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MATHEMATICAL MODELLING AND NUMERICAL ANALYSIS
MODÉLISATION MATHÉMATIQUE ET ANALYSE NUMÉRIQUE

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STABILITY OF SCHEMES FOR THE NUMERICAL TREATMENT OF AN EQUATION MODELLING FLUIDIZED BEDS (*)

by L. ABIA [1], I. CHRISTIE [2] and J. M. SANZ-SERNA [1]

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Abstract. — *We consider a nonlinear partial differential equation arising in fluidized bed modelling which has been numerically studied by Christie and Ganser These authors found that apparently reasonable implicit numerical schemes turn out either to be unconditionally unstable or to perform well only if the time step is suitably* large. *We analyze this strange behaviour and suggest a scheme which does not suffer from stability problems We prove the convergence of the new scheme and provide some numerical illustrations*

Résumé — *Nous considérons une équation aux dérivées partielles non linéaire qui apparait dans la modélisation des lits fluides et qui a été étudiée numériquement par Christie et Ganser Ces auteurs ont trouvé que quelques méthodes « raisonnables » du type implicite ou bien montrent un comportement inconditionnellement instable ou bien ont une bonne performance seulement si le pas Δt est assez grand Nous étudions cet étrange comportement et nous donnons une méthode qui n'offre aucun probleme de stabilité Nous prouvons la convergence de la nouvelle méthode et nous ajoutons des essais numériques*

1. INTRODUCTION

This paper is devoted to the numerical analysis of the periodic initial value problem

$$u_t + u_{xxx} + \beta(u^2)_x + (\gamma/2)(u^2)_{xx} + \varepsilon u_{xx} - \delta u_{tx} = 0, \qquad -\infty < x < \infty,\ 0 < t \leq T < \infty\,, \tag{1.1a}$$

$$u(x,t) = u(x + 2\pi, t), \quad -\infty < x < \infty, \quad 0 < t \leq T\,, \tag{1.1b}$$

$$u(x,0) = q(x)\,, \tag{1.1c}$$

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where β, γ, ε, δ are given real constants with $\varepsilon, \delta > 0$, the unknown function u is real-valued and the given function q is 2π-periodic. The problem (1.1) arises in the theory of flow in a fluidized bed [3], [4] with u representing the value of a spatially periodic small perturbation of the concentration of particles. Christie and Ganser have studied (1.1) numerically by means of finite-difference and modified-Galerkin methods and some of their findings have been collected in [1]. A salient outcome of their work is that many « reasonable » implicit schemes perform in an unexpectedly *unstable* manner, while the application of other implicit schemes leads to stable computations only if the time step used in the integration is *large* enough relative to the mesh-size in space. This should be compared with the more familiar situation where stability requirements set an *upper bound* for the time-step.

In Section 2 of the present paper we consider the linearization of (1.1) near $u = 0$ (i.e. the equation obtained by setting $\beta = \gamma = 0$ in (1.1*a*)). We take up the stability study in [1] and provide insight into the phenomena involved. We show that the instabilities of the schemes are due to the *space* discretization. Of importance is the fact that this instability may be present even in the case of Galerkin space-discretizations. However, we prove that the combination of an unstable space-discretization with a strongly A-stable time-stepping formula may result in a Lax-stable fully discrete scheme. We also suggest a space-discretization which does not suffer from stability problems. A convergence proof for the novel scheme, as applied to the full nonlinear problem (1.1), is given in Section 3. Finally, in Section 4 some numerical illustrations are presented.

2. LINEAR ANALYSIS

2.1. The partial differential equation

In this section we consider the linearization of (1.1*a*) near $u = 0$, given by

$$u_t + u_{xxx} + \varepsilon u_{xx} - \delta u_{tx} = 0, \quad \varepsilon, \delta > 0, \quad -\infty < x < \infty, \quad 0 < t < T. \quad (2.1)$$

A function $u(x, t) = \phi(t)\, e^{imx}$, m integer, satisfies (2.1) if and only if $\phi(t)$ satisfies

$$d\phi/dt = \sigma(m)\, \phi\,,$$

where $\sigma(m)$ denotes the symbol

$$\sigma(m) = m^2[(\varepsilon - \delta m^2) + i(1 + \varepsilon\delta)\, m]/[1 + \delta^2 m^2]\,. \quad (2.2)$$

Thus the modes with wave number m such that $|m| < \sqrt{(\varepsilon/\delta)}$ have $\operatorname{Re} \sigma(m) > 0$ and accordingly grow exponentially in the time evolution.

However, for m outside the bounded interval $[-\sqrt{(\varepsilon/\delta)}, \sqrt{(\varepsilon/\delta)}]$, $\operatorname{Re} \sigma(m) < 0$ and the Fourier modes are damped. As a consequence

$$\sup \{\operatorname{Re} \sigma(m) : -\infty < m < \infty\} < \infty$$

and the 2π-periodic initial-value problem for (2.1) is well-posed in L^2 [9]. The behaviour of $\operatorname{Re} \sigma(m)$ as a function of m is depicted in figure 1, where there is no need to plot the modes with $m < 0$, since $\operatorname{Re} \sigma(m)$ is an even function. Here and later, the arcs which correspond to decaying modes are drawn with dashed lines and shown only in part, as their exact behaviour is not relevant to the issue of stability.

