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## Effect of Statistical Noise on Simulation Results with a Plasma Fluid Code Coupled to a Monte Carlo Kinetic Neutral Code\*

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Power exhaust is one of the major challenges that future devices such as ITER and DEMO will face. Because of the lack of identified scaling parameters, predictions for divertor plasma conditions in these devices have to rely on detailed modelling. Most plasma edge simulations carried out so far rely on transport codes, which most of the times consist of a fluid code for the plasma coupled to a kinetic Monte Carlo (MC) code for neutral particles. One of the main difficulties in interpreting code results is the statistical noise from the MC procedure, which makes it difficult to define a convergence criterion for the simulations. In this work, we elaborate on similarities between noisy transport code simulations and turbulence simulations, and argue that the time averaged solution is a well defined stationary solution for the system. We illustrate these ideas with a simple slab test case with fluid neutrals, to which we add synthetic noise. In this case, the effects of noise are found to be significant only at high noise levels and for large enough correlations times.

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### 1 Introduction

Power exhaust is one of the major challenges that future devices such as ITER and DEMO will face. Because of the lack of identified scaling parameters, predictions for divertor plasma conditions in these devices have to rely on detailed modelling [1]. Most plasma edge simulations carried out so far rely on transport codes, which consist of a fluid code for the plasma coupled to a kinetic Monte Carlo (MC) code for neutral particles (atoms, molecules). An example of such tools is the Soledge2D-EIRENE [2] code developed in our team. One of the main difficulties in interpreting code results is the lack of a proper convergence criterion for the simulations, since statistical noise originating in the kinetic MC calculation precludes, for most coupling procedures in use, residuals to reach machine precision. To solve this issue, one should as a first step take a rigorous look at the various types of errors in the simulations, in order to arrive at a cost effective simulation strategy, as shown by a companion paper [3]. Here, we take a different look at this noise related issues, based on our previous works regarding the proper derivation of transport equations from underlying first-principles fluid equations [2]. In Sec. 1, we argue that these two problems share strong similarities, and that what is usually referred to as the steady state reached by a transport code after convergence bears strong resemblance with the statistically stationary state reached by a turbulence code. This allows us to pinpoint the noise is affecting the problem to be solved, and provides a physical picture of its effects. In order to illustrate these theoretical results, we rely on the neutral fluid model implemented in Soledge2D-EIRENE, in a slab geometry for simplicity. The setup of the simulations is discussed in Sec. 3. In order to mimic the presence of statistical noise from the Monte Carlo simulations, we add synthetic noise to the neutral particle density, using a procedure described in Sec. 4. Section 5 discusses the effects of the noise, evidenced by comparisons with the noise-free solution.

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## 2 Seeing coupled fluid-Monte Carlo transport simulations through the lens of turbulence codes

In presence of statistical noise, coupled fluid-Monte Carlo kinetic transport simulations do not converge to a stationary solution, but rather to a Statistically Stationary State (SSS). It should be pointed out that this is not always the case, sometimes oscillating states of various flavors are reached. We exclude such cases from the discussion below, as a first step). Measuring convergence thus means assessing whether such a SSS has been reached, using a more or less refined metric. The last time step of the simulation is then often taken as the solution provided by the code, even though the system fluctuates. From a statistical physics point of view, the situation is reminiscent of that observed in plasma turbulence simulations. After a relaxation of the initial condition, simulations reach a SSS, the properties of which allows one to calculate the mean fields, their fluctuations levels and correlation coefficients providing turbulent fluxes. We propose to apply the same approach to transport codes, i.e. make use of the SSS to compute various statistical moments of interest. We shall treat the coupled fluid-Monte Carlo kinetic equations as a system of Stochastic Differential Equations (SDE) forced by noise, and define a probability average denoted by  $\langle \cdot \rangle$  over the noise introduced by the Monte Carlo code. Experience suggests that in many cases the system converges to a SSS, e.g. for the mean density  $\langle n \rangle$

$$\partial_t \langle n \rangle = -\nabla \cdot (\langle n u_{\parallel} \rangle \mathbf{b}) + \nabla \cdot (D \nabla_{\perp} \langle n \rangle) + \langle S_n \rangle = 0, \quad (1)$$

