A FINITE DIFFERENCE FORMULA FOR THE DISCRETIZATION OF d^3/dx^3 ON NONUNIFORM GRIDS

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ABSTRACT. We analyze the use of a five-point difference formula for the discretization of the third derivative operator on nonuniform grids. The formula was derived so as to coincide with the standard five-point formula on regular grids and to lead to skew-symmetric schemes. It is shown that, under periodic boundary conditions, the formula is supraconvergent in the sense that, in spite of being inconsistent, it gives rise to schemes with second-order convergence. However, such a supraconvergence only takes place when the number of points in the grid is odd: for grids with an even number of points the inconsistency of the formula results in lack of convergence. Both stationary and evolutionary problems are considered and the analysis is backed by numerical experiments.

1. Introduction

Nonuniform grids may be the only way to numerically solve some practical problems involving partial differential equations and, accordingly, the literature on adaptive/moving meshes has grown enormously in recent years; see, e.g., [1-3, 16-19, 21, 22, 24, 25]. Analyses of finite difference discretizations on nonuniform grids are likely to be considerably more involved than analyses corresponding to constant mesh sizes. In fact, nonuniform grids may give rise to a number of consistency/stability phenomena that have no counterpart on uniform grids. The aim of the present paper is to illustrate such phenomena in the particular case of a five-point formula for the replacement of third derivatives.

It is perhaps useful to give some background on the problems considered here. In [21], one of the present authors and I. Christie suggested a simple moving-grid technique for the numerical solution of one-dimensional evolutionary partial differential equations. The well-known nonlinear Schrödinger equation was used in [21] to illustrate the suggested procedure. The Korteweg-de Vries equation,

$$u_t + uu_x + u_{xxx} = 0,$$

similar in many ways to the Schrödinger equation, appeared to be an obvious candidate to be used in further tests of the technique. Those tests were carried

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out by Fraga and Morris [7], who used the formula

$$v_{xxx}(x_{i}) \cong \frac{6}{h^{i+2}(h^{i+2} + h^{i+1} + h^{i})(h^{i+2} + h^{i+1} + h^{i} + h^{i-1})} v(x_{i+2})$$

$$- \frac{6}{h^{i+2}(h^{i+1} + h^{i})(h^{i+1} + h^{i} + h^{i-1})} v(x_{i+1})$$

$$+ \frac{6}{h^{i-1}(h^{i+1} + h^{i})(h^{i+2} + h^{i+1} + h^{i})} v(x_{i-1})$$

$$- \frac{6}{h^{i-1}(h^{i+1} + h^{i} + h^{i-1})(h^{i+2} + h^{i+1} + h^{i} + h^{i-1})} v(x_{i-2})$$

to discretize the u_{xxx} term on the (highly nonuniform) meshes generated by the regridding strategy employed in [21]. Throughout the paper, h^i denotes the mesh size $x_i - x_{i-1}$. Note that on a uniform grid, (1.1) reduces to the standard five-point, second-order formula

$$(1.2) v_{xxx}(x_i) \cong \frac{1}{2h^3} (v(x_{i+2}) - 2v(x_{i+1}) + 2v(x_{i-1}) - v(x_{i-2})).$$

In fact, (1.1) was found in [7] by imposing the requirements:

- the formula should be consistent;
- the formula should involve five points x_{i+2} , x_{i+1} , x_i , x_{i-1} , x_{i-2} , but, as in (1.2), $v(x_i)$ should carry a zero weight.

These requirements give four linear equations for four unknown weights and lead to (1.1). The order of consistency achieved is, in general, only 1, as there are not enough free parameters to annihilate the coefficient of v_{xxxx} in the relevant Taylor expansion. It is only through the symmetry implicit on a uniform grid that second order of formal consistency can be achieved with four free parameters.

Numerical evidence [7] indicates that, when using (1.1), the resulting moving-grid algorithm is far from being successful. We were thus led to consider the following two problems:

- (1) Account for the poor performance of (1.1).
- (2) Identify an alternative formula.

In connection with problem (1), it has been found [8, 9] that (1.1), in spite of reducing to (1.2) on uniform grids, usually leads to unstable schemes on nonuniform grids.

For problem (2) we set ourselves the following two constraints:

- (i) In order to keep a low bandwidth on the resulting matrices, the alternative formula should be based on a five-point computational molecule.
- (ii) The alternative formula should lead to schemes convergent of the second order (with respect to some standard norm) on arbitrary grids. The insistence

on arbitrary grids is due to the fact that the grids actually produced by the kind of algorithm suggested in [21] are very irregular, so that convergence analyses based on the smoothness of the grid seem inappropriate. In particular, we want to avoid the assumption that, as the grids are refined, the difference $h^i - h^{i-1}$ between two consecutive interval lengths is $O(h^2)$ rather than O(h) (h represents the maximum of h^i over the grid).

In order to obtain the convergence mentioned in constraint (ii) above, the standard approach in finite differences is of course via stability plus consistency. To guarantee stability, we added the requirement:

(iii) The alternative formula should replace, under favorable boundary conditions, the operator d^3/dx^3 by a discrete skew-symmetric operator.

Many attempts to get a five-point formula satisfying (iii) and having second order of consistency failed. The only way to obtain (i)-(iii) appeared to be to resort to the *supraconvergence* phenomenon, i.e., to try and get second order of convergence without having second order of consistency [6, 13, 14, 15, 22]. Generally speaking, the term supraconvergence [13] refers to situations were a finite difference scheme is convergent (in some norm) while not being *formally* consistent, or at least while having a formal order of consistency lower than its order of convergence. Here, *formal* order of consistency means the degree of the leading terms of the truncation error at individual grid points. The word *formal* is used to emphasize that we are considering local truncation errors at individual grid points as distinct from the situation where the order of consistency is measured with respect to some suitable norm. Consistency in the latter sense is norm-dependent [20], while formal consistency is merely an algebraic notion.

The course of events outlined above led us to the investigation of a skew-symmetric, five-point, inconsistent formula that may lead to algorithms with second order of convergence in standard norms. It is this formula which is studied in this article.

