Theoretical and numerical methods for kinetic simulation of plasmas

Filippo Zonta
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Understanding and simulating the dynamics of plasmas in Tokamak devices is a crucial aspect of the plasma physics research, especially with the upcoming ITER device. The development of numerical schemes that possess conservation laws over the vast time scale that covers the dynamics of charged particles in fusion plasmas is an intimidating yet very important task. This thesis presents novel numerical and theoretical techniques to tackle this problem.

First, an overview of the kinetic theory, in particular the derivations of the Vlasov equation, the Fokker-Planck equation and the Vlasov-Maxwell equation in a variational setting, is given. The Euler-Poincaré\(\{\epsilon\}\) reduction, which is a powerful mathematical tool that allows to derive the Vlasov-Maxwell equations in a straightforward way, is presented as well.

A multi-species, marker based, structure-preserving numerical code for the Landau equation is presented. The code is able to preserve energy and momentum to machine precision and leverages GPU-computing to efficiently scale with the dimension of the system. The scheme was validated against relaxation, isotropization and thermalization theoretical estimates for different mass-ratio of the species, including a real electron-deuteron case, showing good agreement in all performed tests.

Finally, the problem of fast ions is tackled by introducing the Backward Monte Carlo (BMC) scheme. The approach aims at increasing the poor statistics of current Forward Monte Carlo simulations by integrating the probability of fast ions backward in time and taking into account deterministically the spread of the Monte Carlo collision operator. The scheme was implemented as a module of the orbit following code ASCOT5, enabling high performance simulations especially with modern supercomputers, and test cases with realistic plasma profiles, magnetic fields and wall geometries. The BMC scheme was applied to a realistic ASDEX Upgrade configuration of beam-ion distributions, with a Fast-Ion Loss Detector (FILD) placed near the divertor. The results show a substantial increase of wall hits compared to a standard Forward Monte Carlo simulation.

Keywords plasma, monte-carlo, gyrokinetics, fast ions, structure-preserving


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At (almost) the end of this big journey, I think it’s a good time to look back for remembering and showing my gratitude to a few people. First, I’d like to thanks my supervisor, Mathias Groth, for the support and for enabling me to pursue this project.

All the insights, support and patience throughout the years from my advisor, Eero Hirvijoki, has been absolutely unforgettable; I would have probably been lost in the middle of my PhD without him.

I would also like to thanks all the people in the department for the good company and support; first of all my PhD journey companion Riccardo for all the support through the years, Fabio, Annika and Rina, Lucia and the ELMFIRE group: Timo, Laurent, Francis and Susan. Taina for her support, for her kindness and for organizing a very nice summer party at her place a while ago. Veera for being the perfect neighbor-turned-italian language prodigy and for all the fun trips, grazie mille!

Thanks for the people, Leevi and Jenna in particular, joining me in those adventures across the Nordics: seeing Lapland, Norway and the hidden places in this beautiful country has been an incredible trip! Päivi for the good company and support throughout all the years.

All the people that are just a couple of kilometers south of Finland: Luca, Max, Diissi, Camp, Pippo, JeJe, Emma and Anna, I’m looking forward to hug you all again!

Last, but not least, I want to give the biggest gratitude to my mom, my sister and Alberto: we are so far away, but the thought of you warms my heart every time.

Dad, even if you are not here anymore, you are still with me every day and I keep thinking about talking and arguing with you about math, physics and fun problems. When the day goes dark, you’re a small, but never ending light.
Finally, I want to dedicate this thesis to the newcomer Pietro. I'm watching the videos of you growing and smile. In a few years, you'll read this thesis and we'll laugh about the old times when humans had yet to solve fusion.

Helsinki, May 10, 2023,

Filippo Zonta
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List of Publications

This thesis consists of an overview and of the following publications which are referred to in the text by their Roman numerals.


Author’s Contribution

Publication I: “Dispersion relation for gauge-free electromagnetic drift kinetics”

The paper examines a new drift-kinetic gauge-free electromagnetic theory and verified tests it against the classic kinetic theory of the dispersion relation of propagating waves in plasmas. The author derived the Vlasov-Maxwell equations for the drift-kinetic Lagrangian using the Euler-Poincarè reduction, co-wrote the appendix sections, and helped with reviewing and correcting the rest of the manuscript. Hirvijoki and Iorio contributed in the formulation of the problem of the study and the interpretation of the results. Burby and Liu contributed in the formulation and interpretation of the theory.

Publication II: “Subcycling of particle orbits in variational, geometric electromagnetic particle-in-cell methods”

The paper deals with an upgrade of the GEMPIC particle-in-cell code to allow for different time steps for different particle species. The author derived the subcycling equations for the push forward in the explicit scheme and wrote the relative section in the paper. Hirvijoki designed and developed the theory of the subcycling schemes and co-wrote the paper. Kormann developed the numerical code, ran the simulations and cowrote the paper.
Publication III: “A Backward Monte Carlo method for fast-ion-loss simulations”

The paper presents a Backward Monte Carlo code for the study of fast ions populations and tested it with Fast-Ion Loss Detector (FILD) in ASDEX Upgrade test cases. The author developed the code, run the simulation with Sanchis and wrote the manuscript with input from all the contributors. Hirvijoki designed the Backward Monte Carlo scheme and contributed in the review and writing of the manuscript. Sanchis prepared the AUG test cases and contributed in performing and reporting the test cases in the manuscript.

Publication IV: “Multispecies structure-preserving particle discretization of the Landau collision operator”

The paper presents a Multi species structure-preserving Landau integrator and tested it with the known analytical theory of thermalization, relaxation and isotorpization. The author extended previous works of the structure-preserving code to account for multiple species, developed the code, run the test cases and wrote the manuscript with inputs from all the coauthors. Hirvijoki designed the single particle scheme and contributed in this work with reviewing, correcting the manuscript, co-writing the response to the reviewers and providing some code samples. Pustzay helped with the review of the manuscript and by providing insights and troubleshooting on the issues of the numerical code.
1. Introduction

The increasing demand for new energy production, as well as the request to reduce the emissions and the environmental impact, the unstable geopolitical scenario, and the increased difficulty in obtain natural gas and oil have put the world in a challenging state.

Thermonuclear fusion is a potential candidate to be one of the leading energy sources of the future, for several reasons: the use of hydrogen as fuel, which is abundant and widely available in nature, has the potential to provide a sustainable source for future generations. Unlike fossil fuels, nuclear reactors do not produce any greenhouse gases or other pollutants. Furthermore, they are considered inherently safe since they cannot suffer catastrophic accidents like fission reactors. While it is true that the activation of exposed materials to high energy neutrons produced by the reactions leads to the creation of nuclear wastes, it is estimated that the radioactivity levels of a commercial fusion power plant after 100 years of its decommissioning are negligible, since the wastes are constituted only by short-lived elements.

However, the remaining scientific and engineering challenges are substantial: open questions remain about the physics of the confinement of the plasma in operational self-sustaining burning condition. Also, designing reactors that can tolerate the power load of a commercial power plant is a big physics and engineering problem.

1.1 Fusion Reactions and confinement

The most common reactions relevant for fusion research are based on the fusion of light nuclei, deuterium, tritium and helium into a heavier element and the release of kinetic energy:
\[ ^2\text{D} + ^2\text{D} \rightarrow ^3\text{He} + ^1\text{n} + 3.27 \text{ MeV} \quad (1.1a) \]

\[ ^2\text{D} + ^2\text{D} \rightarrow \begin{cases} ^3\text{T} + ^1\text{H} + 4.03 \text{ MeV} \\ ^4\text{He} + ^1\text{n} + 17.6 \text{ MeV} \end{cases} \quad (1.1b) \]

\[ ^2\text{D} + ^3\text{T} \rightarrow ^4\text{He} + ^1\text{n} + 18.3 \text{ MeV} \quad (1.1c) \]

These reactions are possible since the binding energy of light nuclei increases with increasing mass number, as depicted in Fig. 1.1, up to Fe\(^{56}\).

![Figure 1.1. Binding energy per nucleon vs mass number](image)

**Figure 1.1.** Binding energy per nucleon vs mass number

While the deuterium-deuterium reaction is used in existing experimental devices due to the advantage of not having to deal with radioactive tritium, the deuterium-tritium (1.1c) reaction is generally considered the most promising one, since the cross-section is the highest at low temperatures, making it an ideal candidate for first-generation power plants. While deuterium is abundant in seawater, tritium must be produced from isotopes of lithium through the following neutron induced fission reactions:

\[ ^6\text{Li} + \text{n} \rightarrow ^4\text{He} + 4.8 \text{ MeV} \quad (1.2a) \]

\[ ^7\text{Li} + \text{n} \rightarrow ^4\text{He} + \text{n} - 2.5 \text{ MeV} \quad (1.2b) \]

The strategy underneath all experimental fusion devices is to confine the particles in a region of space for long enough time for the fusion reactions...
to occur without being lost by elastic scattering. A condition relating the density $n$, the confinement time $\tau_E$ and temperature $T$ is known as the triple-product:

$$n\tau_ET \geq 3 \cdot 10^{21} \text{m}^{-3}\text{sMeV}$$  \hspace{1cm} (1.3)

For typical values of temperature and density, the confinement time should be at least of a few seconds. At temperature of interest, the gases are fully ionized plasmas. The idea to use magnetic fields to induce the charged particles to follow the field lines comes quite natural and it is the main subject of this thesis. However, it is worth mentioning that an alternative approach is given by the inertial confinement method in which a small deuterium-tritium solid target is heated by high energy laser beams which induce the surface of the target to evaporate and the internal part to implode. The subsequent increased density makes fusion reactions possible.

The leading and one of the most advanced design in magnetic fusion research is the Tokamak, in which the magnetic configuration is the results of the superposition of toroidal and poloidal magnetic fields, the first generated by external coils, and the latter is induced by a toroidal current generated through a transformer coil in the center of the device. The results is a helical magnetic field that ensure the confinement of the particles. The toroidal plasma current also heats the plasma resistively. However, as the resistivity of the plasma decreases with increasing electron temperature, alternative heating methods are required in order for the plasma to reach the desired temperature. All of these methods, including the self-heating induced by the fusion reactions, create minority species, fast ions, with temperature much higher than the plasma temperature.

