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Kinetic-diffusion asymptotic-preserving Monte Carlo algorithms for plasma edge neutral simulation

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We develop novel Monte Carlo simulation strategies for the neutral model in plasma edge simulations where both low-collisional and high-collisional regimes are present. To maintain accuracy and reduce simulation costs in high-collisional regimes, we use hybridized particles that exhibit both kinetic and diffusive behaviour, depending on the local collisionality. The method maintains an asymptotically correct distribution and a correct mean, variance, and time correlation for all values of the collisionality. We apply this scheme to a fusion case with a strongly heterogeneous background, prompting the inclusion of a diffusion-induced drift. Our numerical results show a large increase in efficiency at the expense of a minor bias.

KEYWORDS:

plasma edge neutrals, asymptotic preserving, Boltzmann-BGK, Monte Carlo, kinetic-diffusion

1 | INTRODUCTION

A kinetic Boltzmann-BGK-like description captures the physics of neutrals in the plasma edge of fusion devices [1]. In the design of future reactors like ITER and DEMO, a region of increased neutral-plasma interactions reduces the heat load on the plasma-facing components significantly. On the computational side, this increase in collisionality causes the simulation cost of the kinetic description to explode. On the other hand, in that high-collisional limit, the kinetic behaviour converges to a diffusion process [2], which can be simulated cheaply via biased random walk.

Applications in rarefied gases and radiation transport also encounter this challenge, where simultaneously, in part of the domain, a kinetic description is required for accuracy and, in a different part of the domain, its fluid limit is valid and required for computational efficiency. There, coping with this behaviour is mostly achieved by using domain decomposition, where part of the domain is described via the kinetic model and part by the fluid description [3,4]. Separating the density in both a fluid part and a kinetic part throughout the domain is a different strategy that is often used [5–7], also specifically for neutral transport simulation in fusion devices [8,9]. Both types of solutions involve complications in determining the partition in a kinetic and fluid part and in coupling both parts of the model.

A different solution type to solve kinetic equations in the presence of different extreme regimes avoids couplings by using a single method throughout the domain that has the accuracy of the kinetic simulation in the kinetic regions and the efficiency of a fluid simulation in the fluid regions. The first such method was developed in the context of radiation transport [10,11], and for neutron transport [12] and the Boltzmann equation [13]. Most of these methods use a deterministic method that fully resolves the velocity domain, which is unnecessary in the fluid limit. Hence, the more recent class of asymptotic preserving Monte Carlo (APMC) methods [14–16] has been developed that avoid fully resolving the velocity throughout the domain. These APMC methods are dimension independent and easily cope with complex geometries as for instance present in fusion simulations. Additionally,

APMC-like methods based on aggregated collisions have been used to extend the validity of high-collisional plasma energy transport models to lower-collisional cases[17,18].

We present an asymptotic preserving Monte Carlo method for neutral transport and apply it to a fusion-relevant test-case. The Monte Carlo method is based on using the mean and variance of the positional increment during a time step of a kinetically simulated particle. Using these two moments, we replace the kinetic process with a random walk process with matching mean and variance. In the diffusive limit, this matches the model exactly. To capture the kinetic behaviour beyond the first two moments in the low-collisional regime, the random walk is modified with kinetic behaviour that dominates in the low-collisional regime and assures consistency between the velocity sample and the random walk. The resulting schemes function well in low-collisional, high-collisional and intermediate homogeneous settings as shown in[19].

In Sections 2 and 3, we review the kinetic model of the neutral transport and the asymptotic preserving schemes. When the collisionality is changing rapidly as a function of space, the scheme encounters limitations, which are resolved in Section 4, by including an effective drift due to diffusion heterogeneity. In Section 5, we show the results in a fusion-relevant highly heterogeneous test-case.

2 | KINETIC SIMULATION

In this section, we present a particle description of the kinetic model for the neutrals in a nuclear fusion reactor. This description is based on a more complete version in[20]. We restrict ourselves to a single space dimension.

