Multiscale time-integration for particle-in-cell methods.

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Abstract

The simulation of problems in kinetic plasma physics are often challenging due to strongly coupled phenomena across multiple scales. In this work, we propose a wavelet-based coarse-grained numerical scheme, based on the framework of Equation-Free Projective Integration, for a kinetic plasma system modeled by the Vlasov-Poisson equations. A kinetic particle-in-cell (PIC) code is used to simulate the micro scale dynamics for short time intervals. This allows the extrapolation over long time-steps of the behavior of a coarse wavelet-based discretization of the system. To validate the approach and the underlying concepts, we perform two numerical experiments: nonlinear propagation and steepening of an ion wave, and the expansion of a plasma slab in vacuum. The direct comparisons to resolved PIC simulations show good agreement. We show that the speedup of the projective integration scheme over the full particle scheme scales linearly with the system size, demonstrating efficiency while taking into account fully kinetic, non-Maxwellian effects. This suggests that the approach is potentially interesting for kinetic plasma problems with a large separation of scales, especially in higher dimensions.

Keywords: Plasma physics, Coarse-grained time integration, Multiscale numerical methods, Equation Free Projective Integration, Particle In Cell methods

1. Introduction

The importance and complexity of plasma physics makes its simulation a crucial challenge across various domains of science, from astrophysics (stars, solar wind) to efforts in developing nuclear fusion reactors (tokamaks) to everyday human environment (lighting, industrial processes). Plasma phenomena are typically characterized by a complex multiscale character, as physics at scales separated by multiple orders of magnitude in space and time directly influences the global behavior of the plasma. Examples of such phenomena include magnetic reconnection in the solar wind, in which large amounts of magnetic energy are released into the plasma by the breaking and reforming of magnetic field lines at extremely small length scales; or micro-scale plasma turbulence, which is known to have a significant influence on the global transport properties of plasmas in laboratory tokamaks. The direct modeling of such problems still defies numerical methods developed by computational scientists.

In this paper we study the application of an original multiscale computational technique, the Equation-Free Projective Integration method (EFPI) [1, 2, 3, 4], and its application to the simulation of plasmas. A commonly used approach to simulate strongly multiscale systems is to derive and discretize a set of reduced equations for macro-scale phenomenons by analytically averaging the contributions of smaller scales, e.g., using homogenization theory. This procedure typically relies on strong structural assumptions such as periodicity [5], or stationary randomness. In the context of plasmas, reduced fluid models such as magnetohydrodynamics can sometimes be used depending on the physical setting. The EFPI framework, on the other hand, does not rely on discretizing a closed set of reduced equations. Rather, full-scale and highly resolved simulations of the system are computed for short period of times, allowing the recovery of the slow
macroscopic behavior which is then projected forward in time with large timesteps. This approach seeks to account for the effect of micro-scale physics on the macroscopic behavior even when no satisfying upscaling theory is known, assuming only that there is a sufficient separation of scales. Whether this approach can provide accurate, efficient simulations for kinetic plasma problems remains an open question and a question that we shall consider in this work.

In this paper we are particularly concerned with the simulation of collisionless plasmas for which a kinetic description is required. In this context, particle methods, in particular Particle-In-Cell methods [6] have traditionally been preferred to Eulerian (grid-based) methods as they allow a coarse, but reasonably precise description of phase-space. However, standard explicit PIC schemes impose stability conditions to guarantee that space and time steps be sufficiently small to resolve the Debye length and plasma periods which are the typical space and time scales at which the electrostatic force tends to restore local charge neutrality in the plasma. For the majority of applications, these are extremely small when compared to the typical scales of the plasma under investigation. The development of implicit PIC methods, which are free of such constraints, has been the focus point of many recent efforts. Since it is prohibitively expensive to implement a fully implicit resolution of the particle positions and the fields, alternative algorithms have been developed, e.g., the direct implicit method [7, 8, 9] where a two-step predictor-corrector approximation is implemented or semi-implicit methods [10, 11, 12]. In the implicit moment methods [13, 14], moment equations are used to predict the value of the fields. Recently, asymptotic-preserving methods have been introduced [15, 16] to better account for the stiffness due to the quasineutrality constraint. Alternatives include the hybrid method, see e.g. [17], where a particle model is used for some of the particle species and a fluid model for others; or the so-called ‘multiscale’ PIC methods [18, 19] which use different step sizes for different spatial regions, depending on the electric gradient scale in each region.

