Analysis of coupled finite-volume/Monte-Carlo methods for plasma edge simulation in fusion reactors

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Summary. Nuclear fusion reactor design crucially depends on numerical simulation. The plasma can usually be modeled using fluid equations (for mass, momentum and energy). However, the reactor also contains neutral (non-charged) particles (which are important in its operation), of which both the position and velocity distribution is important. This leads to a Boltzmann-type transport equation that needs to be discretized with a Monte Carlo method. One then obtains a coupled finite-volume/Monte-Carlo simulation, of which the results possess both a bias and a variance. We discuss how these Monte Carlo errors affect convergence of steady state computations and reliability of gradient computations (necessary during optimization).

Introduction

Numerical simulations of the plasma edge play a key role in the divertor design of nuclear fusion reactors [1]. The divertor has to be able to handle large power loads and is essential for the power and particle exhaust in a reactor. Two types of particles are modeled in plasma edge models: the plasma, consisting of charged particles (ions and electrons), and the neutral particles. The plasma can usually be described with a Navier-Stokes-like fluid model, discretized in space with a suitable finite volume (FV) method. For the neutrals, however, a more microscopic, kinetic description is necessary, in which the particle distribution is modeled in a position-velocity phase space. Due to the additional dimensions in velocity space, FV simulation of the kinetic equations is computationally prohibitive. Therefore, one turns to Monte Carlo (MC) simulation.
Plasma and neutral particles interact through collisions, which can be charge exchange (an ion and neutral particle collide and exchange charge) or ionization (a neutral particle becomes a plasma particle). Due to these interactions, the plasma and neutral models need to be coupled, leading, for instance, to the B2-EIRENE code [2]. During charge-exchange collisions, momentum and energy are transferred between plasma and neutrals. During ionization, also mass is exchanged. Additionally, neutrals arise from the plasma due to surface and volumetric recombination of ions and electrons. Because of the different nature of the two types of discretizations (MC and FV), the two codes cannot be solved simultaneously, and an iterative procedure is needed. One thus simulates the neutral particles against a fixed plasma "background" and estimates the source terms (mass, momentum and energy) for the plasma equations. One then solves the plasma equations with these estimated sources. This procedure is repeated until no more corrections are required.

Computational bottlenecks

Although B2-EIRENE is used worldwide for the analysis of experimental tokamaks and for the design of ITER, computation time is a serious bottleneck. Using present-day stopping criteria, one simulation may take approximately 1 year to complete. This is due to a number of reasons, of which we now list two important ones:

- The MC simulation introduces *statistical noise* on the computed neutral density, and – via the coupling – also on the source terms in the plasma equations, and hence on the computed plasma solution. The presence of statistical noise excludes stopping criteria based on the computed residuals.
- Large reactors suitable for electricity generation typically operate in a so-called detached regime. In this regime, one aims at an increased interaction of the neutrals with the ions, especially by means of charge-exchange collisions. The goal is to create a kind of neutral "cushion" that prevents the ions to flow immediately to the divertor targets. While this regime is advantageous to avoid a direct interaction between the plasma and the divertor (and thus lengthens the lifetime of the reactor), this has a detrimental effect on the computational cost of the MC simulation, since each individual collision needs to be tracked.

The second problem can be dealt with by the design of a hybrid fluid/kinetic model for the neutral particles, reminiscent of [3]. For the first problem, we need to perform a more detailed analysis of the Monte Carlo statistical errors.

Analysis of statistical noise

There are currently two common ways to control the statistical noise coming from the Monte Carlo part of the simulation: random noise and correlated sampling. We will discuss a numerical analysis of the resulting errors that confirms the numerical observations in [4, 5].

Random noise

With *random noise*, the idea is to use – in every iteration of the coupling between plasma and neutrals – a different set of random numbers in the Monte Carlo simulation of the neutral particles. As a consequence, the residuals of the iteration

will not converge to zero. Instead, the iteration procedure can be show to generate a Markov chain that, upon convergence, samples an invariant distribution for the plasma and neutral states. We will show that the mean of this invariant distribution is close to the exact solution of the coupled FV/MC system: there is a *finite sampling bias* of which the size is inversely proportional to the number of neutral particles in the Monte Carlo simulation. Additionally, the invariant distribution has a variance that is also inversely proportional to the number of simulated neutral particles. Both the size of the bias and the variance (the prefactors) depend on numerical parameters of the iterative coupling (such as the value of the pseudo-time steps or relaxation parameters).

Correlated sampling

An alternative approach is the use of *correlated sampling*. Here, one uses the same sequence of random numbers in every iteration, which allows the iterative plasma-neutral coupling to converge to machine precision. The residuals of the nonlinear equations are thus driven to zero *specifically for the chosen set of random numbers*. We discuss how to implement correlated sampling such that one can ensure that this goal is reached.

Different sequences of random numbers (used consistently throughout the iterations) will result in different converged solutions. We will show that the collection of converged solutions also defines a probability distribution, of which the bias and variance are generally larger than in the random noise case. Nevertheless, correlated sampling may prove useful when estimating gradients in an analysis of sensitivity or an optimization procedure.

Improved Monte Carlo estimation techniques

Also inside the Monte Carlo simulation, there are multiple alternatives possible to estimate the required source terms. The choices affect the variance of the computed results and the conservation properties of the complete scheme.

Source term estimators and modified stochastic processes

The most basic MC estimators for a source term are analog and only count physical events [6]. In this simple case, physical particles are simulated and the contribution of particle collisions is added to the corresponding source term. A first problem with this method is that many collisions are required to obtain a source term estimate with low variance. Second, collision events are not equally distributed in the domain because of the small penetration depth of the particles. To alleviate these problems, more complex and non-analogous estimators have been devised [6]. These estimators count differently and can also count artificial events to reduce the variance without increasing the computational cost or introducing a bias.

Besides changing the estimators for a given particle simulation method, one can also change the stochastic process that governs the evolution of the neutral particles. A typical modification is to attach a weight to the particles, and to implement a reduction of this weight at each collision to mimic the effect of ionization in a way that allows the particle to remain in the simulation. That way, the particle is able to penetrate more deeply in the domain.

We will show that the variance of all these estimators depends on the plasma state in a highly non-trivial way, such that choosing the optimal estimator may become a challenge. We discuss a heuristic to choose a near-optimal estimator (which can be different in different parts of the domain), and provide an analysis of the resulting variance.

Strong and weak conservation and rescaled estimations

All estimators considered above conserve mass, momentum and energy in a weak sense, implying that conservation is achieved in expectation: when repeating a simulation infinitely many times, the average corresponds to the conserved quantity. Only some estimators possess strong conservation properties (i.e., conservation in an individual stochastic simulation). To achieve strong mass conservation (for each) individual simulation, one could rescale the simulation results, at the expense of introducing a (small) bias. This rescaling, however, needs to be done independently for mass, momentum and energy, which makes the resulting source terms inconsistent with each other. We show that the resulting bias is small (again inversely proportional with the number of Monte Carlo particles). It is of the same order as the finite sampling bias one necessarily makes, and it is moreover dominated by the statistical noise. We show how the effect of this bias and effects of non-conservation affect accuracy of the computed results.

References

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