Neutrals in a fusion device arise due to recombination of the plasma, which mostly occurs at the target[1]. The neutrals then fly through a fusion reactor and collide with plasma particles. These collisions result in either an *ionization* event or a *charge-exchange* event. During ionization, the neutral becomes ionized and is hence absorbed by the plasma. Charge-exchanges comprise a situation in which the neutral becomes ionized, but its lost electron is captured by a plasma particle, which then becomes neutralized. Charge-exchanges are typically simulated by keeping the same neutral particle but resampling its velocity according to the velocity distribution of the plasma. In the plasma edge, charge-exchanges occur very frequently and result in the high computational cost. In this paper, we focus solely on these events and consider how the cost associated with the high collision rate can be overcome.

The behaviour of neutrals can be expressed as a velocity jump process, in which the velocity of the particle only changes at discrete times, τ_k, $k \in [1, \dots K-1,]$. The equations for the position $t \mapsto x(t)$ and for the velocity $t \mapsto v(t)$ can be written as

$$\begin{aligned} f\left(x(0), v(0)\right) &\sim Q(x, v)\,, \\ \frac{\mathrm{d}x(t)}{\mathrm{d}t} &= v(t)\,, \\ v(t) &= v_k \text{ for } t \in \left[\tau_k, \dots \tau_{k+1}\right[,\ k \in \{0, 1, \dots\}\ , \end{aligned}$$

where $Q(x, v)$ expresses the recombination density, $\tau_0 = 0$, and the velocity at the final event is unchanged: $v(\tau_K) = v_{K-1}$.

The charge-exchanges occur with a position-dependent rate $R(x)$. Sampling the event times can be done by using standard exponentially distributed samples $\epsilon_k \sim \mathcal{E}(1)$ and solving the equation

$$\int_0^{\Delta\tau_k} R(x(\tau_k + t))\mathrm{d}t = \epsilon_k\,, \tag{1}$$

for the free-flight intervals $\Delta\tau_k$. From which the next event time can be found as $\tau_{k+1} = \tau_k + \Delta\tau_k$.

In practice, the reaction rates $R(x)$ are such that $\Delta\tau_k$ can easily be found from Equation (1), such as piecewise-constant or piecewise-linear functions.

The new velocity at a collision is sampled according to the post collisional velocity distribution, which is a Maxwellian distribution with position dependent mean, μ_v, and variance, σ_v^2, in plasma edge simulations:

$$v_k \sim \mathcal{N}\left(\mu_v\left(x(\tau_k)\right), \sigma_v^2\left(x(\tau_k)\right)\right)\ .$$

The positional increment after K events can be written as

$$\Delta x = \sum_{k=0}^{K} v_k \Delta\tau_k\,.$$

3 | KINETIC-DIFFUSION SCHEMES

Since the number of events in a time step Δt is expected to be $R\Delta t$, the positional increment during Δt will imply taking the sum over a large number of terms when the collisionality is high. From this observation, the validity of using a normally distributed step to replace the kinetic process follows from the central limit theorem. The schemes presented here use diffusion steps with identical mean and variance as the kinetic process.

While such an approach can be expected to be accurate in a high-collisional setting, plainly replacing the kinetic process during a time step by a normally distributed increment with the same mean and variance induces a large error when the collisionality is low. This error arises both due to the large error in the resulting distribution and due to the loss of correlation between subsequent time steps transferred by the velocity in the kinetic process.

This behaviour is resolved with two strategies. The first is only using a diffusion step in between the first and last collision in the time step. That way, the kinetic nature in low collisional regimes is maintained due to the low occurrence of diffusion steps and the correlation is maintained due to maintaining the kinetic velocity behaviour in between time steps. A scheme implementing this concept is presented in algorithm 1, where for the mean and variance during the diffusion step the formulas

$$\mathbb{E}[\Delta x] = \mu_v \Delta t\,, \tag{2}$$

$$\mathrm{Var}(\Delta x) = \frac{2\sigma_v^2}{R^2}\left(e^{-R\Delta t} - 1 + R\Delta t\right)\,. \tag{3}$$

are used. These expressions are exact when the plasma parameters R, μ_v, and σ_v are constants. For non-constant backgrounds that do not change rapidly, the error due to using instantaneous values vanishes with Δt. When the heterogeneity is very severe however a correction has to be used, which will be the topic of the Section 4.

