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Abstract We propose an efficient Markov Chain Monte Carlo method for sampling equilibrium distributions for stochastic lattice models, capable of handling correctly long and short-range particle interactions. The proposed method is a Metropolis-type algorithm with the proposal probability transition matrix based on the coarse-grained approximating measures introduced in [17, 21]. We prove that the proposed algorithm reduces the computational cost due to energy differences and has comparable mixing properties with the classical microscopic Metropolis algorithm, controlled by the level of coarsening and reconstruction procedure. The properties and effectiveness of the algorithm are demonstrated with an exactly solvable example of a one dimensional Ising-type model, comparing efficiency of the single spin-flip Metropolis dynamics and the proposed coupled Metropolis algorithm.

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1 Introduction

Microscopic, *extended* (many-particle) systems with *complex interactions* are ubiquitous in science and engineering applications in a variety of physical and chemical systems, exhibiting rich mesoscopic morphologies. For example, nano-pattern formation via self-assembly, arises in surface processes e.g., in heteroepitaxy, induced by competing short and long-range interactions [6]. Other examples include macromolecular systems such as polymers, proteins and other soft matter systems, quantum dots and micromagnetic materials. Scientific computing for this class of systems can rely on molecular simulation methods such as Kinetic Monte Carlo (KMC) or Molecular Dynamics (MD), however their extensivity, their inherently complex interactions and stochastic nature, severely limit the spatio-temporal scales that can be addressed by these direct numerical simulation methods.

One of our primary goals is to develop systematic mathematical and computational strategies for the speed-up of microscopic simulation methods by developing *coarse-grained* (CG) approximations, thus reducing the extended system's degrees of freedom. To date coarse-graining methods have been a subject of intense focus, mainly outside mathematics and primarily in the physics, applied sciences and engineering literatures [10, 17, 25, 28, 30]. The existing approaches can give unprecedented speed-up to molecular simulations and can work well in certain parameter regimes, for instance, at high temperatures or low density. On the other hand, in many parameter regimes, important macroscopic properties may not be captured properly, e.g. [1, 30, 31]. Here we propose to, develop *reliable* CG algorithms for stochastic lattice systems with complex, and often competing particle interactions in equilibrium. Our proposed methodologies stem from the synergy of stochastic processes, statistical mechanics and statistics sampling methods.

Monte Carlo algorithms provide a computational tool capable of estimating observables defined on high-dimensional configuration spaces that are typical for modeling of complex interacting particle systems at or out of equilibrium. Markov Chain Monte Carlo (MCMC) simulation methods such as the Metropolis algorithm, were first proposed in 1953 by Metropolis and his coauthors [29] for the numerical calculation of the equation of state for a system of rigid spheres. It was generalized in 1970 by Hastings [14] and it is commonly referred to as the Metropolis-Hastings (MH) Monte Carlo method. This method belongs to the family of MCMC methods which generate ergodic Markovian chains with the stationary distribution being the desired sampled probability measure. Metropolis algorithm consists of two main ingredients: (a) the probability transition kernel q; the *proposal*, that generates trial states and (b) the acceptance probability α according to which the proposed trial is accepted or rejected. There are though some drawbacks of this method when applied to large systems, such as a small acceptance probability α, that leads to costly calculations of a large number of samples that are discarded. A way to reduce these costs is to *predict* efficient proposal measures such that the computational cost of calculating a sample is lower and, if possible, increase the acceptance probability. Convergence and ergodicity properties of Metropolis type algorithms are studied extensively in a series of works [7, 8, 32]. The rate of convergence to stationarity

is strongly dependent on the proposal distribution and its relation to the stationary measure ([32] ch. 7). A quantity that measures the speed of convergence in distribution to stationarity is the spectral gap. In order to improve an MCMC method one has to increase its spectral gap by smartly constructing a good proposal.

In this work we propose the Coupled Coarse Graining Monte Carlo (Coupled CGMC) method, a new method of constructing efficient *proposal measures* based on coarse-graining properties of the sampling models. We prove that such approach is suitable for models that include both short and long-range interactions between particles. Long-range interactions are well-approximated by coarse graining techniques [17, 18, 20], and Coarse Graining Monte Carlo (CGMC) are adequate simulation methods with an order of acceleration up to $O(q^2)$ with q a parameter controlling the level of coarse graining [19, 21]. Furthermore, models where only short-range interactions appear are inexpensive to simulate, for example with a single spin-flip Metropolis method. However, when both short and long-range interactions are present the classical MH algorithm becomes prohibitively expensive due to the high cost of calculating energy differences arising from the long-range interaction potential. In [15] we extend our framework for coupled CGMC to the dynamics case, developing Kinetic Monte Carlo algorithms based on coarse-level rates.

Section 2 describes the classical Metropolis-Hastings algorithm and some known mathematical theory for convergence and the rate of convergence for MCMC methods. In Section 3 we present the proposed Coupled CGMC method in a general framework describing its mathematical properties. We state the main theorem that compares the rate of convergence to equilibrium with the rate of the classical MH method. In Section 4 we describe stochastic lattice systems and the coarse-graining procedure in order to prepare for the application of the proposed method in Section 5 to a generic model of lattice systems in which both short and long-range interactions are present.

2 MCMC methods

Before describing the Metropolis-Hastings method we need to introduce some necessary definitions and theoretical facts.

Let X_n be a Markov chain on space Σ with transition kernel $\mathscr{K}$.

Definition 1 *A transition kernel $\mathscr{K}$ has the stationary measure μ if*

$$\mathscr{K}\mu = \mu\,.$$

Definition 2 *$\mathscr{K}$ is called reversible with respect to μ if*

$$(g,\mathscr{K}h)_\mu = (\mathscr{K}g,h)_\mu, \quad \textit{for all } g,h \in L^2(\mu)\,.$$

where $(g,h)_\mu = \int_\Sigma \overline{g(\sigma)}h(\sigma)\mu(d\sigma)$ and $\mathscr{K}g(\sigma) = \int_\Sigma \mathscr{K}(\sigma,d\sigma')g(\sigma'), \forall \sigma \in \Sigma$.

A sufficient condition for μ being a stationary measure of $\mathscr{K}$ is the, often easy to check, detailed balance(DB) condition.