It is perhaps useful to observe that the existence of growing modes can be attributed to the backward heat equation combination $u_t + \varepsilon u_{xx}$ and that, for m large, the effect of this combination is offset by the term δu_{tx}. Linearly unstable modes are frequently present in the modelling of two-phase flows [3], [4] and have a physical origin. In narrow diameter fluidized beds the existence of growing modes is linked to the « slugging » phenomenon.

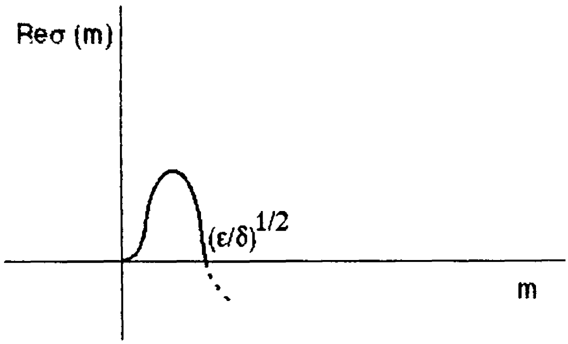

Figure 1. — Partial differential equation symbol.

2.2. Simple space discretization

The simplest finite-difference space discretization of (2.1) is perhaps obtained by replacing the x-derivatives by standard central differences as follows

$$(d/dt)\, U_j + (1/2)\, h^{-3}[U_{j+2} - 2\, U_{j+1} + 2\, U_{j-1} - U_{j-2}] +$$
$$+ \varepsilon h^{-2}[U_{j+1} - 2\, U_j + U_{j-1}] - (1/2)\, \delta h^{-1}(d/dt)[U_{j+1} - U_{j-1}] = 0,$$
$$j = 0, \pm 1, \pm 2, \dots \quad (2.3a)$$

Here, and later, h represents a mesh-size, $h = 2\pi/J$, J a positive integer, and $U_j = U_j(t)$ is an approximation to $u(x_j, t)$, with $x_j = jh$, $j = 0, \pm 1, \pm 2, \ldots$. Of course the scheme (2.3a) will be used together with the periodicity condition

$$U_j = U_{j+J}, \quad j = 0, \pm 1, \pm 2, \ldots \tag{2.3b}$$

Now $U_j(t) = \Phi(t)\exp(imx_j)$, m integer, solves (2.3) if and only if $\Phi(t)$ satisfies

$$d\Phi/dt = \Sigma(m, h)\,\Phi\,,$$

where $\Sigma(m, h)$ is the discrete symbol

$$\begin{aligned}\Sigma(m, h) = h^{-2}(2 - 2\cos z)[\varepsilon - \delta h^{-2}\sin^2 z + i(1 + \varepsilon\delta)h^{-1}\sin z]/\\ [1 + \delta^2 h^{-2}\sin^2 z], \quad z = mh\end{aligned} \tag{2.4}$$

It is then clear that, for m fixed, $\Sigma(m, h) = \sigma(m) + O(h^2)$, in agreement with the fact that (2.3a) is consistent of the second order with (2.1). The behaviour of $\operatorname{Re}\Sigma(m, h)$ as a function of m is given in Figure 2, where the attention has been restricted to the interval $0 \leqslant m \leqslant \pi/h$, as $\operatorname{Re}\Sigma(m, h)$ is even and $2\pi/h$-periodic in m. We observe that now, for $0 \leqslant m \leqslant \pi/h$, there are two intervals of growing modes. The first is given by $(0, (1/h)\arcsin[h\sqrt{(\varepsilon/\delta)}])$ and is therefore of the form $(0, \sqrt{(\varepsilon/\delta)} + O(h^2))$, an approximation to the corresponding interval for $\sigma(m)$. However, there is also a second interval

$$(\pi/h - (1/h)\arcsin[h\sqrt{(\varepsilon/\delta)}], \pi/h)\,,$$

of the form $(\pi/h - \sqrt{(\varepsilon/\delta)} + O(h^2), \pi/h)$, with no counterpart in (2.1). Thus (2.3) possesses *spuriously growing modes*. Moreover

$$\max\{\operatorname{Re}\Sigma(m, h)\,.\, -\infty < m < \infty\} = 4\,\varepsilon/h^2\,,$$

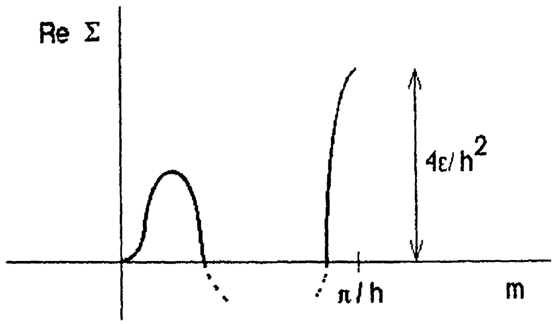

Figure 2. — Symbol of the space discretization (2.3).

