

Chapter 2

Computational Methods for Unsteady Flows

2.1 Introduction

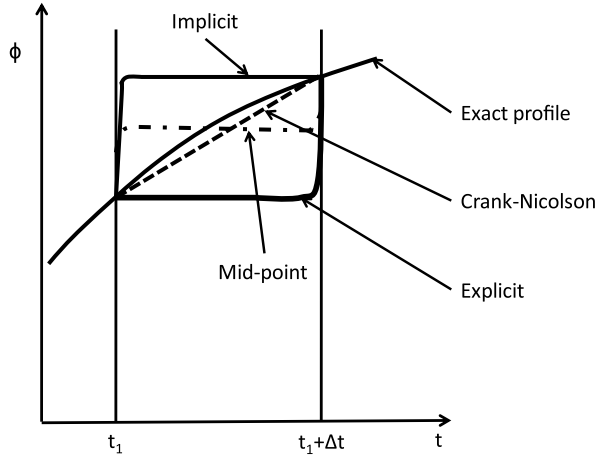
In this chapter various temporal discretization schemes will first be discussed. Then the spatial discretization is considered. Also, peripheral solution approaches will be addressed, such as prediction of the pressure field along with simultaneous equation solvers. Finally, the impact of grid topology on the accuracy of solutions is considered. There is a strong emphasis on LES.

2.2 Overview of Temporal Discretizations

The major element of any CFD procedure is the solution of convection and diffusion transport equations. Like the spatial, the temporal discretization process needs to incorporate assumptions of how variables will change with time and also how this time variation varies over each cell. Generally, the process involves two key initial stages. First, just the spatial terms are discretized (again profile assumptions are involved). These terms are generally represented here by the global symbol A . The temporal derivative remains, giving a semi-discrete Ordinary Differential Equation ($\partial\phi/\partial t = A$).

This process of reducing the full governing equations to semi-discrete Ordinary Differential Equations (ODEs) is called the *Method of Lines*. The second stage involves discretization of the ODEs. There are numerous discretization assumptions and methods originating from general solution procedures for ODEs. The most common procedures, which have found application in CFD, will be described here. Most attention will be focused on schemes widely used in practical CFD. The following generic approaches are presented: two-level, three-level, predictor-corrector and splitting.

Fig. 2.1 Temporal profile assumptions



2.3 Temporal Profile Assumptions for Variables

2.3.1 Dependent Variable Changes with Time

When discretizing the unsteady flow equations an assumption must be made of how dependent variables change with time. Basic profile assumptions are given in Fig. 2.1. These can mathematically be represented as

$$\phi = Wf^{n+1}\phi^{n+1} + Wf^n\phi^n + Wf^{n-1}\phi^{n-1} \quad (2.1)$$

The precise numerical values, for different weighting coefficients, is given later. The discretized transport equations can be written using the method of lines, noted earlier, as below

$$(1 + \eta) \frac{\Delta[\rho_i \phi_i]^n}{\Delta t} - \eta \frac{\Delta[\rho_i \phi_i]^{n-1}}{\Delta t} = A(\phi) \quad (2.2)$$

where A represents the discretized spatial derivatives and source terms. Also,

$$\begin{aligned} \Delta[\rho_i \phi_i]^n / \Delta t &= [(\rho \phi_i)^n - (\rho_i \phi_i)^{n-1}] / \Delta t, \\ \Delta[\rho_i \phi_i]^{n-1} / \Delta t &= [(\rho \phi_i)^{n-1} - (\rho_i \phi_i)^{n-2}] / \Delta t \end{aligned}$$

Equation (2.2) offers the possibility of both two and three-level (involving $\phi^n, \phi^{n-1}, \phi^{n-2}$) schemes. To implement these, values of ϕ *not involved in time derivatives* ($\Delta(\rho_i \phi_i) / \Delta t$) are replaced with Eq. (2.1). The possible number of temporal discretizations available to CFD is extensive. We can define

$$Wf^n = \lambda, \quad Wf^{n-1} = 1 - \lambda - k, \quad Wf^{n-2} = k \quad (2.3)$$

Table 2.1 Values of η , λ and k for commonly occurring time schemes

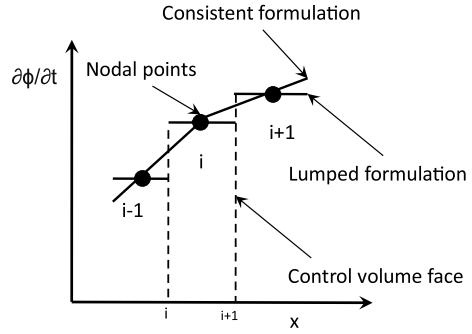
Scheme	η	λ	k	Stability	Order	Other features
Explicit (Euler)	0	0	0	$0 \leq C^2 \leq 2D \leq 1$	1	–
Implicit (Backwards Euler)	0	1	0	Unconditionally stable	1	–
Crank-Nicolson (one-step trapezoidal)	0	1/2	0	Unconditionally stable	2	–
Leapfrog	–1/2	0	0	Unconditionally unstable	2	–
Adams-Moulton	0	5/12	1/12	–	3	–
Galerkin	0	3/5	0	Unconditionally stable	1	–
Exponential	0	$1/(1 - e^{A_{i\phi}\Delta t})$ $- 1/A_{i\phi}\Delta t$	0	Unconditionally stable	1	–
Lax-Wendroff	0	0	0	$0 \leq C^2 \leq 2D \leq 1$	–	Γ augmented by $(\Delta t u^2)/2$
DuFort-Frankel	0	0	0	$C < 1$, for accuracy $C^2 \leq 1$	2	$\phi_i^{n-1} = \frac{\phi_i^n + \phi_i^{n-2}}{2}$ in diffusion terms

Then, some values of η , λ and k , for frequently occurring time schemes are given in Table 2.1. Note, in this table, $C = u\Delta t/\Delta x$ is the Courant number. For compressible flows, this needs to be re-expressed as $C = (|u| + c)\Delta t/\Delta x$ where c is the speed of sound. Hence, for compressible flow the velocity scale is replaced by the maximum acoustic wave speed. The more severe stability constraint is the diffusive. This involves the parameter, $D = \Gamma\Delta t/\rho(\Delta x)^2$ where Γ is a diffusion coefficient. Notice that for the Lax-Wendroff Scheme, Γ is augmented by $(\Delta t u^2)/2$.

2.3.2 Spatial Variation of the Time Derivative

The time derivative, in the governing equations can either be assumed constant over a cell or to vary in some fashion *consistent* with underlying space discretization. With finite volume/difference methods, as used here, the former *lumped approach*, indicated for one-dimension in Fig. 2.2, is adopted. For finite elements, the later *consistent formulation* is common. With this, the time derivative is multiplied by what is called a mass or capacitance matrix. Effectively, this spreads the time derivative over several nodes. For a one-dimensional uniform mesh case, involving linear shape functions/elements the capacitance or mass operators are such that $M_{i-1} = 1/6$, $M_i = 2/3$, $M_{i+1} = 1/6$. This results in the piecewise-linear $\partial(\rho\phi)/\partial t$ profile indicated in Fig. 2.2. The time derivative spreading will introduce extra computational cost. However, there are accuracy benefits (Fletcher 1997). It is possible

Fig. 2.2 Spatial variation of time derivative



to combine differing discretization techniques, such as having a finite element space discretization with finite difference temporal modelling (Segerlind 1976).

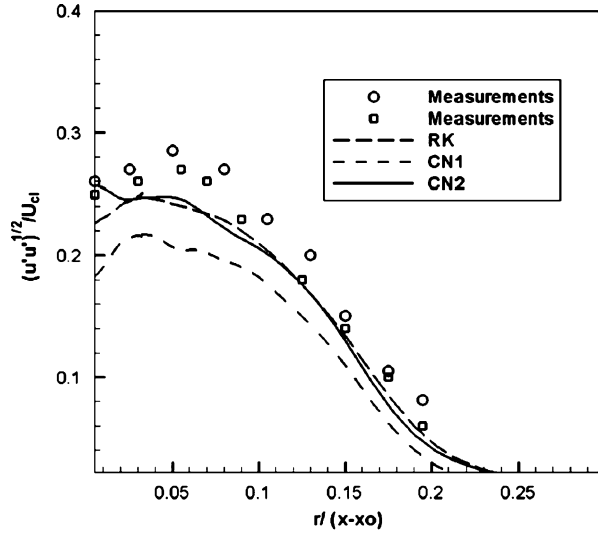
2.4 Two-Level Schemes

A key two-level scheme, finding popularity in more academic LES is the neutrally dissipative Crank-Nicolson (CN) scheme. As with many schemes, it finds different implementations aimed at promoting stability (Giles 2004; Hujeirat and Rannacher 1998) and efficiency (Beam and Warming 1976; Briley and McDonald 1975; Lacor 1999; Jameson 1991). It is possible to use hybridized approaches. For example, in the LES work of Talha (2012) and Manoha et al. (2000) (trailing edge noise) the explicit Adams-Bashforth scheme (see later) is used for the convective terms and CN for diffusive. With regards to CN implementation variants, both one and two-legged discretizations are possible. Here the distinction is being made whether the underlying discretization function is applied to the variable being solved for or some function of it. For LES, all these choices can have a significant impact. For example, as shown in Fig. 2.3, there is an over a 10 % variation in Reynolds stresses, between different CN scheme implementations. The profiles shown are for a free shear flow. The symbols are for two different sets of measurements. The labels, CN1 and CN2 identify the two Crank-Nicolson implementations. CN1 is a stabilized form. Full details for this case can be found in Tucker (2008). Note, for $0.5 \leq \lambda \leq 1$, two-level schemes are unconditionally stable. This does not mean that for $\lambda < 1$ solutions will be physically realistic but instead that errors will reduce with time.

2.4.1 General Explicit Schemes

When $\lambda = 0$ (with $k = \eta = 0$) the explicit forward difference Euler scheme is gained. This first order scheme is stable for $C^2 \leq 2D \leq 1$. The restriction $2D \leq 1$ implies that when the mesh spacing is halved the time-step must be made four times smaller. This is a severe time-step restriction. Therefore, the explicit Euler scheme

Fig. 2.3 Radial variation of streamwise Reynolds stress in self-similar region of a round jet for different temporal schemes (from Tucker 2008). Published with kind permission from Elsevier



is only suitable for problems where high temporal resolution is required and carefully tailored grids can be constructed. The latter requirement avoids needless small cells which place an excessive global time step restriction. For problems where ϕ is changing slowly with time, the time-step restriction makes the scheme inefficient and implicit schemes should be used.

Higher order explicit schemes can be implemented. However, generally the higher the order, the more severe the stability restriction. Explicit methods do not require simultaneous equation solvers. Therefore, they lend themselves to vector and parallel processing.

2.5 Higher-Level Schemes

As termed here, higher-level methods use data stored at several (> 2) levels/points. Generally for industrial CFD applications, no more than 3–4 levels are implemented. The most common multipoint methods are the Adams types. Using polynomial temporal fits both explicit and implicit Adams type schemes can be constructed. The former are referred to as Adams-Bashforth and the latter Adams-Moulton methods. The Adams-Bashforth scheme can be expressed as

$$\phi^{n+1} - \phi^n \simeq \Delta t \sum_{l=0}^p w_{fl} \left(\frac{\partial \phi}{\partial t} \right)^{n-l} \quad (2.4)$$

In the above p defines the number of coefficients that the scheme uses. The application of the Adams-Bashforth method (with CN) to trailing edge noise is given by Manoha et al. (2000). In conjunction with Eqs. (2.2)–(2.3) various Adams multipoint methods can be gained by selecting different values of η , λ and k . Parameter

Table 2.2 Weighting functions for backwards difference schemes

N_{BD}	Wf^{n+1}	Wf^n	Wf^{n-1}	Wf^{n-2}	Wf^{n-3}	Wf^{n-4}
1	1	-1	-	-	-	-
2	3/2	-4/2	1/2	-	-	-
3	11/6	-18/6	9/6	-2/6	-	-
4	25/12	-48/12	36/12	-16/12	3/12	-
5	137/60	-300/60	300/60	-200/60	75/60	-12/60

values, for the implicit 3rd order Adams-Moulton method are given in Table 2.1. Values for other schemes are given by Beam and Warming (1982). Notably, Tam and Webb (1993) optimize the Adams-Bashforth scheme for acoustics problems to minimize dispersion/frequency errors.

The leapfrog (midpoint) scheme, approximates the time derivative using a second order central difference. With stability modifications the scheme is used for meteorological (Hignett et al. 1985) and oceanographic predictions. The DuFort-Frankel is also a three-level, multipoint, second order scheme. It addresses the leapfrog scheme's lack of stability. However, for accuracy there is the severe restriction $C^2 \ll 1$ which limits the scheme's practical use. These schemes find little aerospace application.

2.5.1 Gear Schemes

Gear schemes are implicit backwards difference methods. Hence, for a discretized equation right hand side, A , at a time level $n + 1$ we have the following temporal discretization

$$\left[\frac{\partial \phi}{\partial t} \right]_{BD} = \sum_{n-(N_{BD}-1)}^{n+1} \frac{Wf^n}{\Delta t} = -A^{n+1} \quad (2.5)$$

The weighting functions, Wf , for the different order backwards difference (N_{BD}) schemes are given in Table 2.2.

As can be seen from Appendix A, even for a 5th order Gear scheme the numerical error can be higher than for the CN scheme. Hence, the latter lower storage scheme seems preferable and accuracy grounds. However, stability is lower and, especially in an industrial context, this is important. Higher level schemes can need more careful attention to starting solutions—more data is needed.

2.6 Other Temporal Discretization Methods

Predictor-corrector methods are another key class of temporal scheme. Probably the most widely used temporal integration schemes in aerospace engineering, especially

Table 2.3 Some Runge-Kutta scheme coefficients

Coefficient	SRK4	LDDRK5-BB	LDDRK6-BB	LDDRK4-H	LDDRK5-H	LDDRK6-H
Wf_1	1	1	1	1	1	1
Wf_2	1/2	1/2	1/2	1/2	1/2	1/2
Wf_3	1/6	0.16525035366	0.16591977136	0.162997	0.166558	1/3!
Wf_4	1/24	0.03937258598	0.04091973204	0.040757	0.0395041	1/4!
Wf_5	–	0.00714909644	0.00755570439	–	0.00781071	0.0078100
Wf_6	–	–	0.00089142126	–	–	0.0013214

for acoustics, are explicit Runge-Kutta (RK) schemes. These are used for both unsteady flows and integrating to steady state solutions. Essentially, the RK technique can be considered as using a carefully selected blend of lower order methods. These are intended to give a desired higher order of accuracy or a larger stability ‘foot print’ in a stability diagram. The blend of lower order methods gives rise to multiple stages of solutions with different weighting coefficients— Wf . Explicit Runge-Kutta methods are most common. However, there are implicit variants that allow larger C . Explicit RK schemes offer the potential for high order with low storage. Most RK schemes are tuned to have an enlarged stability foot print. However, optimizing for stability potentially makes them unsuited to computational acoustics. For this, small amplitude, long length waves generally need to be accurately modeled over considerable distances. Also, as will be discussed later (when dealing with spatial discretizations), a scheme can have a high formal order but not be that accurate at practical time step resolutions. Hence, especially for acoustics, potentially high order schemes can be further optimized to reduce dissipation and dispersion to form what are known as LDDRK (Low Dissipation and Dispersion RK) schemes. For a p stage RK scheme, that advances a solution from the n th to the $n + 1$ time step the following can be written

$$\phi^0 = \phi^n \quad (2.6a)$$

$$\phi^l = \phi^n + Wf_l \Delta t A(\phi^{l-1}) \quad \text{for } l = 1, \dots, p \quad (2.6b)$$

$$\phi^{n+1} = \phi^p \quad (2.6c)$$

where Wf_l are the coefficients of the algorithm. Table 2.3 shows the coefficients for a standard 4-stage scheme (SRK4). This is 4th order for linear systems and 2nd for nonlinear. Also given in the table are 5 (LDDRK5-BB) and 6 (LDDRK6-BB) stage schemes from Bogey and Bailly (2004). The table also includes schemes of Hu et al. (1996) for different numbers of stages (LDDRK*-H). These schemes have been optimized for low dissipation and dispersion. They are likely to show clear benefits for aeroacoustics problems or where such problems are combined with LES.

To look at the numerical error in an RK scheme the amplification factor is needed. This is the ratio, in the frequency domain, of predicted values at the current and previous time steps. In what follows, the operation in the frequency domain is identified

using a tilda as an ‘overbar’. In this domain, the RK scheme looks like (Hu et al. 1996)

$$\tilde{\phi}^{n+1} = \tilde{\phi}^n \left(1 + \sum_{l=1}^p Wf_l (-i u w' \Delta t)^l \right) \quad (2.7)$$

In the above u is the convection speed in the following equation $\partial \phi / \partial t + u \partial \phi / \partial x = 0$ and w' is the numerical wave number. The numerical amplification, r_n , factor can be expressed as

$$r_n = \frac{\tilde{\phi}^{n+1}}{\tilde{\phi}^n} = 1 + \sum_{l=1}^p Wf_l (-i \sigma)^l \quad (2.8)$$

where $\sigma = u w' \Delta t$. As noted by Hu et al. the exact amplification factor is $r_e = e^{-i\sigma}$. The numerical factor, as can be seen, is some polynomial approximation to the analytical amplification factor equation. Indeed, the order of the polynomial used to characterize the numerical amplification reflects the scheme’s potential order. Hence, the maximum order of a p stage scheme is p (Hu et al. 1996). Hu et al. optimize $|r_n - r_e|^2$ as a function of $u w' \Delta t$. This optimizes the sum of the dissipation and dispersion errors. This optimization involves the minimization of the following integral

$$\int_0^\beta \left| 1 + \sum_{l=1}^p Wf_l (-i \sigma)^l - e^{i\sigma} \right|^2 d\sigma \quad (2.9)$$

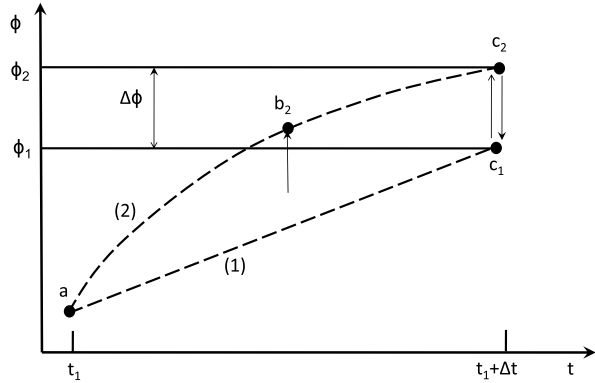
In the above β defines the range of σ for which the optimization applies. Notably, when used in conjunction with high order compact schemes, Kim and Lee (1996) found rather non-monotonic behavior with regards to accuracy benefits and order of RK schemes. Morris et al. (1997) apply the LDDRK scheme of Hu et al. (1996) to the solution of nonlinear disturbance equations (see Chap. 4) when looking at jet noise.

