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A Comparison of Two Numerical Methods for Oscillatory Reaction-Diffusion Systems

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Abstract—Reaction-diffusion systems whose kinetics contain a stable limit cycle are an established class of models for a range of oscillatory biological and chemical phenomena. In this paper, the author compares two numerical methods for calculating the oscillatory wake solutions generated by spatially localized perturbations for one particular reaction-diffusion system, of λ-ω type. The two methods are a semi-implicit, or implicit-explicit, finite difference scheme based on the Crank-Nicolson algorithm, and the method of lines with Gear's method. Though both solutions ultimately converge to a common solution, the approach to this final solution is very different in the two cases. The results provide a clear illustration of the care required in numerical solution of oscillatory reaction-diffusion equations.

Keywords—Gear's method, Crank-Nicolson method, Reaction-diffusion equations, Periodic waves, Traveling waves, Scientific computing.

1. INTRODUCTION

Reaction-diffusion systems whose kinetics contain a stable limit cycle are an established class of models for a range of oscillatory biological and chemical phenomena, including the Belousov-Zhabotinskii reaction [1], the intracellular calcium system [2] and a number of predator-prey interactions [3]. Such oscillatory reaction-diffusion systems have a wide range of solution types, including periodic waves, spiral waves, and spatiotemporal chaos [4]. This paper is concerned with the one-dimensional behaviour that results from a spatially localised perturbation to the unstable steady state inside the kinetics limit cycle. Such an initial condition induces a transition wave front moving outwards from the initial perturbation site, behind which is an oscillatory wake. In some cases, this wake region contains only regular oscillations with the form of periodic traveling waves, while for other equations there are spatiotemporal irregularities behind a leading band of regular oscillations. A typical example of this latter case is illustrated in Figure 1.

I have described the details of this behaviour previously [5,6]; in the present paper, I consider methods of numerical solution. For this purpose, I will focus on the particular equation

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + \left(1 - u^2 - v^2\right)(u - 3v), \tag{1a}$$

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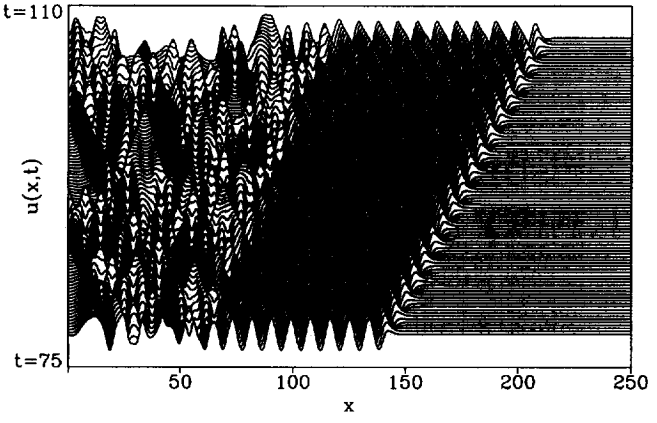

Figure 1. An illustration of the solution of (1). The solution for u is plotted as a function of space x at successive times t, with the vertical separation of the solutions proportional to the time interval.

$$\frac{\partial v}{\partial t} = \frac{\partial^2 v}{\partial x^2} + \left(1 - u^2 - v^2\right)(3u + v), \tag{1b}$$

where u and v are functions of space $x > 0$ and time $t > 0$, and are subject to end conditions

$$\begin{aligned} \frac{\partial u}{\partial x} = \frac{\partial v}{\partial x} &= 0, \qquad \text{at } x = 0 \text{ and} \\ u = v &= 0.01, \qquad \text{at } x = 0, \\ u = v &= 0, \qquad \text{for } x > 0, \text{ at } t = 0. \end{aligned} \tag{1c}$$

This system is in the λ-ω class of equations, which are a commonly-used prototype for more general oscillatory reaction-diffusion systems [7,8]. Figure 1 illustrates the solution of (1); the localised perturbation to $u = v = 0$ induces a transition front, moving across the domain with constant speed. Immediately behind this front are periodic traveling waves, and further back there are irregular spatiotemporal oscillations.

