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Isotropic averaging for cell-dynamical-system simulation of spinodal decomposition

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Abstract. Formulae have been developed for the isotropic averagings in two and three dimensions. Averagings are employed in the cell-dynamical-system simulation of spinodal decomposition for inter-cell coupling. The averagings used in earlier works on spinodal decomposition have been discussed.

Keywords. Isotropic numerical scheme; spinodal decomposition.

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1. Introduction

The paper deals with formula for averaging of a function. Averagings are used in the cell-dynamical-system (CDS) simulation of spinodal decomposition to achieve the inter-cell coupling. An averaging in two dimensions is proposed in [1], which has also been employed by others [2]. On the other hand, various averagings have been employed in three dimensions [3].

We first show that the average of a function over the surface of an n-dimensional 'sphere' around a point, is related to its Laplacian. An averaging formula can therefore be said to be consistent if it leads to discretisation of the Laplacian as given by the above relation. A consistent averaging is necessary to relate the CDS simulations to other simulations, such as a finite-difference simulation. The above relation has been used here to obtain isotropic (rotationally symmetric) averagings in two and three dimensions.

2. A consistency relation

Let $x_1, x_2, \ldots, x_n$ be the coordinates in n-dimension. The average of a function ψ over the surface $\partial\Omega$ of the n-dimensional 'sphere' of radius ε around a point P_0, where ε is small, is obtained from its surface integral,

$$\bar{\psi_0} = \oint_{\partial\Omega} \psi \mathrm{d}s \Big/ \oint_{\partial\Omega} \mathrm{d}s. \tag{1}$$

From a Taylor expansion, ψ in the neighbourhood of the point P_0 is written as

$$\psi = \psi_0 + \sum_{i=1}^{n} \left(\frac{\partial \psi}{\partial x_i}\right)_0 x_i + \frac{1}{2}\sum_{i=1}^{n} \left(\frac{\partial^2 \psi}{\partial x_i^2}\right)_0 x_i^2 + \sum_{\substack{i,j=1 \\ i<j}}^{n} \left(\frac{\partial^2 \psi}{\partial x_i \partial x_j}\right)_0 x_i x_j + \mathrm{HOT},$$

where the suffix 0 refers to the point P_0 and x_i are the coordinates with respect to P_0, and HOT stands for higher order terms. Substituting the above in (1) we get

$$\bar{\psi_0} = \psi_0 + \frac{1}{2}\sum_{i=1}^{n} \left(\frac{\partial^2 \psi}{\partial x_i^2}\right)_0 \oint_{\partial\Omega} x_i^2 \mathrm{d}s \Big/ \oint_{\partial\Omega} \mathrm{d}s + \mathrm{HOT}.$$

In order to evaluate the integral in the above equation, we express the variables $x_1, x_2, \ldots, x_n$ on the surface of the 'sphere' in terms of the angles $\theta_1, \theta_2, \ldots, \theta_{n-1}$, by

$$\begin{aligned}
x_1 &= \varepsilon \cos\theta_1 \\
x_2 &= \varepsilon \sin\theta_1 \cos\theta_2 \\
x_3 &= \varepsilon \sin\theta_1 \sin\theta_2 \cos\theta_3 \\
&\vdots \\
x_{n-1} &= \varepsilon \sin\theta_1 \sin\theta_2 \ldots \sin\theta_{n-2} \cos\theta_{n-1} \\
x_n &= \varepsilon \sin\theta_1 \sin\theta_2 \ldots \sin\theta_{n-2} \sin\theta_{n-1}.
\end{aligned}$$