Tam and Webb (1993) optimise the Adams-Basforth scheme with respect to dissipation and dispersion. When giving a 36 % weighting to dispersion error and 64 % to dissipation they come up with the following Eq. (2.4) weighting factors: $Wf_0 = 2.30255809$; $Wf_1 = -2.49100760$; $Wf_2 = 1.57434093$; $Wf_3 = -0.38589142$.

More precise details of this weighting process between dissipation and dispersion is discussed later when dealing with Dispersion Relation Preserving (DRP) spatial schemes.

Splitting methods are a further key class of temporal integration scheme. A disadvantage of implicit methods is the expense of solving large simultaneous equation sets. For explicit methods this is not necessary, but instead there are greater stability restrictions. With splitting methods, implicit and explicit schemes are combined. In certain circumstances improvements in computational performance are made. The most widely known splitting method is the Alternating Direction Implicit (ADI) scheme of Peaceman and Rachford (1955). With this, in two-dimensions, one full time-step Δt , essentially consists of two $\Delta t/2$ half steps. For the first half time-step,

Fig. 2.4 Schematic of basic time step adaptation approaches



spatial derivatives in say an x coordinate direction are treated implicitly while those in the y direction are treated explicitly. For the second half step, this procedure is reversed. Douglas and Gunn (1964) presents a second order splitting scheme which in three-dimensions is unconditionally stable.

2.7 Elementary Solution Adapted Time-Step Approaches

As noted, through the method of lines, the discretized flow equations can be cast as temporal ODEs. Then, in principle, any standard time adaptive ODE approach (Press et al. 1989; Ascher and Petzold 1998; Brenan et al. 1996) can be applied to the solution of the unsteady flow equations. Possible standard approaches have many similarities to spatial adaptations. Temporal truncation error estimates are here initially grouped into the following four classes:

- (I) Altered Scheme—solutions for schemes of the same order but different natures are made. By analysis of truncated Taylor series terms solution errors can be inferred;
- (II) Altered Step—solutions with one long and two short time-steps are compared and
- (III) Altered Order—solutions of different orders are compared.

Figure 2.4 gives a schematic of two potential comparative solutions (1) and (2). These can be used in assessing the temporal truncation error, where $\Delta t \propto \phi_2 - \phi_1$. Solution Element (1) ($a-c_1$) could involve lower accuracy. Element (2) ($a-b_2-c_2$) either involves two reduced steps or one high order step. Alternatively, elements (1) and (2) can have schemes of the same order but different natures.

Gresho et al. (1984), when using a 1st order forward/backward Euler procedure show from Taylor's series, for a scheme of order $n - 1$, that

$$\Delta t^{new} = C_t \Delta t^{old} \left| \frac{\varepsilon}{E^{old}} \right|^{1/n} \quad (2.10)$$

where the superscripts ‘new’ and ‘old’ refer to solutions for different step sizes, ‘new’ being the latest. The parameter, ϵ , is a pre-set normalised error input value. This enables the maximum temporal solution error to be specified ($\epsilon = 0.001$ corresponds to about a 0.1 % solution error). Also, C_t , is a safety factor. The time step must be spatially constant for all the solution variables (N_ϕ). Hence, $E^{old} \propto \phi_2 - \phi_1$ (the difference in the solution for the two schemes or step lengths), needs to be a spatially averaged (or more conservatively a maximum) normalised (to be consistent with the ϵ definition) value. Gresho et al. propose the following average

$$E^{old} = \left[\frac{1}{N_\phi} \sum_{i=1}^{N_\phi} \left(\frac{1}{N_{P\phi}} \sum_{j=1}^{N_{P\phi}} \left(\frac{E_{P\phi}^{old}}{|\phi_P^{old}| + \phi_o} \right)^2 \right) \right]^{1/2} \quad (2.11)$$

where $N_{P\phi}$ is the number of nodal points for each variable (this is generally the same for all variables) and ϕ_o a reference scale. Evaluation of Eq. (2.11) requires storage of two full solutions. Hence, for a three-dimensional system it gives a significant storage burden. Also, it would seem a more refined volume weighting would be better. Some approaches to overcome this storage burden are outlined in Tucker (2002a).

Equation (2.10) is also arrived at when considering schemes of different order (Press et al. 1989; Skelboe 1977) or solutions of different step length. When using different step lengths three solutions are required, two of these being used in the error estimate. Whether the benefits of being able to adapt time-steps outweigh the significant computational overhead is likely to be problem dependent. As noted by Ascher and Petzold (1998), step-doubling approaches, although easy to implement, can be relatively expensive. When using higher order schemes with adaptive step strategies, instabilities and hence oscillations can occur. To help with this, the order of schemes can be limited (Brenan et al. 1996).

2.7.1 Relating Error Estimate to New Time-Steps

The error estimate is related to Δt through Eq. (2.10). Again, there are many ways in which Eq. (2.10) can be used. For stability reasons (Skelboe 1977), ideally, the maximum *swing* ($(\Delta t^{new} / \Delta t^{old})_{\max}$) should be restricted. According to Ascher and Petzold (1998), Δt^{new} should also be limited to avoid round-off error. Tucker (2001) notes various time-step update protocols used by different workers.

The inferred computed error estimate can be used to effect a Richardson type extrapolation. If the time-steps are sufficiently small, this should yield an improvement to the solution. However, the radius of convergence of the Taylor (power) series is small. Hence, attempting this is probably best avoided. Tucker (2002a) explores the use of subcycling with adaptive time stepping (Gresho et al. 1984). With this, selected data is interpolated from the 1st to the 2nd comparative step. The objective being to make the 2nd step computationally cheaper.

2.7.2 Alternative Techniques

Predictor-corrector methods naturally lend themselves to time adaptation (Ascher and Petzold 1998). Gresho et al. (1980) successfully apply this, to a wake flow, in FIDAP (a commercial CFD program), with a second order Adams-Bashforth predictor step. Further adaptive time step studies for different applications are given by Tu et al. (1992), Reindl et al. (1991) and Hujerir and Rannacher (1998). Crudely, the commercial CFX4 (Glanfield 2000) program adapts time-steps with respect to convergence rates. Muramatsu and Ninokata (1992) apply a novel fuzzy logic based Δt adaptation procedure. Bell and Surana (1994) use temporal adaptation in a space-time finite-element procedure. Based on integral error estimates, element sizes in the time domain are adapted (this is only done after spatial accuracy refinements fail to reduce errors below a specified level). Im (2000) successfully applies an adaptive time integration based around a variable-order, variable-step backwards differentiation formula to the modelling of a transient flame flow.

2.8 Unsteady Adjoint and Time Step Adaptation

The adjoint process has the accuracy of an objective function in mind. Then using a Taylor series we can write an estimate for an exact time domain objective $C_{\Delta t}(\phi_{\Delta t})$ about an estimate $C_{\Delta t}(\phi_{\Delta t}^{\Delta T})$ as

$$C_{\Delta t}(\phi_{\Delta t}) \approx C_{\Delta t}(\phi_{\Delta t}^{\Delta T}) + \left[\frac{\partial C}{\partial \phi} \right]_{\phi_{\Delta t}^{\Delta T}} (\phi_{\Delta t} - \phi_{\Delta t}^{\Delta T}) \quad (2.12)$$

In the above, $\phi_{\Delta t}^{\Delta T}$ represents a variable computed with a coarse time step of ΔT and represented on a finer temporal ‘grid’ of Δt . Similar, to Eq. (2.12) the residual vector, A , can be expressed as

$$A_{\Delta t}(\phi_{\Delta t}) \approx A_{\Delta t}(\phi_{\Delta t}^{\Delta T}) + \left[\frac{\partial A}{\partial \phi} \right]_{\phi_{\Delta t}^{\Delta T}} (\phi_{\Delta t} - \phi_{\Delta t}^{\Delta T}) \quad (2.13)$$

The above can be rearranged as

$$\phi_{\Delta t} - \phi_{\Delta t}^{\Delta T} = [A_{\Delta t}(\phi_{\Delta t}) - A_{\Delta t}(\phi_{\Delta t}^{\Delta T})] \left[\frac{\partial A}{\partial \phi} \right]_{\phi_{\Delta t}^{\Delta T}}^{-1} \quad (2.14)$$

Note, since

$$A_{\Delta t}(\phi_{\Delta t}) = 0 \quad (2.15)$$

Equations (2.12) and (2.14) can be combined to give

$$C_{\Delta t}(\phi_{\Delta t}) = C_{\Delta t}(\phi_{\Delta t}^{\Delta T}) - \left[\frac{\partial C}{\partial \phi} \right]_{\phi_{\Delta t}^{\Delta T}} \left[\frac{\partial A}{\partial \phi} \right]_{\phi_{\Delta t}^{\Delta T}}^{-1} A_{\Delta t}(\phi_{\Delta t}^{\Delta T}) \quad (2.16)$$

The furthest right hand group of terms in Eq. (2.16) are an estimate of the solution error

$$E = - \left[\frac{\partial C}{\partial \phi} \right]_{\phi_{\Delta t}^{\Delta T}} \left[\frac{\partial A}{\partial \phi} \right]_{\phi_{\Delta t}^{\Delta T}}^{-1} A_{\Delta t}(\phi_{\Delta t}^{\Delta T}) \quad (2.17)$$

Alternatively, the above could be viewed as a solution correction. For computational efficiency and convenience the following adjoint variable is defined

$$\Lambda_{\phi_{\Delta t}^{\Delta T}}^T(\phi_{\Delta t}^{\Delta T}) = - \left[\frac{\partial C}{\partial \phi} \right]_{\phi_{\Delta t}^{\Delta T}} \left[\frac{\partial A}{\partial \phi} \right]_{\phi_{\Delta t}^{\Delta T}}^{-1} \quad (2.18)$$

Or, rearranging

$$\left[\frac{\partial A_{\Delta t}}{\partial \phi_{\Delta t}} \right]_{\phi_{\Delta t}^{\Delta T}}^T \Lambda_{\phi_{\Delta t}^{\Delta T}}(\phi_{\Delta t}^{\Delta T}) = - \left[\frac{\partial C}{\partial \phi} \right]_{\phi_{\Delta t}^{\Delta T}}^T \quad (2.19)$$

However, Eq. (2.19) needs solution on the fine time domain and this we seek to avoid. Hence, it is rewritten as

$$\left[\frac{\partial A}{\partial \phi} \right]_{\phi_{\Delta T}}^T \Lambda_{\phi_{\Delta T}} = - \left[\frac{\partial C}{\partial \phi} \right]_{\phi_{\Delta T}}^T \quad (2.20)$$

The above is a simultaneous equation set. It needs to be solved by backwards integration in time. The coarse time domain adjoint is interpolated onto the fine time domain. Of note is the matrix structure in Eq. (2.20). This is given below

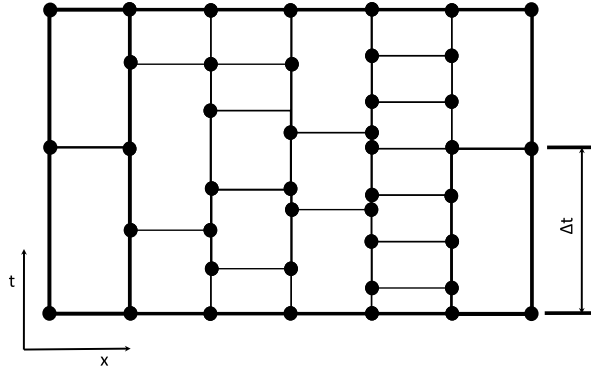
$$\begin{bmatrix} - & & \\ & - & \\ & \left[\frac{\partial A^{n-2}}{\partial \phi^{n-2}} \right] & \left[\frac{\partial A^{n-1}}{\partial \phi^{n-2}} \right] \\ & & \left[\frac{\partial A^{n-1}}{\partial \phi^{n-1}} \right] & \left[\frac{\partial A^n}{\partial \phi^{n-1}} \right]^T \\ & & & \left[\frac{\partial A^n}{\partial \phi^n} \right]^T \end{bmatrix} \begin{bmatrix} - \\ \Lambda_{\phi, \Delta T}^{n-2} \\ \Lambda_{\phi, \Delta T}^{n-1} \\ \Lambda_{\phi, \Delta T}^n \end{bmatrix} = - \begin{bmatrix} - \\ \left[\frac{\partial C}{\partial \phi^{n-2}} \right]^T \\ \left[\frac{\partial C}{\partial \phi^{n-1}} \right]^T \\ \left[\frac{\partial C}{\partial \phi^n} \right]^T \end{bmatrix} \quad (2.21)$$

Once $\Lambda_{\phi, \Delta T}$ has been computed, this field is interpolated onto the fine time ‘mesh’. The error, E , is computed from

$$E = \Lambda_{\phi_{\Delta t}^{\Delta T}}^T A_{\Delta t}(\phi_{\Delta t}^{\Delta T}) \quad (2.22)$$

The backwards integration, needed for the adjoint variable, means that an entire time solution is needed prior to the integration of this equation. Hence, this presents storage challenges (Mani and Mavriplis 2007). Despite this, Rumpfkeil and Zingg (2007) apply the unsteady approach that has just been noted, to the control of a range of unsteady flows. Ad hoc procedures are used to reduce the computational cost. These include storing/using data every other time step.

Fig. 2.5 A typical mesh, with a single spatial dimension



2.8.1 Adjoint Methods for Unsteady Flow Design Optimization

Adjoint methods enjoy most popularity for design optimization. However, the need to store adjoint time histories precludes practical use for unsteady flows. Despite this, Rumpfkeil and Zingg (2007) apply the unsteady approach to the control of a range of unsteady flows. Helpfully, turbomachinery calculations, for example, can involve flows with a discrete unsteadiness frequency(s), ω . Then, harmonic methods can be used where the flow variables, ϕ , are assumed to vary as

$$\phi(x, t) = \bar{\phi}(x) + A(x)\cos(\omega t) + B(x)\sin(\omega t) \quad (2.23)$$

Hence, if ω is specified, the unsteady flow time history is described if $\bar{\phi}(x)$, $A(x)$ and $B(x)$ are defined. Hence, the optimization problem is reduced to one involving *steady* equations. This makes the application of adjoints considerably simpler. The approach, (see Chap. 4) is extendable to multiple harmonics. Using the above harmonic approach, He and Wang (2011) carry out concurrent aerodynamic and aeroelastic adjoint based design optimization for a compressor fan.

2.9 Temporal Adaptation Using Space-Time Elements/Volumes

With space-time methods a mesh that extends into the temporal domain is used. Based on the temporal truncation error, this mesh can be adapted in time (Mani and Mavriplis 2010) or in space also. A key attraction of this approach is that regions of high unsteadiness activity can be treated with smaller time steps than the rest of the domain. The governing equations, in say a finite volume method, are integrated around temporal as well as spatial edges. A typical mesh, with a single spatial dimension, is shown in Fig. 2.5. With time varying, spatial mesh deformation the space-time domain could look as shown in Fig. 2.6.

Fig. 2.6 Mesh, with a single, time-adapting, spatial dimension

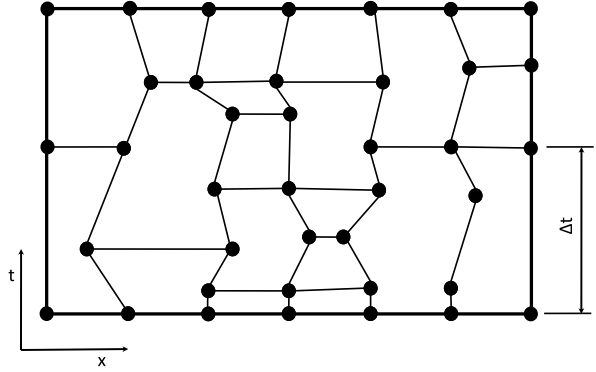
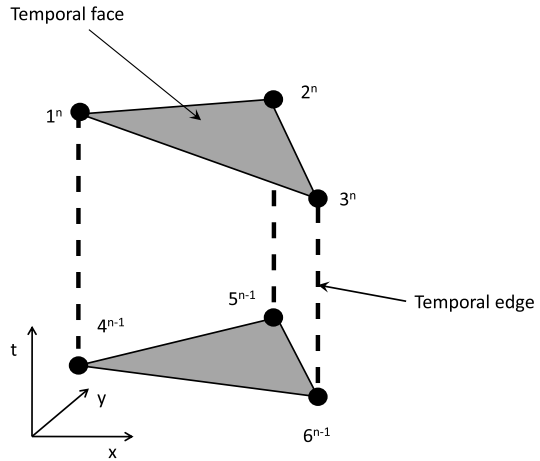


Fig. 2.7 A space-time element at two time locations (shaded zones are the areas of the temporal faces)



For the temporal discretization, the solution variable, ϕ , is assumed to vary in a piece-wise constant fashion. The time derivative is expressed as

$$\int_T \frac{dA\phi}{dt} dt = \frac{dA\phi}{dt} \Delta t \quad (2.24)$$

In the above, Δt is the edge length in the time-domain. Also, the A in the above is the face area normal to the time coordinate. This can be seen in Fig. 2.7. The time derivative is then discretized as the finite difference below

$$\frac{dA\phi}{dt} \Delta t = A^n \phi^n - A^{n-1} \phi^{n-1} \quad (2.25)$$

The n superscripts indicate different time levels. The time domain can essentially be assumed to be treated with upwind type differences. The spatial fluxes are integrated over space-time faces e.g. face 2–3–6–5 in Fig. 2.7. A space-time finite element procedure is outlined by Bell and Surana (1994).

