Numerical error analysis of SOLPS-ITER simulations of EAST

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Abstract

Plasma edge simulations with codes like SOLPS-ITER are widely employed to interpret fusion experiments. However, numerical errors appearing in such simulations are rarely investigated although they can have a large impact on the simulation result. They consist of the statistical error and the bias which both result from the finite number of involved EIRENE Monte Carlo particles and incomplete convergence, and the discretization error due to the finite resolution of the B2.5 and EIRENE grids. In this contribution, the resulting numerical errors on pure deuterium and neon seeded simulations of H-mode EAST discharges are examined. The statistical error can be kept small by averaging the plasma profiles over 45,000 simulation steps, and the bias and discretization errors are investigated using Richardson extrapolation. It is shown that grid refinement and employed Monte Carlo parameters have a significant influence on the result, thus careful choices should be made. This is in agreement with similar studies of an ITER deuterium case. For the first time, numerical error bars on the entire simulated target profiles are determined. By employing a good setup, the largest numerical error is 17.9 %, due to the plasma grid discretization. On top, also numerical errors on simulated neutral pressures are

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investigated in detail, for which the statistical error is dominant. The analysis demonstrates what is needed to keep numerical errors limited using a reasonable computational time: the SOLPS-ITER averaging procedure should be employed in which enough EIRENE particles are included in the last two steps, it has to be ensured that the simulation is in the linear regime, both with respect to the included number of EIRENE particles and to the refinement of the involved grids, and it should be investigated on beforehand which reactions will play an important role in the studied discharge.
Keywords: SOLPS-ITER, numerical errors, statistical, bias, discretization, EAST

1. Introduction

A decrease in power and particle exhaust towards the divertor targets of a tokamak is important for future fusion devices [1]. Current experiments focus on the use of extrinsic impurities to decrease these fluxes [2]. To investigate the effect of such impurities, a good understanding of the physics happening in the plasma edge of a tokamak is needed. Therefore, modeling is often used to examine the plasma edge more in detail [3, 4, 5, 6].

A plasma consists of many particles (both electrons and ions). Each of these particles has a position and a velocity. Starting from the general Boltzmann equation (which is also valid for plasma particles), a collisional plasma can be described by the Fokker-Planck equation [7]. When the collisionality is high, a fluid approximation can be made and the behavior of the electrons and ions in a tokamak plasma can be described by the Braginskii equations, which are conservation laws for density, momentum, and ion and electron energy [8]. In these Braginskii equations, source terms appear due to interaction of plasma with neutrals present in the tokamak edge. As the neutrals collisionality is not everywhere high enough to use a fluid description, they are better described kinetically by solving the Boltzmann equation.

The B2.5 code is a finite volume (FV) code solving these Braginskii equa-

tions for the plasma particles [9]. The EIRENE code is a Monte Carlo (MC) code solving the Boltzmann equation [10], thus it describes macroscopic neutral quantities in a statistical sense. The SOLPS-ITER code package couples these two codes to model plasma and neutral behavior in the tokamak plasma edge [11, 12]. While handling such numerical plasma edge codes, it is important to consider possible errors on the simulation result as they can influence the solution drastically and lead to wrong physical interpretations. Four types of errors can be present: modeling, code, user, and numerical errors [13]. On top, also modeling uncertainties (material parameters, reaction rates...) can influence the result of a simulation.

By employing SOLPS-ITER as a user, the focus is on avoiding user errors and keeping the numerical ones small. User errors appear mostly due to wrong input parameters, while numerical ones depend on the strategy adopted to solve the continuous governing model equations in a discrete setting. By avoiding user errors and keeping numerical ones small, the remaining errors present in the problem are limited to modeling errors and uncertainties. Moreover, the employed numerical strategy plays an important role in balancing the run-time/computational cost versus accuracy [14].

The coupled FV-MC nature of SOLPS-ITER leads to complex interactions and various error contributions, that complicate the analysis compared to standard error estimation for finite volume codes. Only recently these error contributions have been unraveled [14, 15]. In here, Ghoos et al. developed a strategy to compute the numerical errors assessing a trade-off between the resulting error versus code speed. This strategy was successfully applied to simulations of purely deuterium cases for ITER [16, 17] showing that finer grids decreased the estimated discretization error at the divertor targets with a factor of around four (from a discretization error of maximum 60 % to one of maximum 15 %) resulting in significantly higher heat loads on the ITER divertor than predicted with coarser grids.

In the current analysis, the main goal is to show that the numerical errors on the employed simulation setup make physical interpretation possible keeping

a reasonable computing time. This is examined both for an unseeded and a neon seeded simulation. It will be the first time that such an error analysis is performed for simulations with extrinsic impurities present in the tokamak. To ensure a correct comparison with experimental data in a later stage, the errors are analyzed over the entire plasma profiles at the outer midplane and the divertor targets (which are of the highest interest for comparison with experiments). On top, also numerical errors on simulated neutral pressures are examined at the locations of the available pressure gauges.

In ref. [3] Ne seeding experiments performed at the EAST tokamak and initial SOLPS-ITER modeling for an unseeded deuterium discharge were presented. Starting from these simulations, the numerical errors are investigated.

In the next section, the numerical errors appearing on simulation results are described more in detail. Afterwards, the examined SOLPS-ITER setup is discussed in section 3, focusing on the parameters affecting numerical errors. Afterwards, the errors on this particular case are analyzed in section 4. The paper concludes with general recommendations for the numerical setup derived from this study.

2. Numerical errors in SOLPS-ITER

In SOLPS-ITER simulations the numerical error ϵ_{num} appears due to the involved numerics in the B2.5 FV code and in the EIRENE MC code. It is composed of four parts [15]:

$$\epsilon_{num} = \epsilon_d + \epsilon_c + \epsilon_b + \epsilon_s. \tag{1}$$

ϵ_d is the discretization error due to the finite resolution of the grids on which equations are solved. ϵ_c is the error arising from incomplete convergence of the residuals in the FV code (B2.5). ϵ_b is the deterministic (or finite sampling bias) error present in MC codes due to limited number of included particles in combination with the nonlinear coupling of the MC code with the FV one. The statistical error ϵ_s appears as (statistical) noise which is linked with the finite

number of MC particles. This statistical noise has a probability distribution with zero mean and standard deviation dependent on the problem setup.

In the further scope of this paper, the appearing numerical error is examined in three parts: the statistical error ϵ_s, the combination of the convergence error (ϵ_c) and the finite sampling bias (ϵ_b) – together called the bias –, and the discretization error ϵ_d.

The order in which they should be analyzed is predefined. In fact, the discretization error is the error due to the finite grid spacing in case of an infinite amount of MC particles per iteration [15, 18]. This implies that the discretization error is the last to be assessed.

The statistical and bias error represent the influence of the finite number of particles included in an EIRENE simulation. The deviation of the solution in case of an infinite number of particles per iteration causes the bias error, while the random fluctuation with zero mean in comparison with this averaged solution causes the statistical error. Therefore, first this random fluctuation (statistical error) should be investigated, before analyzing the bias error.

In the next section, the simulation approach is first discussed, before a more in dept discussion of the different error contributions.

2.1. Simulation approach

Based on the work of Ghoos et al. [15, 17], a recommended simulation approach was developed for SOLPS-ITER in ref. [19] and is described in this section.

To model a steady-state plasma state with SOLPS-ITER, a typical simulation has first a transient phase, before the plasma and neutral quantities reach their converged values (which are only effected by statistical noise). The transient phase depends on the initial state of the plasma. As the coupling between B2.5 and EIRENE is highly non-linear, this transient phase will typically require several 10s or even 100-thousands iterations.