An outline of the results of the paper is as follows. In §2 we present the five-point supraconvergent formula. Section 3 is devoted to the proof of supraconvergence in the stationary model problem

(1.3)
$$u_{xxx} + u = f, \qquad u, f \text{ L-periodic.}$$

Boundary conditions were chosen to be periodic so as not to complicate the analysis with unwanted details. (Note that with periodic boundary conditions the equation $u_{xxx} = f$ would not have made a suitable model. The operator d^3/dx^3 is singular.) Surprisingly enough, supraconvergence for (1.3) only takes place when using an *odd number of grid points* per period. When using an even number of grid points, the underlying formal inconsistency of the scheme manifests itself in the divergence of the numerical scheme. We shall present numerical results in which this awkward behavior is clearly borne out. The final §4 investigates an evolutionary model problem: the periodic initial value

problem for the equation

$$(1.4) u_t = u_{xxx}.$$

It should be mentioned that, by using the techniques in [12], it would be a simple matter to extend our analysis to periodic problems for equations of the form

$$\begin{aligned} u_{xxx} + L(u) &= f, \\ u_t &= u_{xxx} + L(u) + f(x), \end{aligned}$$

where L(u) denotes a linear operator involving u, u_x , u_{xx} . A forthcoming paper [10] considers the application to the Korteweg-de Vries equation of the formula studied in this paper.

2. The difference formula

Throughout the paper we assume that the (spatial) variable x takes values $x \in (-\infty, \infty)$ and that all functions u = u(x) considered are real-valued and L-periodic. We denote by $\Delta = \{0 = x_0 < x_1 < \cdots < x_J = L\}$ a mesh in the interval [0, L], by h^i the mesh size $x_i - x_{i-1}$, $i = 1, 2, \ldots, J$, and by $x^{i-1/2}$ the center $(x_i + x_{i-1})/2$ of the cell $[x_{i-1}, x_i]$, $i = 1, 2, \ldots, J$. In general, we use subscripts when refering to quantities related to the nodes x_i and superscripts when refering to quantities associated with the cells $[x_{i-1}, x_i]$. Furthermore, sub- and superscripts should be understood in an obvious periodic way, e.g., $x_{J+1} = L + x_1$, $h^0 = h^J$, etc. Discrete functions defined either at the nodes x_1, x_2, \ldots, x_J or at the centers $x^{1/2}, x^{3/2}, \ldots, x^{J-1/2}$ shall be identified with J-dimensional column vectors.

The difference formula studied in this paper was obtained as follows. We first consider the standard divided difference formula

$$v_{xxx}(x^{i-1/2}) \approx -\frac{6}{h^{i-1}(h^{i-1} + h^{i})(h^{i-1} + h^{i} + h^{i+1})}v(x_{i-2}) + \frac{6}{h^{i-1}h^{i}(h^{i} + h^{i+1})}v(x_{i-1}) - \frac{6}{h^{i}h^{i+1}(h^{i-1} + h^{i})}v(x_{i}) + \frac{6}{h^{i+1}(h^{i} + h^{i+1})(h^{i-1} + h^{i} + h^{i+1})}v(x_{i+1}).$$

We then replace in the right-hand side of (2.1) the nodal values $v(x_i)$ by the linear interpolation averages

(2.2)
$$\frac{h^{i+1}}{h^i + h^{i+1}} v(x^{i-1/2}) + \frac{h^i}{h^i + h^{i+1}} v(x^{i+1/2}).$$

This results in the desired five-point formula

$$v_{xxx}(x^{i-1/2}) \approx -\frac{6}{(h^{i-2} + h^{i-1})(h^{i-1} + h^{i})(h^{i-1} + h^{i} + h^{i+1})} v(x^{i-5/2})$$

$$+ \frac{6(h^{i-2} + h^{i-1} + h^{i} + h^{i+1})}{(h^{i-2} + h^{i-1})(h^{i-1} + h^{i})(h^{i} + h^{i+1})(h^{i-1} + h^{i} + h^{i+1})} v(x^{i-3/2})$$

$$- \frac{6(h^{i-1} + h^{i} + h^{i+1} + h^{i+2})}{(h^{i-1} + h^{i})(h^{i} + h^{i+1})(h^{i+1} + h^{i+2})(h^{i-1} + h^{i} + h^{i+1})} v(x^{i+1/2})$$

$$+ \frac{6}{(h^{i} + h^{i+1})(h^{i+1} + h^{i+2})(h^{i-1} + h^{i} + h^{i+1})} v(x^{i+3/2}).$$

On a uniform grid with $h^i = h = \text{constant}$, (2.3) coincides, after an obvious change in notation, with the standard five-point, second-order formula (1.2). However, on arbitrary grids, (2.3) is inconsistent. In fact the leading term in the truncation error is easily found to be

(2.4)
$$\frac{3}{h^{i-1} + h^{i} + h^{i+1}} \frac{1}{4} \left[\frac{h^{i+2} + h^{i+1} + h^{i} + h^{i-1}}{h^{i+1} + h^{i}} - \frac{h^{i+1} + h^{i} + h^{i-1} + h^{i-2}}{h^{i} + h^{i-1}} \right] v_{xx}(x^{i-1/2}),$$

so that the truncation errors will actually grow as the grid is refined.