The confinement of these particles is of primary concern, as its degradation can lead to a substantial decrease of performance of the device or a damage of the plasma-facing components. It is therefore crucially important, specially for the upcoming ITER Tokamak device, to design numerical codes able to simulate accurately the transport losses due to the fast ions and their interaction with the background 3D magnetic fields and with plasma waves and instabilities.

Due to the fact that the dynamics of charged particles in plasmas of fusion interest spans an extremely wide range of time and length scales, current state of the art numerical integrators often suffer of performance degradation in terms of accumulation of energy error or other invariants over time, or a poor statistics of simulated signals. This thesis aims at investigating promising new numerical schemes, as well as the theory
behind them, that can help mitigating the aforementioned issues.

### 1.2 Organization of the thesis

This thesis is organized as follows: first, an overview of the kinetic theory of plasmas, particularly of the Vlasov equation and the collisional operator and its link to the Fokker-Planck equation, is given. Then, it will be shown how to derive the Vlasov-Maxwell equations from a variational principle. This is useful for both the development of structure-preserving codes and for the results obtained in Publication I.

In chapter 3, the attention is shifted towards the physics of fast ions and Monte Carlo schemes for the modelling of wall losses. Particular attention is given to the structure of the numerical code ASCOT5 and the novel Backward Monte Carlo scheme presented in Publication III. Perhaps the main goal of the chapter is making clear what is the logic behind the scheme on one hand, and explaining the code structure and parallelization techniques of the code on the other hand. Both goals are likely useful for decreasing the learning curve of the BMC code.

In chapter 4 the kinetic theory is taking into account and applied to the modeling of structure-preserving schemes for the Vlasov-Maxwell-Landau system. First, the concept of structure-preserving is explained, the metriplectic formulation is described with a fairly good level of details and finally a few examples of structure-preserving codes built from the metriplectic formulation is given.

Finally, in chapter 5 a few numerical results found in Publication III and Publication IV are presented.
2. Kinetic theory

One of the most important topics in fusion physics research is the study of the kinetics of plasmas and the evolution of the distribution function. It is in fact unfeasible to follow the trajectories and states of all single particles in a plasma, due to vast amount of particle interacting with each other. The kinetic theory provides a practical way to describe, through statistics, the probability of particles to occupy a specific 6-dimensional volume in phase-space. In such a way, the usual measurable quantities, e.g. pressure, temperature, density, are obtained as moments of the distribution function. The aim of this chapter is to give a brief overview of the main kinetic equations for the distribution function: the Vlasov equation (section 2.1), the Landau collision operator (section 2.2). This serves as a basis for many numerical schemes and methods, some of which are treated in subsequent chapters. Finally, a description of the variational formulation of the Vlasov-Maxwell system and the Euler-Poincarè reduction is given in section 2.3 and 2.4. These two methods are useful for both numerical structure-preserving schemes, in chapter 4 and for the realization of Publication I

2.1 The Vlasov equation

Consider an ensemble for a system of \( N \) particles for which the configuration of the system is described by a \( 6N \) dimensional \( \Gamma \) – space. The density of states, or in other words, the amount of particles that occupy an infinitesimal region \( dz_1 \ldots dz_N \) is denoted by \( \rho(z_1, \ldots, z_N, t) \). The joint probability to find the first \( k \) particles to be at the same time at the phase-space points \( z_1, \ldots, z_K \) is denoted by \( f_k \) and is derived by integrating over the remaining particles:

\[
f_k(z_1, \ldots, z_K, t) = V^k \int \rho_N d z_{K+1} \ldots d z_N
\]
In particular, the usual one-particle probability distribution is

$$f_1(z, t) = V \int \rho_N dz_2 ... dz_N$$  \hspace{1cm} (2.2)

Given that the density $\rho$ satisfies the Liouville’s equation, it can be proven [41, 9] that $f_1$ satisfies the relation

$$\frac{\partial f_1(z_1, t)}{\partial t} + v_1 \cdot \nabla_x f_1(z_1, t) + n_0 \int dz_2 \frac{F_{12}}{m} \cdot \nabla v_1 f_2(z_1, z_2, t) = 0$$  \hspace{1cm} (2.3)

where $F_{12}$ is the interacting force between the particle 1 and 2 and $n_0$ is the particles density. In the above equation, the distribution $f_1$ depends on the two-particle distribution $f_2$. For every $k$, it can be derived a similar equation in which $f_k$ depends on the next function $f_{k+1}$. In the easiest case, when the particles don’t interact with each other, the joint probability $f_2$ is simply

$$f_2(z_1, z_2, t) = f_1(z_1, t) f_1(z_2, t)$$  \hspace{1cm} (2.4)

Substituting (2.4) into (2.3) gives

$$\frac{\partial f_1(z_1, t)}{\partial t} + v_1 \cdot \nabla_x f_1(z_1) + \frac{F}{m} \cdot \nabla v_1 f_1(z_1) = 0$$  \hspace{1cm} (2.5)

where $F$ is the interacting force averaged over all particles

$$F = n_0 \int dz_2 F_{12} f_1(z_2, t)$$  \hspace{1cm} (2.6)

(2.5) is the well known Vlasov, or the collisionless Boltzmann equation. Although it is one of the most important ones in plasma physics, this equation lacks some important features. A non equilibrium plasma for example is expected to relax itself to an equilibrium with a Maxwellian distribution. This cannot be described by the Vlasov equation alone, but instead it is required to add collisional terms to the equation, in particular to (2.3) and subsequent terms.

### 2.2 The collision operator and the Fokker-Planck equation

The collisional operator for weakly interacting spatially homogeneous plasmas was studied extensively in the past. The first derivation is due to Landau [31], hence the name Landau collisional operator. One of the most important derivation follows the work of Rosenbluth [45] and describes the Coulomb collisions in a Fokker-Planck representation. This is particular attracting for numerical simulation applications, since a number of methods exists for solving the Fokker-Planck equation, including finite element
methods, Monte Carlo schemes and finite difference schemes. A complete
derivation of the Fokker-Planck-Landau equation, for which the reader is
referred for example to [47, 20], is beyond the scope of this work. The main
concepts are however given below.

The individual motion of the particles and their deflections due to Coulomb
scattering are similar to a Brownian motion and its statistical behaviour
can be taken into account as a Markov chain process. Denoting by \( W(z, t, \Delta, \tau) \)
the probability of a particle to jump from the position \( z \) at time \( t \) by an
amount \( \Delta \) in the time interval \( \tau \), the change in the distribution function

\[
f(z, t + \tau) = \int f(z - \Delta, t) W(z - \Delta, \Delta; \tau)
\]

(2.7)

Assuming that the jump probability \( W \) is non negligible only for small de-

\[\Delta\]

flections \( \Delta \), both terms in the R.H.S of the above equation can be expanded
in a Taylor series around \( z \) and \( t \). Keeping only the terms up to second
order in \( \Delta \) and taking the limit \( \tau \to 0 \), the result is:

\[
\frac{\partial f(z, t)}{\partial t} = - \frac{\partial}{\partial v} \cdot \left( K(z, t) f(z, t) \right) + \frac{\partial}{\partial v} \frac{\partial}{\partial v} : D(z, t) f(z, t)
\]

(2.8)

where the coefficients \( K \) and \( D \) are formally defined as:

\[
K(z, t) = \lim_{\tau \to 0} \int \frac{\Delta W(z, t; \Delta, \tau)}{\tau} d\Delta
\]

(2.9)

\[
D(z, t) = \lim_{\tau \to 0} \int \frac{\Delta \Delta W(z, t; \Delta, \tau)}{2\tau} d\Delta.
\]

In practice, since the spatial scale of the collisions, given by the Debye
length \( \lambda_D \), is much smaller than the ones of the velocity, the derivation
of \( K \) and \( D \) requires to compute the expectation value of the mean and
covariance change in velocity induced by the collisions, which is obtained
by integrating though all jumps and weighting with the differential cross
section \( d\sigma/d\Omega \):

\[
K(v) = \sum_\beta \int \int f_\beta(v') |v-v'| \frac{d\sigma(|v-v'|, \Omega)}{d\Omega} (v^* - v) d\Omega d\Omega
\]

(2.10)

\[
D(v) = \frac{1}{2} \sum_\beta \int \int f_\beta(\bar{v}) |v-\bar{v}| \frac{d\sigma(|v-\bar{v}|, \Omega)}{d\Omega} (v^* - v) (v^* - v) d\Omega d\bar{v}
\]

(2.11)

In the above expression, \( v^*(v, \bar{\bar{v}}, \Omega) \) is the final velocity after the scattering
process, function of the velocities \( \bar{\bar{v}} \) of the colliding particles \( \beta \) and the solid
angle element \( d\Omega = \sin\chi d\chi d\phi \), \( \chi \) being the scattering angle. The differential cross section of particles scattering under the Coulomb potential
is:

\[
\frac{d\sigma(|v-v'|, \Omega)}{d\Omega} = \left( \frac{qq_\beta}{8\pi\varepsilon_0 m_e |v-v'|^2} \right)^2 \frac{1}{\sin^4(\chi/2)}
\]

(2.12)
where \( m_r \) is the reduced mass of the two particles. The expressions resulting in substituting (2.12) into (2.10) and (2.11) are divergent when integrated over the solid angle between \( \chi = 0 \) and \( \chi = \pi \). However, the fact that collisions are only possible at distances smaller than the Debye length \( \lambda_D \) provides a lower limit \( \chi_{\text{min}} \) to the scattering angle. The integration then results in:

\[
K(v) = -\sum_{\beta} \frac{q q^2 \ln \Lambda}{8 \pi \varepsilon_0 m^2} \left( 1 + \frac{m}{m_{\beta}} \right) \int f_{\beta}(\vec{v}) \frac{2u}{u^2} d\vec{v},
\]

(2.13)

\[
D(v) = \sum_{\beta} \frac{q q^2 \ln \Lambda}{8 \pi \varepsilon_0 m^2} \int f_{\beta}(\vec{v}) \frac{1}{u} \left( 1 - \frac{uu}{u^2} \right) d\vec{v}
\]

(2.14)

where \( u \) is the relative velocity \( u = v - \vec{v} \) and the Coulomb logarithm \( \ln \Lambda \) is related to the minimum scattering angle with:

\[
\ln \Lambda = -\ln \left( \sin \left( \frac{\chi_{\text{min}}}{2} \right) \right) 
\approx -\ln \left( \frac{ee_{\beta}}{4\pi \varepsilon_0 m_r u^2} \right)
\]

