

A noise-robust Monte Carlo method for electric field calculations in EMC3

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September 24, 2025

Abstract

One of the main codes to analyze and optimize stellarator configurations is the EMC3 code, which implements a state-of-the-art 3D Monte Carlo plasma edge transport code. However, so far, a self-consistent treatment of the $\mathbf{E} \times \mathbf{B}$ drift is absent. This plasma drift is known to significantly impact the particle and heat distribution in the plasma edge. It is desirable to incorporate this drift into EMC3 to improve the predictive capabilities of the code. The calculation of the $\mathbf{E} \times \mathbf{B}$ drift requires the approximation of the electric field \mathbf{E} , which is proportional to the gradient of the electric potential φ . In previous work [2], the gradient was calculated with a least squares method based on a finite difference approximation of the electric potential. However, due to the stochastic nature of EMC3, the output plasma fields computed by the code are inherently noisy. The finite difference method further amplifies the noise, with the amplification growing as the grid size decreases. We continue from [1], which introduced a new noise-robust method for 1D derivatives. We extend the noise-robust method to 2D and apply it to the electric potential. We show that a PDE can be derived that describes the evolution of the electric field in case of a uniform diffusion coefficient. This PDE allows us to approximate the electric field directly with a Monte Carlo simulation, thus avoiding the need for a finite difference approximation. We illustrate the accuracy of the method and the noise robustness with a test case.

Keywords: Monte Carlo, gradient approximation, electric field, noise-robust

1 Introduction

Nuclear fusion reactors have been a research topic for decades now. Over the years, countless of machine design were developed [6]. The most popular machine designs are the tokamak and the stellarator. The stellarator omits the need of an induced plasma current to generate the poloidal magnetic field [7]. Instead, it relies on geometrically complex magnetic coils to induce spiraling magnetic field lines. Therefore, the mathematical models and corresponding numerical solvers have to deal with this complex 3D geometry.

A popular code to perform simulations of the plasma edge in stellarator type devices is the EMC3-EIRENE code. The MC-MC coupled code estimates the density, momentum and energy of the plasma. The plasma edge simulations require an efficient and accurate computation of gradients. Important gradients include the temperature gradient, pressure gradient, gradient of the electrical potential and the magnetic field gradient [3, 9, 10]. Especially the gradient of the electrical potential φ plays an important role in plasma edge simulations, as it directly determines the electric field \mathbf{E} , through the relation $\mathbf{E} = -\nabla\varphi$. The electric field, in turn, is essential for modeling the $\mathbf{E} \times \mathbf{B}$ drift, which is a key mechanism for improving the predictive capabilities of the EMC3 code [4]. The main objective is therefore to obtain an accurate representation of the electric field \mathbf{E} by reliably approximating the gradient of the electric potential φ . The electrical potential itself is approximated by the EMC3 code.

In previous work [2], a least squares method based on a finite difference (FD) approximation of the

gradient was proposed. However, the finite difference method has the downside that it amplifies the noise introduced by the Monte Carlo approximation. We illustrate this with a simple one-dimensional example. Consider the potential, given by $\varphi(t, x)$, which is approximated with a Monte Carlo method. We quantify the variance, or noise, on the finite difference approximation as follows

$$\text{Var} \left[\frac{\varphi_i - \varphi_{i-1}}{\Delta x} \right] = \frac{1}{\Delta x^2} \text{Var} [\varphi_i - \varphi_{i-1}]. \quad (1)$$

In Equation (1), the noise of the MC approximation is given by $\text{Var} [\varphi_i - \varphi_{i-1}]$. It is clear that the variance of the finite difference approximation scales quadratically with the inverse of the grid size Δx . As a consequence, the gradient approximations in EMC3 become too noisy for small grid sizes. In this paper, we propose a new method that is more robust for decreasing grid sizes than the finite difference method. The paper is based on the work in [1], which introduced and discussed the Monte Carlo Gradient Approximation (MCGA) method for general 1D Fokker-Planck equations. In this paper, we extend the method to a specific 2D case.

