

Note

Derivation of Implicit Difference Schemes by the Method of Differential Approximation

In this paper we use the continuum differential approximation of a time discrete difference scheme to show how one can derive simple operators that approximate fully implicit time differencing of a system of partial differential equations. This type of approximation has been considered before and has been called "semi-implicit" [1-3]. It generally involves adding implicitly and subtracting explicitly some simple operator whose matrix form is easy to invert. This modifies the truncation error of the underlying difference scheme and, as far as time error is concerned, results in unconditional linear stability just as for a fully implicit scheme, but for much less work. The question of accurate reproduction of the original continuum system of equations must of course still be considered; however, numerical stability is assured. We show how the method of differential approximation [4-6] can be used to derive semi-implicit operators for any given system of equations. In this way we show explicitly how such operators arise from the truncation error of a "brute force," fully implicit differencing in time. This sheds light on the fundamental meaning of implicit differencing and allows the semi-implicit approximation to be easily evaluated relative to a fully implicit scheme. Unfortunately, the term "semi-implicit" in the literature does not have an accepted meaning. As will be seen, a more descriptive term for this type of procedure is "approximately implicit."

In the method of differential approximation one analyzes a finite difference scheme by converting it to a continuum set of equations by a simple Taylor series expansion keeping an "appropriate" number of truncation error terms. This, the differential approximation, represents the finite difference scheme and shows how it corresponds to the original system to be solved. It is a continuous system of equations and thus allows a direct comparison of the finite difference scheme to the original "primitive" system of equations. The method of differential approximation can be used to study the effects of nonconstant and nonlinear coefficients [4]. In the case of constant coefficients a direct correspondence with the usual Fourier series analysis of difference schemes can be established [5]. Often, instability of an unstable difference scheme will show up as ill-posed diffusion in the lowest order terms of the differential approximation. Some algebraic manipulation may be required to see this [4, 6].

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The answer to the question of how high in degree truncation error terms retained in the differential approximation to a finite difference scheme should be is easily ascertained by the following consideration. For a differential equation to faithfully represent the continuum limit of a discrete difference equation it must require the same initial and boundary data as the difference equation; that is, it must be of the same degree in all of its derivatives. If the difference equation, and thus its differential approximation, is of higher degree than the primitive differential equation it is to represent (usually this is done to obtain a higher order of approximation), then extra numerical boundary or initial conditions are needed. Such schemes will contain spurious computational solutions that have nothing to do with the primitive differential equation. These solutions may influence the stability and accuracy of the difference scheme and may explain why formally higher order difference schemes in some instances give poor results. Since the differential approximation to the difference scheme, as defined above, contains the additional computational solutions, it gives a way of analyzing their properties. Indeed, in this case the differential approximation will contain the primitive differential equation as a factor [7]. In this paper we will be concerned only with difference schemes whose degree is no higher than that of the continuum equations they represent so no spurious computational solutions occur.

To briefly illustrate what has been said about the method of differential approximation consider the first-order accurate, time explicit approximation to the diffusion equation, written as

$$\left(\frac{\partial u}{\partial t}\right)^{n+1/2} = D \left(\frac{\partial^2 u}{\partial x^2}\right)^n. \tag{1}$$

Here the superscript denotes time centering. The l.h.s. of Eq. (1) stands for $(u^{n+1} - u^n)/\Delta t$, and is second-order accurate in time. The spatial differencing of the r.h.s. is taken to be second-order accurate in space and leads to terms of higher degree than the second in the truncation error and is thus suppressed. Since the differential approximation is restricted to require no extra data than the original difference equation (which here matches that of the primitive differential equation) the only possible additional term is $\partial^3 u / \partial t \partial x^2$. Using $u^n = u^{n+1/2} - (\Delta t/2)(\partial u / \partial t)^{n+1/2}$ in the r.h.s. of Eq. (1) yields

$$\left(1 + \frac{D \Delta t}{2} \frac{\partial^2}{\partial x^2}\right) \frac{\partial u}{\partial t} = D \frac{\partial^2 u}{\partial x^2}, \tag{2}$$

as the differential approximation to the difference scheme. Note that a Fourier expansion of the spatial part of Eq. (2) as $\exp(ikx)$ shows that the coefficient of the l.h.s. vanishes when $Dk^2 \Delta t = 2$. Or, using $-4/\Delta x^2$ as the value of $\partial^2/\partial x^2$ in Eq. (2), which is appropriate for the $2 \Delta x$ wave on a uniform spatial grid, this gives the usual stability criterion for an explicit time integration of the diffusion equation. For implicit differencing the superscript n simply goes to $n + 1$ on the r.h.s. of

