

Finite-Difference Schemes for the Diffusion Equation

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Abstract. The Crank-Nicolson scheme is widely used to solve numerically the diffusion equation, because of its good stability properties. It is, however, ill-behaved when large time-steps are used: the short wave-lengths may happen to be *less* damped than the long ones. A detailed analysis of this flaw is performed and an alternative scheme is proposed, which removes this difficulty while preserving all other good properties (unconditional stability and second-order accuracy).

1 Introduction

The diffusion equation plays an important role in many branches of physics, in fields as different as fluid and plasma dynamics, thermodynamics and neutron transport. From the point of view of numerical analysis, diffusive terms are often necessary when solving partial differential equations in order to control the numerical noise at small wave-lengths. Indeed, although a fine resolution is needed to reproduce accurately the larger scales, small scales do not contain any significant physical information. If, however, such small scales are not damped away by some diffusive mechanism, in the long run they can corrupt the entire solution, even at long wave-lengths.

There is a vast literature of numerical methods for the diffusion equation, which we make no attempt to review even partially here (Marchuk 1982; Morton and Mayer 1994; Richtmyer and Morton 1967; Press et al. 1992; Crank 1975; Roache 1972), (Morton and Mayer 1994 provide a list of fourteen finite-difference methods). According to the time-stepping technique used, these schemes can be either explicit or implicit. Explicit schemes are simpler and computationally faster, but often impose a very restrictive upper bound on the maximum time-step, beyond which they are unstable. Implicit schemes are often unconditionally stable, but require the inversion of a (tridiagonal, in one dimension) matrix, which is more time consuming, although not prohibitive.

The scope of this communication is to point out a weakness of a class of widely used implicit, finite-difference techniques, which seems to be generally overlooked. A prototype of such techniques is the Crank-Nicolson (CN)

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scheme (Crank and Nicolson 1947), possibly the most popular of all finite-difference schemes for the diffusion equation. The problem with the CN scheme is that it is extremely ill-behaved for large values of the time-step. By the expression “ill-behaved” we mean that, although the results are of course accurate (to second order) for small time-steps, taking large time-steps radically changes the nature of the equation we are trying to solve. For example, in the limit of very large time-steps, a monochromatic wave is no longer damped (as it should be, according to a diffusion process), but travels with constant phase velocity $\lambda/(2\Delta t)$ (where λ is the wave-length and Δt the time-step). Another, more serious, shortcoming is that, when Δt exceeds a certain value, short wave-lengths can be *less* strongly damped than some long wave-lengths. Bearing in mind that diffusive terms are devised to get rid of the small scale noise, this result can have disastrous consequences.

After recognizing the source of this incorrect behaviour, we propose a class of schemes that does not suffer from this flaw, being “well-behaved” in the limit of large time-steps. These schemes are still second order accurate and unconditionally stable, and only involve the inversion of tridiagonal matrices (just like the CN scheme), but require two matrix inversions rather than one. Therefore, although they are computationally more expensive than CN by a factor of two, they allow the use of an arbitrarily large time-step *without changing the diffusive nature of the equation*.

From the previous discussion it is apparent that “good behaviour” is a crucial property (albeit loosely defined) for many numerical schemes and should be mentioned together with the more familiar notions of accuracy and convergence. Accuracy means that the discrete model closely approximates (in a quantitative sense) the original differential equation when the time-step and grid size are sufficiently small. Good behaviour means that, far away from this limit, the discrete model still preserves qualitatively the most relevant features of the original equation. These notions will become clearer in the following sections, where we work a concrete example.

The remaining material of this paper is organized as follows. In Sect. 2 we briefly review a few schemes for the diffusion equation, then identify the problem with the CN technique and propose an alternative, well-behaved scheme. Section 3 presents a more detailed stability analysis of both CN and our technique, including a numerical example of how CN fails when our scheme succeeds. Finally, in Sect. 4 we draw our conclusions and discuss more extensively the concept of good behaviour of a numerical scheme.