(2.15)

Noting that the \( u \) terms in (2.13) are the derivative of the ones in (2.14), both equations can be rewritten as:

\[
K(v) = \sum_{\beta} \frac{v_{\beta}}{m^2} \left( 1 + \frac{m}{m_{\beta}} \right) \int f_{\beta}(\vec{v}) \frac{\partial}{\partial u} \cdot Q(u) d\vec{v},
\]

(2.16)

\[
D(v) = \sum_{\beta} \frac{v_{\beta}}{m^2} \int f_{\beta}(\vec{v}) Q(u) d\vec{v}
\]

(2.17)

where \( v_{\beta} = (q q^2 \ln \Lambda) / (8 \pi \varepsilon_0^2) \) and \( Q(u) \) is the tensor

\[
Q(u) = \frac{1}{|u|} \left( \frac{u}{u} - \frac{uu}{|u|^2} \right)
\]

(2.18)

Substituting (2.16) and (2.17) into (2.8), the Landau form of the Fokker-Planck equation is retrieved:

\[
\frac{\partial f}{\partial t} = \sum_{\beta} \frac{v_{\beta}}{m} \frac{\partial}{\partial v} \cdot Q(v - \vec{v}) \cdot \left( \frac{f_{\beta}(\vec{v})}{m} \frac{\partial f}{\partial v} - \frac{f(v)}{m_{\beta}} \frac{\partial f_{\beta}}{\partial v} \right) d\vec{v}
\]

(2.19)

Under the condition that the background plasma distributions can be approximated to Maxwellians and that the self-collisions can be neglected, the coefficients \( K \) and \( D \) can be further simplified to

\[
K^i(v) = \kappa_{\beta} v^i,
\]

(2.20)

\[
D^{ij}(v) = D_{\parallel} \frac{v^i v^j}{|v|^2} + D_{\perp} \left( \delta^{ij} - \frac{v^i v^j}{|v|^2} \right),
\]

(2.21)

with \( D_{\parallel}, D_{\perp} \) and \( v \) defined in terms of the function \( \Psi(y) = \pi^{-1/2} \exp(-y^2) + (y + 1/(2y)) \text{erf}(y) \) and evaluated at the particle speed normalized to the
thermal velocities of the species $\beta$, i.e., at $y_\beta = v/\sqrt{2T_\beta/m_\beta}$. The explicit forms (see [2, 47]) are given by

$$\kappa_\beta = \sum_\beta n_\beta \nu_\beta \left( 1 + \frac{m_\beta}{m_\beta} \right) \left( \frac{m_\beta}{2T_\beta} \right)^{3/2} \frac{1}{y} \left( \frac{d^2\Psi(y)}{dy^2} + \frac{2}{y} \frac{d\Psi(y)}{dy} \right) \bigg|_{y=y_\beta}, \quad (2.22)$$

$$D_{\parallel} = \sum_\beta n_\beta \nu_\beta \left( \frac{m_\beta}{2T_\beta} \frac{d^2\Psi(y)}{dy^2} \right) \bigg|_{y=y_\beta}, \quad (2.23)$$

$$D_{\perp} = \sum_\beta n_\beta \nu_\beta \left( \frac{m_\beta}{2T_\beta} \frac{1}{y} \frac{d\Psi(y)}{dy} \right) \bigg|_{y=y_\beta}, \quad (2.24)$$

Another useful way to describe the collisional evolution of particles comes from the Itô formalism. A so-called Wiener process is a stochastic process $W_t$ parametrized by time for which the change in its value for arbitrary $t$ is another stochastic process that obeys a normal distribution with zero mean and variance $\Delta t$:

$$W_{t+\Delta t} - W_t \sim \mathcal{N}(0, \Delta t) \quad (2.25)$$

The values at $t$ is also independent of previous values and $W_0 = 0$. In many cases, for example when studying minority species, the background plasma distributions are approximated as Maxwellians and the self-collisions neglected. The kinetic equation (2.8) then becomes linear, and the collisional evolution of an individual sample particle from $f$ obeys the following stochastic differential equation of Itô kind

$$dv_c^i = K(z_c^i, t) \, dt + \sigma(z_c^i, t) \cdot dW_t, \quad (2.26)$$

where $dW_t$ represent the differential of a standard Wiener process $W_t \sim \mathcal{N}(0, tI)$ with $\mathcal{N}$ being a multivariate normal distribution. The coefficient $K$ is defined in (2.20) while $\sigma \sigma^T = 2D$ where $D$ is the diffusion coefficient defined in (2.21).

In many plasmas relevant for fusion physics, the variations of the electromagnetic fields occur at length scales longer than the gyroradius and time scales slower than the gyrofrequency. In this case, the rapid gyromotion of a charged particle can be decoupled from the guiding-center motion. The sample particles from the distribution $f$ under such conditions still obey an Itô-like equation

$$dz_c^i = \kappa dt + \Sigma \cdot dW_t, \quad (2.27)$$

where the guiding center coordinates $z = (X, u, \xi)$ are the position, $X$, the magnitude of the velocity, $v$, and the pitch with respect to the magnetic field
direction, $\xi = \mathbf{v} \cdot \mathbf{b}/v$. Written component-wise, the collision operator (2.27) takes the form:

$$dX'_i = \sqrt{2D_X} (\delta^{ij} - b^i b^j) dW_X^i, \quad (2.28)$$

$$dv_t = K_v dt + \sqrt{2D_v} dW_v, \quad (2.29)$$

$$d\xi_t = -2\xi_t \frac{D_\perp}{v^2} dt + \sqrt{2(1 - \xi^2)} \frac{D_\perp}{v^2} dW_\xi. \quad (2.30)$$

The spatial diffusion coefficient $D_X$ is defined by the expression

$$D_X = \left[ (D_\parallel - D_\perp) \frac{1 - \xi^2}{2} + D_\perp \right] \frac{1}{\omega_c^2}, \quad (2.31)$$

where $\omega_c = qB/m$ is the cyclotron frequency, and the momentum drift $K_v$ is

$$K_v = \sum_{\beta} \frac{n_\beta v_\beta m_\beta}{2m T_\beta} \left( -\frac{2y}{m_\beta} \frac{d^2 \Psi}{d y^2} + \frac{1}{m} \frac{d^3 \Psi}{d y^3} + \frac{2}{m} \frac{d^2 \Psi}{d y^2} \right) \bigg|_{y=y_\beta}. \quad (2.32)$$

For further details on the derivations of the above coefficients, the reader is referred to [47, 20]. (2.27) can be used for example in pair with Monte Carlo schemes.

### 2.3 The Vlasov-Maxwell variational formulation

It was known since long time that the Vlasov equation (2.5) can be formulated in a variational setting. A pioneering work by Low [33] in fact derived the Vlasov equation coupled with the Maxwell equations starting from a Lagrangian, which is usually referred as the Low Lagrangian. This formulation is of extreme importance: not only one can find the equations for the particles and the fields, but it allows to study the possible energy- and momentum-conservation laws in the system [42, 23, 4]. Additionally, the extension of this method to gyrokinetics [51, 3], and its application to structure-preserving integrators, fueled a consistent part of the research of plasma physics in the last years.

To understand this concept, consider first a set of $N$ charged particles interacting self-consistently with the electromagnetic fields. If the relativistic effects are ignored for simplicity, the Lagrangian of the system can be written as:

$$L(z_t, A, \phi) = \sum_{i=1}^{N} \left[ \frac{m}{2} \left| \dot{z}_i^t \right|^2 - q \int_{\mathbb{R}^3} dx \left( \phi - \frac{z_i^t}{c} \cdot A \right) \right] + \frac{1}{2} \int_{\mathbb{R}^3} \left( \epsilon_0 \left| \nabla A + \nabla \phi \right|^2 - \mu_0^{-1} |\nabla \times A|^2 \right) dx \quad (2.33)$$
where the dependence of the electromagnetic potentials on the coordinates is omitted for simplicity, i.e. $\phi = \phi(x, t)$. The above Lagrangian can be easily generalized to generic particle motions in non canonical coordinates: denoting by $\Gamma(z_t) = \theta \cdot z_t - h(z_t)$ the single particle Lagrangian in non canonical coordinates, (2.33) reduces to:

$$L(z_t, A, \phi) = \sum_{i=1}^{N} [\theta(z_i) \cdot \dot{z}_i - h(z_i)]$$

$$+ \frac{1}{2} \int_{\mathbb{R}^3} \left( \epsilon_0 |\partial_t \mathbf{A} + \nabla \phi|^2 - \mu_0^{-1} |\nabla \times \mathbf{A}|^2 \right) d\mathbf{x}$$

The Low Lagrangian is directly derived from here by transforming the above Lagrangian in the continuum limit by introducing a particle density probability function $f$ and expressing particles trajectories as a function of their initial condition, labeled as $z_0$:

$$L \left( z_t, \partial_t z_t, A, \phi \right) = \int_{\mathbb{R}^3} d\mathbf{z}_0 f(\mathbf{z}_0) [\partial_t(z_t(\mathbf{z}_0))\partial_t z_t(\mathbf{z}_0) - h(z_t(\mathbf{z}_0))] +$$

$$\frac{1}{2} \int_{\mathbb{R}^3} \left( \epsilon_0 |\partial_t A + \nabla \phi|^2 - \mu_0^{-1} |\nabla \times A|^2 \right) d\mathbf{x}$$

It should be noted that the above Lagrangian is expressed in a mixture of Eulerian variables, namely in the electromagnetic part, and Lagrangian variables in the particle contribution, where the trajectories of the particles are functions of the initial conditions.

### 2.4 The Euler-Poincarè reduction

The idea of the Euler-Poincarè reduction is to express the particle contribution in the Vlasov-Maxwell Lagrangian in terms of the velocity of the phase space at fixed points. The Lagrangian is then expressed in terms of new Eulerian variables and the action principle is replaced by the Eulerian action principle and the equations of motion with a set of constrained Euler-Lagrange equations. The Euler-Poincarè procedure has its roots in a famous Poincarè paper [43], and was revamped recently by various authors in the context of geometric mechanics (see for example [25]), and applied later to the Maxwell-Vlasov Lagrangian [8]. Subsequent works then led to a guiding-center [4] and Hamiltonian formulation [50, 5].