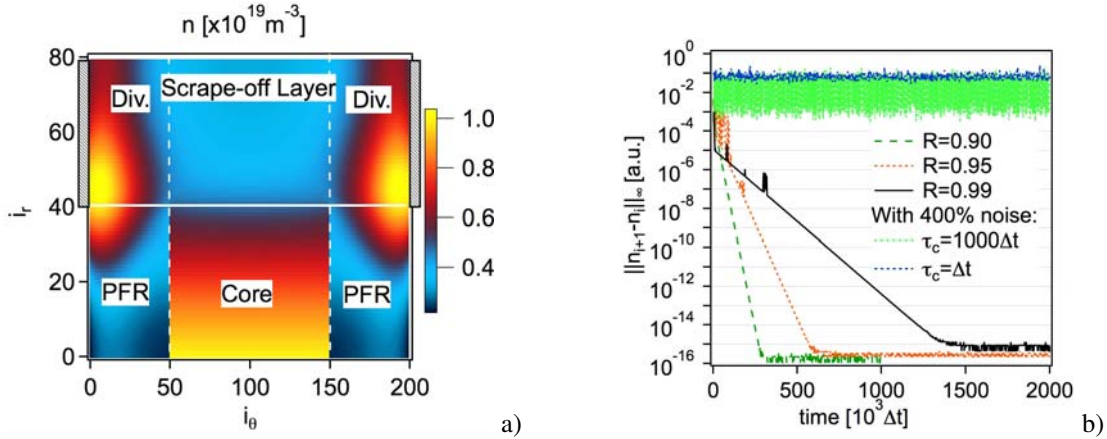
where  $\mathbf{b} = \mathbf{B}/B$ ,  $u_{\parallel}$  is the parallel fluid velocity,  $D_{\perp}$  the turbulent cross field diffusion coefficient and  $S_n$  the particle source from plasma neutrals interactions, through which the noise is entering the equation. In practice, the stationary value of mean fields in the SSS could be estimated by an ensemble average, converging  $N$  simulations with different random seeds and defining  $\langle n(\mathbf{r}, t) \rangle_E = \sum_{i=1, N} n_i(\mathbf{r}, t)/N$ . However, this approach is very demanding, and one can instead rely on the ergodic theorem [4] and use the fact that the time average  $\langle n \rangle_T$  converges in mean square sense towards the probability average as the width of the averaging window  $T \rightarrow +\infty$ . Loosely stated, the difference between  $\langle n \rangle$  and  $\langle n \rangle_T$  goes down with  $\tau_c/T$ , where  $\tau_c$  is the correlation time of the density fluctuations. The latter can be measured in the SSS, so that if the simulation is run in the SSS for a time much larger than  $\tau_c$ ,  $\langle n \rangle_T$  provides a reliable estimate of the probability average. Higher moments of the density fluctuations can be computed from the SSS, and of particular interest is the standard deviation  $\sigma_n = \sqrt{\langle n^2 \rangle_T - \langle n \rangle_T^2}$ . The latter provides a measure of the amplitude of density fluctuations in the SSS. If the Probability Distribution Function (PDF) of the density is gaussian,  $n(\mathbf{r}, t)$  will be within  $\pm 2\sigma_n$  from  $\langle n \rangle_T$  for 95.5 % of the time steps. This also holds for the density at the last time step, so that  $\sigma_n$  gives an indication about the error implied by using the last time step as solution. Now, the essential question is that of the distance between the mean solution and the noise-free solution  $n^{NF}$  (which would be obtained to machine precision by simulating an astronomically large number of trajectories). It obeys

$$-\nabla \cdot (n^{NF} u_{\parallel}^{NF} \mathbf{b}) + \nabla \cdot (D \nabla_{\perp} n^{NF}) + S_n = 0. \quad (2)$$