Eq. (1). This merely changes the sign of the Δt term in Eq. (2). Then the stability restriction due to the l.h.s. of Eq. (2) disappears. Thus we see that the differential approximation to the difference scheme, Eq. (2), does mimic its stability properties, as required.

This example shows that if the difference scheme is not of higher degree ("order" is used in this paper only to denote size of truncation error) than the primitive differential equation it is to approximate, then its differential approximation can only consist of the primitive differential equation (for consistency) and, as truncation error terms, mixed derivatives that are combinations of the terms appearing in the primitive equation. Only these terms require no additional initial or boundary conditions. Note also that in order to directly obtain the differential approximation, Eq. (2), it was necessary to expand Eq. (1) about the $n + \frac{1}{2}$ time level rather than the n level, which would have required an additional transformation to bring it into the form given as Eq. (2).

Next we turn to our main subject—the derivation of approximately implicit difference schemes by means of the method of differential approximation. We will work a simple example in detail and then quickly generalize to more complicated and relevant cases.

Consider the scalar, one-dimensional, second-degree wave equation written as the coupled first-order system

$$\frac{\partial u}{\partial t} = c \frac{\partial v}{\partial x}, \tag{3a}$$

$$\frac{\partial v}{\partial t} = c \frac{\partial u}{\partial x}, \tag{3b}$$

where c is the wave speed. A "brute force" fully implicit first-order accurate time differencing of Eqs. (3) can be written as

$$\left(\frac{\partial u}{\partial t}\right)^{n+1/2} = c \left(\frac{\partial v}{\partial x}\right)^{n+1}, \tag{4a}$$

$$\left(\frac{\partial v}{\partial t}\right)^{n+1/2} = c \left(\frac{\partial u}{\partial x}\right)^{n+1}, \tag{4b}$$

where the superscripts have the same meaning as before and the second-order accurate, centered spatial differencing has once again been suppressed. Since we require that the degree of the difference scheme and its differential approximation agree, only terms of the form $\partial^2/\partial t \partial x$ may be added to Eqs. (4). Taylor expanding the r.h.s. of Eqs. (4) about the $n + \frac{1}{2}$ time level gives as its differential approximation

$$\frac{\partial u}{\partial t} - \frac{c \Delta t}{2} \frac{\partial^2 v}{\partial t \partial x} = c \frac{\partial v}{\partial x}, \tag{5a}$$

$$\frac{\partial v}{\partial t} - \frac{c \Delta t}{2} \frac{\partial^2 u}{\partial t \partial x} = c \frac{\partial u}{\partial x}. \tag{5b}$$

Next we rewrite Eqs. (5) in an equivalent but decoupled form. To this end we time differentiate Eq. (5b) and using Eq. (5a) obtain

$$\left(1 - \frac{c^2 \Delta t^2}{4} \frac{\partial^2}{\partial x^2}\right) \frac{\partial^2 v}{\partial t^2} - c^2 \Delta t \frac{\partial^2}{\partial x^2} \left(\frac{\partial v}{\partial t}\right) = c^2 \frac{\partial^2 v}{\partial x^2}. \tag{6}$$

But this equation can then be rewritten as the coupled system

$$\frac{\partial u}{\partial t} = c \frac{\partial v}{\partial x}, \tag{7a}$$

$$\left(1 - \frac{c^2 \Delta t^2}{4} \frac{\partial^2}{\partial x^2}\right) \frac{\partial v}{\partial t} = c \frac{\partial u}{\partial x} + c^2 \Delta t \frac{\partial^2 v}{\partial x^2}. \tag{7b}$$

Equations (7) are exactly equivalent to Eqs. (5); that is, they represent an approximation to an implicit differencing scheme in the lowest order terms which comprise the differential approximation. Notice that if we had used the primitive system, Eqs. (3), to directly transform the mixed derivatives in Eqs. (5) we would only have obtained the lowest order diffusion terms and would have missed the essential term $\propto \Delta t^2$ in Eq. (7b). This illustrates the important point, stressed in Ref. (5), that one must work directly with the differential approximation to the difference scheme and not use the primitive system to simplify it to a low order nonuniformly.

