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HIGH-RESOLUTION METHODS FOR INCOMPRESSIBLE, COMPRESSIBLE, AND LOW-SPEED VARIABLE DENSITY FLOWS

D. Drikakis†, M. Hahn, S. Patel, E. Shapiro
Fluid Mechanics and Computational Science Group, School of Engineering, Cranfield University, Cranfield, Bedfordshire MK43 0AL, United Kingdom

1 Introduction

The fluid dynamics community has dealt with a number of numerical challenges since the 1950's. These include the development of numerical methods for hyperbolic conservation laws with particular interest in capturing shock wave propagation and related phenomena, solution algorithms for the solution of the incompressible Navier-Stokes equations - a numerical challenge arises here due to the absence of the pressure term from the continuity equation - methods/techniques for the acceleration of the numerical convergence, modelling of turbulence and grid generation techniques. Within each of those areas different numerical approaches have been pursued by various researchers aiming to achieve higher accuracy and efficiency of the numerical solution.

Continuous interest exists in relation to the development of accurate and efficient numerical methods for the computation of instabilities, transition and turbulence. It has been observed for more than a decade that high-resolution methods can be used in (under-resolved) turbulent flow computations without the need to resort to a turbulence model, but this approach has only recently gained some theoretical support and structural explanation for the observed results [3, 15]. Because of this there is a necessary overlap between the classical modelling of turbulence and its computation through high resolution methods [5]. These methods are currently used to simulate a broad variety of complex flows, e.g., flows that are dominated by vorticity leading to turbulence, flows featuring shock waves and turbulence, and the mixing of materials [23]. Such flows are extremely difficult to practically obtain stably and accurately in under-resolved conditions (with respect to grid resolution) using classical linear (both second and higher-order accurate) schemes. Further, new applications at micro-scale, e.g. microfluidics, microreactors and lab-on-a-chip, have raised a number of challenges for computational science methods.

In this paper we provide a brief overview of high-resolution methods in connection with some of the above problems. An extensive description of these methods for incompressible and low-speed flows can be found in [5].

2 Overview of Properties of High-Resolution Methods

We classify as high-resolution methods those with the following properties [11]:

- Provide at least second order of accuracy in smooth areas of the flow.
- Produce numerical solutions (relatively) free from spurious oscillations.
- In the case of discontinuities, the number of grid points in the transition zone containing the shock wave is smaller in comparison with that of first-order monotone methods.

The motivation for the development of high-resolution methods emerges from our effort to circumvent Godunov's theorem [10] that states: *There are no monotone, linear schemes for the linear advection equation of second or higher order of accuracy.* In other words, second-order accuracy and monotonicity are contradictory requirements. The key to circumvent Godunov's theorem lies on the assumption made in the theorem that the schemes are linear. Therefore, if we want to design methods which provide at least second order of accuracy and at the same time avoid spurious oscillations in the vicinity of large gradients, then we need to develop nonlinear methods. The development of high-resolution methods is done in the one-dimensional context due to the lack of adequate theory in multi-dimensions. Even though a numerical scheme can be designed to be second-order accurate for one-dimensional problems its accuracy in multiple dimensions is not guaranteed to be second-order.

To discuss properties of numerical methods it is convenient to consider the hyperbolic conservation law

$$\frac{\partial \mathbf{U}}{\partial t} + \frac{\partial \mathbf{E}(\mathbf{U})}{\partial x} = 0\ . \qquad (1)$$

One can discuss numerical approximations to weak solutions w_i which can be obtained, for example, by $(2k+1)$-point explicit schemes in conservation form, where i denotes cell centered value and $i+1/2$ denotes intercell value.

$$w_i^{n+1} = w_i^n - \frac{\Delta t}{\Delta x}(\tilde{\mathbf{E}}^n_{i+1/2} - \tilde{\mathbf{E}}^n_{i-1/2})\ , \qquad (2)$$

where for the numerical flux $\tilde{\mathbf{E}}$ yields $\tilde{\mathbf{E}}^n_{i+1/2} = \tilde{\mathbf{E}}(w^n_{i-k+1}, ..., w^n_{i+k})$, and n denotes the time level. The numerical flux should also be consistent with the flux $\mathbf{E}$, i.e., $\tilde{\mathbf{E}}(\mathbf{U}, ..., \mathbf{U}) = \mathbf{E}(\mathbf{U})$.

