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The role of statistical noise in edge plasma transport codes based on kinetic Monte Carlo solvers for neutrals: an analogy with turbulent fluctuations

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Abstract:
Power exhaust is a key challenge for future magnetic fusion devices. The modeling tools currently available to predict steady-state heat loads are transport codes, which solve mean field fluid equations for the plasma and often a kinetic Boltzmann equation for neutral particles. In several of the main transport codes available in the community, the latter is solved by a Monte Carlo procedure (implemented in the EIRENE code [4]). This has the adverse effect of introducing statistical noise in the system, whose effect on convergence and on code results have been poorly understood until recently. In this contribution, we highlight the analogy between turbulent fluctuations and statistical noise, from which a theoretical formulation of the problem can be extracted. We then illustrate the practical application of these results on a simple slab case, using a fluid model for neutrals, to which statistical noise is added.

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, 3, 4] 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 in Ref. [5]. Here, we take a different look at these noise related issues, based on our previous works regarding the proper derivation of transport equations from underlying first-principles fluid equations.

2 Theoretical considerations on Monte Carlo noise in transport codes

In the following we consider a standard (i.e. representative of models implemented in transport codes) set of balance equations for plasma density, ion momentum, electron and ion energy, namely

$$\frac{\partial n}{\partial t} + \boldsymbol{\nabla} \cdot \left(nu_\parallel \mathbf{b} - D_\perp \boldsymbol{\nabla}_\perp n\right) = S_n, \tag{1}$$

$$\frac{\partial nu_\parallel}{\partial t} + \boldsymbol{\nabla} \cdot \left(nu_\parallel \left(u_\parallel \mathbf{b} + \mathbf{v}_\perp\right)\right) = -\nabla_\parallel \frac{n(T_i + T_e)}{m} + \boldsymbol{\nabla} \cdot \left(\nu_\perp n \nabla u_\parallel\right) + S_m, \tag{2}$$

$$\begin{aligned}\frac{\partial}{\partial t}\left(\frac{3}{2}nT_e\right) &+ \boldsymbol{\nabla} \cdot \left(\left(\frac{5}{2}nT_e\right)\left(u_\parallel \mathbf{b} + \mathbf{v}_\perp\right)\right) \\ &= \boldsymbol{\nabla} \cdot \left(\kappa_e \nabla_\parallel T_e \mathbf{b} + \chi_\perp n \boldsymbol{\nabla}_\perp T_e\right) + \nabla_\parallel (nT_e) u_\parallel - Q_{ei} + S_{Ee},\end{aligned} \tag{3}$$

$$\begin{aligned}\frac{\partial}{\partial t}\left(\frac{3}{2}nT_i + \frac{1}{2}m_i n u_\parallel^2\right) &+ \boldsymbol{\nabla} \cdot \left(\left(\frac{5}{2}nT_i + \frac{1}{2}m_i n u_\parallel^2\right)\left(u_\parallel \mathbf{b} + \mathbf{v}_\perp\right)\right) = \\ \boldsymbol{\nabla} \cdot \left(\kappa_i \nabla_\parallel T_i \mathbf{b} + \chi_\perp n \boldsymbol{\nabla}_\perp T_i + \nu_\perp n \boldsymbol{\nabla}_\perp \left(\frac{1}{2} m_i u_\parallel^2\right)\right) &- \nabla_\parallel (nT_e) u_\parallel + Q_{ei} + S_{Ei}\end{aligned} \tag{4}$$

where $\mathbf{v}_\perp = -\frac{D_\perp}{n}\boldsymbol{\nabla}_\perp n$, and where the parallel momentum balance has been used to express $E_\parallel$ is terms of $\nabla_\parallel T_e$ (namely, $-enE_\parallel - \nabla_\parallel(nT_e) - R_{ei} = 0$, with R_{ei} the parallel friction force between ions and electrons). Q_{ei} accounts for equipartition between ions and electrons. Here $D_\perp$, $\nu_\perp$ and $\chi_\perp$ are anomalous transport coefficients accounting for turbulent transport in the frame of a gradient diffusion hypothesis [6], that is for example

$$\langle \tilde{n}\tilde{u_\perp} \rangle = -D_\perp \boldsymbol{\nabla}_\perp \langle n \rangle, \tag{5}$$

where angled brackets denote an average over turbulent fluctuations and $\tilde{n}$ and $\tilde{u}_\perp$ are the fluctuating parts of the density and velocity fields. Eq. (1) to (4) are thus mean field equations supplemented by a simple statistical closure accounting for fluctuations. Note that the mean perpendicular flow velocity $\langle u_\perp \rangle$ does not appear in the model, because (mean) drifts are not considered at this point of the discussion (e.g., we assume