We shall pursue the development of a different method, utilizing the equation-free projective integration method with an explicit PIC code as the micro-scale solver. The basic idea is to advance a coarse representation of the solution by lifting the microscopic state of the system throughout a number of microscopic time-steps, recording the macro-state of the system at each step by means of a restriction operator. After a small number of such timesteps, a linear least squares fit is computed for each coarse variable to evaluate its temporal derivative. The coarse representation is then projected forward in time using a large time step.

A first attempt at implementing an equation free procedure in this context was the EFREE procedure developed by Shay et al. [20] and applied to the nonlinear propagation and steepening of an ion-acoustic wave. In EFREE, both electron and ion distribution functions are assumed to be Maxwellian and the electrons are adiabatic. The coarse description is then simply the ion density, mean velocity and pressure discretized on a coarse grid. Despite neglecting all kinetic effects, the EFREE results are promising as the wave propagation is correctly reproduced during the initial phase. However as the wave steepens, kinetic aspects such as trapping and non-Maxwellian phase space structures appear and the assumptions of the EFREE procedure fail to adequately account for these. An effort to include such effects was proposed in [21], by using a coarse discretization of the full inverse cumulative ion distribution function. However, this approach did not show a strong linear scaling for the speedup with the ion acoustic wavelength as the EFREE procedure achieved. Achieving such a scaling appears necessary to establish the usability of the equation free projection integration paradigm in kinetic plasma simulations.

In this paper we propose a new method based on representing the ion distribution function by the use of a multiresolution wavelet analysis. More precisely, the distribution function is discretized using a coarse grid in physical space and a wavelet basis in velocity space. This allows to fully account for kinetic effects by tracking the evolution of macro-scale phase-space structures. In addition, an important concern is the handling of PIC-generated statistical noise by the projective integration procedure [20, 21]. We show that by combining the restriction on a coarse grid in physical space, wavelet thresholding techniques in velocity space, quiet starts and integration with the flow, our proposed method reduces noise dramatically.

We test numerically our proposed method on two well-known problems: the propagation and steepening of an ion acoustic wave, as in [20, 21]; and the expansion of a plasma slab in a vacuum, following [16]. Let us note that at the moment, our method is not necessarily more efficient for either of these problems than a traditional implicit or multiscale PIC methods described above. Rather, its potential lies in the potential of
its extension to strong multiscale problems for which more conventional methods fail. However the method must first be developed and evaluated in simple settings, for which trusted results exist. Our numerical experiments confirm that reference solutions obtained by brute-force PIC simulations are well reproduced by the proposed wavelet-based method. Although smoothing of the shock appears due to the low coarse resolution, ion pressure and phase space features are correctly approximated unlike previous attempts [20].

What remains of the paper is organized as follows. In Section 2, we present the two-fluid Vlasov-Poisson model and the classical PIC scheme. In Section 3, we recall the equation-free projective integration (EFPI) framework and the original EFREE method developed in [20]. From this approach, we develop our proposed wavelet-based method. Section 4 is devoted to the presentation and discussion of the numerical results and a comparison between the brute-force explicit PIC and our proposed schemes is provided. These results show that the scheme is stable and able to deal with multiscale kinetic problems where the stiffness comes from the fast electron scale.

2. Problem presentation

2.1. The Vlasov-Poisson equations

The theoretical modeling of a two-species plasma, comprising electrons and one ion species, usually begins with the two-fluid Vlasov–Poisson system. Each species of ions and electrons is described by a distribution function, respectively $f^i(x, v, t)$ and $f^e(x, v, t)$. The superscripts $i$ and $e$ will refer to the ions and electrons, respectively, throughout the whole paper. The position and velocity variables $x$, $v$ are such that $(x, v) \in \Omega \times \mathbb{R}^d$ with $\Omega \subset \mathbb{R}^d$, $d \leq 3$, and $t \geq 0$ is the time variable. We restrict our attention to the one dimensional case, with $d = 1$, $\Omega = [0, L]$ where $L > 0$ is the size of the system, and periodic boundary conditions are imposed. However, the majority of the developments proposed here can be generalized to the full six dimensional Vlasov–Poisson problem.

