Facilitating the Adoption of Unstructured High-Order Methods Amongst a Wider Community of Fluid Dynamicists

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Abstract. Theoretical studies and numerical experiments suggest that unstructured high-order methods can provide solutions to otherwise intractable fluid flow problems within complex geometries. However, it remains the case that existing high-order schemes are generally less robust and more complex to implement than their low-order counterparts. These issues, in conjunction with difficulties generating high-order meshes, have limited the adoption of high-order techniques in both academia (where the use of low-order schemes remains widespread) and industry (where the use of low-order schemes is ubiquitous). In this short review, issues that have hitherto prevented the use of high-order methods amongst a non-specialist community are identified, and current efforts to overcome these issues are discussed. Attention is focused on four areas, namely the generation of unstructured high-order meshes, the development of simple and efficient time integration schemes, the development of robust and accurate shock capturing algorithms, and finally the development of high-order methods that are intuitive and simple to implement. With regards to this final area, particular attention is focused on the recently proposed flux reconstruction approach, which allows various well known high-order schemes (such as nodal discontinuous Galerkin methods and spectral difference methods) to be cast within a single unifying framework. It should be noted that due to the experience of the authors the review is directed somewhat towards aerodynamic applications and compressible flow. However, many of the discussions have a wider applicability. Moreover, the tone of the review is intended to be generally accessible, such that an extended scientific community can gain insight into factors currently pacing the adoption of unstructured high-order methods.

Key words: high-order, unstructured, mesh generation, time integration, shock capturing

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1. Introduction

Fluid flow problems can be solved numerically using a wide variety of techniques, typically involving the independent discretization of space and time. The discretization of space is often achieved using either:

- A finite difference (FD) method [122], in which the differential form of the governing system is discretized.
- A finite volume (FV) method [77], in which the computational domain is decomposed into cells, and an integral form of the governing system is satisfied within each cell.
- A finite element (FE) method [149], in which the computational domain is decomposed into elements, and a polynomial representation of the solution is required to satisfy a variational form of the governing system within each element.

Throughout the last 50 years numerous implementations of the aforementioned methods have been developed. Typically, such implementations offer at best second-order accuracy in space. For the purposes of this article such schemes will be referred to as low-order. Low-order schemes are on the whole intuitive, geometrically flexible and, due to considerable effort on the part of their original developers, robust and suitably accurate (for many flow problems). In particular a major achievement of the period from 1970 to 1990 was the identification of so called high-resolution shock capturing schemes which are non-oscillatory, whilst also maintaining second-order accuracy almost everywhere except in the vicinity of extrema [46, 47, 66, 130, 131, 132, 133, 134].

As a result of their favorable properties, the use of low-order schemes has become widespread in both academia and industry, and they form the basis of all commercially available fluid flow solvers. However, despite these successes, there exists a range of important flow problems (requiring very low numerical dissipation) for which they are not well suited. These include vortex

dominated flows (*e.g.* flow around rotor-craft blades or flapping wings), as well as problems in aeroacoustics. When solving such problems it may be advantageous to use a high-order spatial discretization (defined in this article as a scheme that is greater than second-order accurate in space). Compared with low-order schemes, high-order methods theoretically offer increased accuracy for a comparable computational cost. Classical spectral methods [12] are one such example of a high-order spatial discretization. These methods involve decomposing the solution into modes (in frequency space), which are defined globally within the domain of interest. Such decomposition is often referred to as a *p-type* discretization, and increasing the number of modes is often referred to as *p-type* refinement. Spectral methods, however, lack the geometrical flexibility of low order FV and FE schemes, since it is often impossible to define continuous global modes within a complex geometry. As such their use is limited. To overcome these limitations a range of so called unstructured high-order methods have been developed which can, theoretically, extend the accuracy of spectral methods to unstructured meshes.

Although unstructured high-order methods potentially offer significant advantages, their use in academia remains limited, and they are used even less (if at all) in industry. There are various reasons for this situation. These include a lack of robust high-order mesh generation software, a lack of simple and efficient time integration schemes tailored specifically for high-order spatial discretizations, a lack of robust and accurate shock capturing algorithms, and finally the complexity (at various levels) of unstructured high-order methods. In this article the aforementioned issues will be discussed, and recent efforts to address the issues will be reviewed. It should be noted that due to the experience of the authors, the review is directed somewhat towards aerodynamic applications and compressible flow. However, many of the discussions have a wider applicability.

The article begins by giving a brief overview of existing unstructured high-order schemes. Barriers to the adoption of unstructured high-order discretizations are then detailed, and efforts to overcome these barriers are reviewed. Finally, simulation results illustrating the potential benefits of unstructured high-order methods are presented, and conclusions are drawn.

2. Existing Unstructured High-Order Methods

2.1. Overview

The objective of unstructured high-order methods is to combine the geometrical flexibility of low-order FV or FE schemes with the superior convergence properties of high-order spectral methods (which cannot be used in complex geometries). Various methods have been developed to achieve this objective. Broadly speaking such methods can be classified as either high-order FV schemes or high-order FE schemes (also referred to as spectral/hp element methods, spectral element methods, or *p-type* methods). However, it should be noted that some newer methods do not (naturally at least) sit in either of these categories.

The most popular high-order FV schemes include *k*-exact methods, FV type essentially non-oscillatory (ENO) methods, and FV type weighted ENO (WENO) methods. The most popular high-order FE methods include high-order continuous Galerkin (CG) methods and high-order dis-

continuous Galerkin (DG) methods. Other more recently developed schemes include spectral volume (SV) methods, which adapt ideas from both k-exact and DG methods, and spectral difference (SD) methods which are similar to DG methods, but based on the governing system in its differential form.

A recent and comprehensive review of all aforementioned methods has been presented by Wang [139]. Also various relevant textbooks are available, including those by Barth and Deconinck [6] and Deville, Fischer, and Mund [29], both of which present a general overview of high-order methods, as well as the textbook by Karniadakis and Sherwin [72], which is primarily focused on high-order FE methods, and the textbooks by Cockburn, Karniadakis, and Shu [18], and Hesthaven and Warburton [51], which focus on DG methods. Given the existence of this literature, a detailed review of various unstructured high-order schemes is omitted from this article. Instead, only a brief overview outlining the essence of each aforementioned scheme is presented.

2.2. High-Order Finite Volume Methods

2.2.1. k-Exact Methods

High-order k-exact methods were first developed by Barth and Frederickson [7]. They can be considered a direct extension of low-order Godunov type FV methods, which solve an integral form of the governing equation within each cell of the computational domain. As such, k-exact schemes hold only solution averages within each cell. Their high-order nature is achieved by constructing a polynomial representation of the solution within each cell of the domain (based on the average solutions within some stencil of surrounding cells). Cell-wise discontinuities between these representations are then used as the input for Riemann solvers at each cell interface. Typically, Riemann problems are solved at some judicious distribution of quadrature points on each cell interface such that accurate numerical integration of the total interface flux can be achieved. Note that such high-order integration of the flux is critical if one is to retain high-order accuracy. Once obtained, the integrated fluxes for each cell face are used to update the cell averaged solutions in time. Note that since the extension to high-order is achieved via an expanded stencil, the schemes are in general not spatially compact. Also note that by definition, a k-exact scheme of degree k will reconstruct the true solution exactly if it is a polynomial of degree k. For examples of how k-exact methods have been applied on unstructured meshes see Barth and Frederickson [7], and Delanaye and Liu [28].

2.2.2. Essentially Non-Oscillatory Methods

FV type ENO methods were first introduced by Harten *et al.* [47], and have been successfully adapted to unstructured grids by various authors including Abgrall [1] and Ollivier-Gooch [95]. Unstructured FV type ENO methods are similar to unstructured high-order k-exact methods. However, ENO schemes associate more than one local polynomial representation of the solution with each cell (by using a range of stencils). The smoothest of the resulting polynomials is then selected and used, in conjunction with the smoothest polynomials from each adjacent cell, to obtain interface fluxes (as in a k-exact scheme) which are then used to update the cell averaged solutions

in time. The purpose of choosing the smoothest reconstruction (identified by some metric such as a norm of the gradient) is to avoid, if possible, using reconstructions that span a discontinuity. Like k -exact methods, the use of an expanded stencil means that ENO schemes are in general not spatially compact. Also, it can be noted that whilst possible, the extension of such schemes to fully unstructured meshes in three-dimensions (3D) is complex and often computationally expensive. For further details of these methods see the textbook by Barth and Deconinck [6].

2.2.3. Weighted Essentially Non-Oscillatory Methods

FV type WENO methods were first introduced by Liu *et al.* [82], and have been successfully adapted to unstructured grids by various authors including Friedrich [38] and Hu and Shu [52]. Unstructured FV type WENO methods are similar to unstructured FV type ENO methods. However, instead of calculating boundary fluxes based on the smoothest of the reconstructed solutions, a weighted average of several reconstructed solutions is used instead. Once again, as for k -exact and ENO methods, the use of an expanded stencil means that WENO schemes are in general not spatially compact. Also, it can be noted that whilst possible, the extension of such schemes to fully unstructured meshes in 3D is complex and often computationally expensive. For further details of these methods see the textbook by Barth and Deconinck [6].