so that the growth can be as fast as $\exp(4\,\varepsilon/h^2)$. Therefore, as the grid is refined, the Cauchy problem for (2.3) is *not* well-posed in L^2 uniformly in h. In other words, the scheme (2.3) is not L^2-stable and, as a result, cannot be convergent for arbitrary L^2 initial data [9], [6], [7]. The fastest rate of growth corresponds to the Fourier mode $\exp(imx_j)$, $m = \pi/h$, i.e. to the saw-tooth mode $(-1)^j$. In fact the δ-term in (2.3*a*) annihilates this wave-number and accordingly, for this mode, the unstable action of the backward heat equation term finds no opposition.

The instability of (2.3) is shared by many other discretizations of (2.1) and related problems. A remarkable instance is provided by the piecewise-linear *Galerkin* space-discretization of the (well-posed) periodic initial value problem for

$$u_t + \varepsilon u_{xx} - \delta u_{tx} = 0, \quad \varepsilon, \delta > 0 .$$

2.3. Time discretization

If the solutions of (2.3) are now advanced in time by means of a standard convergent numerical ODE method, then for h given and Δt very small the fully discrete scheme will reproduce accurately the spuriously growing components. Therefore the values computed in this way cannot be expected to be meaningful approximations to the solutions of (2.1)-(1.1*b*). However we shall show next that, for certain ODE solvers, it is still possible to carry out successful time-integrations of (2.3) provided that Δt *is not too small*, relative to h. This should be compared with the more common situation where stability requirements set an *upper bound* for the time-step. The standard backward Euler rule will be used as an illustration, but analogous considerations can be made for the two-step BDF formulae or, more generally, for any strongly A-stable method, i.e. for any A-stable method whose stability region includes a neighbourhood of infinity [5, p. 102].

A schematic plot of the parametric curve $\zeta = \Delta t\,\Sigma(m, h)$, $0 \leq m \leq \pi/h$, in the complex ζ-plane is given in figure 3. In this plane, the stability region of the backward Euler method consists of the exterior of the circle with radius 1 and centre at 1. The arc BC stems from the spuriously growing semidiscrete modes in the m-interval $(\pi/h - \sqrt{(\varepsilon/\delta)} + O(h^2), \pi/h)$ considered before. The arc OA corresponds to the physically growing modes and the arc AB (not completely drawn) corresponds to the modes damped by the semidiscretization. It seems plausible that if

$$4\,\varepsilon\,\Delta t/h^2 > 2 \quad \text{i.e.} \quad \Delta t/h^2 > 1/(2\,\varepsilon)\,, \tag{2.5}$$

then all offending modes of (2.3) will be damped by the time-integration. In fact, we can prove :

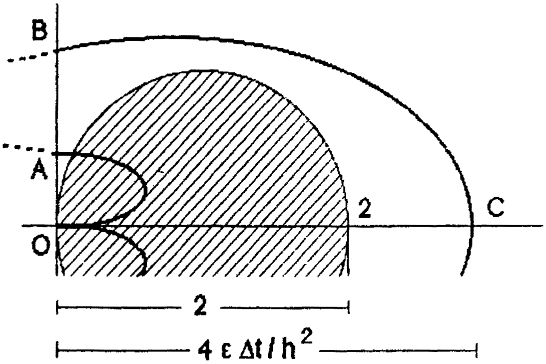

Figure 3. — Instability region of the Backward Euler method and schematic plot of locus $\Delta t\ \Sigma(m, h)$, with $\Sigma(m, h)$ an eigenvalue of the system of ordinary differential equations (2.3) being integrated in time.

THEOREM 2 1 *Let $\lambda > 1/(2\,\varepsilon)$ be a fixed positive number Assume that (2 3) is discretized in time by means of the backward Euler method with a step $\Delta t = \lambda h^2$ Then the resulting fully discrete scheme is Lax-stable in the L^2-norm*

Proof We have to provide, for h sufficiently small, an $1 + O(\Delta t)$ bound for the amplification factor of the scheme, uniformly in m, $0 \leq m \leq \pi/h$ For the modes in the arc OA such a bound exists by consistency For the modes in the arc AB the amplification factor is clearly less than or equal to 1 in magnitude Therefore we are left with the modes corresponding to the arc BC and the proof will be ready if we show that, for $\lambda > 1/(2\,\varepsilon)$, this arc lies completely within the stability region of the backward Euler scheme With $z = mh$, the intersections of the parametric curve $\zeta = \Delta t\ \Sigma(m, h)$ and the stability boundary are the solutions of the equation $|\zeta - 1| = 1$ or

$$0 = [2\cos z - 2] \times$$
$$\times\ [2\,\varepsilon h^2 + \varepsilon^2\lambda h^2 (2\cos z - 2) + \lambda \sin^2 z (2\cos z - 2) - 2\,\delta \sin^2 z] \qquad (2\ 6)$$