In Section 2, we present the electric potential equation. The current approach to calculate the electric field uses a MC method to solve the electrical potential equation and then applies the FD method. Next, Section 3 introduces the Monte Carlo Gradient Approximation method where we derive a new equation that governs the evolution of the electric field directly. We additionally highlight the challenges associated with this equation. Section 4 provides a numerical experiment to illustrate the ability and accuracy of the MCGA method. We also analyse the effect of grid resolution on the variance of both MCGA and FD approximations. Finally, Section 5 summarizes the main findings and presents the conclusions.

2 Electric Potential Equation

In this section, we derive a reduced model for the electrostatic potential φ . Charge conservation requires the current density \mathbf{J} to be divergence-free, i.e.

$$\nabla \cdot \mathbf{J} = 0. \quad (2)$$

The current density is decomposed into parallel and perpendicular components, $\mathbf{J} = \mathbf{J}_{\parallel} + \mathbf{J}_{\perp}$. The parallel current \mathbf{J}_{\parallel} follows from the electron parallel momentum balance,

$$\mathbf{J}_{\parallel} = \frac{\sigma_{\parallel}}{en_e} (\nabla_{\parallel} p_e - en_e \nabla_{\parallel} \varphi + 0.71 n_e \nabla_{\parallel} T_e), \quad (3)$$

where σ_{\parallel} is the parallel conductivity, p_e and T_e denote the electron pressure and temperature, and n_e is the electron density.

The perpendicular current \mathbf{J}_{\perp} accounts for diffusion and non-ambipolar convective drifts,

$$\mathbf{J}_{\perp} = \mathbf{J}_{\text{drift}} - \sigma_{\perp}^{an} \nabla_{\perp} \varphi, \quad (4)$$

with σ_{\perp}^{an} representing the anomalous perpendicular conductivity.

Substituting these expressions into Eq. (2) yields a diffusion equation for the electrostatic potential,

$$\nabla \cdot (-\sigma_{\perp} \nabla_{\perp} \varphi - \sigma_{\parallel} \nabla_{\parallel} \varphi) = S, \quad (5)$$

$$S = -\nabla \cdot \mathbf{J}_{\text{drift}} - \nabla \cdot \left(\frac{\sigma_{\perp}}{e} (T_e \nabla_{\parallel} \ln(n) + 1.71 \nabla_{\parallel} T_e) \right). \quad (6)$$

For boundary conditions at the plates, Bohm boundary conditions of the form

$$\frac{e\varphi}{T_e} = 2.8 + 0.5 \ln \left(\frac{m_i T_e}{m_e T} \right) - \ln \left(1 - \frac{J_{\parallel}}{J_{\text{sat}}} \right), \quad (7)$$

are employed. Other boundary condition, such as reflective boundaries, are also possible. Equation (5) is a stationary diffusion-type equation. However, in Sections 3 and 4, we consider a more general time-dependent diffusion equation. For clarity and simplicity, we adopt classical Dirichlet boundary conditions; however, the approach remains valid if Bohm boundary conditions are used instead. Equation (5) serves as the starting point for deriving a closed evolution equation for \mathbf{E} in the next section.

3 Monte Carlo Gradient Approximation

In this section, we introduce the Monte Carlo Gradient Approximation method for computing gradients in 2D. For both the derivation and the numerical experiments, the electrical potential φ is modeled by a time-dependent linear diffusion equation with spatially varying isotropic diffusion coefficient $D(\mathbf{r})$ in a Cartesian coordinate system. The equation equals

$$\partial_t \varphi(t, \mathbf{r}) = \nabla \cdot (D(\mathbf{r}) \nabla \varphi(t, \mathbf{r})), \quad (8)$$

where $\mathbf{r} = (x, y)^T$ and $\nabla = (\partial_x, \partial_y)^T$. The quantity of interest is the electric field $\mathbf{E} = -\nabla \varphi$. The idea of the Monte Carlo Gradient Approximation method is to derive an evolution equation directly for \mathbf{E} . Taking the gradient of Equation (8) and assuming sufficient smoothness of φ and D to interchange the order of differentiation, we obtain

$$\nabla \partial_t \varphi(t, \mathbf{r}) = \nabla (\nabla \cdot (D(\mathbf{r}) \nabla \varphi(t, \mathbf{r}))). \quad (9)$$