We now wish to dwell on some properties of Eqs. (7). First, note that an explicit time differencing of Eqs. (3) ($n + 1 \rightarrow n$ in Eqs. (4)), known to be numerically unstable, also would lead to Eqs. (7) except that the sign of the dissipative term on the r.h.s. of Eq. (7b) would be negative, indicating instability as ill-posed diffusion. However, if one drops the dissipative term in Eq. (7b) then Eqs. (7) are still unconditionally stable and represent a second-order accurate approximation to Eqs. (3), reminiscent of a time-centered differencing. To see that Eqs. (7) lead to an unconditionally stable scheme consider them differenced by the time-staggered leap-frog scheme with the dissipative term dropped. This gives

$$u^{n+1/2} - u^{n-1/2} = c \Delta t \left(\frac{\partial v}{\partial x}\right)^n, \tag{8a}$$

$$v^{n+1} - v^n = c \Delta t \left(\frac{\partial u}{\partial x}\right)^{n+1/2} + c^2 \frac{\Delta t^2}{4} \left(\frac{\partial^2 v}{\partial x^2}\right)^{n+1} - c^2 \frac{\Delta t^2}{4} \left(\frac{\partial^2 v}{\partial x^2}\right)^n. \tag{8b}$$

The last two terms on the r.h.s. of Eq. (8b) are the usual “semi-implicit” terms—added implicitly and subtracted explicitly. We see that they naturally arise as a piece of the implicit differenced form, Eqs. (4), given directly by Eqs. (7), in fact, as

the only essential part. Leapfrog time differencing on Eqs. (3) yields $c^2 k^2 \Delta t^2 \leq 4$ as a stability criterion. Equations (8) modify this constraint to be

$$\frac{k^2 c^2 \Delta t^2}{1 + k^2 c^2 \Delta t^2 / 4} \leq 4, \quad (9)$$

which is readily seen to always be satisfied independently of Δt . This brings out the important point of implicit difference schemes; namely, they stabilize mainly by means of phase error, diffusion is subsidiary. That is, an implicit difference scheme compresses all time eigenvalues of a system of equations to be inside a radius of $1/\Delta t$ in the complex $1/t$ plane. This always results in a "stabilizing denominator," or in physics terms, a k -dependent mass.¹ The point is that the semi-implicit approximation does the same thing, only Eqs. (8), being more diagonal, are easier to invert than the fully implicit scheme given by Eqs. (4). The diffusion term in Eq. (7b) may be kept to damp unresolved spatial scales or to compensate the ill-posed diffusion that naturally arises from nondiffusive schemes applied to equations with nonconstant coefficients; if so, it should be treated implicitly to avoid a stability restriction due to time differencing of the differential approximation itself. However, a controlled amount of dissipation can always be added in any case. The differential approximation is seen to be "born implicit." The scheme used to difference it must only be conditionally stable in time with respect to the primitive system of equations for the resulting numerical scheme to be unconditionally, linearly stable. What we have shown is that since implicit time differencing compresses eigenvalues anyway, one can just as well do this from the outset by modifying the primitive system of equations appropriately before any discretization is applied (contrast Eqs. (7) and Eqs. (3)).