The first factor in (2 6) gives of course the intersection at the origin Upon setting $c = \cos z$ in the second factor, we derive an algebraic cubic equation for c When $h = 0$, the three values of c are given by $c_1 = 1$, $c_2 = -1$, $c_3 = 1 + \delta/\lambda$ Since these roots are simple, the c-roots, for h sufficiently small, are given as power series in h, with leading terms respectively equal to 1, -1, $1 + \delta/\lambda$ Obviously, the first of those power series corresponds to the intersection in the arc OA, while the third does not lead to a real intersection (the equation $\cos z = c$ cannot possess real solutions for z). The remaining series is easily found to be of the form

$$c = -1 + [(\varepsilon - 2\varepsilon^2 \lambda)/(2\delta + 4\lambda)] h^2 + O(h^4),$$

which again gives rise, if $\lambda > 1/(2\varepsilon)$ and h is small, to a complex intersection. □

In practice and when integrating in a given a spatial grid, the existence of a lowest permissible value for Δt is not appealing. In fact there are several reasons which could recommend a decrease of the time-step below the lowest value allowed by stability. One obvious reason is time accuracy. Also the integration of any nonlinear modification of (2.3) would require that a nonlinear system be iteratively solved at each time-step, and it is well known that the success of the nonlinear solver would be facilitated by a smaller value of Δt.

The foregoing remarks show that it would be advantageous to construct stable time-continuous discretizations of (2.1) and also fully discrete schemes which do not require a lower stability bound on the time step. These constructions are undertaken next.

2.4. Stable space discretizations

In order to arrive at a stable space-discretization of (2.1), we attempted to replace the term $\varepsilon h^{-2}[U_{j+1} - 2U_j + U_{j-1}]$ in (2.3*a*), while retaining the remaining terms. Our rationale for doing so was that the unstable modes found for (2.3) grew like $\exp(4\varepsilon/h^2)$, so that an alteration in the ε term would lead to a change in the rate of growth. If we wish to discretize εu_{xx} to second order of accuracy while using a five-point stencil (so as not to damage the order of accuracy or increase the band-width of the ODE-system (2.3)), then the most general available formula is given by

$$\varepsilon\mu h^{-2}[U_{j+1} - 2U_j + U_{j-1}] + \varepsilon(1-\mu)(2h)^{-2}[U_{j+2} - 2U_j + U_{j-2}], \tag{2.7}$$

with μ a free real parameter. When the term (2.7) is used instead of $\varepsilon h^{-2}[U_{j+1} - 2U_j + U_{j-1}]$ in (2.3*a*), the mode $(-1)^j$ grows in time like $\exp(4\mu\varepsilon/h^2)$, since then the second term in (2.7) obviously vanishes. Therefore $\mu = 0$ provides the only candidate for a stable semidiscretization of the form considered. This choice leads to the formulae

$$\begin{gathered}(d/dt)U_j + (1/2)h^{-3}[U_{j+2} - 2U_{j+1} + 2U_{j-1} - U_{j-2}] + \\ + (1/4)\varepsilon h^{-2}[U_{j+2} - 2U_j + U_{j-2}] - (1/2)\delta h^{-1}(d/dt)[U_{j+1} - U_{j-1}] = 0\,. \\ j = 0, \pm 1, \pm 2, \dots \end{gathered}\tag{2.8}$$

The real part of the symbol of this scheme is readily found to be

$$h^{-2}\sin^2 z[\varepsilon - \delta h^{-2}(2-2\cos z)]/[1+\delta^2 h^{-2}\sin^2 z], \quad z = mh\,. \tag{2.9}$$

Now, for $0 \leq m \leq \pi/h$, (2.9) is nonnegative if m lies between 0 and

$$(1/h)\cos^{-1}[1-(\varepsilon h^2)/(2\,\delta)] = \sqrt{(\varepsilon/\delta)} + O(h^2)$$

and negative otherwise. As a consequence (2.9) is bounded above independently of h, and the Cauchy problem for (2.8)-(2.1b) is well-posed in L^2 uniformly in h, so that (2.8)-(2.1b) provides an L^2-stable scheme. Furthermore, it is clear that, if (2.8)-(1.1b) is integrated in time by means of any A-stable ODE solver, then the resulting fully-discrete scheme is unconditionally stable (i.e. stable under arbitrary refinements of the time and space grids) [8], [11].

