MATHEMATICAL TOOLS FOR ERROR ANALYSIS OF COARSE-GRAINING OF LATTICE SYSTEMS

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Abstract. Coupling microscopic simulations with description at larger scales has been one of the principal tasks in many areas of computational modelling. We discuss some general mathematical issues arising in problems where the microscopic Markov process is approximated by a hierarchy of coarse-grained processes. We provide both analytical and numerical evidence that the hierarchy of the coarse models is built in a systematic way that allows for the error control of quantities that may also depend on the path. We also demonstrate that coarse-grained MC leads to significant CPU speed up of simulations of metastable phenomena, e.g., estimation of switching times or nucleation of new phases. Numerical evidence guided by analytical results suggests that CGMC probes energy landscape in path-wise agreement to MC simulations at the microscopic level.

1. Introduction. In [13, 16] the authors started developing systematic mathematical strategies for the coarse-graining of microscopic models, focusing on the paradigm of stochastic lattice dynamics and the corresponding MC simulators. In these papers a hierarchy of coarse-grained stochastic models–referred to as coarse-grained MC (CGMC) – was derived from the microscopic rules through a stochastic closure argument. The resulting *stochastic coarse-grained processes* involve Markovian birth-death and generalized exclusion processes and their combinations. They share the same ergodic properties with their microscopic counterparts. From the computational complexity perspective, a comparison of CGMC with conventional MC methods for the same real time shows, [12], that the CPU time can decrease approximately as $O(1/q^2)$ where q is the level of coarse-graining, as demonstrated for spin-flip lattice dynamics.

The CGMC algorithms discussed here are related to a number of methods involving coarse-graining at various levels, for instance fast summation techniques, renormalization group theory and simulation and multi-scale computational methods for stochastic systems. Further corrections to the CGMC dynamics from the renormalization group flow given by RGMC and multigrid MC methods [2, 6, 8] will improve approximation properties of CGMC. Various coarse-graining approaches may yield explicitly derived stochastic coarse models such as CGMC or [9, 11, 18], or can be statistics-based [19] or may rely on on-fly simulations, e.g., equation-free [17], heterogeneous multi-scale [7] or multi-scale FEM methods [10]. A systematic approach to upscaling of stochastic systems has been developed in [1, 4, 3, 5]. The authors proposed multilevel techniques that allow for efficient multi-scale simulations using Monte Carlo methods.

2. Microscopic lattice models. The presented analysis applies to the class of Ising-type lattice systems. For the sake of simplicity we assume that the computational domain is defined as the discrete periodic lattice $\Lambda_N = \frac{1}{n}\mathbb{Z}^d \cap \mathbb{T}$ which represents discretization of the d-dimensional torus $\mathbb{T} = [0,1)^d$. The microscopic degrees of freedom or the microscopic order parameter is given by the spin-like variable $\sigma(x)$ defined at each site $x \in \Lambda_N$. In this paper we discuss only the case of discrete spin variables, i.e., $\sigma(x) \in \Sigma$ with $\Sigma = \{-1,1\}$, $\Sigma = \{0,1\}$ (Ising model) or $\Sigma = \{0,1,\dots s\}$ (Potts models). We denote $\sigma = \{\sigma(x) \,|\, x \in \Lambda_N\}$ a configuration of spins on the lattice, i.e., an element of the configuration space $\mathcal{S}_N = \Sigma^{\Lambda_N}$. The interactions between spins at a given configuration σ are defined by the microscopic

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Hamiltonian

$$H(\sigma) = -\frac{1}{2}\sum_{x\in\Lambda_N}\sum_{y\neq x} J(x-y)\sigma(x)\sigma(y) + \sum_{x\in\Lambda_N} h(x)\sigma(x)\,, \tag{2.1}$$

where $h(x)$ denotes the external field at the site x. The two-body inter-particle potential J accounts for interactions between individual spins. We consider the class of potentials with the given interaction range L

$$J(x-y) = \frac{1}{L^d} V\left(\frac{n}{L}|x-y|\right)\,, \quad x, y \in \Lambda_N\,, \tag{2.2}$$

$$V : \mathbb{R} \to \mathbb{R}\,, \quad V(r) = V(-r)\,, \quad V(r) = 0\,, \quad \text{if } |r| \geq 1. \tag{2.3}$$