Since it was seen that only dispersion is needed for the differential approximation of an implicit scheme to be linearly stable we present a simplified derivation of Eqs. (7) that, although it does not exactly match the differential approximation given as Eqs. (5), still retains the essential dispersive truncation error terms. Suppose we simply substitute Eq. (5a) into Eq. (5b), then the differential approximation becomes

$$\frac{\partial u}{\partial t} - \frac{c \Delta t}{2} \frac{\partial^2 v}{\partial t \partial x} = c \frac{\partial v}{\partial x}, \quad (10a)$$

$$\left(1 - \frac{c^2 \Delta t^2}{4} \frac{\partial^2}{\partial x^2}\right) \frac{\partial v}{\partial t} = c \frac{\partial u}{\partial t} + \frac{c^2 \Delta t}{2} \frac{\partial^2 v}{\partial x^2}. \quad (10b)$$

By simply dropping terms linear in Δt in Eqs. (10) we obtain the same system as given by Eqs. (7) with the diffusion in Eq. (7b) also dropped. Since the terms linear

¹ Note that the stabilizing denominator must be spatially global, like a Fourier k mode. For example, the implicit scheme $u_j^{n+1} = u_j^n + (D \Delta t / \Delta x^2)(u_{j+1}^n - 2u_j^{n+1} + u_{j-1}^n)$ for Eq. (1) is useless because it is not spatially global.

in Δt only serve to make Eqs. (7) or (10) a first-order approximation to Eqs. (3) and do not contribute to stability it is just as well to drop them. The point here is that it does not matter whether the terms dropped are small compared to those retained in manipulating the differential approximation. We are concerned only about stability and consistency with respect to the primitive system we wish to solve.

The vector analog of the coupled scalar wave equations, Eqs. (3), can be written as

$$\frac{\partial \mathbf{u}}{\partial t} = -c \nabla \times \mathbf{v}, \tag{11a}$$

$$\frac{\partial \mathbf{v}}{\partial t} = c \nabla \times \mathbf{u}. \tag{11b}$$

Following the same steps as before we find as the analog of Eqs. (7) for the differential approximation to a fully implicit time differencing of Eqs. (11) the result

$$\frac{\partial \mathbf{u}}{\partial t} = -c \nabla \times \mathbf{v}, \tag{12a}$$

$$\left(1 + \frac{c^2 \Delta t^2}{4} \nabla \times \nabla\right) \frac{\partial \mathbf{v}}{\partial t} + c^2 \Delta t \nabla \times \nabla \times \mathbf{v} = c \nabla \times \mathbf{u}. \tag{12b}$$

Again dropping the dissipative term linear in Δt and also considering a solenoidal \mathbf{v} field, we see that the term to be added implicitly and subtracted explicitly to the r.h.s. of Eq. (11b), given any conditionally stable differencing approximation to Eqs. (11), is simply $(c^2 \Delta t/4) \nabla^2 \mathbf{v}$. The resulting scheme will be unconditionally stable and is completely analogous to that given in Eqs. (8). The order of the scheme used to difference the differential approximation to a primitive system should not be higher than that of the differential approximation itself, else that higher order scheme should be used to construct the differential approximation.

Finally, consider the MHD equations for the magnetic field \mathbf{B} and the velocity field \mathbf{v} written in a simplified form with the pressure neglected and all diagonal terms dropped. This system becomes

$$\frac{\partial \mathbf{B}}{\partial t} = \nabla \times (\mathbf{v} \times \mathbf{B}), \tag{13a}$$

$$\frac{\partial \mathbf{v}}{\partial t} = -\mathbf{B} \times (\nabla \times \mathbf{B}). \tag{13b}$$

The linearized version of Eqs. (13) describes Alfvén waves. We implicitly difference this nonlinear system by placing only \mathbf{v} and $\nabla \times \mathbf{B}$ on the r.h.s. of Eqs. (13a) and

(13b), respectively, at the $n + 1$ time level. Then expanding about the $n + 1/2$ time level yields as the differential approximation

$$\frac{\partial \mathbf{B}}{\partial t} - \frac{\Delta t}{2} \nabla \times \left(\frac{\partial \mathbf{v}}{\partial t} \times \mathbf{B} \right) = \nabla \times (\mathbf{v} \times \mathbf{B}), \tag{14a}$$

$$\frac{\partial \mathbf{v}}{\partial t} + \frac{\Delta t}{2} \mathbf{B} \times \left(\nabla \times \frac{\partial \mathbf{B}}{\partial t} \right) = -\mathbf{B} \times (\nabla \times \mathbf{B}). \tag{14b}$$