2. NUMERICAL METHODS

The purpose of this paper is to compare two different numerical methods for calculating the solution illustrated in Figure 1. The methods are based on the Crank-Nicolson and Gear algorithms, and I will show that although they converge to a common solution, the details of convergence are quite different in the two cases. I will begin by describing the methods, starting with the Crank-Nicolson scheme. This is a simple finite difference method in which a uniform discretisation is used in both space and time:

$$\begin{aligned} \frac{u_i^{j+1} - u_i^j}{\delta t} = &\frac{u_{i+1}^{j+1} - 2u_i^{j+1} + u_{i-1}^{j+1}}{2\,\delta x^2} + \frac{u_{i+1}^{j} - 2u_i^{j} + u_{i-1}^{j}}{2\,\delta x^2} \\ &+ \left[1 - \left(u_i^j\right)^2 - \left(v_i^j\right)^2\right]\left(u_i^j - 3v_i^j\right), \end{aligned} \tag{2}$$

and similarly for (1b). Here u_i^j denotes the solution for $u(x,t)$ at space point i and time iteration j. I use an uniform space-time grid, with space interval δx and time step δt; I have not investigated the use of adaptive grids.

A method of type (2) is known as semi-implicit because the terms on the right-hand side are evaluated partly at the new time step $j + 1$ and partly at iteration j. Such methods were introduced by Crank and Nicolson [9], and for the scalar, linear diffusion equation exact convergence conditions can be derived quite easily. In this case, the value $\theta = 1/2$ gives particularly high

accuracy, and I have used this value in my computations. For reaction-diffusion equations, numerical schemes of the form (2) are in widespread use, although convergence results are restricted to a few specific cases [10,11].

The second method I consider is the method of lines and Gear's method. The "method of lines" simply converts the PDEs into a system of coupled ODEs, using a central difference representation of the second derivative:

$$\frac{d}{dt}u_i(t) = \frac{u_{i+1} - 2u_i + u_{i-1}}{\delta x^2} + \left[1 - (u_i)^2 - (v_i)^2\right](u_i - 3v_i), \tag{3}$$

and similarly for (1b). Here $u_i(t)$ denotes the solution as a function of time t at space point i; again I use a spatial grid with uniform separation δx. Together with an appropriate representation of the boundary conditions, this gives a system of $2N$ coupled ODEs, where N is the number of space points. I solve these using Gear's method, which is a variable order, variable step-size scheme for stiff ODE systems, that was proposed by Gear [12]. The term "stiff" refers to the fact that there are typically a range of different time scales involved in the solution of (3), with rapidly decaying transients forcing very small time-steps for stability in simple numerical schemes. I use the implementation of the method of lines and Gear's method in the NAG library, which is described in detail by Dew and West [13]. Of particular importance is that this code contains a parameter ε which bounds the estimated local error at each step of the time integration; the method of estimation of the local error is described in [14].

3. NUMERICAL SOLUTIONS

I have used both of these numerical methods to calculate the solution of (1). The problem (1) is posed on an infinite domain, but of course numerical solution must be done on a finite domain, and I solve numerically on $0 < x < L$ with $u = v = 0$ imposed at $x = L$; provided L is sufficiently large, its value has no significant effect on the solution. As δx and either δt or ε are decreased, the solutions of the two numerical methods converge to the same form. That is, in both cases the solution has the qualitative form illustrated in Figure 1, and the speed of the front, the form of the regular oscillations, and the position at which the behaviour becomes irregular all converge to values that are common to the two methods. However, the form of the irregular oscillations does not converge in either case. This is entirely expected: I have presented evidence elsewhere [15], that the region of irregular behaviour is, in fact, temporally chaotic, so that a numerical solution cannot represent more than its qualitative form. However, we can expect the numerical solution to represent quantitatively the point at which the oscillations become irregular, as well as the details of the regular part of the solution.