Visual inspection of key plasma quantities shows when the state of the plasma is only changing due to the MC behavior of the EIRENE code. At

this point, the initial transient phase is over. Key plasma quantities monitored in this phase are: temperature at the outer midplane, and upper outer and inner target separatrix ($T_{e,sep}^{OMP}$, $T_{e,sep}^{UOT}$ and $T_{e,sep}^{UIT}$), density at the outer midplane, and upper outer and inner target separatrix ($n_{e,sep}^{OMP}$, $n_{e,sep}^{UOT}$ and $n_{e,sep}^{UIT}$), and maximum temperature and density at the targets.

Afterwards, the simulation is in statistically steady state [19], and it is still ran for several thousands iterations. The plasma state is averaged over these iterations resulting in a smaller statistical error. This strategy allows using less MC particles during both the transient and averaging phase. In that way it speeds up the code to reach a converged solution [16]. In the presented simulations, 45,000 iterations are involved in this averaging procedure, in which only plasma quantities are stored and averaged to save memory. Therefore, two purely EIRENE iterations with increased number of MC particles are necessary to guarantee a small statistical error on the neutral parameters. In the present case, 10,000 times more EIRENE particles are used in these last two iterations.

As a result, the presented simulations are composed of three parts: an initial transient phase, 45,000 iterations over which the plasma state is averaged, and two purely EIRENE iterations in the end in which the fixed averaged plasma state is employed. The convergence criteria from section 3.1 are applied to the quantities obtained in this final state.

2.2. Statistical error

Statistical noise as defined here has a probability distribution with mean value 0 and standard deviation σ^s which acts as estimate for ϵ_s [20]. It is linked with the number of EIRENE particles (P), but also averaging over multiple iterations (I) influences it: $\sigma^s \propto \frac{1}{PI}$ [15]. This means that the 45,000 iterations over which the plasma state is averaged will decrease the statistical error on the plasma quantities, while the involved number of MC particles in the last two, purely EIRENE, iterations determines an additional statistical error on the examined neutral parameters.

For the plasma quantities, the central limit theorem for dependent variables

leads to:

$$\sigma^s = \frac{\sigma^s_{500}}{\sqrt{\frac{R}{T_{500}}}} \tag{2}$$

in which σ^s_{500} is the standard deviation on a batch of 500 iterations (the 45,000 iterations are divided into batches of 500 iterations), R is the number of such batches, and T_{500} is the correlation time between them. More information about these parameters and how they are calculated can be found in ref. [15, 19].

As recommended in ref. [17], the estimated σ^s is multiplied by three to account for inaccuracies in the calculation of T_{500} and the stochastic particles behavior.

In contrast to the statistical error on the plasma quantities, the statistical errors on the EIRENE quantities computed during the final two iterations do not have any link with their value on the previous time step. This means that the statistical error on the EIRENE quantities is dominated by the last two, purely EIRENE simulation steps, although the (small) statistical error from the 45,000 coupled simulation steps will have an influence on the neutral source terms. This last contribution is neglected in this work.

For one single EIRENE iteration, a root mean square value is defined in the code as approximation for the standard deviation [21]:

$$\sigma^s \approx \widetilde{\sigma^s}(N) = \sqrt{\frac{1}{N-1}\sum_{i=1}^{N}(X_i - \bar{X})^2} \tag{3}$$

in which N is the number of included particles per iteration, X_i the simulated quantity for particle i, and $\bar{X}$ the averaged quantity over all particles. In the EIRENE code, the relative form of equation 3 can always be calculated [21] and acts as the estimate for the relative statistical error (in percentage):

$$\epsilon_{s,rel.} \approx \frac{\widetilde{\sigma^s}(N)}{\widetilde{R_g}(N)} \cdot 100 \tag{4}$$

with $\widetilde{R_g}(N)$ the MC estimate for the studied EIRENE quantity R_g, the average over N MC histories for this quantity scaled with the source strength (more details about the calculation of $\widetilde{R_g}(N)$ can be found in ref. [21]).

2.3. Bias

The bias on the plasma quantities is estimated using Richardson extrapolation [22, 23] by comparing three simulations in which the number of EIRENE particles is increased by the same factor (simulations with a –the original amount–, na –n times more– and n^2a –n^2 times more– particles) [15]. Richardson extrapolation was originally developed to study the discretization error, but in ref. [15] it is demonstrated by Ghoos that it can also be used to estimate the bias, as this is proportional to the inverse of the involved number of EIRENE particles $\epsilon_{bias} \propto \frac{1}{P}$.

Richardson extrapolation results in the following estimate of the bias (ϵ_{bias}) for quantity f_a in which a MC particles are involved:

$$\epsilon_{bias} \approx \frac{f_a - f_{na}}{1 - n^{p_d}} \tag{5}$$

with p_d the order of convergence equal to [23]:

$$p_d = \frac{log(\frac{f_{na} - f_a}{f_{n^2a} - f_{na}})}{log(n)} \tag{6}$$

and to the following estimate for ϵ_{bias} on the simulation with na MC particles:

$$\epsilon_{bias} \approx \frac{n^{p_d} \cdot (f_a - f_{na})}{1 - n^{p_d}} \tag{7}$$

This means that, if p_d is known, only two simulations are required to estimate the bias. In order to use these formulas, the bias should be the dominant error. Therefore, it can only be determined after eliminating the statistical error trough post processing averaging.

As recommended in ref. [17], a safety factor two is applied on the estimated bias to account for the remaining statistical error on the solution and because of possibly not reaching the theoretical $\epsilon_{bias} \propto \frac{1}{P}$ scaling.

As the neutral parameters are defined by a purely MC process, there is a bias only in non-linear cases, as in linear cases the cross-correlation between the

MC particles is zero [15, 14]. As will be shown later on in this work, the effect of non-linear neutral-neutral interactions in the studied simulations is negligible, and so is their bias. Nevertheless, as for the statistical error, the bias on the coupled B2.5-EIRENE iterations will influence the neutral source terms, and in that way the final simulation result for the neutrals.

2.4. Discretization error

The last error which is investigated is the discretization error, due to the discretized equations solved on a finite grid. In SOLPS-ITER two grids are involved: the B2.5 plasma grid, and the EIRENE neutral one. This means that both of them cause a discretization error. As for the bias, they are analyzed using Richardson extrapolation.

As recommended in ref. [17] by Ghoos et al. and in ref. [22] by Roach, a safety factor 1.25 is applied to the error estimate to take into account inaccuracies in the estimate of p_d.

3. Setup and result of the SOLPS-ITER simulation

In the presented work, the numerical errors introduced in the previous section, are analyzed for two EAST discharges which are currently investigated with SOLPS-ITER [3]: a purely deuterium H-mode discharge, and one with Ne-seeded to achieve detachment trough extrinsic impurity seeding. To both discharges an external heating power of 2.25 MW is applied. Through a feedback, the separatrix density at the outer midplane is kept constant: $n_{e,sep}^{OMP} \approx 0.910^{19} m^{-3}$. The gas puff injection and pumps location is indicated in figure 1.

While setting up the SOLPS-ITER simulations analyzed in this work, special attention is put on making te setup compatible for drift simulations. In the presented analysis drifts are not present, but it is aimed to include them in a later stage.