The Vlasov-Poisson equations is expressed as

$$\begin{align*}
\partial_t f^i + v \cdot \nabla_x f^i - \frac{e}{m_i} (\nabla_x \phi) \cdot \nabla_v f^i &= 0, \\
\partial_t f^e + v \cdot \nabla_x f^e + \frac{e}{m_e} (\nabla_x \phi) \cdot \nabla_v f^e &= 0,
\end{align*}$$

where we denote $e > 0$ as the positive elementary charge, by $m_i$ and $m_e$, respectively, the ion and electron masses, and by $\phi$ the electric potential. The electrostatic potential $\phi$ is recovered by

$$\nabla^2 \phi = \frac{e}{\varepsilon_0} (n^i - n^e)$$

where $\varepsilon_0$ is the vacuum permittivity, and $n^i$, $n^e$ are the ion and electron densities, respectively, given as

$$n^i(x, t) = \int_{\mathbb{R}^d} f^i(x, v, t)dv, \quad n^e(x, t) = \int_{\mathbb{R}^d} f^e(x, v, t)dv.$$ 

Two very important physical scales for this model are the Debye length $\lambda$ and the electron plasma frequency $\omega_p$, given as:

$$\lambda = \sqrt{\frac{\varepsilon_0 k_B T_0}{e^2 n_0}}, \quad \omega_p = \sqrt{\frac{n_0 e^2}{\varepsilon_0 m_e}},$$

where $n_0$ is the plasma density scale, $T_0$ is the electron temperature scale and $k_B$ is the Boltzmann constant. In problems of interest, both the Debye length and the electron plasma period become very small compared to the macroscopic scales.
2.2. Classical particle-in-cell scheme

In order to numerically solve the Vlasov-Poisson equations, the particle-in-cell (PIC) method, discussed at length in [6], is widely used due to its strong parallel scaling and relatively low computational cost compared to traditional Eulerian methods. This is particularly true for problems in high dimensions. The basic idea of the PIC method is to discretize the phase-space distribution function \( f^{i,e}(t, x, v) \) with weighted macro-particles:

\[
f^{i,e}(t, x, v) \approx f_{N_p}^{i,e} = \sum_{j=1}^{N_p} \omega_j^{i,e} \delta(v - V_j^{i,e}) \psi(h^{-1}(x - X_j^{i,e})),
\]

where \( N_p \) is the number of particles, \( \psi \) is a shape function, \( X_j^{i,e}(t) \), \( V_j^{i,e}(t) \) is the location of the \( j \)-th particle in phase space and \( \omega_j^{i,e} \) is a weight which is defined at initialization. One should not consider each particle as a physical particle but rather as particle clouds. Each of these particles follows Newton’s equations:

\[
\begin{align*}
\dot{X}_j^{i}(t) &= V_j^{i}(t), & \dot{V}_j^{i}(t) &= -\frac{e}{m_i} \nabla_x \phi_{N_p,h} (X_j^{i}(t), t), \\
\dot{X}_j^{e}(t) &= V_j^{e}(t), & \dot{V}_j^{e}(t) &= -\frac{e}{m_e} \nabla_x \phi_{N_p,h} (X_j^{e}(t), t).
\end{align*}
\]

These equations are then discretized in time. The potential \( \phi_{N_p,h} \), approximating the electrostatic potential \( \phi \), is determined at the particle locations by the following procedure, repeated at each time step. Given a fixed spatial grid of space step \( h \), the nodal values of the density of each species is computed by projecting every particle using a weighting procedure to the grid nodal locations using a simple model for the shape of the particle [6]. The total charge density is then used to determine the nodal values of the electrostatic potential on the mesh by solving the Poisson equation (2.2) numerically, using either finite differences or the fast Fourier transform. Field values at each particle location are then determined by an interpolation procedure.

2.3. Advantages and limitations

Due to their efficiency and simplicity, PIC-based numerical methods are a dominating tool used in the modeling of kinetic plasma physics phenomena. While the mathematical literature on PIC methods is limited, some a priori convergence results have been obtained, see e.g. [22, 23, 24]. Typically, the error scales with the number of particles, as \( 1/\sqrt{N_p} \) as would be expected. The independence of this rate with respect to dimension is a great advantage of the method, since Eulerian grid-based methods become extremely costly in dimension 4 or higher. Nevertheless, it is well-known that to ensure stability, explicit PIC codes must resolve the local Debye length and the electron plasma period everywhere in the computational domain [6].