$\langle u_\perp \rangle = 0$). The terms S_n, S_m, S_{Ee} and S_{Ei} stand respectively for the particle, ion momentum, electron and ion energy sources (sinks) related to interactions with the neutral species (atoms, molecules). Neutrals are ubiquitous in edge plasmas, and are often treated kinetically (because of their potentially very long mean free paths and/or first flights) by the mean of a Monte Carlo approach. The latter is well suited to handle the geometrical and chemical complexity of the plasma edge, and does not require full phase resolution (6D) to calculate moments of the velocity distributions of the various neutral species involved. The con of the method is that it introduces statistical noise, i.e. it provides estimates of the source terms with a statistical error which cannot - by far - be reduced to machine precision levels in most of the cases of practical interest. The convergence of the code becomes thus more challenging to assess, and the possibility that noise could strongly affects solutions obtained for the non-linear system of equations considered here cannot be ruled out. While practice can provide a feeling about these issues (by changing the level of noise, etc ...), it would be much safer to rely on a theoretical understanding of these issues. The purpose of the remainder of this section is to propose a theoretical formulation of this problem.

In the presence of Monte Carlo noise, the system of differential equations to be solved becomes a system of stochastic differential equations forced by multiplicative noise (because of the form of the sources related to interaction of neutrals). As a result, each transport code run is a realization of a stochastic process, which in most cases converges to a statistically stationary state (SSS). Different realization can be obtained by changing the seed of the random generator in the Monte Carlo code. It is then natural to average over many of these realizations to obtain a mean solution (i.e. $\langle n(\mathbf{r})\rangle$, $\langle u_\parallel(\mathbf{r})\rangle$... which is time independent because of stationarity). In fact, when dealing with stochastic process, predictions are made on statistical moments, not on the detailed time evolution of the fields. Since converging a large number of runs is resource intensive, it is more practical to rely on ergodicity and estimate the mean fields by time averaging in the SSS. The time averaging window T_{av} should be much larger than the autocorrelation time τ of the field considered (how "much larger" has be determined in practice, knowing that the time average converges in the mean square sense as τ/T_{av} towards the true average). The longer T_{av}, the higher the price to pay in CPU usage, since the code has to be run for a longer time in the SSS. So far the usual practice in the community has been to define the solution as the last time step of a run. The distance between this snapshot and the true mean solution can be estimated by calculating the mean square deviation of the various fields in the SSS. Obviously, it will strongly depend on the noise level. Now, the remaining key question is how much the mean solution differs from the zero noise solution. In order to answer this, we remark that equations for the mean solution can be readily obtained by averaging all equations over noise, exactly in the same way as transport equations are derived from the underlying system describing plasma edge turbulence. This leads to equations similar to Eq. (1) to (4) for the mean fields, with a number of additional terms of the same nature as turbulent fluxes (see Eq. (5)). Due to space restrictions, only some of these terms are given explicitly below. Divergences of fluxes (plus time dependent terms vanishing in the SSS) are denoted by $\mathcal{DF}_i$ and are to be found on l.h.s., while sources $\mathcal{S}$ are on the r.h.s.

$$\mathcal{D}\mathcal{F}_n = \boldsymbol{\nabla} \cdot \left(\langle \tilde{n}\tilde{u_\parallel}\rangle \mathbf{b}\right)\rangle \tag{6}$$

$$\mathcal{D}\mathcal{F}_m = \frac{\partial}{\partial t}\langle \tilde{n}\tilde{u_\parallel}\rangle + \boldsymbol{\nabla} \cdot \left(\langle n\rangle\langle \tilde{u_\parallel}^2\rangle + 2\langle \tilde{n}\tilde{u_\parallel}\rangle\langle u_\parallel\rangle\rangle + \langle \tilde{n}\tilde{u_\parallel}^2\rangle\right) \mathbf{b} \tag{7}$$