Let us consider the operator that associates with a discrete function $[U^1, U^2, \ldots, U^J]^T$ the discrete function $[V^1, V^2, \ldots, V^J]^T$, where V^J denotes the third difference at $x^{j-1/2}$ of the values U^J computed according to (2.3). This operator can be identified with the product $D_{\Delta}^3 P_{\Delta}$ of two $J \times J$ matrices, where P_{Δ} is the matrix that performs the averaging of the U^I 's according to (2.2) and D_{Δ}^3 represents differencing according to (2.1). On introducing the "mass" matrix

$$(2.5) \ M_{\Lambda} = \text{Diag}((h^0 + h^1 + h^2)/3, (h^1 + h^2 + h^3)/3, \dots, (h^{J-1} + h^J + h^{J+1})/3),$$

it is easily seen that the matrix $M_{\Delta}D_{\Delta}^{3}P_{\Delta}$ is skew-symmetric. In other words, the operator $D_{\Delta}^{3}P_{\Delta}$ is skew-symmetric with respect to the following inner product for discrete functions $\mathbf{V} = \begin{bmatrix} V^{1}, V^{2}, \dots, V^{J} \end{bmatrix}^{T}, \mathbf{W} = \begin{bmatrix} W^{1}, W^{2}, \dots, W^{J} \end{bmatrix}^{T}$:

(2.6)
$$(\mathbf{V}, \mathbf{W})_{\Delta} = \sum_{1 \le j \le J} \frac{1}{3} (h^{j-1} + h^j + h^{j+1}) V^j W^j.$$

It should be mentioned that the skew-symmetric matrix $M_{\Delta}D_{\Delta}^{3}P_{\Delta}$ also arises when approximating third derivatives via the Galerkin method based on quadratic splines (see [9] for details).

Before we prove the supraconvergence of model difference schemes based on the operator $D_{\Delta}^{3}P_{\Delta}$, it is expedient to study some properties of the averaging

operator P_{Δ} . It turns out that these properties depend on whether the number J of points in the grid Δ is odd or even.

The case J odd. When J is odd, the averaging operator P_{Δ} is invertible. The inverse operator P_{Δ}^{-1} can be found as follows. Assume that $P_{\Delta}\mathbf{V}=\mathbf{U}$, for grid functions $\mathbf{V}=[V^1,V^2,\ldots,V^J]^T$ and $\mathbf{U}=[U_1,U_2,\ldots,U_J]^T$. The relation $P_{\Delta}\mathbf{V}=\mathbf{U}$ provides J equations to determine the entries of \mathbf{V} from those of \mathbf{U} . Multiply the jth equation, $j=1,2,\ldots,J$, by $(-1)^j((1/h^j)+(1/h^{j+1}))$ and sum all the resulting equations to obtain

(2.7)
$$V^{i} = (-1)^{i} \frac{h^{i}}{2} \left[\sum_{j=i}^{J-1} (-1)^{j} \left(\frac{1}{h^{j}} + \frac{1}{h^{j+1}} \right) U_{j} - \sum_{j=0}^{i-1} (-1)^{j} \left(\frac{1}{h^{j}} + \frac{1}{h^{j+1}} \right) U_{j} \right],$$
$$i = 1, 2, \dots, J.$$

This formula determines V in terms of U, i.e., inverts the operator P_{Δ} .

The right-hand side of (2.7) can be written in a more useful way. To do so, we need the standard first and second divided difference operators D_{Δ}^{1} and D_{Δ}^{2} acting on mesh functions $\mathbf{U} = [U_{1}, U_{2}, \dots, U_{I}]^{T}$:

(2.8)
$$D_{\Delta}^{1}\mathbf{U}^{i} = \frac{U_{i} - U_{i-1}}{h^{i}}, \qquad i = 1, 2, \dots, J,$$

(2.9)
$$D_{\Delta}^{2}\mathbf{U}_{i} = \frac{D_{\Delta}^{1}\mathbf{U}^{i+1} - D_{\Delta}^{1}\mathbf{U}^{i}}{(h^{i} + h^{i+1})/2}, \qquad i = 1, 2, \dots, J.$$

Summation by parts in (2.7) leads to

$$V^{i} = \frac{U_{i-1} + U_{i}}{2} + (-1)^{i} \frac{h^{i}}{2} \left[\sum_{j=i+1}^{J} (-1)^{j} D_{\Delta}^{1} \mathbf{U}^{j} - \sum_{j=1}^{i-1} (-1)^{j} D_{\Delta}^{1} \mathbf{U}^{j} \right],$$

$$i = 1, 2, \dots, J,$$

which, on rearranging, becomes

$$V^{i} = \frac{U_{i-1} + U_{i}}{2} + \frac{h^{i}}{2} \left[\sum_{j=1}^{(i-1)/2} \frac{h^{2j} + h^{2j-1}}{2} D_{\Delta}^{2} \mathbf{U}_{2j-1} + \sum_{j=(i+1)/2}^{(J-1)/2} \frac{h^{2j+1} + h^{2j}}{2} D_{\Delta}^{2} \mathbf{U}_{2j} \right],$$

$$(2.10a)$$

$$i = 1, 3, 5, \dots, J,$$

$$V^{i} = \frac{U_{i-1} + U_{i}}{2} + \frac{h^{i}}{2} \left[\sum_{j=0}^{(i-2)/2} \frac{h^{2j+1} + h^{2j}}{2} D_{\Delta}^{2} \mathbf{U}_{2j} + \sum_{j=(i+2)/2}^{(J-1)/2} \frac{h^{2j} + h^{2j-1}}{2} D_{\Delta}^{2} \mathbf{U}_{2j-1} \right],$$

$$i = 2, 4, 6, \dots, J-1.$$

The case J even. In this case, the matrix P_{Δ} is not invertible. In fact, manipulation of the equations $P_{\Delta}\mathbf{V} = \mathbf{0}$ following the steps of the J odd case shows that the kernel of P_{Δ} is generated by the vector

(2.11)
$$\mathbf{c} = [-h^1, h^2, -h^3, \dots, -h^{J-1}, h^J]^T,$$

which plays an important role in later developments.

3. STATIONARY MODEL PROBLEM

In this section, we study the application to the model problem (1.3) of the operator $D_{\Delta}^{3}P_{\Delta}$ associated with (2.3). Namely, we consider the finite difference equations

$$(3.1) D_{\Delta}^{3} P_{\Delta} \mathbf{U} + \mathbf{U} = \mathbf{F},$$

where $\mathbf{F} = [f(x^{1/2}), f(x^{3/2}), \dots, f(x^{J-1/2})]^T$ and $\mathbf{U} = [U^1, U^2, \dots, U^J]^T$. Here, U^j is an approximation to the cell-centered quantity $u(x^{j-1/2}), j = 1, 2, \dots, J$. As discussed in the preceding section, the scheme (3.1) is formally inconsistent. More precisely, the truncation errors $D_{\Delta}^3 P_{\Delta} \mathbf{u}_{\Delta} + \mathbf{u}_{\Delta} - \mathbf{F}, \mathbf{u}_{\Delta} = [u(x^{1/2}), u(x^{3/2}), \dots, u(x^{J-1/2})]^T$, grow under refinement of the grid.