2 Properties of Some Finite-Difference Schemes

Our objective is to solve numerically the diffusion equation

$$\frac{\partial F}{\partial t} = -\hat{D}F, \tag{1}$$

where $\hat{D} = -\sigma \partial^2 / \partial x^2$ is the diffusion operator (σ is the diffusion coefficient), the discrete approximation of which to second order in the grid size is

$$(\hat{D}F)_j = -\sigma (F_{j-1} - 2F_j + F_{j+1}) / \Delta x^2 + O(\Delta x^3). \quad (2)$$

We use this notation because, with suitable boundary conditions, \hat{D} is a positive, hermitian operator (i.e. all of its eigenvalues are real and positive), which, for all practical purposes can be treated as a real positive number. Equation (1) can be solved formally from $t_n = n\Delta t$ to t_{n+1} , yielding

$$F^{n+1} = e^{-\Delta t \hat{D}} F^n, \quad (3)$$

where $F^n = F(t_n)$. Most numerical schemes can be formally represented as an approximation to some order of the exponential appearing in (3). This exponential is the evolution operator for our problem. Thus we have, respectively for the explicit first-order, implicit first-order and Crank-Nicolson schemes:

$$\exp(-\Delta t \hat{D}) = 1 - \Delta t \hat{D} + O(\Delta t^2) \quad (4a)$$

$$\exp(-\Delta t \hat{D}) = (1 + \Delta t \hat{D})^{-1} + O(\Delta t^2) \quad (4b)$$

$$\exp(-\Delta t \hat{D}) = \frac{1 - \Delta t \hat{D}/2}{1 + \Delta t \hat{D}/2} + O(\Delta t^3). \quad (4c)$$

The explicit scheme (4a) is unstable for $\sigma \Delta t / \Delta x^2 > 1/2$, whereas the implicit and the CN schemes (4b-c) are always stable. This can be checked by verifying that the approximate evolution operators have all eigenvalues smaller than unity in absolute value (heuristically, this is obvious by treating \hat{D} as a real positive number). However, the implicit first-order scheme is also well-behaved since, for large time-steps, its evolution operator goes to zero without changing sign, just like the exact exponential. On the contrary the CN evolution operator approaches, for large time-steps, the negative of the identity operator, thus giving rise to unphysical oscillations while suppressing all damping. For instance a sinusoidal wave would, in this limit, simply change sign at each time-step, which is the same as traveling with a phase velocity equal to $\lambda/(2\Delta t)$. This is the paradox first mentioned in the introduction.

The CN scheme is often considered as an ideal choice for the diffusion equation, since it displays some key good properties: (a) it is second order accurate both in space and in time; (b) it is unconditionally stable; and (c) it requires the inversion of a tridiagonal matrix, which can be performed exactly in $O(N)$ operations, N being the number of grid points (Morton and Mayer 1994; Crank 1975). However, as we have seen, when the time-step exceeds a certain value (which will be specified in the next section), the CN scheme is ill-behaved, and gives qualitatively incorrect results.

The problem discussed above does not seem to be mentioned explicitly in the literature. Roache (1972) rather briefly suggests that “large Δt will cause some Fourier modes to overshoot”. He then correctly recognizes that “the CN

second-order method is less accurate than the first-order implicit method for large enough Δt . He wrongly generalizes this fact to suggest that, for large time-steps, first-order schemes are more accurate than second-order schemes. The results presented in the next paragraph prove that this is not generally true. The authors of *Numerical Recipes* (Press et al. 1992) also acknowledge that small scale structures are not damped for the CN scheme in the limit of large time-steps, but do not give a detailed analysis of why it is so. They also incorrectly suggest that the only possible solution is to turn to a first-order implicit method.

