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

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The comments by Teixeira and Mulder [preceding paper, Phys. Rev. E **55**, 3789 (1997)] on the cell dynamics schemes are augmented with respect to (1) the relation between the cell dynamics scheme and the partial differential equation, (2) the optimal form of the discretized Laplacian, and (3) the stability of the scheme. [S1063-651X(97)03802-6]

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The comments by Teixeira and Mulder [1] are all constructive, so that I do not have anything to ''respond'' against them, but wish to add some remarks or to augment their comments on the following three points: (1) the relation between the cell dynamics scheme (CDS) and the partial differential equation (PDE), (2) the optimal form of the discretized Laplacian, and (3) the stability of the scheme.

(1) When the increments are small, the scheme is a simple Euler scheme, as can be seen by inspection and as is noted in the preceding paper. The main question is why the CDS works even if the increments are large. In the case of spinodal decomposition, I explain this with the universality of the form factors [2]. Increasing the time increment size corresponds to modifying the free-energy functional form. However, the form factors and other observables I am interested in are invariant under this change (this invariance is, however, not proved but only numerically empirical). In the actual simulation it is convenient to exploit this universality to use a map whose metastable region is as small as possible [3], as mentioned below.

(2) The idea proposed in Ref. [1] to use the most symmetric regular lattice in d-space is an excellent one. I have chosen the simplest lattice system in d-space, anticipating (hyper)cubically connected parallel processors. It should be noted that I did not arrive at the proposed discretization of the Laplacian from the PDE side. Rather, I wished to capture the spherical mean value theorem for harmonic functions as much as possible. The needed sphericity depends on the length of the simulation. Our choice in 3-space is admissible for up to 100,000 steps, but not expected to be reliable beyond this order.

(3) A comparison of the stability of various Laplacian discretizations is useful. It should be noted that in the actual CDS simulations the subharmonic stability condition is always satisfied, as is already noted in Ref. [4]. When a CDS model is written in the form of Eqs. (1) and (2) in Ref. [1], the existence of the proportionality constant c in $\langle\langle *\rangle\rangle - * = c\nabla^2 *$ should not be forgotten. For example, for the simple cubic lattice approximation in d-space (such as the five-point star in Ref. [1]), the proportionality constant is $1/2d$. In 2-space our choice (Oono and Puri's choice in Ref. [1]) is with the proportionality constant 1/6. These scaling factors effectively reduce D and increase Δt. Hence $\Delta x = \Delta t = 1$ is stable for $D = 0.5$ and $A = 1.3$ [4]. The stability analysis of the 3-space CDS model has been done in Ref. [3]. As has been noted there, the stability condition in the already segregated domain is less stringent than the condition around the zero solution. Needless to say, stability does not guarantee the reliability of a scheme. We still need a consideration on the reliability as mentioned in Ref. [1] above.

Finally, I wish to add a comment on simulations of binary fluid [3]. In this case, choosing large increments can cause registering of the interfaces to lattice planes if not very isotropic schemes are chosen. This tendency is enhanced if the metastable region of the phase diagram corresponding to the chosen map is wide. Hence the practical advice to accelerate fluid simulations is to (1) use a reasonably sphericalized Laplacian and (2) choose a map whose spinodal curve is as close as possible to the coexistence curve (exploiting the universality mentioned above). A similar advice should be effective for PDE simulations as well. Perhaps a good example exhibiting the state of the art of CDS is Ref. [5].

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