The main drawback of PIC methods is the well-known statistical sampling noise due to the low number of numerical particles in each cell [25] - a number that by design is orders of magnitudes smaller than the true number of particles in the plasma. As we shall see, this so-called ’shot noise’ has a significant impact on the use of PIC solvers as a micro-solver in the projective integration framework [20, 21]. Various noise-reduction techniques have been developed to reduce its impact on computations. We will in particular make use of the classical quiet start procedure [6, 24], which helps to ensure that the initial noise is small. Instead of sampling randomly, similar to that of a Monte Carlo method, or on a regular grid in phase space as studied in [22], a given number of particles are initialized in each cell: the (conditional) inverse cumulative distribution function of the distribution is used to assign the particle velocities, and the particle locations inside the cell are scrambled using a pseudo-random sequence to reduce correlations.

3. Projective integration scheme

In this section, we present the equation-free projective integration (EPFI) framework and we develop a new method for the solution of plasma problems. The major issues in the design of such a multiscale scheme, based on the PIC method, are the choice of a set of appropriate macroscopic variables, and the handling of the PIC-generated statistical noise. In the following, we describe the standard EPFI idea and the method proposed by Shay et. al. [20]. We the follow this by introducing our proposed scheme, utilizing wavelets in velocity-space.
### 3.1. Presentation of EFPI schemes

The simulation of strongly coupled multiscale systems remains a major challenge due to the coupling of physics, often known at the fine scale, and the dynamics of interest which may emerge at the macroscale. Often, direct computation of the solution of the original problem is out of reach due to the necessity for the discretization to resolve the smallest or fastest scales in the system. Traditional approaches for the simulation of systems that exhibit a significant separation of scales usually involve two stages. First, a set of reduced equations is derived to describe the system at the coarse or macroscopic scale. These reduced equations are solved numerically and their solutions analyzed. For plasmas, such equations exist in the form of fluid closures which reduce the dimensionality of the problem, such as the equations of magnetohydrodynamics. However, these rely on assumptions which are not always satisfied and leave out important microscale physics [26]. Furthermore, for many problems, the macroscopic equations may not be known.

When such closed-form equations are not available, the equation-free approach, originally proposed by Kevrekidis et al. [1, 2, 3, 4], sidesteps the need for an explicit reduced model. Instead, the approach relies on short bursts of microscopic simulations to determine the time derivatives of a coarse representation of the system. Even though macro-scale level equations may not be necessary, it is worth stressing that an efficient application of the equation-free procedure requires the system to be parameterizable by a set of coarse variables for which the evolution evolves on a slow manifold [2]. However, if the dynamic behavior of the system can be coarse-grained by a representation that is smooth at macroscopic scales in time and space, then it is conceivable that the full system need only be simulated for a small number of microscopic time steps to to advance the coarse variables over a much larger time interval.

The success of the method depends critically on the correct choice of the coarse description of the system, as we discuss below in more detail. Low dimensionality is clearly important as the primary purpose is computational speedup. A restricting operator, allowing the transition between the fine to the coarse representation of the data, as well as a lifting operator to go from coarse to fine scale, must be determined. Of course, the use of a coarse representation implies that some microscale information is lost through the restricting process. This data must be reconstructed when lifting to initialize the fine-scale solver, typically through interpolation techniques and physical knowledge of the system.

**Remark 3.1.** Ultimately, a goal should be to develop error estimators to validate the fidelity of the coarse representation during the time integration. This is in particular the case in the context of plasma simulations, since one may not be able to assume that the relaxation properties on which the EFPI framework is based [2, 3] hold at all times. For example, quasineutrality or Boltzmann equilibria can be violated as shocks develop or kinetic effects become dominant. Such techniques would allow the adaption of the macroscopic projection timestep as well as the coarse resolution, or revert to full-scale simulations when, for example, short transitions are detected during which no scale separation can be exploited.

![Equation free projective integration cycle](image-url)
The basic forward Euler projective integration cycle is presented in Figure 1. This cycle comprises three main parts:

Initialization. At the beginning of the step, only the coarse representation of the system is available. This data is used to recover, by the lifting operator, a consistent micro-state, which is used to initialize the fine-scale time stepper.

Micro-scale evolution. After its initialization, the fine-scale time solver is advanced forward \( N_e \) steps. After each step, the corresponding coarse variables are obtained by restricting the data.