We now show that it is possible to devise a scheme which, while preserving most or all of the CN advantages, is also well-behaved for $\Delta t \rightarrow \infty$. The Padé approximation to the exponential appearing in (3) is

$$\exp(-\Delta t \hat{D}) = (1 + \Delta t \hat{D} + \Delta t^2 \hat{D}^2/2)^{-1} + O(\Delta t^3). \quad (5)$$

The scheme resulting from this approximation is still second order accurate and unconditionally stable and also well-behaved, but, due to the term \hat{D}^2 , requires the inversion of a non-tridiagonal matrix. This property may not be crucial since in more than one dimension the matrix is more complicated even for the CN scheme. However, the multi-dimensional diffusion equation can always be reduced to a sequence of one-dimensional equations by the time splitting technique (Yanenko 1971) and, therefore, tridiagonality can be an important issue.

Let us write the formal solution corresponding to (5)

$$\hat{M}F^{n+1} = F^n, \quad (6)$$

where \hat{M}^{-1} is given by the right hand-side of (5). One could split the matrix $\hat{M} = \hat{M}_1 \cdot \hat{M}_2$, where $\hat{M}_{1,2}$ are linear in \hat{D} (and therefore tridiagonal). The solution is then obtained in two steps

$$\hat{M}_1 F^* = F^n \quad (7a)$$

$$\hat{M}_2 F^{n+1} = F^*. \quad (7b)$$

Unfortunately \hat{M} can only be factored by introducing complex coefficients $\hat{M} = (1 + a_+ \Delta t \hat{D})(1 + a_- \Delta t \hat{D})$, with $a_{\pm} = (1 \pm i)/2$, which would unduly complicate the scheme. We can try a more general approximation of the evolution operator:

$$\exp(-\Delta t \hat{D}) \simeq \frac{1 + \alpha \Delta t \hat{D}}{(1 + \beta_+ \Delta t \hat{D})(1 + \beta_- \Delta t \hat{D})}. \quad (8)$$

We call $g(z) = (1 + \alpha z)/(1 + \beta_+ z)(1 + \beta_- z)$ the *response function*. By expanding both sides of (8) in a Taylor series, we obtain

$$1 - z + z^2/2 - z^3/6 =$$

$$1 + (\alpha - \beta_+ - \beta_-)z + [\beta_+^2 + \beta_-^2 + \beta_+\beta_- - \alpha(\beta_+ + \beta_-)]z^2 - \quad (9)$$

$$[\beta_+^3 + \beta_-^3 + \beta_+\beta_-^2 + \beta_-^2\beta_+ - \alpha(\beta_+^2 + \beta_-^2 + \beta_+\beta_-)]z^3 + O(z^4),$$

where $z = \Delta t \hat{D}$. Matching the coefficients at first and second order we can express β_{\pm} as a function of α

$$\beta_{\pm} = \frac{1 + \alpha \pm \sqrt{\alpha^2 - 2\alpha - 1}}{2}. \quad (10)$$

The truncation error $E(\alpha)$ is the modulus of the coefficient of the third order term in (9). After some algebra, it can be shown that $E(\alpha) = \alpha/2 + 1/6$.

We have thus obtained a family of numerical schemes parameterized by the real number α . However, some conditions must be satisfied for the scheme resulting from (8) to be meaningful. First of all it must have $\beta_{\pm} \geq 0$ so that the response function $g(z)$ remains finite. This condition implies $\alpha \geq -1/2$. Note that, for $\alpha = -1/2$ (yielding $\beta_- = 0, \beta_+ = 1/2$), we recover the Crank-Nicolson scheme. In order to have real coefficients the argument of the square root in (10) must be non-negative, which requires $\alpha \leq 1 - \sqrt{2}$ or $\alpha \geq 1 + \sqrt{2}$. Furthermore, if $\alpha \geq 0$, the response function is positive and decreases monotonically for positive values of z . The special case $\alpha = 0$ yields the Padé approximation (5), as can easily be checked. Finally, by taking $\alpha = -1/3$, we obtain $E = 0$ and the scheme is third order accurate in time.

