# Neutral sampling vs. particle-identity conservation in a coupled fluid-kinetic Monte-Carlo code environment

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## Introduction

The main purpose of plasma edge code packages such as EMC3-EIRENE is to provide detailed bookkeeping in the multi-physics and multi-scale edge plasma problem. In order to isolate numerical from real (physical) dissipative effects in complex geometries, the code resorts to a (Lagrangian) particle scheme in which fluid parcels or individual particles retain their identify whenever possible, minimizing grid interpolation and resampling to capture also subtle cancellation effects with high precision.

Preparing and enforcing the code for future applications in even stronger dissipative conditions, such as tokamak divertor detachment with the ionisation–recombination fronts, we extend this particular conserving scheme now also to the interface between the neutral and ionised components. We show here that these first steps are implemented and working properly, by verification in well characterized benchmark cases, which do not yet have the complexity of ionisation-recombination fronts in the divertor.

## Eulerian vs. Lagrangian specification of flow fields

The Eulerian specification considers a fixed location in space through which a fluid flows as the time passes [1]. A typical example is a guy and/or girl sitting on a bench, looking at a river and counting all the boats passing. On the contrary, the Lagrangian specification can be summarised as following an individual fluid parcel as it moves through space and time. Coming back to the river example, it can be compared to a guy and/or girl sitting on one of the boats travelling along the river. The flow velocity in Eulerian specification is described as $\vec{u}(\vec{r},t)$, with position $\vec{r}$ and time $t$, whereas in Lagrangian specification one would use $\frac{\partial \vec{R}}{\partial t}(\vec{r}_0,t)$, with the parcel location $\vec{r}_0$ at initial time $t_0$ and position $\vec{R}$ of parcel "$\vec{r}_0$" at time $t$. The aforementioned parameters are connected via the relation

$$\vec{u}\left(\vec{R}(\vec{r}_0,t),t\right) = \frac{\partial \vec{R}}{\partial t}(\vec{r}_0,t)\,. \tag{1}$$

**EMC3**

The edge plasma Monte-Carlo code in three dimensions (EMC3) [2] is designed to deal with complex scrape-off layer geometries of magnetically confined fusion devices. It describes the plasma edge transport by solving a reduced set of Braginskii equations [3] utilising a diffusion-advection Monte-Carlo algorithm [4, Ch. 4.1]. When considering the two specifications of flow fields discussed above, one can describe the EMC3 algorithm as treating fluid parcels (momentum and energy) in the Lagrangian specification: a parcel is started at a given location and followed through the numerical grid until it terminates at a wall component. While the parcel is propagating it scores on a numerical grid to extract information on plasma properties like density and temperature from the fluid parcel's path. This obviously is done in an Eulerian specification. The plasma properties are needed, on the one hand, for internal iterations to capture the non-linearity in the Braginskii equations and, on the other hand, as output for comparison with experiments.

**EIRENE**

EIRENE's [5, 6] key feature is the simulation of neutral gas transport in arbitrary geometries. Designed for plasma–wall interaction purposes, its database focusses on typical plasma parameters near fusion device wall components. It solves the linearised Boltzmann equation by utilising a Monte-Carlo algorithm. The particles are treated in a Lagrangian specification. Similar to the case of EMC3 the resulting gas properties like density or ionisation sources are scored on a numerical grid in Eulerian specification as such quantities are the required outputs.

**Interface**

Internally, the EMC3 solver for the electron and ion energy balance and the solver for particle and momentum balance are coupled iteratively by exchanging the scored temperature values on the one hand and density and flow velocity on the other hand.

EMC3 and EIRENE are also coupled iteratively: besides the typical plasma properties ion density, electron and ion temperature, and flow velocity, EIRENE also requires a quantity that specifies the start properties of the neutral particles. Up to now, a particle deposition distribution has been transferred from EMC3 to EIRENE for this purpose. EIRENE, then, needs to sample the neutral particle start locations from that distribution. An obvious disadvantage of this approach is the artificial dissipation added via the sampling process as well as the numerical overhead of creating the distribution (by binning particle intersections) and sampling from it. In our revised formulation, particle positions and weights are handed over from EMC3 to EIRENE directly, so far retaining the energy and flow velocity parameters from the binned

EMC3 solutions in nearby grid cells, same as in the standard approach. In other words, the neutral particles simply continue from the location where ions hit the wall components and surface-recombination took place. The advantage is that one can avoid a change between the Lagrangian and Eulerian specification in the interface from EMC3 to EIRENE.