The canonical equilibrium state is given in terms of the Gibbs measure

$$\mu_{N,\beta}(d\sigma) = \frac{1}{Z_{N,\beta}} e^{-\beta H(\sigma)} \mathrm{P}_N(d\sigma)\,, \qquad Z_{N,\beta} = \int_{\mathcal{S}_N} e^{-\beta H(\sigma)} \mathrm{P}_N(d\sigma)\,, \tag{2.4}$$

where $\mathrm{P}_N(d\sigma) = \prod_{x\in\Lambda_N} \rho(d\sigma(x))$ is the product measure on $\mathcal{S}_N$ and the spins $\sigma(x)$ are independent identically distributed (i.i.d.) random variables with the common distribution ρ. Typically for the Ising model the prior distribution on $\Sigma = \{0, 1\}$ would be $\rho(0) = \rho(1) = 1/2$.

The microscopic dynamics is defined as a continuous-time jump Markov process that defines a change of the spin $\sigma(x)$ with the probability $c(x, \sigma; \xi)\Delta t$ over the time interval $[t, t + \Delta t]$. The probability that over the time interval $[t, t + \Delta t]$ the spin at the site $x \in \Lambda_N$ spontaneously changes from $\sigma_t(x)$ to a new value in the state space $\xi \in \Sigma$ is $c(x, \sigma; \xi)\Delta t + O(\Delta t^2)$. We denote the resulting configuration $\sigma^{x,\xi}$. In the case of the Ising-type state space and spin-flip dynamics we omit ξ in this notation. The generator $\mathcal{L} : L^\infty(\mathcal{S}_N) \to L^\infty(\mathcal{S}_N)$ of the Markov process acting on a bounded test function $f \in L^\infty(\mathcal{S}_N)$ defined on the space of configurations is given by

$$(\mathcal{L}f)(\sigma) = \sum_{x\in\Lambda_N} \int_\Sigma c(x, \sigma; \xi)\left(f(\sigma^{x,\xi}) - f(\sigma)\right)\, d\xi\,. \tag{2.5}$$

We require that the dynamics is of the relaxation type such that the invariant measure of this Markov process is the Gibbs measure (2.4). The sufficient condition is known as *detailed balance* and it imposes condition on the form of the rate

$$c(x, \sigma; \xi)e^{-\beta H(\sigma)} = c(x, \sigma^{x,\xi}; \sigma(x))e^{-\beta H(\sigma^{x,\xi})}\,. \tag{2.6}$$

The widely used class of Metropolis-type dynamics satisfies (2.6) and has the rate given by

$$c(x, \sigma; \xi) = G(\beta \Delta_{x,\xi} H(\sigma))\,, \text{ where } \Delta_{x,\xi} H(\sigma) = H(\sigma^{x,\xi}) - H(\sigma), \tag{2.7}$$

and G is a continuous function satisfying: $G(r) = G(-r)e^{-r}$ for all $r \in \mathbb{R}$. Such dynamics are often used as samplers from the canonical equilibrium Gibbs measure. However, the kinetic Monte Carlo method is also used for simulations of non-equilibrium processes. The dynamics in such a case is known as *Arrhenius dynamics*, the rates are usually derived from transition state theory or obtained from molecular dynamics simulations.

To avoid unnecessary generality from now we restrict the description to the Ising-type model with $\Sigma = \{0, 1\}$ used for modeling adsorption/desorption processes. We also omit ξ in the notation. The Arrhenius rate is defined as follows $c(x, \sigma) = d_0$ if $\sigma(x) = 0$ and $c(x, \sigma) = d_0 e^{-\beta U(x,\sigma)}$ if $\sigma(x) = 1$, where $U(x, \sigma) = \sum_{y\in\Lambda_N y\neq x} J(x-y)\sigma(y) - h(x)$. Furthermore the spin-flip rule is given by $\sigma^x(y) = 1 - \sigma(x)$ if $y = x$ and $\sigma(y)$ otherwise.

