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LETTER TO THE EDITOR

A new numerical scheme for the Fisher equation

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Abstract. In the context of the one-dimensional Fisher equation, we study a new numerical scheme for reaction-diffusion equations (proposed by Oono and Puri). We find that this scheme enables a reasonable simulation of the Fisher equation at high values of the time increment, where conventional schemes are not applicable. For lower values of the time increment, the new scheme compares favourably with conventional schemes.

Many important physical phenomena are described by reaction-diffusion equations, namely

$$\frac{\partial u(\boldsymbol{r}, t)}{\partial t} = f(u(\boldsymbol{r}, t)) + \nabla^2 u(\boldsymbol{r}, t) \tag{1}$$

where $u(\boldsymbol{r}, t)$ is a field variable (e.g. order parameter, population density) which depends on space (denoted by $\boldsymbol{r}$) and time (denoted by t). In (1), $f(u(\boldsymbol{r}, t))$ is some function (usually nonlinear) which models the local contribution to the temporal change in $u(\boldsymbol{r}, t)$ (namely reaction). The diffusion term $(\nabla^2 u(\boldsymbol{r}, t))$ in (1) models the temporal change in $u(\boldsymbol{r}, t)$ as a result of diffusion from neighbouring regions. Examples of phenomena described by reaction-diffusion equations are population dynamics [1-2], chemical turbulence [3], phase-ordering dynamics in thermodynamically unstable (quenched) systems [4], etc. For most interesting physical applications, $f(u(\boldsymbol{r}, t))$ is a complicated nonlinear function of $u(\boldsymbol{r}, t)$. In these cases, (1) is not analytically tractable and must be solved numerically on a spacetime lattice with (typically) time and space increments denoted by Δt and Δx. Conventional numerical schemes are the 'explicit discretization scheme' and the 'implicit scheme' [5], both to be described shortly. These schemes are stable (i.e. errors do not grow exponentially in time) for only small (to be quantified soon) values of Δt, because of instabilities introduced by the function $f(u(\boldsymbol{r}, t))$. In a recent work, Oono and Puri [6] have proposed a new numerical scheme for the solution of reaction-diffusion equations. This new scheme eliminates the instability present in the conventional schemes at high values of Δt and is claimed to enable reasonable simulations of (1), even at high values of Δt. In this letter, we apply the new scheme to the one-dimensional (1D) Fisher equation (proposed by Fisher [1] as a model of mutant gene propagation),

$$\frac{\partial u(x, t)}{\partial t} = u(x, t)[1 - u(x, t)] + \frac{\partial^2 u(x, t)}{\partial x^2} \tag{2}$$

where $u(x, t)$ refers to the population density at a point x at time t. Our results are in accordance with the claims of Oono and Puri [6].

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We mention briefly that there are only a few analytical results available on the Fisher equation, emphasizing the need for efficient numerical simulations. Kolmogorov *et al* [7] found that (2) has a travelling wave solution (called a 'cline'), which is a wall travelling in the $+x$ direction with velocity $v \geqslant 2$ and $u(-\infty, t) = 1$, $u(\infty, t) = 0$ (or a wall travelling in the $-x$ direction with $v \leqslant 2$ and $u(-\infty, t) = 0$, $u(\infty, t) = 1$). They did not provide analytic forms for the cline solutions. As far as we know, these are not yet known in general. Subsequently, Aronson and Weinberger [8] demonstrated that a broad class of initial conditions for (2) asymptotically converge to the cline solution with $v = \pm 2$. Puri *et al* [9] have studied approximations of the cline solution for $v = \pm 2$, though (as mentioned earlier) the exact analytic form is not known.