Definition 3 *A Markov chain with transition kernel $\mathscr{K}$ satisfies the detailed balance condition if there exists a function f satisfying*

$$\mathscr{K}(\sigma,\sigma')f(\sigma) = \mathscr{K}(\sigma',\sigma)f(\sigma'). \tag{1}$$

Here we focus on the Metropolis-Hastings algorithm [32]. The algorithm generates an ergodic Markov chain X_n in the state space Σ, with stationary measure $\mu(d\sigma)$. Let $f(\sigma)$ be the probability density corresponding to the measure μ and $X_0 = \sigma_0$ be arbitrary. The n-th iteration of the algorithm consists of the following steps

Algorithm 1 (Metropolis-Hastings Algorithm)

Given $X_n = \sigma$

Step 1 *Generate* $Y_n = \sigma' \sim q(\sigma'|\sigma)$
Step 2 *Accept-Reject*

$$X_{n+1} = \begin{cases} Y_n = \sigma' \text{ with probability } \alpha(\sigma,\sigma') \\ X_n = \sigma_n \text{ with probability } 1-\alpha(\sigma,\sigma') \end{cases}$$

where

$$\alpha(\sigma,\sigma') = \min\left\{1, \frac{f(\sigma')q(\sigma',\sigma)}{f(\sigma)q(\sigma,\sigma')}\right\}$$

We denote $q(\sigma'|\sigma)$ the proposal probability transition kernel, and $\alpha(\sigma,\sigma')$ the probability of accepting the proposed state σ'. The transition kernel associated to MH algorithm is

$$\mathscr{K}_c(\sigma,\sigma') = \alpha(\sigma,\sigma')q(\sigma,\sigma') + \left[1 - \int \alpha(\sigma,\sigma')q(\sigma,\sigma')d\sigma'\right]\delta(\sigma'-\sigma). \tag{2}$$

Convergence and ergodicity properties of the chain $\{X_n\}$ depend on the proposal kernel q, and they are studied extensively in [32]. $\mathscr{K}_c$ satisfies the DB condition with f ensuring that it has stationary measure μ. $\mathscr{K}_c$ is irreducible and aperiodic [32], nonnegative definite, and reversible, thus the Markov chain with transition kernel $\mathscr{K}_c$ converges in distribution to μ.

2.1 Mixing times and speed of convergence

It is known [7] that for a discrete-time Markov chain X_n with the transition kernel $\mathscr{K}$ and the stationary distribution f, the rate of convergence to its stationarity can be measured in terms of kernel's second largest eigenvalue, according to

$$2||\mathscr{K}^n(\sigma,\cdot)-f||_{TV} \leq \frac{1}{f(\sigma)^{1/2}}\beta^n$$

where $\beta = max\{|\beta_{min}|,\beta_1\}$ and $-1 \leq \beta_{min} \leq \cdots \leq \beta_1 \leq \beta_0 = 1$ are the real eigenvalues of $\mathscr{K}$. The spectral gap of kernel $\mathscr{K}$ is defined by $\lambda(\mathscr{K}) = \min\left\{\frac{\mathscr{E}(h,h)}{\mathrm{Var}(h)}; \mathrm{Var}(h) \neq 0\right\}$ which for the self-adjoint kernel $\mathscr{K}$, because of reversibility, is $\lambda(\mathscr{K}) = 1-\beta_1$. With the Dirichlet form $\mathscr{E}$ and the variance defined by

$$\mathscr{E}(h,h) = \frac{1}{2}\sum_{\sigma,\sigma'}|h(\sigma)-h(\sigma')|^2\mathscr{K}(\sigma,\sigma')f(\sigma)\,,$$
$$\mathrm{Var}(h) = \frac{1}{2}\sum_{\sigma,\sigma'}|h(\sigma)-h(\sigma')|^2 f(\sigma')f(\sigma)\,.$$

Between two algorithms producing Markov chains with identical equilibrium distributions *better* in terms of the speed of convergence is the one with the *smaller second eigenvalue in absolute value* or equivalently with the *larger spectral gap*.

3 The Coupled CGMC method

The proposed algorithm is designed to generate samples from the microscopic probability measure μ with density f on a space Σ, coupling properly states of the microscopic space Σ with states on a *coarse* space $\bar{\Sigma}$ having less degrees of freedom. A properly constructed coarse measure on $\bar{\Sigma}$ will be the basis for constructing efficient proposal kernels for MH algorithms sampling large systems.

The *coarsening* procedure is based on the expansion of the target measure μ to a coarse and a finer part. Abstractly we write $f(\sigma) = f(\eta,\xi)$ and $\Sigma = \bar{\Sigma}\times\bar{\Sigma}'$, where $\eta \in \bar{\Sigma}$ represents the coarse variables.

We denote the projection operator on the coarse variables

$$T : \Sigma \to \bar{\Sigma},\ \ T\sigma = \eta\,.$$

The exact coarse marginal is

$$\bar{f}(\eta) = \int_{\bar{\Sigma}'} f(\eta,\xi)d\xi\,.$$

To obtain an explicit formula of the coarse marginal is as difficult as sampling the original target distribution since space $\bar{\Sigma}'$ remains high dimensional. Therefore use of approximating distributions of $\bar{f}$ becomes necessary. Such approximations have been proposed in [17, 21] for stochastic lattice systems and are abstractly described in Section (4) and for complex macromolecular systems see [4, 11, 13, 35].

Denote $\bar{f}_0$ an approximation of $\bar{f}$ on $\bar{\Sigma}$. This distribution, combined with a reconstruction distribution $f_r(\xi|\eta)$ corresponding to the finer variables ξ, will construct a candidate for proposal distribution in MH algorithms performed in order

to sample from f at the original space Σ. An example of a 'good' proposal distribution is $f_0(\sigma) := \bar{f}_0(\eta) f_r(\xi|\eta)$. For notational simplicity we write $f_r(\sigma|\eta)$ instead of $f_r(\xi|\eta)$. In terms of the Metropolis-Hastings algorithm this means that $q(\sigma,\sigma') = f_0(\sigma')$, or that $f_0(\sigma')$ is the stationary measure of the proposal kernel $q(\sigma,\sigma')$.

The coupled CGMC algorithm is composed of two coupled Metropolis iterations, the first generating samples from the proposal distribution and the second samples from the target measure. The first Metropolis step samples the coarse approximating marginal $\bar{f}_0(\eta)$, using an arbitrary proposal transition kernel $\bar{q}_0(\eta,\eta')$ to produce trial samples η'. The second step is performed if the coarse trial sample is accepted, and consists of the reconstruction from the coarse trial state and a Metropolis criterion designed to ensure sampling from the correct microscopic density f. If a trial coarse sample is rejected, then we go back to the first step to rebuild a new coarse trial, so that the fine Metropolis step is not performed and no computational time is wasted on checking fine trial samples that are most likely to be rejected.