3. Approximation of the coarse-grained process.. The coarse-graining is defined in a geometric way introducing the coarse-grained observables as block-spin variables. We define the coarse-graining operator $\mathbf{T} : \mathcal{S}_N \to \mathcal{S}^c_{M,q}$, where the coarse configuration space $\mathcal{S}^c_{M,q}$ is defined on the coarse lattice Λ^c_M, and with the new state space Σ^c, i.e., $\mathcal{S}^c_{M,q} = (\Sigma^c)^{\Lambda^c_M}$. The coarse configuration $\eta = \mathbf{T}\sigma \in \mathcal{S}^c_{M,q}$ is defined on a smaller lattice with M lattice sites and with the coarse state space Σ^c for the new lattice spins $\eta(k)$. The parameter q defines the coarse-graining ratio. The operator $\mathbf{T}$ induces an operator $\mathbf{T}_*$ on the space of probability measures

$$\mathbf{T}_* : \mathcal{P}(\mathcal{S}_N) \to \mathcal{P}(\mathcal{S}^c_{M,q}) \,, \quad \mu(\sigma) \mapsto \mu^c(\eta) := \mu\{\sigma \in \mathcal{S}_N \,|\, \mathbf{T}\sigma = \eta\} \,.$$

Ising-type spins. To be more specific we analyze the following case of Ising spin-flip dynamics $\mathcal{S}_N = \{0,1\}^{\Lambda_N}$. Each coarse lattice site $k \in \Lambda^c_M$ represents a cube C_k that contains q sites of the microscopic lattice Λ_N. The projection operator defines the block spin at the coarse site k is defined as $(\mathbf{T}\sigma)(k) := \sum_{x \in C_k} \sigma(x)$. Given the Markov process $(\{\sigma_t\}_{t\geq 0}, \mathcal{L})$ with the generator $\mathcal{L}$ we obtain a coarse-grained process $\{\mathbf{T}\sigma_t\}_{t\geq 0}$ which is *not*, in general, a Markov process. From the computational point of view this may cause significant difficulties should sampling of such a process be implemented on the computer. Therefore we derive an *approximating* Markov process $(\{\eta_t\}_{t\geq 0}, \bar{\mathcal{L}}^c)$ which can be easily implemented once its generator is given explicitly.

We define the configuration δ_k defined on the coarse state space is equal to zero at all sites except the site $k \in \Lambda^c_M$ where it is equal 1, i.e., $\delta_k(j) = 1$ for $j = k$ and $= 0$ otherwise. The exact generator for the coarse process can be written in the form

$$\mathcal{L}^c\psi(\eta) = \sum_{k \in \Lambda^c_M} c_a(k)\,[\psi(\eta + \delta_k) - \psi(\eta)] + \sum_{k \in \Lambda^c_M} c_d(k)\,[\psi(\eta - \delta_k) - \psi(\eta)] \,, \tag{3.1}$$

where the new rates

$$c_a(k) = \sum_{x \in C_k} c(x,\sigma)(1 - \sigma(x)) \,, \qquad c_d(k) = \sum_{x \in C_k} c(x,\sigma)\sigma(x) \,, \tag{3.2}$$

correspond to the adsorption and desorption processes. Now it is reasonable to propose an approximating Markov process, which for the case of desorption/adsorption is a *birth-death* process $\{\eta_t\}_{t\geq 0}$ defined on the state space $\Sigma^c = \{0, 1, \ldots q\}$.