The expression

$$\oint_{\partial\Omega} x_1^2 \mathrm{d}s \Big/ \oint_{\partial\Omega} \mathrm{d}s = \frac{2^n \varepsilon^{n+1} \int_0^{\pi/2} \ldots \int_0^{\pi/2} \cos^2\theta_1 \sin^{n-2}\theta_1 \sin^{n-3}\theta_2 \ldots \sin\theta_{n-2} \mathrm{d}\theta_1 \mathrm{d}\theta_2 \ldots \mathrm{d}\theta_{n-1}}{2^n \varepsilon^{n-1} \int_0^{\pi/2} \ldots \int_0^{\pi/2} \sin^{n-2}\theta_1 \sin^{n-3}\theta_2 \ldots \sin\theta_{n-2} \mathrm{d}\theta_1 \mathrm{d}\theta_2 \ldots \mathrm{d}\theta_{n-1}}$$

is simplified by using the relation [4]

$$\int_0^{\pi/2} \sin^m\theta \cos^n\theta \mathrm{d}\theta = \frac{\Gamma(\frac{m+1}{2})\Gamma(\frac{n+1}{2})}{2\Gamma(\frac{m+n}{2}+1)},$$

which gives

$$\begin{aligned}
\oint_{\partial\Omega} x_1^2 \mathrm{d}s \Big/ \oint_{\partial\Omega} \mathrm{d}s &= \frac{2\varepsilon^{n+1}\pi^{n/2}}{n\Gamma(n/2)} \Big/ \frac{2\varepsilon^{n-1}\pi^{n/2}}{\Gamma(n/2)} \\
&= \varepsilon^2/n.
\end{aligned}$$

Equation (1) therefore leads to

$$\bar{\psi}_0 = \psi_0 + \frac{\varepsilon^2}{2n}\left(\nabla^2\psi\right)_0 + \text{HOT}. \tag{2}$$

The average of ψ over the surface of the 'sphere' is thus related to its Laplacian.

Equation (2) can be used to check the consistency of an averaging formula. An averaging is seen to be related to the discretisation of the Laplacian by

$$\left(\nabla^2\psi\right)_0 = \frac{2n}{h^2}\left(\bar{\psi}_0 - \psi_0\right),$$

where h is the unit step size, the smallest length scale in the computational problem. We find that the averaging formula given in [1] is not consistent with any discretisation of the Laplacian. Similarly, the averagings in three dimensions used in [3] are also not consistent.

Equation (2) can also be used to obtain an averaging formula from a discretisation of the Laplacian. Consistent isotropic averagings in two and three dimensions are obtained below.

3. Isotropic averaging in two dimensions

We consider the following discretisations of the Laplacian:

$$(\nabla^2_{\text{NN}}\psi)_0 = \frac{1}{h^2}\left(\sum_{\text{NN}}\psi_i - 4\psi_0\right),$$

$$(\nabla^2_{\text{NNN}}\psi)_0 = \frac{1}{2h^2}\left(\sum_{\text{NNN}}\psi_i - 4\psi_0\right),$$

where NN stands for the four 'next-neighbour' points along the axes, NNN for the four 'next-next-neighbour' points along the diagonals, and h the unit step size. From a Taylor expansion we see that the discretisation

$$(\nabla^2_I\psi)_0 = \alpha(\nabla^2_{\text{NN}}\psi)_0 + \beta(\nabla^2_{\text{NNN}}\psi)_0,$$

where $\alpha + \beta = 1$, represents

$$(\nabla^2_I\psi)_0 = (\nabla^2\psi)_0 + \frac{h^2}{12}(\nabla^4\psi)_0 + \text{HOT}$$

for $\beta = 1/3$, and hence it is isotropic up to $O(h^2)$. Its expanded form is,

$$(\nabla^2_I\psi)_0 = \frac{1}{6h^2}\left(4\sum_{\text{NN}}\psi_i + \sum_{\text{NNN}}\psi_i - 20\psi_0\right). \tag{3}$$

The above discretisation of the Lapalacian has been employed in the literature [5].