B2.5 solves the Braginskii equations in the edge of the plasma –in the scrape off layer and a narrow region inside the core– on a rectangular grid aligned with

the magnetic field. At the core boundary, the continuity boundary condition is of Dirichlet type: a constant electron density ($n_e = 2.8 \cdot 10^{19}\,\mathrm{m}^{-3}$) is imposed based on the experimental profile. A constant heat flux ($P_e = P_i = 1.025\,MW$ in the purely deuterium case, and $P_e = P_i = 0.9\,MW$ for the Ne seeded simulation) is imposed for the energy boundary condition. The energy crossing the core boundary is in agreement with the experimental $P_{in} - P_{rad}$. The Bohm-Chodura condition is applied at target boundaries for all conservation equations. Details about the specific (drift-compatible) implementation for the continuity, momentum, electron energy, and ion energy equations, can be found in ref. [24, 25]. At the boundary of the private flux zone and the radially outermost scrape-off layer boundary, a leakage boundary conition is imposed for continuity (leakage factor of $-1.0 \cdot 10^{-2}$) and energy conservation (leakage factor of $-1.0 \cdot 10^{-2}$ for ions and $-1.0 \cdot 10^{-4}$ for electrons), and a zero gradient boundary condition for momentum. The choice of these factors is based on previous simulation setups made by Dekeyser et al. [4, 26]. The density at the outer midplane separatrix is determined by a feedback loop keeping the density at $n_{e,sep}^{OMP} = 0.9\,m^{-3}$ which agrees with the experimental setup as indicated earlier. Making the setup drift-compatible resulted in a lower resolution grid in comparison with the one of ref. [3]. As indicated in ref. [4] too narrow grid cells do not work in drift cases.

To guarantee numerical stability and accuracy, the size of neighboring plasma grid cells should not differ too much and large cells should only be present in regions of shallow gradients of the plasma quantities. This results in three main requirements for the B2.5 grid: a symmetric grid around the X-point, smooth transitions between the different grid cells, and small grid cells at the divertor targets (due to the expected steep plasma gradients at these locations). These conditions are fulfilled in the 93x42 grid (93 grid cells in the parallel direction following the separatrix, and 42 in the perpendicular one) which is shown in figure 1.

The neutrals are treated with the EIRENE code. The model and reactions employed in the purely deuterium simulations can be found in ref. [27]. On top, some neutral-neutral interactions from the AMMONX database are included

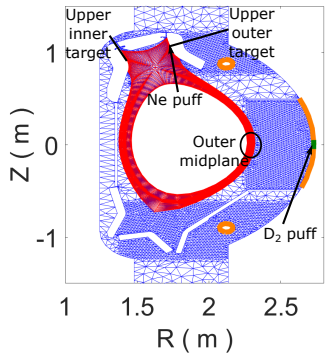


Figure 1: The employed grids for the SOLPS-ITER simulations. The B2.5 grid is indicated in red and the EIRENE grid in blue. The pumping surfaces are given in orange and the deuterium injection location at the outer midplane is indicated as well as the neon injection location. Also the locations where the plasma parameters are analyzed (upper targets and outer midplane) are shown in the figure.

[28]. These neutral-neutral interactions together with their reference to the AMMONX database are summarized in table 1.

Reaction	Reference
$D + D \rightarrow D_2^+ + e$	AMMONX H.2 R-H-H
$D + D_2 \rightarrow D_3^+ + e$	AMMONX H.2 R-H-H2
$D_2 + D \rightarrow 3\ D$	AMMONX H.2 R-H2-H
$D_2 + D_2 \rightarrow D_2 + D + D$	AMMONX H.2 R-H2-H2

Table 1: The included neutral-neutral reactions in the EIRENE model.

In the neon seeded simulations extra reactions from the ADAS [29] and AMJUEL databases are added which are summarized in table 2 [1]. In the neon seeded simulations an additional constant puff of $7.2 \cdot 10^{18}$ Ne particles s^{-1} and the same injection of D_2 take place and are included in the simulation. For both species, the puffing location is located at the outer target strike point.

Chemical and physical sputtering are not taken into account.

[1] The reactions between the higher charge states of neon are covered by the B2.5 code

Reaction	Reference
$e + Ne \rightarrow e + Ne^+ + e$	AMJUEL H.2 2.10B0
$Ne^+ + e \rightarrow Ne$	ADAS H.4,10 acd96,prb96

Table 2: Additional reactions in the EIRENE model for Ne-seeded simulations.

The EIRENE code employs a triangular grid. There will be steep gradients in the concentration of neutrals around the pumping (indicated in orange in figure 1) and puffing (indicated in green) locations. Therefore, the grid is refined at these locations. The initial triangles are generated with a maximal triangle side size of 8 cm. At the locations with steep gradients, this maximal triangle side size is reduced to 2 cm. A view of the resulting EIRENE grid is given in figure 1. The grid is extended below and above the figure: the top of the grid is at the upper pressure gauge which is ~ 2.5 m above the vessel wall, and the bottom of the grid is at the lower pressure gauge which is ~ 3.0 m above the vessel wall.

The included number of EIRENE particles highly influences the statistical noise on the simulation, the bias, and the required computing time. When 10 CPU's are used, the computing time increases with nearly a factor two when 10 times more EIRENE particles are included. Fewer particles, on the other side, change only slightly the needed computing time if 10 CPU's are involved illustrating that the available computational resources influence the choice of number of EIRENE particles.

The particles originate from three sources: deuterium molecules puff at the outer midplane (OMP), volumetric recombination in the plasma, and the surface recycling at the walls of the B2.5 grid. An overview of the included number of particle histories in the setup is given in table 3.

For all presented simulations a time step of $5.0 \cdot 10^{-5}$ s is employed.

The numerical error on the plasma quantities is determined by the 45,000 coupled iterations mentioned in section 2.1 while the error on the neutral quantities consists of the influence of these coupled 45,000 iterations – which determines the neutral source terms originating from the interactions with the

Place in the EIRENE grid	Number of EIRENE particles
Deuterium puff at outer midplane (OMP)	500
Additional deuterium puff at UOT in Ne-seeded case	500
Ne puff at UOT in Ne-seeded case	500
Volumetric recombination	700
Recycling at the target surfaces	500 (for each target)
Recycling at the other walls of the B2.5 grid	100 (for each wall)

Table 3: The number of EIRENE particles per iteration involved in the simulations.

plasma – and the last two purely EIRENE simulations.

3.1. Convergence criteria

For all presented simulations, the following convergence criteria are applied:

- Error on the global particle balance smaller than 1.5 %
- Error on the global energy balance smaller than 1 %
- Statistical error on analyzed plasma quantities ($T_{e,sep}^{OMP}$, $n_{e,sep}^{OMP}$, $T_{e,max}^{UOT}$...) obtained with the techniques of the earlier introduced SOLPS-ITER averaging smaller than 0.5 %

4. Errors for the examined cases

4.1. Statistical error

In the employed 3.0.7 master version of SOLPS-ITER, the statistical error on the plasma quantities can be calculated automatically leading to the errors listed in table 4.

Two key quantities are examined in this table: the electron density (n_e) and temperature (T_e). The analyzed locations are the outer midplane (OMP) and the upper outer target (UOT). These locations, which are indicated in figure

1, are the most interesting to examine in simulations as experimental data are available over here making a comparison between experiments and simulations possible. At each location the maximal simulated quantity is investigated in detail as well as the quantity at the separatrix.

