Numerical Simulation of Mesoscale Patterns Using Maximum Entropy Method for the Boundary Condition

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ソフトマターなどのように複雑な空間構造を有する系を計算機で探索するにあたり、その大きな障害となるものの一つが境界条件である。系の自発的な空間秩序に抵触しない境界条件を開発することが、複数の特徴的長さを持つ高次の空間構造を探る上で不可欠である。本研究は、バルクの情報を元にして最大エントロピー法 (MEM) によって空間パターンのフーリエ級数の振幅を求め、境界部分の情報を外挿するものである。この方法は従来の方法の弱点を原理的に克服する。今回は、バルクの情報を入力として与えたときに、MEM によって出力した外挿が適切であることを示す。

1 Introduction

When performing numerical simulation to study spatial structures of soft condensed matters, the treatment of the boundary condition is one of the most difficult problems. Suppression of the finite size effect is an essential mission to equilibrate complex structures with multiple intrinsic lengthscales. Parrinello and Rahman [1] developed a constant pressure numerical scheme by adjusting the size and shape of the simulation box using the periodic boundary condition. Such a method is successful in reproducing patterns with a single periodicity, but is not compatible for the systems with multiple incommensurate periods. Another solution is to introduce a specially modified dynamic equation for the boundary sites [2]. However, the validity of this method is limited to nearly equilibrium systems.

Here we propose an alternative boundary scheme making use of maximum entropy method (MEM). The MEM gives the most probable Fourier spectrum of the whole system, with which we can calculate the information of the boundary sites. In this presentation, we demonstrate that the extrapolated boundary information (output) reasonably reproduces the original bulk information (input).

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2 Method and Result

As a simple example, we consider a single order parameter ψ. The bulk region (denoted as $\mathbf{B}$) and the boundary region (denoted as $\mathbf{b}$) areas are defined in Fig.1. Our mission is to estimate the most probable information $\bar{\psi}(\mathbf{r} \in \mathbf{B} \cup \mathbf{b})$ from the bulk information $\psi(\mathbf{r} \in \mathbf{B})$. We introduce the following MEM free energy

$$F_{\mathrm{MEM}} = \frac{1}{2\delta^2} \int_{\mathbf{B}} d\mathbf{r} \, |\psi - \bar{\psi}|^2 + \frac{1}{2} \sum_{\mathbf{k}_c} \alpha^c_{\mathbf{k}_c} c^2_{\mathbf{k}_c} + \frac{1}{2} \sum_{\mathbf{k}_s} \alpha^s_{\mathbf{k}_s} s^2_{\mathbf{k}_s}$$
$$\left(\bar{\psi} = \sum_{\mathbf{k}_c} c_{\mathbf{k}_c} \cos \mathbf{k}_c \cdot \mathbf{r} + \sum_{\mathbf{k}_s} s_{\mathbf{k}_s} \sin \mathbf{k}_s \cdot \mathbf{r} \right), \tag{1}$$

and minimize this free energy. Here the first term is a penalty for the difference between ψ and $\bar{\psi}$ with an error scale δ, and the second and third terms are entropy associated with the uncertainty of pridiction of the structure outside the bulk area. The set of planar wave modes $\{\mathbf{k}_c, \mathbf{k}_s\}$ is determined according to the bulk Fourier spectrum. This kind of MEM free energy form and the value of the entropy coefficients $\alpha^c_{\mathbf{k}_c}, \alpha^s_{\mathbf{k}_s}$can be derived using the Gaussian random field model [3]. By choosing an appropriate set of $\{\alpha^c_{\mathbf{k}_c}, \alpha^s_{\mathbf{k}_s}\}$, we find that the extrapolation of the order parameter towards outside of the bulk works for various typs of the input bulk morphologies, such as a Model-A-like disordered pattern, a lamellar structure with a single periodicity, and a checkerboard pattern.

In this work, we have confirmed the efficiency of the MEM approach to the boundary condition problem for static structures. Our next study shall be directed to dynamic patterns envolving time.

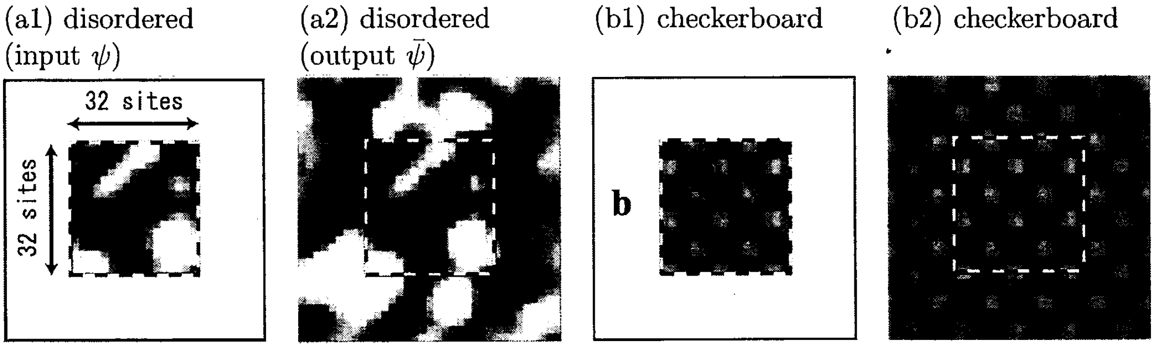

Fig.1. Extrapolations of ordered/disordered patterns

References

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