In [9] Efendiev et.al., propose the Preconditioning MCMC, a two stage (coarse and fine) Metropolis MCMC method, applied to inverse problems of subsurface characterization. The coarse and fine models are finite volume schemes of different resolutions for a PDE two-phase flow model. Our algorithm shares the same idea and structure with the Preconditioning MCMC of constructing a proposal density based on meso/macro-scopic properties of the model studied and taking advantage of the first stage rejections. In terms of the MC method 'coarsening' corresponds to enriching the range of the sampling measure based on coarse-scale models proposed by multiscale finite volume methods. The major difference of the Preconditioning MCMC and the proposed algorithm is that the latter alternates between different state spaces during each MC iteration, the coarse and the finer, whether in the former the state space remains the same since coarse and fine problems are solved independently. Thus, at the end of a simulation we will have both fine-scale and "compressed", coarse-grained data. The performance of the coarse proposals in our case can be further estimated based on a systematic error analysis such as (14).

The proposed procedure has also some common features with the modified Configurational bias Monte Carlo (CBMS) where the trial density is built up sequentialy with stage-wise rejection decision described in [27], applied effectively in quantum mechanical systems [5]. There are also some similarities with simulated sintering and transdimensional MCMC, see [27] and references therein. However, in our method, the construction of the variable dimensionality (and level of coarse-graining) state spaces and the corresponding Gibbs measures relies on statistical mechanics tools that allow a systematic control of the error from one level of coarse-graining to the next, e.g. (14).

3.1 The algorithm

We describe in detail the coupled CGMC Metropolis algorithm outlined in the previews section.

Algorithm 2 (Coupled CGMC Algorithm)

Let $X_0 = \sigma_0$ *arbitrary, for* $n = 0, 1, 2, \ldots$
Given $X_n = \sigma$

Step 1 *Compute the coarse variable* $\eta = T\sigma$
Step 2 *Generate a coarse sample* $\eta' \sim \bar{q}_0(\eta, \eta')$
Step 3 *Coarse Level Accept-Reject*
Accept η' *with probability:*

$$\alpha_{CG}(\eta, \eta') = \min\left\{1, \frac{\bar{f}_0(\eta')\bar{q}_0(\eta', \eta)}{\bar{f}_0(\eta)\bar{q}_0(\eta, \eta')}\right\}.$$

If η' **is accepted then proceed to Step 4**
else generate a new coarse sample Step 2
Step 4 *Reconstruct* σ' *given the coarse trial* η'*,*

$$\sigma' \sim f_r(\cdot|\eta')$$

Step 5 *Fine Level Accept-Reject*
Accept σ' *with probability*

$$\alpha_f(\sigma, \sigma') = \min\left\{1, \frac{f(\sigma')\bar{f}_0(\eta)f_r(\sigma|\eta)}{f(\sigma)\bar{f}_0(\eta')f_r(\sigma'|\eta')}\right\}.$$

Steps 2 and 3 generate a Markov chain $\{Z_n\}$ in the coarse space $\bar{\Sigma}$ with the transition kernel

$$\mathscr{Q}(\eta, \eta') = \alpha_{CG}(\eta, \eta')\bar{q}_0(\eta, \eta') + \left[1 - \int \alpha_{CG}(\eta, z)\bar{q}_0(\eta, z)\right]\delta(\eta' - \eta).$$

The stationary measure of kernel $\mathscr{Q}$ is $\bar{f}_0(\eta)$. Combination of this kernel and Steps 1 and 4 constructs the desired proposal transition kernel $q_0(\sigma, \sigma')$ on the fine level space Σ,

$$q_0(\sigma, \sigma') = \mathscr{Q}(\eta, \eta')f_r(\sigma'|\eta').$$

According to the MH algorithm in order to sample from f, the fine level acceptance probability should be $\alpha_f(\sigma, \sigma') = \min\left\{1, \frac{f(\sigma')q_0(\sigma', \sigma)}{f(\sigma)q_0(\sigma, \sigma')}\right\}$, but since $\mathscr{Q}$ satisfies the Detailed Balance condition $\mathscr{Q}(\eta, \eta')\bar{f}_0(\eta) = \mathscr{Q}(\eta', \eta)\bar{f}_0(\eta')$, α_f is equal to

$$\begin{aligned}\alpha_f(\sigma, \sigma') &= \min\left\{1, \frac{f(\sigma')\mathscr{Q}(\eta', \eta)f_r(\sigma|\eta)}{f(\sigma)\mathscr{Q}(\eta, \eta')f_r(\sigma'|\eta')}\right\} \\ &= \min\left\{1, \frac{f(\sigma')\bar{f}_0(\eta)f_r(\sigma|\eta)}{f(\sigma)\bar{f}_0(\eta')f_r(\sigma'|\eta')}\right\}.\end{aligned}$$

The chain X_n produced by Coupled CGMC algorithm is a Markov chain on the fine space Σ, with the transition kernel

$$\mathscr{K}_{CG}(\sigma,\sigma') = \alpha_f(\sigma,\sigma')q_0(\sigma,\sigma') + \left[1 - \int \alpha_f(\sigma,\sigma')q_0(\sigma,\sigma')d\sigma'\right]\delta(\sigma'-\sigma). \tag{3}$$

The Markov chain X_n generated by the Coupled CGMC algorithm converges to the correct stationary distribution f and is ergodic, which ensures that $\frac{1}{n}\sum_{j=1}^{n} h(X_j)$ is a convergent approximation of the averages $\int h(\sigma)f(\sigma)d\sigma$ for any $h \in L^1(f)$. Ergodicity and reversibility properties are satisfied ensuring that the algorithm generates samples from the correct measure.We state this fact as a separate theorem proof of which is given in detail in [15].

We denote $E = \{\sigma \in \Sigma; f(\sigma) > 0\}$, $\bar{E} = \{\eta \in \bar{\Sigma}; \bar{f}_0(\eta) > 0\}$.

Theorem 1 *For every conditional distribution $\bar{q}_0$, and f_r such that the support of $q_0 f_r$ includes E,*

i) The transition kernel satisfies the detailed balance (DB) condition with f

$$\mathscr{K}_{CG}(\sigma,\sigma')f(\sigma) = \mathscr{K}_{CG}(\sigma',\sigma)f(\sigma')$$

ii) f is a stationary distribution of the chain.
iii) if $q_0(\sigma,\sigma') > 0$, $\forall \sigma,\sigma' \in E$ and $E \subseteq supp(f_0)$ then X_n is f-irreducible
iv) is aperiodic

3.2 The rate of convergence

The calculation of the rate of convergence to stationarity is a hard problem since it is model dependent as argued earlier. What we can prove though for the proposed method is that it is comparable to the classical Metropolis-Hastings algorithm described in Algorithm 1. This fact is stated rigorously in the following theorem which we prove in [15].