Next, we swap the order of ∇ and ∂_t , and substitute $\mathbf{E} = -\nabla \varphi$. This results in

$$\partial_t \mathbf{E}(t, \mathbf{r}) = \nabla (\nabla \cdot (D(\mathbf{r}) \mathbf{E}(t, \mathbf{r}))). \quad (10)$$

Finally, we reformulate Equation (10) back into a standard diffusion formulation

$$\partial_t \mathbf{E}(t, \mathbf{r}) = \nabla \cdot (D(\mathbf{r}) \nabla \mathbf{E}(t, \mathbf{r})) + \underbrace{\nabla \cdot (\nabla D(\mathbf{r}) \otimes \mathbf{E}(t, \mathbf{r}))}_{S(t, \mathbf{r})}. \quad (11)$$

Equation (11) is a vector diffusion equation with a source term $S(t, \mathbf{r})$.

We aim to solve Equation (11) with a Monte Carlo method. However, at present time the writers are not familiar with any Monte Carlo method that can directly approximate vector quantities. Instead, we decompose Eq. (11) into scalar equations for the components E_x and E_y

$$\begin{cases} \partial_t E_x(t, \mathbf{r}) = \nabla \cdot (D(\mathbf{r}) \nabla E_x(t, \mathbf{r})) + \nabla \cdot (\partial_x D(\mathbf{r}) \mathbf{E}(t, \mathbf{r})) \\ \partial_t E_y(t, \mathbf{r}) = \nabla \cdot (D(\mathbf{r}) \nabla E_y(t, \mathbf{r})) + \nabla \cdot (\partial_y D(\mathbf{r}) \mathbf{E}(t, \mathbf{r})) \end{cases} \quad (12)$$

Thus, two coupled scalar equations must be solved to approximate the electric field \mathbf{E} .

We illustrate how these equations are coupled. Consider the source term of the x -component

$$\nabla \cdot (\partial_x D(\mathbf{r}) \mathbf{E}(t, \mathbf{r})) = \partial_x (\partial_x D(\mathbf{r}) E_x(t, \mathbf{r})) + \underline{\partial_y (\partial_x D(\mathbf{r}) E_y(t, \mathbf{r}))}. \quad (13)$$

The underlined term couples different components of the electric field through the source term, which poses difficulties. The term $\partial_y E_y$ is unknown, and cannot be incorporated in the simulation in a straightforward way. Estimating $\partial_y E_y$ with finite differences would reintroduce the original problem we seek to resolve. In this work, the term $\partial_y E_y$ is neglected in numerical experiments, assuming that it introduces a small bias in the simulation. Further work is required to develop a consistent approximation strategy including these source terms.

4 Numerical Experiments

In this section, we present two experiments to evaluate the accuracy and robustness of the method. We utilize the method of manufactured solutions to construct reference solutions [8]. All experiments are performed in 2D on a rectangular, uniformly discretized grid.

4.1 Numerical Verification

As a first test, we validate the Monte Carlo method on a simple 2D problem on a square domain. We consider the following equation for the electrical potential:

$$\partial_t \varphi(t, x, y) = \nabla \cdot (Dx^2 \nabla \varphi(t, x, y)) + S(t, x, y), \quad D \in \mathbb{R}^+. \quad (14)$$

This differs from the electrical potential equation in Section 2 because Eq. (14) is time-dependent, the diffusion coefficient is isotropic, and the source term (6) is neglected. To improve readability, we omit the explicit function arguments in the following equations. We employ the method of manufactured solutions to determine the source term $S(t, x, y)$. We propose an exact solution $\varphi(x, y, t) = \exp(-(x + y)) \exp(-Dt)$, from which the source term follows as

$$S = (-D + 2Dx - 2Dx^2) \varphi \quad (15)$$

The corresponding exact electrical field components are

$$E_x(t, x, y) = -\exp(-(x + y)) \exp(-Dt), \quad E_y(t, x, y) = -\exp(-(x + y)) \exp(-Dt). \quad (16)$$

