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ORIGINAL ARTICLE

Accuracy and convergence with coupled finite volume - Monte Carlo codes for time-dependent plasma edge simulations

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With state-of-the-art plasma edge codes, which consist of coupled finite volume (FV) - Monte Carlo (MC) codes, it is challenging to obtain accurate results for time-dependent simulations in a feasible computational time. For steady-state simulations, it has been recently demonstrated that the speed and accuracy can be drastically improved by choosing more suitable numerical parameters and including post-processing averaging[1]. This paper extends the methodology for accuracy assessment to time-dependent simulations. For a simplified 1D plasma edge model, we compare the numerical accuracy of solutions obtained with an implicit approach, where the code system is fully solved in each time step, to those with a mixed implicit/explicit approach, where only the FV code is converged in each time step. We demonstrate the importance of choosing the numerical parameters adequately in both approaches.

KEYWORDS:
accuracy, convergence, Monte Carlo, errors

1 | INTRODUCTION

State-of-the-art plasma edge codes, such as B2-EIRENE/SOLPS, are computationally expensive and have a limited numerical accuracy. While plasma transport is modeled with fluid equations and implemented with a finite volume (FV) code, neutral transport requires a kinetic equation, implemented with a Monte Carlo (MC) code. In this strongly coupled, iteratively solved FV-MC system, the statistical noise of the MC code hinders strict convergence in the FV code.

A recently developed accuracy framework for steady-state FV-MC simulations classifies the numerical error into its contributions originating from statistical noise, discretization, correlations and incomplete convergence[2]. With a more suitable numerical parameter choice, drastic improvements in speed and accuracy have been achieved applying this framework to a B2-EIRENE simulation of an ITER divertor case. First, an order of magnitude speed up has been obtained by applying post-processing averaging, which allowed to reduce the number of MC particles per iteration without losing statistical accuracy[3]. Then, by increasing the grid resolution, the error could be decreased from up to 60% for peak values to approximately 15%[1]. These results indicate the importance of a thorough numerical error analysis and suggest a large potential for similar improvements in time-dependent simulations.

In this paper, the framework for accuracy assessment, previously developed for steady-state simulations, will be extended to time-dependent simulations. With a simplified transient plasma edge model, we compare an implicit coupling approach where the FV-MC code system is fully converged within each time step with a mixed explicit/implicit coupling approach where for each time step the MC code is only solved once and the FV code is fully converged. The first approach is not frequently used

in practice because it is often thought to be too time-consuming to iterate in each time step. However, this method may become competitive when post-processing averaging is used.

The simplified 1D model and its implementation are described in section 2. In section 3, all error contributions are discussed and evaluated for the two coupling approaches. In section 4, the efficiency of both approaches will be compared by examining the accuracy that can be reached in a fixed computational time. Finally, the main conclusions are summarized.

2 | MODEL DESCRIPTION AND IMPLEMENTATION

We solve a set of plasma edge equations on a one-dimensional numerical domain representing a flux tube in the poloidal cross section of a tokamak. The domain starts at an upstream position 10 cm before the target, where a fixed plasma density is imposed. Plasma reaches sound speed at the target, where a recycling coefficient of 0.99 is taken. The plasma is described with a time-dependent continuity and momentum equation. The neutrals are described with a stationary kinetic equation. It is thus assumed that the neutral state adapts immediately to the changing plasma conditions. More details on the model can be found in [2,4,5], in which it has been previously used.

Starting from a steady-state solution, a sudden increase from $10^{20}\mathrm{m}^{-3}$ to $1.2 \cdot 10^{20}\mathrm{m}^{-3}$ in upstream plasma density is applied. Due to this step, the density at the target peaks after approximately $4 \cdot 10^{-5}$s at $1.24 \cdot 10^{20}\mathrm{m}^{-3}$ before settling in a new steady-state condition. In the following accuracy analysis, we examine the accuracy on this peak density value at the target. Reference solutions with a high grid resolution (10^4 cells) have been obtained without the influence of MC noise using an FV implementation for the kinetic equation.