2.3. High-Order Finite Element Methods

2.3.1. Continuous Galerkin Methods

High-order CG methods are a natural extension of low-order CG FE schemes that utilize a high-order polynomial expansion within each element. As such they involve solving a variational form of the governing equation, and elemental coupling is achieved by enforcing that the approximate solution is C_0 continuous. The polynomial basis used to represent the solution within each element is often classified as either modal or nodal. A modal basis is hierarchical in nature *i.e.* in one-dimension (1D) a modal basis of order $k + 1$ contains all functions from a similar basis of order k plus one new polynomial of degree $k + 1$. Legendre polynomials, for example, can be used to form a modal basis in 1D. A nodal basis is not hierarchical in nature *i.e.* in 1D a nodal basis of order $k + 1$ in general contains no basis functions from a similar basis of order k . Lagrange polynomials, defined by a set of nodal points, can be used to form a nodal basis in 1D. It can be noted that unstructured high-order CG methods are compact in nature, since the polynomial expansions are contained within individual elements (*c.f.* high-order FV schemes, in which an expanded stencil of surrounding elements is required to achieve high-order). It can also be noted that the requirement of C_0 solution continuity explicitly couples all elements of the domain together. This results in a global system having to be solved at each time-step. Various strategies (such as the use of basis sets with a distinct boundary-interior decomposition) have been developed to minimize inter-element coupling, and hence make this process as efficient as possible.

Numerous variants of the CG approach exist. A full discussion of all variants is beyond the scope of this review. However, a particular class, referred to as streamline upwind Petrov Galerkin (SUPG) methods, deserve a specific mention due to their popularity. Such schemes, which were

first developed by Hughes *et al.* [53, 54, 57, 56] and Brooks and Hughes [11], are designed specifically to suppress oscillations (and hence maintain stability) when modeling convection dominated flows using a CG approach. For further details of high-order CG methods see articles by Sherwin and Karniadakis [117], Sherwin, Warburton and Karniadakis [119], and Sherwin and Ainsworth [116], in addition to the textbook by Karniadakis and Sherwin [72].

2.3.2. Discontinuous Galerkin Methods

High-order DG methods, which were first proposed by Reed and Hill in 1973 [111] to solve the neutron transport equation, are perhaps the most widely used type of unstructured high-order scheme for computational fluid dynamics applications. In many regards high-order DG schemes are similar to high-order CG schemes, since they entail solving a variational form of the governing equation, and a high-order polynomial approximation is utilized within each element of the domain. Also, it can be noted that like CG schemes (and for the same reasons), DG schemes are compact in nature. However, as the name suggests, DG methods do not require the approximate solution to be piecewise continuous between elements. Instead, elements are coupled via the calculation of common interface fluxes (obtained using a Riemann solver, for example).

Numerous variants of the DG approach exist. A full discussion of all variants is beyond the scope of this review. However, it can be noted that many have been specifically developed to treat elliptic viscous terms [3]. Of these, so called local DG (LDG) methods, originally proposed by Cockburn and Shu [21], are perhaps the most popular. LDG schemes are formulated by casting the second-order viscous system in terms of two first order systems, via the introduction of an additional variable. This additional variable can in fact be eliminated by judicious choice of inter-element fluxes. However, the resulting scheme is no longer compact in nature for 2D and 3D problems. To address this issue so called compact DG schemes have been developed by Peraire and Persson [100]. These schemes are similar to LDG schemes (in fact they are identical in 1D). However in 2D and 3D they retain a favorable compact stencil. Other popular DG type schemes for treating viscous terms include the interior penalty method [32] and the Bassi-Rebay-2 method [8]. Both of these approaches treat the second order viscous term directly, and are compact in nature for 2D and 3D problems. Finally, it is pertinent to highlight a relatively new class of so called hybridized DG (HDG) methods, which were recently proposed by Cockburn, Gopalakrishnan, and Lazarov [16], and developed further by Nguyen, Peraire and Cockburn [92, 93, 94] amongst others. HDG schemes are advantageous when an implicit temporal discretization is employed, since they result in a globally coupled system with a (relatively) low number of degrees of freedom (DOF). Specifically the global DOF are defined only at element interfaces (and moreover, the global DOF are single valued at element interfaces).

For more information about DG schemes see the textbook by Cockburn, Karniadakis, and Shu [18], and the textbook by Hesthaven and Warburton [51].

2.4. Other Methods

2.4.1. Spectral Volume Methods

SV methods, which were first proposed by Wang *et al.* [138, 141, 142, 143], adapt ideas from both DG methods and high-order k-exact schemes. To implement a SV method the computational domain is decomposed into elements (referred to as spectral volumes) and each spectral volume is further sub-divided into what are essentially standard FV sub-cells (referred to as control volumes). Solution averages stored within each control volume are then used to reconstruct a high-order polynomial representation of the solution within each spectral volume. Like in the DG method, this reconstructed solution is in general discontinuous between adjacent spectral volumes. Fluxes across control volume interfaces (internal to each spectral volume) are then calculated analytically using the reconstructed solution polynomial, and fluxes across spectral volume interfaces are obtained via a numerical flux function, such as a Riemann solver, that utilizes the solution on either side of the interface. Once all interface fluxes have been obtained, the control volume averages can be updated in time via a suitable temporal discretization. Like CG and DG schemes (and for the same reasons), SV schemes are compact in nature.

2.4.2. Spectral Difference Methods

The foundation for SD schemes was first put forward by Kopriva and Kolas [76] in 1996 under the name of “staggered grid Chebyshev multidomain” methods. However, several years later in 2006 Liu, Vinokur and Wang [83] presented a more general formulation for both triangular and quadrilateral elements, which they termed the SD method (a name which has been retained to the present). The methods are similar to DG schemes that employ nodal basis functions (so called nodal DG schemes). However, SD methods are based on the governing system in its differential form. Specifically, interlocking sets of so called solution points and flux points are defined within each element of the computational domain (with some number of flux points located on element boundaries). Values of the solution are stored at each solution point, and used to construct an element-wise discontinuous polynomial representation of the solution via Lagrange interpolation within each element. This representation of the solution is then evaluated at each flux point. Flux values at internal flux points are then obtained directly from these solution values, and flux values at the boundary flux points are obtained using an interface flux formula, such as a Riemann solver (that takes solution values from both elements sharing the interface). Lagrange interpolation is then once again employed, this time to reconstruct a polynomial representation of the flux (from flux values at the flux points) that is one degree higher than the solution polynomial. The divergence of this flux is then evaluated at the solution points, and used to update the solution values in time via a suitable temporal discretization. Like CG and DG schemes (and for the same reasons), SD schemes are compact in nature. The intuitive nature of these methods, their apparent efficiency, and the presentation of formalized stability analysis by Van den Abeele, Lacor and Wang [129], and Jameson [63], has made SD schemes increasingly popular in recent years. For examples of their use see Liang, Jameson and Wang [79] and Ou *et al.* [98].

3. Facilitating the Adoption of Unstructured High-Order Methods

3.1. Overview

In the following section four major issues that have hitherto inhibited the widespread adoption of unstructured high-order methods are identified and discussed. Specifically, these issues are:

- A lack of robust high-order mesh generation software.
- A lack of simple time-integration schemes that work efficiently with high-order spatial discretizations.
- A lack of robust and accurate shock capturing algorithms.
- The overall complexity (at various levels) of unstructured high-order spatial discretizations.

Recent efforts to address the aforesaid issues are reviewed, and directions for future research are suggested.

3.2. Mesh Generation

3.2.1. Overview

Compact unstructured high-order methods, such as high-order FE methods, as well as SV and SD methods, hold multiple DOF per element. As a consequence, meshes for use with compact high-order schemes are typically far coarser than those for use with low-order schemes (for an equivalent total number of DOF). The requirement of relatively large elements, and the existence of multiple DOF per element, leads to various issues when generating suitable computational meshes. In particular:

- To ensure that a coarse mesh can conform to (or at least reasonably approximate) complex boundaries one may need to use elements with curved surfaces.
- Optimally distributing degrees of freedom throughout the mesh is no longer a trivial task. In some regions it may be better to have a coarse mesh of large elements that contain very high-order polynomials, whereas in other regions it may be better to have a fine mesh of small elements that contain relatively low-order polynomials. One must consider an optimal distribution of both element sizes and polynomial orders when generating the mesh.

The complexity of these issues, and a lack of any specifically tailored commercial or open-source software, can lead to severe difficulties generating suitable meshes, especially in 3D. As a result, when using a compact unstructured high-order method to simulate flow within the vicinity of a complex 3D geometry, the process of mesh generation is often a significant bottleneck.

In the following sections several aspects of unstructured high-order mesh generation are detailed. To begin, practical strategies for generating meshes with curved surface elements are discussed. Following this review, efforts to avoid generation of invalid elements are presented. Finally an overview of so called isogeometric approaches is given.

3.2.2. Practical Strategies for Generating Meshes with Curved Surface Elements

In order to generate a coarse high-order curved element volume mesh, one must start with an initial surface definition. Such a definition may take several forms. For example, if obtained from a computer aided design (CAD) package, it will likely be cast in terms of non-uniform rational B-splines (NURBS). However, if obtained by other means, such as via segmentation of medical image data, then it may take the form of a fine linear surface triangulation. It has been shown by various authors [9][40] that creating a coarse high-order curved element mesh that conforms to, or at least reasonably approximates, the true surface definition is important in terms of flow solution accuracy when using a compact unstructured high-order spatial discretization. Dey [30] suggests two practical routes by which such a coarse curved element mesh can be obtained. The first involves directly meshing the original surface definition with coarse triangles or quadrilaterals that have been curved (in some fashion) such that they conform to, or at least approximate, the surface. From this curved element surface mesh, a volume mesh is then generated that respects the curved nature of the surface faces. Dey refers to this approach as a ‘direct approach’ [30].

