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Simulation with Fluctuating and Singular Rates

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Abstract. In this paper we present a method to generate independent samples for a general random variable, either continuous or discrete. The algorithm is an extension of the Acceptance-Rejection method, and it is particularly useful for kinetic simulation in which the rates are fluctuating in time and have singular limits, as occurs for example in simulation of recombination interactions in a plasma. Although it depends on some additional requirements, the new method is easy to implement and rejects less samples than the Acceptance-Rejection method.

AMS subject classifications: 65C05, 82B80, 82D10

Key words: Sampling, Monte Carlo, Acceptance/Rejection method, plasma, recombination.

1 Introduction

Kinetic transport for a gas or plasma involves particle interactions such as collisions, excitation/deexcitation and ionization/recombination. Simulation of these interactions is most often performed using the Direct Simulation Monte Carlo (DSMC) method [1] or one of its variants, in which the actual particle distribution is represented by a relatively small number of numerical particles, each of which is characterized by state variables, such as position x and energy E. Interactions between the numerical particles are performed by random selection of the interacting particles and the interaction parameters, depending on the interaction rates. Correctly sampling these interactions involves several computational challenges: First the number N of particles can be large (e.g., $N=10^6$) and the number of possible interaction events can be even larger (e.g., N^k for $k=2$ or 3). Second, the interaction probabilities vary throughout the simulation since interactions

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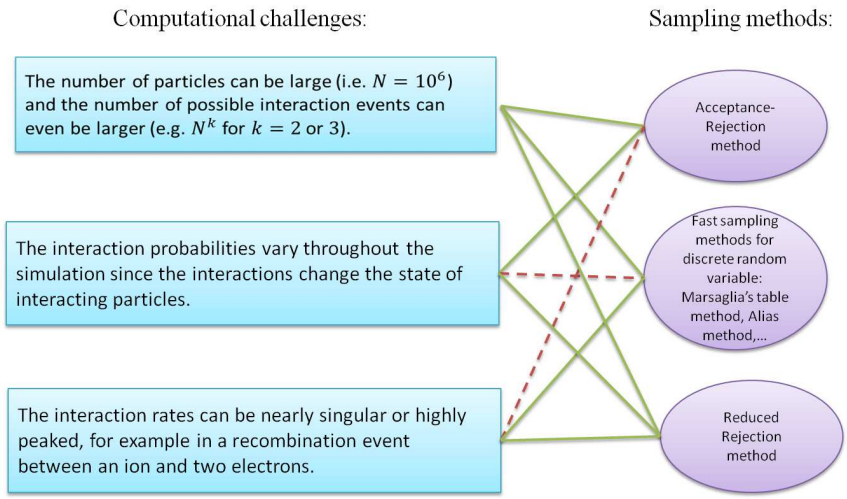

Figure 1: This figure illustrates the computational challenges involved in sampling interactions of numerical particles, and how different methods can handle them. Broken line represents challenges for which the method becomes computationally inefficient, whereas, the solid line represents the challenges for which the method is still computationally efficient.

change the state of the interacting particles. These two difficulties are routinely overcome using Acceptance-Rejection sampling. Third, the interaction rates can be nearly singular, for example in a recombination event between an ion and two electrons (described in more detail in Section 5). This creates a wide range of interaction rates that makes Acceptance-Rejection computationally intractable. Fig. 1 illustrates these challenges and how different methods can handle them. The sampling method presented here, which we call Reduced Rejection, was developed to overcome the challenges of a large number of interaction events with fluctuating and singular rates.

Simulation of kinetics requires sampling methods that generate independent samples. This rules out Markov Chain Monte Carlo schemes, such as Metropolis-Hastings, Gibbs sampling, and Slice sampling. Although these methods are very powerful and are used very often, this paper focuses on sampling methods that generate independent samples.

There are several efficient algorithms for simulation of discrete random variables, notably Marsaglia's Table method [11] and the Alias method [19, 20]. However, these methods require pre-processing time and, therefore, are not efficient for sampling from a random variable whose probability function changes during the simulation. For continuous random variables there are several different algorithms; nevertheless, each of these algorithms has its own constraints. For example, Inverse Transform Sampling method requires knowledge of the cumulative distribution function and evaluation of its inverse, Box-Muller only applies to a normal distribution, and Ziggurat algorithm [12] can be used for random variables that have monotone decreasing (or symmetric unimodal) density function.

The algorithm of choice for general (both continuous and discrete) random vari-