LES) these conflicting requirements are expressed by coarsening the description on the one hand and subgrid modeling on the other hand. The coarsening is achieved by spatial filtering[2] which externally specifies the physical detail that will ideally be retained in the LES solution. Maintaining the dynamical properties of the resolved large scales is approached by introducing subgrid modeling to deal with the closure problem that arises from filtering the nonlinear terms.

In the filtering approach to incompressible flow the specification of the basic convolution filter L is all that is required to uniquely define the relation between the unfiltered and filtered flow field as well as the closure problem for the so-called turbulent stress tensor τ_{ij}. This situation is in sharp contrast with actual present-day large-eddy modeling in which the specification of the subgrid model for τ_{ij} as well as the comparison with reference direct numerical simulation (DNS) results is performed largely independent of the specific choice of the filter L.

In this paper we will formulate an alternative approach to large-eddy simulations which completely restores the two central roles of the basic filter L, i.e., providing an interpretation of LES predictions in terms of filtered DNS results as well as fully specifying all details of the subgrid model. The key elements in this new formulation are a "regularization principle," a filter L and its (formal) inverse operator denoted by L^{-1}.[3]

A regularization principle expresses the smoothing of the dynamics of the Navier–Stokes equations through a specific proposal for direct alteration of the nonlinear convective terms. This modeling differs significantly from traditional, less direct approaches, e.g., involving the introduction of additional eddy-viscosity contributions.[4] The latter are clearly of a different physical nature and do not fully do justice to the intricate nonlinear transport structure of the filtered Navier–Stokes equations. The regularization principle gives rise to a basic mixed formulation involving both the filtered and unfiltered solution. Application of L and L^{-1} then allows to derive an equivalent representation solely in terms of the filtered solution. This provides a unique identification of the implied subgrid model without any further external (*ad hoc*) input or mathematical-physical considerations of the closure problem. The regularization modeling approach is not only theoretically transparent and elegant, but it also gives rise to accurate LES predictions. In particular, we consider the implied subgrid model that arises from Leray's regularization principle.[5] A comparison between the Leray model and dynamic subgrid modeling (e.g., Ref. 6) will be made for turbulent mixing flow, both at moderate and at high Reynolds numbers.

In the filtering approach one assumes any normalized convolution filter L: $u_i \rightarrow \bar{u}_i$ where $\bar{u}_i$ (u_i) denotes the filtered (unfiltered) component of the velocity field in the x_i direction. Filtering the Navier–Stokes equations yields

$$\partial_t \bar{u}_i + \partial_j (\bar{u}_j \bar{u}_i) + \partial_i \bar{p} - (1/\text{Re})\, \partial_{jj} \bar{u}_k = -\partial_j \tau_{ij}, \qquad (1)$$

where the turbulent stress tensor $\tau_{ij} = \overline{u_i u_j} - \bar{u}_i \bar{u}_j$ represents the closure problem and Re denotes the Reynolds number. Both the relation between u_i and $\bar{u}_i$ as well as the properties

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of τ_{ij} are fully specified by L. In actual subgrid modeling for LES, the next step is to introduce a subgrid model $m_{ij}(\bar{\mathbf{u}})$ to approximate τ_{ij}. A variety of subgrid models has been proposed to capture dissipative, dispersive, or similarity properties of τ_{ij}.

