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Efficient Sampling in Event-Driven Algorithms for Reaction-Diffusion Processes

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Abstract. In event-driven algorithms for simulation of diffusing, colliding, and reacting particles, new positions and events are sampled from the cumulative distribution function (CDF) of a probability distribution. The distribution is sampled frequently and it is important for the efficiency of the algorithm that the sampling is fast. The CDF is known analytically or computed numerically. Analytical formulas are sometimes rather complicated making them difficult to evaluate. The CDF may be stored in a table for interpolation or computed directly when it is needed. Different alternatives are compared for chemically reacting molecules moving by Brownian diffusion in two and three dimensions. The best strategy depends on the dimension of the problem, the length of the time interval, the density of the particles, and the number of different reactions.

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1 Introduction

It is of interest in many fields of physics, chemistry, biology, and medicine to simulate the dynamical evolution of particles diffusing independently in three dimensional space according to Brownian dynamics and interact with each other when they are adjacent to each other in kinetic Monte Carlo (KMC) algorithms. Each particle is tracked individually and they may coalesce with a certain probability when they collide or are close together and can split into two products. Examples are found e.g. in [1, 5, 8, 12, 13, 16, 17].

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The simulation technique is usually categorized as either *time-driven* or *event-driven* [7]. In a time-driven algorithm, the particles in the system are advanced in time by small time steps Δt, processing events such as collisions and reactions at the end of the time step. The time step is usually longer in an event-driven simulation where Δt is the time between two events in the system but there is also more computational work in each step. The situation is somewhat similar in the numerical integration of stiff ordinary differential equations. An explicit method is easy to program but needs small Δt for stability and an implicit method is more complicated but allows longer Δt. A new event or the new position of a particle is found by sampling a probability distribution. This distribution is Gaussian for a particle in free space but for two particles in the neighborhood of each other with a risk of collision or reaction between them, the distribution is more complicated. The cumulative distribution function (CDF) is required for the sampling using the inverse transform sampling algorithm and it is sometimes known analytically. Since the number of time steps is large and there may be many particles, the sampling has to be computationally efficient.

In this paper, we compare different ways of sampling the distribution in an event-driven process for simulation of biochemical reactions and diffusion. The molecules are assumed to be hard and spherical and are partitioned into single molecules and pairs of molecules as in the Green's Function Reaction Dynamics (GFRD) algorithm by van Zon and ten Wolde [19]. The mathematical model for the diffusing and reacting molecules was proposed by Smoluchowski [14]. The probability density function (PDF) for the positions of two molecules in a pair satisfies a parabolic partial differential equation (PDE). The boundary conditions for the PDE are given by Collins and Kimball [6]. If the molecules react, then an associative event has occurred and a new molecule is created. Another event is when a molecule dissociates into two molecules. Single molecules move inside protective spheres where the risk of collision with other molecules is very small.

While random sampling for a single molecule is simple, it is more complicated for a pair of molecules. The center coordinates of a pair are found by sampling a normal distribution and the PDF of the distance between the molecules is determined by the Smoluchowski equation. The differential operator in this PDE is split into two or three parts corresponding to the coordinate directions in [9]. The sampling is considerably simplified in this way at the cost of a numerical splitting error. The CDF in each step may be known analytically or can be computed numerically from an analytically known or numerically determined PDF. If the CDF is expensive to compute every time it is needed, then it can be tabulated and the relative position of the molecules in the pair is computed by interpolation in the table. In principle, these are the alternatives for the computational procedure in every event-driven algorithm based on sampling of a CDF.

Different strategies are evaluated for sampling of the radial distance and the angular direction between two molecules in two and three dimensions (2D and 3D). The accuracy in the alternatives is at the same level and the computing time is measured and compared. The algorithms are implemented in MATLAB and executed on a laptop. The difference is