In the analysis, we denote by \wp the set of all grids $\Delta = \{0 = x_0 < x_1 < \cdots < x_J = L\}$ in the interval [0, L] and by \wp_o (respectively \wp_e) the sets of all such grids having odd (respectively even) number J of points. For each $\Delta \in \wp$, the notations $h = h(\Delta)$ and $h_{\min} = h_{\min}(\Delta)$ refer to the maximum and minimum mesh sizes $\max_{1 \le i \le J} h^i$, $\min_{1 \le i \le J} h^i$, respectively. With each L-periodic real function v and each $\Delta \in \wp$ we consider the restrictions

$$\mathbf{v}_{\Delta} = [v(x^{1/2}), v(x^{3/2}), \dots, v(x^{J-1/2})]^{T},$$

$$\mathbf{v}_{\Delta}^{*} = [v(x_{1}), v(x_{2}), \dots, v(x_{J})]^{T},$$

to the cell centers and nodes, respectively.

In the remainder of the paper we shall refer to discrete functions defined at the nodes (resp. at the cell centers) as grid functions (resp. cell functions). Thus, \mathbf{v}_{Λ} is a cell function and \mathbf{v}_{Λ}^{*} a grid function.

The following discrete norms are employed. If $\Delta \in \wp$ and \mathbf{V} is a discrete function (i.e., either a cell function or a grid function), we denote by $\|\mathbf{V}\|_{\infty}$ the standard maximum norm. For grid functions $\mathbf{V} = \begin{bmatrix} V_1, V_2, \dots, V_J \end{bmatrix}^T$ we also

use the discrete Sobolev norms

(3.2)
$$\|\mathbf{U}\|_{m,\infty} = \sum_{1 \le k \le m} \|D_{\Delta}^{k}\mathbf{U}\|_{\infty}, \qquad m = 0, 1, 2,$$

where D_{Δ}^{1} , D_{Δ}^{2} denote the divided difference operators introduced in (2.8)–(2.9) and D_{Δ}^{0} represents the identity operator. Finally, $\|\cdot\|_{\Delta}$ denotes the L^{2} -norm corresponding to the discrete inner product (2.6).

As in the previous section, the cases J odd and J even must be addressed separately.

J odd: supraconvergence. The following stability theorem is the main analytical result of this paper. The proof uses techniques due to Grigorieff [11, 12]. We require the summation operator \sum_{Δ} that maps each grid function $\mathbf{V} = [V^1, V^2, \dots, V^J]^T$ into the grid function defined by

(3.3)
$$\left(\sum_{\Delta} \mathbf{V}\right)_{i} = \sum_{j=1}^{i} \frac{h^{j-1} + h^{j} + h^{j+1}}{3} V^{j}, \qquad i = 1, 2, \dots, J.$$

This is a discrete counterpart of the integration operator

(3.4)
$$\sum v(x) = \int_0^x v(\xi) d\xi.$$

Theorem 3.1. There exist positive constants h_0 , β , γ such that for each grid $\Delta \in \wp_o$ with $h(\Delta) < h_0$, and for each cell function $\mathbf{V} = [V^1, V^2, \dots, V^J]^T$ and each grid function $\mathbf{V}^* = [V_1, V_2, \dots, V_J]^T$ the following inequalities hold:

(3.5)
$$\gamma(\|\mathbf{V}^*\|_{2,\infty} + \|\mathbf{V}\|_{\infty}) \le \left\| \sum_{\Delta} (D_{\Delta}^3 \mathbf{V}^* + \mathbf{V}) \right\|_{\infty} + \|P_{\Delta}^{-1} (P_{\Delta} \mathbf{V} - \mathbf{V}^*)\|_{\infty} \\ \le \beta(\|\mathbf{V}^*\|_{2,\infty} + \|\mathbf{V}\|_{\infty}).$$

Proof. We begin with the first inequality. If the result were not true, a subfamily of odd grids \wp_o^* could be found such that $\inf\{h(\Delta): \Delta \in \wp_o^*\} = 0$ and for each $\Delta \in \wp_o^*$ there exist a cell function $\mathbf{V}_{\Delta} = [V^1, V^2, \dots, V^J]^T$ and a grid function $\mathbf{V}_{\Delta}^* = [V_1, V_2, \dots, V_J]^T$ satisfying

(3.6)
$$\|\mathbf{V}^*\|_{2,\infty} + \|\mathbf{V}\|_{\infty} = 1$$
,

(3.7)
$$\left\|\sum_{\Delta}(D_{\Delta}^{3}\mathbf{V}^{*}+\mathbf{V})\right\|_{\infty}\to 0, \qquad h\to 0,$$

(3.8)
$$||P_{\Delta}^{-1}(P_{\Delta}\mathbf{V} - \mathbf{V}^*)||_{\infty} \to 0, \qquad h \to 0.$$

Furthermore, the relation (3.6) and a compactness result due to Grigorieff [11] imply that it may be assumed that

$$\|\mathbf{V}^* - \mathbf{v}_{\Delta}^*\|_{1,\infty} \to 0, \qquad h \to 0,$$

for a certain C^1 periodic function v. (Recall that \mathbf{v}_{Δ}^* denotes the restriction of v to the nodes of Δ .)