Comparing Eqs. (1) and (2), it becomes clear that the difference between  $\langle n \rangle$  and  $n^{NF}$  is partly rooted in correlation terms which are analogous to turbulent fluxes. Namely, we have  $\langle n u_{\parallel} \rangle = \langle n \rangle \langle u_{\parallel} \rangle + \langle \delta n \delta u_{\parallel} \rangle$ . The second term on the r.h.s is a parallel particle flux driven by fluctuations, which vanishes if  $n$  and  $u_{\parallel}$  are uncorrelated. The second difference is related to non-linearities in the particle source  $S_n$ . Considering only ionisation, we have  $S_n = n n_0 \bar{\sigma} v(n, T_e)$ , where  $n_0$  is the neutral particle density and  $\bar{\sigma} v$  the ionisation rate coefficient. By splitting the densities between mean and fluctuating parts,  $\langle S_n \rangle$  can be rewritten as a sum of several correlation coefficients, plus  $\langle n \rangle \langle n_0 \rangle \langle \bar{\sigma} v(n_e, T_e) \rangle$ . The fact that  $\langle \bar{\sigma} v(n_e, T_e) \rangle \neq \bar{\sigma} v(\langle n_e \rangle, \langle T_e \rangle)$ , essentially because of the non-linearity of  $\bar{\sigma} v$  with temperature, introduces an additional bias related to the presence of noise. However, it should be noted that obtaining large differences between  $\bar{\sigma} v(\langle n_e \rangle, \langle T_e \rangle)$  and  $\langle \bar{\sigma} v(n_e, T_e) \rangle$  requires fluctuation levels of several tens of percents [5]. To summarize, a time independent solution can be extracted from the SSS reached by the coupled fluid Monte Carlo code, and this solution differs from the solution without noise because of additional fluxes/source terms similar to those obtained by deriving mean field transport equations from the underlying turbulent equations. The key point to be illustrated in Sec. 5 is that these spurious terms can be estimated from the SSS.

### 3 Soledge2D test case with fluid neutrals

In order to illustrate the developments of the previous section, we rely on the Soledge2D code (see Ref. [2] for a description of the code) and its simple neutral fluid model. This allows one to solve for the noise free solution  $n^{NF}$ ,  $u^{NF}$ ,  $T_e^{NF}$ ,  $T_i^{NF}$ , which will be compared to mean solutions in presence of noise in Sec. 5. The neutral fluid model currently implemented in Soledge2D is a simple diffusive model, namely  $\partial_t n_0 - D_N \nabla^2 n_0 = -S_n$ , where  $D_N$  is constant in space ( $D_N = 10^3 \text{m}^2 \cdot \text{s}^{-1}$  in the following). For simplicity, we consider a slab case with  $R = 2$  m,  $r = 0.5$  m,  $q = 4$ ,  $B_{tor} = 2$  T and  $B_{pol} = 0.2$  T. The radial extent of the simulation domain is  $\Delta r = 10$  cm. In the simulations discussed here, the density at the core-edge interface is set to  $10^{19} \text{m}^{-3}$  and the temperatures to  $T_e = T_i = 100$  eV. The boundary conditions for neutrals is such that the only sources and sinks of neutrals are at the target plates, with a specified recycling coefficient  $R$ . The size of the mesh is  $80 \times 200$  points, and typical time steps are  $\Delta t \simeq 10^{-8}$  s (because Soledge2D relies on a mixed explicit/implicit scheme). The density field obtained for  $R = 0.95$  is shown on Fig. 1 as an illustration. The simulations are run until the residuals (defined as the maximum norm  $\|n_{i+1} - n_i\|_\infty$ , where  $n_i = n(t_i)$  for the density) reach machine precision, see Fig. 1 b) for  $R=0.9, 0.95$  and  $0.99$ . The particle balance  $\Gamma_{in} + S - \Gamma_{out} = 0$  is satisfied to machine precision (where  $\Gamma_{in}$  is the particle influx from the core,  $\Gamma_{out}$  the outflow on the target plates and  $S = \int \int \int dV S_n$  the volume integrated particle source from neutrals). By construction, we have  $S = R\Gamma_{out}$ , and when particle balance holds  $\Gamma_{out} = 1/(1-R)\Gamma_{in}$ . The total particle content  $\mathcal{N}$  evolves on a time scale  $\tau^* = \tau_0/(1-R)$ , where  $\tau_0 = \mathcal{N}/\Gamma_{out}$  is a particle confinement time. So as  $R$  approaches 1, we come to a situation where  $\tau^* \gg \tau_0$  (and, incidentally,  $\Gamma_{in} \ll \Gamma_{out}$ ). This explains why the convergence time increases sharply with  $R$  on Fig. 1 b).