There are two important conventional schemes for simulating (2) numerically on a spacetime lattice [5]. In the explicit (or Euler) scheme, partial derivatives are approximated by their simple difference forms. (Higher-order schemes use more elaborate approximations for the derivatives and are more accurate than the Euler scheme. However, we do not discuss these here.) Thus, in the explicit scheme, (2) takes the form

$$u(x, t+\Delta t) = u(x, t)[1+\Delta t(1-u(x, t))] + \alpha[u(x+\Delta x, t) - 2u(x, t) + u(x-\Delta x, t)] \quad (3)$$

where Δt and Δx are the time and space increments and $\alpha = \Delta t/(\Delta x)^2$. The stability properties of (3) are studied by considering fluctuations $\delta u(x, t)$ about the flat solution $u_0 = 1$, which is a stable solution of (2). Linearizing in $\delta u(x, t)$, we have

$$\delta u(x, t+\Delta t) = [1-\Delta t]\delta u(x, t) + \alpha[\delta u(x+\Delta x, t) - 2\delta u(x, t) + \delta u(x-\Delta x, t). \quad (4)$$

Taking the discrete Fourier transform of (4), we have (assuming periodic boundary conditions)

$$\delta u(k, t+\Delta t) = [1-\Delta t - 4\alpha \sin^2(k\Delta x/2)]\delta u(k, t) \quad (5)$$

where k is the wavevector associated with the fluctuation. It can take values $k = n(2\pi/L)$, where L $(= N\Delta x)$ is the length of the lattice and n goes from 0 to $N-1$. For (3) to be stable, all fluctuations must decay exponentially in time. This requires that

$$\Delta t \leqslant 2 \qquad \alpha \leqslant (2-\Delta t)/4. \quad (6)$$

The restriction on α in (6) can be relaxed by invoking the so-called implicit scheme, in which the discretized diffusion term is taken at time $t+\Delta t$ rather than at time t (as in the explicit scheme). The implicit scheme for (2) takes the form

$$-\alpha u(x-\Delta x, t+\Delta t) + (1+2\alpha)u(x, t+\Delta t) - \alpha u(x+\Delta x, t+\Delta t)$$
$$= u(x, t)[1+\Delta t(1-u(x, t))]. \quad (7)$$

A linear stability analysis of (7) (similar to that done for (3)) yields

$$\delta u(k, t+\Delta t) = \frac{1-\Delta t}{1+4\alpha \sin^2(k\Delta x/2)}\, \delta u(k, t). \quad (8)$$

Thus, the only requirement for stability is $\Delta t \leqslant 2$. In the context of the Fisher equation, we now quantify what we mean by 'small' and 'high' values of Δt. We will refer to values of $\Delta t \leqslant 2$ as 'small' and $\Delta t > 2$ as 'high'.

Clearly, the implementation of the implicit scheme requires the solution of a matrix equation at each time-step, rather than an algebraic equation as in (3). In the 1D case, this is not difficult as the equations are in a tridiagonal form. However, the numerical solution of the equations for the implicit scheme is much harder in higher dimensions.

Apart from the stability criterion, there are also numerical errors introduced by the approximation of derivatives by their difference forms in (3) and (7). Thus, these schemes give good approximations for solutions of (2) only for very small Δt, Δx values (e.g. $\Delta t \approx O(0.002)$ and $\Delta x \approx O(0.1)$ for the explicit scheme). However, it is worth noting that qualitatively correct solutions can be obtained for higher mesh sizes. These are not accurate numerically but they reproduce the correct qualitative features, which is often enough for most physical applications.

Recently, Oono and Puri [6] have proposed a new numerical scheme for reaction-diffusion equations. In this new scheme, the homogeneous part of (1) is integrated (analytically or numerically). The solution thus obtained is used to define the evolution scheme for (1). We demonstrate the usage of this scheme by applying it to (2). Thus, the homogeneous part of (2) is

$$du/dt = u(1-u). \tag{9}$$

This can be solved analytically as (say)

$$u(t+\Delta t) = \frac{u(t)}{u(t)+[1-u(t)]\exp(-\Delta t)} \equiv F_{\Delta t}(u(t)). \tag{10}$$

Then, the evolution scheme proposed by Oono and Puri [6] takes the form

$$u(x, t+\Delta t) = F_{\Delta t}(u(x, t)) + \alpha[u(x+\Delta x, t) - 2u(x, t) + u(x-\Delta x, t)] \tag{11}$$

where α has the same meaning as previously, namely $\alpha = \Delta t/(\Delta x)^2$. This scheme is claimed (by Oono and Puri [6]) to have two major advantages over conventional schemes (like (3) and (7)) as follows.

