Commun. Comput. Phys.
doi: 10.4208/cicp.OA-2023-0224

Vol. **36**, No. 5 , pp. 1186-1218
November 2024

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

Bert Mortier[1], Martine Baelmans[2] and Giovanni Samaey[1,*]

[1] *NUMA, Dept. Computer Science, KU Leuven, Celestijnenlaan 200A, B-3001 Leuven.*
[2] *TME, Dept. Mechanical Engineering, KU Leuven, Celestijnenlaan 300, B-3001 Leuven.*

Received 18 August 2023; Accepted 4 March 2024

Abstract. In many applications, such as plasma edge simulation of a nuclear fusion reactor, a coupled PDE/kinetic description is required, which is usually 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 paper, we perform a systematic (analytical and numerical) comparison of the variance and computational cost of source term estimations using track-length based simulation techniques and track-length and next-event estimation procedures. We analyze in detail a scenario with forward-backward scattering in a one-dimensional slab. For this test case, we perform a parametric study of the expected statistical error and computational cost, revealing the large differences in performance of the estimation procedures depending on the problem parameters. The analytical part of 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 a simplified setting.

AMS subject classifications: 65C05, 65L12
Key words: Monte Carlo, reaction rate estimation, invariant imbedding, survival biasing, collision estimator, track-length estimator, next-event estimator.

1 Introduction

For many applications, an accurate description of the relevant processes requires coupling a partial differential equation (PDE) of reaction-advection-diffusion type to a

*Corresponding author. *Email addresses:* `bertmortier@hotmail.com` (B. Mortier), `martine.baelmans@kuleuven.be` (M. Baelmans), `giovanni.samaey@kuleuven.be` (G. Samaey)

Boltzmann-type kinetic equation that models a distribution of particles in position-velocity space. Examples of such applications range from bacterial chemotaxis [19], over rarified gas dynamics [26], to plasma physics [18, 24, 27]. Simulating such a coupled model is computationally challenging due to the different dimensionality of both parts of the model.

This work focuses on particle-tracing methods for the Boltzmann-BGK kinetic equation, which are used in the neutral particle transport codes EIRENE [18] and DEGAS2 [25] for nuclear fusion applications. These codes are coupled to solvers for the plasma PDEs, such as the deterministic B2 [18] or UEDGE [5] codes or the stochastic EMC3 code [4]. Such coupled codes are used for plasma edge calculations to evaluate fusion reactor designs and operational conditions. The performance of the coupled simulation depends crucially on the performance of these particle tracing methods. For that reason, we study these particle tracing methods at length in this paper series.

We consider a prototypical model of this type that appears in plasma edge simulations in nuclear fusion reactors, such as ITER [28]. In [17], this model has been presented together with standard and a modified simulation. In this paper, we briefly review the standard simulation and present a different modification in Section 2. The neutral model contains interactions with the plasma and 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 them is the aim of the neutral model simulation. To extract these source terms from the simulation, estimators are used, of which we have seen two types in [17]. In Section 3 of this paper, we will add two more advanced estimators to this set: the track-length estimator and the next-event estimator.

The different source term estimation procedures result in a different statistical behaviour and a different computational cost. Selecting the best estimator forms a fundamental way of reducing the variance and simulation cost of the Monte Carlo procedure [9]. Currently, only a few works are available that compare the performance of these estimation procedures, usually in a very restrictive setting, leaving the choice of estimation procedure to the preference or experience of the user. A first important comparison of the estimation procedures was conducted in [15], where an invariant imbedding methodology [2] is used to derive ODEs for the statistical error of a limited set of estimation procedures in a one-dimensional forward scattering scenario. In this degenerate scenario, neutrals always have the same velocity and do not change direction, leading to very simple particle paths. Indira [6] performed a similar study that included forward-backward scattering, but limited the study to estimation procedures for leakage, the number of particles that leave the domain. Both the setting in [15] and [6] allowed for significant simplifications, resulting in ODEs for the statistical error with a comprehensive analytical solution. We also refer to the work of Lux for approximate formulas for the variance of the most commonly used estimators [13], and for sufficient conditions for one estimator to outperform an other one [12]. While useful, Lux' results do not capture the highly non-trivial behaviour at high scattering rates and low absorption rates, where