Backward Monte Carlo method for fast-ion-loss simulations

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In fusion devices, the fast-ion population plays a crucial role in the plasma performance as it provides one of the primary sources of plasma heating. It is therefore of vital interest to predict the behaviour and the possible confinement losses of such particles with tested and validated models [1–3]. The standard approach, based on the Forward Monte Carlo method (FMC) [4, 5], often suffers of poor statistics and low accuracy when analyzing small target domains of interest, wasting a large amount of resources for markers that do not contribute to the fast-ion loss signal. As a remedy, with the Backward Monte Carlo (BMC) algorithm [6–8], the probability of a marker reaching a specific area is tracked backwards in time starting at the region of interest. The calculation of the probability involves an iterative process in which, during every step, points in phase-space are advanced according to their forward equations of motion and the statistical spread from the Monte Carlo collision operator taken into account deterministically. In the present work, we propose a novel 5D guiding-center BMC-based scheme for simulation of fast-ion losses, integrated into the Monte Carlo orbit-following code ASCOT [4, 5]. The escape probability obtained with the BMC-scheme is used as information for importance sampling of the initial distribution of markers mitigating the artificial diffusion error that was shown previously in [8] and at the same time solving the statistics problem of the standard FMC scheme.

Backward Monte Carlo method

Discretizing time as the regularly spaced ordered set $\{0,\Delta t,...,m\Delta t,...,M\Delta t\}$, the function Φ is used to describe the probability of a particle at phase-space position $\boldsymbol{z}$ and time index m to reach the target domain Ω during a time interval $\tau\in[m\Delta t,M\Delta t]$. The probability Φ can be evaluated formally with the following recursive formula [8]

$$\Phi(\boldsymbol{z},m-1)=\int_{\mathbb{R}^d}\Phi\left(\varphi^{\Delta t,(m-1)\Delta t}(\boldsymbol{z},\boldsymbol{r}),m\right)\frac{\exp\left[-\boldsymbol{r}^2/2\right]}{(2\pi)^{d/2}}d\boldsymbol{r},\tag{1}$$

where $(\boldsymbol{z},t)\mapsto(\varphi^{\Delta t,t}(\boldsymbol{z},R),t+\Delta t)$ is the particle integrator map combining both the Hamiltonian motion $\varphi_{\boldsymbol{U}}^{\Delta t,t}(\boldsymbol{z})$ and the collisional contribution, evaluated with the Euler-Maryama scheme

$$\varphi_{\boldsymbol{C}}^{\Delta t,t}(\boldsymbol{z},R)=\boldsymbol{z}+K(\boldsymbol{z},t)\Delta t+\boldsymbol{\Sigma}(\boldsymbol{z},t)\cdot R\sqrt{\Delta t},\tag{2}$$

*See the author list of H. Meyer et al 2019 Nucl. Fusion 59 112014 where $K(z,t)$ and $\mathbf{\Sigma}(z,t)$ are the guiding center friction and diffusion coefficients [9, 5], and $R \sim \mathcal{N}(0,\mathbf{I})$ is a random variable following a standard multivariate distribution. In the numerical implementation of the BMC scheme, a 5D phase-space mesh is constructed to represent the probability Φ. Since the particle push-forward map is continuous, the function Φ is represented as a linear interpoland $\Phi(z,m) = \sum_i \Phi_i^m \Lambda^i(z)$. Eq. (1) is then discretized by integrating the stochastic part numerically with a Gauss-Hermite quadrature

$$\Phi_i^{m-1} = \pi^{-1/2} \sum_k w_k \sum_j \Phi_j^m \Lambda^j(\varphi_i^{\Delta t}(\sqrt{2} r_k)), \tag{3}$$

where r_k and w_k are the standard nodes and weights for the Gauss-Hermite integration of the type $\int_{-\infty}^{\infty} \exp(-r^2) f(r) dr \approx \sum_k w_k f(r_k)$. Fast-ion loss signals are then computed as an integral of the source distribution weighted with the event probability of hitting the target domain Ω in the given time interval $[0,t]$

$$I(\Omega,t) = \int S(z') \mathbb{E}\left[P(z_\tau;\Omega,t) \mid z_0 = z'\right] dz', \tag{4}$$

In principle, the BMC scheme could be used directly in (4). In the present work, it is adopted for performing importance sampling of the source distribution to improve the statistics of an existing FMC simulation.

Test cases for the new algorithm

the BMC scheme is applied to an AUG H-mode discharge where the fast-ion source (fig. 1) is introduced by means of the neutral beam injector (NBI) system. In particular, the magnetic and kinetic profiles correspond to the shot AUG33143 with the beams Q7 and Q8 produced by the BBNBI code [10], assuming an energy of 93 keV and power of 2.5 MW for each beam. For this example, the target domain is set to a small subset of the wall near the divertor. The target hit probability is computed with both the BMC and FMC schemes, with different total integration time. The result is illustrated in Fig. 2. Where BMC manages to produce a meaningful-appearing evolution for the probability backwards in time, FMC seems to produce only Monte Carlo noise, i.e., insufficient statistics. The benefits of the new BMC-IS method are made apparent by the hit rate statistics in Table 1.