Let us first consider the cell function $P_{\Delta}^{-1}(P_{\Delta}\mathbf{V}_{\Delta}-\mathbf{V}_{\Delta}^{*})=\mathbf{V}_{\Delta}-P_{\Delta}^{-1}\mathbf{V}_{\Delta}^{*}$. The expression for P_{Δ}^{-1} found in (2.10) shows that the *i*th entry of the vector $P_{\Delta}^{-1}\mathbf{V}_{\Delta}^{*}$ differs from $(V_{i}+V_{i-1})/2$ by terms bounded by $(Lh/2)\|D_{\Delta}^{2}\mathbf{V}_{\Delta}^{*}\|_{\infty}$, i.e., by terms of O(h) (see (3.6)). Therefore, (3.8) and (3.9) yield

$$\|\mathbf{V} - \mathbf{v}_{\Lambda}\|_{\infty} \to 0, \qquad h \to 0.$$

We now turn to the grid function $\mathbf{W}_{\Delta} := \sum_{\Delta} D_{\Delta}^{3} \mathbf{V}^{*} - D_{\Delta}^{2} \mathbf{V}^{*}$. On the one hand, for each $\Delta \in \wp_{o}^{*}$, \mathbf{W}_{Δ} is constant (i.e., all entries of the vector \mathbf{W}_{Δ} are equal); this fact is the discrete counterpart of the identity

$$\int_0^x d^3v/d\xi^3 d\xi - d^2v/dx^2 = \text{constant}.$$

On the other hand, W_{Λ} can be rewritten as

(3.11)
$$\mathbf{W}_{\Delta} = \sum_{\Delta} (D_{\Delta}^{3} \mathbf{V}^{*} + \mathbf{V}) - \sum_{\Delta} \mathbf{V} - D_{\Delta}^{2} \mathbf{V}^{*}.$$

In the right-hand side of this expression, the first term tends to 0 according to (3.7), the third is bounded by (3.6), and the second satisfies, in view of (3.10) and [12],

$$\left\|\sum_{\Delta} \mathbf{V} - \sum_{\Delta} \mathbf{v}_{\Delta}\right\|_{\infty} \to 0, \qquad h \to 0.$$

Here, $\sum \mathbf{v}_{\Delta}$ denotes the restriction to the nodes of the antiderivative $\sum v(x)$ defined in (3.4). Putting together all our findings on the grid functions \mathbf{W}_{Δ} , we see that they are constant and bounded. Without loss of generality these constants can be assumed to converge to a real number w. Going back now to (3.11), we see that the left-hand side and the first two terms in the right-hand side converge. Hence the same must be true for $D_{\Delta}^2\mathbf{V}^*$, a result that, when combined with (3.9), reveals that the function v is actually C^2 and that

$$\|\mathbf{V}^* - \mathbf{v}_{\Lambda}^*\|_{2,\infty} \to 0, \qquad h \to 0.$$

We take limits in (3.11) to conclude that $w=-\sum v-v_{xx}$, an expression that, when differentiated, reads $v=-v_{xxx}$. Since v is L-periodic, v vanishes identically, and this contradicts (3.6) and (3.9). The first inequality in (3.5) has now been proved. The proof of the second, with $\beta=3+L$, $h_0<4$, is a simple exercise. \square

We can now turn to the proof of the supraconvergence of (3.1) when J is odd. On introducing the vector of averages $\mathbf{U}^* = [U_1, U_2, \dots, U_J]^T$ defined by $\mathbf{U}^* = P_\Delta \mathbf{U}$, (3.1) can be recast in the form of a system,

$$(3.12) D_{\Delta}^{3}\mathbf{U}^{*} + \mathbf{U} = \mathbf{F}_{\Delta}, P_{\Delta}\mathbf{U} - \mathbf{U}^{*} = 0.$$

For a grid that is sufficiently fine, the unique solvability of this system for U, U^* is an obvious consequence of the first inequality in (3.5). We consider U to approximate \mathbf{u}_{Δ} , i.e., u at the centers of the cells, and U^* to approximate \mathbf{u}_{Δ}^* , i.e., u at the nodes x_i .

Theorem 3.2. Assume that the (periodic) datum f in (1.3) is of class C^2 . Then, when using grids with an odd number of points, the solution of (3.12) satisfies, as $h \to 0$,

$$\|\mathbf{U}^* - \mathbf{u}_{\Delta}^*\|_{2,\infty} + \|\mathbf{U} - \mathbf{u}_{\Delta}\|_{\infty} = O(h^2).$$

Proof. It is clear that the true solution u is C^5 . Introduce the discrete functions of errors $\mathbf{E} = \mathbf{u}_{\Delta} - \mathbf{U}$, $\mathbf{E}^* = \mathbf{u}_{\Delta}^* - \mathbf{U}^*$. If we use the first inequality in (3.5) to estimate the size of $\|\mathbf{E}^*\|_{2,\infty} + \|\mathbf{E}\|_{\infty}$, then it is enough to show that

$$(3.13) \qquad \left\| \sum_{\Delta} (D_{\Delta}^{3} \mathbf{u}_{\Delta}^{*} + \mathbf{u}_{\Delta}) \right\|_{\infty} + \left\| P_{\Delta}^{-1} (P_{\Delta} \mathbf{u}_{\Delta} - \mathbf{u}_{\Delta}^{*}) \right\|_{\infty} = O(h^{2}), \qquad h \to 0.$$

Note that $T1 := D_{\Delta}^3 \mathbf{u}_{\Delta}^* + \mathbf{u}_{\Delta}$ and $T2 := P_{\Delta} \mathbf{u}_{\Delta} - \mathbf{u}_{\Delta}^*$ are the truncation errors arising from substitution in (3.12) of the true solution. Now Taylor expansion implies that the *i*th entry of T1 is given by $\frac{1}{4}(h^{i+1}-h^{i-1})u_{xxxx}(x^{i-1/2})+O(h^2)$. Thus, T1 is only O(h). However, we are really interested in $\sum_{\Delta} T1$, a grid function which, upon summation by parts, can be shown to be $O(h^2)$. As far as T2 goes, Taylor expansion implies that its *i*th component is given by $(h^i h^{i+1}/8)(u_{xx}(x_i) + O(h^2))$. We are interested in $P_{\Delta}^{-1}T2$, whose components can be found via (2.7). Summation by parts is again needed to show that $P_{\Delta}^{-1}T2$ is actually $O(h^2)$. \square

Remark 1. We emphasize the we have shown that, when using an odd number of grid points, the solutions U of (3.1) converge with second order, in spite of the formal inconsistency of that scheme. This provides an approximation to u at the centers of the cells. Furthermore, if approximations U^* at the nodes are computed by linearly interpolating the entries of U, then the U^* are convergent of the second order, together with their first and second divided differences.