Weak solutions of (1) should satisfy the inequality $\tilde{\mathbf{U}}_t + \mathcal{F}_x \leq 0$ (entropy condition), where $\tilde{\mathbf{U}}$ is a convex function of $\mathbf{U}$, i.e. $\tilde{\mathbf{U}}_{\mathbf{UU}} > 0$, and $\tilde{\mathbf{U}}$ satisfies $\tilde{\mathbf{U}}_{\mathbf{U}}\mathbf{E}_{\mathbf{U}} = \mathcal{F}_{\mathbf{U}}$, where $\mathcal{F}$ is the entropy flux [11]. The solution (2) converges to a weak solution of (1) when the following conditions are satisfied:

1. The total variation of the solution (defined below) with respect to x is uniformly bounded with respect to t, Δt and Δx.
2. The scheme (2) satisfies the entropy condition.

†Corresponding author, d.drikakis@cranfield.ac.uk

3. The entropy condition implies unique solution of the initial value problem.

Conditions 1 and 2 can be satisfied by the addition of artificial viscosity to the numerical scheme. This will possibly provide non-oscillatory solutions at the expense of loss of physical information thus deteriorating the overall computational accuracy.

Below we review some of the basic properties that are considered in the design of high-resolution schemes. The total variation of a function $u(x)$ is defined as

$$\mathrm{TV(u)} = \lim_{\epsilon \to 0} \sup \frac{1}{\epsilon} \int_{-\infty}^{+\infty} |\mathrm{u(x+\epsilon) - u(x)}| \, \mathrm{dx} \ . \quad (3)$$

If $u(x)$ is smooth then (3) can be written

$$\mathrm{TV(u)} = \int_{-\infty}^{+\infty} |\mathrm{u'(x)}| \, \mathrm{dx} \ . \quad (4)$$

If u is a function of space and time, $u(x,t)$, then we define the total variation of u at a fixed time, t. In a discretised domain, u is a function of the mesh and its total variation at a time instant indicated by the index n is defined as

$$\mathrm{TV(u^n) \equiv TV(u(t))} = \sum_{\mathrm{i}=-\infty}^{+\infty} |\mathrm{u^n_{i+1} - u^n_i}| \ . \quad (5)$$

The function u is assumed to be either 0 or constant as the index i approaches infinity, in order to obtain finite total variation.

The monotonicity property is defined for a scalar conservation law as

$$\frac{\partial u}{\partial t} + \frac{\partial f(u)}{\partial x} = \frac{\partial u}{\partial t} + \alpha(u)\frac{\partial u}{\partial x} = 0 \ , \quad (6)$$

where $\alpha(u) = \mathrm{d}f/\mathrm{d}u$, $u(x,0) = \phi(x)$, $-\infty < x < \infty$, and $\phi(x)$ is assumed to be of bounded total variation.

An important property of the weak solution of the scalar initial value problem is the *monotonicity property* according to which:

- No new local extrema in x may be created.
- The value of a local minimum increases, i.e., it is a nondecreasing function [11], and the value of a local maximum decreases, i.e., it is a nonincreasing function [11].