According to our definition the numerical scheme is well-behaved if the response function $g(z)$ qualitatively preserves some of the relevant properties of the exact exponential *for all values of z* . What is meant by ‘relevant properties’ depends on the problem under study: in our case it is crucial that $g(z)$ be positive and decreasing for $z > 0$ since this property guarantees that smaller wave-lengths be more damped. If, in addition, we want all coefficients to be real, we need $\alpha \geq 1 + \sqrt{2}$. The minimum truncation error compatible with this choice is obtained when taking the equality sign in the previous expression. This case will be analyzed in detail in the remainder of the article. Other choices are possible, however. For example, if reducing the truncation error is important, the Padé approximation ($\alpha = 0$) is more convenient, although complex numbers must be used in that case.

With our choice ($\alpha = 1 + \sqrt{2}$) we obtain $\beta_{\pm} \equiv \beta = 1 + 1/\sqrt{2}$ and the scheme can be written in a two-step form (each involving the inversion of the same tridiagonal matrix)

$$(1 + \beta \Delta t \hat{D})F^* = (1 + \alpha \Delta t \hat{D})F^n \quad (11a)$$

$$(1 + \beta \Delta t \hat{D})F^{n+1} = F^*. \quad (11b)$$

This is the scheme that we propose in order to circumvent the bad properties of the CN scheme. It is second-order accurate in space and time, unconditionally stable and well-behaved for large time-steps.

3 Stability Analysis and a Numerical Example

The CN scheme can be written explicitly as follows

$$-\frac{s}{2}F_{j-1}^{n+1} + (1+s)F_j^{n+1} - \frac{s}{2}F_{j+1}^{n+1} = \frac{s}{2}F_{j-1}^n + (1-s)F_j^n + \frac{s}{2}F_{j+1}^n, \quad (12)$$

where $s = \sigma \Delta t / \Delta x^2$. Stability can be checked with the Von Neumann method by taking $F_j^n = F^n \exp(ikx_j) = \exp(i\xi j)$, $\xi = k\Delta x$. Substitution into (12) yields

$$\frac{F^{n+1}}{F^n} = \frac{1 - s(1 - \cos \xi)}{1 + s(1 - \cos \xi)} \equiv G, \quad (13)$$

where $G(\xi)$ is the so-called amplification factor. The scheme is unconditionally stable because $|G| < 1$ for every value of s and ξ . In the limit $\xi \ll 1$ (which simply means that we have enough points to describe every wave-length) the amplification factor becomes

$$G = \frac{1 - s\xi^2/2}{1 + s\xi^2/2}. \quad (14)$$

A fundamental property of G to guarantee the good behaviour of the numerical scheme is that its modulus be monotonically decreasing with wave-number: this implies that the damping increases with increasing wave-number. However, from the plot of $|G(\xi)|$ for a given (large) value of s (Fig. 1), we see that this is not true for the CN technique. Indeed, to the right of its zero $\xi = \sqrt{2/s}$, $|G(\xi)|$ increases with wave-number. Let us study the efficiency of the scheme for different values of s . Obviously the well-behaved region is the one for which $0 < \xi < \sqrt{2/s}$. If $s \ll 1$, then the zero of the function $G(\xi)$ will be much larger than unity: the restriction $\xi < 1$ then means that we are exploiting only a small fraction of this region. When $s \simeq 1$, the scheme is well-behaved for all waves satisfying $\xi < 1$. However, we have not gained much with respect to the explicit scheme, the upper bound of which for stability is $s < 1/2$. When $s \gg 1$, $\sqrt{2/s} \ll 1$ and waves with $\xi > \sqrt{2/s}$ are still sufficiently sampled by the spatial grid, but, for these waves, the damping *decreases* with wave-number, giving completely incorrect results. We must therefore conclude that the interesting region $s > 1$ (i.e. $\Delta t > \Delta x^2/\sigma$), which, if accessible, would free us from the restriction of explicit schemes, is still forbidden for the CN method.

