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The relationship of MPDATA to other high-resolution methods

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SUMMARY

High-resolution methods have produced the ability to conduct large eddy simulations without the benefit of an explicit subgrid model. This capability is known as implicit large eddy simulation (ILES). A number of high-resolution methods have been shown to have this property. There are notable exceptions where high-resolution method do not work as ILES, particularly methods that have a leading $\mathcal{O}(h^2)$ dissipative term. On the other hand, MPDATA is an effective ILES method with a leading $\mathcal{O}(h^2)$ dissipative term. This dichotomy has played a key role in the discovery of the key role of conservation or control volume form in producing ILES results. In the process of this analysis, I describe a variant of the method leading to a useful alternative form of sign-preserving limiters. This form is proposed as an extension of the basic MPDATA methodology allowing some flexibility in the choice of effective high-order methods. This multistage version of the algorithm removes the leading order nonlinear dissipative error. I rediscover the recursive form of the MPDATA iteration through modified equation analysis (MEA). Finally, returning to the original purpose of the analysis, I describe how the different principles used in MPDATA have been an important contributor to the recent theoretical understanding of ILES.

MPDATA is compared with monotone high-resolution methods both analytically and computationally. The numerical comparison focuses on the validation of ILES methods for high Reynolds number decaying isotropic turbulence. Copyright © 2005 John Wiley & Sons, Ltd.

KEY WORDS: implicit large eddy simulation; modified equation analysis; sign-preserving; nonoscillatory; order of accuracy

1. INTRODUCTION TO IMPLICIT LARGE EDDY SIMULATION (ILES)

High-resolution methods are characteristically nonlinear in the coefficients used to define the difference stencil [1, 2]. This means that the stencil defined by the method is a function

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of the solution rather than being fixed coefficients even for solving linear equations. Generally, the solutions produced by high-resolution methods are nonoscillatory. The use of nonoscillatory methods has been a major revolution in computational physics and opened many new vistas for numerical simulations including turbulence. The criteria used to define the nonlinear coefficients of the stencil determine the characteristics of each method. The MPDATA method [3] is distinguished by using a different mechanism to determine the nonlinear stencil coefficients than other high-resolution methods. The procedure used to define the stencil uses the concept of upwinding the numerical error as compared with the basic upwind method (donor cell differencing). MPDATA can also be applied iteratively in multiple steps, another clear methodological difference. MPDATA is a sign-preserving method (positive-definite solutions are maintained). This differs from the property of monotonicity used to define nonlinearity with many other high-resolution methods.

Despite these clear differences, MPDATA has been demonstrated to be effective on large-scale simulations including turbulent flows through the technique of implicit large eddy simulation (ILES), a property of many other high-resolution methods [4–13]. Originally a number of researchers had independently come to the conclusion that their high-resolution methods produced effective LES simulations. In these original works on ILES all of the methods used shared monotonicity-preservation as a common thread [4, 5]. This resulted in the original terminology for this simulation approach as MILES for monotone-integrated LES. More recently this relatively common observation has led to the search for unifying principles to explain this good fortune. I report on how the unique design of the MPDATA method helped to provide evidence on the essential elements of ILES leading to the results seen by many researchers. Key to this study has been the differing nature of MPDATA from other methods that has removed the focus from monotonicity as the seminal property of the methods for ILES. Instead this focus has been placed on conservation form and nonlinear stability resulting from a broader definition of nonoscillatory differencing [7–11].

Large eddy simulation (LES) is a turbulence simulation approach where only the large scales of the flow are simulated and the effects of small scales associated with viscous dissipation are modelled. LES originated in the weather simulation community with the work of Smagorinsky [14] who produced the classical and archetypal LES subgrid model based on an extension of Von Neumann–Richtmyer shock viscosity [15]. The state-of-the-art in LES has now been extensively developed as documented by Sagaut and Germano [16] and other recent surveys [17, 18]. Traditionally, LES requires high-accuracy, low-dissipation numerical integration for the fluid equations so that numerical errors do not interfere with the modelling. Unfortunately, LES simulations are limited in applicability to (nearly) incompressible turbulence and simulations where the mesh density is close to that required to conduct a direct numerical simulation of the flow where the viscous dissipation is completely resolved.

These limitations can be overcome with a newer and philosophically distinct approach to simulating turbulence. The ability of some numerical methods to produce large eddy simulations without explicit models was first identified by Boris [4] who dubbed the approach MILES for monotone integrated LES. The method Boris used, FCT is based on a monotonicity principle. Soon other researchers reached the same conclusions with similar, but with different methods. The common thread in all these methods was the use of monotonicity-preservation in the methods loosely referred to as high-resolution methods. During the later part of the 1990s calculations with a different, but related method began to evidence the same behaviour as MILES. This method was MPDATA. The problem was that this method is not monotone, it is sign preserving, a different design principle than monotonicity. The nonlinearity of the scheme used to enforce sign-preservation makes MPDATA a high-resolution method. It gradually became clear that the term MILES was too restrictive because of its basis in monotonicity, and ILES was born. There was also the mystery of what unified the methods with this property. As I will show, the diversity represented by MPDATA allowed us to more easily unravel some of the secrets of ILES.