Starting from a particle trajectory $z_t$, the Eulerian vector field is formally defined by computing the Eulerian derivative at a fixed point:

$$\xi_t = \partial_t z_t \circ z_t^{-1}$$
Also, it is noted that the distribution function \( f_0 \) is advected along the particle trajectory in phase-space:

\[
f_t(z_t(z_0))dz_t(z_0) = f_0(z_0)dz_0
given \text{ (2.37)}
\]

Under this condition, the integration labels \( z_t \) and \( z_0 \) can be exchanged and as a result the particle contribution of the Vlasov-Maxwell system is expressed in terms of a reduced Lagrangian, function of the Eulerian velocity and the distribution function at the fixed point \( t \):

\[
l_P(\xi_t, f_t) = \int_{\mathbb{R}^n} f(z) [\Theta_t(z)\xi_t - h(z)]
given \text{ (2.38)}
\]

The critical thing to understand is that the Vlasov-Maxwell system is recovered by varying the action of the Lagrangian (2.35) with respect to arbitrary variations of the particles trajectories and fields. It should not come as a surprise that, by expressing the system with respect to a new set of vector fields, the variations are not arbitrary anymore, but they are constrained to the original variations. If \( \eta_t^i \) denotes a variation of the trajectory \( z_t^i \), the variations of \( \xi \) and \( f_t \) are then linked with:

\[
\delta f_t = -\partial_i(\eta_t^i f_t) 
given \text{ (2.39)}
\]

\[
\delta \xi_t^i = \partial_t \eta_t^i + \xi_t^j \partial_j \eta_t^i - \eta_t^j \partial_j \xi_t^i
\given \text{ (2.40)}
\]

With this set of constraints, the action variation with respect to variations of \( f_t \) and \( \xi_t \) is computed as:

\[
\delta S = \int_{t_1}^{t_2} \int_{\mathbb{R}^n} \left( \frac{\delta \ell}{\delta f_t} \delta f_t + \frac{\delta \ell}{\delta \xi_t^i} \delta \xi_t^i \right) dtdz \delta S =
given \text{ (2.41)}
\]

\[
= \int_{t_1}^{t_2} \int_{\mathbb{R}^n} (\delta f_t (\partial_t \xi_t^i - h) + f_t \partial_i \delta \xi_t^i) dtdz
\]

\[
= \int_{t_1}^{t_2} \int_{\mathbb{R}^n} \left[ -\partial_i(\eta_t^i f_t) (\partial_t \xi_t^i - h) + f_t \partial_i \left( \partial_t \eta_t^i + \xi_t^j \partial_j \eta_t^i - \eta_t^j \partial_j \xi_t^i \right) \right] dtdz
\]

\[
\text{which is rewritten, using integration by parts, as}
\]

\[
\delta S = \int_{t_1}^{t_2} \int_{\mathbb{R}^n} \left( \partial_t (f_t \partial_i \eta_t^i) + \partial_j \left[ f_t \partial_i \left( \eta_t^i \xi_t^j - \xi_t^i \eta_t^j \right) + f_t h \eta_t^j \right] \right) dtdz
\]

\[
+ \int_{t_1}^{t_2} \int_{\mathbb{R}^n} \left( f_t \eta_t^j \left( (\partial_j \theta_t - \partial_t \theta_t) \xi_t^i - \partial_j h - \partial_t \theta_t \right) \right) dtdz \given \text{ (2.42)}
\]

\[
\text{Finally, since variations of the trajectories, and hence the vector field } \eta_t, \text{ are null at the time boundaries, the above relation is simplified to}
\]

\[
(\partial_j \theta_t - \partial_t \theta_t) \xi_t^i - \partial_j h - \partial_t \theta_t = 0 \given \text{ (2.44)}
\]

which are the Hamilton’s equations for the Hamiltonian \( h \). The Vlasov equation is then recovered by imposing the advection condition (2.37). Similarly, the Maxwell equations are found by varying the action with respect to variations of the fields.
3. Fast ions modeling

In this chapter, the theory of the collisional operator presented in chapter 2 is applied to the study of fast ions dynamics. A brief introduction of the importance of the topic is given in section 3.1. In the same section, a description of the code architecture of ASCOT5, one of the leading tools for fast ion analysis, is reported. ASCOT5 is also used by the Backward Monte Carlo, a promising tool to study fast ions signals by integrating the loss probability backward in time starting from a given target section of the wall. In section 3.2, the logic behind the BMC scheme is described, while in section 3.3 its architecture with a stress on the parallelization scheme and its integration into ASCOT5 is given.

3.1 Fast ions and the ASCOT framework

In the upcoming ITER fusion experiment, the understanding of the physics underneath the heating of the plasma is a major challenge faced by the research community. In fact, the self-sufficiency of the plasma is guaranteed by the generated 3.5 MeV alpha particles in the deuterium-tritium reactions. Other energetic or fast ions, also in the MeV range, generated by the neutral beam injector (NBI) or by ion cyclotron resonant heating (ICRH) are expected to play a major role in the heating of the plasma. It is therefore of primary concern the confinement of these particles, as its degradation can lead to both a reduction of the device performance and a substantial damage in the plasma-facing components in the form of incident heat fluxes, risking the integrity of the device. Moreover, the long mean free-path and slowing-down times of fast ions can results in significant interactions with the background 3D magnetic field and with plasma waves and instabilities, resulting in a number of new phenomena along with an expected change in the confinement losses. It is therefore of
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vital interest to predict the dynamics of such particles and their loss rate across the device wall.

In the standard Forward Monte Carlo (FMC) approach, test particles are usually generated from a fast-ion source, for example a Neutral Beam Injector (NBI), and they are followed in time by integrating the equations of motion until they are either thermalized with the background plasma or they hit the wall. This is the case of the orbit following code ASCOT, which was developed by the Aalto University and the VTT Technical Research Centre of Finland since the 90's. ASCOT is able to integrate the trajectories in guiding center or full orbit coordinates.

At the end of the simulations, the trajectories of the markers are stored in a multidimensional grid, representing the steady-state slowing-down distribution of the fast ions. Also, the end state of the markers that hit the wall is recorded, which offer a direct way to compute the power load of fast ions lost to the wall.

In order to run properly, ASCOT needs a number of information about the plasma and the vessel as input from the user. First, temperature, density and the background fields are given in terms of discrete points on multidimensional grids and the inner routines of the code are responsible of interpolating the data. This allows for simulations of arbitrary full 3-D magnetic fields. The first wall of the device can be either be described by a set of two dimensional segments, assuming the shape of the wall to be constant along the toroidal dimension, or a set of 3D triangles generated typically from CAD data of the device. The code is able to generate input markers for example from an ICRH source or from an NBI source.

The last iteration of the code, ASCOT5, fully exploits the modern high performance computing (HPC) techniques in order to parallelize the integration of the markers. The parallelization happens in three separate layers: first, the input markers are distributed along the computational nodes with the MPI library. In the second layer, the markers are distributed with openMP to multiple threads based on the amount of physical or logical core if hyper-threading is available. Finally, the markers are partitioned in SIMD data structures, allowing for an additional layer of parallelization through vectorization.

All these aforementioned features constitutes a strong foundation for studying the dynamics of fast ions. However, there are cases of interest in which a plain Monte Carlo simulation aimed at solving the particle push forward (2.27) with the friction and diffusion coefficients (2.28), (2.29)
and (2.30) suffers from severe statistics accuracy issues due to Monte Carlo noise. For example, when simulating the signal of Fast-Ions Loss Detectors (FILD) which are usually small compared to the spatial scale of the vessel, the recorded wall hits can be very low or zero, even when the birth distribution is constituted of hundred of thousands or even million of markers, the majority of which hits the wall in regions outside the detector or are slowed down in a steady state configuration. Under these conditions, estimating a realistic value of wall loads is practically impossible.

One possible approach to improve the resolution is to tackle directly the probability function by solving the adjoint Fokker-Planck equation. This path was followed in a series of papers by N.J.Fisch and other authors (see i.e. [26, 13, 32] for studying current drives and runaway electrons. An alternative idea is the constituted by the Backward Monte Carlo. The idea of the method is to avoid wasting unnecessary resources for markers that might not reach the detector. The probability to reach a specific area is tracked backwards in time starting from the region of interest with an iterative process in which, during every time step, markers placed on a mesh are advanced according to their equation of motion. The statistical spread of the Monte Carlo collisional operator is resolved numerically and the result is convoluted at each step in order to find a probability map for arbitrary times. The Backward Monte Carlo was used in quantitative finance [1] and in plasma physics in the context of runaway electrons [55], and lastly, of fast-ion dynamics [18].

### 3.2 The Backward Monte Carlo method

To intuitively visualize the method, a simplified one dimensional problem is depicted in Fig. 3.1, where the aim is to determine the probability of particles to reach a certain end condition, in this case the point \( z = 2 \), in a given time. In a real scenario, the end condition, or target domain, can be for example a Fast-ion loss detector (FILD). At the final time \( 3\Delta t \), the probability is trivially vanishing everywhere except at the target domain. Going backwards in time, assuming, e.g., that a marker at a point has equal probability to jump to any nearest points or to stay put, the probability to reach the target from a specific initial location in the given total time interval is built recursively, utilizing the probabilities of the marker particles to move forward in time. In the figure, for example, the probability to reach the target \( z = 2 \) starting from the point \( z = 1 \) at time \( t = 1\Delta t \) is the
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sum of the two possible paths and it is therefore $P = \frac{1}{2} \cdot \frac{1}{2} + \frac{1}{2} \cdot \frac{1}{3} = \frac{5}{12}$. The generalization to a realistic case follows the same philosophy, with some additional key features.

Similarly to the above simplified method, a mesh is defined on the phase-space, either the full orbit 6D space or the reduced guiding center 5D space. Markers are then placed on the mesh nodes in order to find the jump probability. However, as the trajectories of the markers are now continuous, it is necessary to linearly interpolate their position onto the mesh.

Moreover, as the statistical spread of the Monte Carlo operator is regulated by a multivariate Gaussian random variable (2.26), the probability for a marker to reach the end target domain is not a sum of discrete paths, but it is rather found by integrating over the continuous spectrum of the random variables. However, assuming the pitch-angle contribution to be dominant over the other terms, which is reasonable for fusion physics applications, the integration can be efficiently computed numerically with a one-dimensional Gauss-Hermite quadrature.

