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The design and construction of implicit LES models[§]

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SUMMARY

We offer preliminary thoughts on the design of a modified equation and the construction of a corresponding numerical algorithm, which may be intended for use in an implicit large eddy simulation. The principle of design here is based on ensuring a form for the energy dissipation that is not significantly dissipative on the resolved scales of the numerical mesh, but is strongly dissipative when the solution is unresolved and so provides strong nonlinear stability in the simulation. The construction process is modelled on the composition (hybridization) of two flux approximations by means of a nonlinear, flow-dependent switch. Published in 2004 by John Wiley & Sons, Ltd.

KEY WORDS: nonoscillatory methods; implicit turbulence modelling

1. INTRODUCTION

Recently there has been an increased interest in implicit large eddy simulation (ILES) where nonoscillatory finite volume (NFV) methods provide effective modelling of the unresolved dynamics of turbulence in high Reynolds number fluid flows [1, 2]. ILES is a simple and computationally efficient approach, and has been successfully applied to complex engineering and geophysical flows. Further, the absence of explicit parameters holds the promise of increased predictiveness in simulations. ILES methods offer a more automatic approach to modelling complex, general systems of equations beyond those where classical turbulence theory is grounded.

NFV methods are based on a variety of constructions, both algebraic and geometric. Many of these have been exploited for ILES. The common features of all these schemes are nonlinearity and finite volume approximation. The combination leads to flow-dependent dissipation

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and nonlinear computational stability. Despite this commonality, individual algorithms differ in their details and consequent effectiveness. In Reference [3] we used modified equation analysis [4] to find the equivalent partial differential equations (i.e. modified equations) of several common NFV algorithms, exhibiting the distinct form of the nonlinear dissipative terms in each case. We remark that many (but not all) of these forms can be shown through analysis to correspond to explicit subgrid scale closures used in large eddy simulation (LES).

Suppose for the sake of argument that one could devise an optimal method (with its corresponding modified equation) to describe a turbulent flow. Could one construct a numerical algorithm that corresponds to that particular equation? Further, what principles and constraints would one choose to define optimality? Would these principles and constraints be generic, or be flow specific?

This paper is a first effort to address these questions. In Section 2, we discuss a particular principle of design, namely that the algorithm must be appropriately dissipative on the resolved length scales of the computation mesh. In Section 3, we describe a general construction process based on a composition of high-order and low-order fluxes by a nonlinear, flow-dependent switch. We examine the result of this reverse engineering process in the context of the one-dimensional Burgers' equation for specific choices of the fluxes and of the switch. The emphasis in this paper will be on the dissipative character of the effective model. We provide some discussion in Section 4.

2. ENERGY DISSIPATION

The form and magnitude of energy dissipation is a principal concern in the design of a numerical algorithm. Essentially all physical processes, including fluid flow, are dissipative. However in many cases of practical interest, the length scales at which energy is dissipated are too small to be resolved in numerical simulation. For example, this is the situation in such diverse problems as large Reynolds number turbulence, and high-speed compressible flows with shocks. This similarity can be exploited in the development of implicit turbulence models.

The fact that the dynamics of the dissipative scales are too small to be resolved does not imply that the process of energy dissipation can be ignored. Consider the case of a turbulent fluid forced at the large scales of motion. Because of the nonlinearity of the convective processes, energy cascades down in scale—e.g. to smaller and smaller eddies. Physically, this cascade process continues until it reaches length scales where molecular viscosity becomes effective at converting the kinetic energy into heat. However in numerical simulations where the viscous length scales are not resolved, energy will simply build up at the smallest resolved scales if dissipation is absent from the numerical algorithm, producing a qualitatively incorrect solution.

This conundrum has been long recognized in the turbulence modelling community. The conventional solution has been to augment the governing equations by explicit terms (i.e. subgrid scale models) whose main function is to model turbulent effects and in particular to provide appropriate energy dissipation. On the other hand, advocates of the ILES approach rely on the dissipative properties of the numerical algorithm itself to provide the requisite energy dissipation. In ILES, the particular form of the energy dissipation usually results from the imposition of monotonicity constraints. But suppose we wish to take a more

active role by designing an algorithm with a particular form of dissipation. On what basis would one attempt to choose that form?

The most satisfying basis would be the analytic form of the finite volume-averaged equation. An attempt to derive this form for the one-dimensional Burgers' equations was made in Reference [1]. However there remain unresolved issues in the averaging process. Specifically, there is a lack of uniqueness in the process that cannot be resolved mathematically, and so requires additional input from physical argument (i.e. thermodynamics).

A more practical alternative is to draw on the experience of the turbulence modelling community by prescribing a subgrid scale model as a regularizing term. Many subgrid scale models have been devised and undergone extensive testing and validation against experimental and field data. Their success and continued use in engineering and geophysical flow simulations imply their utility. At the same time, the existing diversity of such models casts doubt on the existence of an optimal model.