Extrapolation. At the completion of the micro-steps, the evolution of the coarse variables is known at \( N_e + 1 \) instants corresponding to the fine time steps. For each of the degrees of freedom, the best fit for the rate of change of the corresponding variable \( \psi \) is computed e.g. by a least squares algorithm. The macroscopic variables are projected forward by the macroscopic timestep \( \Delta t \) by the forward Euler formula

\[
f(t + \Delta t) = f(t) + \Delta t \dot{f}(t).
\]

Remark 3.2. We note that it is possible to adapt this procedure to increase the accuracy of the time integration, i.e., we could also consider a trapezoidal leapfrog method as described in [20].

3.2. Choice of macroscopic variables: EFREE approach

The core of the method is the distinction between a coarse-scale (macroscopic) and a fine-scale (microscopic) model representations. In this study as in [20, 21], the fine representation consists in a fully kinetic description of the plasma, resolving the smallest relevant scales of space and time and using a PIC scheme. A second step is then to choose a coarse representation to approximate the system.

We first discuss the original so-called ‘EFREE’ approach proposed in [20], to model ion-acoustic wave propagation and steepening. In EFREE, both ion and electron distribution functions are assumed to be shifted Maxwellian distributions, the electrons are assumed to be adiabatic, and the plasma is quasineutral. Thanks to these physical assumptions, the system is parameterized by the ion and electron densities \( n^{i,e} \), mean velocities \( V^{i,e} \) and temperatures \( T^{i,e} \) (or equivalently the pressures \( P^{i,e} = n^{i,e} T^{i,e} \)). More precisely, the ion variables are chosen as ‘active’ variables, i.e. directly integrated in time.

However, electron variables are ‘passive’ variables, determined from the ion variables. Due to adiabaticity, the electron temperature is assumed to be constant at all times:

\[
T^e = T^e_0.
\]

Also the electron density is a function of the electrostatic potential \( \psi \):

\[
n^e = n_0 \exp \left( \frac{e \psi}{k_B T^e_0} \right),
\]

where \( n_0 \) is a renormalization constant. Assuming that \( n^i \approx n^e \) by quasineutrality, one deduces from (3.3) the potential \( \psi \) as a function of \( n^i \). Using (2.2) the electron density is then given as

\[
\begin{align*}
\psi &= \frac{k_B T^e_0}{e} \log \left( \frac{n^i}{n_0} \right), \\
n^e &= n^i - \frac{e_0}{e} \Delta \psi,
\end{align*}
\]

i.e.

\[
n^e = n^i - \chi^2 \frac{\partial}{\partial x} \left( \frac{n_0}{n^i} \frac{\partial n^i}{\partial x} \right).
\]
Finally the electron mean velocity is recovered by

\[ V^e = V^i. \]  

(3.6)

The spatial discretization of the 'active' variables (in EFREE, \( n^i, V^i \) and \( P^i \)) uses a two-scale grid structure which is essential for the acceleration properties of the scheme [20]. The coarse representation of the data is defined as the values of the ion variables at nodes of a coarse grid, which resolves the macroscopic phenomenon. The data is then lifted to the fine grid which corresponds to the mesh employed for the PIC algorithm. This grid typically has a much finer resolution as it must resolve the Debye length \( \lambda \). The 'passive' electron variables are then determined using Eqs. (3.2–3.6), and the particle positions are initialized on the fine-scale grid using the usual PIC weighting scheme.

Increasing and decreasing the resolution by moving the data between the coarse and fine grids is realized in two steps:

**Lifting operator.** Let \( n_c \) be the number of nodes in the coarse grid, and \( n_m \) the number of nodes in the fine grid. For simplicity, both numbers are assumed to be powers of 2, and the interpolation procedure is done in successive factors of 2, repeated over \( l \) levels such that \( n_m = 2^n n_c \). Let \( f_i = f^{(0)}_i \) be the values of a variable \( f \) at the coarse grid points \( i = 1, \ldots, n_c \). The first level of interpolation is:

\[ f^{(1)}_{2i} = f_i^{(0)}, \quad f^{(1)}_{2i-1} = 0.5 \left( f_i^{(0)} + f_{i+1}^{(0)} \right), \quad \forall i = 1, \ldots, n_c, \]  

(3.7)

where we assume periodic boundary conditions: \( f^{(0)}_0 = f^{(0)}_{n_c} \). This step is repeated \( l \) times to obtain the fine data \( f^{(1)}_i, i = 1, \ldots, n_m \).