Differentiating Equation (14) with respect to x and y yields the governing equations for the electric field components. For E_x , we obtain

$$\partial_t E_x + \nabla \cdot \left(\begin{bmatrix} -2Dx \\ 0 \end{bmatrix} E_x \right) = \nabla \cdot (Dx^2 \nabla E_x) + S_{E_x}, \quad (17)$$

with the source term S_{E_x} given by

$$S_{E_x} = (2D - 4Dx) \varphi + (-D + 2Dx - 2Dx^2) E_x + \underline{2Dx \partial_y E_y}. \quad (18)$$

The underlined term is again problematic, as it introduces a coupling with the derivative of the y -component. The equation for E_y is simpler, since the diffusion coefficient depends only on the x -direction. We have

$$\partial_t E_y = \nabla \cdot (Dx^2 \nabla E_y) + S_{E_y}, \quad (19)$$

with S_{E_y} equal to

$$S_{E_y} = (-D + 2Dx - 2Dx^2) E_y. \quad (20)$$

Dirichlet boundary conditions are imposed for φ , E_x and E_y with boundary values calculated from the exact solution. The initial condition is likewise taken from the exact solution evaluated in $t = t_0$. All three equations (14), (17) and (19) are simulated with identical parameter values, namely

$$N = 500\,000, \quad t_0 = 0, \quad T^* = 1, \quad \Delta t = 0.001, \quad D = 0.1, \quad (21)$$

where N denotes the number of particles per simulation, t_0 the simulation start time, T^* the end time and Δt the time step. The domain is $[0, 1] \times [0, 1]$ discretized with $M_x = M_y = 15$ grid points. In the source term (18), we utilize the Monte Carlo approximation of φ . The MC approximation of φ is computed jointly with E_x and E_y , such that three equations are solved in parallel. The source terms are incorporated using an operator-splitting method [5]. A detailed description on the treatment of source terms can be found in [1].

Regarding the underlined term in Equation (18), two approaches are considered. Since the manufactured solution is known, $\partial_y E_y$ can be evaluated exactly. When an exact solution is missing, this term is set to 0 under the assumption that it has a minor contribution to the dynamics.

Figure 1 presents the electrical field \mathbf{E} and the norm $\|\mathbf{E}\|_2$, approximated using both the MCGA method and a first-order FD method. For the MCGA method, we additionally show the results obtained when $\partial_y E_y$ is either set to zero or given by the exact source term. The Monte Carlo approximation exhibits significantly less noise compared to the finite difference approximation. Additionally, neglecting the term $\partial_y E_y$ does not introduce a significant bias in the approximation, likely because in this test case the term contributes negligibly to the overall dynamics.

Figure 2 shows the relative error of the MCGA method, both when neglecting $\partial_y E_y$ and when the exact term is used, and the relative error of the FD method. The FD method displays a consistently higher relative error across the domain. When $\partial_y E_y$ is neglected, the relative error is of the same order of magnitude and the approximation remains equally accurate.