Because MPDATA is so different from other high-resolution methods, analysing its effective model in comparison to other methods provides a path towards understanding the ability of all high-resolution methods to model turbulent flows. We have conducted a systematic analysis of high-resolution methods using the technique of modified equations [7, 19]. The modified equation analysis is particularly well suited towards uncovering the nonlinear structure of a method. MPDATA produces a strong dissipation at $\mathcal{O}(h^2)$ with a structure like that of Von Neumann–Richtmyer artificial shock viscosity [20]. This method is the original nonlinear (high-resolution) method. The ILES capability of MPDATA should not be surprising as the Smagorinsky LES model is an extension of the original artificial shock viscosity [15].

Some other high-resolution methods with $\mathcal{O}(h^2)$ dissipation are too dissipative for ILES. These methods are typified by the minmod limiter that will be analysed in the next section. Most high-resolution methods used successfully with ILES have $\mathcal{O}(h^3)$ dissipation with stronger dissipation being triggered by monotonicity violations that indicate a locally under-resolved flow [21]. Monotonicity violations trigger dissipative mechanisms that are $\mathcal{O}(h)$ like upwinding. MPDATA is also a conservation form (control volume) method. I believe that this is one of the two key aspects of MPDATA that leads to ILES success. Conservation form leads to important physical terms in the finite scale governing equations essential to modelling large-scale flows via ILES as shown in Equation (16). Finite volume methods produce these terms through the use of the conservation form and its presence is not a consequence of using a high-resolution method. The high-resolution aspects of the method are essential for the fundamental stability and physical realizability of the simulation.

In the next section we analyse existing methods for suitability as ILES methods. These results also suggest how new methods can be designed with better properties similar to iterative versions of the MPDATA algorithm. I then provide some computational evidence to support the analysis.

2. ANALYSIS AND NEW METHOD DESIGN

There are several main approaches to analysing numerical methods. Fourier stability analysis is limited to linear methods and equations. Because nonlinearity plays the key role in turbulence and high-resolution methods are intrinsically nonlinear, linear analysis methods yield little of value for the purposes of this study. I will adopt an approach that can examine the nonlinear aspects of both the governing equations and the numerical method used to solve them. A major tool in our investigation of MPDATA is modified equation analysis (MEA). MEA derives the effective differential equation solved by the numerical method. This effective differential equation includes terms usually called truncation error terms and represents the equation that the method actually approximates with greater accuracy than the original PDE.

The modified equation is useful for determining the physical meaning of the terms associated with truncation error. As an example consider upwind differencing of

$$\frac{\partial u}{\partial t} + a\frac{\partial u}{\partial x} = 0 \tag{1}$$

where a is greater than zero. For brevity of presentation, I will only examine spatial derivatives. Upwind differencing produces the following discrete approximation with errors:

$$a\frac{\partial u}{\partial x} = a\frac{u_j - u_{j-1}}{\Delta x} - \frac{a\Delta x}{2}\frac{\partial^2 u}{\partial x^2} + \text{H.O.T.} \tag{2}$$

The first term in the truncation error is second-order and diffusive like physical dissipative mechanisms and H.O.T. refers to higher order terms that have been truncated. This is an analysis that reveals the common numerical diffusion typically associated with first-order upwinding.

The basic MPDATA method is defined as a two-step method starting with an upwind step

$$\widetilde{u_j} = u_j^n - \frac{a\Delta t}{\Delta x}(u_j^n - u_{j-1}^n) \tag{3}$$

followed by a correction step that 'upwinds' the truncation error

$$u_j^{n+1} = \widetilde{u_j} - \frac{\Delta t}{\Delta x}(f_{j+1/2} - f_{j-1/2}); \quad f_{j+1/2} = \frac{\Psi_{j+1/2}}{2}(\widetilde{u_j} + \widetilde{u_{j+1}}) - \frac{|\Psi_{j+1/2}|}{2}(\widetilde{u_{j+1}} - \widetilde{u_j}) \tag{4}$$

where the pseudo-velocity is based on the difference in truncation error between upwind and Lax–Wendroff differencing (between first- and second-order)

$$\Psi_{j+1/2} = \frac{1}{2}\left(a - \frac{\Delta t a^2}{\Delta x}\right)\frac{\widetilde{u_{j+1}} - \widetilde{u_j}}{\widetilde{u_j} + \widetilde{u_{j+1}}} \tag{5}$$