Many subgrid models are arrived at through a physical or mathematical reasoning which is only loosely connected to a specific filter L. As an example, the well-known Smagorinsky model[4] is given by $m_{ij}^{S} = -(C_{S}\Delta)^{2}|S_{ij}(\bar{\mathbf{u}})|S_{ij}(\bar{\mathbf{u}})$ where the rate of strain tensor $S_{ij} = \partial_{i}\bar{u}_{j} + \partial_{j}\bar{u}_{i}$ and $|S_{ij}|^{2} = S_{ij}S_{ij}/2$. The only explicit reference to the filter, made in this model, is through the filter width Δ. In actual simulations Δ is specified in terms of the grid spacing h rather than in terms of L. Furthermore, the Smagorinsky constant C_{S} is determined independent of L, which further reduces any principal role for the filter. The situation is comparable for the "tensor-diffusivity" model $m_{ij}^{TD} = C_{TD}\Delta_{k}^{2}\partial_{k}\bar{u}_{i}\partial_{k}\bar{u}_{j}$, with Δ_{k} the filterwidth in the x_{k}-direction.[7] The coefficient C_{TD} is usually related to the normalized second moment $(L(x^{2}) - x^{2})/\Delta^{2}$ of the filter L. For various popular filters such as the top-hat or the Gaussian filter one finds $C_{TD} = 1/12$, i.e., independent of the actual filter used. The role of the filter is in principle fully explicit in Bardina's similarity model $m_{ij}^{B} = \overline{\bar{u}_{i}\bar{u}_{j}} - \bar{\bar{u}}_{i}\bar{\bar{u}}_{j}$.[8] In actual simulations, however, one frequently adopts a wider explicit filter or a filter of a different type, to enhance smoothing properties of this model.[1] Moreover, the model is sometimes multiplied by a constant C_{B} which is specified independently of any presumed filter.[9] Finally, the successful dynamic subgrid modeling requires only the explicit specification of the so-called test filter.[10] To retain the central Germano identity the test filter can in principle be chosen independent of L, mainly requiring the specification of the filterwidth of the test filter relative to Δ. Additional averaging over homogeneous directions, "clipping" steps to stabilize actual simulations, and the fact that the assumed base models are themselves only loosely connected to L, also make the dynamic procedure rather insensitive to the specific assumed filter.

In contrast to these popular LES models, the regularization approach involves the introduction of a pair (L, L^{-1}) to fully specify the implied subgrid model as well as the interpretation of LES predictions in terms of reference DNS results. The selection of any other pair $(\mathcal{L}, \mathcal{L}^{-1})$ directly leads to its corresponding DNS interpretation and the associated subgrid model consistent with the regularization principle. This modeling strategy has a number of important benefits, addressing directly the nonlinear convective contributions and requiring no additional "external" information such as model coefficients or the width of the test filter. The regularization principle allows a transparent modeling in which the modeled system of equations can be made to share a number of fundamental properties with the Navier–Stokes equations, such as transformation symmetries, Kelvin's circulation theorem, etc. The implied subgrid model is quite simple to implement, with some technical complications arising from the construction of an accurate inverse operator L^{-1}.

To illustrate the approach we consider the intuitively appealing and particularly simple Leray regularization in which

the convective fluxes are replaced by $\bar{u}_{j}\partial_{j}u_{i}$, i.e., the solution $\mathbf{u}$ is convected with a smoothed velocity $\bar{\mathbf{u}}$. Consequently, the nonlinear effects are reduced by an amount governed by the smoothing properties of L. The governing equations in the Leray formulation can be written as[5]

$$\partial_{j}\bar{u}_{j} = 0; \quad \partial_{t}u_{i} + \bar{u}_{j}\partial_{j}u_{i} + \partial_{i}p - (1/\mathrm{Re})\,\partial_{jj}u_{i} = 0. \quad (2)$$

Uniqueness and regularity of the solution to these equations have been established rigorously.[5] The Leray formulation contains the unfiltered Navier–Stokes equations in the limiting case $L \to Id$, e.g., as $\Delta \to 0$ (Id denotes the identity). The unfiltered solution can readily be eliminated from (2) by using the inversion operator $u_{j} = L^{-1}(\bar{u}_{j})$. After some calculation (2) can be written in the same way as the LES "template" (1) in which τ_{ij} on the right hand side is replaced by the asymmetric, filtered similarity-type Leray model m_{ij}^{L} given by

$$m_{ij}^{L} = L\big(\bar{u}_{j}L^{-1}(\bar{u}_{i})\big) - \bar{u}_{j}\bar{u}_{i} = \overline{\bar{u}_{j}u_{i}} - \bar{u}_{j}\bar{u}_{i}. \quad (3)$$

This model requires the explicit application of both L and L^{-1}. The tensor m_{ij}^{L} is not symmetric. However, the flow is governed by the divergence $\partial_{j}m_{ij}^{L}$ which can be shown to transform covariantly under Galilean transformations and under a change to a uniformly rotating reference frame, as does $\partial_{j}\tau_{ij}$. For properly chosen filter, Leray solutions of the regularized Navier–Stokes equations behave better with respect to smoothness and boundedness. Correspondingly, the subgrid model (3) can be expected to yield similar benefits in a large-eddy context. The straightforward model $m_{ij} = L(L^{-1}(\bar{u}_{i})L^{-1}(\bar{u}_{j})) - \bar{u}_{i}\bar{u}_{j}$ does not provide sufficient smoothing and leads to unstable LES on coarse grids, at high Re.