To be specific, let us consider the following one-dimensional PDE for velocity u:

$$\frac{\partial u}{\partial t} + \frac{\partial f(u)}{\partial x} = \nu \frac{\partial^2 u}{\partial x^2} \tag{1}$$

Here $f(u)$ is a convex flux function and ν is the physical viscosity. We wish to solve this PDE numerically on a grid with cell size δx. We suppose that the viscosity is small in the sense that $(U\delta x)/\nu \gg 1$ where U is some measure of velocity, e.g. from the initial or boundary conditions of the problem. Then, as described above, (1) is not suitable as a model equation for the numerical simulation and it is necessary to add a term that is dissipative on the scale δx in order to ensure numerical stability. We will choose this term from among the explicit subgrid scale models.

For the sake of definiteness, here we will focus attention on one subgrid scale model that is both simple and widely used. The Smagorinsky model [5] was first developed for use in atmospheric simulations. It is closely related to the artificial viscosity of von Neumann and Richtmyer [6]. In one dimension the artificial stress has the form $(C\delta x^2 |\partial u/\partial x| \partial u/\partial x)$ where C is a dimensionless constant. Then the modified equation that we seek is

$$\frac{\partial u}{\partial t} + \frac{\partial f(u)}{\partial x} = C\delta x^2 \frac{\partial}{\partial x}\left(\left| \frac{\partial u}{\partial x} \right| \frac{\partial u}{\partial x} \right) \tag{2}$$

The specifics of the numerical flux $f(u)$ will determine the bounds on the value of C. Here we have omitted the physical viscosity as being inconsequential to the numerical simulation. Multiplying (2) through by the velocity, we derive the associated equation for kinetic energy $K = \frac{1}{2} u^2$

$$\frac{\partial K}{\partial t} + \frac{\partial F(u)}{\partial x} = -C\delta x^2 \left| \frac{\partial u}{\partial x} \right|^3 + C\delta x^2 \frac{\partial}{\partial x}\left(u \left| \frac{\partial u}{\partial x} \right| \frac{\partial u}{\partial x} \right) \tag{3}$$

where $\partial F/\partial u \equiv u \partial f/\partial u$. Integrating this equation over the entire mesh clearly shows the dissipative nature of the modified equation.

3. REVERSE ENGINEERING

In this section we describe a process to construct an algorithm for simulating (1) whose modified equation matches a specified form, e.g. Equation (2). We term this process reverse engineering (RE). RE does not necessarily have a unique result. Although we have not required that the RE algorithm be nonoscillatory, it appears reasonable to attempt to model the RE process on similar ideas used to build NFV methods. One such idea is the melding of low-order and high-order fluxes (e.g. FCT [7], MPDATA [8], TVD [9]). This melding or hybridization is accomplished by means of a nonlinear, flow-dependent switch θ.

We write the algorithm in the conservation (finite volume) form

$$u_j^{n+1} = u_j^n - \frac{\delta t}{\delta x}(f_{j+1/2}^n - f_{j-1/2}^n) \tag{4}$$

where in common notation the superscript n indicates the time level, the subscript j is a spatial index identifying the centre of the cell, and δt is the computational time step. Further, we write the fluxes generically as

$$f_{j+1/2} = \theta_{j+1/2} f^{\mathrm{LO}} + (1 - \theta_{j+1/2}) f^{\mathrm{HO}} \tag{5}$$

The high-order flux, f^{HO}, is chosen to given accurate solutions in smooth regions of the flow. A common choice is the Lax–Wendroff flux

$$f_{j+1/2}^{\mathrm{LW}} = \frac{1}{2}(f_j^n + f_{j+1}^n) - \frac{1}{2}\lambda \frac{\partial f}{\partial u}(u_{j+1}^n - u_j^n), \quad \lambda \equiv \frac{\partial f}{\partial u}\frac{\delta t}{\delta x} \tag{6}$$

where λ is the dimensionless Courant number. The low-order flux f^{LO} is chosen to ensure sufficient energy dissipation in regions of rapidly varying flow. The most common choice is simple upwinding

$$f_{j+1/2}^{\mathrm{up}} = \frac{1}{2}(f_j^n + f_{j+1}^n) - \frac{1}{2}\left|\frac{\partial f}{\partial u}\right|(u_{j+1}^n - u_j^n) \tag{7}$$

As regards the switch, we will require $\theta \in [0, 1]$. This ensures that the composite scheme (4) is stable for at least the more restrictive of the time step conditions associated with the individual flux models F^{HO} and F^{LO}. Furthermore, this limitation of θ also ensures flux consistency

$$f(u_j, u_{j+1}) = f(u) \quad \text{if } u_j = u_{j+1} = u$$

assuming that the individual fluxes have this property. We also want $\theta \to 0$ as the flow becomes smooth, to ensure an accurate solution in these regions. A simple way to characterize smoothness on the mesh scale is through the dimensionless ratio $(\delta x/u\partial u/\partial x)$. For example, one might define

$$\theta_{j+1/2} \equiv \min\left(1, C\left|\frac{u_{j+1} - u_j}{u_{j+1} + u_j + \varepsilon}\right|\right) \tag{8}$$

where the small (properly dimensional) constant $\varepsilon \equiv \delta x/\delta t \times 10^{-15}$ avoids division by zero. Another effective form for the switch is $(\delta x(\partial x/\partial u)\partial^2 u/\partial x^2)$ which closely corresponds to the minmod limiter [3].