This process is defined by the generator $\bar{\mathcal{L}}^c$ of the form (3.1) where the rates c_a and c_d are replaced by approximate rates $\bar{c}_a(k,\eta) = d_0(q - \eta(k))$, and $\bar{c}_d(k,\eta) = d_0\eta(k)e^{-\beta\bar{U}(\eta)}$. The new interaction potential $\bar{U}(\eta)$ represents the approximation of the original interaction $U(\sigma)$,

$$\bar{U}(l,\eta) = \sum_{\substack{k \in \Lambda^c_M \\ l \neq k}} \bar{J}(l,k)\eta(k) + \bar{J}(0,0)(\eta(l) - 1) - \bar{h}(l) \,. \tag{3.3}$$

The coarse-grained interaction potential $\bar{J}$ is computed as the average of pair-wise interactions between microscopic spins between the coarse cells C_k and C_l

$$\bar{J}(k,l) = \frac{1}{q^2} \sum_{x \in C_k} \sum_{y \in C_l} J(x - y) \,, \quad \text{for all } k, l \in \Lambda^c_M \text{, such that } k \neq l \text{, and} \tag{3.4}$$

$$\bar{J}(k,k) \equiv J(0,0) = \frac{1}{q(q-1)} \sum_{x \in C_k} \sum_{y \in C_k, y \neq x} J(x - y) \,. \tag{3.5}$$

We have the error bound for the approximation of the coarse-grained potential $\bar{U}$ (see [14])

$$\Delta_{q,N}(\bar{U},U) \equiv |\bar{U}(k,\mathbf{T}\sigma) - U(x,\sigma)| = \mathrm{O}\left(\frac{q}{L}\right)\,, \quad \text{for all } x \in C_k. \tag{3.6}$$

The coarse interaction Hamiltonian is then given explicitly in terms of $\bar{J}$ and $\bar{h}$ as

$$\bar{H}(\eta) = -\frac{1}{2}\sum_{l\in\Lambda_M^c}\sum_{k\neq l}\bar{J}(k,l)\eta(k)\eta(l) - \frac{1}{2}\bar{J}(0,0)\sum_{l\in\Lambda_M^c}\eta(l)(\eta(l)-1) + \sum_{l\in\Lambda_M^c}\bar{h}(l)\eta(l)\,. \tag{3.7}$$

A direct calculation shows that the invariant measure of the Markov process $\{\eta_t\}_{t\geq 0}$ generated by $\bar{\mathcal{L}}^c$ is again a canonical Gibbs measure

$$\mu^c_{M,q,\beta}(d\eta) = \frac{1}{Z_{M,q,\beta}}e^{-\beta\bar{H}(\eta)}\mathrm{P}_{M,q}(d\eta)\,,$$

where the product measure $\mathrm{P}_{M,q}(d\eta)$ is the coarse-grained prior distribution. Note that the prior distribution is altered by coarse-graining procedure and different CG projections may yield prior distributions that are computationally intractable.

In summary, the coarse-graining procedure described here has the following characteristics: (i) error control on a finite-time interval $[0,T]$. In particular, the derived coarse-grained stochastic process $\{\eta_t\}_{t\geq 0}$ approximates a pre-specified observable on a finite-time interval $[0,T]$, e.g. the block-spin. In particular, time-dependent error estimates such as (4.2) can rigorously demonstrate that the process $\{\eta_t\}_{t\geq 0}$ keeps track of fluctuations from the microscopic level so expected values of certain path dependent (global) quantities can be properly estimated. More precisely, we can characterize approximation properties of $\{\mathbf{T}\sigma_t\}_{t\geq 0}$ by $\{\eta_t\}_{t\geq 0}$ using a suitable probability metric on the path space;
(ii) approximation of the invariant (equilibrium) measure. More specifically, the invariant measure $\mu^c_{M,q,\beta}(d\eta)$ for the process $\{\eta_t\}_{t\geq 0}$ defined on $\mathcal{S}^c_{M,q}$ is close in a suitable probability metric to the projection of the microscopic measure $\mathbf{T}_*(\mu_{N,\beta}(d\sigma))$; in particular the error estimates in (4.1) below, demonstrate that the coarse-grained process can preserve the ergodicity properties of the microscopic process within a prescribed tolerance. If the approximating process follows the basic principles (i) and (ii) we observe as a result of the error estimates presented here and in [14], that both the transient, as well as the long time dynamics are expected to be captured accurately by the coarse-graining.

