COMMENTS

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Comment on ''Study of phase-separation dynamics by use of cell dynamical systems. I. Modeling''

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The cell dynamical systems method of Oono and Puri [Phys. Rev. A **38**, 434 (1988)] for modeling phase-ordering dynamics is reexamined. We show how some rather puzzling features of this method can be analyzed on the basis of its relation to conventional partial differential equations. [S1063-651X(97)03702-1]

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A few years ago an alternative method was proposed for modeling the phase-ordering and phase-separation dynamics of thermodynamically unstable systems [1]. This scheme, later called the cell dynamical system (CDS) method [2,3], is no less realistic, and computationally more efficient, than the more usual analytical formulation in terms of partial differential equations (PDEs) [4,5]. This allows easier exploration of the late-time regime of phase ordering or spinodal decomposition, which is the focus of much current research aimed at verifying several dynamical scaling hypotheses [4,6]. Furthermore, it has been shown that the CDS method has essentially the same dynamical scaling properties as the Cahn-Hilliard (CH) equation [7–13] and is therefore a reliable tool for their elucidation [14–16].

However, the very success of the CDS approach remains somewhat mysterious. It has been described as a semigroup discretization of the CH equation that allows a far larger time step to be used in the numerical integration than the usual finite-difference schemes [2,17]. In this context, different time and space increments correspond to different solution semigroups, which, in turn, are determined by different free-energy functionals. In the limit of small increments the method reduces to the simplest Euler scheme; nevertheless, it seems to be successful even when increments are larger than allowed by stability analysis (see below). Hence general properties such as structure factors seem to be fairly independent of the form of the free-energy [18]. In particular, it has been noted that the usual formulation of the CDS model can be interpreted as governed by an underlying PDE of the CH type associated with a modified free-energy functional [16]. Moreover, the rather surprising forms of the discrete CDS Laplacians have received some justification [19,20], but have not, to our knowledge, been studied in detail.

In this Comment we show that the CDS equations do indeed formally reduce to the usual CH equation in a very simple way, which, we believe, had not been fully appreciated before. In addition, we shall argue that isotropy could be further improved by using a Laplacian containing only nearest neighbors on a *triangular*, rather than square, two-dimensional (2D) lattice. Finally, we investigate the stability of different discrete 2D Laplacians [21].

Let us consider the fundamental equations of the CDS method [1,2], where time and space are measured in units of time step and mesh size, respectively:

$$\psi(\mathbf{r},t+1)=\mathcal{F}[\psi(\mathbf{r},t)]-\langle\langle\mathcal{F}[\psi(\mathbf{r},t)]-\psi(\mathbf{r},t)\rangle\rangle, \quad (1)$$

$$\mathcal{F}[\psi(\mathbf{r},t)]=f(\psi(\mathbf{r},t))+D[\langle\langle\psi(\mathbf{r})\rangle\rangle-\psi(\mathbf{r},t)], \quad (2)$$

where $f(x)$ is the nonlinear map (which we leave unspecified for the moment); $\langle\langle * \rangle\rangle - *$ is the isotropized discrete ''Laplacian'' on a square lattice, with

$$\langle\langle\psi(\mathbf{r},t)\rangle\rangle=\frac{1}{6}\sum_{i\in\{\mathrm{NN}\}}\psi(\mathbf{r}_i,t)+\frac{1}{12}\sum_{i\in\{\mathrm{NNN}\}}\psi(\mathbf{r}_i,t), \quad (3)$$

NN and NNN denoting nearest and next-nearest neighbors, respectively; and D sets the time scale of phase separation. This last quantity is identified with the phenomenological diffusion constant [2]. Subtracting $\psi(\mathbf{r},t)$ from both sides of Eq. (1) and making the identifications $\psi(\mathbf{r},t+1)-\psi(\mathbf{r},t)\approx\partial\psi(\mathbf{r},t)/\partial t$, $\langle\langle * \rangle\rangle - * \approx \nabla^2 *$, we immediately obtain

$$\frac{\partial\psi}{\partial t}=\nabla^2\psi-\nabla^2[f(\psi)+D\nabla^2\psi]. \quad (4)$$

This reduces to the CH equation in nondimensional form [26] if $2\psi-2f(\psi)=-\psi+\psi^3$ and $D=\frac{1}{2}$, whence

$$f(\psi)=\frac{3}{2}\psi-\frac{1}{2}\psi^3, \quad (5)$$

which is just $\frac{3}{2}\tanh\psi$ to order ψ^3. Now the preferred form of the map in Oono and Puri's original papers [1–3] is $f_1(\psi)=A\tanh\psi$, with $A=1.3$ and $D=0.5$ ($A=1.5$ in later, 3D, work [20]). An alternative choice [see [2], Eq. (2.11)] is $f_3(\psi)=A\psi/[1+\psi^2(A^2-1)]^{1/2}$; for small ψ and $A=1.3$, $f_3(\psi)\approx 1.3\psi-0.4485\psi^3$, again not very far from Eq. (5).

Also note that setting $D=0$ transforms Eq. (4) into a nonlinear diffusion equation and need not lead to a freezing of the dynamics. Thus the identification of D with a diffusion constant appears less than warranted.