Thus the total variation, TV(u(t)), is a decreasing function of time

$$\mathrm{TV(u(t_2)) \leq TV(u(t_1))} \quad \forall \quad \mathrm{t_2 \geq t_1} \ . \quad (7)$$

The explicit scheme of (2) can also be written in a shorter form as

$$w_i^{n+1} = H(w^n_{i-k}, w^n_{i-k+1}, ..., w^n_{i+k}) = L \cdot w_i^n \ , \quad (8)$$

where L is an operator. We say that the scheme (8) is *total variation nonincreasing* (TVNI) if for all w

$$\mathrm{TV(L \cdot w) \leq TV(w)} \ . \quad (9)$$

The scheme (8) is monotonicity preserving if the finite difference operator L is monotonicity preserving, that is, if w is a monotone mesh function, so is $L \cdot w$. Moreover, the scheme (8) is a monotone scheme if H is a monotone increasing function of each of its $2k+1$ arguments. The hierarchy of these properties can be stated as follows: the set of monotone schemes is contained in the set of TVD schemes and this is in turn contained in the set of monotonicity preserving schemes. Monotone schemes can be constructed as upwind or centered. TVD and Essentially Non-Oscillatory (ENO) [12] schemes can also be designed to be monotone in the one-dimensional context. However, the set of monotone schemes is the smallest set of schemes and is a subset of the set of TVD schemes.

For a constant coefficient $\alpha(u) = \alpha$, we obtain the linear advection equation. Well known schemes such as the Godunov first-order upwind scheme [10] and the Lax-Wendroff scheme [14], among others, can cast in the general form

$$w_i^{n+1} = \sum_{l=-k_L}^{l=k_R} b_l w^n_{i+l} \ , \quad (10)$$

where k_L and k_R are two non-negative integers and b_l are constant coefficients. Harten [11] has shown that the linear finite difference approximation (10) is monotonicity preserving if the coefficients b_l are non-negative, i.e., $b_l \geq 0$, $\quad -k_L \leq l \leq k_R$.
Thus any linear monotonicity preserving scheme is a monotone, first-order, accurate scheme.

3 Instabilities and Bifurcation Phenomena

The study of separated flows through suddenly expanded geometries is a classic yet complex area of research. These type of flows can feature instabilities which may lead to bifurcation. Nonlinear bifurcation phenomena is of great importance when considering hydrodynamic stability and the mechanism of laminar-to-turbulent flow transition. We have considered the problem of flow through a rectangular channel with a suddenly-expanded and suddenly-contracted part and have conducted a computational investigation to examine numerical effects on the prediction of flow instabilities and bifurcation phenomena. Three different high-resolution (Godunov-type) methods [4, 8, 21] in conjunction with first-, second- and third-order accurate interpolation schemes have been employed.

The computational results obtained were compared to the experimental results of [18, 17]. At low Reynolds numbers the flow separates symmetrically. As Reynolds numbers is increased a critical Reynolds number is reached and symmetry breaking bifurcation occurs. For this particular geometry it was found that as Reynolds number was further increased the recirculation regions extended to the full length of the expanded part and a second critical Reynolds number was reached upon which the separation regions became symmetric again. The results obtained revealed that the solution of the flow depended on the numerical method employed.

The effect of the order of interpolation used in the discretisation of the wave-speed dependent term (non-linear dissipation term) and averaged part of the intercell flux, was examined for Reynolds numbers within the critical region of symmetry breaking bifurcation. It was found that computations using first-order discretisation for the calculation of the flux components resulted in symmetric stable flow for all numerical schemes except one (the characteristics-based scheme), whereas second- and third-order discretisation lead to symmetry breaking bifurcation for all schemes. Figures (1)-(3) show the numerical solution using the three different Godunov-type methods for a Reynolds number of 120 using third-order interpolation accuracy. It is clear to see that the three different methods give different solutions. The difference between the Rusanov scheme [21] and the HLLE scheme [8] lies in the way the wave-speed dependent term is calculated. The Rusanov scheme employs the definition given by [2] and only considers the maximum wave speed and hence cannot recognise the slowest moving acoustic waves thus causing a larger amount of dissipation. It should be noted that the wave speed dependent term encompasses information about the eigenstructure of the system of equations and is also responsible to adapt the discretisation according to the local solution data.