In the sequel we consider invertible numerical quadrature approximating the top-hat filter. In one dimension the numerical convolution filtering $\bar{u} = G*u$ corresponds to kernels

$$G(z) = \sum a_{j}\delta(z - z_{j}); \quad |z_{j}| \leqslant \Delta/2. \quad (4)$$

In particular, we consider three-point filters with $a_{0} = 1 - \alpha$, $a_{1} = a_{-1} = \alpha/2$ and $z_{0} = 0$, $z_{1} = -z_{-1} = \Delta/2$. Here we use $\alpha = 1/3$ which corresponds to Simpson quadrature of the top-hat filter. In actual simulations the resolved fields are known only on a set of grid points $\{x_{m}\}_{m=0}^{N}$. The application of L^{-1} to a general discrete solution $\{\bar{u}(x_{m})\}$ can be specified using discrete Fourier transformation as[11]

$$L^{-1}(\bar{u}_{m}) = \sum_{j=-n}^{n} \left(\frac{\alpha - 1 + \sqrt{1 - 2\alpha}}{\alpha} \right)^{|j|} \frac{\bar{u}_{m + rj/2}}{(1 - 2\alpha)^{1/2}}, \quad (5)$$

where the subgrid resolution $r = \Delta/h$ is assumed to be even. An accurate and efficient inversion can be obtained with only a few terms, recovering the original signal to within machine accuracy with $n \approx 10$. The invertibility of L only refers to invertibility on the LES grid. Injection from a fine DNS grid to a coarse LES grid is not invertible. At fixed Δ, variation of the subgrid resolution r allows an independent control over flow smoothing and numerical representation.[12] Simulation results obtained in this way are properly smoothed for $k\Delta$

$<2\pi$. At constant Δ the inclusion of modes with higher wavenumber k in case $r>1$ allows to approach the grid-independent solution to the "fixed-Δ" problem. However, the modes with $k>2\pi/\Delta$ are not properly smoothed in the sense of Leray; the Fourier transform of the kernel G does not reduce in amplitude for large $k\Delta$ but rather, it oscillates between fixed limits. To achieve a genuine PDE result, Leray analysis requires correct smoothing of the filter also at high wavenumber. The present results are limited to the modes with $k\Delta<2\pi$ and in subsequent illustrations we restrict ourselves to this range.

To assess the Leray model the turbulent mixing layer is simulated in a volume ℓ^3 at various Re adopting a fourth order accurate spatial discretization and explicit Runge–Kutta time stepping. We compare predictions with those obtained using the dynamic subgrid model, which was shown to be among the most accurate models in a comparative study of the same turbulent mixing layer reported in Ref. 6.

A first introductory test of the Leray model is obtained by studying instantaneous solutions. As a typical illustration of the mixing layer the DNS prediction of the normal velocity u_2 is shown in the turbulent regime in Fig. 1(a). We used Re$=50$ based on the initial momentum thickness and free-stream flow properties. The filtered u_2 can be seen in Fig. 1(b) establishing a significant smoothing due to the "Simpson" filter at $\Delta=\ell/16$. The Leray prediction [Fig. 1(c)] appears to capture the main "character" as well as some of the details of the filtered DNS solution. A slight underprediction of the influence of the small scales is, however, apparent. Further visualization showed that the instantaneous Leray predictions display much better overall agreement with filtered DNS than the dynamic model, which relative to the Leray model significantly overpredicts the smoothing.[6] Of course, assessing the quality of LES predictions in this way is difficult to quantify and we consider more specific measures next.