Consider now the discrete Laplacian, Eq. (3). This rather unconventional form is dictated by the requirement that patterns should be as isotropic as possible in order to yield good scaling of the structure factors [1–3,19,20]. To see this in a more systematic way, let us write down several different versions of the discretized Laplacian in Fourier space $\Gamma(k)$. In all that follows we restrict ourselves to two dimensions: (i) the usual five-point star (5P) (see [22], Eq. 25.3.30) on the square lattice, NN only:

$$\begin{aligned}\Gamma_{5\mathrm{P}}(k)&=\frac{2}{(\Delta x)^2}[\cos(k_x\Delta x)+\cos(k_y\Delta x)-2]\\&=-(k_x^2+k_y^2)+\frac{(\Delta x)^2}{3}(k_x^2+k_y^2)^2\\&\quad-\frac{2(\Delta x)^2}{3}k_x^2k_y^2+O(k^6);\end{aligned}\tag{6}$$

(ii) the 9-point star (9P) (see [22], Eq. 25.3.31) on the square lattice, NN and NNN along axes:

$$\begin{aligned}\Gamma_{9\mathrm{P}}(k)&=\frac{1}{(\Delta x)^2}\left\{\frac{8}{3}[\cos(k_x\Delta x)+\cos(k_y\Delta x)]\right.\\&\quad\left.-\frac{1}{6}[\cos(2k_x\Delta x)+\cos(2k_y\Delta x)]-5\right\}\\&=-(k_x^2+k_y^2)+O(k^6);\end{aligned}\tag{7}$$

(iii) Oono and Puri's choice (OP), Eq. (3), on the square lattice, NN and NNN with relative weights 1 and $\frac{1}{2}$ [23]:

$$\begin{aligned}\Gamma_{\mathrm{OP}}(k)&=\frac{1}{2(\Delta x)^2}\{2\cos(k_x\Delta x)+2\cos(k_y\Delta x)\\&\quad+\cos[(k_x+k_y)\Delta x]+\cos[(k_x-k_y)\Delta x]-6\}\\&=-(k_x^2+k_y^2)+\frac{(\Delta x)^2}{12}(k_x^2+k_y^2)^2\\&\quad+\frac{(\Delta x)^2}{12}k_x^2k_y^2+O(k^6);\end{aligned}\tag{8}$$

(iv) the triangular lattice (tri), NN only:

$$\begin{aligned}\Gamma_{\mathrm{tri}}(k)&=\frac{2}{3(\Delta x)^2}\left[2\cos(k_x\Delta x)+2\cos\left(\frac{1}{2}k_x\Delta x+\sqrt{\frac{3}{2}}k_y\Delta x\right)\right.\\&\quad\left.+2\cos\left(\frac{1}{2}k_x\Delta x-\sqrt{\frac{3}{2}}k_y\Delta x\right)-6\right]\\&=-k_x^2+k_y^2-\frac{(\Delta x)^2}{16}(k_x^2+k_y^2)^2+O(k^6),\end{aligned}\tag{9}$$

where Δx is the mesh size. Although Oono and Puri's form is more isotropic than the ''naive'' five-point star, both are inferior to the Laplacian containing only nearest neighbors on the triangular lattice, which is isotropic to order k^4 due to the higher symmetry of that lattice. OP is in fact the projection onto two dimensions of the Laplacian containing only nearest neighbors on the face-centered hypercubic lattice, as used in lattice-gas [24] and lattice-Boltzmann [25] simulations, where the choice of a sufficiently isotropic lattice is essential for recovering the correct hydrodynamic behavior. However, the nine-point star on the square lattice also performs quite well; we will discuss this further below.

Rogers *et al.* [26] have investigated the stability of the Euler-discretized CH equation with respect to time step and mesh size. Their analysis is based on Fourier-transforming the linearized equation and therefore carries through with minor changes: basically only the discrete Laplacians will be different. The linearized CDS equation with the tanh map is, from Eq. (4),

$$\frac{\partial\psi}{\partial t}=\nabla^2[(1-A)\psi-D\nabla^2\psi].\tag{10}$$

Note that, *for stability considerations*, the detailed form of the map $f(\psi)$ is irrelevant beyond the linear term. We also naturally recover the CDS requirement that $A>1$. The condition for the subharmonic bifurcation now becomes [see [26], Eq. (3.9)]

$$(1-A)\Delta t\Gamma(k)-D\Delta t\Gamma^2(k)<-2,\tag{11}$$

where Δt is the time step used in the numerical integration. It then follows that the subharmonic bifurcation can be avoided, for all k modes, by maintaining the inequalities

$$\Delta t<\frac{(\Delta x)^4}{32D-4(A-1)(\Delta x)^2}\quad(5\mathrm{P}),\tag{12}$$

$$\Delta t<\frac{(\Delta x)^4}{50D-5(A-1)(\Delta x)^2}\quad(9\mathrm{P}),\tag{13}$$

$$\Delta t<\frac{(\Delta x)^4}{18D-3(A-1)(\Delta x)^2}\quad(\mathrm{OP}),\tag{14}$$

$$\Delta t<\frac{(\Delta x)^4}{32D-4(A-1)(\Delta x)^2}\quad(\mathrm{tri}).\tag{15}$$

For $A=1.3$, $D=0.5$, and $\Delta x=1.0$ as before, this gives $\Delta t<0.067$ (5P and tri), $\Delta t<0.042$ (9P), and $\Delta t<0.12$ (OP). Indeed OP has the best stability properties, i.e., admits the largest time step, for a given choice of A, D, and Δx. Conversely, for values of Δt and Δx that do not satisfy the above stability requirements, as is the case in most CDS modeling, OP leads to the least severe violation. On the other hand, the nine-point Laplacian requires the smallest time step and is perhaps less convenient for extensive numerical work, in spite of its excellent isotropy.

We have investigated some of the features of the CDS method by exploring its relation to PDEs. It appears that the form of the CDS Laplacian can be best justified by its better stability properties, but it should be possible to improve isotropy by going to a triangular lattice.

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