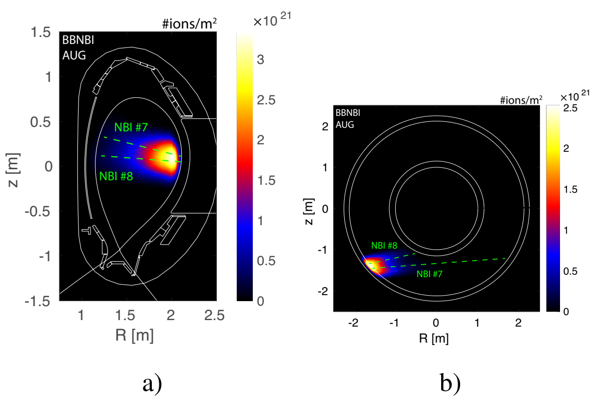
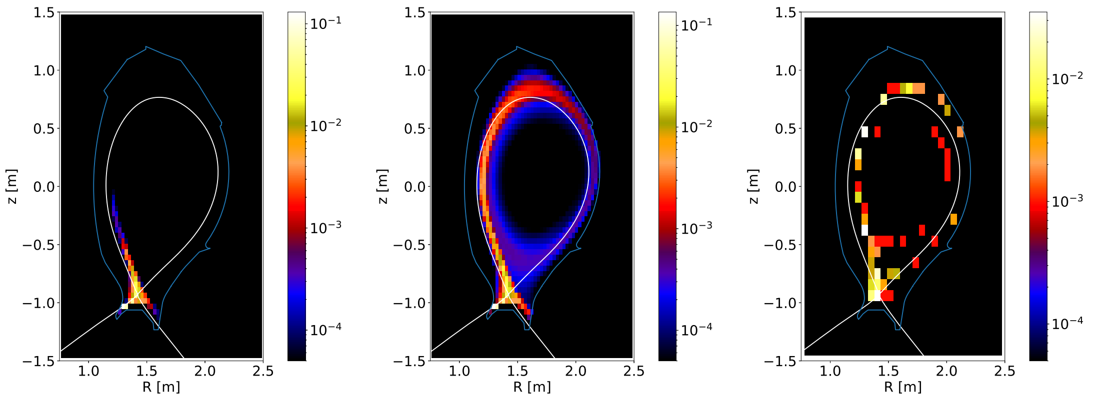


Figure 1: Initial distribution of beams Q7 and Q8 projected onto the toroidal (a) and toroidal (b) cross sections.



a) BMC, $T = 5\times10^{-6}$ s b) BMC, $T = 5\times10^{-4}$ s c) FMC, $T = 5\times10^{-4}$ s

Figure 2: Comparison of the probability from BMC and FMC for different total times T. Time step is $\Delta t = 1\times10^{-6}$ s with 100 sub-cycles. Grid size is 64 nodes in all dimensions. The illustrated quantity is the mean value of Φ over the $\phi, p_{\parallel}$ and $p_{\perp}$ dimensions.

	Mesh elements	T=2×10^{-5}s	T=1×10^{-4}s	T=5×10^{-4}s
FMC	—	10	10	11
BMC-IS	32^5	485	188	86
BMC-IS	64^5	920	853	829
BMC-IS	128^5	1909	1101	1097

Table 1: Number of recorded hits as a function of the total simulation times T for FMC and BMC-IS, using 10^5 input markers. Major time step is $\Delta t = 1\times10^{-6}$ s with 100 sub-cycles.

While the FMC manages only a few hits to the target, the BMC-IS provides a significantly larger number of recorded hits. These results are likely to improve if irregular meshes mimicking the field lines and the shape of the target domain are adopted.

In order to check quantitatively the consistency of the BMC scheme, the probability matrix has been computed for different mesh sizes and then compared to a FMC simulation using markers on a few common nodes. Figure 3 shows the resulting mean error of each mesh refinement after 5 major time steps with respect to the benchmark FMC solution. The error is consistently reduced by increasing the mesh density, indicating that the probability from the BMC calculation converges consistently towards the reference solution.

Summary and conclusions

This paper introduced a novel Backward Monte Carlo scheme to improve statistics in simulations of fast-ion losses, especially to small targets. The method was implemented within the

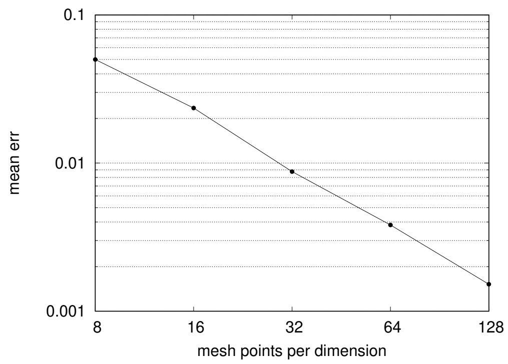


Figure 3: Convergence test for the BMC scheme.

ASCOT suite of codes and tested in realistic AUG configurations using NBI particle distributions. In the test cases considered, the approximate target hit probability from the fast Backward Monte Carlo calculation was used to perform importance sampling of the initial marker population. Using the re-sampled markers in Forward Monte Carlo simulations then significantly improved the statistics of target hits in comparison to not using the information from the Backward Monte Carlo calculation. These encouraging results are anticipated to improve further if irregular meshes, that adapt to target and plasma geometry, are explored.

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