With the space-time approach, where there are moving wake or shock zones, for example, the extent of the element faces in time can be reduced. It can be extended in the calmer (more steady) flow zones.

2.10 Convective Schemes for Unsteady Flow

In unsteady flows, particularly high gradients of variables can arise. This places greater demands on convective differencing schemes. As shown by Orkwis et al. (2002) and also noted by Fritsch and Giles (1992) unsteady flow related numerical artifacts can account for a significant proportion of predicted energy losses in turbomachinery blade rows. Also, (see Fritsch and Giles) numerical smoothing can erroneously drain unsteady flow energy from the main turbine passage zone (outside boundary layers). Therefore, for unsteady flows the use of specialized spatial schemes can be important.

It is also important to understand the spatial schemes interaction with the temporal (Kim and Lee 1996). For example, the accuracy of QUICK (a quadratic upstream biased interpolation—Leonard 1979) with first order forward Euler time differencing is essentially no better than when first order spatial upwinding is used (Nasser and Leschziner 1985). Therefore, it is best adapted, in a similar fashion to Leith's (1964) central difference based scheme, with extra terms that extend control volume face interpolations to include forward in time (linear in the case of Leith's scheme) estimates. This is the essence of QUICKEST (QUICK with Estimated Streaming Terms (EST)). Davis and Moore (1982) present a multi-dimensional version of QUICKEST, showing that a third order temporal integration is effectively gained from the lower order temporal scheme. Glass and Rodi (1982), Roache (1992), and Wallis and Manson (1997) present schemes which to varying degrees (the former loosely) are related to the EST approach. Glass and Rodi make use of a cubic Hermitian interpolation. These are also made use of in compact schemes (see later) by Tang and Baeder (1998).

The above EST related methods are also members of a family called semi-Lagrangian methods. This name arises because they can be partly derived by considering the Lagrangian trajectories of scalars on an Eulerian grid. Staniforth and Côté (1991) give a thorough review of semi-Lagrangian approaches, noting that, in one-dimension, the Eulerian Lax-Wendroff scheme can be considered as a special case of the semi-Lagrangian schemes.

An unusual, semi-Lagrangian related approach—ICED-ALE—is presented by Hirt et al. (1974). A similar technique called LINC is given by Butler (1971). These schemes are extensions to an earlier ALE (Arbitrary-Lagrangian-Eulerian) method devised by Hirt, in which grid nodes can be held fixed (Eulerian), move with the fluid (Lagrangian) or in any prescribed manner. Clearly, moving the grid with the flow, reduces the magnitude of the problematic convective terms. However, severe grid distortion can occur. It seems appropriate to mention here the fully Lagrangian vortex method (Khatir 2000). With this, vortex blobs or elements are convected with the flow in a Lagrangian fashion. Such approaches remove the convective term modelling problem but accounting for diffusion then becomes problematic.

Gresho et al. (1984) presents the Balancing Tensor Diffusivity (BTD) scheme (previously described by Dukowicz and Ramshaw 1979 and Crowley 1967). This involves adding a contribution to the physical diffusion term. This cancels the negative false contribution arising from the forward Euler scheme. For three-dimensional flows, to apply BTD, cross-stream diffusion terms are necessary and 19 stencil points are needed. The aforementioned schemes see little aerospace use being more of historical and academic interest.

For especially high spatial accuracy, *spectral* methods (generally involving a Fourier series based discretization, the order of which increases with the number of grid points) can be used. However, for complex geometries, these methods are of limited use. To extent these geometrical restrictions are overcome using *spectral element* techniques (Patera 1984) or compact difference schemes (Lele 1992) that have spectral like behaviour.

An interesting class of schemes is the kinetic energy (Jameson 2008b) and energy (Jameson 2008a) conserving. Kinetic energy conservation properties are ideal for LES and DNS. In practical terms, the approach seems to offer substantial gains in stability—even for flows with shocks (Allaneau and Jameson 2010a). The kinetic energy conserving scheme is simple to implement. It just needs a localized change in the way variables are averaged at the control volume interface straddled by the adjacent nodes. Hence, if L and R are nodes of cells adjacent to face LR, for kinetic energy conservation the momentum flux should satisfy the following condition

$$[\rho u_i u_j]_{LR} = \frac{1}{2}(\rho u_i)_{LR}(u_{j,L} + u_{j,R}) \quad (2.26)$$

The boundary conditions also need, ideally, to be reformulated to ensure global energy conservation and care needed with the pressure and other stress terms. The potential formulations for $(\rho u_i)_{LR}$ are discussed by Allaneau and Jameson (2010a). Modification (2.26) essentially means that the skew-symmetric form (see later) of the convective term is being solved for. This, on fine enough grids, results in the need for little smoothing—if any (giving a useful computational time saving). Later, tests are presented, showing the impact of unstructured cell topology for homogeneous decaying turbulence. Although results are not shown here, for these cases, the kinetic energy conserving scheme dramatically reduces the sensitivity of results to cell topology. The use of the approach in a DNS study for a plunging aerofoil is given by Allaneau and Jameson (2010b). Note, the use of staggered grids also ensures energy conservation (Kim and Moin 1985). However, this approach is considerably more complex to implement even in a basic structured solver.

2.11 Classical High-Order Approaches

2.11.1 Compact Schemes

Compact (or Pade) schemes are attractive in that they allow use of a relatively small finite difference stencil to gain high order accuracy. Broadly speaking they allow

better resolution at higher waves numbers and offer the potential of spectral type accuracy but with greater geometrical flexibility. With regards to modern parallel computing, the smaller stencil of the compact scheme, has the attraction that the overlap at halo cells, at the grid interfaces, is smaller. Hence, there is less data flow. On the other hand, if applied in an implicit framework a tri-diagonal matrix inversion is required in every coordinate direction, for every variable and derivative for every iteration. In explicit mode the matrix inversions just need to be carried out every time step. Hence, even then this is costly. For a function, ϕ , a compact scheme, for a first derivative, on a uniform grid, can be expressed as

$$Wf_{i-1}\phi'_{i-1} + Wf_i\phi'_i + Wf_{i+1}\phi'_{i+1} = \alpha \frac{\phi_{i+1} - \phi_{i-1}}{2\Delta x} + \beta \frac{\phi_{i+2} - \phi_{i-2}}{2\Delta x} \quad (2.27)$$

Hence, it is not just the nodal values that are unknowns but also the derivatives at these nodal points. The coefficients in the above can be evaluated from Taylor series expansion about node i and some manipulation. Equation (2.27) can be expressed symbolically as

$$(A\phi')_i = (S\phi)_i \quad (2.28)$$

On a uniform grid, the compact scheme will have better resolution (Note, resolution of a scheme is often defined as the minimum number of grid points per wavelength that a scheme needs to resolve a wave to reasonable accuracy and will be discussed further later) than the a finite difference scheme of equivalent order. For 2nd derivatives, the following equation can be used

$$\begin{aligned} & Wf_{i-1}\phi''_{i-1} + Wf_i\phi''_i + Wf_{i+1}\phi''_{i+1} \\ &= \alpha \frac{\phi_{i+1} - 2\phi_i + \phi_{i-1}}{\Delta x^2} + \beta \frac{\phi_{i+2} - 2\phi_i + \phi_{i-2}}{4\Delta x^2} + \gamma \frac{\phi_{i+3} - 2\phi_i + \phi_{i-3}}{9\Delta x^2} \end{aligned} \quad (2.29)$$

Table 2.4 gives the coefficients for different 4th and 6th order accuracy compact schemes. Note, the final table elements are for a 6th order compact scheme. This is designed to be dissipative at higher waves numbers (Laizet and Lamballais 2009). The dissipation is intended to reduce aliasing errors. Hence, as with DRP schemes, the resolution of a scheme can be improved at the potential sacrifice of order. For example, Lele (1992) imposes the constraint that, at selected wave numbers, the scheme gives an exact correspondence between the actual and computed wave number. Kim and Lee (1996) used a more refined optimization approach connected to the concepts used for DRP. They also explore the complex relationship between solution accuracy and RK temporal integration order—finding this to be non-linear. Tang and Baeder (1998) use Hermetian polynomial and trigonometric series based approaches to perform further optimizations of compact schemes. To reduce the potential stencil size, in the matrix inversion embodied in Eq. (2.28), Hixon (2000) proposes a pre-factorization stage. Hence, a pentadiagonal system can be replaced, for example, by the product of tridiagonal systems. This approach, evidently, also makes the enforcement of boundary conditions more straightforward and is tested for a range of benchmark acoustic problems.

Table 2.4 Coefficients for different compact schemes

Derivative	Order	Wf_{i-1}	Wf_i	Wf_{i+1}	α	β	γ
ϕ'_i	4	—	1	—	3/2	0	0
ϕ''_i	4	1/10	1	1/10	6/5	0	0
ϕ'_i	6	1/3	1	1/3	14/9	1/9	0
ϕ''_i	6	2/11	1	2/11	12/11	3/11	0
ϕ'''_i	6	0.479598	1	0.479598	0.42090	1.70207	−0.1637

Compact schemes can also be used for filtering (Lele 1992). Joo and Durbin (2009) use them, to gain stability when making hybrid RANS-LES (see Chap. 4) type computations of an idealized turbine blade.

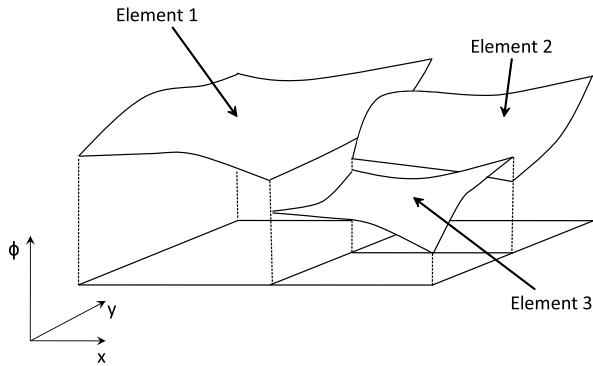
2.11.2 Discontinuous Galerkin Scheme

Another means of getting high order on a compact stencil is through use of the Discontinuous Galerkin (DG) method. The method is similar to the Galerkin finite element method in that a shape function is used. The discontinuous shape function fields are (weakly) connected at boundaries through boundary conditions. The discontinuous shape function fields are shown in Fig. 2.8. At the discontinuous interfaces concepts from approximate Riemann solvers are used. The cells have multiple degrees of freedom. Hence, in LES/DNS grid node count terms, it is not straightforward to make direct comparisons when trying to explore computational performances. Interestingly, Broeckhoven et al. (2007), point out that unstructured triangular grids have better dissipation and dispersion properties for this approach than quadrilateral cells. This aspect is very different to when conventional finite volume methods are used. However, Broeckhoven et al. (2007) note that increased computational cost is to be expected relative to more conventional approaches. For the discontinuous Galerkin method, the mass or capacitance matrix is no longer global and evidently this is computationally convenient (Broeckhoven et al. 2007). An obvious key advantage of discontinuous Galerkin methods is that the small stencil will ensure low communication time when performing distributed parallel processing.

de Wiart et al. (2012) apply the DG method to the DNS for a low-pressure turbine. Wave number against modified wave number plots (real and imaginary) are presented in this work. These suggest the scheme has accurate dispersion properties. However, the dissipative, at high wave numbers, are larger than conventional high order finite difference schemes.

Atkins and Lockard (1999) apply the discontinuous Galerkin method to noise scattering from a two-dimensional slat and a three-dimensional generic wing-body configuration. The linearized Euler equations are solved. In 5th order mode the approach is found to be able to model the propagation of a wave to 100 wavelengths with just 3 % error and just 2 points per wavelength. The approach is

Fig. 2.8 Broken functions of high order polynomials used for the shape functions in the discontinuous Galerkin method (Adapted from de Wiart et al. 2012)



also found to give good parallel speedup and accuracy to be resilient to grid expansion. Stanescu et al. (2002) apply the discontinuous Galerkin method to sound propagation from an engine with a wing and fuselage. The non-linear Euler equations are solved. Birkefeld and Munz (2012) observe that without careful formulation, the discontinuous Galerkin method can be sensitive to grid quality and instabilities can arise after long integration periods. When solving the linearized Euler equations they utilize a hybrid approach. With this, near complex geometrical surfaces the unstructured discontinuous Galerkin method is used. This is linked to high order structured Cartesian grid zones away from surfaces. These have greater computational economy. The complete system is solved to 4th order in space and time.

2.11.3 Spectral Difference, Volume and CPR Methods

The spectral difference (SD) method is intended to be a simpler, more computationally economical alternative to DG (Wang et al. 2007), Spectral Volume (SV), and other high order methods for unstructured grids. The SD and SV (Liu et al. 2006) methods are similar to DG making use of piece-wise discontinuous polynomials. The DG, SV and SD methods are analogous to Galerkin finite element, finite volume and finite difference (Wang et al. 2007) techniques. The SD method of Wang et al. stores discrete variables within each cell in a rigid structured fashion. Thus it hybridizes some of the advantages of structured and unstructured approaches. The SV has a similar sub-cell structuring. Liu et al. demonstrate the application of SV to wave propagation. The correction procedure via reconstruction (CPR) scheme evidently unifies the above along with DG (Haga et al. 2011). The preliminary application of this approach to an ILES of an SD7003 aerofoil with transitional flow is given by Vermeire et al. (2013).

2.11.4 ENO/WENO

The ENO (Essentially Non Oscillatory—see Harten et al. 1987) and WENO (Weighted Essentially Non-Oscillatory—see Liu et al. 1994) schemes are an important class of method. They can be extended to arbitrary order. With them, a combination of stencils/polynomials of equal order and hence equal number of stencil points are used. However, the stencil points used have different levels of upwind and downwind bias. In smooth regions, a weighted combination of all stencils is used. For ENO, where oscillations are detected, one member of the family of stencils is used. The least oscillatory is selected. For WENO, at oscillations, the full family is used but with altered weightings. Typically, a smoothness indicator—based on pressure gradients—is used to activate the stencil/blending control. As noted by Hadjadj (2012), in LES terms the experiences of WENO performance are mixed. For example, when exploring shock/boundary layer interactions, Hadjadj just uses the WENO scheme around the shock. A standard centered scheme is used elsewhere.

2.12 High Resolution Spatial Schemes

2.12.1 DRP Schemes

Typically with numerical methods we first think of the order of a scheme. This can be established from use of the Taylor series. However, we also need to consider the resolution of a method. This relates to considering the dissipation and dispersion errors of schemes (both spatial and temporal). The can be ascertained through Fourier analysis. The DRP schemes look at both the accuracy and resolution of schemes. They seek a best compromise between these two aspects to yield the potentially most efficient scheme. Hence, we might approximate a first order derivate as below

$$\left. \frac{\partial \phi}{\partial x} \right|_i = \frac{1}{\Delta x} \sum_{k=-N}^N Wf_k \phi_{i+k} \quad (2.30)$$

With DRP (Tam and Webb 1993) the coefficients in the above are compromised from what they would be for a standard high order scheme so that the scheme's resolution is improved. Since the scheme of Tam and Webb is a 4th order centered/symmetric, just the dispersion error is optimized through considering the integral below

$$E = \int_{-\beta}^{\beta} |w\Delta x - w'\Delta x|^2 d(w\Delta x) \quad (2.31)$$

where w is the true wave number, w' the computed and β the optimization range. Tam and Webb optimize for wavelengths greater than $4\Delta x$. Lockard et al. (1995)

Table 2.5 DRP scheme coefficients from Broeckhoven et al. (2007)

Source	Wf_0	$Wf_1 = Wf_{-1}$	$Wf_2 = Wf_{-2}$	$Wf_3 = Wf_{-3}$
Tam and Webb (1993)	0	0.79926643	-0.18941314	0.02651995
Tam and Shen (1993)	0	0.77088238	-0.16670590	0.20843142

optimize for wavelength greater than $7\Delta x$. They consider the value of Tam and Webb too restrictive a constraint, corrupting accuracy in the low wave number range. Table 2.5 gives some DRP scheme coefficients, for Eq. (2.30) as summarized in Broeckhoven et al. (2007). Because the DRP scheme is centered and non-dissipative some smoothing can be required for stability. Another way of looking at this is that although the DRP schemes will precisely model long wave components they can also support short waves. Hence, point-wise oscillations can be found, as with standard centered finite difference schemes. These waves can propagate at extremely high velocities relative to the short wave components. Indeed, as noted by Tam et al. (1993) for the wave velocity, c , the following can be written

$$c \approx \frac{dw'}{dw} \quad (2.32)$$

Although Fig. 2.12a relates to standard compact and finite difference schemes it has a typical shape. The application of Eq. (2.32) to this curve will show that the numerical wave speed will become high at high wave numbers. The differentiation of the Fig. 2.12a curves will give a zone where $c \approx 1$ corresponding to long and well-resolved waves. There is also a zone where $0 < c < 1$ corresponding to dispersive waves. Finally, there is a zone where $c < 0$. This corresponds to what Tam et al. call ‘parasite waves’. These travel at high speed and relate to the point-wise oscillations often observed in CFD with centred schemes. Tam et al. observe that these waves can be generated by non-smooth initial data.

To deal with these contaminating waves, Lockard et al. (1995) develop an asymmetric DRP scheme i.e. it has an offset or upwind type stencil. The dissipation means that w' has an imaginary part. Hence, when optimizing the scheme both the real and imaginary parts need to be considered and also the sign of the imaginary part. Hence, a weighting must be assigned to these two components in the optimization

$$E = \int_{-\beta}^{\beta} [Wf[\Re(w\Delta x - w'\Delta x)]^2 + (Wf - 1)(\Im(w'\Delta x))^2] d(w\Delta x) \quad (2.33)$$

In the above, Wf is a weighting function to change the emphasis between controlling dissipation and dispersion. Also, $\Re$ and $\Im$ identify the real and imaginary parts, respectively. However, the imaginary part can have differing signs and the negative part corresponds to dissipation. To ensure a negative imaginary part Lockard et al.