3. NONLINEAR ANALYSIS

Returning now to the nonlinear problem (1.1), it is reasonable to consider the formulae

$$\begin{aligned}
&(d/dt)\,U_j + (1/2)\,h^{-3}[U_{j+2} - 2\,U_{j+1} + 2\,U_{j-1} - U_{j-2}] \\
&+ (1/2)\,\beta h^{-1}[U_{j+1}^2 - U_{j-1}^2] + (\gamma/8)\,h^{-2}[U_{j+2}^2 - 2\,U_j^2 + U_{j-2}^2] \\
&+ (1/4)\,\varepsilon h^{-2}[U_{j+2} - 2\,U_j + U_{j-2}] - (1/2)\,\delta h^{-1}(d/dt)[U_{j+1} - U_{j-1}] = 0, \\
&\qquad\qquad j = 0, \pm 1, \pm 2, \ldots
\end{aligned} \tag{3.1}$$

whose linearization around $U_j = 0$ coincides with (2.8). The system (3.1) is supplemented with the boundary conditions (2.3b).

It is expedient to introduce the following notation : if J is a positive integer we denote by $X(J)$ the vector space of all sequences of real numbers V_j, $j = 0, \pm 1, \pm 2, \ldots$ satisfying the periodicity condition $V_j = V_{j+J}$, $j = 0, \pm 1, \pm 2, \ldots$ Each element in $X(J)$ is represented by a real vector $\mathbf{V}$ with J components $V_1, V_2, \ldots, V_J$. Expressions like $\mathbf{VW}$ or $\mathbf{V}^2$ must be understood componentwise. In $X(J)$ we employ the norms

$$\|\mathbf{V}\| = \left\{\sum_{j=1}^{J} hV_j^2\right\}^{1/2}$$

$$\|\mathbf{V}\|_\infty = \max_{1 \leq j \leq J}|V_j|\,,$$

and the inner product (,) associated with the norm $\|.\|$. The symbol T_+ denotes the forward shift $T_+\,[V_1, V_2, \ldots, V_J]^T = [V_2, V_3, \ldots, V_1]^T$, and

$T_- = T_+^{-1}$ represents the backward shift. We require the divided-difference operators

$$\begin{aligned} D_0 &= (T_+ - T_-)/(2h), \\ D_+ &= (T_+ - I)/h, \\ D_- &= (I - T_-)/h, \\ D^2 &= (T_+ - 2I + T_-)/h^2 . \end{aligned}$$

With these notations the equations (3.1)-(1.1*b*) can be written in the more compact form

$$(d/dt)\,\mathbf{U} + D^2 D_0 \mathbf{U} + \beta D_0 \mathbf{U}^2 + (\gamma/2)\, D_0^2 \mathbf{U}^2 + \\ + \varepsilon D_0^2 \mathbf{U} - \delta (d/dt)\, D_0 \mathbf{U} = \mathbf{0}\,, \quad (3.2a)$$

a system of ordinary differential equations which is integrated subject to an initial condition

$$\mathbf{U}(0) = \mathbf{Q}_h, \quad (3.2b)$$

where $\mathbf{Q}_h$ is an approximation to $[q(x_1), q(x_2), \dots, q(x_J)]^T$.

The following *stability* result holds (*cf.* [2]).

PROPOSITION 3.1 : *To each positive constant R there corresponds a positive constant C, which depends only on R, T, β, γ, ε, δ, such that if t^* is a positive number, $t^* \leq T$ and $\mathbf{V}$ and $\mathbf{W}$ are continuously differentiable $X(J)$-valued functions of the variable t, $0 \leq t \leq t^*$, which satisfy*

$$\|\mathbf{V}(t) + \mathbf{W}(t)\|_\infty + \|D_+(\mathbf{V}(t) + \mathbf{W}(t))\|_\infty + \|D_0^2(\mathbf{V}(t) + \mathbf{W}(t))\|_\infty < R, \\ 0 \leq t < t^*\,, \quad (3.3)$$

then

$$e(t) \leq C\left\{e(o) + \max_{0 \leq s \leq t^*} \|\mathbf{F}(s) - \mathbf{G}(s)\|^2\right\}, \quad 0 \leq t \leq t^*\,, \quad (3.4)$$

where, by definition,

$$e(t) = \|\mathbf{V}(t) - \mathbf{W}(t)\|^2 + \delta^2 \|D_0(\mathbf{V}(t) - \mathbf{W}(t))\|^2, \quad 0 \leq t \leq t^*\,, \quad (3.5)$$

and $\mathbf{F} = \mathbf{F}(t)$ and $\mathbf{G} = \mathbf{G}(t)$ denote the residuals defined for $0 \leq t \leq t^*$ by the formulae

$$\mathbf{F} = (d/dt)\,\mathbf{V} + D^2 D_0 \mathbf{V} + \beta D_0 \mathbf{V}^2 + \\ + (\gamma/2)\, D_0^2 \mathbf{V}^2 + \varepsilon D_0^2 \mathbf{V} - \delta (d/dt)\, D_0 \mathbf{V}, \quad (3.6)$$

$$\mathbf{G} = (d/dt)\,\mathbf{W} + D^2 D_0 \mathbf{W} + \beta D_0 \mathbf{W}^2 + \\ + (\gamma/2)\, D_0^2 \mathbf{W}^2 + \varepsilon D_0^2 \mathbf{W} - \delta (d/dt)\, D_0 \mathbf{W}\,. \quad (3.7)$$