$$\begin{aligned}
\mathcal{D}\mathcal{F}_{Ei} = \frac{\partial}{\partial t}&\left[\langle \tilde{n}\tilde{T_i}\rangle + \frac{1}{2}m_i\left(\langle n\rangle\langle \tilde{u_\parallel^2}\rangle + 2\langle \tilde{n}\tilde{u_\parallel}\rangle\langle u_\parallel\rangle + \langle \tilde{n}\tilde{u_\parallel^2}\rangle\right)\right] \\
&+ \boldsymbol{\nabla} \cdot [\frac{5}{2}\left(\langle n\rangle\langle \tilde{T_i}\tilde{u_\parallel}\rangle + \langle \tilde{n}\tilde{u_\parallel}\rangle\langle T_i\rangle + \langle \tilde{n}\tilde{T_i}\rangle\langle u_\parallel\rangle + \langle \tilde{n}\tilde{T_i}\tilde{u_\parallel}\rangle\right)\mathbf{b} \\
&- \frac{5}{2}D\left(\langle n\rangle\langle \tilde{T_i}\boldsymbol{\nabla}\tilde{n}\rangle + \langle \tilde{n}\boldsymbol{\nabla}\tilde{n}\rangle\langle T_i\rangle + \langle \tilde{n}\tilde{T_i}\rangle\boldsymbol{\nabla}\langle n\rangle + \langle \tilde{n}\tilde{T_i}\boldsymbol{\nabla}\tilde{n}\rangle\right) \\
&+ \frac{1}{2}m_i\left(3\langle n\rangle\langle u_\parallel\rangle\langle \tilde{u_\parallel}^2\rangle + \langle n\rangle\langle \tilde{u_\parallel}^3\rangle + 3\langle u_\parallel\rangle^2\langle \tilde{n}\tilde{u_\parallel}\rangle + 3\langle u_\parallel\rangle\langle \tilde{n}\tilde{u_\parallel}^2\rangle + \langle \tilde{n}\tilde{u_\parallel^3}\rangle\right)\mathbf{b} \\
&- \frac{1}{2}m_i D(2\langle n\rangle\langle u_\parallel\rangle\langle \tilde{u_\parallel}\boldsymbol{\nabla}\tilde{n}\rangle + \langle n\rangle\langle \tilde{u_\parallel}^2\rangle\boldsymbol{\nabla}\langle n\rangle + \langle n\rangle\langle \tilde{u_\parallel}^2\boldsymbol{\nabla}\tilde{n}\rangle + \langle u_\parallel\rangle^2\langle \tilde{n}\boldsymbol{\nabla}\tilde{n}\rangle + 2\langle \tilde{n}\tilde{u_\parallel}\rangle\langle u_\parallel\rangle\boldsymbol{\nabla}\langle n\rangle \\
&+ 2\langle u_\parallel\rangle\langle \tilde{n}\tilde{u_\parallel}\boldsymbol{\nabla}\tilde{n}\rangle + \langle \tilde{n}\tilde{u_\parallel}^2\rangle\boldsymbol{\nabla}\langle n\rangle + \langle \tilde{n}\tilde{u_\parallel}^2\boldsymbol{\nabla}\tilde{n}\rangle]
\end{aligned} \tag{8}$$

In SSS, these terms can be interpreted as the divergence of spurious fluxes resulting from noise, more precisely from the random fluctuations of the various fields and their correlations. In other words, the effect of noise is similar to that of turbulence. Note that mean drifts are not included in Eq. (1) to (4), so that there are is no "direct" contribution (that is through advection) of noise to cross field transport here. There are however contributions to cross field transport from gradients of correlations or mean fields. We do not discuss here the ordering between these terms, and point out that since $\langle u_\parallel\rangle$ can be almost zero in large parts of the domain, the fluctuation level of the parallel velocity could potentially be large (that is, markedly larger than that of other fields - precluding an analysis based on the smallness of the fluctuation level). Expressions of the r.h.s. terms ("sources" $\mathcal{S}$) are similar, we note that $\mathcal{S}_n = 0$ and that e.g.