4. Information theory estimates.. The principal idea proposed in [16] is to control *the specific loss of information* quantified by the relative entropy $\mathcal{R}\left(\mu^c_{M,q,\beta}\,|\,\mathbf{T}_*\mu_{N,\beta}\right)$ between the coarse-grain equilibrium measure $\mu^c_{M,q,\beta}$ and the projected equilibrium measure $\mathbf{T}_*\mu_{N,\beta}$ of the microscopic process.

PROPOSITION 4.1 ([16], *A priori estimate*).

$$\begin{aligned}&\frac{1}{N}\mathcal{R}\left(\mu^c_{M,q,\beta}\,|\,\mathbf{T}_*\mu_{N,\beta}\right) := \\ &\frac{1}{N}\sum_{\eta\in\mathcal{S}^c_{M,q}}\log\left(\frac{\mu^c_{M,q,\beta}(\eta)}{\mu_{N,\beta}(\{\sigma\in{\mathcal{S}_N}^{\Lambda_N}\,|\,\mathbf{T}\sigma=\eta\})}\right)\mu^c_{M,q,\beta}(\eta) = O\left(\frac{q}{L}\right)\,.\end{aligned} \tag{4.1}$$

This a priori estimate quantifies the dependence of the information distance, the specific relative entropy $\mathcal{R}\left(\mu\,|\,\nu\right)$, in terms of the coarse-graining ratio q and the interaction range L.

For the comparison of the processes $\{\mathbf{T}\sigma_t\}_{t\geq 0}$ and $\{\eta_t\}_{t\geq 0}$ we need to carry out a similar a priori analysis on the coarse path space $\mathcal{D}(\Sigma^c)$. We denote $Q_{\sigma_0,[0,T]}$ the measure on $\mathcal{D}(\Sigma)$

for the process on the interval $[0,T]$, $\{\sigma_t\}_{t\in[0,T]}$ with the initial distribution σ_0. Similarly $Q^c_{\eta_0,[0,T]}$ denotes the measure on the coarse path space $\mathcal{D}(\Sigma^c)$. With a slight abuse of notation we also use $\mathbf{T}_*Q$ to denote the projection of the measure Q on the coarse path space, i.e., the exact coarsening of the measure Q.

PROPOSITION 4.2 ([15]). *Suppose the process $\{\eta_t\}_{t\in[0,T]}$, defined by the coarse generator $\bar{\mathcal{L}}^c$ is the coarse approximation of the microscopic process $\{\sigma_t\}_{t\in[0,T]}$ then for any $q<L$ and N, $Mq=N$ the information loss as $q/L\to 0$ is*

$$\frac{1}{N}\mathcal{R}\left(\mathbf{T}_*Q_{\mathbf{T}_*\sigma_0,[0,T]}\,|\,Q^c_{\eta_0,[0,T]}\right)=T\,O\left(\frac{q}{L}\right) \tag{4.2}$$

It is worth noticing that the relative entropy estimates clearly demonstrate limitations of the coarse-graining method since it gives the order one error for short-range interactions (the nearest neighbour interaction $L=1$). On the other hand the analysis using the relative entropy (information) distance identifies the small parameter in the asymptotic expansion of the blocking error, namely the ratio q/L.