Proof: We employ the abbreviations $\mathbf{E} = \mathbf{V} - \mathbf{W}$, $\mathbf{L} = \mathbf{F} - \mathbf{G}$. On subtracting (3.7) from (3.6) taking the inner product of the result and $\mathbf{E} - \delta D_0 \mathbf{E}$ and rearranging, we arrive at

$$\begin{aligned}
((d/dt)\,\mathbf{E}, \mathbf{E}) + \delta^2((d/dt)\,D_0\,\mathbf{E}, D_0\,\mathbf{E}) = \\
= \delta((d/dt)\,D_0\,\mathbf{E}, \mathbf{E}) + \delta((d/dt)\,\mathbf{E}, D_0\,\mathbf{E}) \\
- (D_0\,D^2\,\mathbf{E}, \mathbf{E}) + \delta(D_0\,D^2\,\mathbf{E}, D_0\,\mathbf{E}) - \varepsilon(D_0^2\,\mathbf{E}, \mathbf{E}) + \delta\varepsilon(D_0^2\,\mathbf{E}, D_0\,\mathbf{E}) \\
- \beta(D_0[\mathbf{V}^2 - \mathbf{W}^2], \mathbf{E} - \delta D_0\,\mathbf{E}) - (\gamma/2)(D_0^2[\mathbf{V}^2 - \mathbf{W}^2], \mathbf{E}) \\
+ (\gamma\delta/2)(D_0^2[\mathbf{V}^2 - \mathbf{W}^2], D_0\,\mathbf{E}) + (\mathbf{L}, \mathbf{E} - \delta D_0\,\mathbf{E}), \quad 0 \leqslant t < t^* . \qquad (3.8)
\end{aligned}$$

The definition (3.5) shows that the left hand side of (3.8) is $(1/2)(d/dt)\,e$. We successively consider each of the ten terms in the right hand side. The first two terms cancel each other, since the operator D_0 is skew-symmetric. The third term vanishes because the operator $D^2\,D_0$ is also skew-symmetric. On taking into account that D_+ is the adjoint operator of $-D_-$, the fourth term can be transformed as follows

$$\begin{aligned}
\delta(D^2\,D_0\,\mathbf{E}, D_0\,\mathbf{E}) &= \delta(D_+\;D_-\;D_0\,\mathbf{E}, D_0\,\mathbf{E}) \\
&= -\,\delta(D_-\;D_0\,\mathbf{E}, D_-\;D_0\,\mathbf{E}) = -\,\delta\,\|D_-\;D_0\,\mathbf{E}\|^2 \leqslant 0 .
\end{aligned}$$

For the fifth term, on noting again the skew-symmetry of D_0, we can write

$$-\,\varepsilon(D_0^2\,\mathbf{E}, \mathbf{E}) = \varepsilon\,\|D_0\,\mathbf{E}\|^2 \leqslant Ce .$$

Here and later C denotes a constant which depends only on the allowed quantities and not necessarily the same at each occurrence. We invoke once more the skew-symmetry of D_0 to show that the sixth term vanishes. Next, the Cauchy-Schwartz inequality leads to

$$-\,\beta(D_0(\mathbf{V}^2 - \mathbf{W}^2), \mathbf{E} - \delta D_0\,\mathbf{E}) \leqslant C\,(\|D_0(\mathbf{V}^2 - \mathbf{W}^2)\|^2 + e) . \qquad (3.9)$$

On employing in (3.9) the identity

$$\begin{aligned}
2\,D_0(\mathbf{V}^2 - \mathbf{W}^2) = 2(\mathbf{V} + \mathbf{W})\,D_0(\mathbf{V} - \mathbf{W}) + D_+\,(\mathbf{V} + \mathbf{W})\,T_+\,(\mathbf{V} - \mathbf{W}) + \\
+ D_-\,(\mathbf{V} + \mathbf{W})\,T_-\,(\mathbf{V} - \mathbf{W})
\end{aligned}$$

and recalling (3.3), we conclude that the seventh term in the left hand-side of (3.8) possesses a bound of the form Ce. The eighth, after the rearrangement

$$-\,(D_0^2[\mathbf{V}^2 - \mathbf{W}^2], \mathbf{E}) = (D_0[\mathbf{V}^2 - \mathbf{W}^2], D_0\,\mathbf{E}) ,$$

can be manipulated as in (3.9) to show that is bounded by Ce. For the ninth we write

$$(D_0^2[\mathbf{V}^2 - \mathbf{W}^2], D_0 \mathbf{E}) =$$
$$= (D_0^2[\mathbf{V} + \mathbf{W}]\,\mathbf{E}, D_0 \mathbf{E}) + (T_+ \; D_0[\mathbf{V} + \mathbf{W}]\,T_+ \; D_0 \mathbf{E}, D_0 \mathbf{E}) +$$
$$+ (T_- \; D_0[\mathbf{V} + \mathbf{W}]\,T_- \; D_0 \mathbf{E}, D_0 \mathbf{E}) + ([\mathbf{V} + \mathbf{W}]\,D_0^2 \mathbf{E}, D_0 \mathbf{E}) . \quad (3.10)$$