Algorithm 1 A diffusion-kinetic simulation resolving low-collisional behaviour with a kinetic first and last flight.

function DIFFUSIONKINETIC_KDK($x, v, \Delta t, R(x), \mu_v(x), \sigma_v(x)$)
  $\Delta\tau_0 \leftarrow$ SAMPLECOLLISION($x, v, R(x)$)
  if $\Delta\tau_0 \leq \Delta t$ **then**
    $x \leftarrow x + v\Delta\tau$
    $\Delta\tau_K \leftarrow$ SAMPLECOLLISION($x, v_K, R(x)$)
    if $\Delta\tau_0 + \Delta\tau_K \leq \Delta t$ **then**
      $x \leftarrow x + \mathcal{N}(\text{eq.}(2), \text{eq.}(3))\big|_{\substack{\Delta t=\Delta t-\Delta\tau_0-\Delta\tau_K, v_0=v,\\ R=R(x), \mu_v=\mu_v(x), \sigma_v=\sigma_v(x)}}$
      $v \leftarrow \mathcal{N}(\mu_v, \sigma_v^2)$
      $x \leftarrow x + v\Delta\tau_K$
    else
      $v \leftarrow \mathcal{N}(\mu_v, \sigma_v^2)$
      $x \leftarrow x + v(\Delta t - \Delta\tau_0)$
    end if
  else
    $x \leftarrow v\Delta t$
  end if
  return x, v
end function

The second way is to insert part of the kinetic behaviour into the diffusion part by conditioning the mean and variance on the final velocity. It can be derived[19] that the mean and variance of the positional increment of a kinetic process conditioned on the exiting velocity equalling ν are

$$\mathbb{E}[\Delta x] = \mu_v \Delta t + (\nu - \mu_v)\frac{1}{R}\left(1 - e^{-R\Delta t}\right)\,, \tag{4}$$

$$\mathrm{Var}(\Delta x) = \frac{2\sigma_v^2}{R^2}\left(2e^{-R\Delta t} + R\Delta t + R\Delta t e^{-R\Delta t} - 2\right) + \frac{\left(\nu - \mu_v\right)^2}{R^2}\left(1 - 2R\Delta t e^{-R\Delta t} - e^{-2R\Delta t}\right)\,, \tag{5}$$

again for constant plasma parameters. Combined with an initial kinetic step, this conditioning captures the kinetic behaviour in the low-collisional regime, while maintaining efficiency in the high-collisional case. The resulting algorithm is given as algorithm 2.

Algorithm 2 A diffusion-kinetic simulation with (x, v)-consistency

function DIFFUSIONKINETIC_KD($x, v, \Delta t, R(x), \mu_v(x), \sigma_v(x)$)
  $\Delta\tau \leftarrow$ SAMPLECOLLISION($x, v, R(x)$)
  if $\Delta\tau \leq \Delta t$ **then**
    $x \leftarrow x_0 + v\Delta\tau$
    $v \leftarrow \mathcal{N}(\mu_v(x), \sigma_v^2(x))$
    $x \leftarrow x + \mathcal{N}\left(\text{eq.(4)}, \text{eq.(5)}\right)\Big|_{\substack{\Delta t=\Delta t-\Delta\tau, v_0=v,\\ R=R(x), \mu_v=\mu_v(x), \sigma_v=\sigma_v(x)}}$
  else
    $x \leftarrow x + v\Delta t$
  end if
  return x, v
end function