Finally, ionisation, energy, and momentum sources are transferred from EIRENE to EMC3 to close the loop in the iterative coupling of the two codes.

**Results**

An ITER sample case in a dissipative regime serves as an example for comparing the two interface modes. Figure 1 compares the down-stream electron density (left) and the down-stream electron temperature (right) for the so far used sampling interface (red dashed) and the developed particle-identity conserving interface (blue solid).

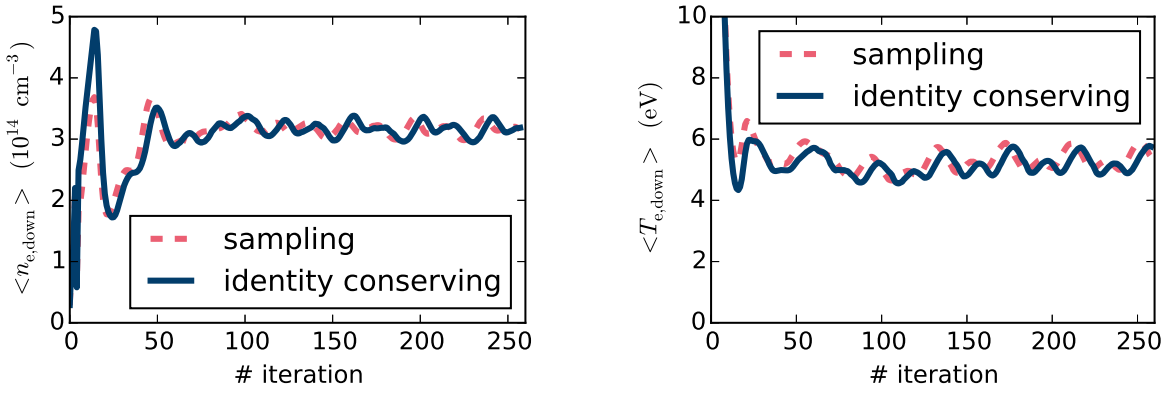


**Figure 1:** Comparing the old sampling interface with the new particle-identity conserving interface for the down-stream electron density (left) and the down-stream electron temperature (right). A similar behaviour can be observed while code iterations are performed, independent on the interface used.

No significant difference in the results can be observed. The observable oscillations while iterating the codes are likely a consequence of the missing volume-recombination processes in this simulations. However, this strict particle conserving scheme may become particularly relevant in a recombining plasma, to remove statistical sampling noise from the anyway challenging near cancellation of source and sinks due to recombination. It needs further investigation and will be part of future work; see section “Remaining issues”.

A crucial computational limitation of a three-dimensional code package like EMC3-EIRENE that is expected to simulate full machines, is its memory consumption. Here, one has to pay the prize for retaining particle-identities. With the sampling approach 28 B of memory are required per wall element on which the sampling takes place. In the ITER sample case considered here it sums up to about 157 kB. In contrast, 72 B need to be stored in memory for each particle if

particle-identity should be conserved. In total this results in about 1.85 MB for the used set-up. However, these total numbers are extremely case dependent. With the new interface one has a flexible control of the additional memory consumption by balancing iteration number vs. particle number. In the old interface the memory consumption was defined by the grid.

**Remaining issues**

Currently, there are still unnecessary changes from the Lagrangian into the Eulerian specification in the interface from EIRENE to EMC3 that can be avoided. Instead of scored sources of ionisation, momentum, or energy, fluid parcels can be handed over from EIRENE to EMC3.

Furthermore, one can implement volume-recombined of neutrals using particle-identity conservation. This avoids any numerical inaccuracy due to sampling.

**Conclusions**

The described work results in a more natural interface from the plasma edge transport code EMC3 to the neutral gas transport code EIRENE. It reduces the number of changes between Lagrangian and Eulerian specification and hence the artificial dissipation in the system. The trade-off for this increase in particle conservation is a higher memory consumption, which, however, on modern cluster architectures is of no obvious relevance and should be treated via shared-memory approaches within the codes (so-far fully absent).

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