The second approach suggested by Dey involves initially constructing a coarse flat sided volume mesh, with nodes located on the initial curved surface definition. External faces of this mesh are then curved (in some fashion) to conform to, or at least approximate, the surface definition. Dey refers to this approach as an ‘*a posteriori* approach’ [30]. The major advantage of this method is that during the first stage of the process one can directly leverage existing low-order mesh generation technology, which is well developed and robust. Unfortunately, however, the approach is likely to result in the generation of so called invalid elements that are self intersecting, or have tangent faces. This is because when the initial flat sided volume mesh was generated, no information was provided as to how the surface elements would be deformed *a posteriori*. Fig. 1 from the study of Sherwin and Peiró [118] shows four stages of an *a posteriori* meshing approach. Specifically, Fig. 1(a) shows contours of an arterial surface definition (extracted from a medical image data set). Fig. 1(b) shows a surface definition, defined in terms of spline patches, that is based on the contours depicted in Fig. 1(a). Fig. 1(c) shows a coarse linear flat sided mesh, with mesh nodes located on the curved surface depicted in Fig. 1(b). Finally, Fig. 1(d) shows the mesh obtained when the surface faces depicted in Fig. 1(c) are curved to approximate the surface definition depicted in Fig. 1(b). Although not visible in the images, invalid elements have been generated as a result of the *a posteriori* meshing approach.

Figure 1: Illustration of stages in an *a posteriori* meshing approach from the study of Sherwin and Peiró [118]. Contours of an arterial surface definition (extracted from a medical image data set) are shown in (a). A surface definition, based on the contours depicted in (a), and defined in terms of spline patches, is shown in (b). A coarse linear flat sided mesh, with mesh nodes located on the curved surface, is shown in (c). The final mesh is shown in (d). Faces of surface elements in (c) have been curved to approximate the surface definition in (b). Although not visible in the images, invalid elements have been generated as a result of the *a posteriori* meshing approach. Image courtesy of S. J. Sherwin and J. Peiró. Copyright John Wiley and Sons [118].

3.2.3. Efforts to Avoid Invalid Elements

Various studies have investigated ways of avoiding invalid elements when using an *a posteriori* meshing approach. In particular, Sherwin and Peiró discuss three methods [118]. The first is to optimize the way in which the flat sided elements are deformed to the curved surface, the second is to use prismatic elements on the surface of the volume mesh, and the third is to refine the linear mesh (based on surface curvature) such that when curved, no invalid elements are generated. Persson and Peraire [104] have also outlined an interesting approach to avoid invalid elements. Specifically, they suggest modeling the linear flat sided coarse mesh as a non-linearly elastic solid. The idea is that when faces of the coarse mesh are deformed (to approximate the underlying geometry) other elements in the mesh will also deform in such a fashion that no invalid elements are generated (if possible). Fig. 2 from the study of Persson and Peraire [104] shows images of a coarse linear flat sided mesh before and after deformation onto an underlying curved surface. It can be noted that no invalid elements are generated when the mesh is distorted.

Figure 2: Images illustrating the curved mesh generation approach of Persson and Peraire [104]. The linear flat sided coarse mesh is shown in (a), along with the true surface definition (blue line). The resulting curved element mesh is shown in (b). Note that interior as well as exterior faces have been deformed in order to avoid generation of invalid elements. Images courtesy of P. Persson. Copyright P. Persson and J. Peraire [104].

Finally, the approach adopted in Gmsh [42] (an open source mesh generation package) should be highlighted. Gmsh utilizes an *a posteriori* approach to generate (up to) fifth-order curved element meshes (making no direct efforts to avoid generation of invalid elements). However, once the mesh has been created the quality/validity of all elements is checked. Low quality elements are then enhanced, and invalid elements are corrected (if possible).

To conclude discussions it is pertinent to note that, despite all the efforts outlined above, generation of some invalid elements is often unavoidable when an *a posteriori* meshing approach is employed. Usually, the only practical option is to remove or modify such elements by hand.

3.2.4. Isogeometric Approaches

In general, curved mesh elements may only approximate the initial surface definition. However, in an isogeometric approach the mesh elements must conform exactly to the initial surface *i.e.* there is only one true geometry that is respected at all times. In practice this implies using NURBS to define the curved element faces, since any underlying CAD geometry is most likely represented with NURBS. A interesting isogeometric approach, referred to as the NURBS enhanced FE method (NEFEM) has recently been proposed by Sevilla, Fernández-Méndez, and Huerta [115][114]. The NEFEM uses NURBS to define curved boundary faces such that they can conform exactly to a CAD definition, and NURBS to enhance the solution basis functions within each *curved element*. However, within each flat sided element (internal to the domain) a standard FE basis is employed. The efficiency of the standard FE approach is, therefore, preserved within the majority of the domain.

A holistic isogeometric approach, known as isogeometric analysis, has recently been developed by Hughes [55, 27]. Isogeometric analysis employs NURBS to define the shape of element faces, and as the basis functions (used to represent the solution) within each element. The aim of

isogeometric analysis is to fully integrate the processes of surface definition, volume mesh generation, and flow calculation within a single all-encompassing framework, removing the bottleneck between geometric definition and flow solution. To date most applications of isogeometric analysis have been in the field of solid mechanics. However, more recently, various fluid flow problems have also been studied [146].

3.2.5. Summary

There have been various attempts to advance high-order mesh generation technology. However, despite these efforts, an integrated solution capable of robustly creating optimal curved element meshes in 3D does not exist. Development of such a meshing tool, that can be used by a non-specialist, is absolutely essential if compact unstructured high-order schemes such as DG, SV and SD methods are ever to become popular within a wider fluid dynamics community.

3.3. Time Integration

3.3.1. Overview

When solving time-dependent problems one can choose to employ either an explicit or implicit time integration scheme. Explicit schemes such as multi-stage Runge-Kutta (RK) methods are simple to implement, have low memory requirements, and offer arbitrarily high orders of temporal accuracy. Well known variants include the four stage fourth-order RK scheme popularized by Jameson [66], or one of the so called strong stability preserving RK schemes originally developed by Shu [120] and Shu and Osher [121], and generalized by Gottlieb, Shu and Tadmor [43]. Unfortunately, however, when using an explicit time integration scheme the time-step size is limited by a stability constraint, termed the Courant-Friedrichs-Lewy (CFL) limit, which is often more restrictive than any limit imposed by temporal accuracy requirements. When using an implicit time integration scheme no such stability constraint exists. Instead, for time-dependent problems the step size is limited by accuracy requirements. As a result one can typically take far larger time-steps with an implicit scheme. However, the cost of an implicit time-step is far greater than the cost of an explicit time-step. In fact, one has to effectively solve a modified form of the steady-state problem at each implicit time-step (with the notable consequence that a prerequisite of an efficient time-accurate implicit scheme is an efficient steady-state solver). Also, memory requirements are often far higher for implicit schemes, and they can be significantly more complex to implement. As a result, despite the lack of a stability limit, it is not obvious that implicit schemes are more efficient than explicit ones, especially when a low-order spatial discretization is employed.

When solving steady state problems one can again choose to use either an explicit or implicit time integration scheme, potentially in conjunction with a convergence acceleration procedure such as local time-stepping, residual averaging [64] or a multigrid method [62, 67, 14, 2]. When integrating explicitly, since time accuracy is no-longer an issue, one is able to use a low-accuracy high-CFL limit scheme, such as one of the multi-stage methods developed by Jameson [62]. These schemes, which do not fall within the RK framework, are specifically designed using Fourier analysis to have a large CFL limit and provide significant damping of high-frequency errors (a

property that is crucial if they are to be used with a multigrid approach, as will be discussed shortly). Similarly, when using an implicit scheme, since time accuracy is no longer important, one is free to choose time-steps in a fashion that expedites relaxation to steady state, without any regard for whether the scheme approaches steady state in a physical manner.

The majority of research into high-order methods has focused on spatial discretization techniques. It is only recently that significant attention has turned to the critical issue of how one should efficiently integrate the schemes in time (either in a time accurate fashion, or to obtain a steady state solution). This topic is discussed in some detail within the general review article of Wang [139]. More recently, reviews specifically on this topic by Iacono and May [60] and Iacono, May and Wang [61] have been presented, along with a book chapter by May and Jameson [90]. Based on this literature, it is apparent that two major issues are inhibiting the efficient temporal integration of unstructured high-order spatial discretizations. Specifically:

- For explicit integration of high-order spatial discretizations the allowable time-step size (based on stability considerations) typically scales with the inverse of the order squared [50]. This limit can become prohibitively severe for high orders of accuracy, especially if one uses thin elements to resolve, for example, a viscous boundary layer. As a result the use of explicit time integration schemes can become prohibitively expensive with unstructured high-order spatial discretizations.
- For implicit integration of high-order spatial discretizations, the memory requirements associated with large scale 3D problems can become prohibitively large.

In the followings sections three topic are discussed, all of which are intimately related to the above issues. Specifically, these are the use of implicit time integration schemes in an unstructured high-order context, the use of geometric multigrid and so called p-multigrid schemes in an unstructured high-order context, and finally the use of local time stepping to develop efficient time-accurate explicit schemes in an unstructured high-order context.