(i) It gives the exact solution in the homogeneous case, by construction. This is not true for conventional schemes (like (3) and (7)).

(ii) For large values of Δt, conventional schemes (like (3) and (7)) exhibit oscillatory (or chaotic) behaviour in the local mapping. This causes spurious results and limits the value of Δt for which accurate simulations are possible. In the new scheme, the local mapping is always one-to-one and can never be oscillatory (or chaotic), regardless of the value of Δt. Thus, the new scheme can be used with much higher values of Δt then the conventional schemes, enabling a more efficient simulation.

The first claim is trivially seen to be correct. However, the second claim is not quite accurate. For the specific case of the Fisher equation, the local mapping in (3) or (7) shows oscillatory (or chaotic) behaviour for $\Delta t > 2$. But, for $\Delta t > 2$, both (3) and (7) are unstable (as we have already seen). Thus, it is not possible to perform a simulation with a value of Δt for which the local mapping in (3) or (7) is oscillatory (or chaotic). (Actually, this is a more general result. For the reaction-diffusion equation (1), the value of Δt at which the local mapping (in the corresponding explicit or implicit scheme) becomes oscillatory is the same as the value of Δt for which the scheme becomes unstable. This is because both of these result from the same source, namely the destabilization of the fixed point in the local mapping.) However, the second claim of Oono and Puri [6] is still valid in the sense that the new scheme gives qualitatively correct results for the Fisher equation for $\Delta t > 2$. (We will shortly present results which demonstrate this.) Thus, we can gainfully use the new scheme for values of Δt which are too large (because of instability rather than locally oscillatory behaviour) for the conventional schemes.

Before we present our numerical results, consider the results of a linear stability analysis (about $u_0 = 1$) for (11). This yields

$$\delta u(k, t+\Delta t) = [\exp(-\Delta t) - 4\alpha \sin^2(k\Delta x/2)]\delta u(k, t) \tag{12}$$

where all symbols have the same meaning as previously. For (11) to be stable, we must have

$$\alpha \leqslant (1+\exp(-\Delta t))/4 \tag{13}$$

which can always be satisfied, regardless of the value of Δt. Thus, the instability in the local mapping has disappeared because of the introduction of the exact solution for the homogeneous case. (Notice that a 'new implicit' scheme, in which spatial derivatives are taken at time $t+\Delta t$ rather than at time t, has the further advantage of being unconditionally stable. However, we do not wish to introduce the added complication of solving a matrix equation at each time step.)

For our numerical results (presented below), we need the exact solution of the Fisher equation. The analytic form of this exact solution is unknown, as mentioned earlier. We numerically found the 'exact' solution of the Fisher equation by iterating (3) with a step function initial condition, namely

$$\begin{aligned} u(x, 0) &= 1 \qquad \text{if } x \leqslant x_0 \\ &= 0 \qquad \text{if } x > x_0 \end{aligned} \tag{14}$$

where x_0 is the location of the step. For the Fisher equation, this initial condition is expected [8] to converge to the $v = 2$ cline solution. Numerically, we found this cline solution by using (3) with $\alpha = 0.1$ (fixed) and by reducing Δt till there is no change in the numerical solution on further reduction of Δt. This was found to occur for $\Delta t = 0.00025$ and $\Delta x = 0.05$. With these mesh sizes, we iterate (3) with the initial condition (14). The profile obtained after 0.05 time units (200 iterations) is taken as the 'exact' solution profile and is denoted by $u_e(x, 0)$. This profile then translates as a travelling wave with $v = 2$ and we denote this by $u_e(x, t)$.