To measure convergence of the solution, it is convenient to represent the solution not in terms of u or v, but rather in terms of $r = (u^2 + v^2)^{1/2}$. In a system of the form (1), standard theory [8] shows that periodic traveling waves have constant amplitude r. Replotting the solution illustrated in Figure 1 in terms of r shows a simple transition front, with irregular oscillations behind this (Figure 2). In Figure 1, the values of δx, δt, and ε are sufficiently small that the two numerical methods agree very closely; however, lower accuracy solutions have rather different qualitative forms in the two schemes. Figure 2 illustrates the way in which the solutions change as δt and ε are decreased, with fixed δx. Here, I plot r as a function of x at time $t = 76$, and I use this time point (chosen arbitrarily) in all my numerical tests. In the finite difference scheme, the various aspects of the numerical solution converge at approximately the same rate. That is, the speed of the leading front, the amplitude of the regular oscillations, and the point at which these become irregular all approach their final values at approximately the same rate. In contrast, for the Gear code, the front speed and amplitude of the periodic waves converge rapidly, at relatively low values of ε, while the transition point between regular and irregular behaviour converges much more slowly.

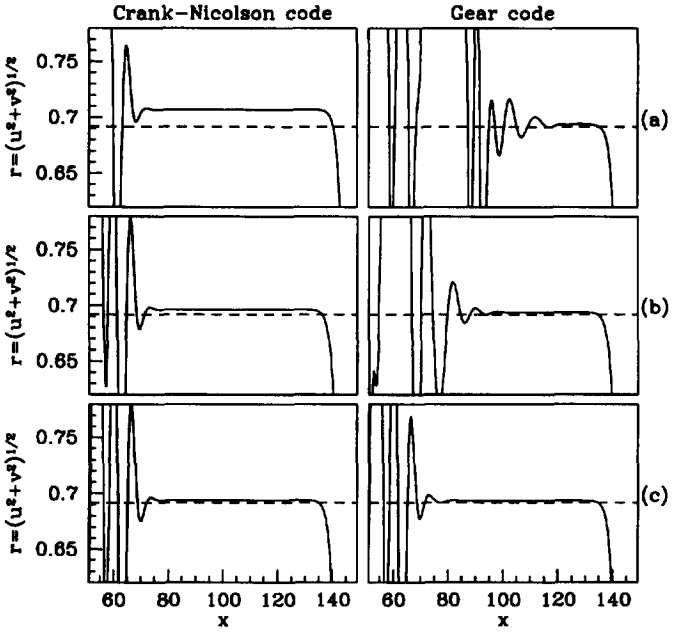

Figure 2. An illustration of convergence in the two numerical schemes. The solutions for r are plotted as functions of x at $t = 76$, with $L = 250$, which is a suitable value for the finite domain length in numerical solutions. In all cases, $\delta x = 0.4$. For the Crank-Nicolson scheme, δt = (a) 0.01; (b) 0.002; (c) 0.0004, and for the Gear method, ε = (a) 10^{-4}; (b) 10^{-6}; (c) 10^{-8}. Only a limited portion of the r-axis is used, in order to show clearly the convergence of the periodic wave amplitude.

