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Computational Techniques for Fluid Dynamics 1

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4. Theoretical Background

In practice the algebraic equations that result from the discretisation process, Sect. 3.1, are obtained on a finite grid. It is to be expected, from the truncation errors given in Sects. 3.2 and 3.3, that more accurate solutions could be obtained on a refined grid. These aspects are considered further in Sect. 4.4. However for a given required solution accuracy it may be more economical to solve a higher-order finite difference scheme on a coarse grid than a low-order scheme on a finer grid, if the exact solution is sufficiently smooth. This leads to the concept of computational efficiency which is examined in Sect. 4.5.

An important question concerning computational solutions is what guarantee can be given that the computational solution will be close to the exact solution of the partial differential equation(s) and under what circumstances the computational solution will coincide with the exact solution. The second part of this question can be answered (superficially) by requiring that the approximate (computational) solution should converge to the exact solution as the grid spacings Δt, Δx shrink to zero (Sect. 4.1). However, convergence is very difficult to establish directly so that an indirect route, as indicated in Fig. 4.1, is usually followed. The indirect route requires that the system of algebraic equations formed by the discretisation process (Sect. 3.1) should be consistent (Sect. 4.2) with the governing partial differential equation(s). Consistency implies that the discretisation process can be reversed, through a Taylor series expansion, to recover the governing equation(s). In addition, the algorithm used to solve the algebraic equations to give the approximate solution, T, must be stable (Sect. 4.3). Then the pseudo-equation

$$\text{CONSISTENCY} + \text{STABILITY} = \text{CONVERGENCE} \tag{4.1}$$

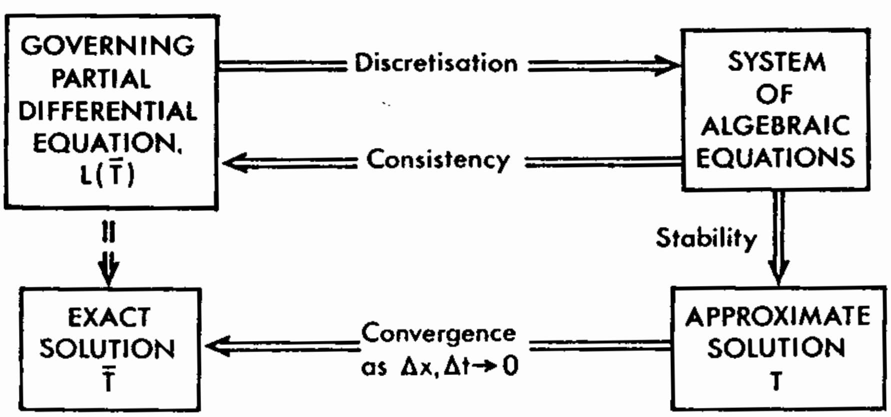

Fig. 4.1. Conceptual relationship between consistency, stability and convergence

is invoked to imply convergence. The conditions under which (4.1) can be made precise are given by the Lax equivalence theorem (Sect. 4.1.1).

It is very difficult to obtain theoretical guidance for the behaviour of the solution on a grid of finite size. Most of the useful theoretical results are strictly only applicable in the limit that the grid size shrinks to zero. However the connections that are established between convergence (Sect. 4.1), consistency (Sect. 4.2) and stability (Sect. 4.3) are also qualitatively useful in assessing computational solutions on a finite grid.

4.1 Convergence

A solution of the algebraic equations (Fig. 4.1) which approximate a given partial differential equation is said to be convergent if the approximate solution approaches the exact solution of the partial differential equation for each value of the independent variable as the grid spacing tends to zero. Thus we require $T_j^n \rightarrow \bar{T}(x_j, t_n)$, as Δx, $\Delta t \rightarrow 0$.

The difference between the exact solution of the partial differential equation and the exact solution of the system of algebraic equations is called the solution error, denoted by e_j^n; that is

$$e_j^n = \bar{T}(x_j, t_n) - T_j^n \ . \tag{4.2}$$

The exact solution of the system of algebraic equations is the approximate solution of the governing partial differential equation. The exact solution of the system of algebraic equations is obtained when no numerical errors of any sort, such as those due to round-off, are introduced during the computation. The magnitude of the error, e_j^n, at the (j, n)-th node typically depends on the size of the grid spacings, Δx and Δt, and on the values of the higher-order derivatives at that node, omitted from the finite difference approximations to the derivatives in the given differential equation.

Proof that a solution to the system of algebraic equations converges to the solution of the partial differential equation is generally very difficult, even for the simplest cases. For the approximate solution to the diffusion equation, using the very simple FTCS algorithm (3.41), a proof of convergence for $s \leqq \frac{1}{2}$ is given by Noye (1984, pp. 117–119). Convergence is very difficult to show when the given partial differential equation is more complicated than the diffusion equation and the method of discretisation is less direct.

A few flow problems possess exact solutions so that, for these cases, convergence can be inferred by obtaining computational solutions on progressively refined grids (Sect. 4.1.2).

4.1.1 Lax Equivalence Theorem

For a restricted class of problems convergence can be established via the Lax equivalence theorem (Richtmyer and Morton 1967, p. 45): “Given a properly posed linear initial value problem and a finite difference approximation to it that satisfies the consistency condition, stability is the necessary and sufficient condition for convergence".

