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Efficient kinetic Monte Carlo method for reaction–diffusion problems with spatially varying annihilation rates

Karsten Schwarz, Heiko Rieger *

Theoretische Physik, Universität des Saarlandes, 66041 Saarbrücken, Germany

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ABSTRACT

We present an efficient Monte Carlo method to simulate reaction–diffusion processes with spatially varying particle annihilation or transformation rates as it occurs for instance in the context of motor-driven intracellular transport. Like Green's function reaction dynamics and first-passage time methods, our algorithm avoids small diffusive hops by propagating sufficiently distant particles in large hops to the boundaries of protective domains. Since for spatially varying annihilation or transformation rates the single particle diffusion propagator is not known analytically, we present an algorithm that generates efficiently either particle displacements or annihilations with the correct statistics, as we prove rigorously. The numerical efficiency of the algorithm is demonstrated with an illustrative example.

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1. Introduction

Kinetic Monte Carlo simulations are frequently used in various fields to analyze the spatio-temporal evolution of systems consisting of many freely diffusing particles that can collide, react, transform or annihilate. Spatial as well as stochastic aspects are important when diffusion is not sufficiently fast to make the system well-stirred and the number of reactants within diffusion range is small. In this case a mean-field description, for instance with a set of coupled reaction–diffusion equations, is inappropriate. Moreover, in the limit of extreme dilution methods using a discretization of the underlying stochastic reaction–diffusion system, either in time [1] or in space [2,3], become computationally inefficient.

The currently most efficient methods to simulate extremely diluted reaction–diffusion systems are Green's function reaction dynamics [4,5] and first-passage kinetic Monte Carlo methods [6–8]. In essence they avoid the small diffusion hops of a conventional random walk or Brownian dynamics simulation by propagating particles over long distances through a sequence of large displacements. The latter are generated stochastically according to the exactly known Green's function for a freely diffusing particle within so-called protective domains that are free from other particles. The typical size of these protective domains is inversely proportional to the particle density and the larger these domains are (i.e. the smaller the particle density is) the more efficient the algorithm is.

In general, during the free diffusion the particle can also be annihilated or transformed with a rate k into a different species, in which case the Green's function is still exactly know. In this paper we address the question how to propagate the particles when the annihilation rate varies in space and time, denoted as $k(\mathbf{r},t)$. This problem arises for instance in the context of motor-driven intracellular transport, where particles (or cargos) can in addition to diffusion and reaction also attach to a cytoskeleton filament and move ballistically with a constant speed in the direction of the filament. A continuum description of the diffusive and ballistic modes of motion [11,12] involves the filament density $\rho(\mathbf{r},t)$ which determines the local rate with which freely diffusing particles make a transition into the ballistic state. In a typical cell the filament density is

* Corresponding author. Tel.: +49 681 302 3969; fax: +49 681 302 4899.
E-mail addresses: kschwarz@lusi.uni-sb.de (K. Schwarz), h.rieger@mx.uni-saarland.de (H. Rieger).

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spatially inhomogeneous and thus has to be taken into account during the propagation of particles on large scales. Analogous examples arise in systems in which the annihilation of particles depends on a spatially inhomogeneous concentration field of an abundant reaction partner (i.e. whose density is much larger such that a continuum description is appropriate for it).

Green's function reaction dynamics and first-passage time Monte Carlo methods reduce the simulation of a many-particle reaction–diffusion system to individual particles that diffuse freely as long as other particles are sufficiently distant (i.e. outside the interaction range), and perform a reaction event once a particle pair reaches a minimum distance. Algorithmically one can ensure free diffusion for instance by estimating the maximum diffusion distance [4,5] until a reaction is scheduled or by the definition of protective domains for each particle [6–8] depending on the actual arrangement of neighboring particles. In both cases one then utilizes the free diffusion propagator within predefined domains to generate stochastically a time when either the maximum distance is underrun or a protective domain boundary is reached. For free diffusion this is achieved using the analytically known Green's function, but for free diffusion with spatially varying annihilation rates this propagator is unfortunately not analytically available.