Using Eq. (14a) in Eq. (14b) and dropping terms linear in Δt , as illustrated by the discussion of Eqs. (10), yields

$$\frac{\partial \mathbf{B}}{\partial t} = \nabla \times (\mathbf{v} \times \mathbf{B}), \tag{15a}$$

$$\frac{\partial \mathbf{v}}{\partial t} + \frac{\Delta t^2}{4} \mathbf{B} \times \nabla \times \nabla \times \left(\frac{\partial \mathbf{v}}{\partial t} \times \mathbf{B} \right) = -\mathbf{B} \times (\nabla \times \mathbf{B}). \tag{15b}$$

This gives $(-\Delta t/4) \mathbf{B} \times \nabla \times \nabla \times (\mathbf{v} \times \mathbf{B})$ as the term to be added implicitly (only with respect to \mathbf{v} ; \mathbf{B} is taken as known at the n time level) and subtracted explicitly from the r.h.s. of Eq. (15b). This is the semi-implicit MHD term originally derived by Harned [1, 2].

As discussed in Ref. [3], the eigenvectors of the simplified “semi-implicit” system may not be the same as those of the primitive system. However, this is not always true and, in fact, arises only if the semi-implicit term is further simplified as was the case in Ref. [3] with the complicated term given in Eq. (15b). To explore this consider Eqs. (3) written in matrix form as

$$\frac{\partial y}{\partial t} = Ly; \quad L = \begin{pmatrix} 0 & c \frac{\partial}{\partial x} \\ c \frac{\partial}{\partial x} & 0 \end{pmatrix}, \tag{16}$$

where $y = (u, v)$. Then the differential approximation given as Eqs. (5) is

$$\frac{\partial y}{\partial t} = Ly + \frac{\Delta t}{2} \frac{\partial}{\partial t} Ly. \tag{17}$$

When rewritten in the equivalent form as Eqs. (7) it becomes

$$\frac{\partial y}{\partial t} = Ly + Gy; \quad G = \begin{pmatrix} 0 & 0 \\ 0 & \frac{c^2 \Delta t^2}{4} \frac{\partial^3}{\partial t \partial^2 x} + c^2 \Delta t \frac{\partial^2}{\partial x^2} \end{pmatrix}, \tag{18}$$

which is desired, since G has lower rank than L and is thus easier to invert. The eigenvectors of L , defined by $L\xi = \lambda\xi$, $\xi = (\xi_u, \xi_v)$ readily give for Eq. (18) the result

$$\frac{\partial \xi_u}{\partial t} = \lambda \xi_u, \tag{19a}$$

$$\left(1 - \frac{\lambda^2 \Delta t^2}{4}\right) \frac{\partial \xi_v}{\partial t} = (1 + \lambda \Delta t) \lambda \xi_v, \tag{19b}$$

which shows that the eigenvectors of L still remain uncoupled so that the semi-implicit approximation can be used to faithfully compute eigenvectors of the primitive system of equations.

We now wish to briefly discuss how other implicit schemes fit in and, in fact, are a subset of the procedure just outlined [8]. In particular, we now show how the ICE algorithm of Harlow and Amsden [9] and the scheme of Robert [10], which he calls "semi-implicit," fit into our framework. (These appear to be very similiar, if not identical, numerical methods.) A second-order accurate ICE scheme applied to Eqs. (3) consists in first center differencing them as

$$u^{n+1} = u^n + \frac{c \Delta t}{2} \left(\frac{\partial v^{n+1}}{\partial x} + \frac{\partial v^n}{\partial x} \right), \tag{20a}$$

$$v^{n+1} = v^n + \frac{c \Delta t}{2} \left(\frac{\partial u^{n+1}}{\partial x} + \frac{\partial u^n}{\partial x} \right), \tag{20b}$$

and then putting Eq. (20a) into (20b) to obtain

$$v^{n+1} = v^n + c \Delta t \left[\frac{\partial u^n}{\partial x} + \frac{c \Delta t}{4} \left(\frac{\partial^2 v^{n+1}}{\partial x^2} + \frac{\partial^2 v^n}{\partial x^2} \right) \right]. \tag{21}$$

Then one first solves Eq. (21) for v^{n+1} (implicit step) and then solves Eq. (20a) explicitly for u^{n+1} to advance a timestep.