**Fig. 1** a) 2D map of the plasma density illustrating the setup of the slab case, for  $R=0.95$  b) Decrease of residuals to machine precision for noise free cases with  $R=0.9, 0.95$  and  $0.99$ . Residuals in the SSS for cases with  $\mathcal{R}_0 = 400\%$  of noise discussed in Sec. 5, for  $\tau_c = \Delta t$  (dark blue) and  $1000\Delta t$  (green dotted). Note that this figure is made using 1000 points in time per simulation, so that time scales faster than  $1/1000$ th of the simulation length are filtered out.

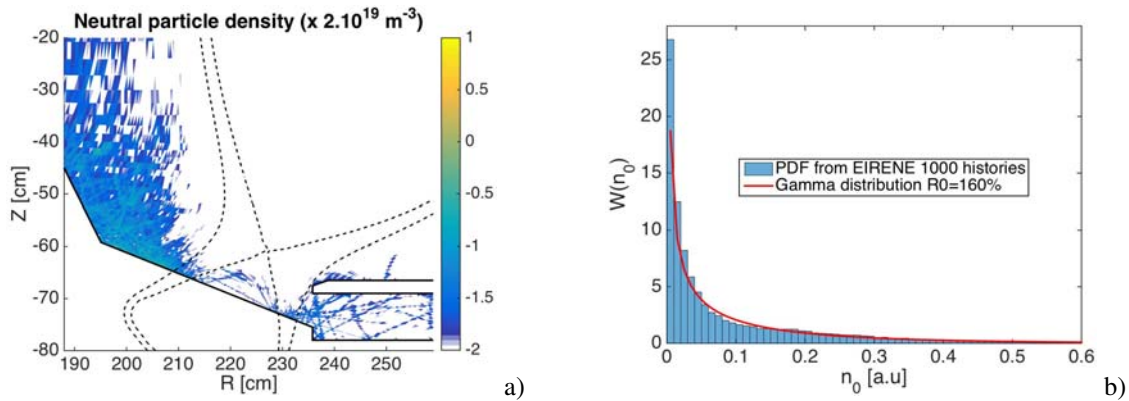
### 4 Properties of the synthetic noise added to the neutral particle density

We now define the properties of the synthetic noise  $\eta = \delta n_0(\mathbf{r}, t)$  which will be added to the neutral particle density  $n_0(\mathbf{r}, t)$  in order to mimic the statistical noise introduced by a Monte Carlo code such as EIRENE. This noise should have zero mean, so as to avoid introducing biases, and should guarantee  $n_0(\mathbf{r}, t) > 0$  even at large relative fluctuation levels. In previous works (e.g. [6]), we often relied on the gamma distribution to satisfy the latter condition. The gamma PDF is defined by

$$W(n_0) = \frac{1}{\Gamma(\beta)\alpha^\beta} n_0^{\beta-1} \exp\left(-\frac{n_0}{\alpha}\right), \quad (3)$$

where  $\alpha$  and  $\beta$  are respectively the scale and shape parameters, related to the mean and the variance  $\sigma_0^2$  through  $\langle n_0 \rangle = \alpha\beta$  and  $\sigma_0^2 = \alpha^2\beta$ . The relative fluctuation level  $\mathcal{R}_0 = \sigma_0/\langle n_0 \rangle$  is given by  $\mathcal{R}_0 = \beta^{-1/2}$ . For low