How serious the above restriction is in practice will of course be determined by the physical problem under consideration. When studying two-dimensional fluid turbulence, for example, the time-step is generally determined by other terms in the equations, typically the convective terms, and must obey $\Delta t \lesssim \Delta x/u$, where $u = O(1)$ is a typical velocity of the flow. On the other hand, since the physical Reynolds number is generally much larger than what can be afforded in the computation, the diffusion coefficient is chosen mainly for numerical reasons. In order for wave-lengths comparable

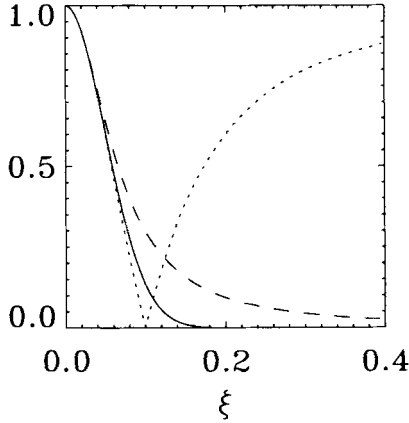


Fig. 1. Modulus of the amplification factor $G(\xi)$ as a function of $\xi = k\Delta x$ for the exact solution (solid line), the Crank-Nicolson scheme (dotted line) and our proposed scheme (dashed line). The curves are plotted for $s = 200$. For the CN case, the curve has a zero at $\xi = (2/s)^{1/2}$.

to the grid size to be damped quickly, one must have $\sigma \simeq u\Delta x^2/a$, where $a = O(1)$ is a macroscopic length scale. The stability parameter then becomes $s \simeq \Delta x/a \ll 1$, which ensures stability even for explicit schemes. We conclude that, in two-dimensional turbulence, the use of a more costly implicit scheme to treat the diffusive terms is hardly justifiable.

In other physical situations the restriction can be less severe. Let us consider a purely diffusive process, in which we only want to isolate a few dominant modes allowed by the boundary conditions, which are all long wavelength modes. This imposes a less strict bound on Δt . Suppose that we want to treat correctly all modes in the range $k_0 < k < k_1$, where the fundamental mode is $k_0 = 2\pi/L$. The maximum mode present is $k_{max} = 2\pi/\Delta x$. It is crucial to require that all modes larger than k_1 should be more damped than k_1 itself. The maximum k that satisfies this condition can be found by solving the algebraic equation $|G(\xi_1)| = |G(\xi_{max})|$, where we recall that $\xi = k\Delta x$. The result, expressed as an upper bound for the time-step, is

$$\sigma \Delta t < \frac{2}{k_1 k_{max}} = \frac{\Delta x}{\pi k_1}. \quad (15)$$

Thus, for this very particular case, Δt scales as Δx instead of Δx^2 , as for the explicit scheme. However, for large values of k_1 , the above upper limit can still be very stringent: in the next paragraph it will be shown that, with our technique, all restrictions on the time-steps are lifted.

Turning to the scheme that we propose (11) we have

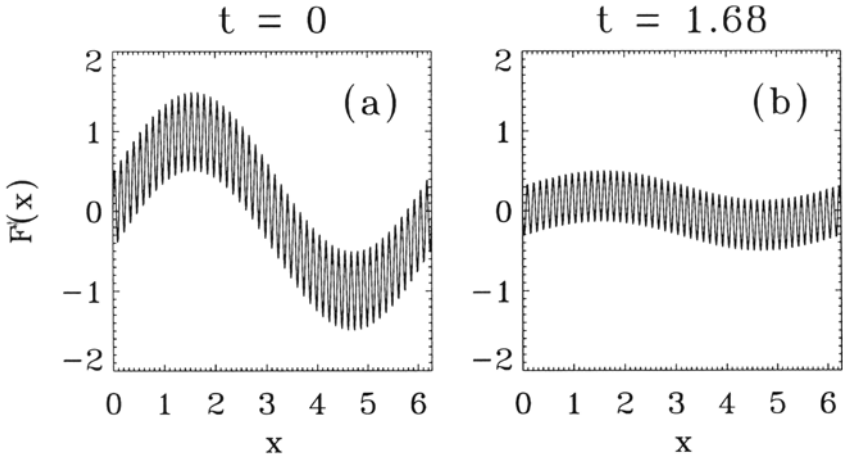


Fig. 2. Plot of $F(x)$ at different times (a) $t = 0$, (b) $t = 1.68$, from a numerical solution with the Crank-Nicolson scheme. The long wave-length is more strongly damped than the short wave-length