Variable	Mean value no	ϵ_s	$\epsilon_{s,rel.}$ (%)	Mean value Ne	ϵ_s	$\epsilon_{s,rel.}$ (%)
$T_{e,sep}^{OMP}$	107 eV	0.0182 eV	0.017	96.8 eV	0.0126 eV	0.013
$n_{e,sep}^{OMP}$	$9.00\frac{10^{18}}{m^3}$	$2.97\frac{10^{15}}{m^3}$	0.033	$9.00\frac{10^{18}}{m^3}$	$2.71\frac{10^{15}}{m^3}$	0.030
$T_{e,sep}^{UOT}$	12.2 eV	0.0414 eV	0.34	4.00 eV	0.0102 eV	0.26
$n_{e,sep}^{UOT}$	$6.36\frac{10^{19}}{m^3}$	$2.04\frac{10^{17}}{m^3}$	0.32	$1.43\frac{10^{20}}{m^3}$	$3.62\frac{10^{17}}{m^3}$	0.25
$T_{e,max}^{UOT}$	53.9 eV	0.0261 eV	0.048	46.6 eV	0.0171 eV	0.037
$n_{e,max}^{UOT}$	$1.03\frac{10^{20}}{m^3}$	$3.01\frac{10^{17}}{m^3}$	0.29	$1.67\frac{10^{20}}{m^3}$	$3.28\frac{10^{17}}{m^3}$	0.20

Table 4: Overview of the statistical error on key plasma quantities. On the left the values in the simulation with no impurities are indicated, on the right the ones with added neon seeding.

On top, the statistical error on the entire T_e profile at the OMP is calculated. This analysis indicates that the maximum statistical error on the T_e profile at the OMP remains below $\sim 0.6\%$.

Based on table 4 it is clear that a small statistical error on the plasma quantities is obtained employing the averaging method. For a small statistical error on the neutral quantities, the number of involved MC particles in the last two, purely EIRENE simulation steps determines the solution, while the number of particles per iteration employed during the averaging does not play a significant role on the neutral quantities.

The EIRENE quantities which are analyzed in the presented error analysis are the neutral pressures. It is chosen to analyze the neutral pressures at three locations –the ones where pressure gauges are located in EAST and until where the SOLPS-ITER grid is extended: 2.5 meters above the vessel (P_{up}), 3.0 meters below the vessel (P_{down}), and around the outer midplane at the same location where the D_2 injection is located (P_{mid}, see figure 1). The neutral pressure

depends on two EIRENE quantities, namely the atom and molecule energy density, and it is approximated as $\frac{2}{3}$ of the sum of these quantities. As a result, also the estimate for the statistical error on the neutral pressure is the sum of the estimated errors on each quantity multiplied with $\frac{2}{3}$ (assuming that there is no correlation between them).

The locations above and below the vessel where the neutral pressures are analyzed are far away from the neutral sources. This means that only a few MC particles will reach these surfaces, so that the expected statistical error is large and significantly more EIRENE particles are needed to reduce this error.

It was verified whether it was sufficient to multiply the number of EIRENE particles in the two last steps with a factor 100. To study this, the number of followed particles in the MC process is further multiplied with 1,000, 10,000 and 100,000. The result for the studied neutral pressures in the purely deuterium simulation is shown in figure 2a indicating that the simulation outcome is significantly affected by using more MC particles. From the figure it is clear that at least 1,000 times more EIRENE particles are required in the last two simulation steps. In case of Ne seeding, on the other hand, 100 times more particles in the last two simulation steps are sufficient as can be seen in figure 2b. However, it should be noted that more gas sources are present in the Ne seeded simulation resulting in more involved EIRENE particles as indicated in section 3.

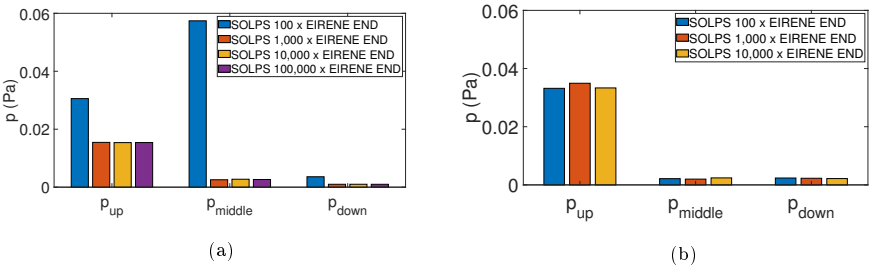


Figure 2: The influence of the number of EIRENE particles in the last two (purely EIRENE) simulation steps on the calculated neutral pressures in the purely deuterium (a) and neon seeded (b) simulation.

The estimated statistical errors on the pressures for the purely deuterium

case are given in table 5. Due to the inactivity of the lower divertor, the particle sources will be the most far away from this location so that fewer particles will reach the bottom measuring surface, resulting in the largest statistical error. Even when using 100,000 more EIRENE particles, the estimated statistical error on the neutral pressure is 17.4 %.

For a large number of particles N, the root mean square estimate for the relative standard deviation scales as $\widetilde{\sigma^s}(N) \sim \frac{1}{\sqrt{N}}$ [21]. In this case the product of this estimate and $\sqrt{N}$, converges to a constant value. These values ($\epsilon_s \cdot \sqrt{N}$) are indicated in table 5 and plotted in figure 3. They help to determine if the final solution will improve while increasing the number of EIRENE particles. This is confirmed by the curves of figure 3 which saturate towards high N.

Variable	P_{up}	P_{mid}	P_{down}
P_{100} [Pa]	0.0306	0.0574	$3.59\,10^{-3}$
$\epsilon_{s,rel.}$ [%]	29.6	16.8	55.8
$\epsilon_s \cdot \sqrt{100}$	9.06	9.64	2.00
$P_{1,000}$ [Pa]	0.0155	0.00256	$9.97\,10^{-4}$
$\epsilon_{s,rel.}$ [%]	10.4	27.6	35.2
$\epsilon_s \cdot \sqrt{1,000}$	5.10	2.23	1.11
$P_{10,000}$ [Pa]	0.0154	0.00274	$1.01\,10^{-3}$
$\epsilon_{s,rel.}$ [%]	3.51	8.82	41.4
$\epsilon_s \cdot \sqrt{10,000}$	5.41	2.42	4.18
$P_{100,000}$ [Pa]	0.0154	0.00265	$9.95\,10^{-4}$
$\epsilon_{s,rel.}$ [%]	1.11	2.96	17.4
$\epsilon_s \cdot \sqrt{100,000}$	5.41	2.48	5.47

Table 5: The simulation result and statistical error on the studied neutral pressures caused by the two last EIRENE simulation steps.

Table 5 and figure 3 indicate that for P_{up} and P_{mid} at least 10,000 times more EIRENE particles are required to ensure convergence in the purely deuterium simulation. If this number of EIRENE particles is employed, the value for

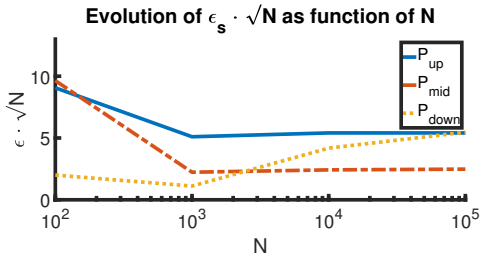


Figure 3: The evolution of $\epsilon_s \cdot \sqrt{N}$ with increasing N.

$\epsilon_s \cdot \sqrt{N}$ has come to a constant value. For P_{down}, however, it is not clear if the simulation with a multiplication factor of 100,000 has already a converged $\epsilon_s \cdot \sqrt{N}$. For the further analysis in this work, 10,000 more particles were used in the last two simulation steps.