Fig. 3.2 gives an idea of these concepts: the red marker is evolved by the map $\varphi$, which follows the Hamiltonian equations of motion and the diffusion terms evaluated with a fixed set of Gauss-Hermite knots, represented by the variable $r_k$, and the final position is then interpolated onto the mesh. The probability is then computed multiplying the weights of the quadrature $w$, the weights of the interpolation $\Lambda$ and the probability of the
Figure 3.2. Push forward evolution of mesh markers in the Backward Monte Carlo scheme and linear interpolation to neighbors nodes. The two paths represent two sample trajectories with two different random variable $r$.

Relative nodes at the previous time step $m$. The result is:

$$\Phi_i^{m-1} = \pi^{-1/2} \sum_k w_k \sum_j \Phi_j^m \Lambda_j (\varphi_i^{\Delta t} (\sqrt{2}r_k))$$

where $i$ and $m$ labels the mesh node and time step respectively and the numerical factors are added in order to ensure the proper normalization of the quadrature. It is also worth noticing that the probability at a specific time step depends only on the previous step, hence in the implementation the probabilities can be safely overwritten when the time is advanced.

### 3.3 Implementation and parallelization

The Backward Monte Carlo scheme was implemented as two standalone modules in the ASCOT5 suite. The first, which is explained now, is the BMC core module that computes the probability map on a mesh as anticipated in the previous section. The second, dubbed as BMC important sampling (BMC-IS) and explained later in the section, produces an efficient birth distribution from the pre generated BMC probability map and runs a forward Monte Carlo simulation on top of it.
Algorithm 1 Backward Monte Carlo algorithm flow

1. Read the input parameters from the ASCOT5 hdf5 input file
2. Initialize the phase-space mesh and put markers $z_i^0$ on the vertices.
3. Set initial mesh probabilities $\Phi_i^0$ to 0
4. $t \leftarrow T$
5. while $t > 0$ do
6.   Distribute markers $z_i$ across MPI nodes and threads
7.   Markers Push-Forward, $z_i^1 \leftarrow \varphi^\Delta t(z_i^0, t)$
8.   Compute interpolation weights and wall hits
9.   Compute new probabilities $\Phi_i^1$ using (3.1)
10. Collect probabilities $\Phi_i^1$ from nodes and shift: $\Phi_i^0 \leftarrow \Phi_i^1$
11. $t \leftarrow t - \Delta t$
6. end while

The flow chart of the BMC scheme follows the steps listed in Algorithm 1. The numerical implementation reuses the ASCOT5 code base as much as possible, in order to reduce maintenance costs and to lower the learning curve for both developers and end users. In the initialization phase, the BMC scheme reads the simulation parameters from the ASCOT5 hdf5 input file and the probability mesh is constructed by reusing the diagnostic histogram data. The scheme is able to work with both 2D and 3D wall structures, and with the fields and plasma profiles used by ASCOT5. However, some small notable changes in the particle data structure and the marker simulation functions were necessary in order to take into account the Gauss-Hermite quadrature and hence the possibility to have the diffusion random variables $r_k$ as fixed parameters.

The most important steps are the markers push forward routine, which is illustrated in Fig. 3.3, and the weights computation. After partitioning the markers in MPI nodes and threads, the markers are further divided in SIMD blocks for vectorization. The main particularity is that, in order to avoid wasting unnecessary computational resources, the markers are first pushed-forward with the Hamiltonian vector field, regardless of their $r_k$ realizations. Later, in the stochastic push-forward, each marker is duplicated $K$ times, where $K$ is the number of Gauss-Hermite points, rearranged in a new SIMD vectors structure, and finally evolved according to the equations of motion for the pitch-angle diffusion. Since the number of sub-cycles are in the order of thousands for practical applications, this kind of optimization is very beneficial.
Figure 3.3. Push forward implementation and parallelization strategy of the BMC scheme. The $r_k$ parameters represent the different pitch-angle coefficients in the diffusion evolution terms.

In the interpolation step, for each marker in the stochastic SIMD structure an array of 32 closest neighbors interpolation data is stored. Each contains the information of: the index $j$ of the neighbor, the interpolation weight $\Lambda_j$ and a flag indicating whether the marker has hit the target domain. The Gauss-Hermite weight is stored instead in the marker structure. The wall hit information is taken into account in the probability computation (3.1) in three different cases:

- **Target domain hit in the Hamiltonian push-forward:** the probability of the marker $\phi_i^{m-1}$ is trivially 1.

- **Target domain hit in the Stochastic push-forward with Gauss-Hermite knot $r_k$:** the interpolation is skipped and the hit contributes with a factor $w_k$.

- **The linear interpolation intersects the target domain:** the contribution is $w_k \Lambda_j(q_i^M(\sqrt{2r_k}))$. This happens when the trajectory is inside, but still close to the wall.
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Since for typical BMC simulation the number of markers can possibly be in the order of $10^8$, it is important to optimize the available computational resources. In case the push-forward maps can be approximately considered time-independent, the computational effort lowers substantially. In fact, the push-forward and the weight computation routines can be precomputed before the main time loop. The problem then reduces to the computation of one major time step, or equivalently $N_{RK4}$ sub-cycles, and the time loop turns out to be at least one order of magnitude faster and hence negligible.

The memory performance is important as well, given the large amount of particles. The algorithm listed in 1 shares the whole probability histogram to all computational nodes, while the other data, including the markers and the precomputed interpolation weights, are efficiently partitioned among the nodes. Fig. 3.4 shows how the probability histogram, the precomputed interpolation weights and the markers structure memory scales with the number of computational nodes. It is clear that the scheme is capped by the probability histogram memory occupation when the number of nodes is sufficiently high. In order to scale beyond 400 nodes, a better domain decomposition of the probability histogram is therefore much needed.

![Figure 3.4. Memory scaling of the main data structure of the BMC scheme. The values shown are Bytes per number of total markers](image)

Figure 3.4. Memory scaling of the main data structure of the BMC scheme. The values shown are Bytes per number of total markers.
3.3.1 Importance sampling

One promising application of the BMC scheme is the possibility to improve the statistics of Forward Monte Carlo simulations by generating an important sampling distribution from a given birth distribution. To do so, a simple marker duplication scheme follows these steps:

- For each marker $i$ in the original birth distribution, the BMC probability is interpolated in the marker position. An importance sampling weight is then assigned to the marker: $\lambda_i = \sum_j \Lambda_j \Phi_j$

- the weights are normalized to the required total number of markers for the new birth distribution: $\lambda_i = \frac{\lambda_i N}{\sum \lambda_i}$

- The new birth distribution is built by placing $\lambda_i$ numbers of markers for each marker of the original distribution, rounded to the closest integer. Note that in cases of interest, where the wall hit rate of the old distribution is very low, the majority of the markers will be discarded completely.

- Each marker usually carries a physical particle weight, $w_i$, needed for computing a signal, for example the power load of lost ions to the detector. The weights of the new distribution are updated according to the importance sampling weights: $w_i \rightarrow \frac{w_i}{\lambda_i}$
4. The geometric structure of kinetic models

The huge difference in timescales that characterizes the dynamics of charged particles in plasmas forces to develop techniques to either simplify the problem or ensure high accuracy or global conservation properties of the numerical schemes. This is specially true for simulations aimed at discretizing the Vlasov-Maxwell-Landau system for which high fidelity of the algorithm is critical, from time scales of the electron cyclotron motion \((10^{-11} \text{ s})\) up to timescales important for macroscopic transport \((10^{-6} \text{ s})\).

In section 4.1 a brief introduction on the concept of structure-preserving integrator is given. In section 4.2 it will be shown how the Vlasov-Maxwell-Landau system can be derived from a geometric principle. Lastly, in section 4.3, some basic notions of structure-preserving discretization for the Vlasov-Maxwell-Landau system will be given, with particular attention to marker based discretization methods of the Landau collision operator, which constitutes the basis of Publication IV, and the GEMPIC scheme, which is the topic of Publication II.

4.1 Basic notions of structure-preserving integrators

To better understand the tasks described in this chapter and what is meant by the term "structure-preserving", consider first a simple mechanical system described by an Hamiltonian \(H(p,q) = \frac{|p|^2}{2m} + V(q)\) and regulated by the Hamilton’s equations of motion:

\[
\dot{z} = J^{-1} \nabla H(z) \tag{4.1}
\]

where \(z = (q,p)\) and \(J\) is the canonical symplectic matrix:

\[
J = \begin{pmatrix}
0 & I \\
-I & 0
\end{pmatrix}
\tag{4.3}
\]
The geometric structure of kinetic models

If a generic algorithm is applied to the equations of motion (4.2), an error on the momentum coordinate $p$ is expected at every time step:

$$ p_{\Delta t} = p_{\text{exact}} + \delta p $$  \hspace{1cm} (4.4)  

It is easy to show that the error is inherited by the kinetic energy and it is accumulated over time. In fact:

$$ K_{\Delta t} = |p_{\text{exact}}|^2 + |\delta p|^2 + 2p_{\text{exact}} \cdot \delta p $$ \hspace{1cm} (4.5)  

The second term is always positive and accumulated over time, while the third usually averages to $0$. It is therefore clear that more sophisticated algorithms are required in order to obtain some conservation of quantities. This purpose can be achieved, for single particle dynamical systems, with symplectic integrators. It is well known that solution trajectories $\varphi_t$ of Hamiltonian systems are symplectic maps or, more precisely:

$$ \omega(\varphi'(z)\xi, \varphi'(z)\eta) = \omega(\xi, \eta) $$ \hspace{1cm} (4.6)  

where $\omega$ is a bilinear form that measures the area of the phase-space parallelogram spanned by vectors $\xi$ and $\eta$:

$$ \omega(\xi, \eta) = \sum_i (\xi_i^p \eta_i^q - \xi_i^q \eta_i^p) = \xi^T J \eta $$ \hspace{1cm} (4.7)  

A simple, and perhaps one of the first examples in history of structure-preserving integrator is due to de Vogelaere [12] and it is known as the symplectic Euler scheme:

$$ z^{n+1} = z^n + \Delta t \cdot J \cdot \nabla H(p^{n+1}, q^n) $$ \hspace{1cm} (4.8)  

By differentiating the above equation (4.8) with respect to $z^n$, one can immediately prove that the symplectic Euler scheme is indeed a symplectic map [15]. The direct consequence of this conservation property is the fact that notable quantities, i.e. the kinetic energy, are exactly conserved or bounded indefinitely over time. The typical evolution of the energy error over time for a symplectic method over a non structure-preserving one is sketched in Fig. 4.1.