I am interested in expressing the method in a form where a limiter function is defined. For this purpose I will suppress the multistep form of the base MPDATA method. Next, I will assume that our low-order method is upwinding for $a > 0$, leading to $u_{j+1/2}^{\text{low}} = u_j$ and the high-order method is Lax–Wendroff (second-order centred difference without the time-accurate terms), $u_{j+1/2}^{\text{high}} = (u_j + u_{j+1'})/2$. With these steps in place, one can rearrange this method into a form that isolates the limiter by making the observation that Equation (5) can be expressed as the ratio of the difference between high- and low-order over the high-order

$$\Psi_{j+1/2} = \frac{1}{2}\left(a - \frac{\Delta t a^2}{\Delta x}\right)\frac{u_{j+1/2}^{\text{high}} - u_{j+1/2}^{\text{low}}}{u_{j+1/2}^{\text{high}}} \tag{6}$$

Inserting Equation (6) into Equation (4) and simplifying plus adding in the first step gives an expression for a single step MPDATA scheme in cell j

$$u_{j+1/2} = u_{j+1/2}^{\text{low}} + \phi_{j+1/2}(u_{j+1/2}^{\text{high}} - u_{j+1/2}^{\text{low}}) \tag{7}$$

At the same edge in cell $j+1$ the expression is the same, but a low-order approximation projected toward that cell edge from cell $j+1$ will be, $u_{j+1/2}^{\text{low}} = u_{j+1}$, thus

$$u_{j+1/2} = u_{j+1} + \phi_{j+1/2}(u_{j+1/2}^{\text{high}} - u_{j+1}) \tag{8}$$

where for simplicity I have dropped the time dependence. The final value can be determined through applying upwind (i.e. the Riemann problem at the cell interface). This limiter can either be applied iteratively to get higher order methods, or as the original MPDATA can be applied repeatedly using the same high order objective value for the flux.

This form allows us to compare the 'limiter' from MPDATA with similar forms from TVD and Godunov-type methods based on monotonicity [22]. The one iteration version of MPDATA is more dissipative than the form based on Monotone limiters, but the iterative version of MPDATA will produce smaller dissipations for two or more iterations especially when coupled with a higher than second-order, high-order flux. If one simplifies each limiter, the difference between the two forms reduces to MPDATA being approximately, $\phi_{j+1/2} \approx u^{\text{low}}_{j+1/2}/u^{\text{high}}_{j+1/2}$ where the monotone form is $\phi_{j+1/2} \approx u^{\text{low}}_{j+1/2}/(u^{\text{high}}_{j+1/2} - u^{\text{low}}_{j+1/2})$. I will examine a fourth-order approximation in the following. It is interesting that the work in this meeting includes efforts to bridge MPDATA to monotone methods by producing a version that has many of the characteristics of monotone limiters [23]. Together these efforts provide a fuller picture of MPDATAs place among high-resolution method.

This provides the observation that MPDATA produces leading order dissipation like that introduced by Von Neumann and Richtmyer and therefore like Smagorinsky eddy diffusion, the original LES model. By applying MEA to a nonlinear conservation law and a single MPDATA iteration, the leading order error is

$$\frac{\partial f}{\partial x} \approx \frac{\partial f}{\partial x} - \frac{\partial}{\partial x}\left(\frac{\Delta x^2}{6}\frac{\partial f}{\partial u}\left(\frac{\partial u}{\partial x}\right)^2 + \frac{\Delta x^2}{6}\left|\frac{\partial f}{\partial u}\right|\frac{\partial^2 u}{\partial x^2} + \frac{\Delta x^2}{4|u|}\left|\frac{\partial u}{\partial x}\right|\left(\frac{\partial u}{\partial x}\right) + \text{H.O.T.}\right) \tag{9}$$

As I will discuss later, it is the presence of the other terms without the absolute value term that actually contributes most greatly to MPDATA prowess as a LES method. When included as an explicit model this term produces a scale-similarity model and together with the dissipative term constitutes what is known as a mixed model in the LES community. The form of the truncation error produces a similar impact with the MPDATA method. The second key point is that the nonlinear dissipative error with MPDATA does not interfere with the proper scaling of dissipation in a turbulent flow. This form will be produced for whatever MPDATA method I use. The second truncation error term is the dispersion error. For either an iteratively defined MPDATA or high-order MPDATA, the leading order nonlinear dissipative term can be raised to higher than second-order in Δx, but the conservation form of the differencing assures that the first term is retained.