4.2. Bias

An important condition to use Richardson extrapolation introduced in section 2.3, is that the three simulations required by this method are in the linear regime so that a correct estimate of the order of convergence – p_d – is possible. Therefore, simulations with 10 and 100 times more EIRENE particles are employed for the purely deuterium case, as a simulation with 10 times less particles is not in the linear regime as can be seen in figures 4 and 5. In this last one the separatrix saturation current is plotted towards the multiplication factor of the involved number of EIRENE particles. This plot illustrates that even the current used number of EIRENE particles is on the limit of being in the linear regime. Also a simulation with 10 times less particles in the neon seeded case is not in the linear regime. Because the additional EIRENE particles in the neon seeded study slow down the simulation, no convergence could be reached for a simulation with 100 times more EIRENE particles. Therefore, the bias is analyzed based on the original simulation and one with 10 times more EIRENE particles. As a consequence, assumptions about the order of convergence are made as discussed later on.

The bias on the plasma profiles is examined at the OMP and at the divertor

targets. At the OMP, the influence of a changed number of EIRENE particles is negligible on the entire profile (both in the purely deuterium case as in the case with neon impurities) as the density at the OMP separatrix is fixed for all simulations.

As indicated in figure 4 for the profile of the ion saturation current (j_s) at the UOT in the purely deuterium case, the calculated p_d does not result in a usable estimate in each simulation point: where the influence of the bias is too small, the statistical error dominates and formula 6 cannot be used. At these locations the order of convergence is set to 0.5.

Since there are only two simulations available for the estimate of the bias in the neon seeded simulation, the worst case estimate from the deuterium case is used everywhere. Based on figure 4, this means $p_d = 0.5$.

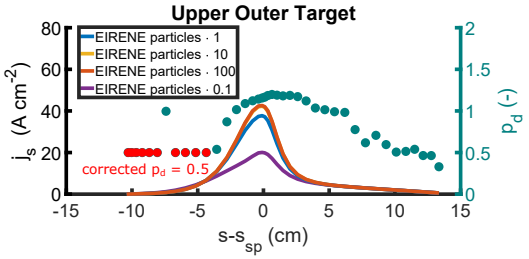


Figure 4: The outcome of the simulations with different number of EIRENE particles (left axis) and the estimated order of convergence for the bias (right axis) for the j_s profile at the upper outer target in the purely deuterium case. The points in red indicate the estimates which resulted in an imaginary number, and were therefore corrected to 0.5.

The resulting bias for the inner and outer target in the purely deuterium simulation, and the one for the outer target in the neon seeded case are shown in figure 6. The curve with the original number of EIRENE particles is clearly lower than the plots of the cases in which the number of involved EIRENE particles was multiplied with 10 and 100, while the curve with 10 times less particles is out of the linear regime.

This resulting bias for the plasma quantities at the inner and outer target helps to determine whether enough MC particles are involved in the 45,000 steps

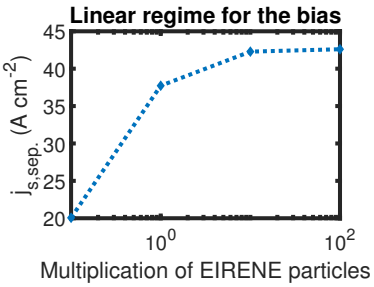


Figure 5: The separatrix values of the saturation current of figure 4 versus the multiplication factor of the number of EIRENE particles indicating the most left point (EIRENE particles · 0.1) is not in the linear regime to study the bias.

of the coupled simulation. On the figure it can be seen that the maximal bias is obtained on the density profiles. At the upper outer target, the maximum density in the purely deuterium simulation is increased by 41.5 % on the bias-corrected solution and at the upper inner target even by 44.7 %. As indicated before, figure 5 illustrates that the current number of EIRENE particles is on the limit of being in the linear regime. Because of these reasons, ten times more EIRENE particles are included in the simulations which are used to determine the discretization error. This results in a significant decrease of the estimated bias on the maximum density for the purely deuterium simulation down to 3.17 % at the outer target, and 3.08 % at the inner target. However, it should be kept in mind that this increases the required computing time by 50 %. This illustrates the difficult balance between accuracy and required computing time. Increasing the number of EIRENE particles, also reduces further the statistical errors of table 4 below 0.15 % for the examined quantities. The profiles of figure 6 show that the bias is small at the locations where p_d could not be estimated accurately. This, in combination with the small statistical error, allows the assumption for p_d which was made before.

The bias on the neutral parameters is mainly caused by the influence of the bias on the coupled iterations which determines the neutral sources. Therefore, the effect of increasing the number of EIRENE particles in the coupled iterations is shown in figure 7 for the purely deuterium case (a) and the neon seeded case

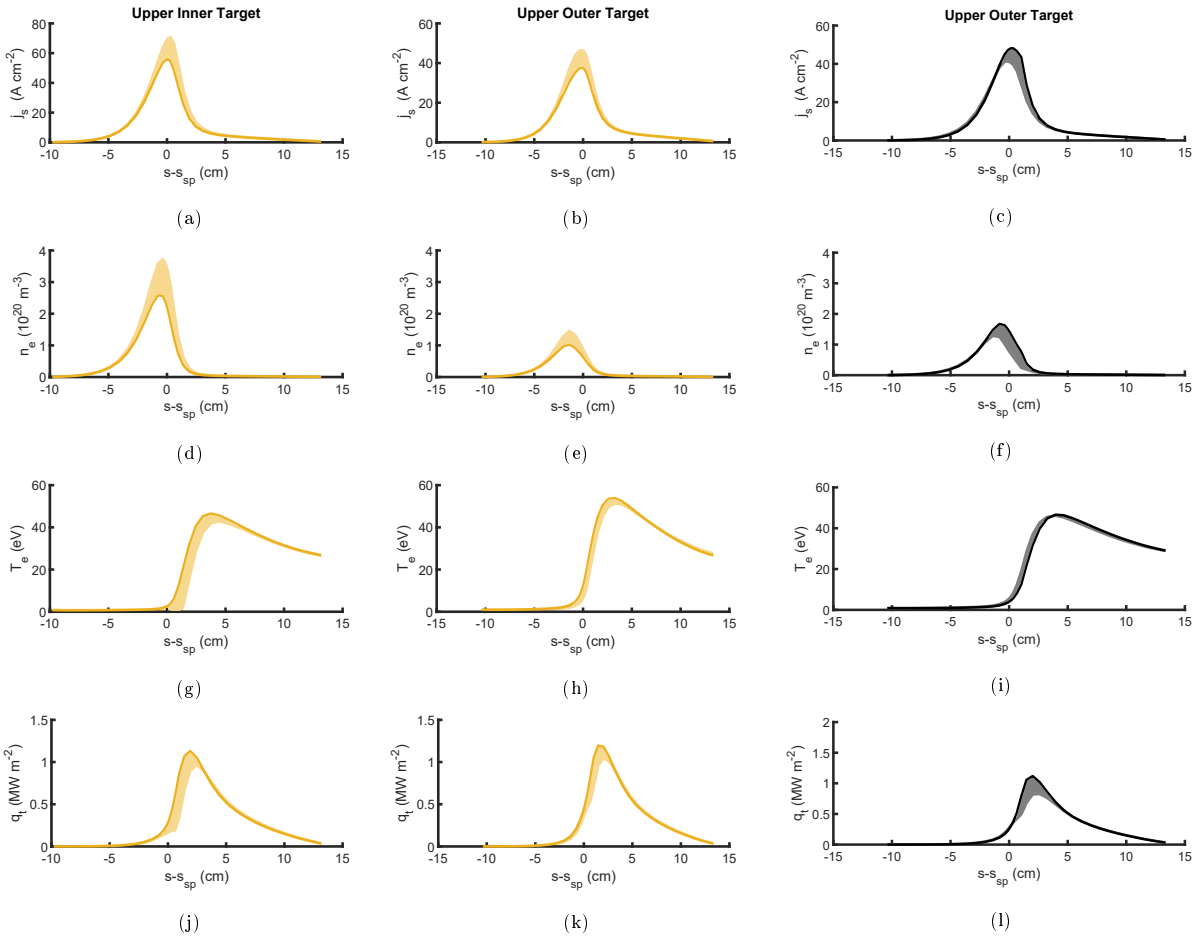


Figure 6: The outcome at the inner (left) and upper outer target (middle and right) for the analyzed purely deuterium (yellow) and neon seeded (black) simulation is shown including a shaded region which represents the error due to bias (including safety factor).