(1995) modify the equation above to

$$E = \int_{-\beta}^{\beta} [Wf[\Re(w\Delta x - w'\Delta x)]^2 + (Wf - 1)(\Im(w'\Delta x) - Wf_1 \sin^{Wf_2}(w\Delta x/2))^2] d(w\Delta x) \quad (2.34)$$

where Wf_1 and Wf_2 are further control parameters. With Wf_1 negative (or zero) and Wf_2 a positive integer, dissipation (negative w') can be enforced.

The alternative to the approach of Lockard et al. is to specifically add a smoothing term. Again, the order of this can be controlled but also the wave number components that are damped. This strategy is similar to the well-known approach adopted by Jameson et al. (1981) who use 2nd and 4th order derivatives. Tam et al. (1993) produce a selective damping that is only active at high wave numbers. Also, crude explicit filtering can be used.

Notably, Morris et al. (1997) apply Tam and Webb's 4th order DRP scheme to the solution of nonlinear disturbance equations (see Chap. 4) when looking at jet noise. Agarwal and Morris (2000) use the approach to explore acoustic scattering from a ROBIN rotorcraft fuselage. Again, the 4th order DRP scheme is used but this time it is applied to the linearized Euler equations.

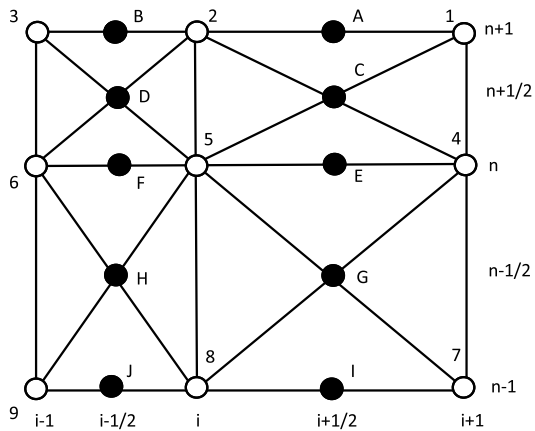
2.12.2 CABARET

CABARET (Compact Accurately Boundary-Adjusting high-REsolution Technique) is a distinctive, explicit, upwind, leapfrog based, second-order method (Karabasov and Goloviznin 2007, 2009). It extends the original work of Iserles (1986) and others. CABARET uses dual staggered variables in a compact space-time computational stencil. The scheme has low dispersion and dissipation error. The dispersion error is as low as that of the fourth order optimized—six order central schemes (Colonius and Lele 2004), for a wide range of wave and CFL numbers. Use is made of the CABARET scheme in Chap. 6. The data structure/stencil is shown in Fig. 2.9. The solid symbols give the locations of variables ϕ . The open symbols identify the location of $f(\phi)$. Unlike standard practice, here the whole indices identify faces and the half the cells. Considering the scalar conservation law $\partial\phi/\partial t + \partial f(\phi)/\partial x = 0$ and the Fig. 2.9 nomenclature the following can be written

$$\frac{\phi_C - \phi_E}{0.5\Delta t^{n+1/2}} + \frac{f_4 - f_5}{\Delta x_{i+1/2}} = 0 \quad (2.35)$$

where $\Delta t^{n+1/2} = t^{n+1} - t^n$ and $\Delta x_{i+1/2} = x_{i+1} - x_i$. The above assumes that all variables are known at the n th time level. Hence, the first stage is a space centred explicit in time predictor step. The time step is a half-step. The next stage involves another half step. However, this is a corrector step. Again it is space centred but this

Fig. 2.9 CABARET data structure for a one-dimensional spatial domain (the solid circles represent the conservation variables and the open flux variables)



time backwards difference in time as given below

$$\frac{\phi_A - \phi_C}{0.5\Delta t^{n+1/2}} + \frac{f_1 - f_2}{\Delta x_{i+1/2}} = 0 \quad (2.36)$$

However, the fluxes f_1 and f_2 need to be determined. These are estimated using a linear extrapolation. Hence, for $f_1 = f_1(\phi)$

$$\phi_1 = 2\phi_c - \phi_5 \quad (2.37)$$

2.13 Convective Schemes for Density Based Solvers and Related Aspects

The convective schemes used in density based solvers can differ quite substantially to those used in pressure based solvers. This is because as well as resolving ‘waves’ convecting at the fluid speed (vortical and entropy) they also capture acoustic waves. For best efficiency there is the need to account for these differing wave speeds. The schemes in density-based codes also generally include some capability to deal with shocks.

Of note is the two-stage Flux Corrected Transport (FCT) SHASTA (Sharp And Smooth Transport Algorithm) of Boris and Book (1973) extended by Book et al. (1975). The first stage involves integrating the governing equations using a strongly diffusive method (incidentally, for this stage, Boris and Book’s scheme has a semi-Lagrangian element), which gives, rise to a monotone solution. The second involves correcting this solution (by correcting fluxes), reducing the diffusive error by introducing an anti-diffusive element. Ideally, the anti-diffusive component is made smaller than the initial diffusive component, leaving, if possible, a residual diffusive component large enough in principal to cancel any dispersive error. The method easily extends to three-dimensions. Unlike SHASTA, to damp shock-induced oscillations, traditional methods can introduce levels of artificial viscosity, which based

on diffusive stability limits, produce severe time-step restrictions. SHASTA has the key disadvantage that the initial diffusive stage can damp out maxima that will not be recovered in the anti-diffusion stage, thus giving rise to erroneous solution clipping. Motivated by this, Chapman (1981) presents the explicit FRAM (Filtering Remedy and Methodology) monotone solution approach. This has three stages. In the first, a higher order scheme is used to give a provisional time advanced solution. During the second stage, based on a local Lagrangian solution, bounds are calculated for the provisional solution. Where the initial solution is outside these bounds sufficient local dissipation is introduced to yield a monotone solution. For the first stage, several predictions presented by Chapman use the second order scheme of Crowley (1967) noted earlier.

By far the most popular density based solver convective scheme is the so-called flux-difference splitting scheme of Roe (1981). This is a Godunov-type scheme. It is based on the solution of a Riemann type problem. A key characteristic is that the control volume face flux interpolation is based on upstream and downstream interpolations to the face. The average of these two interpolations is taken. Also, the level of smoothing is controlled by a matrix of Eigen values. These are based on the difference between the fluid speed and the speed of sound. Notably, Roe's scheme sees wide spread use in LES. However, it was never designed with this purpose in mind. A related approach is flux vector splitting (Steger and Warming 1981). Another, relatively popular density based solver scheme is the Advection Upstream Splitting Method (AUSM)—see Liou and Steffen (1993).

2.13.1 The MUSCL Scheme

The MUSCL scheme (Monotone Upstream-centred Schemes for Conservation Laws) extends the Roe scheme to higher orders (Van Leer 1979). This is achieved through using higher order interpolations both upstream and downstream of the control volume face. This scheme is discussed in more detail later. Since, quite a few of the later results are MUSCL based further details are given below. An inviscid convective flux, E^{inv} , at a control volume face can be approximated as below

$$E_l^{inv} = \frac{1}{2} [E^{inv}(\phi_L) + E^{inv}(\phi_R) - |A|(\phi_R - \phi_L)] \quad (2.38)$$

The subscripts L and R represent left and right control volume face values. These values reside immediately to the left and right of a control volume face. Also, $A = \partial E / \partial \phi$ and ϕ represents primitive variables. The left and right interpolations can be expressed as

$$\begin{aligned} \phi_L = & \phi_{i-1} + [Wf_{i+2}\Delta_{i+2}^\phi l_{i+2} + Wf_{i+1}\Delta_{i+1}^\phi l_{i+1} + Wf_i\Delta_i^\phi l_i \\ & + Wf_{i-1}\Delta_{i-1}^\phi l_{i-1} + Wf_{i-2}\Delta_{i-2}^\phi l_{i-2} + Wf_{i-3}\Delta_{i-3}^\phi l_{i-3}] \end{aligned} \quad (2.39)$$

Table 2.6 Coefficients of ϕ_L for different schemes

ϕ_L	Wf_{i+3}	Wf_{i+2}	Wf_{i+1}	Wf_i	Wf_{i-1}	Wf_{i-2}	Wf_{i-3}
$m = 1$	0	0	0	0	0	0	0
$m = 3$	0	0	0	2/6	1/6	0	0
$m = 5$	0	0	-3/60	24/60	11/60	-2/60	0
$m = 7$	3/420	-22/420	79/420	180/420	-34/420	4/420	0

Table 2.7 Coefficients of ϕ_R for different schemes

ϕ_L	Wf_{i+3}	Wf_{i+2}	Wf_{i+1}	Wf_i	Wf_{i-1}	Wf_{i-2}	Wf_{i-3}
$m = 1$	0	0	0	0	0	0	0
$m = 3$	0	0	0	2/6	1/6	0	0
$m = 5$	0	0	-3/60	24/60	11/60	-2/60	0
$m = 7$	3/420	-22/420	79/420	180/420	-34/420	4/420	0

and

$$\begin{aligned} \phi_R = \phi_i &+ [Wf_{i+3}\Delta_{i+3}^\phi l_{i+3} + Wf_{i+2}\Delta_{i+2}^\phi l_{i+2} + Wf_{i+1}\Delta_{i+1}^\phi l_{i+1} \\ &+ Wf_i\Delta_i^\phi l_i + Wf_{i-1}\Delta_{i-1}^\phi l_{i-1} + Wf_{i-2}\Delta_{i-2}^\phi l_{i-2}] \end{aligned} \quad (2.40)$$

In the above

$$\Delta_{i+n}^\sigma = (\sigma_{i+n} - \sigma_{i+n-1}) \quad (2.41)$$

and

$$l_{i+n} = \frac{L_i}{L_{i+n}}, \quad L_{i+n} = \sqrt{(\Delta_{i+n}^x)^2 + (\Delta_{i+n}^y)^2 + (\Delta_{i+n}^z)^2} \quad (2.42)$$

The values of Wf_{i+n} for various upwind schemes are given in Tables 2.6 and 2.7, where m gives the scheme's order. Note, i is the index in the coordinate direction being considered.

For LES type simulations to control smoothing, Eq. (2.38) is modified to

$$E_l^{inv} = \frac{1}{2} \left[\underbrace{E^{inv}(\phi_L^{cen}) + E^{inv}(\phi_R^{cen})}_{\text{central}} - \epsilon_1 |A| \underbrace{(\phi_R^{dis} - \phi_L^{dis})}_{\text{dissipation}} \right] \quad (2.43)$$

where ϵ_1 is a variable parameter (discussed later) and a value of zero would give a pure central difference. Values above this introduce dissipation. To provide a second-order ($n = 2$) centred term ϕ_L^{cen} and ϕ_R^{cen} use $m = 1$ weighting coefficients. For a 6th order central term the $m = 5$ coefficients are needed. Smoothing terms use $m = 3$ coefficients for the $n = 2$ scheme, and $m = 7$ coefficients for the $n = 6$ scheme. This leads to smoothing to the 4th and 8th power of the derivative being considered for $n = 2$ and $n = 6$ schemes, respectively.

2.13.2 Monotonicity

A desirable numerical scheme property is that it is Total Variation Diminishing (TVD). TVD's basis can be appreciated by considering a one-dimensional convection equation— $\partial\phi/\partial t + u\partial\phi/\partial x = 0$. For a solution, over a domain of length L , a variable called the *total variation*

$$TV = \int_0^L \left| \frac{\partial\phi}{\partial x} \right| dx \quad (2.44)$$

should ideally not increase with time. Based on this correct physical behaviour, TVD schemes are constructed so that

$$\int_0^L \left| \frac{\partial\phi^{n+1}}{\partial x} \right| dx \leq \int_0^L \left| \frac{\partial\phi^n}{\partial x} \right| dx \quad (2.45)$$

Or, if the above differentials are expressed as central differences, the following can be written

$$\sum_{x=0,L} |\phi_{i+1}^{n+1} - \phi_i^{n+1}| = \sum_{x=0,L} |\phi_{i+1}^n - \phi_i^n| \quad (2.46)$$

Enforcing the TVD constraint (introduced by Harten 1983) removes erroneous solution oscillations. TVD schemes are monotonicity preserving. This means that they do not produce any new extrema in a domain of L . Also, all local minima and maxima do not decrease or increase, respectively. To enforce monotonicity, for high order schemes flux or slope limiters are used. These limiters only become active in non-smooth flow regions. Basically, they allow blending of a low-order, high-resolution scheme with a high order but lower resolution scheme. There are numerous limiters. Relatively well known ones are the minmod, superbee (Roe 1986; Van Albada et al. 1982; Van Leer 1977). Limiters are necessary for the proper implementation of MILES schemes. For example, a 3rd order limiter (Drikakis and Rider 2004) results in accurate turbulence energy spectrums.

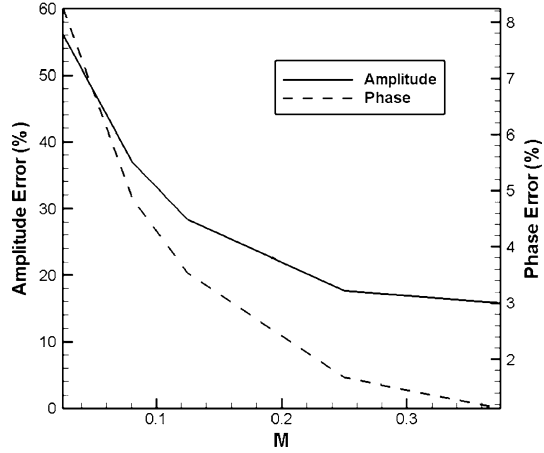
2.14 Preconditioning

It seems worth stressing here that when using a compressible flow solver, at low Mach numbers the smoothing can become excessive and thus damp out flow unsteadiness. As already noted, for compressible flow solvers, as well as being scaled by ε_1 , essentially, the smoothing term is also scaled by a matrix of Eigen values. These have the form

$$\lambda = (u, u, u \pm c) \quad (2.47)$$

The latter Eigen value scales pressure. When, the Mach number is low the magnitude of this Eigen value can become large thus smoothing the pressure field. In

Fig. 2.10 Amplitude and phase errors for different Mach numbers. Published with kind permission from the ASME



practical terms this seems to have a knock on effect for the rest of the flow variables. This is shown in Fig. 2.10 which gives the phase and amplitude errors for a subcritical Tollmien-Schlichting wave. The case setup is discussed in Appendix A. We can see substantial errors with decreasing Mach number.

The essential form of the compressible flow equations can be expressed as

$$\frac{\partial Q}{\partial t} + \frac{\partial E}{\partial x} + \frac{\partial F}{\partial y} = \text{Viscous Terms} \quad (2.48)$$

where $Q = [\rho, \rho u, \rho v, e]^T$, $E = [\rho u, \rho u u + p, \rho u v, e u + p u]^T$, $F = [\rho v, \rho u v, \rho v v + p, e v + p v]^T$. In the forgoing, p is pressure, ρ density, u and v the velocity components and e total energy per unit volume. Using the Jacobian matrix below

$$\Gamma = \frac{\partial Q}{\partial Q_R} \quad (2.49)$$

Equation (2.48) can be re-expressed as

$$\Gamma \frac{\partial Q_R}{\partial t} + \frac{\partial E}{\partial x} + \frac{\partial F}{\partial y} = \text{Viscous Terms} \quad (2.50)$$

where now $Q = [p, u, v, T]^T$ and following Choi and Merkle (1991), after some rearrangement the following can be gained

$$\Gamma = \begin{pmatrix} 1/\beta M^2 & 0 & 0 & 0 \\ u/\beta M^2 & \rho & 0 & 0 \\ v/\beta M^2 & 0 & \rho & 0 \\ \frac{e+p}{\rho\beta M^2} - 1 & \rho u & \rho v & -\frac{\gamma p R}{\gamma - 1} \end{pmatrix} \quad (2.51)$$

In the above, R is the specific gas constant and T temperature, $\beta = \gamma RT$ and γ is the ratio of specific heats. The Eigen values for the above are now

$$\lambda = \left(u, u, \frac{u(1 + \frac{\beta M^2}{\gamma RT}) \pm c'}{2} \right) \quad (2.52)$$

However, in the above a key step is the introduction of the pseudo acoustic speed, c' . This is given below

$$c'^2 = u^2 \left(1 - \frac{\beta M^2}{\gamma RT} \right)^2 + 4\beta M^2 \quad (2.53)$$

where now $\beta = k\gamma RT$ and k is chosen to ensure that the acoustic wave speed is similar to the particle speed. Hence, in the above we have changed the scaling of the time derivative in the compressible solver through introduction of the Jacobian. The latter, with c' maintains well conditioned Eigen values at low speeds. However, the time accuracy has been lost.

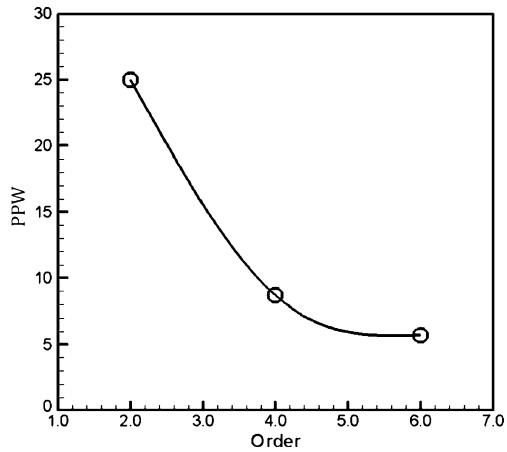
The most popular form of preconditioning is that of Weiss and Smith (1995). For unsteady flows the scheme must be used in an implicit temporal framework with pseudo inner time step iterations. Otherwise, as with the Choi and Merkel approach above, if used explicitly time accuracy is lost. In an implicit solution framework (where the preconditioning is applied to a pseudo time term) although the preconditioning cures the excessive damping the problem is shifted. The number of inner iterations becomes large. Also, most preconditioning strategies seem to neglect that in a three-dimensional flow there are three key Mach number components. Amalgamating these into one resolved component neglects the tensorial nature of the discretized equations. Hence, for highly anisotropic Mach number fields preconditioned results can be inaccurate. Then it seems better to switch, if possible, to pressure based solver technology. A specialist DNS scheme—flux entropy splitting—for compressible flow solvers is outlined by Sandham et al. (2002). A key point is that near walls the Mach number will always tend to zero. This is highly problematic for LES. The increased dissipation will kill the structures in the key turbulent production zone (at around 20 wall units from surfaces). Then a potential option is to use a near wall RANS layer. Such hybrid RANS-LES approaches are discussed in the next chapter. For example, for typical gas turbines beyond 60 wall units the Mach numbers are sufficiently high for a compressible flow solver to be effective.

