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An error indicator for finite difference methods using spectral techniques with application to aerofoil simulation

Christian T. Jacobs*, Markus Zauner, Nicola De Tullio, Satya P. Jammy, David J. Lusher, Neil D. Sandham

Aerodynamics and Flight Mechanics Group, Faculty of Engineering and the Environment, University of Southampton, University Road, Southampton SO17 1BJ, United Kingdom

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ABSTRACT

This work introduces a new error indicator which can be used to determine areas of insufficient numerical resolution in unfiltered finite difference simulations. The background behind the methodology is that smaller scales (i.e. the flow features with higher wave numbers) are physically characterised by a smaller energy content in comparison with larger scales. This energy should decrease with increasing wavenumber at a minimum rate; if this rate is not attained it likely means that the smaller scales are not being properly resolved on the computational grid of solution points. An approach using spectral techniques is used to formulate two varieties of the error indicator – one integer-valued and one floating point-valued. These values are computed at a finite number of 'blocks' which span the domain. The indicator is implemented within the OpenSBLI finite difference-based modelling framework, and evaluated in the context of a three-dimensional Taylor-Green vortex problem and flow past a V2C laminar flow aerofoil.

1. Introduction

Computational grids are at the core of many numerical models. They comprise a set of points upon which the governing equations are solved. One of the crucial constraints of grid generation is that small-scale structures must be sufficiently well resolved by the grid, since any errors (introduced through numerical dispersion and dissipation, as well as nonlinear effects such as aliasing) can cause the simulation to become inaccurate and unstable [1]. Adopting a uniformly-fine grid to ensure this constraint is satisfied often results in a large number of superfluous grid points, which is detrimental to the model's computational efficiency. At the same time, it is often not possible to know *a priori* exactly where high resolution needs to be placed in the domain, particularly when dealing with transient and turbulent dynamics frequently encountered in real-world applications. The formulation of *a posteriori* error estimators and indicators [2–6], and their coupling with adaptive grid refinement methods [7–13], has therefore attracted a considerable amount of attention over the last few decades.

The current work is focussed on finite difference solutions of the compressible Navier–Stokes equations in the absence of explicit filtering or artificial dissipation. Such an approach is commonly used for DNS [14]. A feature of under-resolved regions of flow is the appearance of grid-to-grid point oscillations, usually first apparent in derivative quantities such as vorticity or dilatation rate. Typically the appearance of such numerical errors/oscillations is used to decide when and where grid refinement is required. This work aims to quantify and calibrate these features of under-resolution such that the grid refinement process can ultimately be automated.

A new error indicator, based on spectral techniques using small-domain Fourier transforms, is presented herein. It does not attempt to quantify the solution error, but instead estimates the severity of any under-resolution that occurs in the solution field. The indicator is implemented in the OpenSBLI finite difference modelling framework [15]. Section 2 describes the error indicator in further detail. It is then evaluated in Section 3 by considering three-dimensional simulations of the Taylor–Green vortex problem [16] and flow past a V2C laminar aerofoil (see e.g. [17]). Some conclusions are drawn in Section 5.

2. Error indicator

The error indicator considers a finite number of small cubes which together span the whole 3D domain. For each N_e^3 block, and for each line of N_e points within it, various Fourier amplitudes of

* Corresponding author.
E-mail address: christian@christianjacobs.uk (C.T. Jacobs).

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a user-specified solution field are computed. These amplitudes are subsequently averaged over N_e^2 lines to determine the anisotropic error 'severity' values.

The first step to computing the error indicator is to apply a Hamming window to the solution field y, in order to ensure its smoothness and periodicity for Fourier analysis. Thus for each line of N_e solution points in each direction:

$$y_j = y_j \frac{\left(0.54 - 0.46\cos\left(\frac{2\pi j}{N_e}\right)\right)}{0.54}, \tag{1}$$

where y_j is the jth component of the solution field y in the line of solution points under consideration.

The Fourier amplitudes (proportional to the square root of the spectral energy) for selected modes/wavenumbers $N_e/2$, $N_e/4$ and $N_e/8$ of the solution field are then computed, for each N_e^3 block. In order to avoid doing a computationally intensive Fourier transform each time, the amplitudes are reconstructed by using simple summations, S:

$$S_2 = \sum_{j=0}^{N_e-1} (-1)^j y_j, \tag{2}$$

$$S_4 = \sum_{j=0}^{N_e-1} (-\mathrm{i})^j y_j, \tag{3}$$

$$S_8 = \sum_{j=0}^{N_e-1} \exp\left(-\frac{\pi}{4}\mathrm{i}\right)^j y_j, \tag{4}$$

where $\mathrm{i} = \sqrt{-1}$. These values were checked for correctness against a fast Fourier transform.

With an increasing mode/wavenumber k, we desire the spectral energy $E(k)$ (and therefore the mode amplitude $Y(k)$) to decrease at a minimum rate, such that the smallest scales have the lowest energy content. An increase in $E(k)$, for example due to aliasing errors arising from non-linear terms, is likely to mean that we are not resolving the small scales well enough. Determining where this increase occurs in the domain facilitates the dynamic focussing of resolution in that area. To this end, the error indicator presented here is based on detecting whether the spectrum decay rate is worse than some prescribed value.