3.3.2. Implicit Methods

The result of an implicit temporal discretization is a globally coupled non-linear system that must be solved at each time-step. In order to solve this system it is often linearized. For practical problems direct inversion of the resulting linear system is not feasible (due to its size), thus iterative solution methods must be employed. Various approaches are used in practice, including Newton-Krylov methods such as GMRES, block Jacobi methods, line Jacobi methods, Gauss-Seidel (GS) methods, symmetric GS (SGS) methods, and lower-upper SGS (LU-SGS) methods (developed by Jameson and Yoon [68] and Yoon and Jameson [145]). For full details of all aforementioned approaches the reader is referred to the review of Wang [139], and the book chapter of May and Jameson [90]. However, we will note two important points here. Firstly, the efficiency of Newton-Krylov type methods can be greatly enhanced by preconditioning the system. It is often found that the choice of an effective preconditioner is problem dependent. This is an issue which has recently been discussed by Persson and Peraire [103] in an unstructured high-order context. Secondly, various so called matrix free implementations of the aforementioned algorithms have been developed

in an effort to limit memory requirements, which can become excessive for 3D unstructured high-order discretizations.

Linearization of the implicit temporal discretization is not the only approach that can be adopted. A notable technique based on solving the non-linear system directly has been developed by Jameson and Caughey [65] and Chen and Wang [15]. The method is known as a non-linear LU-SGS method. This approach has proved to be particularly popular in a high-order context due to its efficiency and limited memory requirements (since it is effectively explicit at a mesh level, and only implicit at an element level). In particular Sun, Wang and Liu [124] implemented the approach in 3D for hexahedral elements in a SD context, Haga, Sawada and Wang [45] implemented the approach in 3D for tetrahedral elements in a SV context, and Premasathan, Liang and Jameson [108] implemented the approach in two-dimensions (2D) in a SD context. In all cases where the non-linear LU-SGS approach was employed, the rate of convergence to steady-state was orders of magnitude faster than when an explicit RK time integration scheme was used. However, it appears that none of the test cases were particularly large, and hence it is currently an open question as to whether such an approach is feasible for real-world 3D problems (due to memory requirements).

3.3.3. Geometric Multigrid and p-Multigrid Methods

Geometric multigrid algorithms for convergence acceleration were made popular by Jameson [62] and others in the early 1980's. Details of such schemes can be found elsewhere [62, 67, 14, 2], and are hence omitted from this article. The basic idea is to obtain a correction to a 'fine' mesh solution by advancing a related problem on a coarser mesh. This procedure can be applied recursively using successively coarser meshes. Often so called 'V' or 'W' cycles are employed (following standard terminology) to advance through multiple mesh levels. While available theorems related to multigrid methods generally assume ellipticity, it is apparent that the multigrid principle also leads to accelerated steady state convergence of hyperbolic systems, since coarser meshes allow larger time-steps to be taken, which in turn expedite the expulsion of disturbances through outer boundaries of the domain. A critical aspect of the approach is the underlying scheme used to advance the solution (often referred to as the smoothing algorithm). It is necessary that this smoothing algorithm can rapidly damp high-frequency errors that manifest when coarse corrections are transferred back to finer grids. Without such a property these high frequency errors, which cannot be rapidly expelled from the fine mesh, will degrade the rate of convergence. Either an explicit or an implicit smoothing algorithm can be used. One of the most successful geometric multigrid schemes was implemented by Jameson and Caughey [65], who achieved steady state convergence of the Euler equations in just 3-5 multigrid cycles using a nonlinear LU-SGS algorithm as the smoother at each multigrid level.

The so called p-multigrid approach was first proposed by Rønquist and Patera in 1987 [113], and subsequently analyzed further by Maday and Munoz in 1988 [86]. The approach can be considered a natural extension of geometric multigrid that is well suited for use with unstructured high-order spatial discretizations. The major difference is that with a p-multigrid approach successively lower order polynomial spaces are employed on the same mesh (instead of successively coarser meshes). As such the approach might more appropriately be labeled multi-p or multi-order.

In all other regards the approach is similar to the geometric multigrid method. In particular an efficient and suitably tuned smoothing algorithm is required at each p-multigrid level. As with a geometric multigrid approach, both explicit and implicit smoothers can be used. In recent years there has been significant interest in the p-multigrid approach and its application to unstructured high-order schemes. An approximately chronological overview of various recent studies in this area is given below.

In 2005 Fidkowski *et al.* [36] presented a p-multigrid algorithm in a DG context for solving the Navier-Stokes equations. The scheme utilized an element line Jacobi smoother. Element lines were formed by determining the strongest directions of inter-element coupling (using a first order discretization of a scalar convection diffusion equation). It was found that the element line Jacobi smoother offered improved performance over block Jacobi smoothers, especially when the meshes were highly anisotropic. It was also found that such an approach lead to convergence rates independent of solution polynomial order. In 2006 Nastase and Mavriplis [91] developed a mixed geometric/p-multigrid approach that utilized various implicit smoothers. Specifically, when the zeroth order p-multigrid level was reached a geometric multigrid approach was employed to further coarsen the discretization. Convergence rates independent of both order and mesh size were achieved. Also in 2006, Luo, Baum and Lohner [85] developed a p-multigrid scheme for compressible inviscid flow on unstructured grids. They investigated using a mix of explicit RK smoothers (for the highest-order multigrid levels) and matrix free implicit SGS and LU-SGS smoothers (for low-order multigrid levels), such that the scheme converged quickly, yet had reasonable memory requirements. Once again order-independent convergence rates were observed. In 2007 Van den Abeele, Broeckhoven and Lacor [127] applied a p-multigrid algorithm with an explicit RK smoother in a SV context in 1D. Also in 2007 Wolkov, Hirsch and Leonard [144] applied a p-multigrid algorithm in a DG context to solve the 3D Euler and Navier-Stokes equations on unstructured hexahedral grids. In 2008 Helenbrook and Atkins [49] investigated using a p-multigrid approach in an DG context to solve the Poission equation. In particular they studied the final p-multigrid step (the restriction from first to zeroth order discontinuous solution polynomials), and determined that this step degraded convergence. To rectify the issue an alternative approach was suggested in which the final zeroth-order discontinuous p-multigrid level was replaced by a first order continuous space. Discussions of how to extend p-multigrid to even coarser discretizations using a geometric multigrid approach were also presented. In 2009 Kannan and Wang [70] employed a p-multigrid method using an implicit LU-SGS smoother in a SV context to solve the Navier-Stokes equations. Also in 2009, Premasathan *et al.* [108] investigated using a p-multigrid approach with an explicit RK smoother. Performance was compared with an implicit non-linear LU-SGS approach and a fully explicit time accurate RK scheme. Although the implicit non-linear LU-SGS approach offered the fastest convergence, memory requirements for the p-multigrid scheme (with an explicit smoother) were far lower, implying that the latter may better suited for large scale 3D calculations. Finally in 2009, Liang, Kannan and Wang [80] presented a p-multigrid algorithm in a SD context to solve the Euler equations. The scheme utilized a mix of implicit and explicit smoothers at different multigrid levels (similar to the approach of Luo, Baum and Lohner [85]). Specifically, explicit smoothers were used at the highest-order levels to limit memory requirements, and implicit smoothers were used for the low-order levels to expedite

convergence. In 2010 Parsani et al. [99] employed a p-multigrid approach in a SV context and compared the effect of using implicit LU-SGS smoothers and explicit RK smoothers. It was found that the rate of convergence could be increased by a factor of 5-10 when using an implicit smoother (relative to using an explicit RK smoother). Also in 2010, Mascarenhas, Helenbrook and Atkins [87] extended their previous study [49] to investigate the coupling of p-multigrid and geometric multigrid in a DG context when solving the convection diffusion equation. Once again they focused particular attention on the performance of the first to zeroth order p-multigrid step. As in their previous study [49], performance was improved if the zeroth order discontinuous space was replaced by a first order continuous space. However, due to the additional convective term being analyzed, it was also necessary to employ ideas from the SUPG method, in order to ensure that an upwind bias (and thus stability) was retained when this continuous space was employed.

It can be noted that in all of the aforementioned studies, use of a p-multigrid approach typically accelerated convergence by orders of magnitude relative to using a simple explicit RK scheme alone.

3.3.4. Local Time-Stepping Methods

As has been discussed, when using an explicit integration scheme the time-step size is limited by a CFL stability constraint. This constraint depends in part on element size. It is therefore clear that in an unstructured context, use of a domain wide time-step may be extremely inefficient, since its size will be limited by the size of the smallest element. To circumvent this issue various recent studies have developed time-accurate local time-stepping approaches in an unstructured high-order context. In particular Lörcher, Gassner and Munz [84] used a DG space-time expansion to enable local time-stepping when solving the Euler equations, and Gassner, Lörcher and Munz [41] utilized a similar approach when solving the Navier-Stokes equations. Also Liu, Li and Hu [81] have recently developed a time accurate RK discontinuous Galerkin (RKDG) scheme with local time-stepping, which they applied to both linear and non-linear test problems. Finally, in a variant on the theme, Doleana *et al.* [31] recently developed a locally implicit DG method, in which the majority of elements were treated explicitly using a leap-frog scheme, whereas smaller, problematic elements, were treated implicitly using a Crank-Nicolson scheme.