Although the theorem is expressed in terms of a finite difference approximation it is applicable to any discretisation procedure that leads to nodal unknowns, e.g., the finite element method. The Lax equivalence theorem is of great importance, since it is relatively easy to show stability of an algorithm and its consistency with the original partial differential equation, whereas it is usually very difficult to show convergence of its solution to that of the partial differential equation.

Most "real" flow problems are nonlinear and are boundary or mixed initial/boundary value problems so that the Lax equivalence theorem cannot always be applied rigorously. Consequently the Lax equivalance theorem should be interpreted as providing necessary, but not always sufficient, conditions. In the form of (4.1) the Lax equivalence "equation" is useful for excluding inconsistent discretisations and unstable algorithms.

4.1.2 Numerical Convergence

For the equations that govern fluid flow, convergence is usually impossible to demonstrate theoretically. However, for problems that possess an exact solution, like the diffusion equation, it is possible to obtain numerical solutions on a successively refined grid and compute a solution error. Convergence implies that the solution error should reduce to zero as the grid spacing is shrunk to zero.

For program DIFF (Fig. 3.13), solutions have been obtained on successively refined spatial grids, $\Delta x = 0.2, 0.1, 0.05$ and 0.025. The corresponding rms errors are shown in Table 4.1 for $s = 0.50$ and 0.30. It is clear that the rms error reduces like Δx^2 approximately. Based on these results it would be a reasonable inference that refining the grid would produce a further reduction in the rms error and, in the limit of Δx (for fixed s) going to zero, the solution of the algebraic equations would converge to the exact solution.

The establishment of numerical convergence is rather an expensive process since usually very fine grids are necessary. As s is kept constant in the above example the timestep is being reduced by a factor of four for each halving of Δx. In Table 4.1 the solution error is computed at $t = 5000$ s. This implies the finest grid solution at $s = 0.30$ requires 266 time steps before the solution error is computed.

For the diffusion equation (3.1) with zero boundary values and initial value $T(x, 0) = \sin(\pi x)$, $0 \leqq x \leqq 1$, the rms solution error $|e|_{\mathrm{rms}}$ is plotted against grid

Table 4.1. Solution error (rms) reduction with grid refinement

	rms error			
$s = \alpha \Delta t / \Delta x^2$	$\Delta x = 0.2$	$\Delta x = 0.1$	$\Delta x = 0.05$	$\Delta x = 0.025$
0.50	1.658	0.492	0.121	0.030
0.30	0.590	0.187	0.048	0.012

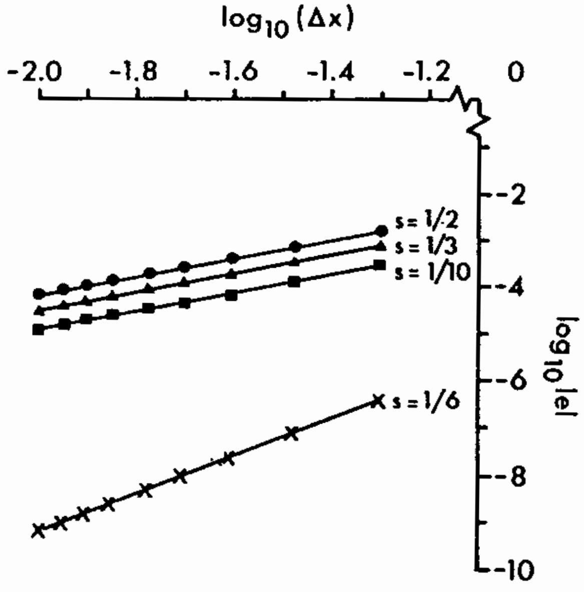

Fig. 4.2. Numerical convergence for the FTCS method

spacing Δx in Fig. 4.2. The increased rate of convergence (fourth-order convergence) for $s=\frac{1}{6}$, compared with other values of $s \leq \frac{1}{2}$ (second-order convergence), is clearly seen, i.e. the convergence rate is like Δx^4 for $s=\frac{1}{6}$, and like Δx^2 otherwise. As will be demonstrated in Sect. 4.2, the superior convergence rate for $s=\frac{1}{6}$ is to be expected from a consideration of the leading term in the truncation error. Typically, for sufficiently small grid spacings Δx, Δt, the solution error will reduce like the truncation error as $\Delta x, \Delta t \rightarrow 0$.

4.2 Consistency

The system of algebraic equations generated by the discretisation process is said to be consistent with the original partial differential equation if, in the limit that the grid spacing tends to zero, the system of algebraic equations is equivalent to the partial differential equation at each grid point.

Clearly, consistency is necessary if the approximate solution is to converge to the solution of the partial differential equation under consideration. However, it is not a sufficient condition (Fig. 4.1), for even though the system of algebraic equations might be equivalent to the partial differential equation as the grid spacing tends to zero, it does not follow that the solution of the system of algebraic equations approaches the solution of the partial differential equation. For instance, choosing $s > \frac{1}{2}$ in program DIFF causes the solution using the FTCS algorithm (3.41) to diverge rapidly. Thus as indicated by the Lax equivalence theorem (Sect. 4.1.1), both consistency and stability are required for convergence.

The mechanics of testing for consistency requires the substitution of the exact solution into the algebraic equations resulting from discretisation, and the expansion of all nodal values as Taylor series about a single point. For consistency the resulting expression should be made up of the original partial differential equation plus a remainder. The structure of the remainder should be such that it reduces to zero as the grid is refined.