Let us apply these choices: (6) for the high-order flux, (7) for the low-order flux, and (8) for the switch, to the case of Burgers' equation where the flux function $f(u)=u^2$. In the limit $\delta t \to 0$, we find the modified equation:

$$\frac{\partial u}{\partial t}+\frac{\partial(\frac{1}{2}u^2)}{\partial x}=\delta x^2\,\frac{\partial}{\partial x}\left(-\frac{1}{6}\,u\,\frac{\partial^2 u}{\partial x^2}-\frac{1}{6}\left(\frac{\partial u}{\partial x}\right)^2+\frac{C}{4}\left|\frac{\partial u}{\partial x}\right|\frac{\partial u}{\partial x}\right) \tag{9}$$

The terms not present in our original modified equation are related to linear dispersion (which can be removed with a third-order base scheme) and a nonlinear term associated with control volume differencing. The corresponding equation for kinetic energy is

$$\frac{\partial K}{\partial t}+\frac{\partial(\frac{1}{3}u^3)}{\partial x}=-\frac{\delta x^2}{6}\,\frac{\partial}{\partial x}\left(u^2\,\frac{\partial^2 u}{\partial x^2}-u\left(\frac{\partial u}{\partial x}\right)^2\right)-\delta x^2\left(\frac{C}{4}\left|\frac{\partial u}{\partial x}\right|^3-\frac{1}{6}\left(\frac{\partial u}{\partial x}\right)^3\right) \tag{10}$$

which is dissipative for $C>\frac{2}{3}$.

Comparing (10) with (3), we see that they have qualitatively the same form of energy dissipation. Our RE equation does not treat rarefying and compressing regions symmetrically, a modification that is now preferred for the artificial viscosity in shocks as well.¶ Also, the RE equation has extra dispersive terms that move energy around, but do not change the dissipative properties of the equation. The effect of this dispersion has been discussed in Reference [11].

We note that the modified equation (9) is very similar to that for MPDATA [1], even though the motivation for its derivation is much different. MPDATA in its basic form [12], as well as our RE method, is sign-preserving but not monotonicity preserving. In our case, this is a direct result of the form for the switch θ, which is not gauge invariant (i.e. depends explicitly on where the zero of velocity is set). Other forms for the switch that are monotonicity preserving are proposed in Reference [13] through the use of modified equation analysis.

MPDATA is derived as a multipass method, where truncation errors are compensated with upwind approximations. In this approach, it is possible to eliminate unwanted dispersive errors, as appear in (9). The elimination of unwanted second-order dispersion in MPDATA is discussed in Reference [14].

Our limiter (8) was designed to emphasize the use of the accurate flux f^{HO} for smooth flow. An alternate idea is to completely turn off any contribution of f^{LO} wherever possible, while strongly dissipating flows that are not sufficiently resolved. This implies a more nonlinear switch. One common switch that has this characteristic is based on the monotone limiting such as that used in MUSCL or FCT methods, e.g. a minmod limiter. To illustrate, first define the monotone bound

$$\delta f_{j+1/2}=2\,\mathrm{minmod}(f_{j+1}-f_j, f_j-f_{j-1}) \tag{11}$$

This is a first-order accurate approximation to the flux. Now we define a final flux similarly,

$$f_{j+1/2}=f_j+\mathrm{minmod}(\delta f_{j+1/2}, f^{\mathrm{HO}}_{j+1/2}-f_j) \tag{12}$$

where the $f^{\mathrm{HO}}_{j+1/2}$ can be any second-order or higher flux.

¶For artificial viscosity this is the result of work by Marshall Rosenbluth while at Los Alamos in 1955 [10].

4. DISCUSSION

In this paper we have explored the design of model equations for ILES, and the construction of a corresponding algorithm. The underlying principle for the design of a model equation is that of ensuring energy dissipation on the smallest resolved scales of the computational mesh. We note that a similar strategy is employed in the variational multiscale methods [15] through the use of a spectral viscosity. In spectral space, the quantification of scale size in the numerical solution is explicit and so it is possible to design a wavenumber dependent viscosity that damps the smallest resolved scales without affecting the larger scales of motion. The situation is more complex in finite difference algorithms, where all computational cells have the same length scale, and there is no readily accessible local quantification of scale size in the numerical solution. Instead, in conventional turbulence simulations explicit scale-dependent dissipative terms are added to the equations, while in ILES simulations dissipation results from the constraint of preserving monotonicity. In Reference [3] we demonstrated the equivalence of these approaches.

In the current paper, we have exploited this equivalence to design new algorithms for modelling turbulent flow by using explicit subgrid scale models to regularize the evolution equations. We note that these subgrid scale models are independent of the physical viscosity ν of the fluid. This is an indication that the details of the small scales of fluid motion where physical viscosity is operating do not matter, or more precisely that the small scales are enslaved by the larger scales of motion. It is this enslavement that underlies the success of both LES techniques and of ILES.

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