While this concept of preservation of symplectic forms is general, it is not straightforward to find structure-preserving schemes that are of practical interest. On one hand, dynamical systems in plasma physics are often described by non canonical Hamiltonian equations of motion, for example in the case of the motion of single particles in guiding center coordinates. On the other hand, the Vlasov-Maxwell-Landau system is described by an infinite set of degrees of freedom and this poses an additional complication.
4.2 The Metriplectic formulation

The starting point to find structure-preserving schemes for kinetic models is perhaps the following question: what is the geometric structure underlying the kinetic equations? It was already shown by Low [33] and reported here in section 2.3 that the Vlasov-Maxwell system can be derived from a variational principle. In other words, the Vlasov equation and the Maxwell equations can be seen as solutions of the Euler-Lagrange equations for the Lagrangian (2.35). However, a complete formal geometrical description of the kinetic equations that includes both the non-collisional and the Landau collisional operator was made by P. Morrison and various authors in a series of works [37, 38, 39, 28, 27, 35, 34], and it is known as metriplectic formulation. The theory was developed in a few ways later on, most notably by extending it to gyrokinetic theories [22, 21], to the MHD theory [10] and to structure-preserving integrators [36, 29].

The foundation of the metriplectic formulation is the fact that the complete dynamics of the system can be described by a Poissonian part, which is essentially equivalent to the above-mentioned variational formulation of the Maxwell-Vlasov equations, and a dissipative part that describes the collisions. Formally, the evolution of functionals can be written as a sum of a Poisson bracket and a symmetric, positive, semi-definite metric bracket:

$$\dot{U} = \{U, \mathcal{F}\} + (U, \mathcal{F})$$  \hspace{1cm} (4.9)

where $\mathcal{F} = H + S$ is the sum of the Hamiltonian and the Entropy of the
system and with the additional requirement that the Hamiltonian and Entropy are Casimir functionals of the metric and Poisson bracket respectively. Dissipation is typical of a few important physical systems, including viscous fluids, heating and thermal diffusion. Likewise, the Landau operator dissipates entropy, as it will be proved shortly, while conserving other quantities, such as momentum and energy. To prove that the Landau operator can effectively be derived from this formalism, the entropy functional is first defined as:

\[ S = - \sum_s \int f_s \ln f_s \, dz \]  

(4.10)

Given two functional \( \mathcal{A} \) and \( \mathcal{B} \), the metric bracket is then given as:

\[ (\mathcal{A}, \mathcal{B}) = \sum_{s, \bar{s}} \frac{1}{2} \int \Gamma_{s\bar{s}}(\mathcal{A}, z, \bar{z}) \cdot W_{s\bar{s}}(z, \bar{z}) \cdot \Gamma_{s\bar{s}}(\mathcal{B}, z, \bar{z}) \, dz \, d\bar{z} \]  

(4.11)

where \( W_{s\bar{s}} \) and \( \Gamma_{s\bar{s}} \) are:

\[ W_{s\bar{s}}(z, \bar{z}) = \nu_{s\bar{s}} \delta(x - \bar{x}) f_s(z) f_{\bar{s}}(z) Q(v - \bar{v}) \]  

(4.12)

\[ \Gamma_{s\bar{s}}(\mathcal{A}, z, \bar{z}) = \frac{1}{m_s} \frac{\partial}{\partial v} \frac{\delta \mathcal{A}}{\delta f_s}(z) - \frac{1}{m_{\bar{s}}} \frac{\partial}{\partial \bar{v}} \frac{\delta \mathcal{A}}{\delta f_{\bar{s}}}(z) \]  

(4.13)

In the above equations, \( \nu_{s\bar{s}} = q_s^2 q_{\bar{s}}^2 \ln \Lambda_{s\bar{s}} / (8\pi \varepsilon_0^2) \), the tensor \( Q \) is defined in (2.18) and satisfying \( (v - \bar{v}) \cdot Q(v - \bar{v}) = 0 \), and \( W \) is symmetric when exchanging particles and species. It is straightforward from here to prove all the properties deriving from the bracket. To begin, using (4.9) and remembering that the Hamiltonian is a Casimir function of the metric bracket, the collisional evolution of a functional \( \mathcal{A} \) is then:

\[ \left. \frac{d\mathcal{A}}{dt} \right|_{\text{coll}} = \frac{d}{dt} \sum_s \int A_s(z) f_s(z) \, dz \]

\[ = \sum_{s, \bar{s}} \frac{1}{2} \int \left( \frac{1}{m_s} \frac{\partial A_s(z)}{\partial v} - \frac{1}{m_{\bar{s}}} \frac{\partial A_{\bar{s}}(z)}{\partial \bar{v}} \right) \cdot W_{s\bar{s}}(z, \bar{z}) \cdot \Gamma_{s\bar{s}}(\mathcal{A}, z, \bar{z}) \, dz \, d\bar{z} \]  

(4.14)

The expression (4.13) is clearly antisymmetric for exchange of particles and species, hence when summed through all the particles and species the first term of the above expression can be simplified to give:

\[ \frac{d}{dt} \sum_s \int A_s(z) f_s(z) \, dz = \sum_{s, \bar{s}} \int \frac{1}{m_s} \frac{\partial A_s(z)}{\partial v} \cdot W_{s\bar{s}}(z, \bar{z}) \cdot \Gamma_{s\bar{s}}(\mathcal{A}, z, \bar{z}) \, dz \, d\bar{z} = \]

\[ = - \sum_s \int A_s(z) \sum_{\bar{s}} \nu_{s\bar{s}} \frac{\partial}{m_s} \int W_{s\bar{s}}(z, \bar{z}) \cdot \Gamma_{s\bar{s}}(\mathcal{A}, z, \bar{z}) \, dz \, d\bar{z} \]  

(4.15)

where the last step is obtained with an integration by parts. This is the expression for the evolution for a generic functional \( \mathcal{A} \). However, if one is
interested in the evolution of the distribution function, then \( A := \delta ( z - z' ) \) and the expression reduces to:

\[
\frac{\partial f_s}{\partial t}_{\text{coll}} = -\sum_s \frac{v_{ss}}{m_s} \frac{\partial}{\partial v} \int \delta ( x - \mathcal{F} ) f_s ( z ) f_s ( \mathcal{F} ) Q ( v - \mathcal{F} ) \cdot \Gamma_{ss} ( S, z, z ) d \mathcal{Z} \quad (4.16)
\]

which, after substituting the expression for \( \Gamma_{ss} ( S, z, z ) \) using (4.13), is the Landau form of the Fokker-Planck equation found in the theory section 2.2. Proving the conservation of energy, momentum and the dissipation of the entropy is immediate from here. In fact:

\[
\frac{d}{dt} S = ( S, S ) = \sum s, s' \frac{1}{2} \int \Gamma_{ss} ( S, z, z ) \cdot W_{ss} ( z, z ) \cdot \Gamma_{ss} ( S, z, z ) d z d z \geq 0 \quad (4.17)
\]

where the last inequality is a consequence of the matrix \( Q ( v - \mathcal{F} ) \) appearing in \( W_{ss} \) being positive semi-definite. The easiest way to check this is perhaps by direct computation:

\[
\Gamma \cdot Q \cdot \Gamma = \frac{1}{| \xi |} \left( | \Gamma |^2 - \frac{| \Gamma \cdot \xi |^2}{| \xi |^2} \right) \geq 0 \quad (4.18)
\]

Defining the momentum and kinetic energy as:

\[
P = \sum_s m_s \int v f_s ( z ) d z \quad (4.19)
\]

\[
K = \sum_s \frac{m_s}{2} \int | v |^2 f_s ( z ) d z \quad (4.20)
\]

it follows immediately from (4.11) that the Landau operator conserves both operators. In fact, \( \Gamma_{ss} ( P, z, z ) \) is trivially 0 and \( \Gamma_{ss} ( K, z, z ) = ( v - \mathcal{F} ) \) is in the kernel of the \( Q \) matrix.

This section is concluded completing the discussion about the Poisson part of the metriplectic bracket (4.9). While an action principle for the Vlasov-Maxwell system is given in section 2.3, obtaining a Poisson bracket from the action is non trivial and outside the scope of this work. The reader is referred to the original derivation by Morrison [37] for further details, while here the final result is given:

\[
\{ A, B \} = \sum_s \int \frac{f_s}{m} \left\{ \frac{\delta A}{\delta f_s}, \frac{\delta B}{\delta f_s} \right\} d z + \sum_s \int \frac{q_s}{m^2} f_s B \cdot \left( \frac{\partial v}{\partial f_s} \times \frac{\partial v}{\partial f_s} \right) d z + \sum_s \int \frac{q_s}{m_s \epsilon_0} f_s \left( \nabla_v \frac{\delta A}{\delta f_s} \cdot \frac{\delta B}{\delta f_s} - \nabla_v \frac{\delta B}{\delta f_s} \cdot \frac{\delta A}{\delta f_s} \right) d z + \frac{1}{\epsilon_0} \int \left( \frac{\delta B}{\delta B} \cdot \nabla \times \frac{\delta A}{\delta E} - \frac{\delta A}{\delta B} \cdot \nabla \times \frac{\delta B}{\delta E} \right) d x \quad (4.21)
\]
In the above equation, the bracket appearing in the integral is the single particle canonical Poisson bracket. The following Hamiltonian functional, sum of the kinetic functional (4.20) and the fields energy:

$$H = \sum_s m_s \frac{1}{2} \int |v|^2 f_s(z) dz + \frac{1}{2} \int \left( \epsilon_0 |E|^2 + \frac{1}{\mu} |B|^2 \right) dx$$  \hspace{1cm} (4.22)

together with the Poisson bracket (4.2) is enough to obtain the Vlasov-Maxwell equations by evaluating the bracket with respect to the Hamiltonian and the distribution function or the electromagnetic fields.