3.3.5. Summary

Further research is needed in order to develop time integration schemes specifically tailored to work efficiently with unstructured high-order spatial discretizations (both for cases where time accuracy is critical, and for cases where only a steady state solution is required). With regards to developing efficient time-accurate schemes, several avenues of research should be pursued. These include developing time-accurate local time stepping schemes for high-order unstructured spatial discretizations, and identification of time accurate implicit schemes with manageable memory requirements (even for high-order large scale 3D simulations). Also, it may prove useful to further investigate the development of spatial discretizations that do not suffer from a severe order-dependent CFL time-step restriction. With regards to developing efficient steady-state solvers, p-multigrid approaches seem to offer promising results. However much further work is needed before their efficiency is

on a par with that of the best geometric multigrid approaches. Studies to date indicate that using a judicious choice of explicit and implicit smoothers at various multigrid levels may help to circumvent memory related issues whilst maintaining a suitable rate of convergence [85][80]. Also, studies indicate that a combination of both p-multigrid and geometric multigrid may be beneficial [91].

Only when effective time integration schemes have been identified will unstructured high-order spatial discretization be able to compete with well established low-order methods in terms of efficiency.

3.4. Shock Capturing

3.4.1. Overview

All of the aforementioned high-order schemes utilize a polynomial representation of the solution. If the solution is smooth this approach can lead to very accurate results. However, if the solution contains discontinuities, such as shock waves, problems arise. Specifically, representing a discontinuous solution with a high-order polynomial can lead to the formation of spurious oscillations. These may cause strictly positive quantities such as fluid density to become negative (non-physical), and may eventually cause the solution to blow up. Such a problem is significant since shock waves, or other discontinuities such as contact surfaces, are present in many flows of practical importance.

Various approaches have been developed to stabilize unstructured high-order schemes when solutions become discontinuous. For example ENO and WENO schemes, by design, attempt to avoid constructing a polynomial representation of the solution that spans a discontinuity (in an effort to avoid spurious oscillations). As such they are naturally suited to modeling flows containing shock waves. However, as has been mentioned, the extension of ENO and WENO schemes to highly unstructured 3D meshes is complex and computationally expensive. For other methods, such as DG, SV and SD schemes, it is necessary to employ special treatment if shocks are present. In general, such treatments act to ensure that the solution remains non-oscillatory near discontinuities, either by applying a slope limiter or by adding a tuned artificial viscosity term to the system, such that the shock is smeared out over a suitably resolvable distance. In the following sections both approaches are discussed, as are automatic mesh adaptation procedures designed to improve shock resolution.

3.4.2. Limiter Based Approaches

Numerous flux and slope limiters have been developed in the past fifty years for use with low-order spatial discretizations; allowing second order accuracy when the solution is smooth, yet reducing the scheme to first order in the vicinity of discontinuities, and thus avoiding spurious oscillations. The resulting schemes often have a so called ‘local extremum diminishing’ (LED) property *i.e.* no new maxima or minima can be created as the approximate solution evolves. In the past decades similar limiters (in particular slope limiters) have been applied to unstructured high-order schemes. The most famous example of such an approach is the so called RKDG method

developed by Cockburn *et al.* [20, 19, 17, 22] and reviewed by Cockburn and Shu [23]. This method combines a DG spatial discretization with an explicit RK time integration scheme and, critically, a generalized slope limiter. The resulting fully discrete scheme is theoretically stable for any non-linear flux function, and hence stable in the presence of shocks. In subsequent studies slope limiters have been combined with DG schemes in various ways, for similar purposes. A full review of all such combinations is beyond the scope of this article. However, a notable example is the application of WENO type limiters in a DG context by Qiu and Shu [109] and Zhu *et al.* [148].

Slope limiter based approaches have proved to be robust. However, it should be noted that use of a slope limiter precludes sub-cell resolution of shocks, which is a significant drawback if one wishes to use large high-order elements. In addition, issues regarding steady state convergence have been raised [135], and the use of a slope limiter may adversely effect the ability of a scheme to resolve fine scale turbulent structures.

3.4.3. Artificial Viscosity Based Approaches

The idea of using artificial viscosity to capture shocks was first proposed by von Neumann and Richtmyer in 1950 [137]. Numerous variants of the approach have been used to stabilize second-order discretizations. For example the well known Jameson-Schmidt-Turkel (JST) scheme [66] utilizes a blend of low and high order artificial diffusion in order to remain LED. In recent decades artificial viscosity approaches have been adapted by various authors to stabilize high-order discretizations when discontinuities are present. For example, in 1989 Tadmor [125] developed the spectrally vanishing viscosity approach, which was extended and applied by various authors including Karamanos and Karniadakis [71], and Kirby and Sherwin [74]. This approach directly applies viscosity to high-frequency components of the solution, which are energized when steep gradients such as shocks are present. Another high-wavenumber biased scheme is that of Cook and Cabot [25], who employ a mesh dependent artificial shear viscosity scaled by the gradient (or higher derivatives) of the solution. This approach was extended by the same authors to include both artificial shear and bulk viscosity terms (so called hyperviscosity) [26], and then further extended by Cook [24] to include an artificial thermal conductivity term. Recently, the work of Cook and Cabot [25, 26], and Cook [24], has been extended to non-uniform curvilinear grids by Kawai and Lele [73], and further extended by Bhagatwala and Lele [10] to include an additional flow sensor, which allows artificial viscosity to be focused in regions of strong negative dilatation (likely coincident with shock structures). Even more recently, the work of Kawai and Lele [73] and Bhagatwala and Lele [10] has been adapted by Premasathan, Liang and Jameson [106, 107] for use in a fully unstructured SD flow solver.

It should be noted that none of the approaches discussed above, as implemented, result in sub-cell resolution of shocks. However, a significant advance that offers the potential to resolve discontinuities *within* a single high-order element has been proposed by Persson and Peraire [102]. The approach applies a element-wise constant (and order dependent) artificial viscosity to elements in which discontinuities are present. Specifically, artificial viscosity is added to elements in which the highest frequency components of the solution are significant relative to all other components. Critically, the artificial viscosity is tuned such that shock structures are smeared over a distance that

can be resolved by the polynomial expansion within each element (without spurious oscillations). As a result, the scheme offers sub-cell shock resolution that improves as the polynomial order within each element is increased. Fig. 3 shows results obtained using the approach of Persson and Peraire [102]. Specifically, in Fig. 3(a) contours of local Mach number within the vicinity of a NACA0012 airfoil are shown (for inviscid supersonic flow at Mach 1.5). It is clear that shock structures are resolved within elements. Fig. 3(b) shows the corresponding contour plot of artificial viscosity, applied to stabilize the scheme. The artificial viscosity is element-wise constant, and only applied in the vicinity of shocks.

Figure 3: Contours of local Mach number within the vicinity of a NACA0012 airfoil are shown in (a). Flow is inviscid and supersonic at Mach 1.5. The result was obtained using a DG flow solver combined with the sub-cell shock capturing approach of Persson and Peraire [102]. Fourth order solution polynomials were used within each element. Note that shock structures are resolved within elements. A color map of the element-wise constant artificial viscosity applied in order to capture the shock is shown in (b). The gray color indicates that no artificial viscosity was applied. Images courtesy of P. Persson. Copyright P. Persson and J. Peraire [102].

Finally, it should be noted that a recent extension of the technique developed by Persson and Peraire [102] has been suggested by Barter and Darmofal [4, 5], who recognized that use of an

element-wise constant artificial viscosity may induce oscillations in state gradients; which may pollute the downstream flow solution. To rectify this problem, Barter and Darmofal proposed a more complex formulation, which involves solving an additional partial differential equation to obtain a smooth artificial viscosity profile.

3.4.4. Automatic Mesh Adaptation

Other than the method of Persson and Peraire [102], and its extension by Barter and Darmofal [4, 5], the approaches detailed above (at least as applied) do not result in sub-cell resolution of shocks. This can be a significant problem if the mesh contains relatively large high-order elements.

Figure 4: Contours of pressure within the vicinity of a circular bump are shown in (a). Flow is inviscid and supersonic at Mach 1.4. The result was obtained using a SD flow solver combined with the automatic mesh refinement approach of Premasuthan, Liang and Jameson [107]. Third order solution polynomials were used within each element. The refined mesh is shown in (b). In the case presented, two levels of mesh refinement were used. Images courtesy of S. Premasuthan. Reprinted with permission of the American Institute of Aeronautics and Astronautics. Copyright American Institute of Aeronautics and Astronautics [107].

To overcome this issue various automatic mesh refinement strategies have been developed, with the objective of automatically reducing element size in the vicinity of discontinuities. For example Premasuthan, Liang and Jameson [107] adapted an artificial viscosity based shock capturing scheme (in an SD context), such that mesh refinement was applied in regions where the artificial viscosity rose above a certain threshold. A result obtained using this approach is shown in Fig. 4. Specifically, in Fig. 4(a) contours of pressure above a circular bump are shown (for inviscid supersonic flow at Mach 1.4. In Fig. 4(b) the corresponding automatically refined mesh is shown. It is clear that more elements are located where shock structures are present.

Other more involved methods of mesh refinement, exploiting output based error estimation techniques, have also been used in an unstructured high-order context. Such methods often employ adjoint-based approaches, for example see Hartmann [48], Fidkowski and Roe [37], and Li, Premasuthan and Jameson [78]. Although in general such output based error estimation schemes are not designed specifically to refine the mesh near shocks, it is often the case that such refinement does occur, since an under-resolved shock may cause errors in the output of interest. A review of such approaches has recently been given by Fidkowski and Darmofal [35].