Remark 2. By considering only uniform grids, it is easy to show that the exponent 2 in the right-hand side of (3.13) cannot be improved. Combining this with the second inequality in (3.5), we prove rigorously that, in Theorem 3.2, the order of convergence cannot be higher than 2.

The case J even: divergence. The scheme (3.1) diverges (i.e., does not converge) when used with grids having an even number J of points. This is so regardless of the smoothness of the datum f and even if attention is focused not on arbitrary grids but only on quasiuniform grids, i.e., grids that are refined so that the ratio h/h_{\min} remains bounded. This divergence is particularly remarkable after recalling that on uniform grids the scheme (3.1) involves the standard five-point formula for the third derivative and therefore is convergent of the second order.

Divergence will be proved in the L^2 -norm $\|\cdot\|_{\Delta}$. Note that this implies divergence in the maximum norm. We begin by noticing that, by (1.3) and (3.1),

$$D_{\Delta}^{3}P_{\Delta}\mathbf{U}+(\mathbf{U}-\mathbf{u}_{\Delta})=\mathbf{u}_{xxx\Delta}.$$

(Recall that $\mathbf{u}_{xxx\Delta}$ denotes restriction of u_{xxx} .) We take the scalar product (defined in (2.6)) of this equality and the vector \mathbf{c} in (2.11). The result is

$$(\mathbf{c}, \mathbf{U} - \mathbf{u}_{\Lambda})_{\Lambda} = (\mathbf{c}, \mathbf{u}_{\chi \chi \chi \Lambda})_{\Lambda}$$

This is because c lies in the kernel of P_{Δ} and hence in the kernel of the skew-symmetric matrix $M_{\Lambda}D_{\Lambda}^{3}P_{\Lambda}$. From (3.14) we can write

$$||\mathbf{U} - \mathbf{u}_{\Delta}||_{\Delta} \ge |(\mathbf{c}, \mathbf{u}_{xxx\Delta})_{\Delta}|/||\mathbf{c}||_{\Delta}.$$

The denominator in (3.15) is bounded above by $(\sqrt{L})h$. We shall show that the numerator is at best O(h), and divergence will follow.

Choose a real number λ , $0 < \lambda < 1$, and for each positive integer N set $h = L/(2N(1+\lambda))$. Consider the grid $\Delta_N = \{0 = x_0 < x_1 < \cdots < x_{4N} = L\}$ defined by

$$(3.16) x_{2j} = j(1+\lambda)h, j = 0, 1, ..., 2N, x_{2j+1} = j(1+\lambda)h + h, j = 0, 1, ..., N-1, x_{2j+1} = j(1+\lambda)h + \lambda h, j = N, N+1, ..., 2N-1.$$

Note that the grid is symmetric with respect to the point $L/2 = x_{2N}$ and that in [0, L/2] the odd-numbered lengths h^1, h^3, \ldots are all equal to h and the even-numbered lengths are all equal to λh . We are going to show that, for $u_{xxx} = \sin(2\pi x/L)$ and N large, the numerator in (3.15) is bounded below by νh , for a suitable constant ν . To do so, we note that by the symmetry with respect to L/2, the numerator in question can be written as

$$\frac{2}{3} \frac{2\lambda + \lambda^2}{1 + \lambda} h \sum_{j=1}^{N} (1 + \lambda) h \sin\left(\frac{2\pi}{L} \left(j(1 + \lambda)h - \frac{\lambda h}{2}\right)\right)$$
$$-\frac{2}{3} \frac{1 + 2\lambda}{1 + \lambda} h \sum_{j=0}^{N-1} (1 + \lambda) h \sin\left(\frac{2\pi}{L} j(1 + \lambda)h + \frac{h}{2}\right).$$

On viewing each summation as a quadrature formula, the result follows easily.

Remark. By writing a more general solution u as a Fourier series, it can be shown [9] that for the grids (3.16) divergence actually takes place for all smooth solutions, not only for $u = \sin(2\pi x/L)$.

Numerical tests. The rather surprising difference between the analyses of the cases J odd and J even led us to perform some numerical experiments to back up our findings. In the interval [0, 1], we selected the datum f in (1.3) so as to have $u = \cos 2\pi x$. We implemented the scheme (3.1) on random grids, calling the IMSL library for carrying out the linear algebra. The random grids

were generated by means of the following algorithm:

```
x_0 = 0

i = 1

h^1 = \text{random number (uniform distribution in } [0, \delta])

x_1 = x_0 + h^1

do while x_i < 1

i = i + 1

h^i = \text{random number (uniform distribution in } [0, \delta])

x_i = x_{i-1} + h^i

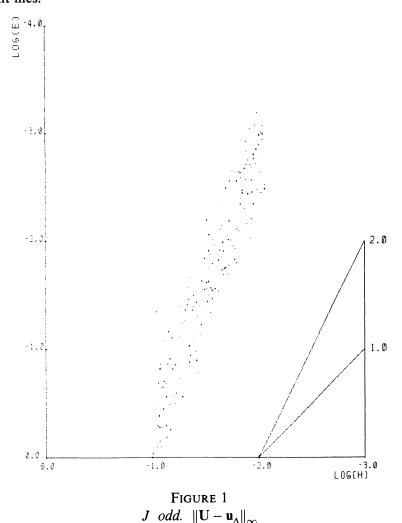
end do

J = i

x_J = 1

h^J = x_J - x_{J-1}.
```

The parameter δ that governs the maximum step length varied in the range $0.01 \le \delta \le 0.1$. Results coming from grids with J odd and even were kept in different files.