4.3 Metriplectic Structure-preserving schemes

Consider first the problem of the discretization of collisions. A natural way to approach the problem is that of binary-collision schemes. The spatial domain is typically divided in collisional cells of size of the Debye length $\lambda_D$ and, in each cell, $N_s$ markers are placed for each species. For each time step, collision pairs are selected and the change of relative velocity of the markers is computed according to some Monte Carlo collision operator. Examples of these types of algorithms, which can be found in the literature for example in [52, 40], are usually very fast and allow for the conservation of energy and momentum to be imposed at every collisional process. However, when these schemes are extended to allow for arbitrary marker weights, as it is customary in Monte Carlo simulations, the energy and momentum conservation properties are broken. It has become more clear in the last decades that numerical integrator able to exploit the geometry and symmetries of the system are necessary in order to accurately discretize the collisions over long times.

One attractive approach for the discretization of the Landau operator is constituted by particle discretization methods, in which the distribution function is treated as a sum of delta-shaped markers:

$$f_{h,s}(z)dz = \sum_{p \in s} w_p \delta(x - x_p) \delta(v - v_p) \, dz$$  \hspace{1cm} (4.23)

where either the marker weights $w_p$ or the marker positions $(x_p, v_p)$ can be chosen as the degrees of freedom of the system. In this way, solving the original equation is effectively equivalent of solving ordinary differential equations for both $w_p$ and the markers positions. While this approach has many advantages, including the ability to be coupled easily with particle-in-cell (PIC) codes, it is known that the Landau equation, when the
The geometric structure of kinetic models
discretization (4.23) is used, doesn’t usually converge to the correct solution (see for example [7]). Various regularization methods were proposed in the last decades, for example, in [11, 46]. However, it is only in the last few years that a new regularization method, able to conserve the geometric structure of the system, emerged. This new idea, first found in [7] and further developed in [6, 19], is based on the understanding that the velocity field of the Landau equation is determined by the functional derivative of the entropy functional, as demonstrated in the previous section. It has been realized that the same metric structure and gradient flow can be achieved in the discretization approach by first regularizing the entropy and then computing all the necessary equations from the metric bracket. Precisely, the entropy functional (4.10) is discretized using (4.23) and then regularized as follows:

$$S_\epsilon = -\sum_s \sum_p \int w_p \psi_\epsilon_s (v - v_p) \ln \left( \sum_{p'} w_{p'} \psi_\epsilon_s (v - v_{p'}) \right) dv$$ (4.24)

Here, the function $\Psi_\epsilon$ acts as a mollifier function that converges to the Dirac-delta in the limit $\epsilon \to 0$:

$$\psi_\epsilon(v) = \frac{1}{2\pi \epsilon_s} \exp \left( -\frac{|v|^2}{2\epsilon_s} \right)$$ (4.25)

After choosing the markers trajectories $(x_p, v_p)$ as the degrees of freedom of the system, the metric bracket and the equations of motion are found using (4.11) after linking the functional derivatives to the new set of variables $(x_p, v_p)$:

$$\frac{\partial}{\partial v} \delta A \bigg|_{f_S} = \frac{1}{w_p} \frac{\partial A (\{Z_s, W_s\})}{\partial v_p}.$$ (4.26)

The conservation of the discrete momentum and energy, defined respectively as:

$$P = \sum_s \sum_p w_p m_s v_p$$ (4.27)

$$K = \sum_s \sum_p \frac{w_p m_s}{2} |v_p|^2$$ (4.28)

is an immediate consequence of (4.26): as in the continuous case, the derivative of the momentum results in the vector $\Gamma_{ss} (P, z, \bar{z})$, defined in (4.13), being 0 and the derivative of $K$ results in $\Gamma_{ss} (K, z, \bar{z}) = v_p - v_{\bar{p}}$, still in the kernel of $Q(v_p - v_{\bar{p}})$, as before.

This section is concluded with a short introduction to structure-preserving Vlasov-Maxwell integrators, which were developed extensively in the last
decade [48, 53, 16, 44, 54] and culminated in the Geometric Particle-in-cell (GEMPIC) scheme [49, 30], which is perhaps the current state of the art of the structure-preserving numerical integrators for the Vlasov-Maxwell system. In the GEMPIC scheme, the distribution function is discretized as in (4.23), with the markers positions chosen as degrees of freedom as in the above studied collisional case. The electromagnetic potentials are then represented in some suitable basis function:

\[ A(x, t) = a^i(t)W_i(x) \]  
\[ \phi(x, t) = \phi^i(t)W_i^0(x) \]

From here, the Vlasov-Maxwell action functional is discretized by substituting the expression of the potentials and the distribution function in the original action:

\[ S[x_p, \phi_k, A_k] = \int dt L(x_p, x_p, \phi_k, A_k, A_k) \]  

where \( x_p, \phi_k \) and \( A_k \) represent the sets of the degrees of freedom for the markers and the fields in the basis representation (4.29). After discretizing the time in \( N \) time steps:

\[ S = \sum_{n=0}^{N-1} S_{n,n+1} \]

the minimization results in a system of equations which is by construction conservative and possesses an Hamiltonian structure. However, the additional outstanding feature of the GEMPIC scheme is in the particular forms of the basis functions (4.29) that allow to obtain discrete version, \( \text{curl}_i^j \) and \( \text{grad}_i^j \) of the vector operators with the desired properties \( \text{curl}_i^k \text{grad}_j^l = 0 \) and \( \text{div}_k^l \text{curl}_j^i = 0 \), which are satisfied by construction. Some notable electromagnetic properties then hold automatically, for example the null divergence of the magnetic field at every time, given that it is set to 0 initially. Subsequent efforts on the GEMPIC code have tried, with promising results so far, to improve the performance of the scheme by skipping the cyclotron motions of the particles while suitably averaging the fields, which is of great importance since the timescale of electrons cyclotron motion is typically in the order of \( 10^{-11} \) s, as opposed to the typical timescale of the macroscopic transport, \( 10^{-6} \) s. This can be achieved by further dividing the markers degrees of freedom in the discrete action (4.32) in \( V \) substeps, i.e.:

\[ S_{n,n+1} = S[x_i^n, x_i^{n+1/V}, \ldots, x_i^n, \phi_k^n, \phi_k^{n+1}, A_k^n, A_k^{n+1}] \]
and assuming straight trajectories between subsequent nodes \((v, v+1)\) when computing the time derivative \(\dot{x}\):

\[
x_{i}^{n,v}(\tau) = (1 - \tau)x_{i,n+1}^{v,v+1} + \tau x_{i,n+1}^{v,v}
\]  

(4.34)

A set of discrete Euler-Lagrange equations of motion is then derived perturbing each degree of freedom \(x_{p,n}^{\phi}, \phi_{n,k}^{\phi}\) and \(A_{n,k}^{A}\) and minimizing the discrete action (4.32). For example, the resulting equation for the marker degrees of freedom formally reads

\[
\partial_{\epsilon}|_{\epsilon=0} S_{n,n+1} \left[ x^{n} + \epsilon \delta x^{n} \right] + \partial_{\epsilon}|_{\epsilon=0} S_{n-1,n} \left[ x^{n} + \epsilon \delta x^{n} \right] = \]

(4.35)

Similarly, the minimization of the discrete action with respect to variations of the electromagnetic fields produces discrete relations for the Ampère-Maxwell equation and the Gauss’ law. The discrete equivalent of the Faraday law is provided by construction from the particular choice of the fields basis functions of the GEMPIC scheme. These relations form a recipe for a substepping integrator, in which the equations for the degrees of freedom of the fields are advanced at every major time-step, while the markers are advanced in each \(V\) substep. The simple trajectory temporal discretization (4.34) provides an explicit map for the fields solver and an implicit map for the markers push forward map. Alternative, more refined, temporal trajectory discretizations that make the markers evolution map explicit can be found in [24].
5. Numerical Results

The main end goal of this thesis work is to apply the kinetic theory of plasmas to the development of improved numerical schemes for relevant applications for plasma and fusion physics. This was achieved in two main ways: in Publication III a Backward Monte Carlo scheme was developed as a module integrated in the ASCOT5 orbit following code. The BMC scheme was tested and compared to a standard Forward Monte Carlo simulation of a slowing down fast-ion population in ASDEX Upgrade (AUG). The results are presented in section 5.1. In Publication IV a Multi species structure-preserving scheme for the Landau collisional operator was developed and tested against realistic cases of thermalization, isotropization and relaxation. The results are presented in section 5.2.

5.1 Improving fast-ion losses resolution in AUG

The Backward Monte Carlo scheme, described in chapter 3, was applied to the ASDEX Upgrade H-mode discharge AUG#33143, correspondent to a high $\beta_N = 2.4$, low collisionality $\nu^* = 0.2$, a toroidal magnetic field $B_t = -1.8$ T and a fast-ion birth population generated by a neutral beam injector (NBI) through the ASCOT5 module BBNBI. The AUG NBI systems consists of 8 beams in total, of which the Q7 and Q8 beams was used in Publication III for the numerical experiments. The flux density in the poloidal plane of the two beams is illustrated in Fig. 5.3a, while the safety factor, density and temperature profiles are sketched in Fig. 5.1. In Fig. 5.2a, a Monte Carlo simulation is performed using the Q8 beam as birth population and the times when markers hit the wall are recorded in a histogram. The first peak appearing at approximately $10^{-5}$ s is constituted by prompt-losses of markers that escape the plasma before being slowed down. The second peak is due to collisions and is therefore the primary concern of this work.
The prompt losses are in fact entirely deterministic and can be easily simulated with a Forward Monte Carlo simulation without any noise. The time step for the stochastic push-forward of the BMC scheme can therefore skip the quick prompt-losses timescale and be set to some longer time scale that can models the collisions accurately. On the other hand, it is desirable to minimize the number of collisional steps that introduce an interpolation error, or numerical diffusion, every time they are performed. For this reason, a time step of $\Delta t = 8 \times 10^{-4}$ s turns out to be a good and accurate compromise. The Hamiltonian push-forward, as Fig. 3.3 illustrates, is computed dividing the major time step in sub-cycles, in order to have an effective time step of $\Delta t = 1 \times 10^{-8}$ s needed to integrate accurately the Hamiltonian equations of motion.

With reference to Fig. 5.3, the BMC scheme was used assuming a FILD detector located near the divertor and indicated with a green box. The phase-space probabilities of markers reaching the target domain after a total time $T = 2 \times 10^{-2}$ s were computed by the BMC scheme. As the simulation was run in time-independent mode, the computational power needed is equivalent to compute the evolution of marker for one collisional time step, $\Delta t = 8 \times 10^{-4}$ s, or 8000 sub-cycles, as explained in section 3. The original NBI birth distribution is reconstructed by the BMC scheme using the simple marker duplication importance sampling scheme. The result is plotted in Fig. 5.3d, and clearly shows that the areas in the center of the plasma that are unlikely to reach the wall are completely discarded, and more markers are put in the areas with higher probability.