(b). The number of EIRENE particles in the last two steps of these simulations was always multiplied with 10,000 in comparison with the original number of EIRENE particles.

The error itself is quantified for the upper pressures in table 6. For the neon seeded case, the same order of convergence as for the unseeded simulation is assumed ($p_d = 1.0$). However, figure 7b indicates that the simulation with the original number of EIRENE particles might be not in the linear regime

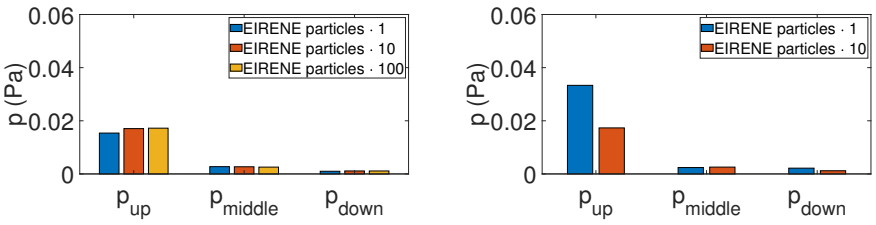


Figure 7: The influence of the number of EIRENE particles in the coupled SOLPS-ITER simulation steps (the bias of the coupled simulation) on the calculated neutral pressures in the purely deuterium (a) and neon seeded (b) simulation.

(as only two simulations are available, this cannot be verified in detail), so the estimate for the neon seeded case should be addressed carefully. As for the plasma parameters, a safety factor of two is applied on the final result.

In section 2 it was indicated that first the influence of the statistical error should be investigated to ensure its influence is smaller than the influence of the bias. Comparing estimates for the upper pressure statistical error from table 5 and the bias from table 6, indicates the statistical error is higher than the bias when 10 times more EIRENE particles are included. The statistical error is an upper limit as it was calculated with fewer particles in the coupled simulation, but it might cause a wrong bias estimate. That is also why the bias for middle and lower pressures cannot be estimated with the current setup.

Multiplication of particles	D simulation		Ne simulation	
(coupled simulation)	P_{up} (Pa)	$\epsilon_{bias,rel.}$ (%)	P_{up} (Pa)	$\epsilon_{bias,rel.}$ (%)
1	0.015	22.5	0.033	205
10	0.017	2.14	0.017	20.5
100	0.017	0.210	/	/

Table 6: Overview on the bias for the upper pressure for the different number of EIRENE particles.

As for the bias on the plasma parameters this bias estimate indicates that

involving ten times more EIRENE particles in the coupled simulation decreases the bias (for the neutral pressures with a factor of ~ 10 as $p_d = 1.0$). For the neon seeded simulations, the estimated bias stays high, but from figure 7b it is clear that involving 10 times more EIRENE particles changes the pressure drastically. However, as long as no simulation with 100 times more EIRENE particles is performed, it is not possible to verify if P_{up} with the original number of EIRENE particles is in the linear regime, and the bias estimate can be wrong.

It was indicated before that the bias on the neutral quantities in the last two purely EIRENE steps was neglected due to the small effect of neutral-neutral interactions, which causes non-linear effects. The chance that the involved neutral-neutral reactions take place during the studied discharge is determined by the mean free path for elastic collisions (λ_{el}) [21]:

$$\lambda_{el} = \frac{1}{\sqrt{2}\sigma_{el} n_N} \tag{8}$$

in which σ_{el} is the typical collision cross section ($\sigma_{el} = \pi \frac{d^2}{4}$ with d the diameter of the atom/molecule) and n_N the gas density. Using the maximum density in the EIRENE simulation for D_2 and D, the self collision mean free path is calculated for both substances. This results in a mean free path of $\sim 4.61\,\mathrm{m}$ for the D self collision and one of $\sim 0.84\,\mathrm{m}$ for the D_2 self collision. This means that their influence on the final simulation outcome is small as the calculated mean free path is large in comparison with the size of EAST. These findings are in agreement with the JET results of ref. [27] and the TCV ones of ref. [30] indicating that these neutral-neutral effects only play a role for large tokamaks like ITER.

4.3. Discretization error

Similarly to the bias, Richardson extrapolation is employed to study the effect of spatial discretization. For the discretization error, only one additional simulation (with a different grid) is involved. The numerical scheme of the SOLPS-ITER code is a hybrid between first- and second-order numeri-

cal schemes [9, 25]. This results in p_d between 1 and 2. Therefore, the most conservative one ($p_d = 1$) is taken everywhere, and only two grids are required.

For this extra simulation, the already existing grid from ref. [3] is used. In here, the B2.5 grid is refined with a factor of 1.66 in comparison with the original grid, while the EIRENE neutral grid outside the plasma domain stays similar. Inside the plasma domain, each B2.5 grid cell is divided into two EIRENE grid cells.

In order to determine the discretization error, also the bias on this further refined grid is computed in the same way as for the coarser grid.

The discretization error is only analyzed for the purely deuterium case as the solved equations are the same for the neon seeded case, resulting in a similar error contribution.

The combination of the discretization error and the bias on the original simulations at the upper outer target is shown in figure 8 for the standard (coarser) grid and for the refined grid. As the statistical error was less than 0.15 % for all analyzed parameters, this is not included in the given error bars.

Based on these simulation results, the maximum error due to a combination of the bias and discretization can be examined. As for the bias, the maximum effect is observed on the difference in peak density. The estimated total error on the coarser grid is maximum 17.9 % where the maximum estimated total error on the refined grid is 5.66 %. This indicates that finer grids result indeed in smaller errors for the studied EAST cases. However, by refining the grid by a factor of 1.66, the required computing time more then doubles. Running 10,000 simulation steps using 10 CPU's takes ~ 5 hours for the coarser grid, but ~ 12 hours for the refined grid using the same time step in both simulations. On top, this is the maximum error. As can be seen in figure 8 the other errors (especially on the q_t and T_e profiles) are much smaller. Therefore, coarser B2.5 grids are used for analyzing the plasma and neutral quantities.

