A link between energy conserving schemes and LES models of tensor-diffusivity type

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Large-eddy simulation (LES) mainly consists of a "projection": an effective "truncation" to much fewer modes than what is required to perform a direct numerical simulation (DNS). This can be done in different ways: using a reduced set of discrete field values (formally equivalent to sampling, on the coarse grid, of the continuous DNS field), or using a reduced set of continuous functions, etc. One can also first assume a filtering of the DNS field (using an regular filter of effective width Δ; this is basically the view in the method of finite volumes, where the filter is a top hat of width $\Delta = h$), but this step is necessarily followed by the projection step.

The main property of a projector is that applying the projector twice is like applying it once. Letting $\tilde{u}$ be the LES projection of u (i.e., the u field as "seen" on the coarse LES grid), one indeed has that $\tilde{\tilde{u}} = \tilde{u}$: projection is idempotent. The product of the LES fields is also captured on the LES grid. Thus, in LES, one really solves a "tilde" equation (as all terms have the same status):

$$\partial_t \tilde{u}_i + \partial_j \widetilde{\tilde{u}_i \tilde{u}_j} + \partial_i \tilde{P} + \partial_j \tilde{\tau}_{ij} = \nu \, \partial_j \partial_j \tilde{u}_i \tag{1}$$

with $\tilde{\tau}_{ij} = \widetilde{u_i u_j} - \widetilde{\tilde{u}_i \tilde{u}_j}$ the effective subgrid-scale stress (SGS): the product of DNS quantities minus the product of LES quantities, projected on the LES grid. The effect of this term must be modelled.

As mentioned previously, one can do LES with regular filtering of effective width Δ before the projection step, such filtering being explicitely added or implicitely assumed (as in finite volumes) and not idempotent ($\overline{\overline{u}} \neq \overline{u}$). One then solves LES equations for $\widetilde{\overline{u}}$: the projection/truncation of the filtered field $\overline{u}$. There is a then a subfilter-scale stress (SFS) and a subgrid-scale stress (SGS). All terms in the effective LES equation still have a "tilde" status (see, e.g., JFM (2001), vol. 441, pp. 119-138). This added filtering concept can also be used in spectral methods (see e.g., Phys. Fluids (2001), vol. 13(5), pp. 1385-1403), yet with little added value (due to the almost perfect numerical behavior of spectral methods). It appears that the potential interest of filtering lies more in grid-based methods. Once the filter is characterized (not an easy step with implicit filtering), one can use "deconvolution tools" to recover the SFS stress: high level deconvolution using van Cittert iterative method or the direct SFS reconstruction series (limited to second order filters); low level deconvolution using the tensor-diffusivity model (TDM, which is the first term of the direct reconstruction series, and is same for all second order filters of same effective width, see e.g., JFM 2001), or the scale-similarity model, or one van Cittert iteration.

Second, it is also important to recognize that the numerics can be seen as a filter acting on the scales of the LES grid (from $k = 0$ to $k = \pi/h$): the concept of modified wavenumber. The numerical evaluation of a derivative can be expressed as effective filtering of the exact derivative or, equivalently, as the exact derivative of a filtered function. The effective numerical filter then depends on the order of the derivative and on the method used (order and type). Recall also that spectral methods have a perfect wavenumber behavior: no numerical filter.

Third, the equations being non-linear, the discrete energy conservation (in absence of viscosity and/or SGS model, of course) is strongly affected by the discretization of the non-linear convective term. Dealiased spectral methods are also efficient in that respect, as they lead to discrete energy conservation. The same property is desirable for the simulation of turbulent flows (DNS and LES) using grid-based methods: it is important to have schemes with good discrete energy conservation properties. For LES, this also guarantees to better distinguish between the effects of the added SGS model and the numerics.

We here first consider the simplest grid-based method: second order finite differences. We consider the different ways to discretize the non-linear convective term (advective, divergence and mixed forms), and we focus on the discrete energy conservation.

We first consider the case of Burger's equation in 1-D. The energy conservation properties of second order finite differences are then shown to be related to the discrete skewness which is negative in the "turbulent" regime (as for the 3-D Navier Stokes equations). One then obtains that:

- the advective form produces energy;
- the divergence form evaluated using a compact stencil produces energy (yet four times less than the advective form). We here call it the "compact divergence form";
- the divergence form evaluated using a wide stencil dissipates energy. We here call it the "wide divergence form".

For each form, a correction term is developed that leads to an enhanced scheme with good energy conservation properties (exact conservation in the cases of the enhanced advective and compact divergence forms). It is noted that the added term is similar to various forms (advective or divergence) of the "non-linear deconvolution model" (i.e., TDM when in 3-D) used in some LES approaches with explicit filtering to partially recover the SFS stress (e.g., as in Phys. Fluids 2001).

The correction term that appears in the enhanced compact divergence form (also the most natural discretization form) is seen to be formally equivalent to the TDM with $\Delta = h$: the filter width Δ to use in the TDM correction term is thus equal to the grid size h. In the present context, this supports the view that this correction term essentially amounts to *partial deconvolution of the SFS stress corresponding to an implicit filter of effective width equal to the grid size.*

We also notice that one must remain limited to the lowest order correction term: the TDM term; using more terms of the SFS reconstruction series would degrade the performance of those corrected schemes. We also remark that deconvolution methods that are based on "refiltering the LES field" (such as the van Cittert iteration, or the scale-similarity model) cannot be used here, as any filter applied in physical space necessarily has an effective width greater than the grid spacing. The TDM-like approach is thus also special in that respect.

An new link is also made between the proper numerical evaluation of the non-linear convective derivative (i.e., proper evaluation of the "product rule" for derivatives) and the TDM-like term. This also relates to the concept of numerical filter (effect of modified wavenumber behavior on the product rule). We believe that this new formalism constitutes a tool for better understanding and/or deriving energy conserving scheme. Its extension to higher order finite difference methods is ongoing work.

The case with added (explicit) filtering, thus of effective width $\Delta > h$, is considered next. So is the case of LES: thus with added truncation and SGS modelling.

Supporting numerical results are presented, using the forced Burger's equation (white noise forcing) with fixed mesh and for different viscosities: DNS ranging from very well-resolved to much under-resolved, and also LES. Cases with added (explicit) filtering are also presented. The results are compared to solutions obtained using the reference method: the spectral method with dealiasing.

Finally, the case of the 3-D Navier Stokes equations is also considered, with respect to the existing second order schemes used to discretize the non-linear convective term. Starting from non energy conserving schemes, it is shown that one can again recover energy conserving schemes by adding TDM-like elements. The results obtained so far are presented.