fluctuation levels, the Gamma PDF is very close from a Gaussian PDF, which is a desirable property here because the Central Limit Theorem shows that Monte Carlo noise should be gaussian when a large number of histories score in the cell of interest. For higher fluctuation levels the distribution becomes more and more positively skewed (its skewness is  $S = 2\mathcal{R}_0$ ). For  $\mathcal{R}_0 = 100\%$ ,  $W(n_0)$  reduces to the exponential distribution (hence  $W(n_0 = 0) = 1/\alpha$ ) and for higher fluctuation levels  $W(n_0) \rightarrow \infty$  as  $n_0 \rightarrow 0$ . This is again a desirable property, since the density map calculated by the Monte Carlo code using only few histories will have holes with  $n_0 = 0$  in cells where no trajectory scored. This is illustrated on Fig. 2 a), which shows the neutral particle density calculated with only 1000 particles on a converged WEST [7] Soledge2D-EIRENE solution. White regions correspond to  $n_0 = 0$ . The PDF of  $n_0$  in this case has been calculated for a limited number of cells in the grid, by running the simulation for  $7 \times 10^4$  time steps calling EIRENE at each time step. The result is shown on Fig. 2 b), for a point in the outer divertor leg. In order to compare to the gamma distribution, the parameters  $\alpha$  and  $\beta$  are recalculated from the time series (that is, from  $\langle n_0 \rangle$  and  $\sigma_0$ ) and the gamma PDF is plotted on Fig. 2 b) (solid red line). The agreement is excellent, and this observation holds also for the limited number of other cases we have studied. This points towards more than a coincidence. In fact, for integer values of  $\beta$ , the gamma distribution is the distribution of the sum of  $\beta$  exponentially distributed numbers. As a result, if the probability for a particle to score in a given cell is an exponential distribution (which is conceivable, e.g. law of rare events), then the neutral particle density should indeed be gamma distributed. In any case, our findings have implications on the estimation of the confidence level for  $n_0$  in MC runs (because the PDF, whatever it is, is clearly non-gaussian). For simplicity, we assume that the fluctuation level is spatially homogeneous in the whole domain. After the  $i^{\text{th}}$  time step of the fluid neutral code, at every point in space a gamma distributed density  $n_0^s(\mathbf{r}, t_i)$  of mean  $n_0(\mathbf{r}, t_i)$  and standard deviation  $\mathcal{R}_0 n_0(\mathbf{r}, t_i)$  is sampled and used to compute the particle, momentum and energy sources. We do not attempt to introduce spatial correlations here (as was done in ref. [8]), since the realizations of the neutral density fields are very spatially inhomogeneous (as shown on Fig. 2). The noise  $\delta n_0 = n_0^s - n_0$  can be frozen for a number  $k$  of time steps  $\Delta t$  (hence retaining in particular its spatial structure) in order to introduce time correlations, with a correlation time  $\tau_c = k\Delta t$ .

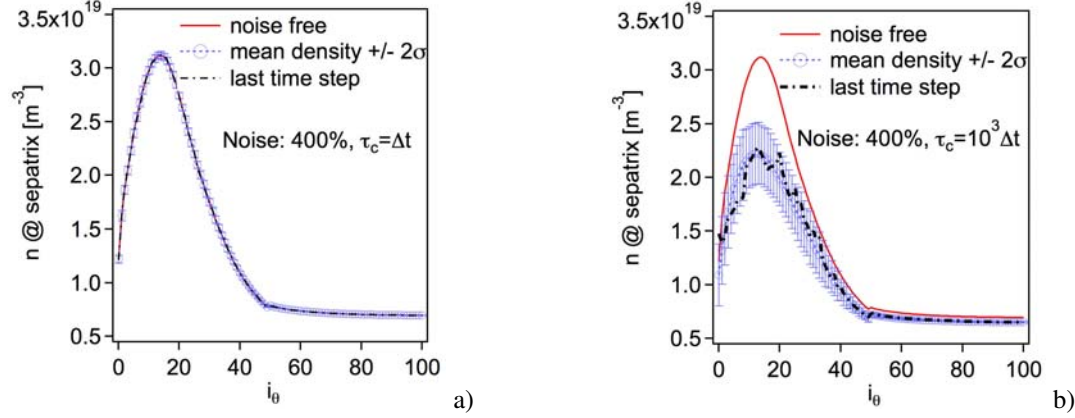


**Fig. 2** a) Atom density from EIRENE in a WEST case, with 1000 histories. The trajectories of recycled atoms are clearly visible through their scores into cells b) PDF of the neutral particle density in a cell located in the outer divertor leg (histogram). Red line: corresponding gamma PDF, with  $\mathcal{R}_0 = 160\%$ .