To examine the influence of the EIRENE grid, two additional simulations were performed decreasing the maximum triangle side size by a factor two each time. No change was observed on the plasma profiles at the targets and outer

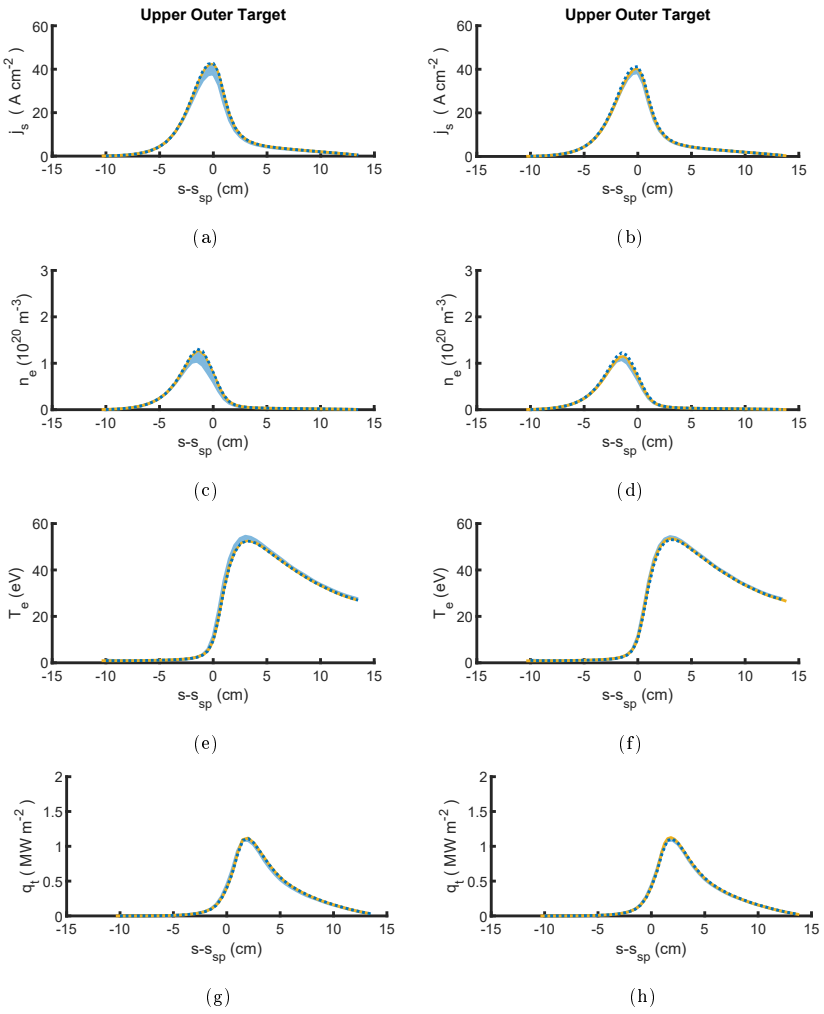


Figure 8: Outcome at the UOT for the analyzed simulation on the original grid (left) and on the refined one (right) including the numerical error. In yellow the original simulation result is shown, the bias-corrected one is indicated with the dotted blue curve. The shaded blue region indicates the numerical error due to the bias and the finite B2.5 grid on the simulated profiles. The shown outcome is the one with 10 times more EIRENE particles.

midplane indicating that the influence of the EIRENE triangle size outside the plasma domain is limited on these profiles.

The effect of finite grid spacing on the neutral pressures is shown in figure 9 in which the simulated neutral pressures are shown for a coarser EIRENE grid

(∼ 4 times larger grid cells outside the B2.5 grid) and a more refined B2.5 grid in comparison with the original simulation result.

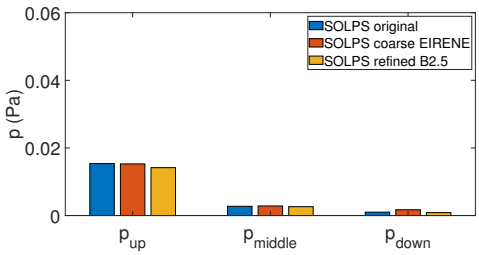


Figure 9: The simulated neutral pressures of the reference simulation (with 10,000 times more EIRENE particles in the last two simulation steps), of a simulation with a four times as coarse EIRENE grid, and of one with a 1.66 times refined B2.5 grid.

It is clear from the discussion before, and from figure 9 that refinement of the EIRENE grid has a negligible impact on both plasma and neutral quantities. This agrees with the negligible bias caused by the two last pure EIRENE steps, and is explained again by the small contribution of nonlinear neutral-neutral collisions in the cases at hand. Whenever such contribution becomes important, a finer EIRENE grid would be required to resolve these non-linearities.

The effect of the B2.5 grid on the plasma pressures, on the other hand, is larger. For P_{up} the difference between using the coarse and refined B2.5 grid, is 20.4 % for the purely deuterium case. Following a similar procedure as for the plasma quantities would lead to an estimated error of 63.8 %. It should be mentioned that, as no averaging is applied, a larger statistical error will influence this estimate making a correct interpretation difficult. For the refined grid, this error stays large, but decreases to 38.3 %. Although the possible inaccuracies on this estimate, this illustrates the importance of a fine B2.5 grid to examine the appearing neutral pressures in detail.

4.4. Discussion

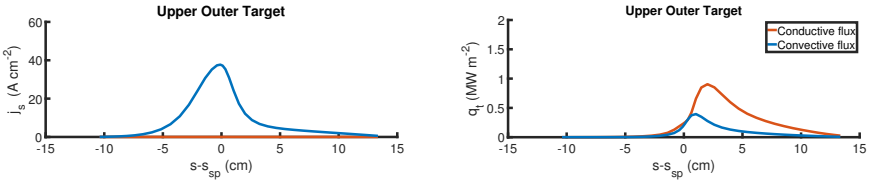
In this section, insight is given on how errors on state quantities translate to errors on derived quantities. All derived quantities in SOLPS-ITER are a

combination of a convective and a diffusive term as below for the velocity in the poloidal direction x [9]:

$$V_x = b_x V_{||} - \frac{D_\perp^{na}}{n} \frac{1}{h_x} \frac{\partial n}{\partial x} \tag{9}$$

in which $b_x = B_x/B$, $h_x = 1/||\nabla x||$, V the velocity and $D_\perp^{na}$ the anomalous particle diffusion of the species.

Some plasma quantities are mainly dominated by the convective contribution, while others are dominated by the diffusive one. This is shown in figure 10 for the simulation results of j_s and q_t. The particle flux is nearly completely convective, and the conductive part has the major contribution to the heat flux.



(a) (b)

Figure 10: Conductive and convective part of the SOLPS-ITER result -without any error correction- for j_s (a) and q_t (b).

When we compare this with the bias of figure 6 and the total error of figure 8, it is clear that the numerical error is larger when the quantity is dominated by the convective term. This is in agreement with the findings of ref. [31] where it is demonstrated for the discretization error that the magnitude of this is depending on the convective/conductive behavior of the examined quantity.

To summarize, all the different error contributions to the main plasma target quantities and examined neutral pressures are given in table 7. As the statistical errors on the saturation current and heath flux are not calculated automatically by the averaging tool built-in in SOLPS-ITER, they are not quantified. The discretization error is only calculated in detail for the purely deuterium simulation. On its own, the discretization error on the maximum density at the outer target is larger than the total error shown in figure 8. This comes because bias

and discretization shift the plasma profiles in opposite directions. Figure 6, on the other side, indicates that the bias for the Ne seeded simulation shifts the plasma profiles in the similar direction as the discretization error. For this, it is assumed that the discretization error on the neon seeded simulation is similar to the one on the purely deuterium simulation. This is originating from the fact that the solved equations are in both cases the same, and that the same B2.5 and EIRENE grids are employed. As table 7 also shows a larger bias for the Ne seeded simulation, the total error can be up to $\sim 28\,\%$ for the maximum density at the outer target. The resulting errors at the inner target are smaller in comparison with the ones at the outer target.