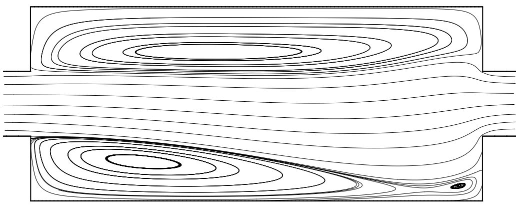

Figure 1: Re=120 Characteristics-based scheme in conjunction with third-order interpolation accuracy.

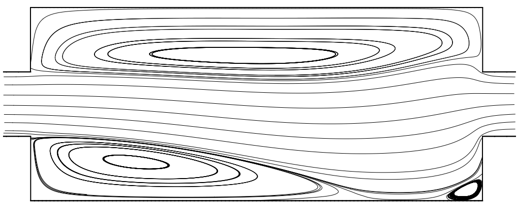

Figure 2: Re=120 Rusanov's scheme in conjunction with third-order interpolation accuracy.

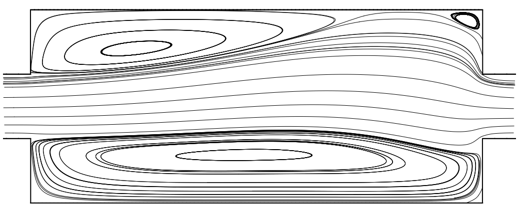

Figure 3: Re=120 HLLE scheme in conjunction with third-order interpolation accuracy.

Comparing the computational results obtained to the experimental results of [18] (see table 1 below), show that the characteristics-based scheme is the most accurate of the three numerical schemes employed. Also its ability to predict symmetry breaking bifurcation even when using first-order interpolation accuracy is something that neither of the other two schemes could predict. The present results show how important it is to further understand the properties and numerical behaviour of computational methods, especially in relation to instabilities and flow transition.

Table 1: Comparison of solutions with previously published experimental results [18] for symmetric (S) and asymmetric (A) cases.

Re	Exp	CB	Rusanov	HLLE.
80 (S)	Bubble size =0.0278m	Bubble size =0.028m	Bubble size =0.0265m	Bubble size =0.027m
116 (A)	Δx =0.019m	Δx =0.02m	Δx =0.0215m	Δx =0.021m

4 Compressible Flows

Previous computations for turbulent flows have suggested that high-resolution schemes appear to achieve many of the properties of sub-grid models used in LES, e.g. [3, 9, 16, 19, 23]. The idea to use these methods as an implicit way to numerically model turbulent flows is referred to as MILES or Implicit Large Eddy Simulation (ILES). We have employed three high-resolution schemes for solving the compressible Euler and Navier-Stokes equations in the context of ILES:

- Flux Vector Splitting Scheme (FVS) [25]: This is a modified Steger-Warming FVS scheme.
- Godunov-type characteristic flux averaging scheme (Godunov-type) [7]: The scheme provides third-order of accuracy in smooth flow regions and second-order of accuracy in discontinuities.
- Hybrid total variation diminishing (TVD) scheme [25]: It combines the Godunov-type characteristic flux averaging and FVS schemes through a flux limiting approach.

The following examples investigate under-resolved simulations of decaying turbulence in a triply periodic cube and compressible flow around open cavities, both for low and high Reynolds numbers, at transonic and supersonic speeds.

4.1 Decaying turbulence

ILES of homogeneous decaying turbulence – a generic problem in turbulence studies [13, 16, 23] – has been carried out in a three-dimensional cube applying periodic boundary conditions in each spatial direction. The compressible Euler equations have been employed on uniformly spaced grids of three different resolutions 32^3, 64^3, and 128^3 with initial conditions similar to [13] (corresponding, in the present simulations, to a reference Mach number $M = 0.1$). The analysis of the computational results has been performed by transforming the kinetic energy into Fourier space via a power spectrum estimation.