To investigate this difference in convergence further, I have calculated two numbers from each numerical solution. The first of these, r_{test}, represents the periodic wave amplitude, and is calculated by using linear interpolation to determine the value $x = x_{0.4}$ at which $r = 0.4$; r_{test} is the value of r at $x = x_{0.4} - 15$. The second quantity I calculate is x_{test}, which represents the point at which the oscillations become irregular, and is defined as the largest value of $x < x_{0.4} - 15$ at which $|r - r_{\text{test}}| > 0.02$; again this is determined by linear interpolation. The details of these definitions are quite arbitrary, but together they give a good representation of these two basic properties of the numerical solution. Table 1 lists the values of r_{test} and x_{test} for the two numerical methods, for a range of values of δx, δt, and ε. The difference in convergence between the two schemes can also be seen clearly in this table. In the finite difference scheme, r_{test} and x_{test} converge at approximately the same rate. In contrast, in the Gear code convergence of r_{test} is very rapid, with the error primarily dependent on δx, while x_{test} converges much more slowly, as a function of both δx and ε. This difference between the methods can be made precise by calculating the product-moment correlation coefficient between r_{test} and x_{test}; for the Crank-Nicolson method this correlation coefficient is 0.69 while for the Gear scheme it is 0.40.

4. DISCUSSION

Scientific computing plays a fundamental role in the study of oscillatory reaction-diffusion systems, for which analytical study is restricted to particular solution forms. The results I have presented underline the great importance of careful tests of numerical methods for such systems. In particular, I have shown that although the Gear scheme gives very good accuracy in the amplitude of the periodic waves, it is significantly worse than the Crank-Nicolson method at calculating the point at which the oscillatory wake becomes irregular. This may be because the variable time-step of Gear's method is chosen to limit the estimated local error at each iteration, but provides no mechanism for controlling the growth of these local errors, which will grow

Table 1. The values of r_{test} and x_{test} for the Crank-Nicolson and Gear schemes as δx, δt, and ε are varied. The definitions of r_{test} and x_{test} are given in the main text. All results are for the system (1) at $t = 76$.

	r_{test} for Crank-Nicolson code				x_{test} for Crank-Nicolson code			
$\delta t =$	10^{-2}	2×10^{-3}	4×10^{-4}	8×10^{-5}	10^{-2}	2×10^{-3}	4×10^{-4}	8×10^{-5}
$\delta x = 1.60$	0.73539	0.72560	0.72357	0.72317	82.94	83.55	83.73	83.75
$\delta x = 0.80$	0.71329	0.70288	0.70075	0.70032	69.21	71.96	72.12	72.19
$\delta x = 0.40$	0.70698	0.69641	0.69424	0.69381	66.08	67.74	68.09	68.15
$\delta x = 0.20$	0.70537	0.69476	0.69258	0.69215	66.00	67.81	68.21	68.29
$\delta x = 0.10$	0.70501	0.69440	0.69223	0.69179	63.99	65.72	66.07	66.15
$\delta x = 0.05$	0.70499	0.69438	0.69221	0.69177	61.67	65.80	66.19	66.27
	r_{test} for Gear code				x_{test} for Gear code			
$\varepsilon =$	10^{-4}	10^{-6}	10^{-8}	10^{-10}	10^{-4}	10^{-6}	10^{-8}	10^{-10}
$\delta x = 1.60$	0.72323	0.72307	0.72306	0.72306	125.10	95.63	83.82	83.76
$\delta x = 0.80$	0.70058	0.70022	0.70021	0.70021	110.90	85.64	72.12	72.21
$\delta x = 0.40$	0.69423	0.69370	0.69370	0.69370	103.25	82.93	67.98	68.16
$\delta x = 0.20$	0.69175	0.69204	0.69204	0.69204	106.21	82.11	66.26	68.33
$\delta x = 0.10$	0.69204	0.69170	0.69168	0.69168	102.21	77.00	66.11	66.16
$\delta x = 0.05$	0.69206	0.69167	0.69166	0.69166	101.67	75.14	65.62	66.32

to eventually dominate the solution in a case such as (1) in which the long-term behaviour is temporally chaotic. However, from a practical viewpoint, the difference in convergence between the two numerical schemes I have described is, in fact, rather beneficial, since the methods only agree when they have both converged. Thus, comparison of the solutions given by the two methods provides a simple test for convergence.

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