Figure 1 shows the results obtained in a simulation using the new scheme with $\Delta t = 3.364$, $\Delta x = 5.8$ and lattice size $N = 50$. We compare (for times 25, 50 and 75) the results obtained using the new scheme (shown by a full curve) with the 'exact' solution $u_e(x, t)$ (shown by a broken curve). The initial condition used in the simulation of (11) is the 'exact' solution profile $u_e(x, 0)$ obtained as described earlier. These results show that, even for a very high value of Δt (for which (3) and (7) are unstable), a reasonable simulation is possible using the new scheme. In figure 1, it is interesting to note that the shape of the solution obtained using the new scheme is approximately the same as that of the 'exact' solution. The only difference is that the asymptotic velocity of the solution from the new scheme is somewhat less than 2, the theoretically predicted asymptotic velocity for the 'exact' solution [8]. We are currently studying the dependence of the asymptotic velocity (of solutions obtained using the new scheme) on the time increment Δt.

A quantitative estimate of the error in the simulation is obtained by considering the 'distance function' $d[u, u_e]$ defined by

$$d[u, u_e] = \sum_x [u(x, t) - u_e(x, t)]^2 \tag{15}$$

where x is defined on the lattice. The rate of increase of this distance gives a measure of the numerical inaccuracy. Figure 2 shows the distance $d[u, u_e]$ as a function of time for the previous case. The major contribution to this 'distance function' is from the drifting apart of the result obtained using the new scheme from the 'exact' solution.

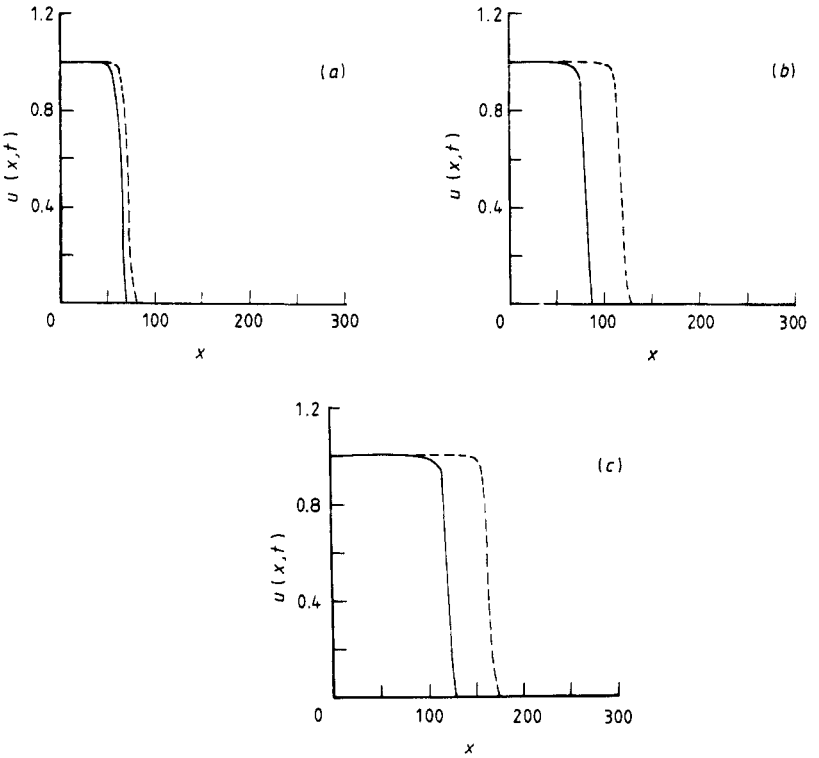

Figure 1. Numerical results for the 1D Fisher equation, obtained using the new scheme with $\Delta t = 3.364$, $\Delta x = 5.8$ and lattice size $N = 50$. We compare results from the new scheme (shown by a full curve) with the 'exact' solution $u_e(x, t)$ (shown by a broken curve) at times (*a*) 25, (*b*) 50 and (*c*) 75. The initial condition for the simulation is the 'exact' solution profile $u_e(x, 0)$.