2.15 Spatial Order and Solution Accuracy

An open question, especially with LES is the influence of numerical order on results. There are many successful LES and DNS that make use of schemes with 2nd order accuracy. Clearly the numerical order/scheme will influence the grid requirements.

It is straightforward, using Fourier based modified wave number analysis to study the accuracy of numerical differentiation. The property of interest can be expressed as $\phi(x) = e^{iwx}$ where w is the wave number. On differentiation this becomes

Fig. 2.11 PPW against scheme order for a wave number error of 1 %



$d\phi(x)/dx = iw e^{iwx} = iw\phi(x)$. The discrete scheme will give $iw'\phi(x)$ here w' is the, less accurate, modified wave number. We could quantify the error in the wave number as

$$\text{Error} = \frac{(w' - w)}{w} \quad (2.54)$$

For a spectral scheme the error in the above equation will be zero. Using the above noted analysis it is possible to estimate the ratio of say an eddy scale, l , (or wave length) to the grid spacing Δx . Hence, the points needed per wave length (PPW) for a specified error can be calculated. Figure 2.11, takes tabulated data from Lele (1992). However, it is plotted as the PPW for an error of 1 % based on Eq. (2.54) for different scheme orders. The lines are curve fits to Lele's data the symbols being the actual data. Substantial benefits appear for schemes of up to 4th order. It does not seem worth going beyond 6th order. Note, that the results discussed are for, uniform grid, and central difference schemes. Hence, there is no dissipative error (unless the grids are stretched) to consider. From Fig. 2.11, the use of high order schemes in LES/DNS might look promising. However, dissipation is more of a critical issue for LES and DNS. The dispersion can assist in yielding resolved scales and hence in an erroneous sense can perhaps be useful. However, for LES there is a lot of resolved energy at the interface between the resolved and modelled scales (this is especially so at high Reynolds numbers). Relative to DNS, the grid is coarse at this interface and then the theoretical justification for a high order scheme is compelling. As shown by Ghosal (1996), even for a scheme of order eight, the numerical contribution will be higher than the LES model contribution. The alternative to high order scheme use, to correct this theoretical problem would be to use a finer grid embedded under an explicit LES filter. However, this approach comes at an extreme cost. A compromise, according to Ghosal is to have a 4th order scheme with grid spacings under the filter of half the filter width. Then the LES model contribution will outweigh that of the numerical scheme. However, even this compromise gives almost a factor of ten increase in computational cost. The most concrete example of where

high order is shown to be of benefit for LES is perhaps the work of Spyropoulos and Blaisdell (1998). In this LES of a spatially evolving supersonic boundary layer is performed. Strong theoretical justification is given by Chow and Moin (2003) for high order schemes in LES. Potential benefits for combustion modelling, where characterization of small-scale behaviour is more critical, are identified by Pitsch (2006). The benefits of a high order spectral scheme for modelling a basic boundary layer using DNS are identified by Laizet and Lamballais (2009). However, the substantial improvements are only evident in the fluctuating vorticity. Of note, it appears that more serious work on LES model development makes use of higher order schemes or larger filters with grid resolution under the filter (Geurts and Holm 2003).

2.15.1 Grid Stretching

Lele's analysis is for uniform grids. However, for practical industrial applications non-uniform grids are essential. Chung and Tucker (2003) repeat Lele's analysis for non-uniform hyperbolic sine and tangent grids. The ratio of largest to the smallest grid spacings is 100. This is consistent with typical DNS (where $\Delta y_{\min} = 0.1$ and $\Delta y_{\max} = 10$) and also for LES where typically $\Delta y_{\min} = 1$ and $\Delta y_{\max} = 100$). Hyperbolic sine grids are relatively popular for free shear layers and tanh boundary layers. Figure 2.12 plots dispersion and dissipation errors for compact and finite difference schemes on tanh grids with $N = 32$. The dotted line gives the exact result that a spectral scheme would provide. The other lines are for different levels of grid stretching and are as identified in the figure caption. Figure 2.12(a) shows how the wave number overshoots for a compact 6th order scheme when the grid becomes more stretched.

However, the key thing that happens for a non-uniform grid is that there is a finite imaginary component to w' representing dissipation. This is zero for uniform grids. As can be seen from Fig. 2.12(b), as the grid is stretched, for a compact scheme, the dissipation error (negative w' zone) becomes large. However, as Fig. 2.12(c) shows, for the centred scheme (2nd order) this error is much smaller. Hence, since finite difference schemes are more economical there is an attraction in staying with them for industrial flows.

This is further illustrated in Fig. 2.13. This plots the PPW for a 10 % dispersion error. The results are for a stretched sinh grid and a 4th order standard finite difference scheme (explicit) and compact scheme (implicit). The largest grid stretching, in the plot, is consistent with typical expansion ratios for LES/DNS. Figure 2.13 shows that for practical problems, where the grid needs stretching, the compact and standard finite difference schemes have similar accuracy. However, the latter needs less computational effort.

Figure 2.14 plots contours of instantaneous axial velocity for a round jet. The plot is intended to show the shear layer development for high and low order centred schemes (with higher order smoothers). Frame (a) is the solution for a 2nd order

Fig. 2.12 Dispersion and dissipation errors for compact and finite difference schemes on tanh grids: (a) dispersion error for 6th order compact scheme; (b) dissipation error for 6th order compact scheme and (c) dissipation error for 2nd order central difference scheme (from Chung and Tucker 2003)

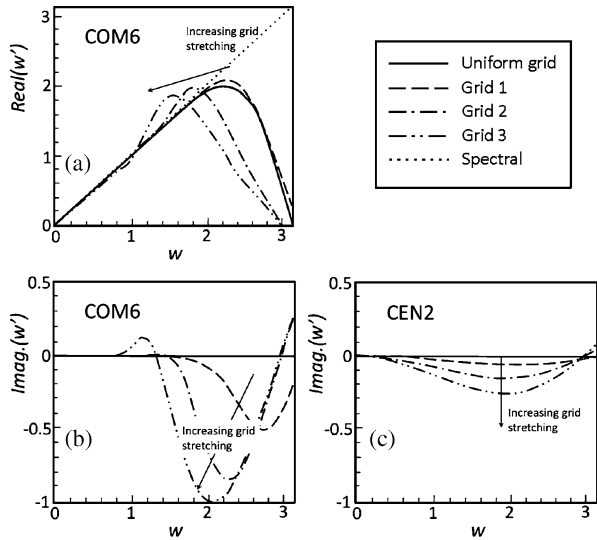
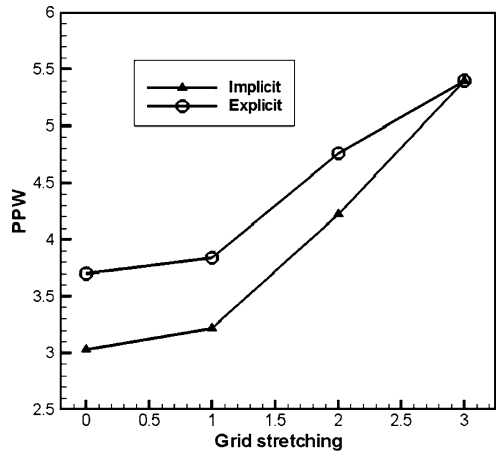


Fig. 2.13 Points per wave length (PPW) (for a 10 % dispersion error) with grid stretching for a 4th order standard finite difference scheme (explicit) and compact scheme (implicit)



scheme and (b) for a 6th order scheme. The solution is made on a modest 5 million cell grid for a jet Reynolds number of around 2×10^5 . The high order scheme seems to show the development of more plausible structures in the near nozzle region. Notably, Ozyoruk and Long (1997) use 4th order central difference scheme solutions to predict fan noise emanating from an engine intake. They gain encouraging agreement with far field noise data.

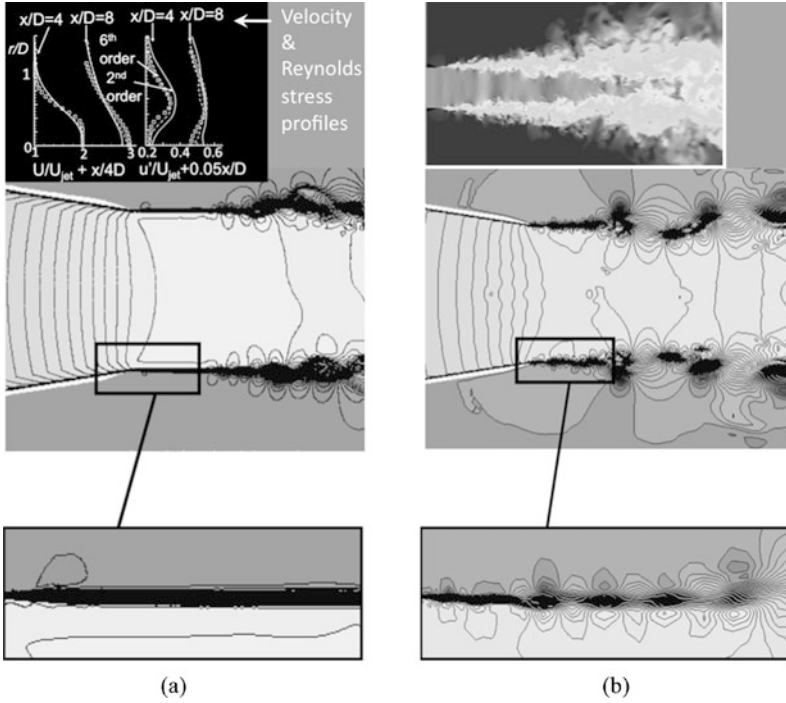


Fig. 2.14 Shear layer development in a jet for high and low order centred schemes: (a) 2nd order scheme and (b) 6th order scheme

2.15.2 High Order Upwinding

The stability of high order upwinding schemes makes them appear attractive for LES. However, as shown in the Fig. 2.15, the energy spectrum, even with 7th order upwinding results in a substantial damping of energy at the higher frequencies. Indeed for the Fig. 2.14 plot—with 5th order upwinding (Tucker 2004) the shear layer development is even more delayed (in fact it is totally suppressed) than for the 2nd order scheme.

2.15.3 Aliasing and Numerical Order

The shortest wavelength that can be resolved by a grid is twice the grid spacing. From Fourier analysis, flows can be seen to consist of a range of wave components. Because of the non-linear convective terms, without significant dissipation this range, with time, will grow. Energy from wavelengths that cannot be resolved by the grid (sub-grid scale wavelengths) can erroneously become combined with longer wavelengths. This is called aliasing.

Fig. 2.15 Predicted energy spectrum for homogeneous decaying turbulence with various order upwind and central difference schemes. Published with kind permission from the ASME

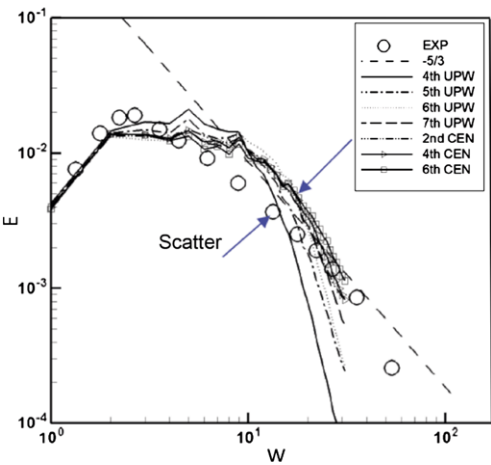


Table 2.8 Various forms of convective term in the Navier-Stokes equations

Title	Tensor form	Source
Non-conservation	$u_j \frac{\partial u_i}{\partial x_j}$	—
Conservation	$\frac{\partial (u_j u_i)}{\partial x_j}$	—
Skew-symmetric	$\frac{1}{2} \left(\frac{\partial (u_j u_i)}{\partial x_j} + u_j \frac{\partial u_i}{\partial x_j} \right)$	Arakawa (1966)
Rotational form	$u_j \left(\frac{\partial u_i}{\partial x_j} - \frac{\partial u_j}{\partial x_i} \right) + \frac{1}{2} \frac{\partial (u_j u_j)}{\partial x_i}$	Deardorff (1970)

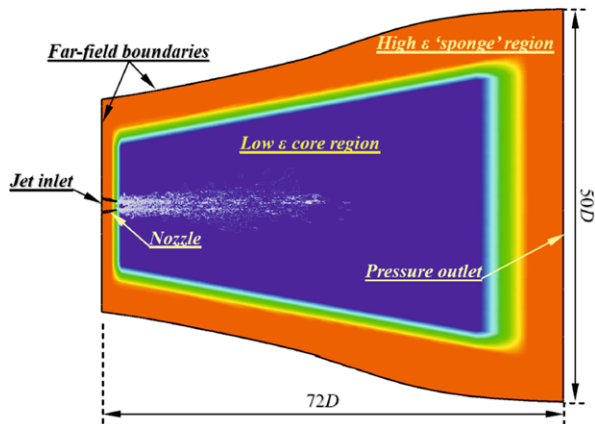
According to Arakawa (1966), aliasing divergence is characterized by a smooth fluid flow structure degenerating into eddies. Evidently, once formed, the eddies intensify without limit. As a result, there is an explosive growth of kinetic energy. This results in the solution diverging. The convective term in the Navier-Stokes equations can be expressed in a range of forms. Some well-known forms are given in Table 2.8.

It is widely reported that discretization of skew-symmetric form results in substantially less aliasing error (see, for example, Blaisdell et al. 1996). On the other hand, the rotational form is observed to show substantial dissipation of turbulence. Horiuti and Itami (1998) attribute this to the discretization error when using low order schemes. From the chain rule of differential calculus, given below

$$\frac{\partial (u_j u_j)}{\partial x_i} = u_j \frac{\partial u_j}{\partial x_i} + u_j \frac{\partial u_j}{\partial x_i} \tag{2.55}$$

it can be seen that the last two terms in the rotational form should cancel. However, because of numerical truncation error in low order schemes they will not (Horiuti and Itami 1998). Ducros et al. (2000) show that in finite volume form the 2nd order central difference discretization naturally provides a skew-symmetric form. Hence, this could reflect why the 2nd order central difference scheme seems to perform well for LES. Joo and Durbin (2009) use the skew-symmetric form of the convective term

Fig. 2.16 Contours of ε_1 for a jet flow LES (blue zone corresponds to low ε_1). Published with kind permission from Elsevier



to gain stability when making hybrid RANS-LES type simulations for the cutback film cooling flow on a turbine blade representation.

When using spectral methods aliasing is prevented through use of the so-called 2/3 rule. With this, for $w > 2n/3$, where n is the number of resolved Fourier components, the modes are set to zero. For more dissipative schemes aliasing becomes less of a problem. The damping from upwinding suppresses the growth of the high wave number components. The substantial density variations accompanying compressible flow gives rise for further non-linearity but little is known regarding the implications of this for aliasing errors.

2.16 Smoothing Control

For high-speed flows, unless the grids are extremely fine it is necessary to introduce some numerical smoothing. Hence, typically centred fluxes, J_{ctr} , might be used with an additional smoother, J_{smth} . Generally, with 2nd order centred codes and shock free flow, this smoother would involve fourth order derivatives.

$$J_{conv} = J_{ctr} + \varepsilon_1 J_{smth} \quad (2.56)$$

The smoother is typically pre-multiplied by a scaling parameter, ε_1 . This can be reduced around a target zone of interest (Shur et al. 2003). To assist in damping reflections, it can become higher, in a smooth fashion, near boundaries. This is shown in Fig. 2.16 for a jet LES. Note, in the work of Shur et al. the blending is made between higher order upwinding and central differences but the two approaches are mathematically equivalent.

An alternative approach developed by Mary and Sagaut (2002) is to have a ε_1 field, which is flow dependent. Where there are excessive point-wise oscillations (dispersion error) ε_1 is increased. Where no dispersion error is detected it is decreased.

The approach works by taking a stencil of four nodes for an arbitrary control-volume interface. Wiggles in the primitive variables (p , u , v , w) are checked for by looking for the coexistence of a minimum and a maximum along the stencil. If a wiggle is detected, the local value of ε_1 is increased; otherwise it is decreased according to Eq. (2.57) below

$$\varepsilon_1^{new} = \begin{cases} \min[(\varepsilon_1^{old} + \Delta_\varepsilon), \varepsilon_1^{\max}] & \text{if wiggle is detected} \\ \max[(\varepsilon_1^{old} - \Delta_\varepsilon), \varepsilon_1^{\min}] & \text{if wiggle is not detected} \end{cases} \quad (2.57)$$

Here Δ_ε , $\varepsilon_1^{\max}$ and $\varepsilon_1^{\min}$ correspond to the increment in ε_1 , the maximum allowable ε_1 and the minimum allowable ε_1 . A parameter also controls the number of updates per time step when inner iterations are used. An investigation of this scheme can be found in Jefferson-Loveday (2008). Its performance for decaying homogeneous isotropic turbulence is explored with and without a standard Smagorinsky model. The scheme is found to be effective in keep solutions running with the lowest amount of dissipation in an average sense.