4 | HETEROGENEITY CORRECTION

The diffusion part of algorithms 1 and 2 effectively consists of replacing a large amount of free flights by an advection-diffusion step of the form

$$\Delta x = \mu_x \Delta t + \sqrt{\sigma_x^2 \Delta t}\,\chi\,,$$

with $\mu_x \Delta t = \mathbb{E}[\Delta x]$, $\sigma_x^2 \Delta t = \mathrm{Var}(\Delta x)$, and $\chi \sim \mathcal{N}(0, 1)$. This corresponds to an Itô discretization of the SDE corresponding to the limiting Fokker-Planck equation of the density [2],

$$\frac{\partial \rho(x,t)}{\partial t} + \frac{\partial}{\partial x}\left(\mu_x \rho(x,t)\right) - \frac{\partial^2}{\partial x^2}\left(\frac{1}{2}\sigma_x^2 \rho(x,t)\right) = \text{sources}\,.$$

The limiting model of the neutral particle behaviour is Fick's diffusion equation [2],

$$\frac{\partial \rho(x,t)}{\partial t} + \frac{\partial}{\partial x}\left(\mu_x \rho(x,t)\right) - \frac{\partial}{\partial x}\left(\frac{1}{2}\sigma_x^2 \frac{\partial}{\partial x}\rho(x,t)\right) = \text{sources}\,,$$

which differs from the Fokker-Planck equation when the background is heterogeneous. We correct for this difference with an additional drift term in the numerically integrated equation of the form

$$\frac{1}{2}\frac{\partial \sigma_x^2}{\partial x}\Delta t\,,$$

with the partial derivative computed numerically. To furthermore cope with the strong heterogeneity, the diffusion step uses the background values at the intermediate location $x + \mu_v \frac{1}{2}\Delta t$

In the next section we evaluate this correction for heterogeneity in the context of a detached fusion case.

5 | NUMERICAL EXPERIMENTS AND ALGORITHMIC IMPROVEMENTS

In this section the diffusion-kinetic simulation is applied to a one-dimensional fusion test-case based on the case studied in [21]. The neutrals all arise at the reflective right boundary, being the location of the divertor plates towards which the hot plasma flows. To retain the focus on the relevant aspects, we simplify the case of [21] by taking constant $\mu_v = 500$, $\sigma_v = 10000$, and by ignoring absorption. We furthermore rescale space to resolve the neutral behaviour at the edge. The resulting collision rate is

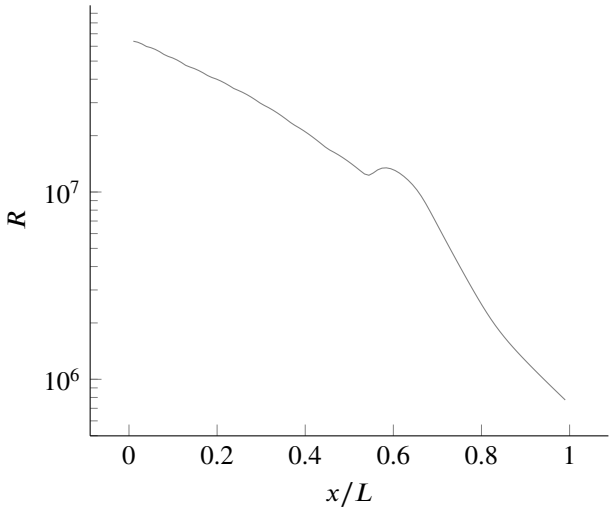

FIGURE 1 The collision rate in the detached fusion case.