The isotropic averaging in two dimensions, from (2) and (3), is given by

$$\bar{\psi}_0 = \frac{1}{6}\psi_0 + \frac{1}{6}\sum_{\text{NN}}\psi_i + \frac{1}{24}\sum_{\text{NNN}}\psi_i. \tag{4}$$

Note that the isotropic averaging formula for $\bar{\psi}$ at the point P_0, given by (4), also involves the value of ψ at P_0.

4. Isotropic averaging in three dimensions

Similar to two dimensions, we consider the following discretisations of the Laplacian in three dimensions:

$$(\nabla^2_{\mathrm{NN}}\psi)_0 = \frac{1}{h^2}\left(\sum_{\mathrm{NN}}\psi_i - 6\psi_0\right),$$

$$(\nabla^2_{\mathrm{NNN}}\psi)_0 = \frac{1}{4h^2}\left(\sum_{\mathrm{NNN}}\psi_i - 12\psi_0\right),$$

$$(\nabla^2_{\mathrm{NNNN}}\psi)_0 = \frac{1}{4h^2}\left(\sum_{\mathrm{NNNN}}\psi_i - 8\psi_0\right),$$

where, in three dimensions, NN stands for the six 'next-neighbour' points along the axes, NNN for the twelve 'next-next-neighbour' points along the edges of the finite-difference stencil, and NNNN for the eight 'next-next-next-neighbour' points at the corners of the stencil. We consider the discretisation

$$(\nabla^2_I\psi)_0 = \alpha(\nabla^2_{\mathrm{NN}}\psi)_0 + \beta(\nabla^2_{\mathrm{NNN}}\psi)_0 + \gamma(\nabla^2_{\mathrm{NNNN}}\psi)_0,$$

where $\alpha+\beta+\gamma=1$. From a Taylor expansion the above can be shown to represent

$$(\nabla^2_I\psi)_0 = (\nabla^2\psi)_0 + \frac{h^2}{12}(\nabla^4\psi)_0 + \mathrm{HOT}$$

for $\beta+2\gamma=2/3$. We then have one parameter family of isotropic discretisation of the Laplacian. The parameter γ can be chosen, e.g., to maximise the stability limit of the diffusion equation $\partial\psi/\partial t = \nabla^2\psi$, which gives $0 \le \gamma \le 1/12$. The cases $\gamma = 0$ and 1/12 are considered below.

4.1 *Case*: $\gamma = 0$

For $\gamma = 0$ we get the 19-point discretisation,

$$(\nabla^2_I\psi)_0 = \frac{1}{6h^2}\left(2\sum_{\mathrm{NN}}\psi_i + \sum_{\mathrm{NNN}}\psi_i - 24\psi_0\right).$$

The above 19-point discretisation is considered in [6]. The corresponding isotropic averaging is

$$\bar{\psi_0} = \frac{1}{3}\psi_0 + \frac{1}{18}\sum_{\mathrm{NN}}\psi_i + \frac{1}{36}\sum_{\mathrm{NNN}}\psi_i.$$

4.2 *Case*: $\gamma = 1/12$

For $\gamma = 1/12$, we get the 27-point discretisation,

$$(\nabla_I^2\psi)_0 = \frac{1}{48h^2}\left(20\sum_{\mathrm{NN}}\psi_i + 6\sum_{\mathrm{NNN}}\psi_i + \sum_{\mathrm{NNNN}}\psi_i - 200\psi_0\right).$$

The corresponding isotropic averaging is

$$\bar{\psi_0} = \frac{11}{36}\psi_0 + \frac{5}{72}\sum_{\mathrm{NN}}\psi_i + \frac{1}{48}\sum_{\mathrm{NNN}}\psi_i + \frac{1}{288}\sum_{\mathrm{NNNN}}\psi_i.$$

5. Conclusions

The average of a function over the surface of an n-dimensional 'sphere' around a point is shown to be related to its Laplacian. This relation has been used to develop isotropic averagings from the isotropic discretisations of the Laplacian in two and three dimensions. Because of the absence of numerical anisotropy, these formulae can provide a better understanding of the research issues in spinodal decomposition.

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