The next estimate provides a lower bound for the loss of information in terms of coarser observables:

PROPOSITION 4.3 ([14]). *Suppose the process $(\{\eta_t\}_{t\in[0,T]},\bar{\mathcal{L}}^c)$, defined by the coarse-graining operator $\mathbf{T}$ with coarse-graining parameters $Mq=N$, is the coarse approximation of the microscopic process $\{\sigma_t\}_{t\in[0,T]}$. Let $\mathbf{T}^{M',q'}$ be another coarse-graining operator, such that $m'\le m$, $M'q'=Mq=N$. Then the following estimate for the invariant microscopic measure $\mu_{N,\beta}$ and the coarse approximation $\mu^c_{M,q,\beta}$ holds*

$$\mathcal{R}\left(\mu^c_{M,q,\beta}\,|\,\mathbf{T}_*\mu_{N,\beta}\right)\ge\mathcal{R}\left(\mathbf{T}^{M',q'}_*\mu^c_{M,q,\beta}\,|\,\mathbf{T}^{M',q'}_*\mu_{N,\beta}\right)\,. \tag{4.3}$$

Moreover, on any finite-time interval $[0,T]$

$$\mathcal{R}\left(\mathbf{T}_*Q_{\mathbf{T}_*\sigma_0,[0,T]}\,|\,Q^c_{\eta_0,[0,T]}\right)\ge\mathcal{R}\left(\mathbf{T}^{M',q'}_*Q_{\mathbf{T}_*\sigma_0,[0,T]}\,|\,\mathbf{T}^{M',q'}_*Q^c_{\eta_0,[0,T]}\right)\,. \tag{4.4}$$

5. Weak convergence estimates.. In many practical MC simulations the main goal is to estimate averages (expected values) of specific observables. Therefore it is natural to analyse the weak approximation properties of the coarse-graining procedure. The weak error is defined as the quantity $e_w:=|\mathbb{E}_S\left[\mathbf{T}\sigma_t\right]-\mathbb{E}_S\left[\eta_t\right]|$, where the expectation $\mathbb{E}_S\left[\mathbf{T}\sigma_t\right]$ is defined for the path conditioned on the initial configuration $\mathbf{T}\sigma_0=S$ and $\mathbb{E}_S\left[\eta_t\right]$ on $\eta_0=S$. In the estimates derived below we deal with a specific class of observables (test functions) $\phi\in L^\infty(\mathcal{S}_N)$ which satisfy the following assumption: (A1) the test function $\phi\in L^\infty(\mathcal{S}_N)$ depends only on the coarse variable $\eta=\mathbf{T}\sigma$, i.e., $\phi(\sigma)=\psi(\mathbf{T}\sigma)$, and $\sum_{x\in\Lambda_N}|\partial_x\phi(\sigma)|\le C$.

THEOREM 5.1 ([14], *Weak error*). *Let $\phi\in L^\infty(\mathcal{S}_N)$ be a test function (observable) on the microscopic space satisfying (A1). Given the initial configuration σ_0 we define the coarse configuration $S=\mathbf{T}\sigma_0$. Assume the microscopic process $(\{\sigma_t\}_{t\ge 0},\mathcal{L})$ with $\mathbf{T}\sigma_0=S$ and its synthetic Markov process $(\{\gamma_t\}_{t\ge0},\mathcal{L}^\gamma)$, then the weak error satisfies for $0<T<\infty$*

$$|\mathbb{E}_S\left[\phi(\sigma_T)\right]-\mathbb{E}_S\left[\phi(\gamma_T)\right]|\le C_T\left(\frac{q}{L}\right)^2\,, \tag{5.1}$$

where the constant C_T is independent of q and L but depends on T. It is worth clarifying the difficulty of comparing the projected process $\{\mathbf{T}\sigma_t\}_{t\ge0}$ with the approximating process $\{\eta_t\}_{t\ge0}$. The projection $\mathbf{T}\sigma_t$ of the microscopic process on the coarse grid does not necessarily defines a Markov process. On the other hand the approximating process $\{\eta_t\}_{t\ge0}$ is constructed as a Markov process $(\{\eta_t\}_{t\geq 0}, \bar{\mathcal{L}}^c)$ with the generator $\bar{\mathcal{L}}^c$ defined by the coarse rates $\bar{c}_a$ and $\bar{c}_d$. To circumvent the technical difficulty we construct an auxiliary process $\{\gamma_t\}_{t\geq 0}$ as an intermediate step, in order to make comparison between observables which depend on Markovian processes $\{\sigma_t\}_{t\geq 0}$ and $\{\gamma_t\}_{t\geq 0}$. The process $\{\gamma_t\}_{t\geq 0}$ can be directly reconstructed from the coarse-grained process $\{\eta_t\}_{t\geq 0}$. The auxiliary process $\{\gamma_t\}_{t\geq 0}$ is defined on the microscopic configuration space by the generator $\mathcal{L}^\gamma : L^\infty(\mathcal{S}_N) \to \mathbb{R}$,