The time-dependent plasma equations are solved using so-called dual time stepping [6], where both a physical and a false time step are used. As the name suggests, the physical time step Δt advances the simulation in the physical time dimension, while the false time step $\Delta\tau$ is used to converge the results within each physical time step. Outer iterations proceed in time with physical time step Δt, while inner iterations will converge the solution using false time stepping with $\Delta\tau$ within each outer iteration. For both time steps, a first order implicit Euler scheme is implemented.

We consider two simulation approaches: one with a fully implicit system in each time step, the other with incomplete or mixed implicit-explicit coupling in each time step. In the implicit solution, the neutral and plasma code are iteratively solved within each outer iteration until convergence is reached (a specified statistical error or number of statistically stationary iterations). Within each outer time step, an iterative procedure with pseudo-transient phenomenon occurs after which a statistically pseudo-converged state within the inner iterations is reached, similar as in a steady-state simulation. We take the post-processing average of these stationary iterations as the initial state for the next outer time step. This Random Noise coupling approach has been demonstrated to be very efficient in steady-state simulations [2,3], compared to the usual approach without post-processing averaging. In the mixed approach, which is more often used in practice, the neutral code is only run once each outer iteration. After the neutral simulation is solved, the plasma code is run until convergence in the inner iterations (until a specified residual is reached). In this approach, averaging within one time step is not relevant.

3 | ERROR CONTRIBUTIONS

We define several error contributions based on their origin. The errors related to the discretization in space and time are respectively defined as the space discretization error ϵ_d and the time integration error ϵ_t. The error due to the statistical noise of the finite number of MC particles is divided into two contributions: a statistical error ϵ_s and a deterministic error, which we call the bias ϵ_b. Each contribution will be discussed in the next subsections for both solution approaches.

3.1 | Space discretization error

The space discretization error originates from truncations made in the discretization schemes w.r.t. the spatial domain. For a chosen discretization scheme, it is, therefore, highly dependent on the number of grid cells X. We analyze this dependency by performing runs with different numbers of grid cells X, while keeping the time step constant ($\Delta t = 10^{-7}$s). The reference solution is obtained with a very high number of grid cells (10^4). Because the MC noise has no influence on the discretization error, the FV code for the neutrals is used to obtain grid-sensitive solutions without MC noise [2]. Figure 1 shows the relative error as a function of the number of grid cells for the implicit and the mixed approach. As can be seen from the coinciding

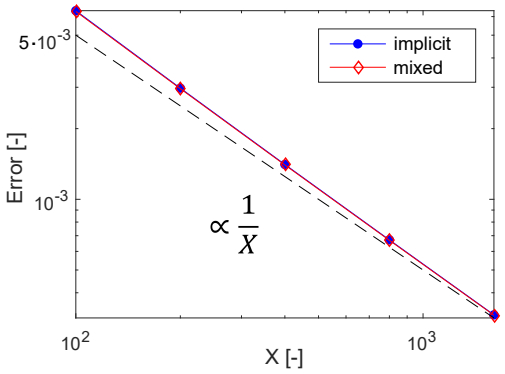

FIGURE 1 The relative space discrezation error ϵ_d as a function of the number of grid cells X for implicit (blue) and mixed (red) simulations with $\Delta t = 10^{-7}$ s.

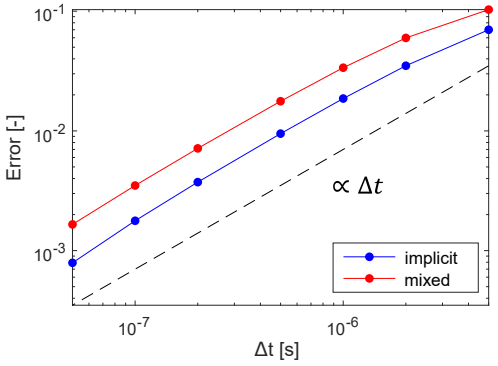

FIGURE 2 The relative time integration error ϵ_t as a function of the time step Δt for implicit (blue) and mixed (red) simulations with $X = 100$.

lines, the discretization error is independendent of the chosen approach. As expected with the chosen discretization schemes, convergence is of first order and the space discretization error can be written as $\epsilon_d = A_d/X$, with A_d a constant w.r.t. the number of grid cells X, the time step Δt and the coupling approach.