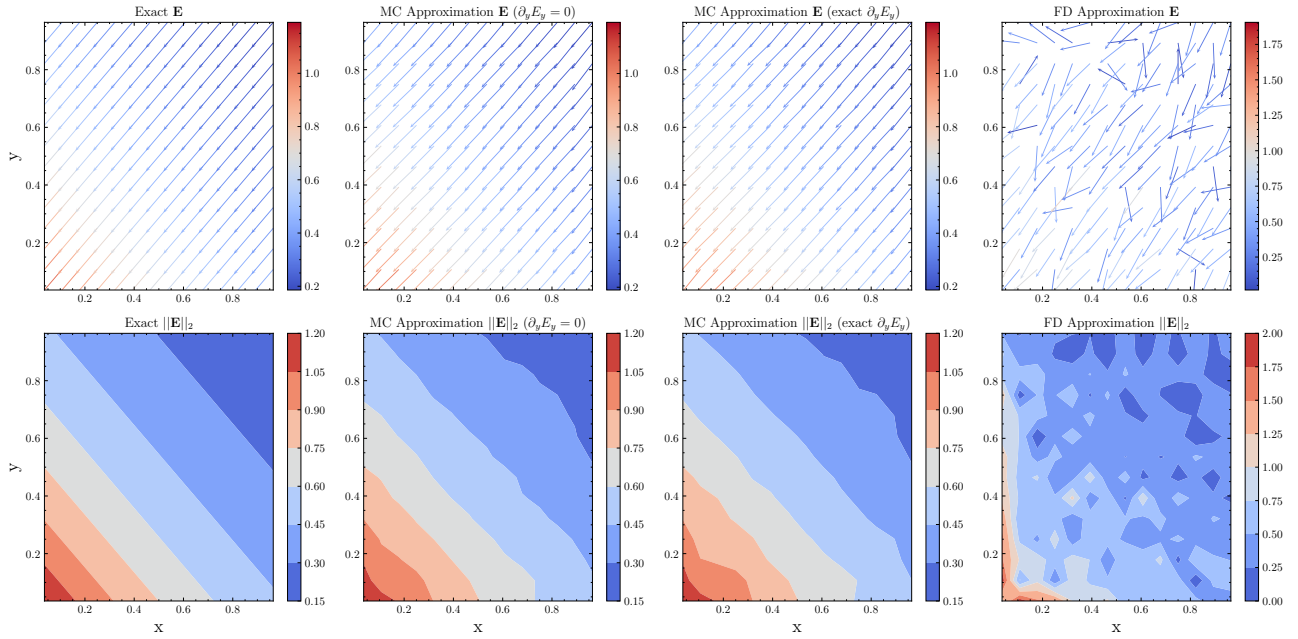


Figure 1: Comparison of the MCGA and finite difference approximation of the electric field \mathbf{E} and the norm $\|\mathbf{E}\|_2$. For the Monte Carlo method, two cases are considered: one where the term $\partial_y E_y$ in Eq. (18) is set to zero, and another where it is given by the exact source term.

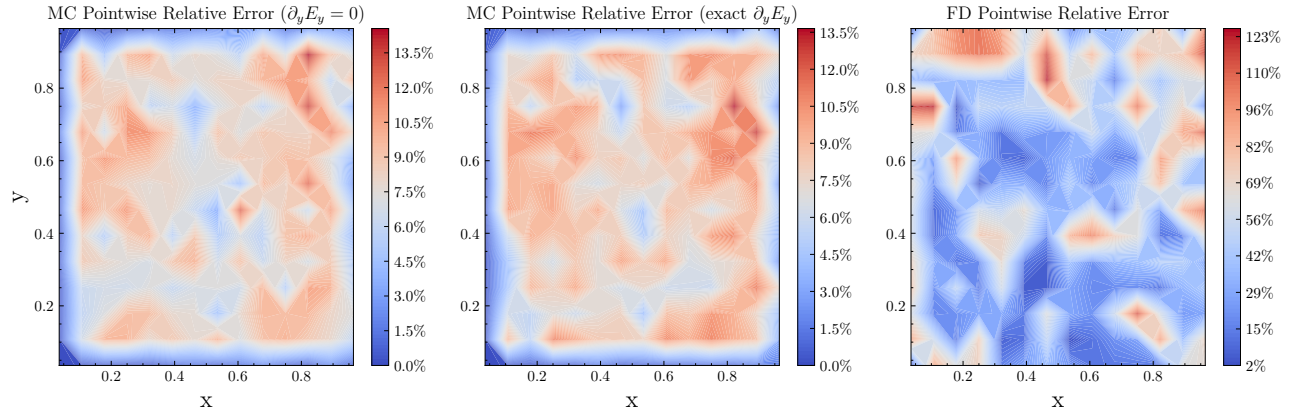


Figure 2: Comparison of the relative error at each grid point for the MCGA and FD methods. As before, the MCGA method is shown both with $\partial_y E_y$ set to zero and with its exact value. Note that the colorbar scales are different between the plots.