The first three terms in the right of (3.10) can be dealt with as above. In the remaining term, we proceed as follows :

$$([\mathbf{V} + \mathbf{W}]\,D_0^2 \mathbf{E}, D_0 \mathbf{E}) = ([\mathbf{V} + \mathbf{W}], \bar{D}_0^2 \mathbf{E} D_0 \mathbf{E})$$
$$= (1/2)([\mathbf{V} + \mathbf{W}], D_0\{D_0 \mathbf{E}\}^2) - (1/4)([\mathbf{V} + \mathbf{W}], D_- \{(T_+ - I)\,D_0 \mathbf{E}\}^2)$$
$$= -\,(1/2)(D_0[\mathbf{V} + \mathbf{W}], \{D_0 \mathbf{E}\}^2) + (1/4)(D_+ [\mathbf{V} + \mathbf{W}], \{(T_+ - I)\,D_0 \mathbf{E}\}^2).$$

It is now clear that (3.10) has a bound of the form Ce. Finally the tenth term in the right of (3.8) satisfies

$$(\mathbf{L}, \mathbf{E} - \delta D_0 \mathbf{E}) \leqslant C\,(e + \|\mathbf{L}\|^2) .$$

To sum up, we have proved that

$$(d/dt)\,e \leqslant C\,(e + \|\mathbf{L}\|^2), \quad 0 \leqslant t < t^* .$$

Now (3.4) is a consequence of Gronwall's lemma. □

We are in a position to prove the convergence of the scheme (3.2). The symbol $\mathbf{u}_h(t)$ denotes the vector $[u(x_1, t), u(x_2, t), \ldots, u(x_J, t)]^T$.

THEOREM 3.1 : *Assume that :* (i) *The problem* (1.1) *possesses a unique solution* u. (ii) *The derivatives* $\partial^5 u/\partial x^5$ *and* $\partial^4 u/\partial t\,\partial x^3$ *exist and are bounded for* $-\infty < x < \infty$, $0 < t < T$. (iii) *The starting vectors* $\mathbf{Q}_h$ *in* (3.2*a*) *satisfy*

$$\|\mathbf{Q}_h - \mathbf{u}_h\| + \|D_0(\mathbf{Q}_h - \mathbf{u}_h)\| = O(h^2), \quad h \to 0 . \quad (3.11)$$

Then for h sufficiently small, the Cauchy problem (3.2) *possesses a unique solution* $\mathbf{U}'$ *defined for* $0 \leqslant t \leqslant T$, *and*

$$\max_{0 \leqslant t \leqslant T} \{\|\mathbf{U}(t) - \mathbf{u}_h(t)\| + \|D_0(\mathbf{U}(t) - \mathbf{u}_h(t))\|\} = O(h^2), \quad h \to 0 . \quad (3.12)$$

Proof: We first note that the operator $I - \delta D_0$ which acts on $(d/dt)\,\mathbf{U}$ in (3.2*a*) is invertible and that therefore (3.2) is a regular Cauchy problem. Thus (3.2) possesses, for each h, a unique solution $\mathbf{U}$ defined, at least, for small values of t, $0 \leqslant t \leqslant t_{\max}(h) > 0$. Next, we set $R = 1 + 2\,M$ with

$$M = \max_{0 \leqslant t \leqslant T} \left\{\|\mathbf{u}_h(t)\|_\infty + \|D_+ \mathbf{u}_h(t)\|_\infty + \|D_0^2 \mathbf{u}_h(t)\|_\infty\right\}$$

and note that

$$\|\mathbf{U}(t) - \mathbf{u}_h(t)\|_\infty + \|D_+(\mathbf{U}(t) - \mathbf{u}_h(t))\|_\infty + \\ + \|D_0^2(\mathbf{U}(t) - \mathbf{u}_h(t))\|_\infty < 1 \quad (3\ 13)$$

implies

$$\|\mathbf{U}(t) + \mathbf{u}_h(t)\|_\infty + \|D_+(\mathbf{U}(t) + \mathbf{u}_h(t))\|_\infty + \|D_0^2(\mathbf{U}(t) + \mathbf{u}_h(t))\|_\infty < R$$