3.2 | Time integration error

The approximations related to the time integration scheme lead to a time integration error. To examine its behavior, simulations with increasing time steps have been performed with both approaches. Noise-insensitive simulations are obtained using the FV code for the neutrals. All simulations are run on a grid with 100 cells such that the discretization error is equal in each simulation. Figure 2 shows the relative error as a function of the time step for the implicit and mixed approach in respectively blue and red. It confirms the expected error reduction rate with a first order time integration scheme, such that the error can be written as $\epsilon_t = A_t \Delta t$, where A_t is a constant w.r.t. Δt. Moreover, by repeating the analysis with a finer grid resolution, it has been demonstrated that A_t is independent of the grid size.

3.3 | Statistical error

The statistical error is defined as the stochastic part of the error originating from the limited number of MC particles. It has a probability distribution with mean 0 and standard deviation σ. The magnitude of σ depends on the number of MC particles per iteration P and the number of iterations over which the solution is averaged I. Approximating the statistical error as its standard deviation σ and following the central limit theorem, we write

$$\epsilon_s \approx \sigma = \frac{\sigma_1}{\sqrt{I/T}} = \frac{A_s}{\sqrt{PI/T}}, \tag{1}$$

where σ_1 is the standard deviation of one iteration, T is the correlation time which takes into account the dependencies between consecutive iterations, and A_s is a constant w.r.t. P and I.

The expected $\propto 1/\sqrt{P}$ is confirmed in the left graph in figure 3 , which shows the standard deviation σ_1 as a function of the number of MC particles per iteration P for both approaches. The magnitude of the constant A_s is dependent on the coupling approach, and also on the chosen Δt and, for the implicit approach, on $\Delta \tau$. The standard deviation σ_1 is calculated as the sample standard deviation $s_1 = \sqrt{\frac{1}{I}\sum_{i=1}^{I}(\Phi_i - \overline{\Phi})^2}$, with Φ_i the result of iteration i and $\overline{\Phi} = \frac{\sum_{i=1}^{I}\Phi_i}{I}$ the post-processing average. We stress that iterations used in the average should be in statistically stationary regime. The iterations in the transient I_{tr} should be discarded. More details on methods to estimate the statistical error in simulations with averaging can be found in [5,7].

In the implicit approach, in which post-processing averaging is used, ϵ_s can be decreased by taking either more particles per iteration P or more iterations I. The number of iterations I can either be fixed or determined on the fly based on a criterion for the statistical error.

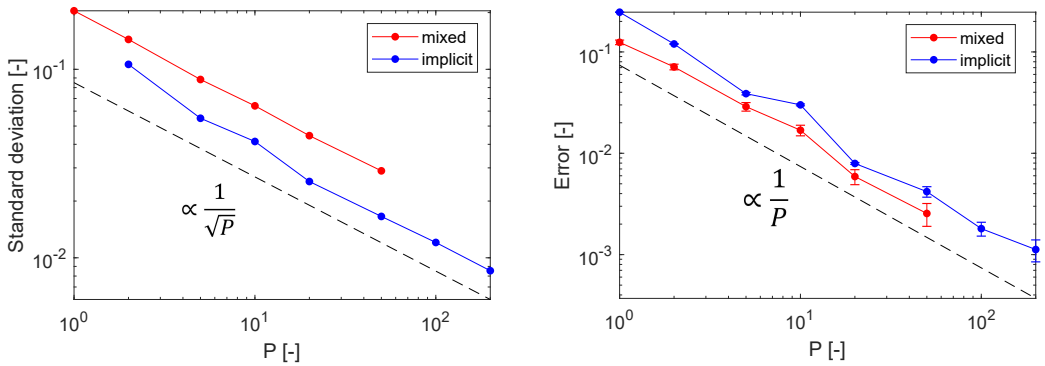

FIGURE 3 The relative standard deviation σ_1 (left) and the relative bias ϵ_b (right) as a function of the number of MC particles per iteration P for implicit (blue) and mixed(red) simulations.

In the mixed approach, averaging is not used, and, therefore, the statistical error ϵ_s can only be decreased by choosing a higher number of MC particles per iteration P ($I = 1, T = 1$). The standard deviation σ_1 is in this case calculated as the sample standard deviation of the solution of at least 30 independent runs.