Let $\lambda(\mathscr{K}_{CG}), \lambda(\mathscr{K}_c)$ be the spectral gap corresponding to the coupled CGMC $\mathscr{K}_{CG}$, (3), and the classical MH $\mathscr{K}_c$, (2), transition kernels respectively.

Theorem 2 *Let $q(\sigma,\sigma')$ be a symmetric proposal transition probability for the classical MH algorithm and $\bar{q}_0(\eta,\eta')$ a symmetric proposal transition probability on the coarse space $\bar{\Sigma}$ for the coupled CGMC algorithm, then for any reconstruction conditional probability $f_r(\sigma|\eta)$*

i)

$$\mathscr{K}_{CG}(\sigma,\sigma') = \mathscr{A}(\sigma,\sigma')\mathscr{B}(\sigma,\sigma')\mathscr{K}_c(\sigma,\sigma') \tag{4}$$

$$\mathscr{B}(\sigma,\sigma') = \begin{cases} \frac{\bar{q}_0(\eta,\eta')f_r(\sigma'|\eta')}{q(\sigma,\sigma')} \\ \frac{\bar{q}_0(\eta',\eta)f_r(\sigma|\eta)}{q(\sigma',\sigma)} \end{cases}$$

Furthermore we define the subsets

$$C_1 = \big\{(\sigma,\sigma') \in \Sigma\times\Sigma : \big\{\alpha<1, \alpha_{CG}<1, \alpha_f<1\big\} \;\; or \;\; \big\{\alpha=1,\alpha_{CG}=1,\alpha_f=1\big\}\big\}$$
$$C_2 = \big\{(\sigma,\sigma') \in \Sigma\times\Sigma : \big\{\alpha=1, \alpha_{CG}<1, \alpha_f=1\big\} \;\; or \;\; \big\{\alpha<1,\alpha_{CG}=1,\alpha_f<1\big\}\big\}$$
$$C_3 = \big\{(\sigma,\sigma') \in \Sigma\times\Sigma : \big\{\alpha=1, \alpha_{CG}=1, \alpha_f<1\big\} \;\; or \;\; \big\{\alpha<1,\alpha_{CG}<1,\alpha_f=1\big\}\big\}$$
$$C_4 = \big\{(\sigma,\sigma') \in \Sigma\times\Sigma : \big\{\alpha<1, \alpha_{CG}=1, \alpha_f=1\big\} \;\; or \;\; \big\{\alpha=1,\alpha_{CG}<1,\alpha_f<1\big\}\big\}$$

$$\mathscr{A}(\sigma,\sigma') = \begin{cases} 1, & if\,(\sigma,\sigma') \in C_1 \\ \min\{\frac{\bar{f}_0(\eta')}{\bar{f}_0(\eta)}, \frac{\bar{f}_0(\eta)}{\bar{f}_0(\eta')}\}, & if\,(\sigma,\sigma') \in C_2 \\ \min\{\frac{f(\sigma')\bar{f}_0(\eta)}{f(\sigma)\bar{f}_0(\eta')}, \frac{f(\sigma)\bar{f}_0(\eta')}{f(\sigma')\bar{f}_0(\eta)}\}, & if\,(\sigma,\sigma') \in C_3 \\ \min\{\frac{f(\sigma')}{f(\sigma)}, \frac{f(\sigma)}{f(\sigma')}\}, & if\,(\sigma,\sigma') \in C_4 \end{cases}$$

ii)

$$\mathscr{A}\underline{\gamma}\lambda(\mathscr{K}_c) \le \lambda(\mathscr{K}_{CG}) \le \bar{\gamma}\lambda(\mathscr{K}_c) \tag{5}$$

where $\mathscr{A} = \inf_{\sigma,\sigma'}\mathscr{A}(\sigma,\sigma')$ *and* $\underline{\gamma}>0, \bar{\gamma}>0$ *such that* $\underline{\gamma} \le \mathscr{B}(\sigma,\sigma') \le \bar{\gamma}$.

4 Extended Lattice Systems

This class of stochastic processes is employed in the modeling of adsorption, desorption, reaction and diffusion of chemical species in numerous applied science areas such as catalysis, microporous materials, biological systems, etc. [3, 26]. To demonstrate the basic ideas, we consider an Ising-type system on a periodic d-dimensional lattice Λ_N with $N = n^d$ lattice points. At each $x \in \Lambda_N$ we can define an order parameter $\sigma(x)$; for instance, when taking values 0 and 1, it can describe vacant and occupied sites. The energy H_N of the system, at the configuration $\sigma = \{\sigma(x) : x \in \Lambda_N\}$ is given by the Hamiltonian,

$$H_N(\sigma) = -\frac{1}{2}\sum_{x\in\Lambda_N}\sum_{y\neq x}[K(x-y)+J(x-y)]\,\sigma(x)\sigma(y) + \sum h\sigma(x)\,, \tag{6}$$

where h, is the external field and J is the inter-particle potential. Equilibrium states at the temperature $\sim \beta^{-1}$ are described by the (canonical) Gibbs probability measure, and Z_{Λ_N} is the normalizing constant (partition function)

$$\mu_{\Lambda_N,\beta}(d\sigma) = Z_{\Lambda_N}^{-1}\exp\big(-\beta H_N(\sigma)\big)P_N(d\sigma)\,. \tag{7}$$

Furthermore, the product Bernoulli distribution $P_N(\sigma)$ is the *prior distribution* on Λ_N.

The inter-particle potentials K, J account for interactions between occupied sites. We consider K corresponding to the short and J to the long-range interactions discussed in detail in Section (4.2). General potentials with combined short and long-range interactions are discussed here, while we can also address potentials with suitable decay/growth conditions [2].

The prior $P_N(d\sigma)$ is typically a product measure, describing the system at $\beta = 0$, when interactions in H_N are unimportant and thermal fluctuations-disorder-associated with the product structure of $P_N(d\sigma)$ dominates. By contrast at zero temperature, $\beta = \infty$ interactions, and hence order, prevail. Finite temperatures, $0 < \beta < \infty$, describe intermediate states, including possible phase transitions between ordered and disordered states. For both on-lattice or off-lattice particle systems, the finite-volume equilibrium states of the system have the structure (7).