Finally, it should be noted that while automatic mesh refinement approaches may significantly improve shock resolution, they do have an associated computational overhead. Also, they will reduce the CFL time-step limit for an explicit scheme, and may result in the generation of non-conforming elements with hanging nodes, which require special treatment.

3.4.5. Summary

High-order ENO and WENO schemes, by design, can be used to model flows with discontinuous solutions. However, extension of these schemes to fully unstructured meshes in 3D can be complex and costly. When using compact unstructured high-order schemes such as the DG method, limiter based approaches have proven to be robust. However, there are questions regarding their accuracy, and they do not offer sub-cell shock resolution. The sub-cell resolution obtained by Persson and Peraire [102] using an artificial viscosity based approach is impressive. However, the extension of this approach by Barter and Darmofal [4, 5] to avoid piecewise discontinuous artificial viscosity (which may generate spurious downstream errors) is somewhat involved. In summary, whilst a range of shock capturing approaches have been identified, there is further scope for identifying even cheaper, simpler and more robust schemes that offer sub-cell shock resolution, and which have a negligible impact on flow features away from shocks.

3.5. Complexity

3.5.1. Overview

Unstructured high-order spatial discretizations exhibit increased complexity (at various levels) compared with low-order schemes. In particular:

- The related mathematical theory is often more complicated.
- Their mathematical formulation is often more complicated.

- They often require more complex data structures, which are best dealt with in practice by adopting an object-oriented programming style.
- They are often less physically intuitive.
- Since the field of unstructured high-order methods is still developing, there is no definitive consensus as to which (of the very many) methods is best suited to a particular problem.

These issues, although fundamentally surmountable through detailed study, act as a significant barrier to the use of unstructured high-order schemes amongst a non-specialist community. In the view of the authors, such issues are best addressed in two ways. The first is to identify and develop schemes that are fundamentally intuitive and straightforward to implement, and that ‘recycle’ various aspects from well known low-order schemes. It is already apparent that such an approach works. For example, the popularity of high-order DG methods can, in part, be attributed to the fact they share many aspects with low-order FV type schemes (in particular the use of Riemann solvers to connect otherwise independent elements). Also SD type schemes, which are similar to nodal DG methods (but based on the governing system in its differential form) have become increasingly popular in recent years due to their comparative simplicity and their intuitive nature. The second way in which the above issues can be addressed is to clearly identify similarities and overlap between existing (and new) schemes. To this end there have been several recent advances. Specifically, it was shown in 2007 by Van den Abeele, Lacor and Wang [128] that SV and SD methods are identical in 1D. Also, in 2008 May [89] demonstrated equivalence between SD type schemes and quadrature free nodal DG schemes, and Dumbser [34] proposed what have become known as PnPm schemes, which unify high-order FV and DG methods [34]. Finally, in 2007 Huynh [58] proposed the so called flux reconstruction (FR) approach, which unifies both nodal DG schemes and SD schemes (at least for a linear flux function) within a single intuitive framework, as well as facilitating the definition of infinitely many new schemes, a range of which appear to have favorable properties.

In the view of the authors the FR approach represents a significant advance in terms of unifying simple, robust, efficient and intuitive unstructured high-order methods. As such, the remainder of this section is devoted to a discussion of the FR approach. To begin, a brief review of FR in 1D is presented (for full details see the original article by Huynh [58]). This review is followed by a summary of recent findings by Vincent, Castonguay and Jameson [136], who were able to identify a special class of FR schemes that are guaranteed to be linearly stable for all orders of accuracy. Finally, a brief overview of FR schemes in multiple dimensions is presented, and the ability of simple FR schemes to model viscous flows is discussed.

3.5.2. The Flux Reconstruction Approach in One-Dimension

Consider solving the following 1D scalar conservation law

$$\frac{\partial u}{\partial t} + \frac{\partial f}{\partial x} = 0 \quad (3.1)$$

within an arbitrary domain Ω , where x is a spatial coordinate, t is time, $u = u(x, t)$ is a conserved scalar quantity and $f = f(u)$ is the flux of u in the x direction. Further, consider partitioning Ω into N distinct elements each denoted $\Omega_n = \{x | x_n < x < x_{n+1}\}$ such that

$$\Omega = \bigcup_{n=0}^{N-1} \Omega_n, \quad \bigcap_{n=0}^{N-1} \Omega_n = \emptyset. \quad (3.2)$$

Finally, having partitioned Ω into separate elements, consider representing the exact solution u within each Ω_n by polynomials of degree k denoted $u_n^\delta = u_n^\delta(x, t)$ (which are in general discontinuous between elements), and the exact flux f within each Ω_n by polynomials of degree $k+1$ denoted $f_n^\delta = f_n^\delta(x, t)$ (which are C^0 continuous between elements), such that a total approximate solution $u^\delta = u^\delta(x, t)$ and a total approximate flux $f^\delta = f^\delta(x, t)$ can be defined within Ω as

$$u^\delta = \bigoplus_{n=0}^{N-1} u_n^\delta \approx u, \quad f^\delta = \bigoplus_{n=0}^{N-1} f_n^\delta \approx f. \quad (3.3)$$

From an implementation perspective, it is advantageous to consider transforming each Ω_n to a standard element $\Omega_S = \{r | -1 \leq r \leq 1\}$ via the mapping

$$r = \Gamma_n(x) = 2 \left(\frac{x - x_n}{x_{n+1} - x_n} \right) - 1, \quad (3.4)$$

which has the inverse

$$x = \Gamma_n^{-1}(r) = \left(\frac{1-r}{2} \right) x_n + \left(\frac{1+r}{2} \right) x_{n+1}. \quad (3.5)$$

Having performed such a transformation, the evolution of u_n^δ within any individual Ω_n (and thus the evolution of u^δ within Ω) can be determined by solving the following transformed equation within the standard element Ω_S

$$\frac{\partial \hat{u}^\delta}{\partial t} + \frac{\partial \hat{f}^\delta}{\partial r} = 0, \quad (3.6)$$

where

$$\hat{u}^\delta = \hat{u}^\delta(r, t) = u_n^\delta(\Gamma_n^{-1}(r), t) \quad (3.7)$$

is a polynomial of degree k ,

$$\hat{f}^\delta = \hat{f}^\delta(r, t) = \frac{f_n^\delta(\Gamma_n^{-1}(r), t)}{J_n}, \quad (3.8)$$

is a polynomial of degree $k+1$, and $J_n = (x_{n+1} - x_n)/2$.

The FR approach to solving Eq. (3.6) within the standard element Ω_S consists of five stages. The first stage is to define a specific form for $\hat{u}^\delta$. To this end, it is assumed that values of $\hat{u}^\delta$ are known at a set of $k+1$ solution points inside Ω_S , with each point located at a distinct position r_i ($i = 0$ to k). Lagrange polynomials $l_i = l_i(r)$ defined as

$$l_i = \prod_{j=0, j \neq i}^k \left(\frac{r - r_j}{r_i - r_j} \right) \quad (3.9)$$

can then be used to construct the following expression for $\hat{u}^\delta$

$$\hat{u}^\delta = \sum_{i=0}^k \hat{u}_i^\delta l_i, \quad (3.10)$$

where $\hat{u}_i^\delta = \hat{u}_i^\delta(t)$ are the known values of $\hat{u}^\delta$ at the solution points r_i .

The second stage of the FR process involves constructing a degree k polynomial $\hat{f}^{\delta D} = \hat{f}^{\delta D}(r, t)$, defined as the approximate transformed discontinuous flux within Ω_S . An expression for $\hat{f}^{\delta D}$ can be written as

$$\hat{f}^{\delta D} = \sum_{i=0}^k \hat{f}_i^{\delta D} l_i \quad (3.11)$$

where the coefficients $\hat{f}_i^{\delta D} = \hat{f}_i^{\delta D}(t)$ are simply values of the transformed flux at each solution point r_i evaluated directly from the approximate solution. The flux $\hat{f}^{\delta D}$ is termed discontinuous since it is calculated directly from the approximate solution, which is in general piecewise discontinuous between elements.

The third stage of the FR process involves calculating transformed numerical fluxes at either end of the standard element Ω_S (at $r = \pm 1$). In order to calculate such fluxes, one must first obtain values for the approximate solution at either end of the standard element via Eq. (3.10). Once these values have been obtained they can be used in conjunction with analogous information from adjoining elements to calculate transformed numerical interface fluxes. The exact methodology for calculating such numerical fluxes will depend on the nature of the equations being solved. For example, when solving the Euler equations one may use a Roe type approximate Riemann solver [112], or any other two-point flux formula that provides for an upwind bias. In what follows the numerical interface fluxes associated with the left and right hand ends of Ω_S (and transformed appropriately for use in Ω_S) will be denoted $\hat{f}_L^{\delta I}$ and $\hat{f}_R^{\delta I}$ respectively.