3.4 | Bias

The bias is defined as the deterministic error due to the finite number of MC particles per iteration P and exist because of non-linearities. Based on previous analysis[2], we expect the following dependency $\epsilon_b = A_b/P$, with A_b a constant w.r.t. P and I. To confirm this, several runs with varying number of MC particles per iteration P are executed, while keeping the time step Δt and number of grid cells X constant. The reference solution is obtained with the FV code for the neutrals. The right graph in figure 3 shows the bias as a function of the number of MC particles per iteration P for both the implicit (in blue) and the mixed approach (in red). The error bars indicate the remaining statistical error on the solution. With the mixed approach, the statistical error can be decreased by taking an average over independent runs (each starting with a different seed). With the implicit approach, the statistical error can be made as low as desired by making use of averaging within each iteration. It is also possible to average the results of several independent runs. It is noticed that the expected scaling is slightly disturbed around $P = 10$. This is due to a bifurcation, which disappears with a higher number of MC particles. More details can be found in[5].

3.5 | Total error

To take into account the total error, we take the sum of all contributions. The following equation comprises the total error in the implicit (with superscript I) and mixed (with superscript M) approach:

$$\epsilon^I = \frac{A_d}{X} + A_t^I \Delta t + \frac{A_b^I}{P} + \frac{A_s^I}{\sqrt{PI/T}} \qquad \text{and} \qquad \epsilon^M = \frac{A_d}{X} + A_t^M \Delta t + \frac{A_b^M}{P} + \frac{A_s^M}{\sqrt{P}}, \tag{2}$$

with X the number of grid cells, Δt the time step, P the number of particles per iteration, I the number of iterations in the average, T the correlation time, A_i the constants of their related errors ϵ_i. The presence of the superscript (I or M) indicates a dependence on the simulation approach.

Without reference solutions available, the constants for the deterministic errors can be estimated by comparing solutions with a different resolution. This method (often referred to as 'Richardson extrapolation') is typically used to determine the discretization error in finite volume codes[8], but can be applied to estimate any deterministic error with a consistent reduction rate. For parameter Y (which can be X, Δt or P for the errors ϵ_d, ϵ_t and ϵ_b respectively), two solutions ϕ^Y and $\phi^{\alpha Y}$ with respectively resolution Y and αY are required, with α the scaling factor. Assuming $\epsilon = A_Y Y^{p_Y}$, with p_Y a known order of convergence ($p_X = -1$, $p_{\Delta t} = 1$ and $p_P = -1$), the error on solution ϕ^Y is than estimated as

$$\epsilon^Y = \frac{\phi^{\alpha Y} - \phi^Y}{1 - \alpha^{p_Y}}. \tag{3}$$

From this, the constant can be easily obtained as $A_Y = \epsilon^Y / Y^{p_Y}$. This method has been applied in[1] to estimate the space discretization error and the bias.

Because time-dependent simulations can be time-consuming, we propose to make a fast estimate of the constants A_d, A_b and A_s using steady-state simulations, which are run with the same Δt and $\Delta \tau$ as the transient simulations. The table in figure 4 summarizes the value of the constants obtained with both transient and steady-state simulations for the 1D case. As expected, the values obtained for steady-state simulations are in the same order of magnitude as those for transient simulations, and can thus be used as a first estimate.

	transient		steady-state	
	implicit	mixed	implicit	mixed
A_t	$1.8\ 10^{4}$	$3.6\ 10^{4}$	-	
A_d	$6.0\ 10^{-1}$		$2.5\ 10^{-1}$	
A_b	$3.7\ 10^{-1}$	$1.2\ 10^{-1}$	$2.7\ 10^{-1}$	$1.1\ 10^{-1}$
A_s	$1.5\ 10^{-1}$	$1.9\ 10^{-1}$	$1.5\ 10^{-1}$	$2.1\ 10^{-1}$

FIGURE 4 Constants for the relative error [-] obtained with the implicit and mixed approach, and with steady-state simulations.