$$\mathcal{S}_m = -\nabla_\parallel \frac{\left(\langle \tilde{n}\tilde{T_e}\rangle + \langle \tilde{n}\tilde{T_i}\rangle\right)}{m} + \boldsymbol{\nabla}\nu_\perp\langle \tilde{n}\boldsymbol{\nabla}\tilde{u_\parallel}\rangle \tag{9}$$

the first term being the contribution of the pressure fluctuations to the mean force balance. An additional source of differences between the mean solution and the zero noise solution is found in the sources related to interactions with neutrals. The latter differences result both from Monte Carlo noise *and* the fact that neutrals see a fluctuating background. The latter effect is substantial only when the fluctuation levels of the density and temperature fields reach several tens of percents and the spatial correlation lengths of the fluctuations are large (see Ref. [7]). The mean sources (e.g. $\langle S_n\rangle = \langle nn_0\overline{\sigma v}(T_e)\rangle$ in the simplest case where only ionization is taken into account - $\overline{\sigma v}$ being the rate coefficient and n_0 the neutral particle density) have to be compared to the sources calculated with the mean fields $S_{mf,i}$ (namely $\langle n\rangle\langle n_0\rangle\overline{\sigma v}(\langle T_e\rangle)\rangle$).

It should be highlighted that all these additional terms, $\mathcal{DF}_i$, $\mathcal{S}_i$ and $\langle S_i\rangle - S_{mf,i}$ (with $i = n, m, T_e, T_i$) can be be calculated numerically by running the code in the SSS (again making use of the ergodic theorem), and compared to other terms in the equations in order to quantify how much noise affects the balance equations. Note that this does not provide a straightforward way of estimating the bias introduced on the solution itself, which is the ultimate goal of this work. In the following we will report on numerical results obtained with Soledge2D coupled to a very simple fluid neutral model, for which a noise-free numerical solution can be obtained (i.e. converged to machine accuracy). Synthetic noise is then added to the neutral particle density n_0 calculated with the fluid model.

3 Synthetic noise in Soledge2D

A simple diffusive model for the neutral particle density n_0 is available in Soledge2D, namely $\partial_t n_0 - D_N\nabla^2 n_0 = -S_n$. Here D_N is constant in space ($D_N = 10^3\mathrm{m}^2.\mathrm{s}^{-1}$ in the results presented later on). For simplicity, a slab case with $R = 2$ m, $r = 0.5$ m, $q = 4$, $B_{tor} = 2$ T and B_{pol}=0.2 T is considered. The simulation domain has a radial extent of 10 cm. The density at the core-edge interface is set to 10^{19} 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, where a recycling coefficient R is specified ($R = 0.99$ in the following). The mesh has 80x200 points, and it has to kept in mind that typical time steps are of the order of $\Delta t \simeq 10^{-8}$ s because Soledge2D relies on a mixed explicit/implicit scheme. This will turn out to be a key point in the discussion of our results. We now would like to add statistical noise $\delta n_0(\mathbf{r}, t)$ to the neutral particle density field. An analysis of the Probability Density Function (PDF) of neutral particle density fluctuations in an actual Soledge2D-EIRENE run shows that it is surprisingly close to a gamma PDF [8]. The latter has a positive support which is appropriate for a density field, and reduces to a Gaussian at low fluctuation levels, which is the expected behavior (because of the Central Limit Theorem, since low fluctuation level means many trajectories are calculated and the density field results from the contribution of a large number of trajectories). This agreement is illustrated on Fig. 1 a). We therefore implemented a post-treatment of the density field n_0 in the code, whereby n_0 is replaced by a realization of a gamma multivariate field with no spatial correlations n_0^g such that $\langle n_0^g\rangle = n_0$. Two examples of such realizations are provided on Fig. 1 b) and c), with different relative fluctuation levels of the noise $R = \sqrt{\langle n_0^2\rangle - \langle n_0\rangle^2}/\langle n_0\rangle$, namely 90 % and 400 % (note that these values are indeed achievable with a real Monte Carlo code run with few particles). Typically, as the fluctuation level increases, the density field becomes more and more patchy. The sources S_n, ..., S_{T_i} are then calculated using n_0^g, feeding noise through the system. An additional parameter is introduced in order to control the time correlation of the noise, e.g. a correlation time measured here in units of time steps Δt. This is made necessary by the fact that Soledge2D is run with short time