Different simulation with different BMC mesh sizes were performed and the wall hit rates are then compared in Fig. 5.4. The results show a clear increase in hit rates, specially when the mesh size is increased. In fact, a
Figure 5.2. Histogram of wall hit times for a Q8 beam birth distribution, using a standard FMC simulation (a) and a BMC-IS birth distribution (b).

more refined mesh implies a more accurate marker linear interpolation at each collisional time step, hence a better estimate of the final probability. Finally, it is worth noticing that the observed increase in wall hit rates is mirrored by an improved resolution of the signal in the FILD detector, which is perhaps the characteristic that is most useful for future applications. Fig. 5.5 shows the energy-pitch spectrum of particles hitting the detector, for a plain Forward Monte Carlo simulation and for a simulation with the birth distribution rebuilt by the BMC importance sampling scheme on a $64^5$ mesh. It is possible to appreciate the improved resolution of markers, specially when zooming-in in the lowest NBI energy band.

5.2 Modelling Multi Species collisions

The ideas behind structure-preserving integrators presented in chapter 4 were applied in Publication IV to build a Multi-Species marker based discretization of the Landau collisional operator. In doing so, the previous works [7, 6, 19] were extended to account for collisions between multiple species. Also, part of the motivation was to leverage parallelization through GPU computing and studying how the integrator performs and how it can scale with the increasing number of markers. Lastly, theoretical examples were replicated with the schemes and the results are presented in this
The algorithm starts by initializing the markers constituting the distribution function \( f_s \) of each species on a rectangular grid. The weights \( w_p \) were set by mimicking the initial desired distribution function of an anisotropic Maxwellian:

\[
  f_s(v, t = 0) = \frac{n_s m_s}{2\pi k_B \sqrt{T_s T_s}} \left[ \exp \left( -\frac{m_s (v^x - u_s^x)^2}{2k_B T_s} - \frac{m_s (v^y - u_s^y)^2}{2k_B T_s} \right) \right]
\]

(5.1)

where \( n_s, u_s \) and \( T_s \) are the discrete density, flow velocity and temperature:

\[
  n_s = \sum_p w_p \tag{5.2}
\]

\[
  u_s = \frac{1}{n_s} \sum_{p \in S} w_p v_p \tag{5.3}
\]
Numerical Results

![Histogram of the number of target hits for three different total integration times and four BMC mesh sizes.](image)

**Figure 5.4.** Histogram of the number of target hits for three different total integration times and four BMC mesh sizes.

![Energy–pitch histogram for the FMC and BMC-IS.](image)

**Figure 5.5.** Energy–pitch histogram for the FMC and BMC-IS. The number of input markers used is $10^5$ in both cases with total integration time of $T = 2 \times 10^{-2} s$. Fig. 9 of PIII.

$$T_s^x = \frac{m_s}{n_s k_B} \sum_{p \in s} w_p (v_p^x - u_s^x)^2$$

(5.4)

The size of the grid is naturally tailored for each species taking care specifically of the thermal speed. For the performed simulations, it was chosen a very safe size of $L_s = 5 v t_s$ and a total number of marker of $N_s = 400$ per species. The mollifier parameter $\epsilon_s$ appearing in the regularized entropy (4.24) is quite important for ensuring proper convergence of the
Numerical Results

equations of motion. After a proper analysis and comparison with the previous work by Carrillo [6], the value for the mollifier parameter was set to \( \epsilon_S = 1.2(L_S/N_S)^{1.98} \). Finally, the time step was set to \( \Delta t = 10^{-8} \) s, which is reasonable considering the fast electron-electron collision time of about \( 10^{-6} \) s.

Before diving into the numerical results, a few notes on the performance of the scheme are stated here. The two computational intensive tasks required by the algorithm are the computation of the \( \Gamma \) vector (4.13) and the equations of motion for the markers degrees of freedom, found by evaluating (4.14) with \( \mathbf{a} = \mathbf{v}_p \). The latter is a set of implicit equations and typically require 5 to 10 fixed-point iteration to reach convergence. As sketched in Fig. 5.6, the scaling time of the two procedures is very similar with a scaling factor of about \( O(N^{1.8}) \), which is comparable with other modern multi species collisional codes [14].

\[ \frac{1}{\tau_{ei}^{\text{eff}}} = \frac{16}{3} \frac{\sqrt{\pi} e^4 \ln \Lambda}{(4\pi\varepsilon_0)^2 \sqrt{m_e}(k_BT_e)^{3/2}} \] (5.5)

Fig. 5.6 shows the results for an electron-ion relaxation simulation, where the mass-ratio of the two species was artificially set to 200. The initial temperature for both species is \( T_0 = 400 \) eV, and the flow velocities are null except for the \( x \) component for the electrons which is set to \( u_{e,x} = -v_{t,e}/2 \). Both total energy and momentum are conserved to machine precision, as expected from the theory, and the relaxation rate for the electrons agrees well with the analytical theory [17]:
Numerical Results

Figure 5.7. Species flow velocity (a), Energy error (b) and momentum error (c) for a velocity relaxation simulation with masses $m_e$ and $m_i = 200 m_e$ with initially isotropic Maxwellian with temperature $T = 400$ eV and $u_{e,x} = 2.1 \times 10^6$ m/s. Fig. 2 of PIV.

When the mass-ratio is set to the real value of electron-deuterons, the results are still in good agreement with the analytical estimates, as Fig. 5.8 shows. In this occasion the two species were initialized with 4 different temperature values for each axis, and null flow velocity. The species are expected to become isotropic following the relations:

$$\frac{dT^x_s}{dt} = -\frac{T^x_s - T^y_s}{\tau_s}$$  \hspace{1cm} (5.6) $$\tau_s^{-1} = \frac{2\sqrt{\pi} e^2 e_s^2 n_s \ln \Lambda_s}{(4\pi\epsilon_0)^2 \sqrt{m_s (k_b T)}^{3/2}} A^{-2} \left[-3 + (A + 3) \frac{\tan^{-1} (A^{1/2})}{A^{1/2}} \right]$$  \hspace{1cm} (5.7)

where $A = T_\perp/T_\parallel - 1$ for $T_\perp > T_\parallel$. Finally, at longer time scales, the two species are expected to thermalize according to:

$$\frac{dT_s}{dt} = -\frac{T_s - T_\infty}{\tau_s^{\perp/\parallel}}$$  \hspace{1cm} (5.8) $$\frac{1}{\tau_s^{\perp/\parallel}} = \frac{8}{3} \sqrt{\frac{2\pi m_s e^2 e_s^2 e^2 n_s \ln \Lambda_s}{(4\pi\epsilon_0)^2 (m_s k_b T + m_5 k_b T_5)^{3/2}}}$$  \hspace{1cm} (5.9)

Both results are verified exceptionally well by the numerical scheme, proving the high fidelity of the algorithm over very long time scales.
Numerical Results

Figure 5.8. Species temperatures (a) for an isotropization and thermalization simulation of electrons and deuterons with an anisotropic Maxwellians as initial distribution. A zoomed-in view is provided in (b). Fig. 3 of PIV.

However, the multi species integrator, in its current state, showed two main issues: first, while energy and momentum are guaranteed to be exactly conserved, the same does not happen for the entropy. Fig. 5.9a shows the evolution of the entropy for a typical simulation. When an equilibrium is reached, the entropy might oscillate, thus violating the H-theorem. The proper dissipation of entropy in fact requires a more sophisticated time discretization, for example by using a discrete-gradient scheme [19]. Finally, some jumps in the energy error were observed in some simulations and reported in Fig. 5.9b. The root cause of this behaviour were found to be the the equations of motion which are non convergent in some situations. However, it must be noted that in all cases the energy relative error remained under very reasonable values, typically $10^{-5}$ or lower. Also, from a preliminary analysis, which is due to be completed in the near future, it seems that by improving the entropy gradient numerical integration by increasing the resolution of the used quadrature is likely to mitigate or completely solve the issue.
Figure 5.9. Entropy evolution for the multi species Landau scheme (a) and energy error jump behaviour (b). Fig. 6 and 3a of PIV.
6. Summary and Future Prospects

In this thesis, some promising novel numerical schemes for the simulation of fast ions and for the Vlasov-Maxwell-Landau system are presented.

First, an energy and momentum preserving multi-species particle discretization of the Landau operator was presented. The code was validated against different test cases, including a relaxation example, for two species with mass-ratio 200, and a thermalization example for electron-deuteron species with a real mass-ratio. The numerical results appear to be in excellent agreement with the theoretical estimates. However, while the total momentum is always conserved to machine precision, sporadic jumps in the energy error was observed. The code was developed in the C programming language and the CUDA library allowing for a future massive parallelization the computational power of existing supercomputers. The code is a proof of concept that works in a two dimensional velocity space, and an extension to the full 3D space is already planned for a future work, as well as the resolution of the energy error jumps issues. Also, in order to guarantee an exact H-theorem, or dissipation of entropy, a more sophisticated time discretization scheme needs to be implemented.

A new Monte Carlo integrator, known as the Backward Monte Carlo (BMC) was presented here. This numerical scheme aims at integrating the probability to reach a certain target domain, for example a Fast-Ion Loss Detector (FILD), backward in time, taking into account deterministically the statistical spread of the Monte Carlo collision operator. In such way, the BMC scheme has proven to improve substantially the simulated hit rates of fast ions, and hence their statistics, in a ASDEX Upgrade (AUG) test case with a Neutral Beam Injector (NBI) source. The code for the BMC scheme was developed inside the orbit following code suite ASCOT5, therefore providing an easy, production ready and parallelized code that can be used with the existing tool chain in use by the research community.
Engineering works on the BMC are still needed. The current version of the code only allows regular rectangular meshes. In the future, it will be important to adapt the code to allow dynamically refined meshes that follow the topology of the field lines and the target domain. Also, the results presented in this work are only for 2D magnetic fields and 2D walls. A future study with a realistic test case, a 3D wall configuration and 3D magnetic fields is being considered and already worked on.
References