This fact can be confirmed through putting the method into an advective form and defining the truncation error. Consider second-order centred differencing in conservation form

$$\frac{\partial f}{\partial x} \approx \frac{f_{j+1} - f_{j-1}}{2\Delta x} - \frac{\partial}{\partial x}\left(\frac{\Delta x^2}{6}\frac{\partial f}{\partial u}\left(\frac{\partial u}{\partial x}\right)^2 + \frac{\Delta x^2}{6}\frac{\partial f}{\partial u}\frac{\partial^2 u}{\partial x^2}\right)$$

and advective form

$$\frac{\partial f}{\partial x} \approx \frac{\partial f_j}{\partial u_j}\frac{u_{j+1} - u_{j-1}}{2\Delta x} - \frac{\partial f}{\partial u}\frac{\partial}{\partial x}\left(\frac{\Delta x^2}{6}\frac{\partial^2 u}{\partial x^2}\right)$$

With the advective form the term associated with scale-self-similarity does not appear in the truncation error. This can be demonstrated through conducting the same analysis with any method, the conservation form results in the scale-self-similar term and the advective form does not. I believe that this produces the scale-self-similar approach to modelling turbulence essential to ILESs success.

As I will demonstrate below applying the MPDATA approach iteratively the leading order nonlinear dissipation can be removed. If we begin with the form defined by Equation (7) defining the first iteration, a second iteration is

$$u_{j+1/2}^{(2)} = u_{j+1/2}^{(1)} + \phi_{j+1/2}^{(2)}(u_{j+1/2}^{\text{high}} - u_{j+1/2}^{(1)}); \quad u_{j+1/2}^{(1)} = u_{j+1/2}^{\text{low}} + \phi_{j+1/2}^{(1)}(u_{j+1/2}^{\text{high}} - u_{j+1/2}^{\text{low}}) \tag{10}$$

here the limiter in the first stage is defined as before, but the second stage limiter is

$$\phi_{j+1/2}^{(2)} = 1 - \left| \frac{u_{j+1/2}^{\text{high}} - u_{j+1/2}^{(1)}}{u_{j+1/2}^{\text{high}}} \right| \tag{11}$$

Similarly, a third or fourth iteration can be defined, each iteration getting closer to the objective of using the high-order edge value, the general form of the nth stage iteration is

$$u_{j+1/2}^{(n)} = u_{j+1/2}^{(n-1)} + \phi_{j+1/2}^{(n)}(u_{j+1/2}^{\text{high}} - u_{j+1/2}^{(n-1)}); \quad \phi_{j+1/2}^{(n)} = 1 - \left| \frac{u_{j+1/2}^{\text{high}} - u_{j+1/2}^{(n-1)}}{u_{j+1/2}^{\text{high}}} \right| \tag{12}$$

As found for the original form of MPDATA [24], this process admits a compact recursive form

$$u_{j+1/2}^{(n)} = u_{j+1/2}^{\text{high}} + (u_{j+1/2}^{\text{low}} - u_{j+1/2}^{\text{high}}) \left| 1 - \frac{u_{j+1/2}^{\text{low}}}{u_{j+1/2}^{\text{high}}} \right| \prod \left(\frac{u_{j+1/2}^{\text{high}} - u_{j+1/2}^{\text{low}}}{u_{j+1/2}^{\text{high}}} \right)^{2^{(n-1)}} \tag{13}$$

In terms of the truncation error, each subsequent iteration pushes the nonlinear dissipative term two orders higher in Δx per iteration. For example, the two iteration form of this approach produces a nonlinear dissipative error at Δx^4 of the form

$$\frac{\partial}{\partial x} \left(\frac{\Delta x^4}{16|u|} \left| \frac{\partial u}{\partial x} \right| \left(\frac{1}{u} \frac{\partial u}{\partial x} \right)^2 \left(\frac{\partial u}{\partial x} \right) \right) \tag{14}$$

I have also examined the behaviour of this method for the case where the high-order value is replaced by a value of higher than second-order. This provides the method with greater flexibility in achieving small truncation errors. The iterative form can be used to remove the lower order linear errors. In this case, for a fourth-order centred high-order edge value, the first iteration produces the following truncation error at leading order:

$$\frac{\partial}{\partial x} \left(\frac{\Delta x^2}{4|u|} \left| \frac{\partial u}{\partial x} \right| \left(\frac{\partial u}{\partial x} \right) \right)$$

The second iteration raises this to

$$\frac{\partial}{\partial x} \left(\frac{\Delta x^4}{16|u|} \left| \frac{\partial u}{\partial x} \right| \left(\frac{1}{u} \frac{\partial u}{\partial x} \right)^2 \left(\frac{\partial u}{\partial x} \right) + \frac{1}{30} \frac{\partial^4 u}{\partial x^4} \right)$$

with the third and higher iterations leave only the leading order truncation error from the linear high-order method.

Another important aspect of many limiters is the property of whether the effect of the limiter is nullified when the flow is resolved. Thus, in resolved regions only the high-order method is used. For the single nonlinear correction of MPDATA, the limiter is always active whether the flow is resolved or not. Most of the methods that have been associated with ILES have the property that the limiting is inactive in resolved flows. High-resolution monotone methods that have limiting that is always active at $\mathcal{O}(h^2)$ such as the minmod limiter do not make effective ILES methods as I discuss next [21].