The evolution of a crucial mean-flow property such as the momentum thickness is shown in Fig. 2. The Leray results compare significantly better with filtered DNS results than those obtained with the dynamic model on 32^3 grid cells. We observe that some of the discrepancies between Leray and filtered DNS results are due to numerical contamination. By increasing the resolution at fixed Δ, a good impression of the grid-independent solution to the modeled equations can be inferred using 64^3-96^3 grid-cells, i.e., $\Delta/h=4$ to 6.[12] Numerical contamination also plays a role in the dynamic model. The grid-independent solution corresponding to the dynamic model appears less accurate than the corresponding Leray result.

A more detailed assessment is obtained from the streamwise kinetic energy spectrum shown in Fig. 3. The dynamic model yields a significant underprediction of the intermediate and smaller retained scales, particularly for the approximately grid-independent solution. The Leray predictions are much better. On coarse grids, an overprediction of the smaller scales is apparent due to interaction with the spatial discretization method. At proper numerical subgrid resolution the situation is considerably improved and the Leray model is seen to capture all scales with high accuracy. A
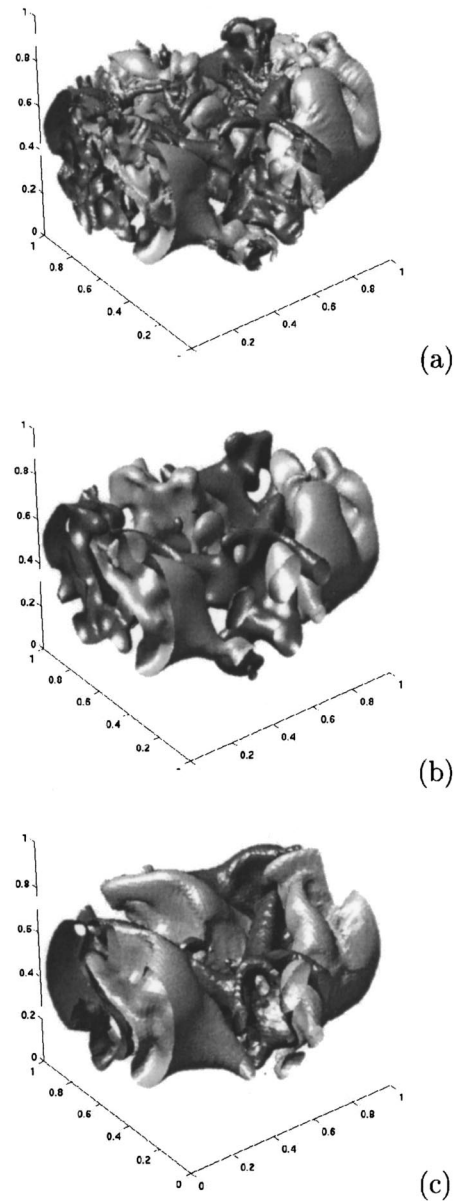

(a)

(b)

(c)

FIG. 1. Normal velocity component u_2 at time $t=80$, (a): DNS, (b): filtered DNS, (c): Leray on 64^3; using a filterwidth $\Delta=\ell/16$. The light (dark) iso-surfaces correspond to $u_2=0.3$ (-0.3).

slight, systematic underprediction of the smaller scales remains, consistent with the impression obtained from Figs. 1(b)–1(c).

A particularly appealing property of Leray modeling is the robustness at very high Reynolds numbers, cf. Fig. 4. This is quite unique for a subgrid model without an explicit eddy-viscosity contribution. Although comparison with filtered DNS data is impossible here, we observe that the smoothed Leray dynamics is essentially captured as $r=\Delta/h\geqslant4$.[12] The tail of the spectrum increases with Re, indicating a greater importance of small scale flow features. Improved subgrid resolution shows a reduction of these smallest scales, consistent with the reduced numerical error. At high Re the spectrum corresponding to the Leray model tends to contain a region with approximately $k^{-5/3}$ behavior,
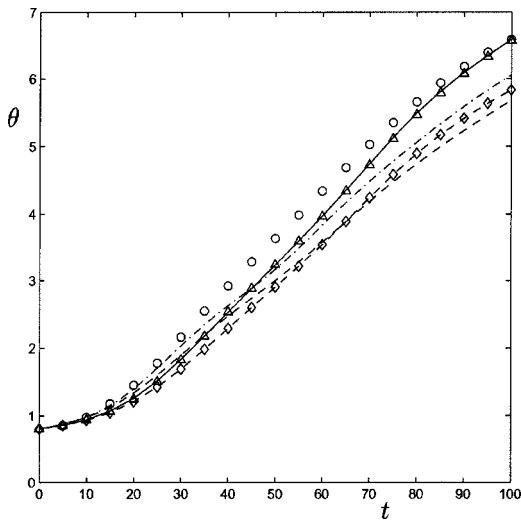
FIG. 2. Momentum thickness θ: filtered DNS ($\bigcirc$), Leray model (32^3: dash–dotted line, 64^3: solid line, 96^3: $\triangle$), dynamic model (32^3: dashed line, 64^3: dashed line, with $\diamond$). A fixed filterwidth of $\ell/16$ was used.