However, the scheme does lack certain sophistication in that the smoothing variable is both increased and decreased in a stepwise fashion. This can be improved through the use of a PI (Proportional and Integral) controller. The difference between the current level of dispersion and that which is desired (some low level) can be defined ψ . A smoothing increment, $\Delta\varepsilon_1$ can then be expressed using a PI controller as

$$\Delta\varepsilon_1(t) = k_p\psi(t) + k_I \int_0^t \psi(\tau) d\tau + k_D \frac{d\psi}{dt} \quad (2.58)$$

In the above k_p , k_I and k_D are tuneable parameters. The integral term avoids a steady state offset developing, thus avoiding the target value being reached. The final term avoids overshoots. Figure 2.17 gives a schematic showing the expected variation of ψ and ε_1 for the original scheme of Mary and Sagaut (Frame (a)) and the one using a PI controller (Frame (b)). As can be seen, from Frame (b), a more smooth variation of ε_1 is expected.

Figure 2.18 shows the performance of the PI scheme when predicting homogeneous decaying turbulence. Details of the case-setup can be found in Jefferson-Loveday (2008). The symbols are measurements. The chain dashed lines are results for a fixed ε_1 scheme. The full line is for the PI controller based scheme. There is evidence of much less dissipation with this scheme.

Strelets (2001) presents a flow physics based dispersion/dissipation control. With this

$$\varepsilon_1 = \varepsilon_{\max} \tanh(A^{c_1}) \quad (2.59)$$

and

$$A = c_2 \max \left\{ \left[\left(\frac{C_{DES}\Delta}{l} \right) / g - 0.5 \right], 0 \right\} \quad (2.60)$$

In the above, Δ , is the LES filter width (see Chap. 3) and l is a turbulence length scale. This has a complex functional form that is not reported here. However, $l =$

Fig. 2.17 Schematic of the expected variation of ψ and ε_1 with time: (a) original scheme of Mary and Sagaut (2002) and (b) PI controller based scheme

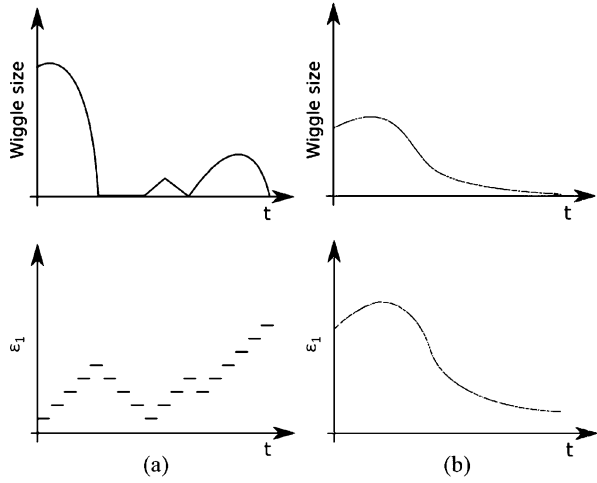
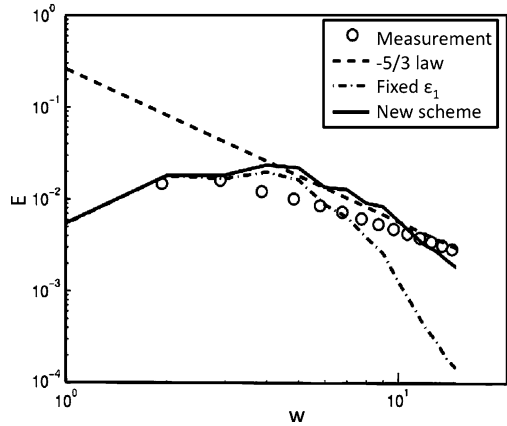


Fig. 2.18 Turbulence energy spectrum for homogeneous decaying turbulence with PI control scheme



$f(\mu_T, S, \Omega, \tau)$ where μ_T is turbulent viscosity, S strain rate, Ω vorticity and τ a convective time scale. The function g is given below

$$g = \tanh \left\{ \frac{c_3 \Omega_{\max}[S, \Omega]}{\max([S^2 + \Omega^2]/2, \varepsilon)} \right\} \quad (2.61)$$

The function g is intended to introduce more smoothing/upwind behaviour in irrotational but disturbed flow zones where $\Omega \ll 1$ and $S > 0$. Clearly, also low smoothing is sought in rotational flow zones. In the above, $\varepsilon \rightarrow 0$, $\varepsilon_{\max} = 1.0$, $c_1 = 3.0$, $c_2 = 1$ and $c_3 = 2$.

2.16.1 Shocks and LES

Around shocks a 2nd order derivative smoother can be activated via a pressure based shock detection switch. This is the most standard CFD procedure. The switch basically detects high pressure gradients. The difficulty when performing LES is that small scale eddies can be misinterpreted as shocks and hence the 2nd order smoother can become excessively active.

The switch of Ducros et al. (1999), given below, assists in alleviating this problem. It attempts to only make the shock smoothing active around shocks and not under-resolved turbulence.

$$\Phi = \frac{(\nabla \cdot \mathbf{u})^2}{(\nabla \cdot \mathbf{u})^2 + \omega^2 + \epsilon} \quad (2.62)$$

In the above ϵ is a small number to prevent division through by zero and ω is the resolved vorticity ($\nabla \times \mathbf{u}$). This function Φ , ranges between zero and unity—tending to unity around shocks.

Bisek et al. (2013) when making compact scheme LES use the Swanson and Turkel (1992) pressure gradient detector.

$$\Phi = \frac{|p_{i+1} - 2p_i + p_{i-1}|}{(1 - \omega)(|p_{i+1} - p_{i-1}|) + \omega(p_{i+1} - 2p_i + p_{i-1})},$$

$$\begin{cases} \Phi > 0.05, & \text{Roe scheme} \\ \Phi \leq 0.05, & \text{Compact scheme} \end{cases} \quad (2.63)$$

In shock zones a flux limited (van Albada) Roe scheme is used, the high order compact scheme being used elsewhere.

2.17 Mesh Related Techniques

Unstructured moving meshes can be used in an ALE formulation. More details on such meshes can be found in Chap. 7. Yang et al. (1997) give a Cartesian, trimmed cell method for moving body problems. Where the geometry is especially complex, the immersed boundary method provides a more flexible alternative for modelling complex moving body cases (Pinelli et al. 2010). However, both the trimmed cell and immersed boundary methods are unsuitable for modelling flows where the prediction of accurate skin friction is important. Vortex methods, that generally do not require the use of grids, (Khatir 2000) naturally lend themselves to moving boundary problems. The mesh-less smooth particle hydrodynamics method (Marongiu et al. 2007, 2010) are also suitable. The smooth particle hydrodynamics methods were originally developed for astrophysics modelling such as modelling the formation of stars. Like most mesh-less methods it has been available for many decades. As originally formulated it is intended for highly compressible problems. Marongiu et al. apply the approach to a free surface Pelton turbine flow.

2.17.1 Body Fitted Grids

For finite volume schemes it is challenging to maintain formally high order numerical discretizations. This is much more straightforward with finite difference and compact schemes. However, then geometrical flexibility is limited. A way round this, to an extent, is to work in transformed coordinates. With this, the governing equations in an (x, y, z, t) coordinate system can be transformed into a (ξ, η, ζ, τ) system using the chain rule of differential calculus. The transformed computational grid is normally uniform and Cartesian. Hence, the application of higher order schemes is made, in a sense, relatively easy. The transformation (Rayner 1993) simply involves making the following substitutions in the governing (x, y, z, t) equations, where $\xi = \xi(x, y, z, t)$, $\eta = \eta(x, y, z, t)$, $\zeta = \zeta(x, y, z, t)$ and $\tau = \tau(t)$

$$\frac{\partial}{\partial x} = \left(\frac{\partial \xi}{\partial x} \right) \frac{\partial}{\partial \xi} + \left(\frac{\partial \eta}{\partial x} \right) \frac{\partial}{\partial \eta} + \left(\frac{\partial \zeta}{\partial x} \right) \frac{\partial}{\partial \zeta} + \left(\frac{\partial \tau}{\partial x} \right) \frac{\partial}{\partial \tau} \quad (2.64)$$

$$\frac{\partial}{\partial y} = \left(\frac{\partial \xi}{\partial y} \right) \frac{\partial}{\partial \xi} + \left(\frac{\partial \eta}{\partial y} \right) \frac{\partial}{\partial \eta} + \left(\frac{\partial \zeta}{\partial y} \right) \frac{\partial}{\partial \zeta} + \left(\frac{\partial \tau}{\partial y} \right) \frac{\partial}{\partial \tau} \quad (2.65)$$

$$\frac{\partial}{\partial z} = \left(\frac{\partial \xi}{\partial z} \right) \frac{\partial}{\partial \xi} + \left(\frac{\partial \eta}{\partial z} \right) \frac{\partial}{\partial \eta} + \left(\frac{\partial \zeta}{\partial z} \right) \frac{\partial}{\partial \zeta} + \left(\frac{\partial \tau}{\partial z} \right) \frac{\partial}{\partial \tau} \quad (2.66)$$

If the grid is moving, the chain rule also needs to be applied to the time derivative

$$\frac{\partial}{\partial t} = \left(\frac{\partial \xi}{\partial t} \right) \frac{\partial}{\partial \xi} + \left(\frac{\partial \eta}{\partial t} \right) \frac{\partial}{\partial \eta} + \left(\frac{\partial \zeta}{\partial t} \right) \frac{\partial}{\partial \zeta} + \left(\frac{\partial \tau}{\partial t} \right) \frac{\partial}{\partial \tau} \quad (2.67)$$

The bracketed derivatives above are called metrics. Variables treated as fixed in the partial differentiations contained in Eqs. (2.64) to (2.67) are indicated using subscripts below

$$\left(\frac{\partial}{\partial x} \right)_{yzt} \left(\frac{\partial}{\partial y} \right)_{xzt} \left(\frac{\partial}{\partial z} \right)_{xyt} \left(\frac{\partial}{\partial t} \right)_{xyz} \left(\frac{\partial}{\partial \xi} \right)_{\eta\zeta\tau} \left(\frac{\partial}{\partial \eta} \right)_{\xi\zeta\tau} \left(\frac{\partial}{\partial \zeta} \right)_{\xi\eta\tau} \left(\frac{\partial}{\partial \tau} \right)_{\xi\eta\zeta}$$

Clearly $\partial\tau/\partial x = \partial\tau/\partial y = \partial\tau/\partial z = 0$ and so grid distortion from boundary movement does not affect transformations (2.64) to (2.66).

Results presented later make use of the artificial compressibility method of Rogers and Kwak (1990). Hence, it seems useful here to outline the transformed equations in combination with this approach. With the artificial compressibility method the following artificial equation of state is used, $p = \beta^{-1}\rho$. In this relationship, β is an artificial compressibility parameter (see later) and τ is a pseudo time. Since the flow is assumed incompressible, the pseudo time derivative is integrated to a steady state. Application of the chain rule above to the Reynolds averaged Navier-Stokes equations, in their strong conservation form, gives (Jefferson-Loveday 2008)

$$\partial_\tau \mathbf{Q} + \partial_\xi \mathbf{E}^{inv} + \partial_\eta \mathbf{F}^{inv} + \partial_\zeta \mathbf{G}^{inv} = [\partial_\xi \mathbf{E}^{vis} + \partial_\eta \mathbf{F}^{vis} + \partial_\zeta \mathbf{G}^{vis}] \quad (2.68)$$

where

$$\mathbf{Q} = J^{-1} \begin{bmatrix} \bar{p} \\ \bar{u} \\ \bar{v} \\ \bar{w} \end{bmatrix}, \quad \mathbf{E}^{inv} = J^{-1} \begin{bmatrix} \beta \bar{U} \\ \bar{u} \bar{U} + \xi_x \bar{p} \\ \bar{v} \bar{U} + \xi_y \bar{p} \\ \bar{w} \bar{U} + \xi_z \bar{p} \end{bmatrix}$$

$$\mathbf{F}^{inv} = J^{-1} \begin{bmatrix} \beta \bar{U} \\ \bar{u} \bar{V} + \eta_x \bar{p} \\ \bar{v} \bar{V} + \eta_y \bar{p} \\ \bar{w} \bar{V} + \eta_z \bar{p} \end{bmatrix}, \quad \mathbf{G}^{inv} = J^{-1} \begin{bmatrix} \beta \bar{U} \\ \bar{u} \bar{W} + \zeta_x \bar{p} \\ \bar{v} \bar{W} + \zeta_y \bar{p} \\ \bar{w} \bar{W} + \zeta_z \bar{p} \end{bmatrix}$$

$$\bar{U} = \xi_x \bar{u} + \xi_y \bar{v} + \xi_z \bar{w}, \quad \bar{V} = \eta_x \bar{u} + \eta_y \bar{v} + \eta_z \bar{w}, \quad \bar{W} = \zeta_x \bar{u} + \zeta_y \bar{v} + \zeta_z \bar{w} \quad (2.69)$$

Note, the overbars, see Chap. 3, represent Reynolds averaging. The viscous flux terms are given by

$$\begin{aligned} \mathbf{E}^{vis} &= J^{-1} (\xi_x \mathbf{E}^{vis} + \xi_y \mathbf{F}^{vis} + \xi_z \mathbf{G}^{vis}) \\ \mathbf{F}^{vis} &= J^{-1} (\eta_x \mathbf{E}^{vis} + \eta_y \mathbf{F}^{vis} + \eta_z \mathbf{G}^{vis}) \\ \mathbf{G}^{vis} &= J^{-1} (\zeta_x \mathbf{E}^{vis} + \zeta_y \mathbf{F}^{vis} + \zeta_z \mathbf{G}^{vis}) \end{aligned} \quad (2.70)$$

where

$$\mathbf{E}^{vis} = \begin{bmatrix} 0 \\ \tau_{xx} \\ \tau_{xy} \\ \tau_{xz} \end{bmatrix}, \quad \mathbf{F}^{vis} = \begin{bmatrix} 0 \\ \tau_{yx} \\ \tau_{yy} \\ \tau_{yz} \end{bmatrix}, \quad \mathbf{G}^{vis} = \begin{bmatrix} 0 \\ \tau_{zx} \\ \tau_{zy} \\ \tau_{zz} \end{bmatrix} \quad (2.71)$$

and

$$\begin{aligned} \tau_{xx} &= (\mu + \mu_t) (4(\xi_x \bar{u}_\xi + \eta_x \bar{u}_\eta + \zeta_x \bar{u}_\zeta) \\ &\quad - 2(\xi_y \bar{v}_\xi + \eta_y \bar{v}_\eta + \zeta_y \bar{v}_\zeta + \xi_z \bar{w}_\xi + \eta_z \bar{w}_\eta + \zeta_z \bar{w}_\zeta)) / 3 \\ \tau_{yy} &= (\mu + \mu_t) (4(\xi_y \bar{v}_\xi + \eta_y \bar{v}_\eta + \zeta_y \bar{v}_\zeta) \\ &\quad - 2(\xi_x \bar{u}_\xi + \eta_x \bar{u}_\eta + \zeta_x \bar{u}_\zeta + \xi_z \bar{w}_\xi + \eta_z \bar{w}_\eta + \zeta_z \bar{w}_\zeta)) / 3 \\ \tau_{zz} &= (\mu + \mu_t) (4(\xi_z \bar{w}_\xi + \eta_z \bar{w}_\eta + \zeta_z \bar{w}_\zeta) \\ &\quad - 2(\xi_x \bar{u}_\xi + \eta_x \bar{u}_\eta + \zeta_x \bar{u}_\zeta + \xi_y \bar{v}_\xi + \eta_y \bar{v}_\eta + \zeta_y \bar{v}_\zeta)) / 3 \\ \tau_{xy} &= (\mu + \mu_t) (\xi_x \bar{u}_\xi + \eta_x \bar{u}_\eta + \zeta_x \bar{u}_\zeta + \xi_y \bar{v}_\xi + \eta_y \bar{v}_\eta + \zeta_y \bar{v}_\zeta) \\ \tau_{yz} &= (\mu + \mu_t) (\xi_y \bar{v}_\xi + \eta_y \bar{v}_\eta + \zeta_y \bar{v}_\zeta + \xi_z \bar{w}_\xi + \eta_z \bar{w}_\eta + \zeta_z \bar{w}_\zeta) \\ \tau_{zx} &= (\mu + \mu_t) (\xi_z \bar{w}_\xi + \eta_z \bar{w}_\eta + \zeta_z \bar{w}_\zeta + \xi_x \bar{u}_\xi + \eta_x \bar{u}_\eta + \zeta_x \bar{u}_\zeta) \end{aligned} \quad (2.72)$$

Note, μ_t is eddy viscosity. Although the transformed differential equations are much larger than the original, they can be solved on a uniform grid computational plane. Hence, high order schemes can be readily applied. A key issue is the formation of the metric terms. Ideally, these must be also expressed at an order consistent with that of

the base finite difference scheme. For highly non-orthogonal grids the formulation of the metric terms can have a critical accuracy impact (Visbal and Gaitonde 2002) as will non-smooth grid stretching (Gamet et al. 1999). Hence, care is needed. Visbal and Gaitonde (2002) contrast standard

$$\begin{aligned}\hat{\xi}_x &= y_\eta z_\zeta - y_\zeta z_\eta \\ \hat{\eta}_x &= y_\zeta z_\xi - y_\xi z_\zeta \\ \hat{\zeta}_x &= y_\xi z_\eta - y_\eta z_\xi\end{aligned}\tag{2.73}$$

and the conservation metric form of Thomas and Lombard (1979)

$$\begin{aligned}\hat{\xi}_x &= (y_\eta z)_\zeta - (y_\zeta z)_\eta \\ \hat{\eta}_x &= (y_\zeta z)_\xi - (y_\xi z)_\zeta \\ \hat{\zeta}_x &= (y_\xi z)_\eta - (y_\eta z)_\xi\end{aligned}\tag{2.74}$$

On skewed grids, they found that the latter held free stream conditions more accurately. Hence, Daude et al. (2012) also adopt this approach in their high-order, finite difference simulations.