When comparing MPDATA with other high-resolution methods I find that the scale-self-similar and dispersion error (for second-order methods) are systematically present. For monotone schemes the dissipative terms are different in form, for example with the minmod limiter

$$\frac{\partial}{\partial x}\left(\frac{\Delta x^2}{4}\left|\frac{\partial f}{\partial u}\right|\frac{|\partial u/\partial x \partial^2 u/\partial x^2|}{\partial u/\partial x}+\cdots\right. \tag{15}$$

differing from the Smagorinsky-like MPDATA term at $\mathcal{O}(h^2)$. Other monotone limiters are completely inactive if the flow field is resolved and the leading order dissipative terms is at $\mathcal{O}(h^3)$ and does not interfere with the control volume term at second-order (the PLM method based on Fromm's method used in the next section is an example).

The key to understanding the differences in the methods is the energy analysis that shows how energy will scale in a computed flow. The analysis proceeds by forming an energy through multiplying the equation by u (the energy is $1/2u^2$) then integrating the modified equation over control volumes and applying integration by parts [21, 25]. Terms that retain conservation form do not contribute to the energy evolution on the average. The dispersion term conserves energy and does not change the energy content of the fluid. The scale self-similar term is not in conservation form and produces the correct scaling for turbulence and shocks

$$\left\langle\frac{\mathrm{d}(1/2u^2)}{\mathrm{d}t}\right\rangle \propto \Delta x^2\left\langle\frac{\partial f}{\partial u}\left(\frac{\partial u}{\partial x}\right)^3\right\rangle \tag{16}$$

and depends on the asymmetry of the field (and stable computation as well) to produce a dissipative result. The angled brackets denote the averaging over the domain of interest. The dissipation in MPDATA produces a positive-definite dissipation that also matches the scaling in theory without depending on the details of the computed field,

$$\left\langle\frac{\mathrm{d}(1/2u^2)}{\mathrm{d}t}\right\rangle \propto \Delta x^2\left\langle\left|\frac{\partial u}{\partial x}\right|\left(\frac{\partial u}{\partial x}\right)^2\right\rangle \tag{17}$$

Monotone limiters produce a result and scaling that is not consistent with theoretical expectations

$$\left\langle\frac{\mathrm{d}(1/2u^2)}{\mathrm{d}t}\right\rangle \propto \Delta x^2\left\langle\left|\frac{\partial u}{\partial x}\right|\left|\frac{\partial^2 u}{\partial x^2}\right|\right\rangle \tag{18}$$

Equation (18) is the key to understanding why some high-resolution methods do not perform well as ILES.

3. COMPUTATIONAL EVIDENCE

The goal of this section is to provide computational support for the analysis in the preceding section of the paper. I will examine three different high-resolution methods: the MPDATA method using a second nonlinear iteration, the minmod limiter TVD method, and the limited Fromm TVD method. These results will clearly demonstrate the relative character of each method especially related to the computation of turbulent flows via the ILES approach. The results are consistent with the expectations resulting from the analysis in the previous section.

3.1. Verification: Riemann invariant

I begin the comparisons using a simple flow that has analytically defined initial conditions, and through nonlinear dynamics produces ever smaller and, ultimately, unresolvable scales. The flow is a one-dimensional case of acoustic wave breaking. This problem was introduced by Cook and Cabot [26] consisting of an initial condition having signal content in a single Riemann invariant. The initial flow is confined to a single wave family, and the other characteristics carry no information until the shock forms. Our calculations are patterned after Cook and Cabot with a comparison shown at a time that is 75% of the time required for a shock to form. The solution remains analytic at that time and the exact solution is available for comparison. I use a grid of 64 uniformly spaced zones in our calculations.

The comparison of the three methods is shown in Figure 1. The upper frame shows the computed spectra for each method. Interestingly, the minmod and limited Fromm method break from the analytic spectrum in a nonmonotonic manner. MPDATA on the other hand, falls from the analytical spectrum in a smooth fashion. As the lower frame demonstrates, the magnitude of the error with the minmod limiter greatly exceeds that associated with the other flows especially in the highest wavenumbers. Moreover, the overly dissipative behaviour of minmod in medium wavenumbers results in an under dissipative result for the highest wavenumbers. In contrast both MPDATA and limited Fromm show their strongest dissipation at the grid resolution limit, an attractive character for a method. For this problem and the simulation in the following subsection a more extensive comparison of MPDATA using different numbers of nonlinear iterations is given in a recent paper [25]. The results in that paper strongly indicate that MPDATA improves significantly as the number of iterations is taken to three and slightly more with four iterations. These results will lay the groundwork for considering a full-fledged turbulent flow as is shown next.