Thus in this paper we consider a freely diffusing single particle in an arbitrary domain $G \in R^n$ that can be annihilated with a time and space dependent rate $k(\mathbf{r},t)$. In general, annihilation means a transition into a different species that is not considered in the present reduced setup. For a particle initially at time t_0 located at $\mathbf{r}_0 \in G$ this diffusion–annihilation process is described by the following diffusion–annihilation equation

$$\frac{\partial P(\mathbf{r},t|\mathbf{r}_0,t_0)}{\partial t} = D\Delta P(\mathbf{r},t|\mathbf{r}_0,t_0) - k(\mathbf{r},t)P(\mathbf{r},t|\mathbf{r}_0,t_0), \tag{1}$$

where $P(\mathbf{r},t|\mathbf{r}_0,t_0)$ is the probability density to find the particle at time t at $\mathbf{r} \in G$. For arbitrary $k(\mathbf{r},t)$ and arbitrary G there is no analytic solution of Eq. (1) available. In principle this equation can be solved numerically, but in the context of a general reaction–diffusion system (involving many particles and several particle species) using for instance the first-passage Monte Carlo method this is unfeasible: Here one needs for each particle hop the whole first-passage time distribution for a particle to reach the protective domain boundary ∂G, which is computationally too demanding to be carried out in the innermost loop of the algorithm.

Therefore we present in this paper an algorithm that samples times $t > t_0$ and positions $\mathbf{r}$ for arbitrary annihilation rates $k(\mathbf{r},t)$ and arbitrary domains for which a particle diffusing according to Eq. (1) either (a) reaches the boundary for the first time ($\mathbf{r} \in \partial G$) or (b) is annihilated ($\mathbf{r} \in G$). In addition, a slightly modified version of the algorithm generates the whole probability density $P(\mathbf{r},t|\mathbf{r}_0,t_0)$ within G, meaning it solves Eq. (1) stochastically.

The paper is organized as follows: Section 2 defines all probability densities and flows used throughout this paper. Based on the ideas of [4–8], Section 3 presents an algorithm for the sampling of $(\mathbf{r},t)$ on arbitrary domains G in the case of a spatially homogeneous but temporally varying annihilation rate $k(\mathbf{r},t) = k(t)$. Section 4 generalizes this method to spatially inhomogeneous rates $k(\mathbf{r},t)$, proves its correctness and discusses its efficiency. Finally Section 5 shows an application example of this method.

2. Definitions

In this section the probability densities and flows used later on are defined. Let $P(\mathbf{r},t|\mathbf{r}_0,t_0)$ be the probability density solving the diffusion–annihilation equation (1) within the domain G with boundary ∂G, possibly partly absorbing, partly reflecting. The particle annihilation generates a probability flow $f_a(\mathbf{r},t|\mathbf{r}_0,t_0)$ out of the system given by

$$f_a(\mathbf{r},t|\mathbf{r}_0,t_0) = k(\mathbf{r},t)\cdot P(\mathbf{r},t|\mathbf{r}_0,t_0). \tag{2}$$

The probability flow $f_b(\mathbf{r},t|\mathbf{r}_0,t_0)$ at the absorbing parts of the boundary at time t at position $\mathbf{r} \in \partial G$ is given by

$$f_b(\mathbf{r},t|\mathbf{r}_0,t_0) = -D\nabla P(\mathbf{r},t|\mathbf{r}_0,t_0)\cdot \mathbf{n}_\mathbf{r}, \tag{3}$$

where $\mathbf{n}_\mathbf{r}$ denotes the outward pointing unity vector perpendicular to the boundary ∂G at $\mathbf{r}$. Consequently $P(\mathbf{r},t|\mathbf{r}_0,t_0)$ is not normalized for $t > t_0$. The corresponding probability density $\rho_e(t|\mathbf{r}_0,t_0)$ for an annihilation or absorption event is given by

$$\rho_e(t|\mathbf{r}_0,t_0) = -\frac{d}{dt}\left[\int_G d\mathbf{r}\, P(\mathbf{r},t|\mathbf{r}_0,t_0)\right] = \alpha(t|\mathbf{r}_0,t_0) + \beta(t|\mathbf{r}_0,t_0) \tag{4}$$

$$\text{with}\quad \alpha(t|\mathbf{r}_0,t_0) = \int_G d\mathbf{r} f_a(\mathbf{r},t|\mathbf{r}_0,t_0)$$

$$\text{and}\quad \beta(t|\mathbf{r}_0,t_0) = \int_{\partial G} dF f_b(\mathbf{r},t|\mathbf{r}_0,t_0),$$

where dF denotes the surface element at position $\mathbf{r} \in \partial G$. Hence, the task is to sample the pairs $(\mathbf{r},t)$ in statistical agreement to $f_a(\mathbf{r},t|\mathbf{r}_0,t_0)$ and $f_b(\mathbf{r},t|\mathbf{r}_0,t_0)$, i.e. the statistic of t will be according to ρ_e.

In the following we also need the probability distribution of a freely diffusing particle $P_D(\mathbf{r},t|\mathbf{r}_0,t_0)$ without annihilation, which obeys

$$\frac{\partial P_D(\mathbf{r},t|\mathbf{r}_0,t_0)}{\partial t} = D\,\Delta P_D(\mathbf{r},t|\mathbf{r}_0,t_0). \tag{5}$$

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