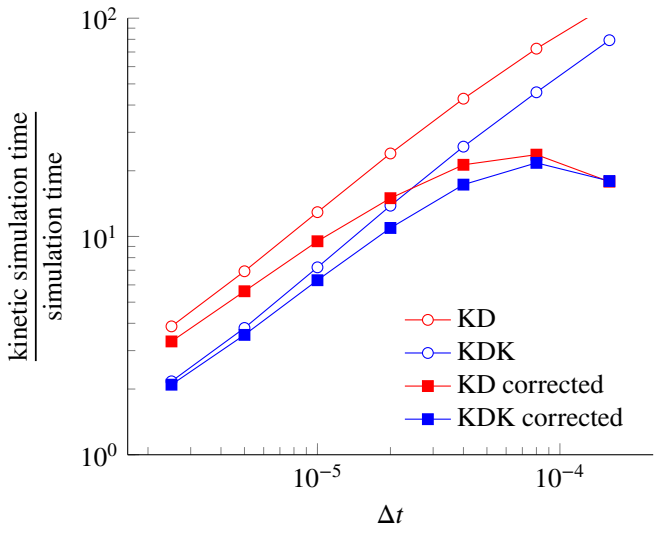

FIGURE 2 The computational gain as a function of Δt.

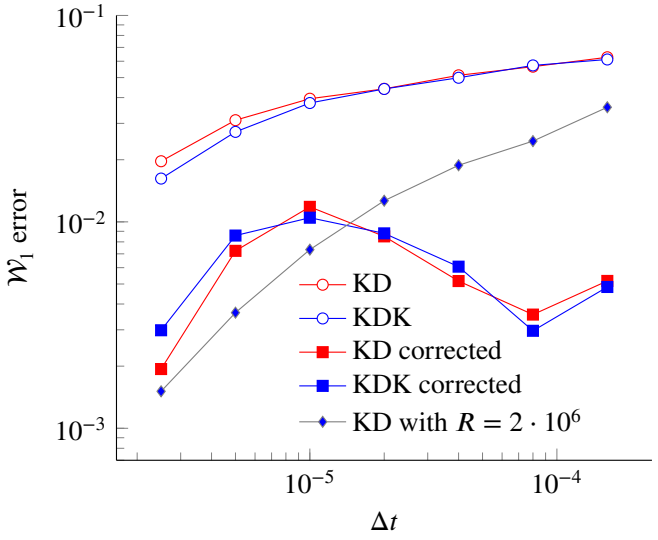

FIGURE 3 The bias as a function of Δt.

given in Figure 1 . This case contains two of the main difficulties present in the neutral simulation of the detached cases: regions of very high collisionality and a rapidly changing intermediate region.

We evaluate the performance of the kinetic-diffusion schemes based on the particle distribution after a simulation time of 0.1s, where the reflective boundary is executed kinetically. Since the rates are approximately $10^6 \mathrm{s}^{-1}$, approximately 10^5 events take place in the kinetic simulation. For the KD scheme in these regimes, only in the order of $0.1/\Delta t$ events take place and for the KDK scheme about twice that amount. The resulting large gains in computational efficiency are shown in Figure 2 . Figure 3 shows the difference in distribution between the kinetic simulation and the kinetic-diffusion simulation. We express this error with the Wasserstein distance[22], the average distance mass should be moved from the kinetic-diffusion distribution to obtain the kinetic distribution. The kinetic-diffusion results from the scheme with drift correction as described in Section 4, results show an acceptable drop in speed-up and a large decrease of the error. In many cases, the correction even outperforms the case with a homogeneous plasma background. In correspondence with the findings in[19], in the high-collisional case, there is no significant difference in error between the two kinetic-diffusion schemes.

6 | CONCLUSION AND OUTLOOK

To overcome high simulation costs in high-collisional regimes and erroneous results in low-collisional regimes present in neutral simulations for the plasma edge, we developed a class of kinetic-diffusion algorithms that captures both limiting behaviours. To apply these schemes to the practical situation with a rapidly changing collision rate, we modified the diffusion part of the schemes in order to capture the emergent flux. The presented numerical results illustrate the effectiveness of the kinetic-diffusion schemes and the heterogeneity correction in terms of computational speed and accuracy. The next step in applying these schemes for steady-state fusion simulations, is developing estimators that function well for both the kinetic parts and the diffusion parts of the algorithm.

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