The assumption (3 11) implies that, at $t = 0$, (3 13) holds, provided that h is sufficiently small Denote by $t(h)$ the largest $s \leq T$ such that $\mathbf{U}$ exists and satisfies (3 13) for $0 \leq t < s$ Note that by continuity either $t(h) = T$ or the left hand-side of (3 13) evaluated at $t(h)$ equals 1 On applying the Proposition 3 1 with $\mathbf{V} = \mathbf{U}$, $\mathbf{W} = \mathbf{u}_h$, $t^* = t(h)$ and noticing that then $\mathbf{F}$ vanishes identically while $\mathbf{G}$ represents the truncation error, we conclude that

$$\max_{0 \leq t \leq t(h)} \left\{ \|\mathbf{U}(t) - \mathbf{u}_h(t)\| + \|D_0(\mathbf{U}(t) - \mathbf{u}_h(t))\| \right\} = O(h^2), \quad h \to 0$$

Therefore the left hand side of (3 13) at $t = t(h)$ is, for h small, less than 1, and as a consequence $t(h) = T$ □

Remark 3 1 The kind of « local » stability estimate in Proposition 3 1 is typically the strongest one that applies in nonlinear problems See [2]

Remark 3 2 The convergence of the implicit midpoint time discretization of (3 2) can be proved with techniques analogous to those used in Theorem 3 1

4. NUMERICAL EXAMPLES

We consider the nonlinear problem (1 1) with the parameter values $\beta = -0\ 45000$, $\gamma = 0\ 37947$, $\delta = 0\ 04216$, $\varepsilon = 0\ 09487$ and the initial condition

$$q(x) = 0\ 1 \sin x, \quad (4\ 1)$$

which represents a small initial periodic disturbance in particle concentration This problem was considered in [1] Since $\sqrt{(\varepsilon/\delta)} = 1\ 5000$, and the wave number in (4 1) is $m = 1$, the linear analysis in Section 2 1 predicts that in the time evolution the initial profile will increase in amplitude while being convected As the amplitude grows, the nonlinear terms start playing a larger role, with the result that the increase in amplitude does not proceed indefinitely In fact, the solution u asymptotically becomes a (non sinusoidal) travelling wave $u(x, t) = g(x - ct)$ [4] For all practical purposes, u behaves like a travelling wave for t larger than, say, 100. In our experiments we therefore set $T = 100$.

Experiment 1 : We simulated (1.1) with implicit midpoint time-stepping in the stable semidiscretization (3.2). The implementation details are as follows. Newton iteration was used to solve the nonlinear equations. The initial guess for Newton's method was taken to be the solution at the previous time level. The Jacobian was updated at each time step, but not within the inner iteration. The linear algebra was done by a banded Gaussian elimination routine which did *not* allow pivoting.

As distinct from the simulations by Chrisite and Ganser [1], no stability problems were encountered, even if the time-step was chosen to be very small relative to h. In Table I we have displayed the computed $\max_j U_j(t)$ at the final time $t = 100$. Note that, with the finest value of Δt the simulation requires 64 000 time steps.

TABLE 1

Stable discretization (3.2). Maximum of computed solution at time $t = 100$.

J \ Δt	0 1	0.025	0.00625	0.0015625
20	1.026	1.023	1.023	1.022
40	1.036	1.034	1.033	1.033

Experiment 2 : We also considered the straightforward central-difference semidiscretization

$$(d/dt)\,\mathbf{U} + D^2 D_0\,\mathbf{U} + \beta D_0\,\mathbf{U}^2 + \\ + (\gamma/2)\,D^2\mathbf{U}^2 + \varepsilon D^2\mathbf{U} - \delta\,(d/dt)\,D_0\,\mathbf{U} = \mathbf{0}\,. \quad (4.2)$$

whose linearization near $\mathbf{U} = \mathbf{0}$ is the unstable scheme (2.3). We employed the stabilizing backward Euler method, implemented as above. All the combinations of h and Δt tried in experiment 1 violate the linear stability condition (2.5) and thus we decided to also perform runs on a finer spatial grid with $J = 80$. We tried each of $J = 20$, 40, 80 with each of $\Delta t = 0.1$, 0.025, 0.00625, 0.0015625. The simulation with $J = 80$ and $\Delta t = 0.1$ satisfies (2.5) and indeed turned out to proceed in a stable manner. However at $t = 29.5$ the integration had to be stopped, due to a zero pivot at the Gaussian elimination. All other simulations violate (2.5) and led to machine overflow. The solution, prior to the overflow, consisted mainly of the $(-1)^j$ mode. The overflow times for the most accurate time-integrations of (4.2) (i.e. $\Delta t = 0.00625$, 0.0015625) are given in Table 2, and clearly suggest an h^2 behaviour. These phenomena can be easily explained. When the

TABLE 2

Unstable discretization (4.2). Overflow time.

J \ Δt	0.00625	0.0015625
20	5.84	5.32
40	1.40	1.46
60	0.30	0.35

integration begins, the nodal values are small and the linear theory applies. Therefore the mode $(-1)^j$ is triggered. Now the solution of (4.2) corresponding to initial data $U_j = c(-1)^j$, c any constant, is given by $U_j = c(-1)^j \exp(4\,\varepsilon t/h^2)$ and therefore consists only of the spatial mode $(-1)^j$ and produces machine overflow after a time interval whose length decreases like h^2 (cf. [10]).

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