3.2. Validation: decaying turbulent flow

Next, I will simulate an experiment by Kang *et al.* [27] utilising the high quality data is available. The decay of isotropic turbulence is an essential benchmark flow for turbulence. The classical experiment of decaying turbulence was conducted by Comte–Bellot–Corrsin and is often used to test turbulence models. Recently a group at John Hopkins University has conducted a similar experiment, but at a much larger Reynolds' number [27]. In the John Hopkins' experiment, a wind tunnel was utilized with an active grid to produce a decaying (nearly) isotropic turbulent field with an initial Taylor microscale Reynolds number in excess of 700. Along the length of the wind tunnel four stations with X-wire probes produced

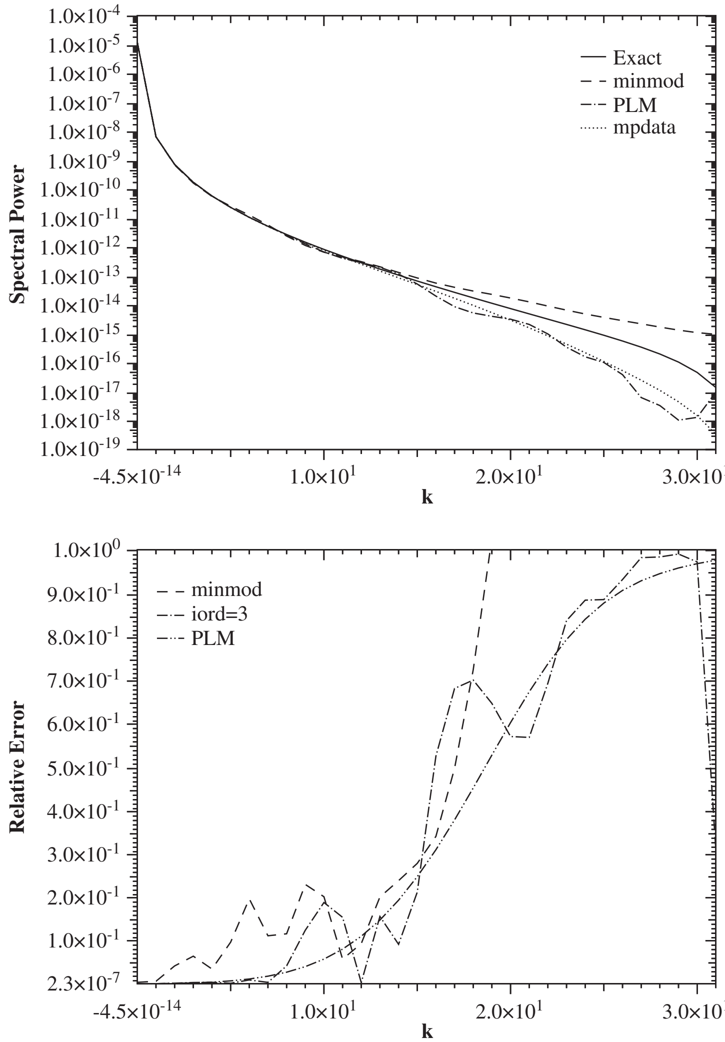

Figure 1. The comparison of the spectral behaviour of the three methods is shown in the upper frame. The relative spectral error is shown in the lower frame.

measurements of the flow field. These stations were placed at $x/M = 20, 30, 40$, and 48 where x is the downstream position and M is the spacing of the grid.

I will use several of the published measurements as a means of comparison between the simulations and the experiment. These measurements include the kinetic energy of the flow, the longitudinal velocity increments, and the transverse velocity increments. These are derived from the experimental data filtered at different length scales. Our initial condition is taken from the conditions given in Reference [27] and time is measured using the flow velocity through the relation, $x = Ut$ where U is the downstream velocity in the experiment. The data plotted