The penultimate stage of the FR process involves adding a degree $k+1$ transformed correction flux $\hat{f}^{\delta C} = \hat{f}^{\delta C}(r, t)$ to the approximate transformed discontinuous flux $\hat{f}^{\delta D}$, such that their sum equals the transformed numerical interface flux at $r = \pm 1$, yet follows (in some sense) the approximate discontinuous flux within the interior of Ω_S . In order to define $\hat{f}^{\delta C}$ such that it satisfies the above requirements, consider first defining degree $k+1$ correction functions $g_L = g_L(r)$ and $g_R = g_R(r)$ that approximate zero (in some sense) within Ω_S , as well as satisfying

$$g_L(-1) = 1, \quad g_L(1) = 0, \quad (3.12)$$

$$g_R(-1) = 0, \quad g_R(1) = 1, \quad (3.13)$$

and, based on symmetry considerations

$$g_L(r) = g_R(-r). \quad (3.14)$$

A suitable expression for $\hat{f}^{\delta C}$ can now be written in terms of g_L and g_R as

$$\hat{f}^{\delta C} = (\hat{f}_L^{\delta I} - \hat{f}_L^{\delta D})g_L + (\hat{f}_R^{\delta I} - \hat{f}_R^{\delta D})g_R, \quad (3.15)$$

where $\hat{f}_L^{\delta D} = \hat{f}^{\delta D}(-1, t)$ and $\hat{f}_R^{\delta D} = \hat{f}^{\delta D}(1, t)$. Using this expression, a degree $k + 1$ approximate total transformed flux $\hat{f}^\delta = \hat{f}^\delta(r, t)$ within Ω_S can be constructed from the discontinuous and correction fluxes as follows

$$\hat{f}^\delta = \hat{f}^{\delta D} + \hat{f}^{\delta C}. \quad (3.16)$$

The final stage of the FR process involves calculating the divergence of $\hat{f}^\delta$ at each solution point r_i using the expression

$$\frac{\partial \hat{f}^\delta}{\partial r}(r_i) = \sum_{j=0}^k \hat{f}_j^{\delta D} \frac{dl_j}{dr}(r_i) + (\hat{f}_L^{\delta I} - \hat{f}_L^{\delta D}) \frac{dg_L}{dr}(r_i) + (\hat{f}_R^{\delta I} - \hat{f}_R^{\delta D}) \frac{dg_R}{dr}(r_i). \quad (3.17)$$

These values can then be used to advance the approximate transformed solution $\hat{u}^\delta$ in time via a suitable temporal discretization of the following semi-discrete expression

$$\frac{d\hat{u}_i^\delta}{dt} = -\frac{\partial \hat{f}^\delta}{\partial r}(r_i). \quad (3.18)$$

The nature of a particular FR scheme depends solely on three factors, namely the location of the solution collocation points r_i , the methodology for calculating the transformed numerical interface fluxes $\hat{f}_L^{\delta I}$ and $\hat{f}_R^{\delta I}$, and finally the form of the flux correction functions g_L (and thus g_R). It has been shown previously that a collocation based (under integrated) nodal DG scheme is recovered in 1D if the corrections functions g_L and g_R are the right and left Radau polynomials respectively [58]. Also, it has been shown that SD type methods can be recovered (at least for a linear flux function) if the corrections g_L and g_R are set to zero at a set of k points within Ω_S (located symmetrically about the origin) [58]. Several additional forms of g_L (and thus g_R) have also been suggested, leading to the development of new schemes, with various stability and accuracy properties. For further details of these new schemes see the article by Huynh [58].

3.5.3. Energy Stable Flux Reconstruction

In a recent study by Vincent, Castonguay and Jameson [136] an infinite number of linearly stable FR schemes were identified (for all orders of accuracy). These schemes, henceforth referred to as Vincent-Castonguay-Jameson-Huynh (VCJH) schemes, are recovered if the left and right corrections functions g_L and g_R respectively are defined as

$$g_L = \frac{(-1)^k}{2} \left[L_k - \left(\frac{\eta_k L_{k-1} + L_{k+1}}{1 + \eta_k} \right) \right], \quad (3.19)$$

and

$$g_R = \frac{1}{2} \left[L_k + \left(\frac{\eta_k L_{k-1} + L_{k+1}}{1 + \eta_k} \right) \right], \quad (3.20)$$

where

$$\eta_k = \frac{c(2k+1)(a_k k!)^2}{2}, \quad a_k = \frac{(2k)!}{2^k (k!)^2}, \quad (3.21)$$

L_k is a Legendre polynomial of order k , and c is a free scalar parameter that must lie within the range

$$\frac{-2}{(2k+1)(a_k k!)^2} < c < \infty. \quad (3.22)$$

If such correction functions are used, then the resulting FR scheme will be linearly stable in a broken Sobolev type norm $\|u^\delta\|_{k,2}$, defined as

$$\|u^\delta\|_{k,2} = \left[\sum_{n=1}^N \int_{x_n}^{x_{n+1}} (u_n^\delta)^2 + \frac{c}{2} (J_n)^{2k} \left(\frac{\partial^k u_n^\delta}{\partial x^k} \right)^2 dx \right]^{1/2}, \quad (3.23)$$

(where the notation of section 3.5.2. has been adopted), *i.e.* it can be shown that

$$\frac{d}{dt} \|u^\delta\|_{k,2}^2 \leq 0. \quad (3.24)$$

It can be noted that several existing methods are encompassed by the new class of VCJH schemes. In particular if $c = 0$ then $\eta_k = 0$ which implies

$$g_L = \frac{(-1)^k}{2} (L_k - L_{k+1}), \quad (3.25)$$

and

$$g_R = \frac{1}{2} (L_k + L_{k+1}). \quad (3.26)$$

These can be recognized as expressions for the right and left Radau polynomials respectively. Thus, following the analysis of Huynh [58] a collocation based nodal DG scheme is recovered. Alternatively, if

$$c = \frac{2k}{(2k+1)(k+1)(a_k k!)^2}, \quad (3.27)$$

then

$$\eta_k = \frac{k}{k+1}, \quad (3.28)$$

which implies

$$g_L = \frac{(-1)^k}{2} \left[L_k - \left(\frac{kL_{k-1} + (k+1)L_{k+1}}{2k+1} \right) \right] = \frac{(-1)^k}{2} (1-x)L_k, \quad (3.29)$$

and

$$g_R = \frac{1}{2} \left[L_k + \left(\frac{kL_{k-1} + (k+1)L_{k+1}}{2k+1} \right) \right] = \frac{1}{2} (1+x)L_k. \quad (3.30)$$

In this case both g_L and g_R have k symmetrically located (and hence coincident) zeros internal to Ω_S . The resulting scheme is therefore an SD method (at least for a linear flux function). It is in fact the only SD type scheme that can be recovered from the range of VCJH schemes. Further, it is identical to the SD scheme that Jameson [63] proved to be stable (the interior flux collocation

points are at zeros of the Legendre polynomial of degree k), which is the same as the only SD scheme that Huynh found to be devoid of weak instabilities [58].

Finally, in the original presentation of the FR approach by Huynh [58], a range of new methods were investigated (in addition to DG and SD type schemes). One of these new methods, which Huynh denoted the g_2 scheme, proved to be particularly stable. It is found that such a scheme can be recovered from the range of VCJH schemes if

$$c = \frac{2(k+1)}{(2k+1)k(a_k k!)^2}, \quad (3.31)$$

which leads to

$$\eta_k = \frac{k+1}{k}, \quad (3.32)$$

and thus

$$g_L = \frac{(-1)^k}{2} \left[L_k - \left(\frac{(k+1)L_{k-1} + kL_{k+1}}{2k+1} \right) \right], \quad (3.33)$$

and

$$g_R = \frac{1}{2} \left[L_k + \left(\frac{(k+1)L_{k-1} + kL_{k+1}}{2k+1} \right) \right]. \quad (3.34)$$

These expressions are consistent with those derived by Huynh for the g_2 method.

The identification of VCJH type schemes offers significant insight into why certain FR schemes are stable, whereas others are not. Also from a practical standpoint the VCJH formulation offers a simple prescription for implementing an infinite range of particularly intuitive and linearly stable high-order methods.

3.5.4. Flux Reconstruction in Multiple Dimensions

All 1D FR schemes can be extended to quadrilateral and hexahedral elements via the construction of tensor product bases as described by Huynh [58]. However, in simplex elements the direct construction of a tensor product basis is not possible, and one must use an alternative methodology. Wang and Gao [140] have indirectly extended the FR approach to triangles, developing the so called lifting collocation penalty (LCP) method, which has also been extended by Haga, Gao and Wang [44] to tetrahedral and prismatic elements in 3D. The present authors and co-workers are currently attempting to extend the energy stable VCJH schemes detailed in section 3.5.3. to simplex elements.

3.5.5. Flux Reconstruction for Viscous Terms

In contrast to DG schemes (for which the treatment of viscous terms is somewhat involved), SD type schemes are able to accommodate viscous terms in a simple fashion [123]. The FR approach potentially offers an equally simple way to treat viscous terms [59]. The present authors and co-workers are currently investigating whether a simple FR based Navier-Stokes flow solver can be developed for 2D and 3D unstructured meshes. Preliminary results are encouraging. However, further testing is necessary to ascertain whether a suitable level of accuracy is achieved.

3.5.6. Summary

We suggest that the complex nature of unstructured high-order methods has inhibited their adoption amongst a wider community of fluid dynamicists. In the view of the authors, this issue is best addressed in two ways. The first is to identify and develop schemes that are fundamentally intuitive and straightforward to implement, and that ‘recycle’ various aspects from well known low-order methods. The second is to clearly identify similarities and overlap between existing (and new) schemes. The FR approach introduced by Huynh [58], which has been discussed in some detail, satisfies all of the aforementioned criteria. Furthermore, the recent identification of VCJH schemes [136] gives significant insight into why certain FR schemes are stable whereas others are not, as well as providing a simple prescription for implementing an infinite range of linearly stable high-order methods. Future studies should further investigate the properties of VCJH schemes, in an attempt to identify if an optimal scheme exists. Also, the extension of VCJH schemes to simplex elements should be investigated, as well as the use of FR schemes to solve real world non-linear inviscid and viscous flow problems.