Two versions of the error indicator, denoted I_i and I_f, were developed; I_i is integer-valued while the other, I_f, is floating-point-valued. These are defined as

$$I_i = \begin{cases} 1, & \text{if } A_2 > A_4 + \varepsilon \\ 0, & \text{otherwise} \end{cases} + \begin{cases} 1, & \text{if } A_4 > A_8 + \varepsilon \\ 0, & \text{otherwise} \end{cases} + \begin{cases} 1, & \text{if } A_2 > A_8 + \varepsilon \\ 0, & \text{otherwise} \end{cases} \tag{5}$$

$$I_f = \log\left(1 + \lfloor\frac{A_2}{A_4 + \varepsilon}\rfloor + \lfloor\frac{A_4}{A_8 + \varepsilon}\rfloor + \lfloor\frac{A_2}{A_8 + \varepsilon}\rfloor\right), \tag{6}$$

where $\lfloor\ldots\rfloor$ is a 'floor' operation, and the values A_2, A_4 and A_8 are defined as

$$A_2 = 2^{-2r}\left|\frac{S_2}{N_e}\right|, \tag{7}$$

$$A_4 = 2^{-r}\left|\frac{2S_4}{N_e}\right|, \tag{8}$$

$$A_8 = \left|\frac{2S_8}{N_e}\right|, \tag{9}$$

which (in the case of a 3D domain) are computed in each direction along N_e^2 lines. The small value ε (set to 10^{-2} in Section 3 and 3×10^{-2} in Section 4) is used to avoid division-by-zero problems in uniform flow conditions. Note that either the maximum or mean of these A values can be taken, thereby generating slightly different variants of I_i and I_f. It was found *a posteriori* that considering the maximum values in each block seems to make the indicators I_i and I_f more sensitive compared to taking the mean values (an operation that likely smears out any under-resolution effects). Therefore, only the maximum values are considered in this paper.

The quantity I_i is an integer in the set {0, 1, 2, 3}, where a value of 3 indicates the worst possible error according to the error indicator, and 0 indicates that no error is present. In contrast, the quantity I_f is a real value bounded below by zero (which indicates that little or no solution error is present). The I_i indicator was devised by partitioning the spectrum decay into 3 spectral amplitude 'pairs' (S_2–S_4, S_4–S_8, S_2–S_8). The ratios of these pairs give a piecewise indication of how the spectrum decays and should satisfy a maximum acceptable deviation/'turn-up' in the spectrum's slope. Any breach of these criteria is penalised accordingly, with a similar approach also being applied to I_f:

$$\left|\frac{S_2}{S_4}\right| \leq 2^r, \tag{10}$$

$$\left|\frac{S_4}{S_8}\right| \leq 2^{r+1}, \tag{11}$$

$$\left|\frac{S_2}{S_8}\right| \leq 2^{2r+1}. \tag{12}$$

Deciding what constitutes an unacceptably high 'turn-up' in the spectrum's slope depends on the specific problem at hand. One of the caveats of the approach is the need to estimate the minimal acceptable slope r of the spectrum. For example, this could be taken to decrease with a slope of r=-5/6 for turbulent dynamics (following Kolmogorov's $k^{-5/3}$ law for the inertial subrange of the spectral energy spectrum), but in practise r will be higher or lower locally; throughout this paper we consider a slope value of $r = -0.5$. If shocks are present, then a slope of -1 (following the k^{-2} law for discontinuities [18]) may be more appropriate. Note also that the slope r may also depend on the behaviour of the solution field/quantity being considered. The typical values mentioned so far correspond to the decay of energy, but it was found *a posteriori* that these values also worked well for vorticity which followed a similar decay pattern. Nevertheless, it is important to remember that the desired slope may vary depending on the chosen quantity and problem.

The current approach is different to error indicators already appearing in the literature. For example, robust indicators that are based on the second derivative (such as the Hessian matrix [19,20]) or interior penalty methods [21] could also be used. However, one potential caveat with second derivative-based methods occurs when the solution has a low second derivative but still shows a 'turn-up' in the Fourier spectrum decay. A flat spectrum without any 'turn-up' in the Fourier amplitude would pass our measure but fail the Hessian measure. Conversely, a steep spectrum with a 'turn-up' would pass the Hessian measure but fail our measure. Moreover, the way our approach analyses solution error mimics the way a user would manually check flow fields for grid-to-grid point oscillations and refine as necessary.

3. Test case: compressible Taylor–Green vortex

A three-dimensional compressible Taylor-Vortex problem (see e.g. [16]) in a periodic cube domain of length 2π was used to evaluate the effectiveness of the error indicator. This considered a fourth-order finite difference solution without additional filtering on computational grids of size $N = 32^3$, 64^3, 128^3 and 256^3. The robustness of the error indicator was improved by considering