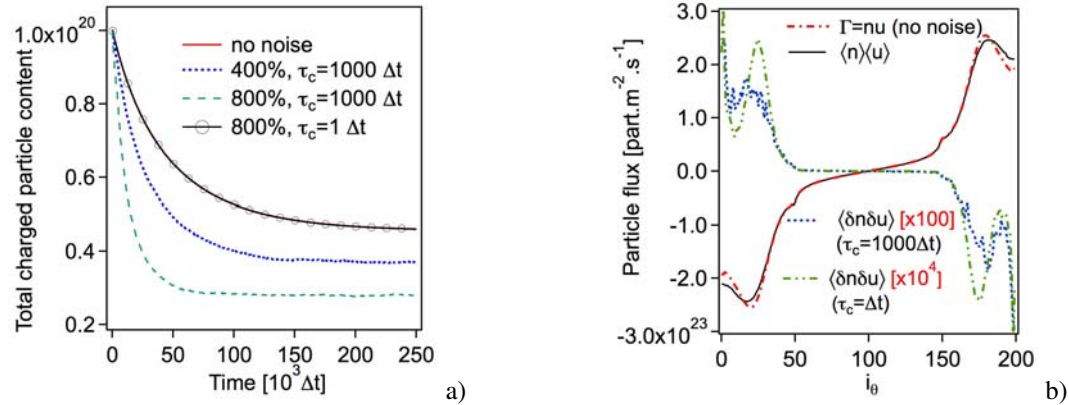
## 5 Effect of the synthetic noise on the test case simulations

In this section we focus on a case with  $R=0.99$ , since it is the most sensitive in terms of particle balance and thus should present a subset of the difficulties encountered in real ITER simulations. As shown on Fig. 3, this case is in a detached regime, so that we expect the particle source  $S_n$  to be a large term in the particle balance, and therefore that the effects of noise can become significant. We start by looking at cases with a time correlation for the noise such that  $\tau_c = \Delta t$ , i.e. refreshing  $\delta n_0(\mathbf{r}, t)$  at each time step, ramping up the relative fluctuation level from 10% to 800%. The overwhelming conclusion of this exercise is that when  $\tau_c = \Delta t$ , the system is extremely robust to noise. Even at  $\mathcal{R}_0 = 400\%$ , differences between the mean density profile and its noise-free counterpart

remain almost immaterial (0.1 % at maximum), see Fig. 3 a) (obtained by averaging over  $5 \times 10^5$  time steps). The relative difference between the mean solution and the last time step is below 2 %. The residual for the continuity equation, plotted on Fig. 1 (dark blue) saturate at a fairly high level, a situation which obviously results from the non-stationarity rather than from a strong deviation from the noise-free solution.



**Fig. 3** Plasma density profiles along the separatrix (half of the domain, because of symmetry), for  $\mathcal{R}_0 = 400\%$  and a correlation time of a)  $\tau_c = \Delta t$  and b)  $\tau_c = 10^3 \Delta t$ . Solid red, noise free solution, blue mean density with  $\pm 2\sigma_n$  error bars, representing the dispersion of profiles in the SSS. Dash dotted black : solution at the last time step



**Fig. 4** a) Relaxation of the total content of the plasma to its steady state (solid red, without noise). In presence of noise, with  $\tau_c = 10^3 \Delta t$  (same  $\Delta t$  as on Fig. 1b), the system relaxes faster to a lower plasma content. This behavior is consistent with changes of the particle confinement time  $\tau_0$ . b) comparison between  $\langle u_{\parallel} \rangle \langle n \rangle$  and  $\langle \delta n \delta u_{\parallel} \rangle$  in the simulations with  $\tau_c = 1000 \Delta t, \Delta t$ .