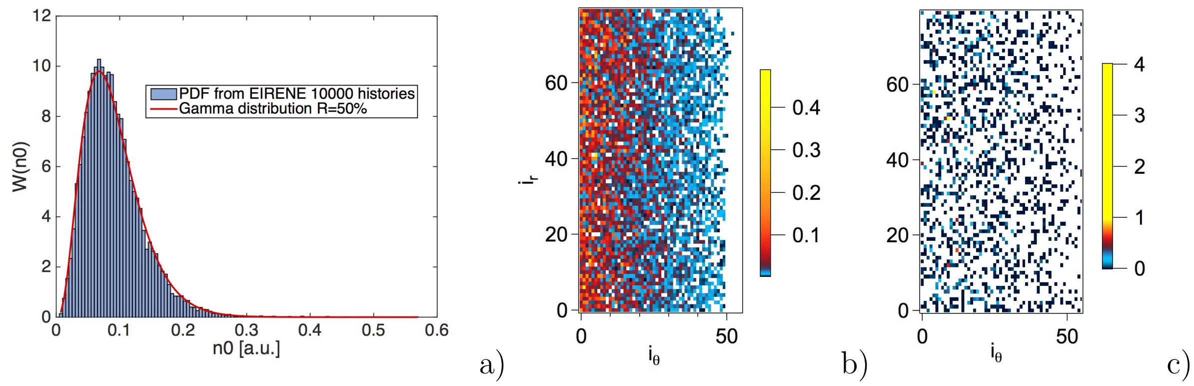
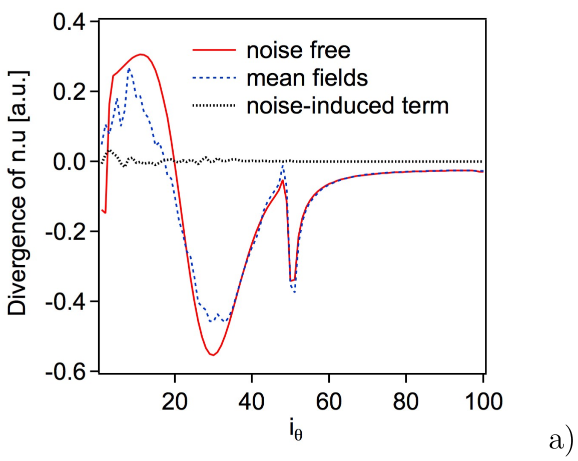


FIG. 1: a) Histogram of the neutral particle density compared to the gamma PDF. The latter is parametrized with the moments of the time series, i.e. the agreement is not improved by fitting. The relative fluctuation level is 50 % here, corresponding to 10^4 *particles in a WEST case. b) Neutral density field close to one of the divertor targets in the slab model, with 90 % of noise c) same with 400 %.*

steps, so that EIRENE is not called at every time steps (”short cycling”). Therefore, the noise is frozen in-between EIRENE calls. Also, some coupling schemes aim at increasing correlations between successive Monte Carlo noise, and can also be emulated by increasing the correlation time of the noise in our toy model system.

4 Effects of noise

We summarize here the findings made by running the slab case with synthetic noise, which have been first presented in Ref. [8], and elaborate further on the results. Perhaps the most striking finding is that when the noise is uncorrelated in time (i.e. refreshed at every time step of the fluid code), the system proves to be extremely resilient to noise. Fig. 3 a) of Ref. [8] shows virtually no effect on the parallel plasma density profile along the separatrix for relative fluctuation levels as high as 400% (see Fig. 1) - in fact the differences between the mean solution and the noise-free solution is at most 0.1%. This is associated to very low fluctuation levels, because the noise is filtered out from the system: the dynamics of the system is too slow to adapt to fluctuations in neutral particle density, so that the systems only sees the average density. Another way to see things is to note that the fluctuation levels of all plasma fields are very low, so that noise-induced spurious terms are negligibly small in the equations. In order for the noise to have a marked impact on results, it is necessary to increase the correlation time of the noise τ_n by several orders of magnitude (compared to Δt). Then, as shown on Fig. 3 b) of Ref. [8] for a correlation time of $\tau_n = 10^3 \Delta t$, the mean parallel plasma density profile along the separatrix deviates markedly from the noise-free solution. At the same time, the residuals of the equations show much larger excursions (following noise re-sampling) than in the $\tau_n = \Delta t$ case and the fluctuation level of the different fields is much larger too. All these observations point to the fact that the system now has time to react to noise, which translate in larger