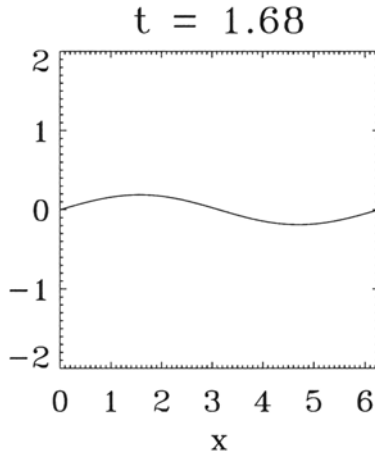


Fig. 3. Plot of $F(x)$ at $t = 1.68$, from a numerical solution with our proposed scheme. The initial condition is the same as shown in Fig. 2a. Now the short wave-length is rapidly damped

$$-\beta s F_{j-1}^* + (1 + 2\beta s) F_j^* - \beta s F_{j+1}^* = -\alpha s F_{j-1}^n + (1 + 2\alpha s) F_j^n - \alpha s F_{j+1}^n \quad (16a)$$

$$-\beta s F_{j-1}^{n+1} + (1 + 2\beta s) F_j^{n+1} - \beta s F_{j+1}^{n+1} = F_j^*. \quad (16b)$$

Using again the Von Neumann method to investigate stability we find that the amplification factor is

$$G = \frac{1 + 2\alpha s(1 - \cos \xi)}{[1 + 2\beta s(1 - \cos \xi)]^2}. \quad (17)$$

It can easily be verified that $|G| < 1$ for any value of ξ and s , if α and β are those of our choice ($\alpha = 1 + \sqrt{2}, \beta = 1 + 1/\sqrt{2}$): this is sufficient to ensure stability. The plot of $|G(\xi)|$, in the case $s \gg 1$, is given in Fig. 1. Note that, in contrast to the CN scheme, the amplification factor decreases monotonically to zero. It is obvious that, even for very large values of s , the property that short wave-lengths be *more* damped than long ones is preserved for the entire spectrum. The scheme is thus, according to our definition, well-behaved.

We now illustrate the results obtained above with a numerical example. We solve the diffusion equation (1), in a periodic domain of extension $L = 2\pi$, with diffusion coefficient $\sigma = 1$. The initial condition is the sum of two waves with very different wave-lengths:

$$F(x, t = 0) = A_1 \sin(k_1 x) + A_2 \sin(k_2 x), \quad (18)$$

with $A_1 = 1, A_2 = 0.5, k_1 = 1, k_2 = 50$. For the numerical solution we take $N = 500, \Delta x = 0.0126$, so that $k\Delta x < 1$ for both waves. Normally, the second wave should decay much faster, leaving only the large scale perturbation. However, for the CN scheme, if we choose the time-step so that $|G(k_1)| = |G(k_2)|$, then the two waves will decay with the same rate. For a still larger time-step the first wave will decay faster than the second one, yielding completely incorrect results. The upper bound for Δt – given by (15) with k_1, k_2 replacing k_1, k_{max} – is in this case $\Delta t_{lim} = 0.04$.

We present a numerical solution with $\Delta t = 0.08$, first using the standard CN scheme. Fig. 2 shows $F(x)$ at two different times: as expected, the large scale wave decays faster. Using the scheme of (11),(16) completely eliminates the problem, as is apparent from Fig. 3, and the small wave-length is now correctly damped faster. Fig. 4 shows the amplitude of the Fourier coefficient of each wave for the two cases. The damping of the first wave ($\gamma_1 = -\sigma k_1^2$) is reproduced accurately in both cases, since $|\gamma_1| \Delta t \ll 1$. However, the CN scheme grossly underestimates the damping rate γ_2 of the second wave, as is apparent from Fig. 2. Moreover, spurious oscillations appear, which are due to the fact that $G(\xi)$ is negative for the value of $\xi = k\Delta x$ corresponding to k_2 . Our scheme also underestimates γ_2 , but automatically preserves the crucial relation $|\gamma_2| > |\gamma_1|$.