A comparison of the energy spectra (ES) using different high-resolution schemes on the 128^3 grid is presented in Figure 4. At high wave numbers the slope of the energy spectra obtained by the Godunov-type scheme is closer to Kolmogorov's $k^{-5/3}$ slope for a broader range of wave numbers compared to the FVS and hybrid TVD schemes. This can be explained by the more dissipative nature of these schemes (the FVS contribution to the hybrid flux accounts for 40% of the total flux value). In the aforementioned cases, the high-resolution schemes produce plausible solutions without resorting to explicit addition of dissipation (e.g., through subgrid scale modelling).

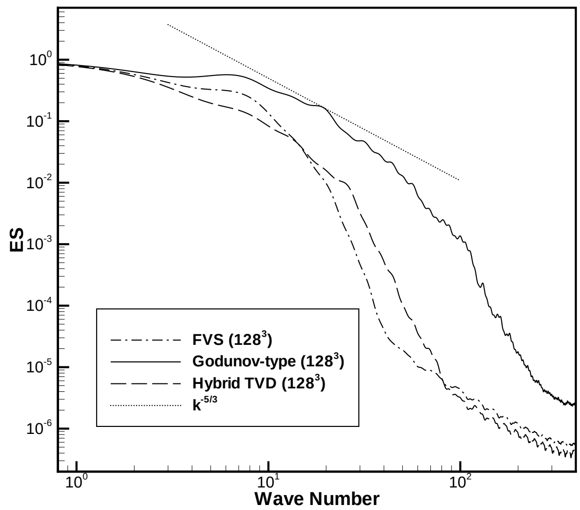

Figure 4: Results for decaying turbulence using different high-resolution schemes on a 128^3 grid.

4.2 Open cavity

Results from the implementation of high-resolution methods in wall-bounded flows [3, 9] show that in principle there is nothing that prevents the use of these methods in near wall flows even without using an explicit turbulence model. Compressible, turbulent flow past an open cavity encompasses a variety of flow phenomena including large and small vortical structures, free shear layers, transitional flow, flow separation and flow re-laminarisation, shock and rarefaction waves. DNS studies with a grid resolution 15 times finer than the present ILES were performed in [20] at low Reynolds numbers to investigate the resonant instabilities in the flow past an open rectangular cavity.‡ Cavity resonance arises from a pressure feedback loop including shear layer instability, separation at the leading edge, vortical structures, noise radiation at the trailing edge and re-attachment, see Figure 5. Further, experimental (and computational) results for cavity flows at high Reynolds numbers and supersonic speeds have been presented in [24].

Table 2 shows results for the Strouhal number as predicted by ILES, DNS of [20] for transonic flows (at low Reynolds numbers) and experimental data of [24] for supersonic flow at high Reynolds number. The comparison of dominant frequencies shows the applicability of ILES for open cavity flows. Simulations for the transonic cases using a SGS (Smagorinsky-type) model have shown no further improvement of the results.

‡The Reynolds number is $Re = 2,500$ based on the cavity depth and free stream velocity, which is equivalent to $Re = 56.8$ based on the momentum thickness at the cavity's leading edge.

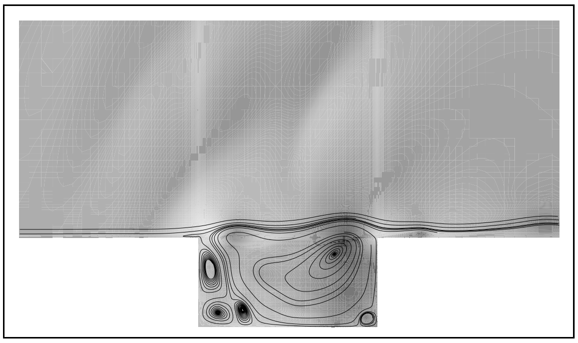

Figure 5: Iso-density contours and streamlines for the transonic cavity flow at $M_\infty = 0.8$ and $Re = 1.813 \times 10^5$.

Table 2: Strouhal number comparisons of ILES with DNS [20] and experimental data [24]. The Re number is based on the cavity's depth and free stream velocity.