4. Practical Utilization

4.1. Overview

In the following section examples are provided of applications where unstructured high-order methods may offer significant benefits over low-order schemes. Specifically, vortex dominated flow in the vicinity of flapping wings, and transitional flow over airfoils are considered. Illustrating the successful application of unstructured high-order methods to such practical problems is an important part of encouraging their adoption. To end the section, the impact of graphical processing units (GPUs) on the future use of unstructured high-order methods is briefly discussed.

4.2. Vortex Dominated Flow in the Vicinity of Flapping Wings

The ability to model vortex dominated flow within the vicinity of flapping wing configurations is essential if one wishes to understand how natural fliers (such as insects, birds and bats) generate lift and propel themselves. It is also essential if one wishes to optimize the design of efficient and maneuverable micro air vehicles (MAVs). Unstructured high-order methods are well suited to modeling such problems for two reasons. Firstly, they offer very low numerical dissipation, allowing vortices to be tracked over significant distances (without non-physically decaying). Secondly, their unstructured nature facilitates meshing of the complex (and deforming) geometries associated flapping wing motion.

High-order 2D simulations of viscous flow over pitching and plunging airfoils have recently been undertaken by various authors including Ou, Liang and Jameson [97], amongst others. Such configurations act as simple flapping wing models, and also allow comparisons to be made with experimental studies, of which there are several for the 2D configurations in question [69]. Fig.

5(a) shows a plot of instantaneous vorticity magnitude in the vicinity of a plunging NACA0012 airfoil obtained using the approach of Ou, Liang and Jameson [97] (a fourth-order SD method), at a Reynolds number of 1850. Fig. 5(b) shows an analogous experimental result obtained by Jones, Dohring and Platzer [69] in a water tunnel. It can be seen that the high-order SD scheme is able to capture very fine vortical structures (observed experimentally) that develop in the wake of the airfoil.

Figure 5: A plot of vorticity magnitude in the vicinity of a plunging NACA0012 airfoil obtained using the approach of Ou, Liang and Jameson [97] is shown in (a). The Reynolds number is 1850. An analogous experimental result from Jones, Dohring and Platzer [69] is shown in (b). The numerical results compare well with the experimental results. In particular, the simulations were able to reproduce the fine structures that develop in the wake of the plunging airfoil. Image (a) courtesy of K. Ou. Copyright K. Ou. Image (b) courtesy of K. Jones. This image is declare work of the U.S. Government and is not subject to copyright protection in the United States [69].

High-order 2D simulations of viscous flow over deforming structures have also recently been undertaken by various authors including, Mavriplis and Nastase [88], Persson, Bonet and Peraire [101], Ou and Jameson [96], and Ou, Liang, and Jameson [97], amongst others. Fig. 6 shows plots of instantaneous vorticity magnitude in the wake of a flexing beam attached to the downstream side of a cylinder obtained by Ou and Jameson [96] using a high-order SD method, at a Reynolds number of 200. The aforementioned studies suggest that both SD and DG methods perform well on deforming grids. The development of efficient and accurate deforming mesh capabilities is critical if flapping wing simulations are to be carried out using such approaches.

Figure 6: Plots of vorticity magnitude in the wake of a flexing beam attached to the downstream side of a cylinder obtained by Ou and Jameson [96] using a high-order SD method, at a Reynolds number of 200. SD methods have been found to perform well with deforming meshes. Images courtesy of K. Ou. Copyright K. Ou and A. Jameson [96].

Finally, we note that high-order fully 3D simulations of viscous flow over a flapping wing configuration have been undertaken by Persson, Willis and Peraire [105] using a DG method. Fig. 7 shows plots of entropy isosurfaces (colored by Mach number) obtained in the vicinity of a flapping wing configuration with a 10 degree angle of attack by Persson, Willis and Peraire [105].

Figure 7: Plots of entropy isosurfaces (colored by Mach number) in the vicinity of a flapping wing configuration with a 10 degree angle of attack obtained by Persson, Willis and Peraire [105] using a DG flow solver, at a Reynolds number of 2000. Images courtesy of P. Persson. Copyright P. Persson [105].

The aforementioned preliminary studies have obtained promising results. However, much future work is needed before unstructured high-order schemes can be used routinely to solve complex 3D flapping wing problems at a useful rate *i.e.* a rate that makes design optimization tenable.

4.3. Transitional Flow Over an Airfoil

Recent studies by various authors including Castonguay, Liang and Jameson [13], Zhou and Wang [147], Uranga *et al.* [126] and Galbraith and Visbal [39] suggest that certain high-order methods are able to model transitional flow over an SD7003 airfoil without explicitly employing a turbulence model, despite the simulation being under resolved. Such under resolution has been termed an implicit large eddy simulation (ILES) approach.

ILES of flow over an SD7003 airfoil at a 4° angle of attack has been performed by Castonguay and Jameson [13] using a 3D viscous compressible SD flow solver. The SD7003 airfoil was selected due to the availability of existing experimental [110] data. Third-order and fourth-order accurate simulations were undertaken on a mesh with with 49,152 high-order SD elements (resulting in 1.3×10^6 degree of freedom for the third-order case and 3.1×10^6 degree of freedom for the forth-order case). Reynolds numbers of 1×10^4 and 6×10^4 were considered. When the Reynolds number was 1×10^4 the flow remained essentially 2D, with close-to-periodic vortex shedding (see Fig. 8(a)). The computed average lift coefficient was 0.372 and the average drag coefficient was 0.0492, which are consistent with those obtained by other similar studies. At a Reynolds number of 6×10^4 , however, transition was observed to take place across a laminar separation bubble (see Fig. 8(b)).

The Q-criterion Q , initially proposed by Dubeif and Delcayre [33], provides a means of visualizing vortex cores and identify turbulent structures. It can be calculated as

$$Q = \frac{1}{2}(\Omega_{ij}\Omega_{ij} - S_{ij}S_{ij}), \quad (4.1)$$

where

$$\Omega_{ij} = \left(\frac{\partial u_i}{\partial x_j} - \frac{\partial u_j}{\partial x_i} \right), \quad S_{ij} = \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \quad (4.2)$$

are the anti-symmetric and symmetric parts of the velocity gradient tensor respectively. Fig. 8 shows instantaneous isosurfaces of Q obtained by Castonguay and Jameson [13] over the SD7003 airfoil for Reynolds numbers of 1×10^4 and 6×10^4 .

While the aforementioned studies offer promising results, further work is required in order to ascertain exactly why they are successful, and whether the successes are repeatable when other geometries and flow configurations are considered. A useful line of investigation would be to compare the above results with those obtained when a sub-grid scale (SGS) turbulence model is also employed *i.e.* compare with a standard large eddy simulation (LES) approach. Understanding the interplay between high-order spatial discretizations and SGS models for LES is potentially a very interesting avenue of future research.

Figure 8: Instantaneous isosurfaces of Q (colored by Mach number) above an SD7003 airfoil at a 4° angle of attack obtained using a fourth-order SD method by Castonguay and Jameson [13]. In (a) the Reynolds number is 1×10^4 , and the flow is essentially 2D and laminar. However, in (b) the Reynolds number is 6×10^4 , and transition takes place across a laminar separation bubble. Images courtesy of P. Castonguay. Copyright P. Castonguay and A. Jameson [13].

4.4. Graphical Processing Units

There has recently been a significant increase in the use of GPUs as general-purpose programmable units to solve computationally intensive problems in a variety of fields. Several algorithms have achieved significant (order of magnitude) speedups when run on a single off-the-shelf GPU *c.f.* CPU implementations of the same method. In particular, compact unstructured high-order methods with limited inter-element communication, such as DG methods, are found to perform particularly well on GPUs [75].

There are two reasons why such high-order schemes perform well on GPUs. Firstly, high-order methods in general require more work per degree of freedom than low-order methods. This increased arithmetic intensity shifts the method from being limited by memory bandwidth to being limited by computing power, which is generally in abundance on a GPU. Secondly, the element-local nature of DG type schemes allows one to make significant use of the GPUs fast on-chip shared memory, leading to considerably improved performance.

The fact that various unstructured high-order methods are well suited to GPUs may well encourage their use in the coming years as the availability of GPU hardware becomes increasingly widespread.

5. Conclusions

In this article four major issues currently inhibiting the adoption of unstructured high-order methods have been identified and discussed. Specifically, the issues were a lack of robust high-order mesh generation software, a lack of efficient time-integration schemes (tailor suited for high-order spatial discretizations), a lack of robust and accurate shock capturing algorithms, and finally the overall complexity (at various levels) of unstructured high-order methods. Recent efforts to address each of these issues were presented, and directions for future research were suggested. Various examples illustrating the potential benefits of unstructured high-order schemes were also given, including their application to the simulation of flapping wing flight, and their application to the simulation of transitional flows using a so called ILES approach. Such results are promising. It is the view of the authors that further concerted effort by academia to address the issues detailed in this article will lead to the eventual adoption of unstructured high-order schemes by industry. This will in turn lead to further enhancements (in terms of accessibility), eventually resulting (where beneficial) in the widespread adoption of unstructured high-order schemes by fluid dynamicists.

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