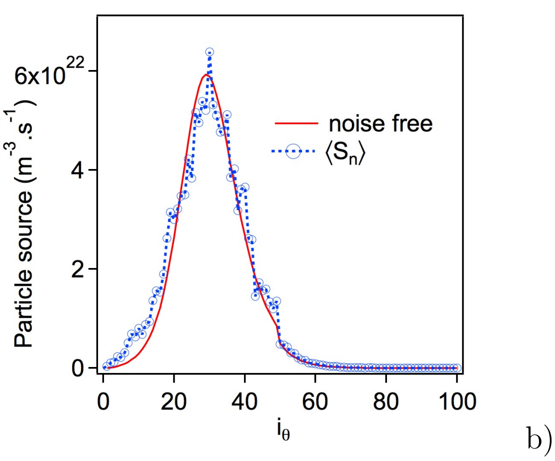


FIG. 2: a) Divergence of $nu_\parallel$ in the noise free case (solid red) compared to the divergence of $\langle n\rangle\langle u_\parallel\rangle$ (dashed blue) and the divergence of $\langle\tilde{n}\tilde{u}_\parallel\rangle$ (dotted black). b) Noise-free particle source S_n (solid red) compared to the mean source $\langle S_n\rangle$ for $\tau_c = 10^3\Delta t$ and $R = 400$ %
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excursions of the time dependent solution and thus larger noise-induced terms. Fig. (2) compares $\mathcal{DF}_n = \boldsymbol{\nabla}\cdot\langle\tilde{n}\tilde{u}_\parallel\rangle\mathbf{b}$ to $\boldsymbol{\nabla}\cdot\langle(n)\langle u_\parallel\rangle\mathbf{b})$, and shows that while $\langle\tilde{n}\tilde{u}_\parallel\rangle$ is typically two orders of magnitude smaller than the mean field contribution (see Fig. 4 b) of Ref. [8]), the actual contribution of the divergence of this flux is only one order smaller because of the larger gradients. The noisy behavior is also seen on the mean sources on Fig. 2 b), and results from the fact that the time averaging window is of the order of 10^3 noise autocorrelation time τ_n. This is not enough to smooth sources because of the very high fluctuation level of the neutral particle density field. However, the mean plasma density and temperature fields are much smoother and do not further evolve if the time averaging window is increased, which means that the requirements in terms of terms of averaging window length for these fields are much less stringent than for sources.

The validity of our conclusions remain to be assessed in more complicated "real life" cases, but recent results suggest that the mean solution obtained for ITER cases with the SOLPS code run with very few particles (several hundreds) show remarkably low biaises compared to simulations run with much higher statistics [9]. This results are very encouraging and could help reducing the computational cost of such simulations by orders of magnitude.

5 Conclusions and perspectives

The conclusions of this work are that: i) time averaged plasma solutions should be used instead of the last time step ii) that the time averaged plasma is solution of equations with noise-induced terms very similar to turbulent fluxes, which can be calculated by running the code in the "converged" state. iii) the effects of noise strongly depend on its randomness in time. Namely very high noise levels are tolerable if there are no correlations in time, i.e. the noise is "refreshed" at every iterations. On the contrary, if the noise is frozen too long (e.g. because the Monte Carlo code is not called at every time step) then eventually marked biases can occur at very high fluctuations levels. We believe that this provides very useful guidelines to run the code efficiently, and could lead to orders of magnitude in reduction of computational time for transport code through a potentially drastic reduction of the number of particle histories calculated in the Monte Carlo solver.

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References

[1] A. S. Kukushkin et al. Fusion Eng. Design 86 2865, 2011.

[2] H. Bufferand et al. Contrib. Plama Phys., 54:378, 2014.

[3] H. Bufferand et al. Nuclear Fusion 55 053025, 2015.

[4] D. Reiter et al., Fusion Sci.Technol. 47 172, 2005.

[5] K. Ghoos et al., Contrib. Plasma Phys. 56 616, 2016.

[6] S. B. Pope *Turbulent Flows*, Cambridge University Press, 2001.

[7] Y. Marandet et al. Plasma Phys. Control. Fusion, 53:065001, 2011.

[8] Y. Marandet et al. Contrib. Plasma Phys. 56 604, 2016.

[9] T. Baelmans et al., 22^{nd} International Conference on Plasma Surface Interactions, Roma, May 30^{th}-June 3^{rd}, submitted to Nuclear Materials and Energy.