4.1 Coarse-graining of microscopic systems

Coarse-graining of microscopic systems is essentially an approximation theory and a numerical analysis question. However, the presence of *stochastic fluctuations* on one hand, and the *extensivity* of the models (the system size scales with the number of particles) on the other, create a new set of challenges. We discuss all these issues next, in a general setting that applies to both on-lattice and off-lattice systems.

First, we write the microscopic configuration σ in terms of coarse variables η and corresponding fine ones ξ so that $\sigma = (\eta, \xi)$. We denote by T the coarse-graining map $T\sigma = \eta$.

The CG system size is denoted by M, while the microscopic system size is $N = Mq$, where we refer to q as the level of coarse graining, and $q = 1$ corresponds to no coarse graining. The exact CG Gibbs measure is given (with a slight abuse of notation) by $\bar{\mu}_{M,\beta} = \mu_{N,\beta} \circ T^{-1}$. In order to write $\bar{\mu}_{M,\beta}$ in a more convenient form we first define the CG prior $\bar{P}_M(d\eta) = P_N \circ T^{-1}$. The conditional prior $P_N(d\sigma|\eta)$ is the probability of having a microscopic configuration σ, given a coarse configuration η. We now rewrite $\bar{\mu}_{M,\beta}$ using the *exact coarse-grained Hamiltonian*:

$$e^{-\beta \bar{H}_M(\eta)} = \mathbb{E}[e^{-\beta H_N}|\eta] = \int e^{-\beta H_N(\sigma)} P_N(d\sigma|\eta), \tag{8}$$

a procedure known as the *renormalization group map*, [12]; $\bar{\mu}_{M,\beta}(d\eta)$ is now rewritten using (8) as

$$\bar{\mu}_{M,\beta}(d\eta) = \frac{1}{\bar{Z}_M} e^{-\beta \bar{H}_M(\eta)} \bar{P}_M(d\eta). \tag{9}$$

Although typically $\bar{P}_M(d\eta)$ is easy to calculate, even for moderately small values of N the exact computation of the coarse-grained Hamiltonian $\bar{H}_M(\eta)$ given by (8) is, in general, impossible.

We have shown in [21] that there is an expansion of $\bar{H}_M(\eta)$ into a convergent series

$$\bar{H}_M(\eta) = \bar{H}_M^{(0)}(\eta) + \bar{H}_M^{(1)}(\eta) + \bar{H}_M^{(2)}(\eta) + \cdots + \bar{H}_M^{(p)}(\eta) + N \times \mathscr{O}(\varepsilon^p), \qquad (10)$$

by constructing a suitable first approximation $\bar{H}_M^{(0)}(\eta)$ and identifying a suitable small parameter ε to control the higher order terms in the expansions. Truncations including the first terms in (10) correspond to coarse-graining schemes of increasing accuracy. In order to obtain this expansion we rewrite (8) as

$$\bar{H}_M(\eta) = \bar{H}_M^{(0)}(\eta) - \frac{1}{\beta} \log \mathbb{E}[e^{-\beta(H_N - \bar{H}_M^{(0)}(\eta))} | \eta]. \qquad (11)$$

We need to show that the logarithm can be expanded into a convergent series, yielding eventually (10), however, two interrelated difficulties emerge immediately: first, the stochasticity of the system in the finite temperature case, yields the nonlinear log expression which in turn will need to be expanded into a series. Second, the extensivity of the microscopic system, i.e., typically the Hamiltonian scales as $H_N = O(N)$, does not allow the expansion of the logarithm and exponential functions into a Taylor series. For these two reasons, one of the mathematical tools we employed is the *cluster expansion method*, see [33] for an overview. Cluster expansions allow us to identify uncorrelated components in the expected value $\mathbb{E}[e^{-\beta(H_N - \bar{H}_M^{(0)}(\eta))} | \eta]$, which in turn will permit us to factorize it, and subsequently expand the logarithm.

The coarse-graining of systems with purely long- or intermediate-range interactions of the form

$$J(x-y) = L^{-1} V\Big((x-y)/L\Big), \quad x, y \in \Lambda_N, \qquad (12)$$

where $V(r) = V(-r)$, $V(r) = 0, |r| > 1$, was studied using cluster expansions in [2, 20, 21]. The corresponding CG Hamiltonian is

$$\bar{H}^0(\eta) = -\frac{1}{2} \sum_{l \in \bar{\Lambda}_M} \sum_{\substack{k \in \bar{\Lambda}_M \\ k \neq l}} \bar{J}(k,l) \eta(k) \eta(l) - \frac{\bar{J}(0,0)}{2} \sum_{l \in \bar{\Lambda}_M} \eta(l)\big(\eta(l) - 1\big) + \sum_{k \in \bar{\Lambda}_M} \bar{h} \eta(k). \qquad (13)$$

$$\bar{J}(k,l) = \frac{1}{q^2} \sum_{x \in C_k} \sum_{y \in C_l} J(x-y), \;\; \bar{J}(k,k) = \frac{1}{q(q-1)} \sum_{x \in C_k} \sum_{y \in C_k, y \neq x} J(x-y)$$

One of the results therein is on deriving error estimates in terms of the specific relative entropy $\mathscr{R}(\mu|\nu) := N^{-1}\sum_\sigma \log\{\mu(\sigma)/\nu(\sigma)\}\mu(\sigma)$ between the corresponding equilibrium Gibbs measures. Note that the scaling factor N^{-1} is related to the extensivity of the system, hence the proper error quantity that needs to be tracked is the loss of information *per particle*. Using this idea we can assess the *information compression* for the same level of coarse graining in schemes differentiated by the truncation level p in (10)

$$\mathscr{R}(\bar{\mu}^{(p)}_{M,\beta}|\mu_{N,\beta}\circ T^{-1}) = \mathscr{O}(\varepsilon^{p+1}), \qquad \varepsilon \equiv \beta\|\nabla V\|_1\big(\frac{q}{L}\big), \tag{14}$$

where $\bar{H}^{(0)}_M(\eta)$ in (10) is given by (13). The role of such higher order schemes was demonstrated in nucleation, metastability and the resulting switching times between phases, [2].