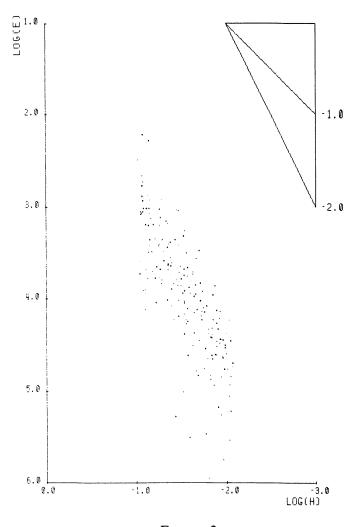


FIGURE 2

J odd. Truncation error

Figure 1 depicts $\log(\|\mathbf{U}-\mathbf{u}_{\Delta}\|_{\infty})$ versus $\log(h)$ for the grids with J odd (log means \log_{10}). Each individual run is represented by a dot, and straight lines with slopes 1 and 2 have been included to facilitate the estimation of the order of convergence. Convergence of the second order manifests itself.

Figure 2 was obtained from the same family of runs used for Figure 1, the difference being that now we give truncation errors $D_{\Delta}^{3}P_{\Delta}\mathbf{u}_{\Delta}+\mathbf{u}_{\Delta}-\mathbf{F}$ rather than global errors $\mathbf{U}-\mathbf{u}_{\Delta}$. The formal inconsistency of the scheme is clearly borne out. Note that for the finer grids the maximum norm of the truncation errors can be as high as 10^{5} .

Figure 3 was obtained with grids with J even. The axes correspond to $\log(\|\mathbf{U} - \mathbf{u}_{\Delta}\|_{\Delta})$ versus $\log(h)$ and to try and help the scheme, the grids actually employed were quasiuniform with $h_{\min} > h/10$. (To generate quasiuniform grids, the algorithm above was used, with h^i taken from a uniform distribution

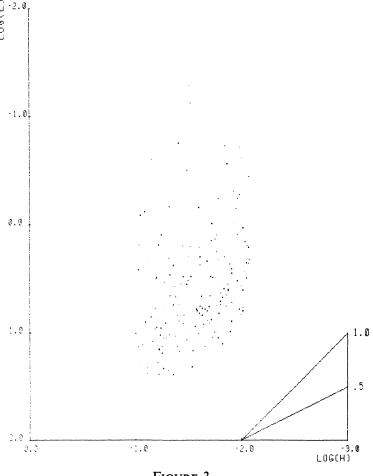


FIGURE 3

J even. $\|\mathbf{U} - \mathbf{u}_{\Delta}\|_{\Delta}$. Quasiuniform meshes

in $[0.1\delta, \delta]$.) Figure 3 should be compared with Figure 1. With the finer grids, the errors in Figure 1 are (in the maximum norm) well below 10^{-2} , while here we find runs with h in the neighborhood of 0.01 and L^2 -errors above 10^1 . This large difference in global error behavior between the cases J odd and J even has no counterpart when truncation errors are considered. In fact, the (not depicted here) truncation errors for the J even runs in Figure 3 were found to behave as the truncation errors depicted in Figure 2 (J odd).

Finally, we solved the problem we have been considering (i.e., $u = \sin(2\pi x)$, L = 1) on the grids (3.16). Errors, given in Table 1, show an O(1) behavior in good agreement with our analysis. We divided the last subinterval of each grid (3.16), with length h, into two subintervals of lengths h/2. The resulting grids have J odd. The corresponding results are given in Table 2, where convergence of the second order is apparent. Note the striking difference in global errors caused by the small change in the grid.

TABLE 1

J	h	$\left\ \mathbf{E}_{\!\scriptscriptstyle\Delta}^{}\right\ _{\!\scriptscriptstyle\Delta}$
32	.05681	.079054
64	.02840	.055207
128	.01420	.054569
256	.00710	.054129

TABLE 2

J	h	$\left\ \mathbf{E}_{\!\scriptscriptstyle\Delta}^{}\right\ _{\!\scriptscriptstyle\Delta}$
33	.05681	.013514
65	.02840	.002253
129	.01420	.000530
257	.00710	.000130

The case J even: average behavior (collaboration with C. Matrán and P. Revész). A family of grids with J even for which divergence takes place has been constructed above. However, it has also been mentioned that uniform grids with J even lead to convergence. It may be asked whether the "typical" case is given by the divergence in the ad hoc grid (3.16) or by the (second-order) convergence on uniform grids. The data in Figure 3 appear to indicate that for J even the global errors, while being large, decrease under grid refinement. To end this section, we provide some indications of the statistical analysis of such a convergence "in the average-grid case."

Recall that the divergence on \wp_e is linked to the presence of a mode \mathbf{c} which lies in the kernel of the averaging operator. The projection $|(\mathbf{c}, \mathbf{u}_{xxx\Delta})_{\Delta}|/\|\mathbf{c}\|_{\Delta}$ of $\mathbf{u}_{xxx\Delta}$ onto the normalized mode $(\|\mathbf{c}\|_{\Delta})^{-1}\mathbf{c}$ was shown in (3.15) to provide an obstacle to the convergence of the method. Such a projection, which was shown to be O(1) for a particular family of grids, can be expected to be on the average $O(h^{1/2})$ on grids randomly generated by the algorithm above. This suggests an order of convergence of 1/2, in agreement with Figure 3.

We begin by noticing that, after summation by parts, for smooth u,

(3.17)
$$(\mathbf{c}, \mathbf{u}_{xxx\Delta})_{\Delta} = \frac{1}{3} \sum_{j=1}^{J} (-1)^{j} (h^{j})^{2} u_{xxx}(x^{j-1/2}) + O(h^{2}).$$

We shall study the behavior of the sum in (3.17), and to this end we consider the simplified model

(3.18)
$$Y = \sum_{1 \le i \le J} (-1)^i (h^i)^2.$$

According to the grid generation algorithm, the h^i are independent random variables uniformly distributed in $[0, \delta]$, and J is also a random variable (stopping time), namely the smallest integer for which $\sum_{1 \le i \le J} h^i \ge 1$, provided

this integer is even. In h^i and J, δ features as a parameter. It is expedient to introduce the random variables $X_i = h^i/\delta$, with uniform distribution in [0, 1] and the variables $Z_i = X_{2i}^2 - X_{2i-1}^2$. Then

$$(3.19) Y = \sum_{1 \le i \le J/2} Z_i,$$

and J is the first integer with

$$(3.20) \sum_{1 \le i \le J} X_i \ge 1/\delta.$$

Now X_i , Z_i do not depend on the parameter δ , while $J=J(\delta)$. It is reasonable to expect that, for δ small, J will be approximately $2/\delta$. More precisely, it can be shown [5, pp. 136–137] that for any sequence $\{\delta_k\}$ with $\lim \delta_k = 0$,

$$(3.21) \delta_{\nu} J(\delta_{\nu}) \to 2,$$

with almost sure convergence.