$$(\mathcal{L}^\gamma \phi)(\sigma) = \sum_{x\in\Lambda_N} c_\gamma(x,\sigma)(\phi(\sigma^x) - \phi(\sigma))\,, \tag{5.2}$$

where the rate function $c_\gamma(x,\sigma)$ is defined in terms of the coarse-grained interaction potential

$$c_\gamma(x,\sigma) = d_0(1-\sigma(x)) + d_0\sigma(x)e^{-\beta\bar{U}(l(x),\mathbf{T}\sigma)}\,.$$

The coarse-grained interaction potential $\bar{U}(l,\eta)$ has been defined in (3.3). The piece-wise constant interpolation is used to extend the function $\bar{U}(.,.)$ from the coarse lattice to the fine lattice. We denote $l(x)$ to be the cell index of the cell to which the site x belongs, i.e., $x \in C_{l(x)}$. The properties of $\{\gamma_t\}_{t\geq 0}$ were studied in [14, 15] and it was proven that: (i) the coarse-grained projection $\{\mathbf{T}\gamma_t\}_{t\geq 0}$ of the Markov process $(\{\gamma_t\}_{t\geq 0}, \mathcal{L}^\gamma)$ is still a Markov process, (ii) the processes $\{\mathbf{T}\gamma_t\}_{t\geq 0}$ and $\{\eta_t\}_{t\geq 0}$ have the same transition rates. Hence, whenever the processes have the same initial distribution they induce the same probability measure on the coarse-grained path space. If we define $Q^c_{\eta_0}(d\eta,t)$ and $Q_{\gamma_0}(d\gamma,t)$ to be the probability measures of the Markov processes $\{\eta_t\}_{t\geq 0}$ and $\{\gamma_t\}_{t\geq 0}$ respectively (conditioned on the initial condition $\eta_0 = \mathbf{T}\gamma_0$) then for all $t>0$ we have the projection

$$Q^c_{\eta_0}(d\eta,t) = \mathbf{T}_* Q_{\gamma_0}(d\gamma,t) \equiv \sum_{\{\gamma\,|\,\mathbf{T}\gamma=\eta\}} Q_{\gamma_0}(d\gamma,t)\,,$$

provided the relation is satisfied at $t=0$. Thus this property allows us to compare the processes in a path-wise way. Furthermore, the microsocpic process $\{\gamma_t\}_{t\geq 0}$ can be reconstructed from the approximating coarse process $\{\eta_t\}_{t\geq 0}$. Such reconstruction is an inverse procedure to the projection from fine to coarse configuration space. In that way we can compare the original microscopic process with the approximation on the coarse configuration space. A simple choice of a reconstruction operator is to distribute spins $\gamma_t(x)$ for $x \in C_k$ uniformly so that $\mathbf{T}\gamma_t|_{C_k} = \eta_t(k)$. It is conceivable that the synthetic process $\{\gamma_t\}_{t\geq 0}$ can be used not only as a technical tool but as a systematic procedure for reconstructing the microscopic process $\{\sigma_t\}_{t\geq 0}$ for the purpose of model refinement, adaptivity etc. As shown in Theorem 5.1 the reconstruction is done under rigorous error estimates. We refer to [14] for more details and proofs as well as numerical simulations that confirm the error analysis and demonstrate also good agreement for quantities that depend on the path.

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