Although CGMC and other CG methods can provide a powerful computational tool in molecular simulations, it has been observed that in some regimes, important macroscopic properties may not be captured properly. For instance, (over-)coarse graining in polymer systems may yield wrong predictions in the melt structure [1]; similarly wrong predictions on crystallization were also observed in the CG of complex fluids, [31]. In CGMC for lattice systems, hysteresis and critical behavior may also not be captured properly for short and intermediate range potentials, [19, 21]. Motivated by such observations, in our recent work we studied when CG methods perform satisfactorily, and how to quantify the CG approximations from a *numerical analysis* perspective, where error is assessed in view of a specified tolerance. Next, we discuss systems with *long range* interactions, i.e., $L >> 1$ in (12). These systems can exhibit complex behavior such as phase transitions, nucleation, etc., however, they are more tractable analytically. At the same time they pose a serious challenge to conventional MC methods due to the large number of neighbors involved in each MC step.

Here we adopt this general approach, however, the challenges when both short and long-range interactions are present, require a new methodology. Short-range interactions induce strong "sub-coarse grid" fine-scale correlations between coarse cells, and need to be explicitly included in the initial approximation $\bar{H}^{(0)}_M(\eta)$. For this reason we introduced in [24] a *multi-scale decomposition* of the Gibbs state (7), into fine and coarse variables, which in turn allows us to describe in an explicit manner the communication across scales, for both short and long-range interactions.

4.2 Multiscale Decomposition and Splitting Methods for MCMC

We first focus on general lattice systems, and subsequently discuss related applications in later sections. We consider (6) where in addition to the long-range potential (12), we add the short-range $K(x-y) = S^{-1}U(N|x-y|/S)$, where $S << L$ and U has similar properties as V in (12); for $S = 1$ we have the usual nearest neighbor

interaction. The new Hamiltonian includes both long and short-range interactions: $H_N = H_N^l + H_N^s$.

The common theme is the observation that long-range interactions $L >> 1$ can be handled very efficiently by CGMC, (14). On the other hand short-range interactions are relatively inexpensive and one could simulate them with Direct Numerical Simulation (DNS) provided there is a suitable *splitting* of the algorithm in short and long-range parts, that can reproduce within a given tolerance equilibrium Gibbs states and dynamics. We return to the general discussion in (10) and outline the steps we need in order to construct the CG Hamiltonian for the combined short and long-range interactions.

Step 1: Semi-analytical splitting schemes. Here we take advantage of CG approximations developed in (14) in order to decompose our calculation into analytical and numerical components, the latter involving only short-range interactions:

$$\begin{aligned}\mu_{N,\beta}(d\sigma) \sim e^{-\beta H_N(\sigma)} P_N(d\sigma) = \\ = e^{-\left(\beta H_N^l(\sigma) - \bar{H}_M^{l,0}(\eta)\right)} \left[e^{-\beta H_N^s(\sigma)} P_N(d\sigma|\eta)\right] e^{-\bar{H}_M^{l,0}(\eta)} \bar{P}_M(\eta)\,,\end{aligned}$$

where $\bar{H}_M^{l,0}$ is the analytical CG formula (13) constructed for the computationally expensive, for conventional MC, long-range part; due to the estimates (14), the first term has controlled error. Furthermore, the dependence of ε on ∇V in these estimates suggests a *rearrangement* of the overall combined short- and long-range potential, into a new short-range interaction that includes possible singularities originally in the long-range component (12), e.g., the singular part in a Lennard-Jones potential, and a locally integrable (or smooth) long-range decaying component that can be analytically coarse-grained using (13), with a small error due to (14). This breakdown allows us to isolate the short-range interactions (after a possible rearrangement!), and suggests the two alternative computational approaches: either seek an approximation $e^{-\beta \bar{H}_M^s(\eta)} = \int e^{-\beta H_N^s} P_N(d\sigma|\eta)$, or use sampling methods to account for the short-range "unresolved" terms.

4.3 Microscopic Reconstruction

The reverse procedure of coarse-graining, i.e., reproducing "atomistic" properties, directly from CG simulations is an issue that arises extensively in the polymer science literature, [30, 36]. The principal idea is that computationally inexpensive CG simulations will reproduce the large scale structure and subsequently microscopic information will be added through *microscopic reconstruction*, e.g., the calculation of diffusion of penetrants through polymer melts, reconstructed from CG simulation, [30]. In this direction, CGMC provides a simpler lattice framework to mathematically formulate microscopic reconstruction and study related numerical and computational issues. Interestingly this issue arised also in the mathematical error analysis in [18, 22].

The mathematical formulation for the reconstruction of the microscopic equilibrium follows trivially when we rewrite the Gibbs measure (7) in terms of the exact CG measure corresponding to (8), defined in (9), [20]:

$$\mu_N(d\sigma) \sim e^{-\beta(H(\sigma)-\bar{H}(\eta))} P_N(d\sigma|\eta)\bar{\mu}_M(d\eta) \equiv \mu_N(d\sigma|\eta)\bar{\mu}_M(d\eta)\,.$$

We can define the conditional probability $\mu_N(d\sigma|\eta)$ as the *exact reconstruction* of $\mu_N(d\sigma)$ from the exactly CG measure $\bar{\mu}_M(d\eta)$. Although many fine-scale configurations σ correspond to a single CG configuration η, the "reconstructed" conditional probability $\mu_N(d\sigma|\eta)$ is *uniquely* defined, given the microscopic and the coarse-grained measures $\mu_N(d\sigma)$ and $\bar{\mu}_M(d\eta)$ respectively.

A coarse-graining scheme provides an approximation $\bar{\mu}_M^{\text{app}}(d\eta)$ for $\bar{\mu}_M(d\eta)$, at the coarse level. The approximation $\bar{\mu}_M^{\text{app}}(d\eta)$ could be, for instance, any of the schemes discussed in Section 4.2. To provide a reconstruction we need to lift the measure $\bar{\mu}_M^{\text{app}}(d\eta)$ to a measure $\mu_N^{\text{app}}(d\sigma)$ on the microscopic configurations. That is, we need to specify a conditional probability $\nu_N(d\sigma|\eta)$ and set $\mu_N^{\text{app}}(d\sigma) := \nu_N(d\sigma|\eta)\bar{\mu}_M^{\text{app}}(d\eta)$. In the spirit of our earlier discussion, it is natural to measure the efficiency of the reconstruction by the relative entropy,

$$\mathscr{R}\left(\mu_N^{\text{app}} \,|\, \mu_N\right) = \mathscr{R}\left(\bar{\mu}_M^{\text{app}} \,|\, \bar{\mu}_M\right) + \int \mathscr{R}\left(\nu_N(\cdot|\eta) \,|\, \mu_N(\cdot\,|\,\eta)\right) \bar{\mu}_M^{\text{app}}(d\eta)\,, \tag{15}$$

i.e., relative entropy splits the total error at the microscopic level into the sum of the error at the coarse level and the error made during reconstruction, [20, 34].