The situation changes when considering larger values of the correlation time for the noise,  $\tau_c$ , at high noise levels ( $\mathcal{R}_0 > 100\%$ ). This is reminiscent of the diabatic/adiabatic regimes introduced in Ref. [10], with  $\tau_c/\tau^*$  being the control parameter (note that here we have in both case  $\tau_c/\tau^* < 1$ ). In actual coupled fluid/Monte Carlo simulations, one would get increased  $\tau_c$  either by introducing correlations between successive Monte Carlo runs, and/or when the Monte Carlo code is not called at each time steps (the so-called short cycling procedure, first introduced in Ref. [9], on which Soledge2D-EIRENE heavily relies). Fig. 3 b) shows that for  $\mathcal{R}_0 = 400\%$  and  $\tau_c = 1000 \Delta t$  the mean density profile becomes quite different from the noise-free solution. The fluctuation level of the density fields also becomes substantial, as evidenced both by the error bars on the mean density representing  $\pm 2\sigma_n$  and the roughness of the profile at the last time step. It is likely that this results from the fact that the plasma has enough time to start adapting to each realization of the noise. This behavior is actually visible on the residuals plotted on Fig. 1 b) (green curve), where the large excursions results from these successive partial relaxation process. Note that while the mean parallel flow (see Fig. 4 b) and mean temperatures are also

affected by fluctuations, but to a smaller extent than density. We now focus on the mean particle balance for this particular case. In the SSS, we should have  $\langle \Gamma_{in} \rangle + \langle S \rangle - \langle \Gamma_{out} \rangle = 0$ . By calculating the time averages over  $2 \times 10^6$  time steps, we get  $(\langle \Gamma_{in} \rangle + \langle S \rangle - \langle \Gamma_{out} \rangle) / \langle \Gamma_{in} \rangle = 4 \times 10^{-3}$  (note that  $\langle S \rangle / \langle \Gamma_{out} \rangle$  is equal to  $R=0.99$  with an accuracy of roughly  $5 \times 10^{-3} \%$ ). The mean values for the three terms in the mean particle balance differ at most by 1% from their values in the noise free case. So, the noise is affecting the global particle balance in a seemingly minor way. But in terms of charged particle content  $\mathcal{N}$ , the effect are substantially stronger, as illustrated on Fig. 4 a), which shows the relaxation of  $\mathcal{N}$  with and without noise (solid red). It is clear that when the noise has significant effects on the mean solution, relaxation is *faster* and the final mean total content is *lower*. The effective recycling coefficient being essentially unaffected by noise, these observations can be interpreted as a reduction of the particle confinement time  $\tau_0$  (the relaxation time is  $\tau^* = \tau_0 / (1 - R)$  and the mean plasma content is  $\langle \mathcal{N} \rangle = \tau^* \langle \Gamma_{in} \rangle$ ). Why this happens is still under investigation. For instance, the term  $\langle \delta n \delta u_{\parallel} \rangle$  is plotted on Fig. 4 b), and is found to be small compared to  $\langle u_{\parallel} \rangle \langle n \rangle$  (but is 2 orders of magnitude larger than when  $\tau_c = 1$ ). Its contribution to the total outflow is of the order of 1%. The continuation of this work will deal with finding ways of identifying the terms responsible for the deviations observed, and practical criteria to judge whether they are small enough in actual simulations.

## 6 Conclusions and perspectives

In this work we have argued, by analogy with turbulence related studies, that the proper choice for the solution of coupled fluid-kinetic Monte Carlo simulations is the time average of the Statistically Stationary State (SSS). In most of the cases, this quantity is time independent, and is solution of a well defined set of equations. The latter exhibits additional terms compared to the initial system, originating from its parametric and/or statistical non linearities. The additional terms can be calculated from the SSS, and provide a physical picture of the effects of the noise, e.g. adding spurious contribution to parallel transport and particle sources in the continuity equation. The standard deviations of the various fields provide estimates for the noise-induced fluctuations in these fields, and in particular on the distance between the solution at the last time step and the mean solution. These ideas have been illustrated on a 2D slab case with the Soledge2D code, relying a simple fluid model for neutrals, to which synthetic noise is added. The mean solution is shown to be a very robust estimator of the noise free solution, even at relative fluctuations of several hundreds percents, provided the correlation time of the noise is short (here, one time step). For larger correlation times, the mean solution deviates from the noise free solution, and the exact mechanism through which noise induce these changes (one manifestation being a reduced particle confinement time) is still under investigation. In particular, the effect of noise on the numerical scheme (in particular for advection) on which the code relies should be investigated in depth, in order to determine whether it plays a role in the discrepancies observed.

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