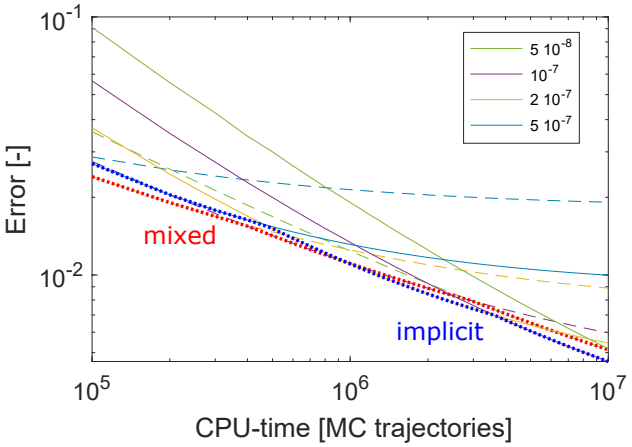

FIGURE 5 Minimal relative error as a function of the computational time for the implicit (dotted blue line) and the mixed (dotted red line) approach. The full and dashed lines are obtained with a fixed time step with respectively the implicit and mixed approach.

4 | OPTIMAL PARAMETERS

In this section, we optimize the numerical parameter choice for both approaches to obtain a minimal error in a specified computational time. The objective is to analyze which approach is optimal. Since the discretization error is equal for each solution approach, it does not influence this choice and, thus, we can exclude this error from the analysis. Of course, when all parameters need to be chosen in preparation of an actual run, it is also important to take this error into account.

We calculate the optimal choice for the numerical parameters Δt, I and P using parametrized expressions for the error and the computational times. For the error, we use equation (2) with the constants specified in table 4 and excluding the first term for the discretization error. The constant for the statistical error is multiplied by 2 to take into account 2σ reliability (approximately 95% chance that the statistical error is smaller than the estimated one). The number of transient iterations I_{tr} and the correlation time T are respectively 10 and 1.3. The computational time is expressed as the total number of MC trajectories required: $CPU^I = P(I + I_{tr})t_{tot}/\Delta t$ and $CPU^M = Pt_{tot}/\Delta t$, for respectively the implicit and the mixed approach, where $t_{tot} = 4 \cdot 10^{-5}$s is the time to reach the peak value for the density at the target. These equations provide a good approximation if the MC code is responsible for the majority of the computational time.

With a small amount of computational time available, the mixed approach gives the smallest error, while with more computational time the implicit approach becomes more beneficial. This can be seen from the red and blue dotted lines in figure 5 , in which we show the the minimal errors as a function of the computational time for respectively the mixed and the implicit approach. The sum of the bias and the statistical error can decrease faster with more computational time when averaging is used. Without averaging, this combined error $\epsilon_b + \epsilon_s$ is dominated by the statistical error ϵ_s, while a compromise between ϵ_b and ϵ_s

is sought with averaging. Another advantage of the implicit approach are the smaller constants for the time integration (A_t) and the statistical error (A_s).

Because the implicit and mixed approach are highly competitive in this example, it is more important to choose the optimal parameters within each approach than to choose the best approach. To demonstrate this, the minimal errors obtained with several choices of the time step Δt are indicated in figure 5 , in which the full and dashed lines are obtained with the implicit and mixed approach, respectively. Because the difference in accuracy between the errors obtained with different time steps is large, we conclude that it is critical to choose the optimal value for the the time step.

The best approach with its optimal choice of parameters highly depends on the magnitude of the constants. To select appropriate parameters, it is, therefore, critical to evaluate all error contributions and estimate the constants, which are expected to be highly case-dependent. Estimating the numerical errors, therefore, does not only provide knowledge on the numerical accuracy, but also allows to select more suitable parameters to speed up and/or improve the accuracy of the simulations.

5 | CONCLUSION

We analysed the numerical accuracy in time-dependent simulations with coupled finite volume (FV) - Monte Carlo (MC) codes. Next to the space discretization error, bias and statistical error, present in steady-state FV-MC simulations [2], an additional time integration error exists. Using a simplified 1D model, an implicit approach, in which the system is solved in a fully coupled way and post-processing averaging is used to reach convergence within each time step, is compared to a mixed implicit-explicit approach, in which the MC code is only run once each outer iteration. The implicit and mixed implicit-explicit approach are competitive, with the implicit getting more advantageous with more computational time available. Within each approach, selecting suitable numerical parameters, based on an error analysis, can bring significant improvements in speed and/or accuracy.

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