FIG. 4. Streamwise kinetic energy spectrum E at $t = 75$ predicted by the Leray model: Re=50 (64^3: dash–dotted line, 96^3: dash–dotted line, $\triangle$), Re=500 (64^3: dashed line, 96^3: dashed line, $\triangle$), Re=5000 (64^3: solid line, 96^3: solid line, $\triangle$). A fixed filterwidth of $\ell/16$ was used. The dotted line represents $k^{-5/3}$.

which is absent at Re=50. Further analysis showed that the solution develops self-similarly at high Re.

The Leray model was presented to illustrate the new regularization approach for LES. It predicts mean flow properties such as momentum thickness very accurately. The model exhibits both positive and negative production of turbulent kinetic energy. The computational overhead associated with the Leray model can be much lower than that of dynamic (mixed) models, especially if quantities are desired which are rather insensitive to the inversion quality. The regularized Leray dynamics shows an appealing robustness at high Re. Further extensions of the regularization approach are presently being considered. Of particular interest is the
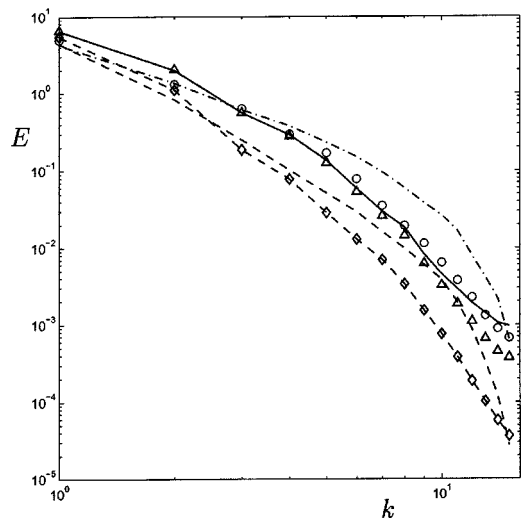
Lagrangian averaged NS$-\alpha$ model[13] which arises in the Euler–Poincaré framework for smoothed flow dynamics.

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FIG. 3. Streamwise kinetic energy spectrum E at $t = 75$: filtered DNS ($\bigcirc$), Leray model (32^3: dash–dotted line, 64^3: solid line, 96^3: $\triangle$), dynamic model (32^3: dashed line, 64^3: dashed line with $\diamond$). A fixed filterwidth of $\ell/16$ was used.
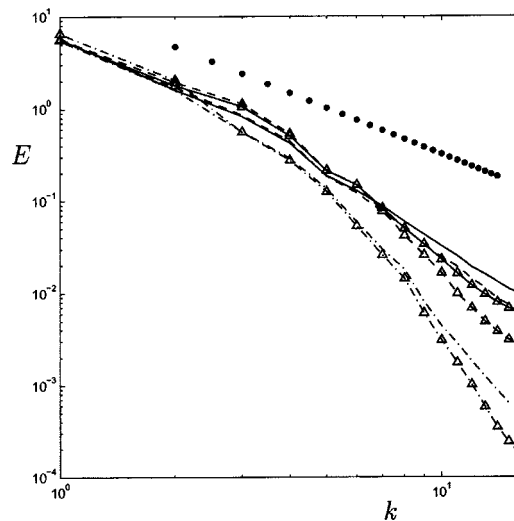
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