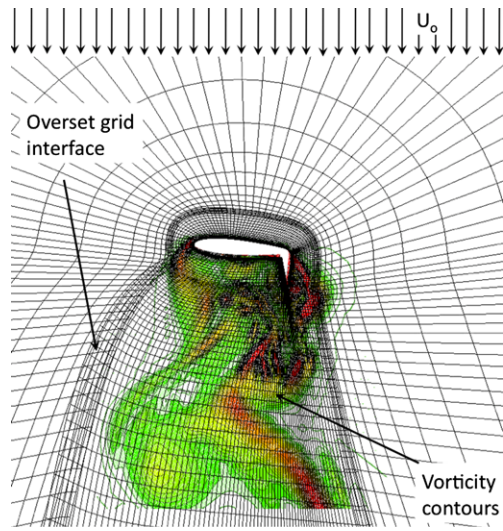
There is an extensive body of literature on the use of high order schemes on curvilinear grids for acoustics. For example, Uzun and Hussaini (2009) use 6th high order compact schemes for complex chevron nozzle jet noise LES. In a related fashion, Lu et al. (2012) use a high order unstructured flux reconstruction method. The unstructured element shape is mapped into a locally regular transformed ξ , η , ζ system—a standard high-order procedure. The method is applied to transonic flow around a VKI-LS59 turbine blade.

2.17.2 Overset Grids

The Chimera (a Chimera is a mythological creature with a goats body, snakes tail and lions head) or overset grid method, described by Chesshire and Henshaw (1990), has seen popularity for modelling moving grid problems. With this, for example, a Cartesian grid often maps the flow domain and the body modelled by moving curvilinear overset grids.

Figure 2.19 shows a simple overset mesh and the isosurfaces of vorticity from a hybrid large eddy type simulation, for a static geometry case. Notably, Paliath et al. (2011) also use a compact overset code for complex chevron geometry nozzle LES. Spalart et al. (2003) use 5th order finite differences on curvilinear overset meshes. They explore flow control over an idealized V22 tilt rotor wing using detached eddy simulation (see Chaps. 3 and 5). Hedges et al. (2002) use the approach for landing gear aerodynamic studies. Rizzetta et al. (2008) apply a 4th order compact scheme (with 6th order smoothing) in an overset grid solver, studying flow control over turbine blades.

Fig. 2.19 Overset mesh and vorticity contours showing the flow field for a generic tilt-rotor wing geometry (from Tucker 2006). Published with kind permission from Wiley and Sons



However, with overset meshes, the key issue is how to produce a high order and sufficiently conservative interpolation between the different overlapping grids. This is compounded by the potential for several overlapping grids at the same point in space. Maintaining order is explored in Lee et al. (2011). Unstructured overset meshes, with relative movement can be a powerful tool for especially complex, moving grid problems (Nakahashi and Togashi 2000). The moving overset component allows a reduction in cell distortion. For distorting meshes, control volume face velocities need to be reformulated to obey space conservation (Demirdžić and Perić 1988). This aspect is discussed further in Chap. 7.

2.18 The Substantial Derivative

When computing unsteady flows, concepts relating to the substantial derivative can be helpful to consider. These can have implications for the numerical scheme. The substantial derivative, $(\partial\phi/\partial t)_{fp}$, is more usually expressed as $D\phi/Dt$. However, here the subscript fp is used. This enforces its meaning. This being the time rate of change in ϕ when a particular fluid particle is followed. The derivative is given below

$$\left(\frac{\partial\phi}{\partial t}\right)_{fp} = \underbrace{\left(\frac{\partial\phi}{\partial t}\right)_g + \left(\frac{\partial\phi}{\partial t}\right)_f}_{\partial\phi/\partial t} + (\mathbf{U} - \mathbf{U}_g) \cdot \nabla\phi + G \quad (2.75)$$

The terms $(\partial\phi/\partial t)_g$ and $(\partial\phi/\partial t)_f$ together are those that would normally be related to unsteadiness i.e. $(\partial\phi/\partial t)$. However, here they are split out with $(\partial\phi/\partial t)_g$

being the component that can be reduced by minimizing $|\mathbf{U} - \mathbf{U}_g|$ where $\mathbf{U}_g$ is the grid/coordinate system velocity. For a rotating system $\mathbf{U}_g$ can be proportional to Ω_g the grid angular velocity. The $(\partial\phi/\partial t)_f$ represents any unsteadiness would potentially remain.

For certain systems (classified as exhibiting unsteady flow), the fluid structure may stay exactly or much the same, but simply translate (at a velocity $\tilde{\mathbf{U}}$) or rotate (at an angular velocity Ω) in space, relative to the coordinate system/grid. The mechanism for this translation or rotation could be fluid dynamic in origin or alternatively as the result of boundary movement. Examples of the former are a wave train moving around a cylindrical domain (Tucker 2002b) with an angular velocity, Ω , about a rotation axis or vortex wakes propagating downstream from aircraft wings (Steger and Kutler 1977). Translational movement of effectively a constant geometrical distortion when viewed in a frame of reference moving with the distortion, will give steady flow ($(\partial\phi/\partial t)_g + (\partial\phi/\partial t)_f = 0$). For some practical flows it is possible to make unsteadiness smaller by minimizing $(\partial\phi/\partial t)_g$ through appropriate choice of coordinate system. Also, reducing the magnitude of temporal terms should bring down some temporal solution errors. This could be achieved through the ALE process. Furthermore, moving coordinate systems can significantly lower convective term magnitudes. These terms, as indicated above, are generally challenging in terms of unsteady flow modelling accuracy. Tucker (1997) gives examples of solution accuracy gains by the use of rotating coordinate systems. The G term, in Eq. (2.75), relates to grid distortion, being applicable to moving boundary cases. For a three-dimensional transformed grid (ξ, η, ζ) system

$$G = \left(\frac{\partial \xi}{\partial t} \right)_g \left(\frac{\partial \phi}{\partial \xi} \right) + \left(\frac{\partial \eta}{\partial t} \right)_g \left(\frac{\partial \phi}{\partial \eta} \right) + \left(\frac{\partial \zeta}{\partial t} \right)_g \left(\frac{\partial \phi}{\partial \zeta} \right) \quad (2.76)$$

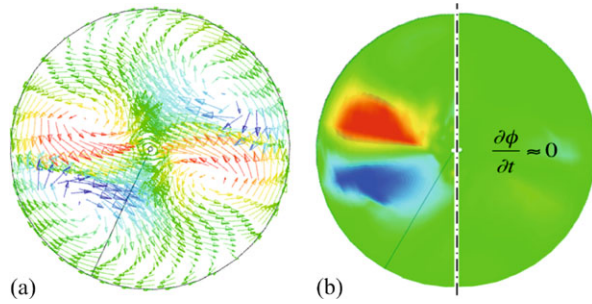
However, as implied earlier, the coordinate system can also be chosen to minimize G . Hence, inaccuracies arising from modelling these extra terms, in whatever form they might appear in the chosen discretization framework, will also be minimized.

To illustrate the alteration of grid velocity to minimize unsteadiness the case of a rotating cavity with an axial through flow is considered. This is representative of the flow in the high-pressure compressor drum of an aero engine. The case is fully reported in Tucker (2002b). Two regions of radial outflow occur for the conditions considered. These emanate from an inner axial through flow of coolant. Figure 2.20, Frame (a) gives cavity mid-axial plane velocity vectors. Frame (b) gives cavity mid-axial contours of $\partial u/\partial t$ (where u is axial velocity). These are for grid angular velocities $\Omega_g = 17.0$ (left hand image) and 16.8 rad/s (right hand image). The larger Ω_g corresponds to the cavity angular velocity. The more uniform, Frame (b), right hand, $\Omega_g = 16.8$ rad/s contours signify greater flow steadiness.

Sliding grid planes can be used to connect rotating to stationary blade zones. These have the advantage that in the rotating frame the relative velocities solved for are smaller and hence Peclet/Reynolds numbers smaller. The latter enables the use of centred schemes or schemes that are more centred in nature. These are less prone

Fig. 2.20 Mid-axial velocity vectors and contours of for rotating cavity with an axial through flow of air:

(a) Velocity vectors and
(b) Contours for $\Omega_g = 17.0$
and 16.8 rad/s (adapted from
Tucker 2002b). Published
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to dissipation and hence allow, for example, better wake preservation. The sliding planes allow appropriate minimization of unsteadiness. Of note, for the rotating wake body force modelling of Loiodice et al. (2010) the blade viscous body forces are cast in a rotating frame to enhance wake preservation. Vorticity confinement (Steinhoff and Underhill 1994) injects energy lost from dissipation back into flows. This approach is potentially useful for maintaining the strength of, for example tip, vortices on under-resolved grids.

2.19 Simultaneous Equation Solution

A discussion on the extensive field of advanced simultaneous equation solver technology is not attempted here. This is partly because for unsteady flows the flow equations become more parabolic and hence this issue is less critical. Hence, except for the Poisson based equations used in pressure-based solvers, efficient simultaneous equation solvers become less critical. Explicit temporal schemes do not require a simultaneous equation solver and can be easily parallelized. However, they have more severe time-step stability restrictions. Consequently they are only suitable when high temporal resolution is required. Implicit techniques essentially require a simultaneous equation solver. This is generally a major solution overhead. Approximate factorization or splitting methods successfully combine explicit and implicit techniques only requiring a one-dimensional solver. ADI is a member of this family. A relatively popular method is the Bi-CGSTAB (biconjugate gradient stabilized method). This is applied to LES of trailing edge noise by Manoha et al. (2000). Strong solvers such as GMRES (Campobasso and Giles 2003) and Recursive Projection Methods (Campobasso and Giles 2004) can force steady solutions where none exist. In an engineering design context, where fast solutions are needed, this can appear attractive. However, as shown by Krakos and Darmofal (2010) such solutions may not correspond to the time average of the unsteady solution.

Multigrid convergence acceleration is an especially efficient procedure and sees widespread use. Brandt (1980) describes a multilevel-based strategy tailored for modelling flows evolving with time. The basis of the method is Brandt's assumption that for evolution processes the high and low frequency (in a spatial sense)

components can be very different. During early time-steps, the high frequency components change rapidly but then settle down. Then, the lower frequency components only need be resolved. The evolution of these can be modelled using coarser grids, the higher frequency component being accounted for by forcing terms originating from the finer grid. Therefore, after an initial period, the solution can mostly be integrated through time on a coarser grid. The fine grid is periodically revisited to update the relationship between the newer low frequency and older high frequency components.

When using Newton methods to compute unsteady flows the Jacobian re-evaluation is expensive. To circumvent this, Gresho et al. (1980) and Engelman and Sani (1986) explore the following two approaches: (a) Use adaptive time-stepping, with a small user defined time truncation error and (b) Use a quasi-Newton approach. With this the Jacobian is only re-evaluated every two or three time-steps. Option (a) results in the need for only one Newton iteration and hence Jacobian up-date per time-step.

To improve solution speed a parallel processing domain decomposition in time is evidently possible (Seidl et al. 1995; Burmeister and Horton 1991). Such approaches are not covered here and as yet do not see widespread use/acceptance.

2.20 Evaluation of the Pressure Field

The evaluation of the pressure field for density and pressure-based solvers is dramatically different. For pressure-based solvers with unsteady flow the PISO (Issa 1986) and fractional step (Kim and Moin 1985) approaches are regarded as the most ideal alternatives to the multitude of SIMPLE variants. However, in the author's experience these schemes do not offer any great performance benefits.

The AVPI scheme described by Jones and Marquis (1985) and Henkes (1990) is of note for unsteady flows. It reduces core memory requirements by avoiding the need to store additional coefficients required in popular projection methods. With AVPI, these coefficients become approximately equal to $\Delta t / \rho_i^{n-1}$ and so can be calculated on the fly. For the 1st order backwards Euler scheme and a constant density system, AVPI gives the following relatively simple Poisson equation for a correction, p' , to the pressure field

$$\nabla^2 p'^{n+1} = \frac{\rho}{\Delta t} \nabla \cdot u^* \quad (2.77)$$

The star superscripted quantities are iteratively approximate. An overview of various techniques for computing p in pressure-based solvers is given in Tucker (2001).

2.20.1 Pressure Subcycling

As previously noted, explicit scheme stability requirements can dictate that smaller time-steps must be used than needed to resolve actual physical processes. In this

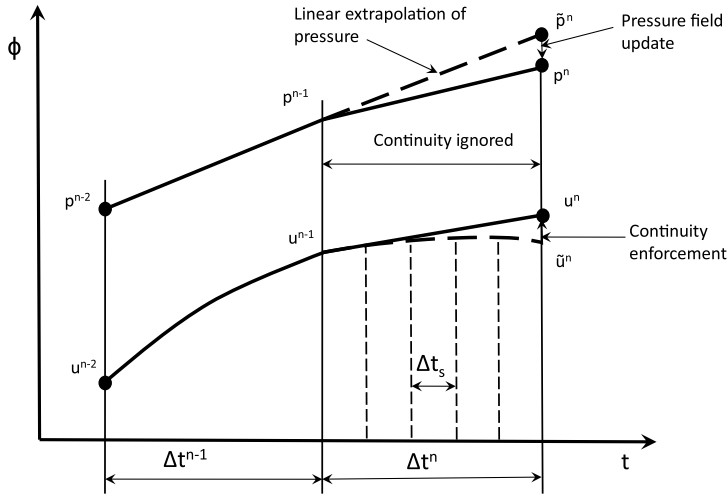


Fig. 2.21 Illustration of the subcycling procedure

situation, to lessen computational expense a procedure called subcycling, described by Gresho et al. (1984) can be used. The premise for the procedure is that, for the momentum equations (and other transport equations), explicit scheme stability is not linked to pressure and continuity constraints. The subcycling procedure, illustrated in Fig. 2.21, is as follows:

- (I) Over a time period Δt^n , solve the momentum equations explicitly using minor steps, Δt_s , governed by stability limits. During this period use extrapolated pressure values.
- (II) At the end of the period Δt^n , by correcting the velocity field, re-enforce continuity.
- (III) Finally, use the continuity satisfying velocity field to update pressures.

By not requiring a pressure update for every minor time-step the above procedure saves computational effort.

2.20.2 Pressure-Velocity Coupling

To avoid the prediction of nonphysical oscillatory pressure fields, for incompressible flow solvers the pressure-velocity coupling has been a considerable area of research. For many years, a popular technique (Harlow and Welch 1965) has been to arrange the grids such that the relevant pressure nodes are coincident with the control volume faces of the momentum variable being solved for. To achieve this, staggered multiple control volumes must be used. Due to programming simplicity, collocated variable arrangements are preferred. The most well known collocated

variable technique, to avoid unrealistic pressure field oscillations, is due to Rhie and Chow (1983). Essentially, this approach involves the introduction of pressure field smoothing. The smoothing properties of this approach, which applies dissipation to the pressure field, depend on time-step and under-relaxation values (Barton and Kirby 2000). The alternative Pressure Weighted Interpolation Method—Corrected (PWIMC) method of Kobayashi and Pereira (1991) is less dependent on under-relaxation parameter values. Barton and Kirby (2000) also present a method where performance is de-sensitized to time-step and under-relaxation values. Clearly these aspects are particularly important for LES/DNS.

2.20.3 Compressible Flow Solvers and Pressure Recovery

A key point to note is that for density based solvers, at low Mach numbers, the density variations in the time derivative of the continuity equation becomes extremely small. It is through these that the pressure field is recovered. This, when combined with the pre-conditioning issues noted earlier creates serious solution accuracy problems. Hence, compressible flow solvers are best used for high Mach number flows, where there are substantial density variations that can be used to recover pressure.

If density variations can be completely neglected the artificial compressibility method of Rogers and Kwak (1990) (based on the approach of Chorin 1967) can be effective. With this, the continuity equation is re-expressed, through a simplified equation of state, as below.

$$\frac{\partial p}{\partial \tau} + \beta \left(\frac{\partial u_j}{\partial x_j} \right) = 0 \quad (2.78)$$

The parameter β is tunable but has a fixed theoretical range (Rogers et al. 1986). The approach is intended to be used in a compressible solver framework. When used in this framework, like all other equations, the above pressure equation has a smoothing term. If β is too large, in steep pressure gradient areas, this will act as a substantial mass source term. However, with reasonable care the method is effective. A simple, alternative, expedient can be to scale down the geometry and increase velocity to preserve the Reynolds number. The higher velocity ensures a higher Mach number. If this is sufficiently high, then the compressible flow solver will have reasonable computational performance. The Mach number required for reasonable compressible solver performance can vary dramatically between different codes. Hence, there is a need to understand the CFD program's traits. However, for many flows this Mach number scaling strategy will give rise to excessive density variations in localized regions. Also, the Mach number tends to zero at walls.

2.21 Boundary Conditions

For unsteady flows the use of both non-reflecting inflow and outflow boundary conditions becomes especially important. If not, the multiple reflections of waves will ultimately lead to solution divergence. The simplest remedy is to do the following:

- (I) Keep the boundaries well away from the key area of unsteadiness activity;
- (II) Coarsen grids towards these boundaries and
- (III) Increase the numerical dissipation towards the boundaries.