4.2 Noise Robustness

Next, we investigate the effect of grid resolution on the variance of the MCGA method, and compare the results with the FD method. While a Monte Carlo method is independent of the grid size, the grid resolution affects the density approximation. In 2D, for a uniform grid and equal scaling in both dimensions, the variance increases with order 2. For the FD method, we expect an increase of order 4, consistent with Eq. (1).

To avoid complications arising from incomputable source terms, we consider the simplified diffusion problem for the electrical potential

$$\partial_t \varphi(t, x, y) = D \nabla^2 (\varphi(t, x, y)), \quad (22)$$

with Dirichlet boundary conditions. An exact solution to Equation (22) is the Gaussian

$$\varphi(t, x, y) = \frac{1}{4\pi Dt} \exp\left(-\frac{x^2 + y^2}{4Dt}\right). \quad (23)$$

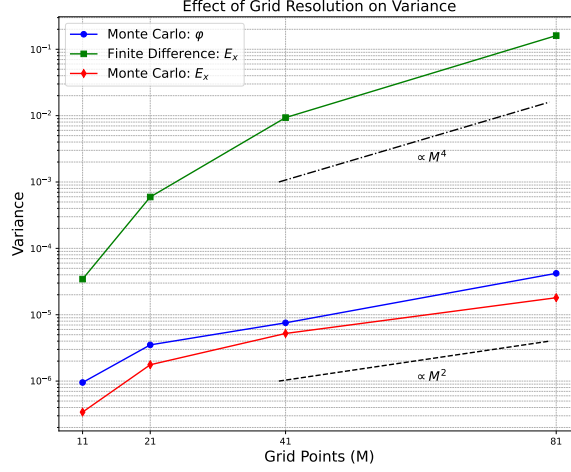


Figure 3: Effect of the grid resolution on the variance. The variance of the FD approximation of E_x grows faster than the MC approximation of E_x . This indicates that the MC method is more robust to noise increase with decreasing grid sizes.

The corresponding exact electric field components are

$$E_x(t, x, y) = -\frac{2x}{4\pi Dt} \exp\left(-\frac{x^2 + y^2}{4Dt}\right), \quad E_y(t, x, y) = -\frac{2y}{4\pi Dt} \exp\left(-\frac{x^2 + y^2}{4Dt}\right), \quad (24)$$

which satisfy the diffusion equations

$$\partial_t E_x(t, x, y) = D \nabla^2 (E_x(t, x, y)), \quad \partial_t E_y(t, x, y) = D \nabla^2 (E_y(t, x, y)), \quad (25)$$

respectively. Equations (22)-(25) are solved on the domain $[0, 2] \times [0, 2]$ using uniform grids with a different number of gridpoints $M = M_x = M_y = \{11, 21, 41, 81\}$. The remaining simulation parameters are chosen as

$$N = 500\,000, \quad \Delta t = 0.01, \quad t_0 = 5, \quad T^* = 6, \quad D = 0.1. \quad (26)$$

The variance for each grid resolution M is computed as

$$\text{Var}_M = \mathbb{E} \left[(\hat{u}_M - \mathbb{E}[\hat{u}_M])^2 \right], \quad (27)$$

where \hat{u}_M denotes the solution, calculated with either MC or FD, in the middle of the grid with M grid points. We ran 20 independent simulations to approximate the expectation values with Welford's online algorithm [11]. The results are displayed in Figure 3. We observe the theoretical predicted order of convergence. Furthermore, they indicate that the MC method exhibits greater robustness with respect to grid refinement than the FD method.

5 Conclusion

In this work, we presented the Monte Carlo Gradient Approximation method for computing the electrical field. We demonstrated how to derive a new equation for the electrical field from the electrical potential and discussed the challenges associated with approximating the source term in this formulation. With a numerical experiment, we illustrated that the method works and achieves a lower relative error than FD, even when we set the $\partial_y E_y$ to zero. Lastly, we showed that the method achieves better robustness to noise compared to finite differences for decreasing grid sizes.

