Asymptotic-preserving and hybrid finite-volume/Monte-Carlo methods for kinetic equations in the plasma edge of a fusion reactor

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<u>Summary</u>. 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 discretised with a Monte Carlo method. In high-collisional regimes, the Monte Carlo simulation describing the evolution of neutral particles becomes prohibitively expensive, because each individual collision needs to be tracked. In this talk, we look into several strategies to overcome this computational bottleneck.

Introduction

Numerical simulations of the plasma edge play a key role in the divertor design of nuclear fusion reactors [1]. The divertor needs 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 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.

Although B2-EIRENE is used worldwide for the analysis of experimental tokamaks and for the design of ITER, computation time is a serious bottleneck. One reason is the number of collisions neutral particles undergo in a realistic setting. 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.

In this presentation, we overview a number of approaches that can alleviate the computational burden associated with the high-collisional regime.

Kinetic-diffusion Monte Carlo methods

One option is to avoid simulating each invididual collision. In the limit of infinite collision rate, the law of large numbers dictates the approach of an advection-diffusion like particle behaviour, in which the accumulated effect of an infinite amount of collisions is aggregated in a Brownian motion (diffusion). To maintain accuracy and remove exploding simulation costs in high-collisional regimes, one can define hybridized particles that exhibit both kinetic behaviour and diffusive behaviour depending on the local collisionality [3]. Features of the method are maintaining an asymptotically correct distribution and a correct mean, variance, and correlation for all values of the collisionality.

Multilevel Monte Carlo methods

An alternative approach is to reduce the number of Monte Carlo particles that needs to be simulated via an appropriate variance reduction technique. One very appealing option is the multilevel Monte Carlo method[5]. Asymptotic-preserving schemes as defined above result in an additional time discretization error, possibly resulting in an unacceptably large bias for larger time steps. To remove this bias, we can define a multilevel Monte Carlo scheme that reduces this bias by combining estimates using a hierarchy of different time step sizes. The multilevel Monte Carlo method relies heavily on the construction of correlated trajectories on two subsequent levels. We demonstrate how to correlate trajectories using different time steps. We also present a strategy for selecting the levels in the multilevel scheme. This approach signifi-

cantly reduces the computation required to perform accurate simulations of the considered kinetic equations, compared to classical Monte Carlo approaches.

Hybrid finite-volume Monte Carlo methods

Finally, one can also reduce the variance of the simulation by using an approximate fluid model for the neutral particles, discretized with a finite volume methods. This deterministic simulation can be used as a control variate, allowing the Monte Carlo simulation to focus on solely the deviation of the kinetic model with respect to the approximate fluid model.

References

- Kukushkin A.S., Pacher H.D., Kotov V., Pacher G.W., and Reiter D. (2011) Finalizing the ITER divertor design: the key role of SOLPS modeling Fusion Eng. Des. 86:2865-2873.
- [2] Reiter D., Baelmans M., and Börner, P. (2005) The EIRENE and B2-EIRENE codes, Fusion Sci. Technol. 47:172-186.
- [3] Mortier B., Samaey G., Baelmans M. (2019) Kinetic-diffusion asymptotic-preserving Monte Carlo algorithms for plasma edge neutral simulation. Contributions to Plasma Physics, in press.
- [4] Horsten N., Samaey G., Baelmans M. (2019) Hybrid fluid-kinetic model for neutral particles in the plasma edge. *Nuclear Materials and Energy* **18**:201-207.
- [5] Løvbak E., Samaey G., Vandewalle S. (2019) A multilevel Monte Carlo method for asymptotic-preserving particle schemes. Submitted. https://arxiv.org/abs/1907.04610.