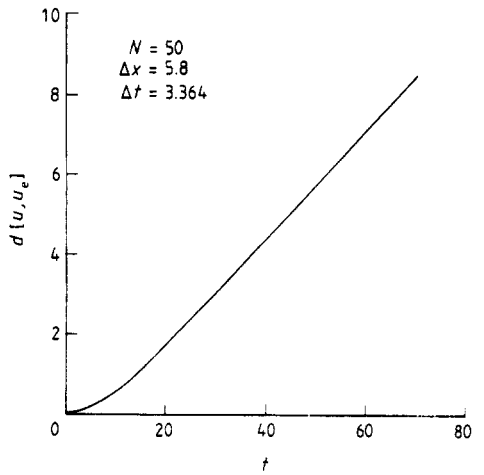

Figure 2. Time dependence of 'distance function' $d[u, u_e]$ for the numerical solution shown in figure 1.

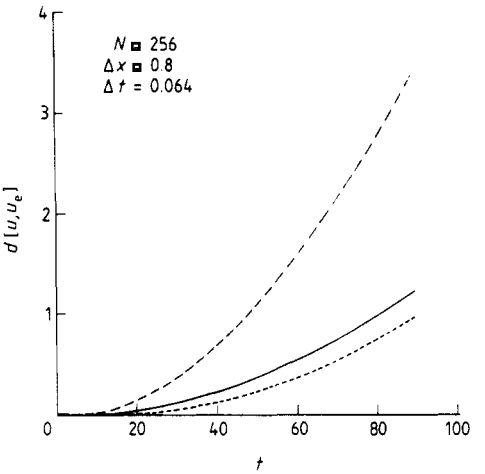

Figure 3. Time dependence of 'distance function' $d[u, u_e]$ for numerical solutions from the conventional (broken curve), implicit (dotted curve) and new (full curve) schemes with $\Delta t = 0.064$, $\Delta x = 0.8$ and $N = 256$. Again, the initial condition for these simulations is the 'exact' solution profile $u_e(x, 0)$.

It is also of interest to compare the results from (3), (7) and (11) for $\Delta t < 2$. Figure 3 shows $d[u, u_e]$ as a function of time for (3) (denoted by a broken curve), (7) (denoted by a dotted curve) and (11) (denoted by a full curve) for $\Delta t = 0.064$, $\Delta x = 0.8$ and $N = 256$. Again, the initial condition used in these simulations is the 'exact' profile $u_e(x, 0)$. Figure 3 shows that (numerical error-wise) the implicit scheme is somewhat better behaved than the new scheme and both of these are much better behaved than the explicit scheme. This is true for all $\Delta t < 2$.

A comparison of figures 2 and 3 gives an idea of the numerical inaccuracy introduced by increasing the mesh size. Thus, the 'distance function' $d[u, u_e]$ for the new scheme with $\Delta t = 3.364$, $\Delta x = 5.8$ (figure 2) is only about ten times larger (at comparable times) than the corresponding $d[u, u_e]$ for the new scheme with $\Delta t = 0.064$, $\Delta x = 0.8$ (denoted by a full curve in figure 3), even though the value of Δt in figure 2 is about fifty times larger than that in figure 3. This, coupled with the robustness of the shape of the interfacial profile against the increase of Δt, indicates that a qualitatively correct simulation of the Fisher equation is possible at high values of Δt if we use the new scheme of Oono and Puri [6].

To summarize: we have applied a new numerical scheme proposed by Oono and Puri [6] to the 1D Fisher equation. We find that this new scheme gives reasonable results for high values of Δt (>2), where the conventional schemes are not applicable because they are unstable. For $\Delta t < 2$, the implicit scheme is marginally better behaved than the new scheme. However, the ease of implementation of the new scheme makes it more attractive than the implicit scheme, at least for dimensions higher than 1.

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