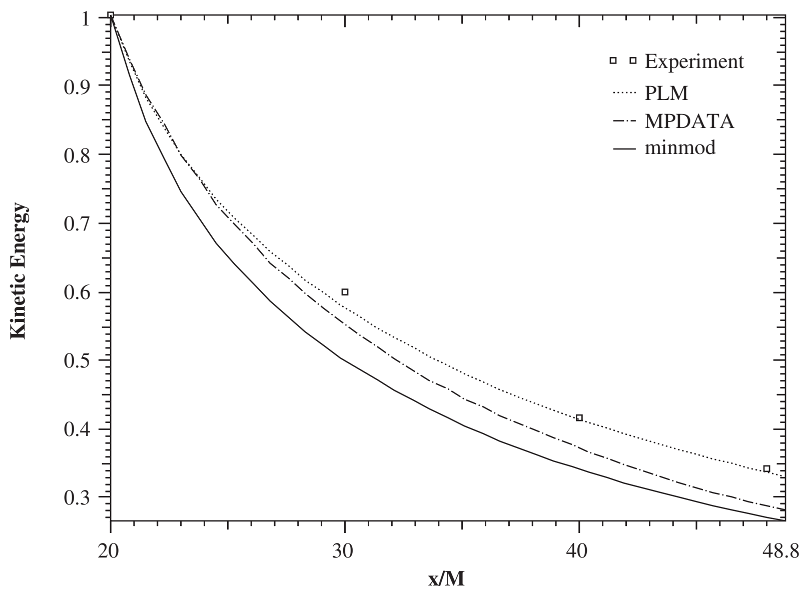

Figure 2. The plot shows a comparison of kinetic energy decay between the experiment and simulation. The kinetic energy levels and times have been normalized to refer to the same dimensionless time.

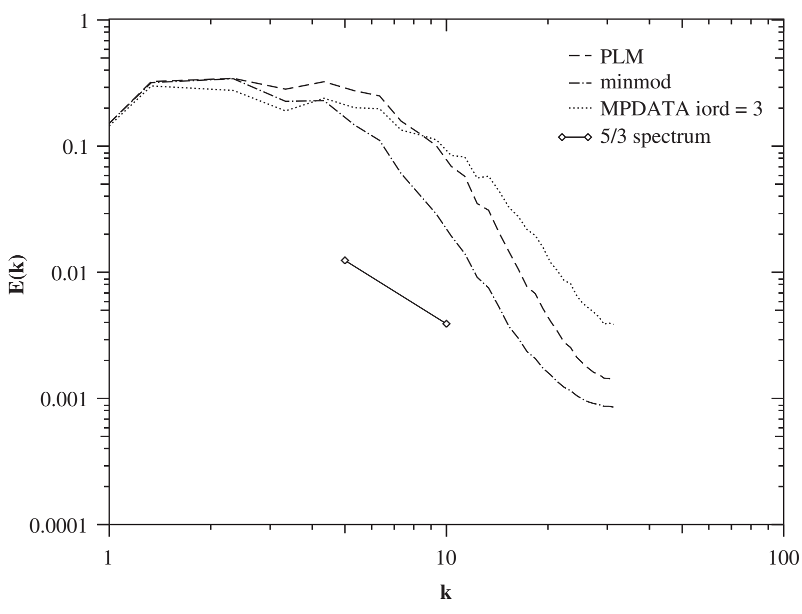

Figure 3. The three-dimensional energy spectra are shown for each of the methods used at $x/M = 48$. The spectra behave in the same manner as the experimentally measured spectra. The three methods are similar in the low wavenumber region. There are significant differences in the manner in which the spectrum behaves at high wavenumbers ($k > 15$).