On the other hand, the Z_i have zero mean, and the central limit theorem guarantees that as $n \to \infty$

(3.22)
$$\frac{\sum_{i=1}^{n} Z_{i}}{\sqrt{\frac{8}{45}}n} \to N(0, 1).$$

In (3.22) the arrow means convergence in law and N(0, 1) denotes normal with 0 mean and standard deviation 1. The factor 8/45 arises as follows. With E denoting mean,

$$E(Z_{i}^{2}) = E(X_{2i}^{4}) + E(X_{2i-1}^{4}) - 2E(X_{2i}^{2})E(X_{2i}^{2}) = \frac{2}{5} - \frac{2}{9} = \frac{8}{45}$$

A theorem due to Doeblin and Anscombe [4, p. 317] can be used to show that (3.21)–(3.22) imply, as $k \to \infty$, and in the sense of convergence in law,

(3.23)
$$\frac{1}{\sqrt{\frac{8}{45}J(\delta_k)/2}} \sum_{i=1}^{J(\delta_k)/2} z_i \to N(0, 1).$$

Finally, since the maximum increment $h=h(\delta_k)$ obviously satisfies $h(\delta_k)/\delta_k\to 1$ (almost sure convergence), in the denominator of (3.23), $J(\delta_k)$ can be replaced by $2/h(\delta_k)$, according to Slutsky's theorem [4, p. 249]. This, and the elimination of the Z_i variables, lead to

$$Y/\sqrt{\frac{8}{45}}h^{3/2} \to N(0, 1), \qquad h \to 0.$$

In conclusion, the model variable Y behaves asymptotically as a normally distributed $O(h^{3/2})$ variable. Thus, $(\mathbf{c}, \mathbf{u}_{xxx\Delta})_{\Delta}$ can be expected to also behave as $O(h^{3/2})$ and the lower bound in (3.15) would be, on the average, $O(h^{1/2})$. This

is not as bad as the O(1) behavior found for the worst possible case, but still far away from the $O(h^2)$ bound shown for the J odd situation.

4. EVOLUTIONARY MODEL PROBLEM

In this section we consider the periodic initial value model problem for (1.4), with the formally inconsistent discretization given by

(4.1)
$$\frac{d}{dt}\mathbf{U} = D_{\Delta}^{3}P_{\Delta}\mathbf{U}.$$

Again, U is meant to approximate the restriction of the true solution to the centers $x^{i-1/2}$ of the cells. Note that, since (4.1) is linear, its solutions are defined for all times. Techniques similar to those used above show that J even leads to divergence [9], and only the case J odd will be considered. For simplicity we assume that the initial value for (4.1), U(0), is taken to be the restriction to the cell centers of the initial condition u(t=0).

Theorem 4.1. Let u be a C^8 solution of (1.4). Then to each positive T there correspond positive constants h_0 and C so that for each grid Δ with an odd number of points J and $h(\Delta) < h_0$, the solution \mathbf{U} of (4.1) with $\mathbf{U}(0) = \mathbf{u}(t=0)$ satisfies

$$\max_{0 < t < T} \left\| \mathbf{u}_{\Delta}(t) - \mathbf{U}(t) \right\|_{\Delta} \le C h^2.$$

Furthermore, h_0 and C only depend on the period L, on T, and on bounds for the derivatives of u (up to the eighth).

Proof. For each positive time t, we introduce the solution W(t) of the problem

$$(4.3) D_{\Delta}^{3} P_{\Delta} \mathbf{W}(t) + \mathbf{W}(t) = \mathbf{u}_{t}(\cdot, t)_{\Delta} + \mathbf{u}(\cdot, t)_{\Delta} = \mathbf{u}_{xxx}(\cdot, t)_{\Delta} + \mathbf{u}_{\Delta}(\cdot, t)_{\Delta}.$$

Theorem 3.2 implies that

$$\|\mathbf{u}(\cdot, t)_{\Lambda} - \mathbf{W}(t)\|_{\infty} \leq Ch^2$$

and a fortiori

$$\|\mathbf{u}(\cdot,t)_{\Lambda} - \mathbf{W}(t)\|_{\Lambda} \le Ch^2$$

with C dependent on t, L, and bounds for the space derivatives of u up to the fifth. Differentiating (4.3) with respect to t and reasoning as above leads to

(4.5)
$$\left\|\mathbf{u}_{t}(\cdot, t)_{\Delta} - \frac{d}{dt}\mathbf{W}(t)\right\|_{\Delta} \leq Ch^{2},$$

where now the constant depends on t, L, and derivatives of u up to the eighth.

We decompose the error $\mathbf{E}=\mathbf{u}_\Delta-\mathbf{U}$ as $\mathbf{E}=(\mathbf{u}_\Delta-\mathbf{W})+(\mathbf{W}-\mathbf{U})$. The first term has already been bounded in (4.4). The evolution of the second is governed by

$$(4.6) \qquad \frac{d}{dt}(\mathbf{W}_{\Delta} - \mathbf{U}) = \frac{d}{dt}(\mathbf{W} - \mathbf{u}_{\Delta}) + \mathbf{W} - \mathbf{u}_{\Delta} + D_{\Delta}^{3}P_{\Delta}(\mathbf{W} - \mathbf{U}).$$

Now (4.2) follows easily by, say, the energy method, because the operator $D_{\Delta}^{3}P_{\Delta}$ is skew-symmetric and the sources $(d/dt)(\mathbf{W}-\mathbf{u}_{\Delta})$, $(\mathbf{W}-\mathbf{u}_{\Delta})$ have been shown, in (4.4) and (4.5), to be $O(h^{2})$. \square

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