Commun. Comput. Phys.
doi: 10.4208/cicp.OA-2022-0303

Vol. **37**, No. 1, pp. 104-136
January 2025

A Study of Source Term Estimators in Coupled Finite-Volume/Monte-Carlo Methods with Applications to Plasma Edge Simulations in Nuclear Fusion: Analog and Collision Estimators

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Received 9 December 2022; Accepted (in revised version) 14 July 2023

Abstract. In many applications, such as plasma edge simulation of a nuclear fusion reactor, a coupled PDE/kinetic description is required. Such systems can be solved with a coupled finite-volume/Monte-Carlo method. Different procedures have been proposed to estimate the source terms in the finite volume part that appear from the Monte Carlo part of the simulation. In this series of papers, we present a systematic (analytical and numerical) comparison of the variance and computational cost of a coherent set of such estimation procedures. The comparison is based on an invariant imbedding procedure, in which systems of ordinary differential equations (ODEs) are derived that quantify the statistical error and computational cost of each estimator. In this paper, we discuss analog and collision simulation and estimation procedures. We analyze in detail a scenario with forward-backward scattering in a one-dimensional slab, uncovering and quantifying the effects determining the performance of the estimation procedures.

AMS subject classifications: 65C05, 65L12

Key words: Monte Carlo, reaction rate estimation, invariant imbedding, survival biasing, collision estimator.

1 Introduction

One often encounters situations in which an accurate mathematical description of the processes under study requires coupling a partial differential equation (PDE) of reaction-

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advection-diffusion type to a Boltzmann-type kinetic equation that models a distribution of particles in position-velocity phase space. Examples can be found in applications that are as diverse as bacterial chemotaxis [21], rarified gas dynamics [28], and plasma physics [20, 26, 29]. The motivating application in the present work is the simulation of the plasma edge in fusion energy devices, which is of crucial importance to evaluate vital aspects of reactor operation: energy and particle exhaust, as well as erosion of the plasma-facing components and the related migration and deposition of material [12, 20, 26]. In this application, the PDE part of the model describes the plasma, whereas the kinetic equation describes the behaviour of neutral particles.

Such a coupled simulation presents a computational problem due to the different dimensionality of both parts of the model. Both the plasma model and the neutral model can be simulated with either deterministic or stochastic methods, including but not limited to Galerkin methods [10], discrete velocity methods [18], particle-in-cell methods [3], and particle-tracing methods [16]. This work focuses on particle-tracing methods for the neutral kinetic model as they are used in the fusion codes EIRENE [20] and DEGAS2 [27]. These codes can be coupled with, for instance, the deterministic B2 [20] or UEDGE [5] codes or the stochastic EMC3 code [4] for the plasma equations.

In this paper, we start from a prototypical model of this type that appears in plasma edge simulations in nuclear fusion reactors, such as ITER [30]. In this model, the plasma is discretized with a finite volume method, whereas the neutral particles are simulated via Monte Carlo method. Plasma and neutral particles interact through *ionization* and *charge-exchange* events [26], of which the rates depend on the plasma state. During ionization, a neutral particle is ionized and is absorbed by the plasma; ionization is therefore also called absorption in this text. Charge-exchange events model collisions of a neutral particle with an ion during which an electron is transferred from the neutral particle to the ion: the neutral particle then becomes ionized, whereas the ion becomes neutral. In a Monte Carlo simulation, this effect can be emulated by keeping the same neutral particle with a newly sampled velocity; charge-exchange events are therefore also called scattering events. The corresponding Monte Carlo particle tracking simulations are described in Section 2.

During these interactions, mass, momentum, and energy are exchanged between plasma and neutral particles. The exchanges between neutrals and plasma are modeled as source terms in the plasma equations and estimating these source terms is the aim of the neutral model simulation. Given the importance of accurate source term estimation, many estimation procedures have been proposed. Because the source term estimation procedures only trace a finite number of particles, they induce a statistical error and a finite sampling bias on the coupled PDE/Monte-Carlo simulation. Both the statistical error and the finite sampling bias scale with the variance on the source term estimation in the Monte Carlo simulation [6]. Selecting the best estimator, that keeps this variance low for a reasonable computational cost, is thus an important objective [11].

Currently, only a few works are available that compare the performance of source term estimation procedures, usually in a very restrictive setting, leaving the choice of