The latter two things ensures that reflected waves cannot be supported by the grid. However, clearly such strategies are computationally wasteful. Hence, if possible, more refined methods should be used. The literature on non-reflecting boundary conditions and potential variants is extensive. Hence, just some of the key approaches, that are used in results presented here, are discussed. The one-dimensional, characteristics based non-reflecting boundary condition of Giles (1990) has seen extensive use for compressible flows. However, the one-dimensional nature of this scheme limits its applicability. The convective boundary condition of Pauley et al. (1990) is simple to implement and given below

$$\frac{\partial \phi}{\partial t} + U_c \frac{\partial \phi}{\partial x} = 0 \quad (2.79)$$

In the above U_c is taken as the bulk mean velocity and ϕ would be the velocity components and other solution variables. The damping approach of Ashcroft and Zhang (2001) is also easy to implement. With this the equation below is used

$$\phi(l) = (1 - s)\phi_{\text{target}}(l) + s\phi(l) \quad (2.80)$$

ϕ_{target} being a target field and ϕ a computed field that is gradually, via a transition zone, pinned to the target field. A potential transition function is given below

$$s = |1 - (l/L)^\beta| \quad (2.81)$$

In the above, L is the width of the sponge/damped layer and $0 < l < L$. Also, $l = 0$ at the domain boundaries and $l = L$ is inside the domain. Following the approach of Shur et al. (2003), and as noted earlier, ideally, for LES etc, a centered scheme, is used in the target zone. This can then be blended with dissipative upwind differences at boundaries or the magnitude of smoothing terms increased. With this strategy, following Shur et al., when centered schemes are being blended with upwind differences, to assist with damping numerical reflections, the order of the upwinding scheme, N_{UP} , can also be reduced towards flow boundaries. This can be achieved through the following equation

$$N_{UP} = \max \left\langle \text{int} \left[\frac{N_{UP,MAX}l}{L} \right], 1 \right\rangle \quad (2.82)$$

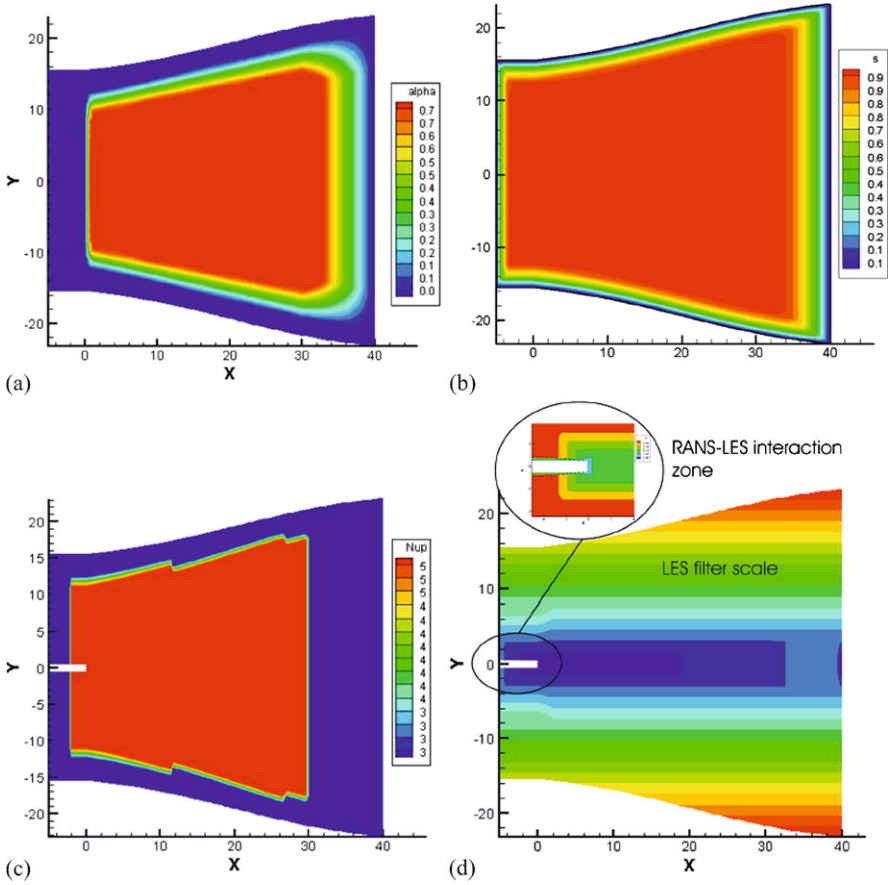


Fig. 2.22 Level set based weighting function distributions used for jet acoustic simulations: (a) upwind/centered scheme blending function (ϵ_1); (b) blending function (s) for sponges; (c) N_{UP} distribution and (d) modelled turbulence scales

where $N_{UP,MAX}$ is the maximum order of the upwind solution component (5 in the simulations of Shur et al.). Also, int represents the rounding up of the bracketed quantity to the nearest integer. The operator $\max$ takes the maximum value.

Figure 2.22 relates to jet LES computations. Level set fields, generated by differential Hamilton-Jacobi (HJ) equations (Sethian 1999) are presented, some after being subjected to further computational operations. For example, Frame (a) gives a blending field that allows a convective flux, J_{conv} , to be expressed as a weighted average of centred, J_{CD} , and upwind fluxes, J_{UP} . This is achieved via a blending parameter ϵ_1 where $J_{conv} = \epsilon_1 J_{CD} + (1 - \epsilon_1) J_{UP}$. The Frame (a) contours are equivalent to those in Fig. 2.16. Similarly, Frame (b) shows HJ computed values for s used in Eq. (2.80). Frame (c) gives the result of the application of Eq. (2.82) to a HJ level set field. Finally, Frame (d) gives length scale fields to model turbulence. This

consists of a near wall distance field propagated to the LES filter scale with the HJ equation solved in its eikonal form. The combined figures show how the HJ equation can be used to yield a more unified hybrid RANS-LES (see Chap. 4) solution approach. This is through providing both non-reflecting boundary properties and also modelled turbulence length scales. Notably, HJ type equations are amenable to parallel solution on unstructured grids. Hence, they offer greater potential for large-scale computations where serial based surface distance search procedures can be slow.

The radiation boundary condition is based on the idea that for acoustic problems asymptotic solutions, at the far field, can be derived. These can be expressed as expansions, typically written as powers of $1/r$ where r is the distance from the sound source to the boundary. Differential equations are derived that satisfy the expansion. These differential equations are imposed as boundary conditions to the Euler equation. The differential equations only have outwards pointing characteristics. Hence, they do not need information at the domain boundary and can be discretized by off-set differences. As a basic example, the far field boundary condition of Tam (1998), for a two-dimensional acoustic problem, is given below.

$$\frac{1}{U(\theta)} \frac{\partial \mathbf{u}}{\partial \tau} + \frac{\partial \mathbf{u}}{\partial \rho} + \frac{\mathbf{u}}{\rho} = 0 \quad (2.83)$$

In the above:

$$U(\theta) = M \cos(\theta) + \sqrt{1 - M^2 \cos^2 \theta} \quad (2.84)$$

where M is the far field Mach number and θ' the angle of the node point relative to the mean flow. The above can be extended to three-dimensions.

With the Perfectly Matched Layer (PML) approach Hu (2001) a perfect mathematical matching is enforced between the core solution zone and the extended grid sponge zone. The extended sponge zone is intended to perfectly damp all acoustic waves at all angles. The approach allows use of a more compact sponge zone. The formulation of Hu (2001) is for the linearized Euler equations.

Aero engine intakes can have acoustic liners. These need to be modelled using impedance boundary conditions. If it is assumed the unsteadiness varies as $e^{-i\omega t}$ then the impedance, $Z = R - iX$, where R is the resistance and X the reactance (imaginary component of acoustic impedance). An impedance boundary condition is used by Muhlbauer et al. (2008), but this time as an outflow condition when exploring pulsed gain combustion engines. A brief overview of impedance boundary conditions is given by Tam (1998).

2.22 Impact of Grid Topology on Solution Accuracy

To further explore the performances of some of the schemes discussed examples are considered for acoustic, vortical and Tollmien-Schlichting (T-S) waves in Appendix A. Here, in relation to grid topology influence, some key points will be sum-

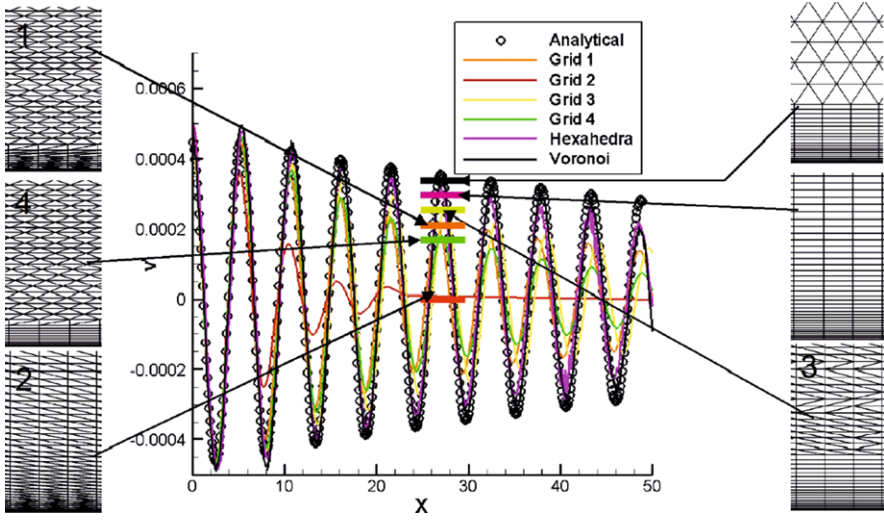


Fig. 2.23 Plot of T-S wave decay with streamwise distance for different grid topologies (from Tucker 2008). Published with kind permission from Elsevier

marized for T-S waves and also homogeneous decaying turbulence. Comparisons are made with an analytical solution for a subcritical T-S wave (Orszag 1971).

As noted above, the most popular options for dealing with complex aerodynamic geometries is either through use of overset curvilinear grids, unstructured grids or for highly complex problems a combination of the two. The former option is considered in Appendix A. It is shown that the overset interface can create a slight discontinuity in the mean flow field. Fortunately, this does not corrupt the T-S wave amplitude relative to the mean field. Unstructured grids allow more severe cell topology changes. These have greater potential solution impact and hence are dealt with here.

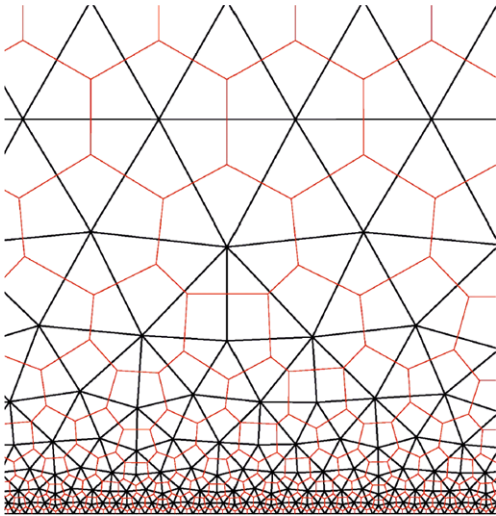
The unstructured grids shown in Fig. 2.23 are considered. Just grid snapshots for a lower channel half, that contains the T-S wave, are shown. Essentially, for these more triangulated grids, where possible, the nodal locations are the same as used for the hexahedral grid shown in the figure. However, due to the inclusion of triangulation the number of edges typically increases by around 30 %. Table 2.9 summarizes the number of edges for the different Fig. 2.23 grids.

The program considered here is an edge-based solver hence computational demands rise with the increasing number of edges. The grid referred to as Voronoi is shown in the top right hand corner of Fig. 2.23. As can be seen, this grid is in fact hybrid. The construction of a pure Voronoi grid, that can capture the sharp near wall velocity gradients, without radically altering the streamwise grid spacing, being impossible. A potential quasi-Voronoi grid, illustrating the aspect ratio problem, is shown in Fig. 2.24.

Table 2.9 Number of nodes and edges for the different unstructured grids

Grid	No. of nodes	No. of edges
Hex	34706	86113
1	35876	124284
2	34706	120169
3	37386	106717
4	35876	114044
Voronoi	24794	65381

Fig. 2.24 Quasi-Voronoi grid refined in the near wall region (from Tucker 2008). Published with kind permission from Elsevier



The graph at the centre of Fig. 2.23 shows the decay of v' (perturbation in vertical velocity) for the T-S wave. The analytic solution to the Orr-Sommerfeld equation is represented by symbols. From Fig. 2.23 it is clear that Grid 2 (lower left hand corner) gives the worst accuracy.

As would be expected, in Fig. 2.23, the modest hexahedral grid shows reasonable agreement with the analytic solution. On the other hand the hybrid-Voronoi grid (even though the linking of the different grid topologies is far from smooth) does well. In fact, it has the highest accuracy. It is important to stress that this grid has around 40 % less nodes and over 30 % less edges than the hexahedral grid.

Figure 2.25 perhaps sheds some light on the computational performance issues. The hexahedral and Voronoi grids do well probably partly because the control volume face is orthogonal to the line connecting the nodes that straddle it. According to Moulinec et al. (2005), this property gives better energy conservation. Also, for the different grids there are different levels of mean flow alignment (and symmetry). Compared to grids 1 and 4, the Grid 2 triangulation appears to be least mean flow aligned. It exhibits the most control volume to node connecting line non-orthogonality. The randomized grid's nature ensures more faces exhibit the desir-

Fig. 2.25 Control volume shapes studied. Published with kind permission from Elsevier

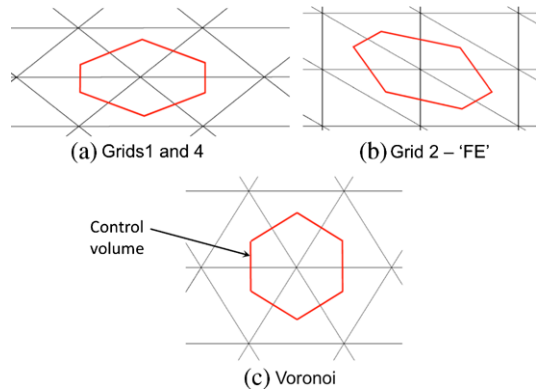
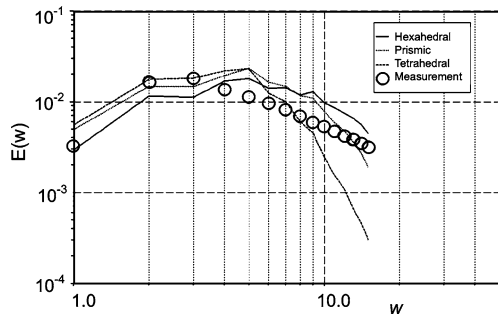


Fig. 2.26 Energy spectrum for homogeneous decaying turbulence computed on different grid topologies



able orthogonal condition i.e. at least one zone of the control volume will be akin to grids 1 & 4. Also, it should be stressed the randomized grids have a bigger accuracy enhancing hexahedral cell zone.

From this discussion it is clear that for LES/DNS the cell shape can potentially strongly influence results. There seems room for research into optimal grid topologies for LES. Based on the above findings, for DNS/LES type simulations it seems sensible to, where possible, use hexahedral cells having as isotropic nature as possible. As discussed by Broeckhoven et al. (2007) it can be critical to have smooth changes in grid spacing at internal boundaries. This is especially so for aeroacoustics, where a mismatch in the vorticity field, between an LES zone and acoustic propagation zone, can act as an artificial sound source. The hybrid Voronoi grid could well give rise to this issue. To avoid this problem, workers have explored carefully decaying the acoustic source term in the vicinity of this interface zone (Broeckhoven et al. 2007).

Figure 2.26 gives energy spectrums for LES type computations of the homogeneous decaying turbulence case explored earlier. The hexahedral grid locations are triangulated in differing ways. Again, the hexahedral grid does well. The prismatic which is like an extruded Voronoi also shows encouraging performance. However, the tetrahedral mesh, that lacks the orthogonality property shows strong numerical dissipation levels. It is worth noting that the kinetic energy scheme, discussed earlier remedies much of the grid sensitivity shown in Fig. 2.26.

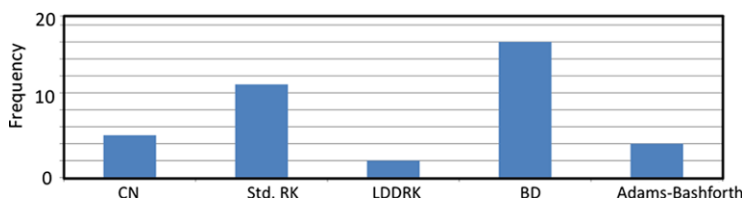


Fig. 2.27 Frequency of use of different temporal schemes

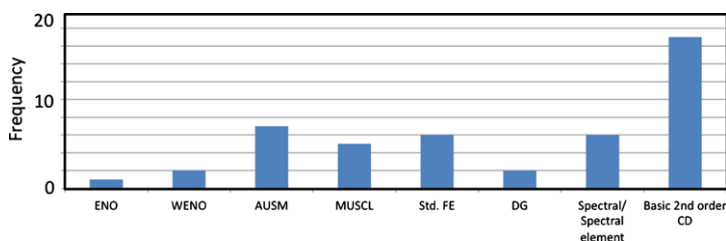


Fig. 2.28 Frequency of use of different spatial schemes

2.23 Frequency of Use of Different Numerical Approaches

The frequency of use, of the different numerical schemes, discussed above, are considered in this section. The statistics are based on the later chapters. In these, the application of such schemes to eddy resolving simulations is mostly overviewed. Figure 2.27 gives the frequency of use of different temporal schemes. The most popular appears to be the implicit backwards BD scheme. This is followed the RK and then the CN. Figure 2.28 gives the frequency of use of different spatial schemes. Like the temporal, it seems that the most popular scheme(s) are the more traditional. The basic 2nd order central difference (CD) scheme is by far the most popular. Although not tabulated, the later chapters shown the finite volume approach is considerably more popular than finite element method, as would be expected. Structured and unstructured grid methods have similar frequencies of use. Chimera grids have a low frequency of use (5 % of simulations). Also, the Roe scheme sees much more application than the Jameson—nearly an order of magnitude in frequency.

2.24 Conclusions

As can be seen from the brief overview of methods given in this chapter there are a wide range of schemes. Just small subsets of these find practical use. In the subsequent chapters further case customized (for different application areas) numerical approaches will emerge. Grid quality can have a strong solution impact as does the numerical scheme. Hence, particularly when making LES computations, attention should be paid to the numerical scheme and grid quality and how these two elements interact. The choice of solution frame of reference can also have a profound

accuracy impact. Assessing when to use high order schemes is complex and again is linked to mesh quality. Increases in computational power allow the use of finer grids and time steps. Hence this helps alleviate accuracy deficiencies in schemes. However, schemes need sufficient order for grid resolution increases to make a worthwhile accuracy impact. Effective non-reflecting boundary conditions help remove the need for excessive numbers of grid nodes.

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