The first term in (15) can be controlled via CG estimates, e.g., (14). However, (15) suggests that in order to obtain a successful reconstruction we then need to construct $\nu_N(d\sigma\,|\,\eta)$ such that (a) $\mathscr{R}\left(\nu_N(d\sigma\,|\,\eta)\,|\,\mu_N(d\sigma\,|\,\eta)\right)$ should be of the same order as the first term in (15), and (b) it is easily computable and implementable.

The simplest example of reconstruction is obtained by considering a microscopic system with intermediate/long-range interactions (12)

$$\bar{\mu}_M^{\text{app}}(d\eta) = \bar{\mu}_M^{(0)}(d\eta)\,, \quad \nu_N(d\sigma\,|\,\eta) = P_N(d\sigma\,|\,\eta)\,. \tag{16}$$

Thus we first sample the CG variables η involved in $\bar{\mu}_M^{(0)}$, using a CGMC algorithm; then we reconstruct the microscopic configuration σ by distributing the particles uniformly on the coarse cell, conditioned on the value of η. Since $P_N(d\sigma|\eta)$ is a product measure this can be done numerically in a very easy way, without communication between coarse cells and only at the coarse cells where an update has occurred in the CGMC algorithm. In this case the analysis in [23] yields the estimates

$$\mathscr{R}\left(\bar{\mu}_M^{(0)} \,|\, \bar{\mu}_M\right) = O(\varepsilon^2)\,,\ \mathscr{R}\left(\mu_N(\cdot\,|\,\eta)\,|\,P_N(\cdot\,|\,\eta)\right) = \frac{\beta}{N}\left(\bar{H}^{(0)}(\eta) - \bar{H}(\eta)\right) = O(\varepsilon^2)\,.$$

Hence the reconstruction is second order accurate and of the same order as the coarse-graining given by (13).

5 Example: Short and long-range interactions

Short and long-range interactions pose a formidable computational challenge. We consider an example that has been explicitly solved by Kardar in [16]. The model considered has state space $\Sigma_N = \{0,1\}^{\Lambda_N}$, where Λ_N is a 1-dimensional lattice with N sites. The energy of the system at configuration $\sigma = \{\sigma(x), x \in \Lambda_N\}$ is

$$\begin{aligned}\beta H_N(\sigma) &= -\frac{K}{2}\sum_x \sum_{|x-y|=1} \sigma(x)\sigma(y) - \frac{J}{2N}\sum_x \sum_{y\neq x} \sigma(x)\sigma(y) - h\sum \sigma(x) \\ &\equiv H_N^s(\sigma) + H_N^l(\sigma) + E(\sigma)\,.\end{aligned}$$

Hamiltonian $H_N(\sigma)$ consists of the short-range term H_N^s, the long-range term H_N^l and an external field E. The interactions involved in H_N^s are of the nearest-neighbor type with strength K, while H_N^l represents a mean-field approximation or the Curie-Weiss model defined by the potential J averaged over all lattice sites. For this generic model Kardar gave in [16] a closed form solution for magnetization $M_\beta(K,J,h)$,for the state space $\{-1,1\}$

$$M_\beta(K,J,h) = \arg\min_m \left(\frac{J}{2}m^2 - \log\left[e^K \cosh(h+Jm) + \sqrt{e^{2K}\sin^2(h+Jm) + e^{-2K}}\right]\right)$$

a simple rescaling of which gives the exact average coverage $m_\beta(K,J,h)$ for the lattice-gas model considered here.

$$m_\beta(K,J,h) = \frac{1}{2}\left(M_\beta\left(\frac{1}{4}K, \frac{1}{4}J, \frac{1}{2}h - \frac{1}{4}J - \frac{1}{4}K\right) + 1\right) \tag{17}$$

We have constructed the classical single spin-flip M-H algorithm and the coupled Metropolis CGMC for the single spin-flip algorithm, both generating samples from the Gibbs measure

$$\mu_{N,\beta} = \frac{1}{Z_N} e^{-\beta H_N(\sigma)} P_N(d\sigma)\,.$$

We denote σ^x the state that differs from σ only at the site x, $\sigma^x(y) = \sigma(y), y \neq x$, $\sigma^x(x) = 1 - \sigma(x)$, the proposal transition kernel is $q(\sigma'|\sigma) = \frac{1}{N}\sum_x \delta(\sigma' - \sigma^x)$, proposing a spin-flip at the site x with the probability $\frac{1}{N}$.

We apply the coupled CGMC method with coarse updating variable

$$\eta := T\sigma = \{\eta(k), k = 1,\ldots,M\}$$

$\eta(k) := \sum_{x\in C_k} \sigma(x)$, $qM = N$ with a coarsening level $q < M$, and for the maximum coarsening $q = N$ where the coarse variable is total magnetization $\eta = \sum_{x\in\Lambda_n} \sigma(x)$. This can be thought as a coarsening procedure constructing a system consisting of one big coarse cell $M = 1$ with $q = N$ sites. Since we want to consider only single

spin-flip updates, for the sake of comparison to the classical Metropolis method, the cell updating can take only the values ± 1 and the reconstruction is chosen uniform in each cell, in the sence described in example at Section 4.3.

Table 1 gives a comparison of the classical single-site updating Metropolis Hastings algorithm with the proposed coupled Metropolis CGMC algorithm, in terms of computational complexity per iteration. By computational complexity here we mean the cost of calculating energy differences involved at the acceptance probabilities. Consider the case that both the microscopic single-site updating Metropolis and the two-step CGMC are run n times. This is reasonable to consider since as stated at Theorem 2 the two methods have comparable mixing times, therefore the number of iterations needed to achieve stationarity are comparable. We denote $\mathbb{E}(\alpha_{CG}) := \int\int \alpha_{CG}(\eta,\eta')\bar{q}_0(\eta,\eta')\bar{f}_0(\eta)d\eta d\eta'$ the average acceptance rate of the coarse proposal. The average number of accepted coarse samples is $n_1 := [\mathbb{E}(\alpha_{CG})n]$ for which $n_1 < n$ since $\mathbb{E}(\alpha_{CG}) < 1$. This means that the reconstruction and fine step acceptance criterion are performed in average only for n_1 iterations.