The approximately implicit result given by Eq. (7) can be differenced in time many ways. Suppose after first dropping the diffusive term $\propto \Delta t$ in Eq. (7b) we difference Eqs. (7) as

$$u^* = u^n + c \Delta t \frac{\partial v^n}{\partial x}, \tag{22a}$$

$$v^{n+1} = v^n + \frac{c \Delta t}{2} \left(\frac{\partial u^*}{\partial x} + \frac{\partial u^n}{\partial x} \right) + \frac{c^2 \Delta t^2}{4} \left(\frac{\partial^2 v^{n+1}}{\partial x^2} - \frac{\partial^2 v^n}{\partial x^2} \right), \tag{22b}$$

$$u^{n+1} = u^n + \frac{c \Delta t}{2} \left(\frac{\partial v^{n+1}}{\partial x} + \frac{\partial v^n}{\partial x} \right). \tag{22c}$$

Thus we explicitly predict u^* , u at the $n + 1$ level, using Eq. (22a); next in differencing Eq. (7b) we use u^* to simply center $\partial u/\partial x$ in time and invert Eq. (22b) to obtain v^{n+1} ; and last, we explicitly advance Eq. (22c) to obtain u^{n+1} to second-order accuracy. This is easily verified to be identical to solving Eqs. (21) and (20a) in the ICE procedure. Thus we see that the approximately implicit form given by Eqs. (7) can be used to arrive at the ICE method, but allows more generality.

Last, we consider higher order accuracy in time. As pointed out in Ref. (2) this can be achieved by iterating on the semi-implicit term. That is, we simply use the last value of v at the $n + 1$ time level in the term that is subtracted on the next iteration step instead of just using data at the time level n . Thus in place of Eq. (8b) we have

$$v^l - v^n = c \Delta t \frac{\partial u}{\partial x} + a_0 c^2 \Delta t^2 \left(\frac{\partial^2 v^l}{\partial x^2} - \frac{\partial^2 v^{l-1}}{\partial x^2} \right), \tag{23}$$

where the iterates $l = 1, 2, \dots$ are all at the $n + 1$ time level and, for $l = 1$, $l - 1$ is replaced by n , the value at the beginning of the timestep. By rewriting $v^l - v^{l-1}$ as $v^l - v^n - (v^{l-1} - v^n)$ on the r.h.s. of Eq. (23) and using $(v^l - v^n)/\Delta t \equiv \partial v^l/\partial t$, it follows by induction that this iterated scheme can be written as

$$\left(1 - a_0 c^2 \Delta t^2 \frac{\partial^2}{\partial x^2} \right) \frac{\partial v^l}{\partial t} = c \frac{\partial u}{\partial x} + \sum_{l'=1}^{l-1} \left(c \frac{\partial u}{\partial x} - \frac{\partial v^{l'}}{\partial t} \right), \tag{24}$$

where the sum is omitted for $l = 1$. The value of a_0 needed for stability is determined by noting that Eq. (24) represents a sequence given by

$$\frac{1}{1 + y}, \frac{1 + 2y}{(1 + y)^2}, \frac{1 + 3y + 3y^2}{(1 + y)^3}, \dots$$

for $l = 1, 2, 3, \dots$, where $y = a_0 c^2 k^2 \Delta t^2$, that multiplies $c^2 k^2 \Delta t^2/4$ when Fourier analyzed for stability. Therefore we have that a set of l iterates is $(\Delta t)^{2l}$ order accurate and must have $a_0 \geq l/4$ to be stable. Thus we must use a larger value of a_0 on all steps if we iterate more times. The iteration method given by Eq. (24) can simply be implemented as indicated and is seen to be a type of defect correction scheme.

In summary, it has been shown how the method of differential approximation can be used to construct simplified implicit schemes that are unconditionally linearly stable so that accuracy is the only remaining consideration. This has been illustrated by a series of worked examples which it is hoped are sufficiently general to suggest how any given system of equations might be investigated via this method. The number of terms to be kept in the differential approximation to any difference scheme has been given a unique definition. This is that the differential approximation require no more initial and boundary data for its solution than does the difference scheme. By use of the method of differential approximation the

precise relation of semi-implicit time differencing as an approximation to implicit differencing is transparent. In addition, how implicit time differencing results in stability is also clarified.

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