Ma	Re	ILES	DNS	Exp.
0.5	2.5×10^3	0.730	0.74	
0.6	2.5×10^3	0.683	0.70	
0.8	2.5×10^3	0.635	0.65	
1.5	4.5×10^5	0.197		0.208

5 Variable Density Incompressible Flows

Variable density incompressible flows are encountered in many practical applications in mechanical, biomedical and chemical industries. Here, we are particularly interested in the application of high-resolution methods in microreactors and microfluidics. This field is rapidly progressing due to factors such as the elimination of scale-up procedures, higher precision of mixing and component contact surfaces, and minimization of processing hazards. The system of equations comprises the Navier-Stokes equations and chemical reaction equations for N species. Although the flow in microdevices remains laminar, computational challenges arise from the stiffness of the numerical solution associated with the different time scales of chemical reaction and fluid flow equations. The vast majority of mixing devices rely on diffusion, which occurs between fluid layers. Due to the laminar flow, large contact surfaces between components and small microdevice dimensions induce small diffusional paths. These short paths reduce the time, with demonstrated speeds in the range of a few milliseconds to as fast as few microseconds.

In relation to the solution of variable density flow through micro reactors, we have employed the artificial compressibility approach [1] combined with a characteristics-based Godunov-type scheme of [4], which has been extended to handle variable density flows [22]. An example of a diffusion broadening study is shown in Figure 6. Currently, the extension of the aforementioned high-resolution methods in the context of multiscale modelling ranging from macro- to nanoscales is pursued by the research group.

Figure 6: Computation of diffusion broadening in a microchannel using the characteristics-based Godunov-type scheme [4, 22].

6 Conclusions

The desire for understanding better the physics encompassed by numerical methods, high-resolution methods in particular, is motivated by the fact that almost all practical computations in engineering are under-resolved. Numerical aspects play an important role in the prediction of instabilities, transition and turbulence in terms of both accuracy and efficiency. Further, emerging fields in science such as nanotechnology pose new challenges in the development of numerical methods.

Numerical methods encompass numerical dissipation which acts to regularize the flow, thereby allowing shock propagation to be captured physically realistically even if it is not fully resolved on the computational mesh. One develops numerical schemes with two competing criteria in mind: a desire for high accuracy coupled with protections against catastrophic failure due to nonlinear wave steepening or unresolved features. Nonlinear mechanisms (limiters) in high-resolution methods guard the methods from such catastrophic failures by triggering entropy producing mechanisms that safeguard the calculation when the need arises. The two key questions are: (i) what criteria should be used to design the nonlinear mechanism that triggers the entropy production, and (ii) to what extent numerical dissipation accounts for turbulent flow effects.

The theory of numerical methods for hyperbolic conservation laws has made significant progress in one-space dimension. However, we need to further understand the nonlinear behaviour of numerical methods in multi-dimensional problems. This nonlinear behaviour is also closely related to the numerical mechanisms underlying the formation of spurious solutions in under-resolved flows. Previous studies [6] seem to indicate that the generation of spurious vortices in under-resolved simulations depends solely on the advective scheme. In particular, it depends strongly on how the numerical dissipation is partitioned between different terms of the advective scheme. Although one can succeed to regain control over deficient (spurious-wise) schemes [6] by modifying the dissipative terms of the schemes the exact numerical mechanism is not yet understood. In particular, the question "why certain schemes evince spurious solutions while others do not" still eludes a scholastic answer. In [6] it was shown that for an idealized finite-difference scheme the definition of the advective velocities in the primitive variable formulation of the equations can induce a truncation error vorticity source. However, a rigorous vorticity analysis of nonlinear approximations such as high-order Godunov-type schemes appears very difficult.

The success of high-resolution methods to compute turbulent flows as well as the issue of spurious solutions in under-resolved flows seem to depend on a delicate balance of truncation errors due to wave-speed-dependent terms (chiefly responsible for numerical dissipation) in the case of Godunov-type fluxes and hyperbolic part of the flux. It is the essence of this balance that needs to be understood.

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