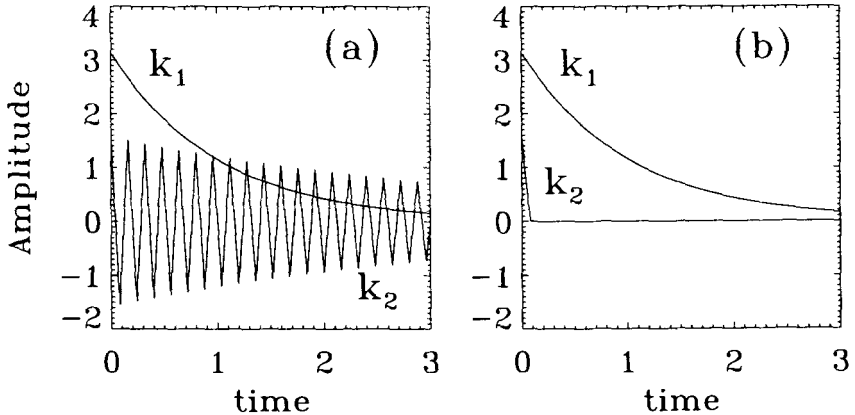


Fig. 4. Time evolution of the Fourier coefficient of both waves for (a) the Crank-Nicolson scheme and (b) our alternative scheme. The damping of the small wave-number k_1 is well reproduced in both cases, but the large wave-number k_2 is poorly treated by the Crank-Nicolson scheme

4 Conclusion

We have identified a flaw occurring in a class of finite-difference, implicit schemes for the diffusion equation, the prototype of which is the Crank-Nicolson scheme. Although the CN is stable for arbitrary values of the time-step, in practice it gives poor results for $\Delta t > \Delta x^2/\sigma$. In particular, short wave-lengths may happen to be less damped than long ones. For problems of fluid turbulence, the constraint on the size of the time-step is virtually as severe as that of explicit schemes ($\Delta t < \Delta x^2/\sigma$), although, for flows at high Reynolds numbers, the convective terms impose a time-step which always falls in the stability region. For purely diffusive problems, the constraint is somewhat less severe (Δt scales as Δx , instead of Δx^2). The possibility of using an even larger time-step is in any case ruled out.

The technique that we propose to overcome this restriction is based on a Padé-like approximation of the exact evolution operator for the diffusion equation. This allows us to construct a new scheme that preserves all the good properties of CN, while avoiding the above shortcoming. For this scheme, short wave-lengths are always more damped than long ones. The only price to pay is that the computation time *per time-step* is roughly twice that of CN, but now a much larger time-step can be used so that the total computation time will in fact be much shorter. We note that our choice, expressed by (8), is not the only one possible. The denominator on the right hand-side does not need to be a perfect square, although this slightly simplifies the resulting scheme since the same matrix is inverted twice.

We have also tried to convey the idea that convergence and stability are often not sufficient for a good numerical scheme. The scheme should also preserve qualitatively some key properties of the original equation over all the range of the discretization parameters: it should be “well-behaved”. For the diffusion equation it should ensure that the damping rate increases with wave-number *for all values of Δt* . Of course good behaviour strongly depends upon the equation to be solved. Take for example the Schrödinger equation, obtained by replacing \hat{D} with $i\hat{H}$ in (1), where $\hat{H} = -\partial^2/\partial x^2 + V(x)$ is the Hamiltonian. The key property of this equation is that \hat{H} is a unitary operator, i.e. the integral of $|F(x)|^2$ is conserved in time. It is easy to show that the CN scheme provides the only discrete approximation to \hat{H} which is both unitary and second order accurate. Both schemes (5) and (11) introduce some numerical damping that violates unitarity. The CN scheme is thus well-behaved for the Schrödinger equation, although not for the diffusion equation.

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