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Multilevel coarse graining and nano-pattern discovery in many particle stochastic systems

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ABSTRACT

In this work we propose a hierarchy of Markov chain Monte Carlo methods for sampling equilibrium properties of stochastic lattice systems with competing short and long range interactions. Each Monte Carlo step is composed by two or more sub-steps efficiently coupling coarse and finer state spaces. The method can be designed to sample the exact or controlled-error approximations of the target distribution, providing information on levels of different resolutions, as well as at the microscopic level. In both strategies the method achieves significant reduction of the computational cost compared to conventional Markov chain Monte Carlo methods. Applications in phase transition and pattern formation problems confirm the efficiency of the proposed methods.

1. Introduction

Our primary goal in this work is to develop a systematic mathematical and computational strategy for accelerating microscopic simulation methods with competing short and long range interactions, arising in numerous physical systems for instance in micromagnetics, models of epitaxial growth, etc. We propose the Multilevel Coarse Graining Monte Carlo (ML-CGMC) method, based on a hybrid statistical mechanics and statistics approach. The method introduces a *hierarchy of Markov chain Monte Carlo methods coupling scales and types of interactions* that can sample the exact or controlled error approximations of Gibbs measures $\mu_{N,\beta}(d\sigma) = Z_N^{-1} e^{-\beta H_N(\sigma)} P_N(d\sigma)$ defined on a high dimensional configuration space $\Sigma_N = \{0,1\}^{\Lambda_N}$, with Λ_N a d-dimensional lattice with $N \gg 1$ sites, that can be easily generalized to any probability measure with similar properties. It is a method of constructing efficient *proposal measures* in Metropolis sampling using coarse-graining techniques, aiming at reducing the rejection rate and the computational complexity. The key idea is a decomposition of the sampling distribution to a product measure

$$\mu_{N,\beta}(d\sigma) = \bar{\mu}^{(0)}_{M,\beta}(d\eta) \nu_r(d\sigma|\eta), \tag{1}$$

with $\eta := \mathbf{T}\sigma$ a variable with less degrees of freedom compared to σ, defined by a projection map $\mathbf{T} : \Sigma_N \to \overline{\Sigma}_M, M < N$. $\bar{\mu}^{(0)}_{M,\beta}(d\eta)$ is a measure with a simple explicit representation approximating the marginal $\bar{\mu}_{M,\beta}(d\eta) = \mu_{N,\beta} \circ \mathbf{T}^{-1}(d\eta)$ and $\nu_r(d\sigma|\eta)$ is a uniquely defined (prior) measure, responsible for *reconstructing* variables σ given η [18]. Such a two-level measure decomposition can be

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trivially extended to a multi-level setting where (1) can include different resolution levels interpolating between a coarser level and the microscopic one σ.

We describe a Monte Carlo step of a two-level CGMC method:

1. Sample η from $\bar{\mu}^{(0)}_{M,\beta}(d\eta)$, using Coarse Grained (CGMC) samplers [17,16]. Appropriate coarse-grained measures have been evaluated in earlier work via cluster expansions that can be easily constructed with available analytical error estimates, ensuring that such approximations are controllable, [19].
2. Conditioned on such η, obtained in Step 1, we sample $\nu_r(d\sigma|\eta)$ using an accept/reject method.

A schematic description of this procedure is seen in Fig. 1. Better proposals constructed in Step 1 will lead to fewer rejections in Step 2, furthermore, there is no need to consider all possible microscopic proposals since at the coarse step we do a first screening.

In comparison to two-level rejection-free CGMC previously discussed in [4], the approach here provides a rigorous mathematical framework and employs a rejection-based type algorithm that is computationally easier to implement and, in contrast to the general belief, more efficient than rejection-free methods under certain conditions (e.g. long range interactions and stiff problems), [33]. Instead of further approximating the sampling measure, as is done with cluster expansion keeping the typically computationally expensive multi-body higher order terms [19,2], we use the hybrid statistical and statistics approach that construct $\nu_r(d\sigma|\eta)$. Even when CGMC provides less accurate approximations, the ML-CGMC approach can refine the results by the accept/reject step in the finer space.

A necessary ingredient for applicability of the method is a decomposition of the form (1), which includes a possibly less accurate coarse-grained measure and the correcting accept/reject Step 2 above. This formulation can make the proposed method extentable to off-lattice systems where various coarse-graining schemes are already available [25,12], although without controlled-error approximations. In such off-lattice systems we typically have two main features: a presence of short and long interactions, as well as comparable energy and entropy, hence fluctuations are expected to be important in the modelling and simulation.

Systems with smooth long or intermediate range interactions are well approximated by coarse-graining techniques [16,18,23], and CGMC are reliable simulation methods with controlled error approximations, both for observables and loss of information [20,19]. Furthermore, models where only short-range interactions appear are inexpensive to simulate with conventional methods. However, when both short and long-range interactions are present, the conventional methods become prohibitively expensive, and coarse-graining error estimates are not applicable. The proposed method can handle such systems efficiently by either (a) compressing only the long range interactions for Step 1 and sample with CGMC with low computational cost, including the short range part at the accept/reject Step 2 (potential splitting), or (b) compress all types of interactions for Step 1, and correct appropriately in Step 2 (corrections).

A wide literature exists on sophisticated Markov chain Monte Carlo (MCMC) methods designed to accelerate simulations for large systems, applying for example parallel techniques and/or constructing good first approximations (proposals) in Metropolis sampling [9,31]. In [10] Efendiev et al., the preconditioning MCMC is proposed, a two stage Metropolis method, applied to inverse problems of subsurface characterization. Our algorithm shares the same idea of constructing a proposal density based on meso or macroscopic properties of the model studied and taking advantage of the first stage rejections. Several methods where the trial density is built up sequentially with stage-wise rejection decision appear [3,27]. There are also some similarities with simulated sintering, and transdimensional MCMC, see [28,27] and references therein. However, the novelty of our method lies in the construction of the variable dimensionality (and level of coarse-graining)

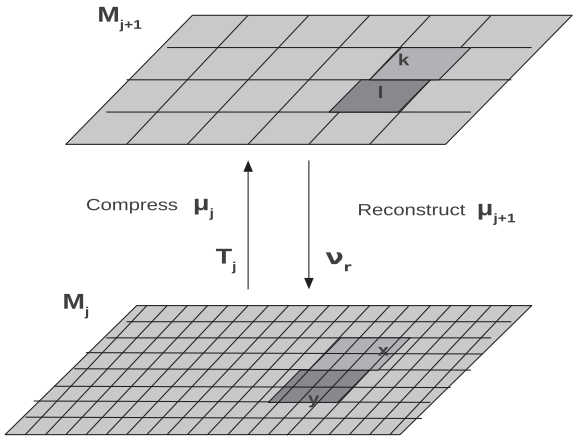

Fig. 1. Schematic of a two-level ML-CGMC. Information exchange between coarser and finer resolutions. Step 1: Sample $\mu_{j+1}(d\eta_{j+1})$, Step 2: Reconstruct with $\nu_r(d\eta_j|\eta_{j+1})$ such that $\mu_j(d\eta_j) = \mu_{j+1}(d\eta_{j+1})\nu_r(d\eta_j|\eta_{j+1})$.