Variable	D simulation			Ne simulation		
	$\epsilon_{s,rel.}$ (%)	$\epsilon_{bias,rel.}$ (%)	$\epsilon_{d,rel.}$ (%)	$\epsilon_{s,rel.}$ (%)	$\epsilon_{bias,rel.}$ (%)	$\epsilon_{d,rel.}$ (%)
$j_{s,max}^{UOT}$	/	1.6	11	/	4.8	~ 11
$n_{e,max}^{UOT}$	0.11	3.2	20	0.070	8.0	~ 20
$T_{e,max}^{UOT}$	0.016	0.34	4.0	0.011	0.34	~ 4.0
$q_{t,max}^{UOT}$	/	0.64	2.4	/	8.5	~ 2.4
$j_{s,max}^{UIT}$	/	1.6	3.0	/	1.3	~ 3.0
$n_{e,max}^{UIT}$	0.068	2.9	4.0	0.045	4.7	~ 4.0
$T_{e,max}^{UIT}$	0.030	0.69	4.3	0.019	2.7	~ 4.3
$q_{t,max}^{UIT}$	/	1.2	2.1	/	7.2	~ 2.1
P_{up}	< 3.5	2.1	~ 64	/	21	~ 64
P_{mid}	< 8.8	/	/	/	/	/
P_{down}	< 41	/	/	/	/	/

Table 7: Overview of the different error contributions to the final simulation results.

For the neutral pressures, the estimates for the statistical error from table 5 are an upper limit for the error in the final simulation setup as simulations with 10 times more EIRENE particles in the coupled iterations are employed. From the table it is clear that also this error is dominated by the discretization error

making it difficult to give an accurate interpretation to the simulated neutral pressures far away from the plasma (where often pressure gauges are placed in fusion experiments).

5. Recommendations for future SOLPS-ITER studies

A big challenge for SOLPS-ITER simulations is finding the correct balance between accuracy and computational effort. The starting question is which numerical error can be tolerated for the investigated problem. In case of comparison with experimental data, their accuracy should be considered, in case only the plasma quantities are examined, less attention will be put on avoiding errors on the neutral quantities. In this section, some general statements to decrease the statistical error, bias, and discretization error are formulated while keeping in mind the required computational cost. They are based on the findings in the presented simulations, but it is aimed to make them as general as possible.

As demonstrated above, and also in ref. [16, 17], it is beneficial to use the SOLPS-ITER averaging to decrease the statistical error, or speed up the code using less EIRENE particles to obtain a similar statistical error. In the current analysis, 45,000 iteration were immediately included in the averaging phase. In the SOLPS-ITER averaging manual [19] it is recommended to use at least 30,000 iterations. From a computational viewpoint, it is better to first check after 30,000 iterations the existing statistical errors, and deciding afterwards if more iteration steps are beneficial for the averaging. By deciding if the statistical errors are small enough, also the convergence criteria introduced in section 3.1 –especially the required statistical error below 0.5 %– should be considered. A small statistical error is also required for a correct investigation of the bias.

In order to guarantee correct neutral quantities, it is of crucial importance to include enough EIRENE particles in the last two, purely EIRENE steps. As only two iterations are needed, the impact on the required computational resources is limited due to the trivial parallelization over multiple processors

and it is better to include too many than too few EIRENE particles. For the examined simulations, it was demonstrated that at least 10,000 times more EIRENE particles are required to study in detail the neutral quantities.

For the bias, the most important is to ensure the simulation is in the linear regime. From figure4 it is clear that too few EIRENE particles can lead to a completely different result. Therefore, it is recommended first to run a simulation with ten times less particles. If the profiles of the original simulation and the one with less EIRENE particles are similar, the linear regime for the bias is reached. If less than ten times fewer MC particles are used, the statistical error should be adequately small to correctly estimate the bias.

A similar effect is observed due to the finite B2.5 grid. A too coarse one will also lead to a simulation result outside the linear regime. In the performed EAST study, two coarser grids were tested. While a 62 x 28 grid is still in the linear regime, a 31 x 14 is not anymore. However, as the largest error contribution is caused by the employed discretization, it is not recommended to use the coarsest possible grid. For EAST simulations, the employed 93 x 42 grid or a more refined one is recommended, as the maximum discretization error on the plasma quantities stays below 20 %. In case the main goal of the simulation is an in-dept analysis of the neutral quantities, it is shown that a more refined B2.5 grid should be considered as the B2.5 discretization error remained the largest one on the neutral quantities in examined case.

For the EIRENE parameters, the important neutral reactions should be investigated before starting a new simulation. In case the expected mean free path of neutral-neutral collisions is large in comparison with the expected system length scale, it is better to neglect them, reducing the computational effort. Besides the studied EAST case, this is also shown in ref. [27] for JET and in ref. [30] for TCV. They will slow down the simulation, and require a refined EIRENE grid. When neutral-neutral collisions are important, on the other hand, the refinement of the EIRENE grid should be investigated in the same way as the one from the B2.5 grid.

6. Summary

In this work the importance of an accurate choice of numerical parameters in plasma edge simulations with SOLPS-ITER is demonstrated for a purely deuterium and a neon-seeded simulation of EAST. Knowledge of this error is required to correctly interpret the simulation results and compare to experimental data.

In SOLPS-ITER the numerical error consists of four contributions: the statistical, bias, and discretization error, and the effect of incomplete convergence. The first two are caused by the involved number of MC particles in the EIRENE code, while the discretization error is caused by the finite grid spacing. Incomplete convergence is originating from residuals in the B2.5 code.

By applying the previously developed SOLPS-ITER averaging scheme, the statistical errors on the results are reduced to negligible values below 0.15 % for the examined plasma quantities in the studied discharges. To examine the statistical errors on the neutral quantities, the performed analysis shows that at least 10,000 times more EIRENE particles are required for the last two, purely EIRENE steps compared to the number of particles employed during the averaging. Nevertheless, the statistical error on the neutral quantities remains significantly larger than on plasma quantities, especially in remote locations reached by few particle trajectories and thus providing poor statistics.

After examining the statistical error, the focus is on investigating the bias. By applying Richardson extrapolation, the bias is examined and the simulation setup modified to reduce this error contribution. This leads to a maximum bias of 3.08 % for the purely deuterium simulation which is observed on the peak density at the inner target. As it is demonstrated that the non-linear effects from neutral-neutral interactions have a negligible effect, also the bias on neutral quantities caused by the last two purely EIRENE iterations is negligible. The coupled iterations on beforehand lead to a bias of 2.14 % on the upper pressure.

Finally, it is shown that the finite B2.5 grid causes the largest error on the plasma profiles resulting in a total numerical error up to 17.9 % for the

examined simulations. As the non-linear effects are negligible in this case, the EIRENE grid has no observable influence and is best taken coarse to decrease the computing time. The employed grids also have an influence on the calculated neutral pressures, but the error on these pressures is dominated by the statistical MC noise. However, after making a decent choice fo the EIRENE particles, the discretization error shows the largest error contribution which is $\sim 64\,\%$ for the examined purely deuterium case.

The performed analysis of the numerical errors on the plasma and neutral quantities shows that a fully converged SOLPS-ITER simulation – errors on the particle and energy balance below $1.5\,\%$ and statistical errors below $0.5\,\%$ – does not mean necessarily that the remaining numerical errors are small and that the simulation result can be used for a physical interpretation. Therefore, in all SOLPS-ITER simulations the appearing numerical errors should be considered before starting with a physical interpretation of the simulation result. This has to be done taking into account the computational cost. Special attention should be put on the required number of EIRENE particles to ensure a simulation is in the linear regime for the bias. The same applies for the involved B2.5 grid. If the mean free path of the neutral-neutral collisions is large in comparison with the tokamak size –which is the case for the studied EAST discharges– computational time can be saved by excluding neutral-neutral reactions and using a coarse EIRENE grid.

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