Table 1 Operations count for evaluating energy differences for n iterations

Cost	Metropolis Hastings	Coupled CGMC $q < N$	Coupled CGMC $q = N$
coarse A-R	–	$n \times O(M)$	$n \times O(1)$
fine A-R	$n \times O(N)$	$n_1 \times O(1)$	$n_1 \times O(1)$

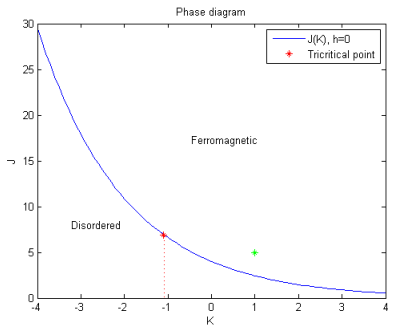

Fig. 1 Phase Diagram [16]

Results of computational implementation are shown in Figure 2 and Table 2 and 3. Figure 2a represents the average coverage versus the external field h for the exact solution m_{ex}, the classical MH result $< m_{cl} >$ and the coupled CGMC $< m >$, for a choice of interaction parameters $K = 1,\ J = 5$ in the ferromagnetic region as is stated at the phase diagram depicted in Figure 1. The exact solution m_{ex} as is ploted in Figure 2a corresponds to the part the full solution (17) up to the point it jumps. Figure 2b is a graph of the average acceptance rates for the classical MH

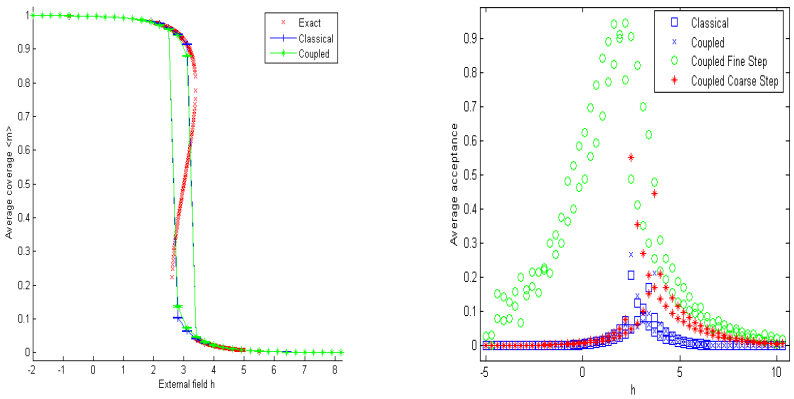

Fig. 2 N= 1028, q=8, K= 1, J= 5: (a) Coverage ; (b) Average acceptance.

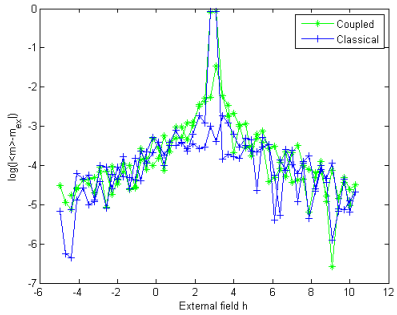

Fig. 3 N= 1028, q=8, K= 1, J= 5: Local error $\log(|<m>-<m_{ex}|)$

algorithm and the coupled CGMC algorithm, that verifies the theoretical proof of the fact that the two algorithms have comparable mixing times since the acceptance rate is strongly related to mixing times. In the same figure we also give the average acceptance rates of the coarse and fine step of the coupled method, noting that the fine acceptance rate is high which means that most of the trial samples entering the fine step are accepted.

Table 2 reports the error between the exact solution and the average coverage obtained from the coupled CGMC algorithm. Error is measured in terms of the pointwise solutions as $\text{Error}_c = \left(\sum_i (m_{ex}(h_i) - <m>(h_i))^2\right)^{1/2}$ and $\text{Error}_{cl} = \left(\sum_i (m_{ex}(h_i) - <m_{cl}>(h_i))^2\right)^{1/2}$ for the coupled and the classical method respectively, where h_i are the different external field parameters for which the average coverages are computed. CPU times are compared for the coarse-graining levels $q = 4$ and $q = 8$. To demonstrate the robustness of the algorithm we present simulations at three different points of the phase diagram plane $K - J$: in the disordered

Table 2 N= 4096

	CG level q	Error_c	CPU(min)
K= -2.0, J=2	4	0.089	93.52
	8	0.302	45.8
K= 1.0, J=5	4	0.003	93.6
	8	0.003	45.9
K= 1, J=1	4	0.027	91.6
	8	0.100	45.5

(($K=-2.0, J=2$) and ($K=1, J=1$)) and ferromagnetic ($K=1.0, J=5$) regions. In table 3 we compare the error between the coupled CGMC average coverage with the exact solution and the corresponding CPU time for $q=4$ and $q=8$, in the ferromagnetic region ($K=1.0, J=5$) for which the classical Metropolis results.

These results demonstrate the efficiency of the coupled CGMC methods in terms of computational time since the run time gain scales almost linearly with the coarsening level. We expect that according to Theorem 2ii, the error should be independent of the coarse graining parameter due to the microscopic nature of the algorithm though this is not evident in the tables since we are using a simplification of the reconstruction procedure for computational ease. We should also mention that a large number of samples (10^5) were considered ensuring the statistical error is small enough.

Table 3 N= 1028, K= 1, J= 5, $\text{Error}_{cl} = 0.003$, Classical CPU = 94.5min

CG level	Error_c	Coupled CPU(min)
q=4	0.01	23.1
q=8	0.04	12.1

6 Conclusions

An advantage of the Coupled CGMC approach over the asymptotics methodology discussed in Section 4.2 is that the trial distribution may even be order one away from the target distribution, however, the method can still perform well. On the other hand, the methods can *complement* each other; for example, for equilibrium sampling considered in this work we use as a trial reconstructed distribution, the conditional measure $\nu(d\sigma|\eta)$ in the multiscale decomposition in [24], see also Section 4.3. Such proposals based on careful statistical mechanics-based approximations provide better trial choices for the MH methods and more efficient sampling, as is proved theroretically and numerically. The example illustrated makes clear that the

coupled CGMC method implements a splitting of the short and long-range interaction terms, into the two Metropolis acceptance criteria involved. The long-range part which is responsible for the expensive calculations at a fully microscopic method, now enters only in the coarse approximation measure where its computational cost is much lower.

Coupling of a coarse and fine step is also effective in the study of dynamic processes of stochastic lattice systems with kinetic Monte Carlo methods, a topic studied in detail in [15].

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