For future work, more realistic test cases need to be considered to further assess the accuracy and applicability of the Monte Carlo Gradient Approximation method. These may include cases with Bohm boundary conditions and non-rectangular grids. Such test cases are necessary to assess whether neglecting $\partial_y E_y$ is justified. If omitting this source term introduces a significant bias, more advanced strategies for handling source terms in the electric field equations are needed.

Author contributions

William De Deyn: Conceptualizations (lead), Writing software, Writing of the original draft. **Ruben De Wolf:** Conceptualizations (support), Helping in writing of Section 2, Review and editing. **Vince Maes:** Conceptualizations (support), Review and editing. **Giovanni Samaey:** Conceptualizations (support), Review and editing.

Acknowledgments

The work of W.D.D is supported by the European Union’s Horizon Europe research and innovation program under the Marie Skłodowska-Curie Doctoral Network Datahyking (Grant No. 101072546).

References

- [1] W. De Deyn. Monte Carlo techniques for noise-robust field calculations in nuclear fusion plasma edge modelling. Master’s thesis, KU Leuven, Leuven, Belgium, 2024.
- [2] R. De Wolf, F. Reimold, Y. Feng, M. Jacobs, W. Dekeyser, G. Samaey, and M. Baelmans. Toward plasma drifts in EMC3: Implementation of gradient, divergence, and particle tracing schemes. *Contributions to Plasma Physics*, page e202300154, 2024.
- [3] K. C. Hammond, Y. Gao, M. Jakubowski, C. Killer, H. Niemann, L. Rudischhauser, A. Ali, T. Andreeva, B. D. Blackwell, K. J. Brunner, B. Cannas, P. Drewelow, P. Drews, M. Endler, Y. Feng, J. Geiger, O. Grulke, J. Knauer, S. Klose, S. Lazerson, M. Otte, F. Pisano, U. Nener, A. P. Sitjes, K. Rahbarnia, J. Schilling, H. Thomsen, G. A. Wurden, and the W7-X team. Drift effects on w7-x divertor heat and particle fluxes. *Plasma Physics and Controlled Fusion*, 61(12):125001, Oct. 2019.
- [4] D. Kriete, A. Pandey, V. Perseo, J. Schmitt, D. Ennis, D. Gradic, K. Hammond, M. Jakubowski, C. Killer, R. König, D. Maurer, F. Reimold, V. Winters, M. Beurskens, S. Bozhnikov, K. Brunner, G. Fuchert, J. Knauer, E. Pasch, and E. Scott. Effects of drifts on scrape-off layer transport in W7-X. *Nuclear Fusion*, 63(2):026022, Feb. 2023.
- [5] S. MacNamara and G. Strang. Operator splitting. In *Splitting methods in communication, imaging, science, and engineering*, Scientific Computation, pages 95–114. Springer, Cham, dec 2016.
- [6] S. Meschini, F. Laviano, F. Ledda, D. Pettinari, R. Testoni, D. Torsello, and B. Panella. Review of commercial nuclear fusion projects. *Frontiers in Energy Research*, 11, June 2023.
- [7] D. Moiraf. Transport and radiation analysis of radiation-limited plasmas in the stellarator wendelstein 7-x. Master’s thesis, Paris-Saclay University, Aug. 2021.
- [8] P. J. Roache. Code Verification by the Method of Manufactured Solutions. *Journal of Fluids Engineering*, 124(1):4–10, Mar. 2002.
- [9] T. Rognlien, G. Porter, and D. Ryutov. Influence of and ∇B drift terms in 2-D edge/SOL transport simulations. *Journal of Nuclear Materials*, 266-269:654–659, Mar. 1999.
- [10] W. M. Stacey. On the physics of the pressure and temperature gradients in the edge of tokamak plasmas. *Nuclear Fusion*, 58(4):046006, Feb. 2018.
- [11] B. P. Welford. Note on a method for calculating corrected sums of squares and products. *Technometrics*, 4:419–420, 1962.