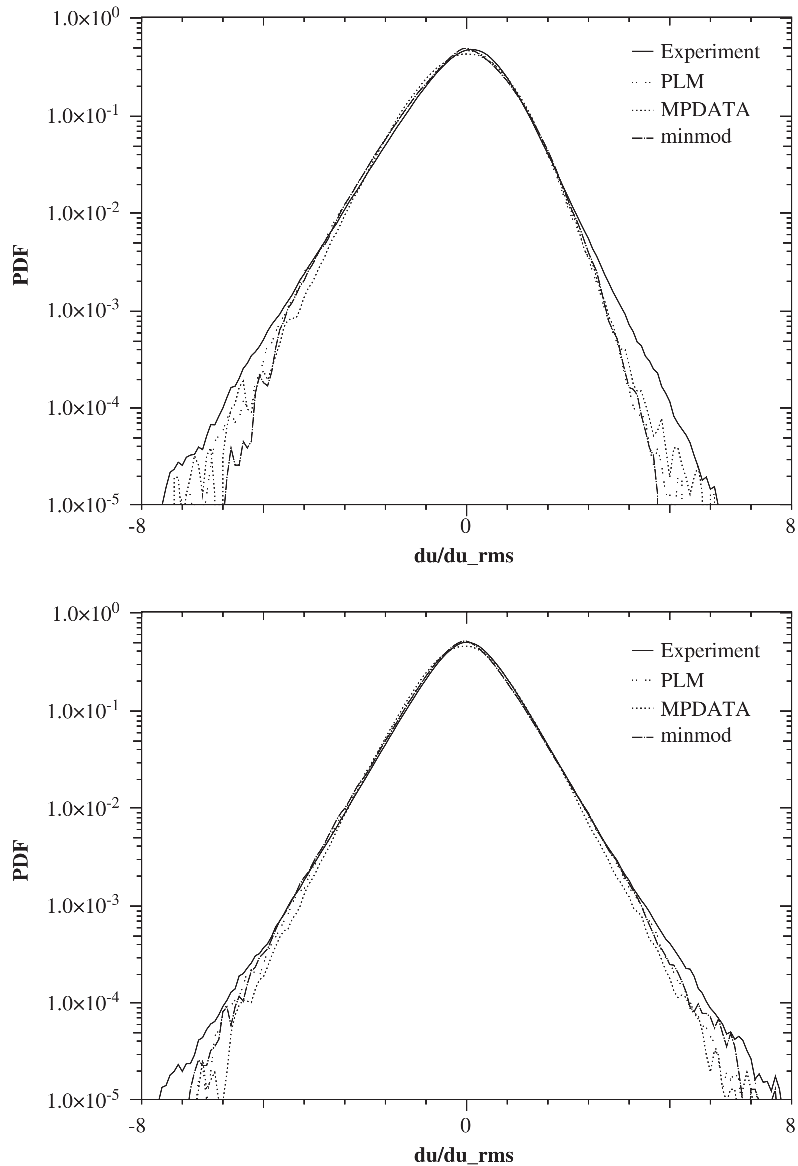

Figure 4. The PDFs of the computed and experimental velocity increments are compared in this figure. The experimentally measured PDFs are quite well reproduced by the ILES methods. This includes the magnitude of the velocity increments in the tails of the PDF.

as the experimental PDFs of the velocity increments can be found online at the website for the Johns Hopkins turbulence research group.

All of my simulations employed a grid of 64^3. Figure 2 shows the decay of kinetic energy computed with our methods compared with the experiment. The limited Fromm (PLM) method produces a good comparison with the experimentally observed energy decay. Both

MPDATA and especially the minmod method are too dissipative on the grid utilized here. The comparison of the simulated power spectra is shown in Figure 3. This measure compliments the kinetic energy comparison with the absolute magnitude of the spectrum at low wave numbers paralleling the total energy content computed with each method. At high wave numbers the results with each method are somewhat different with MPDATA showing the shallowest decay. The minmod method begins to decay strongly at a relatively low wavenumber as might be predicted from the numerical analysis of the method.

In Reference [27] LES comparisons of velocity increments have shown good agreement with the small increments while not capturing the tails of the distribution. This indicates that the simulations do not show the proper intermittency as the data. For our simulations we compute the velocity increments using backward differences. We then construct the PDFs from these differences. The longitudinal velocity increments are $u_i(x_i + \Delta x_i) - u_i(x_i)$, and the transverse velocity increments are $u_i(x_j + \Delta x_j) - u_i(x_j)$, for $i \neq j$. With ILES simulations we find that the intermittency is quite well reproduced in both the longitudinal and transverse velocity increments. We display the comparison between the experiment and simulations in Figure 4. It is important for the reader to note that the experimental data that I compare with has been filtered with a narrower width filter than that shown in earlier comparisons. These results seem to indicate that ILES methods are effective in both simulating the mean behaviour of classical turbulence as well as a superior capability in capturing the turbulence's intermittency.

Despite this generally good behaviour there are differences between the three methods. The minmod method computes the least intermittent flow consistent with other fiducials. Interestingly the MPDATA method compares favourably with the two other methods in the tails of the PDFs. This is despite its more dissipative nature compared with PLM. One could conclude that the reason for the good behaviour of MPDATA is the lack of a monotonicity-based limiter that allows better preservation of high-wavenumber flow structures.

4. CONCLUDING REMARKS

Given the available evidence I conclude that MPDATA works for ILES for two reasons: its use of the conservation form, and the nonlinear dissipation that is consistent with observed turbulent flow (and accepted theory). The relatively low order $\mathcal{O}(h^2)$ dissipation in the base MPDATA algorithm matches the differential form found in turbulent models. This term matches the finite scale terms mod the positive-definite nature of the dissipation. Other lower-order high-resolution methods do not have this type of dissipation. I have hypothesized that the different $\mathcal{O}(h^2)$ dissipation in the other methods is the key difference. Through our combined experience with MPDATA and other high-resolution methods, I further hypothesize that conservation form is essential, and the nonlinear dissipation must either match the observed form, or not interfere with the terms associated with conservation form. This lack of interference can also be achieved by having the nonlinear dissipation work at higher than second-order. Each of these hypotheses is supported by the calculations shown in the previous section.

The analysis shows that this form of the leading order error can be removed through the use of the iterative form of the algorithm. While MPDATA is sign-preserving, the form of the effective limiter does not match sign-preserving methods based on monotonicity-preserving methods. Through the use of higher order differencing, coupled with the iterative form of MPDATA more effective methods can be found. These forms share the property of having the nonlinear dissipative mechanisms associated with limiters be completely inactive should the flow be resolved. This appears to be a highly desirable property for a high-resolution method to exhibit.

MPDATA shows the value of both methodological diversity as well as rigorous asymptotic analysis in uncovering the basic properties of both specific and categories of numerical methods.

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