**Restriction.** To restrict the data obtained by projection from the particle positions on the fine grid, a linear smoothing scheme is employed. Knowing the values \( f^{(l)}_i \) of the variable \( f \) at the fine grid points \( i = 1, \ldots, n_m = 2^n n_c \), the first level of restriction gives the values

\[ f^{(l-1)}_i = 0.25 \left( f^{(l)}_{2i-1} + 2 f^{(l)}_{2i} + f^{(l)}_{2i+1} \right), \quad \forall i = 1, \ldots, 2^{l-1} n_c, \]  

(3.8)

also assuming periodic boundary conditions \( f^{(l)}_{n_m+1} = f^{(l)}_1 \). This operation is repeated until the coarse level is reached.

**Remark 3.3.** Restriction of the data to a coarse grid is essential to realize a speedup through EFPI integration. Here, it also plays a crucial role by smoothing the statistical fluctuations of the variables inherent in the PIC scheme for the fine kinetic representation of the data [20]. As we will illustrate below, random fluctuations in the computed quantities appear to be substantially less pronounced when the EFPI-accelerated schemes is used as compared to a traditional PIC schemes. However, it should be noted that levels of fluctuations in the net charge \( n^i - n^e \), the electric field, or the potential remain too important to allow their use as active variables.

We refer to [20] for more details on this EFREE procedure. The numerical results presented in that work show good agreement with full microscale PIC simulations for the propagation of an ion acoustic wave. In particular, the propagation speed of the wave is very well reproduced and the numerical speedup obtained with the EFREE procedure is promising, particularly since a macroscopic CFL condition, related only to the ion sound speed \( c_s \) and the coarse grid step \( \Delta x_c \), appears as the limiting factor for the coarse time step \( \Delta t \):

\[ 2 c_s \Delta t \lesssim \Delta x_c. \]  

(3.9)

This property enables a linear scaling as one increases the system size, i.e. the wavelength of the ion acoustic wave.

However, problems appear as the wave steepens, a shock forms and the ion distribution exhibits strong non-Maxwellian features due to ion trapping. In particular, large differences in the ion pressure appear relatively fast. As already noted in [20], it is necessary to generalize the description to handle non-Maxwellian distribution functions to address these phenomena.
3.3. A wavelet-based equation-free scheme

To capture the \((x,v)\) phase-space structures emerging during the time evolution of the kinetic PIC experiments, we propose to represent the full ion distribution function \(f\), using a coarse-grained wavelet approximation in the velocity space. The motivation for introducing a multiresolution wavelet analysis, widely used in signal processing, is its multiscale nature which allows the local adaption driven by the smoothness of the function to be approximated [27]. One of their most successful applications has been signal denoising [28]. Wavelet-based density estimation (WBDE) has recently been applied to the estimation of particle distribution functions obtained from plasma simulations with PIC methods [29]. The noise reduction is typically obtained by thresholding the expansion coefficients in a wavelet basis, based on the fact that this expansion is assumed to be sparse, or more precisely, the signal is assumed to be well-approximated by a small number of large expansion coefficients.

The two fundamental properties, sparsity and denoising, appear particularly well suited for application in the equation-free projective integration framework. First, depending on the bin size used for estimation of the ion distribution function, important random fluctuations can appear in the measured coefficients, especially in phase space regions with low particle count. The smoothing operation (3.8) from the fine to coarse grid, introduced in [20], is typically not sufficient to correct for the strong noise in the simulations. On the other hand, the wavelet representation enables the computation of a much smoother approximation as shown in Section 4.

**Remark 3.4.** Note that non-physical negative values of the distribution function can be obtained due to the extrapolation procedure, or due to the non-positivity of the oscillating wavelet functions as observed in [29]. We propose in paragraph 3.3.3 a procedure designed to correct this defect and allow resampling from the approximated distribution function.

Moreover, the sparsity of the representation is naturally connected to the coarse-graining of the data in phase-space. In this first step of the wavelet-based projective integration method, we limit attention to a non-adaptive approach, i.e., the wavelet representation is truncated at some pre-defined level of resolution to reduce the number of active variables. We will also show how noisy data obtained with this approach can be post-processed using adaptive coefficient thresholding as passive denoising [29, 30].

3.3.1. A primer on wavelets

Let us first recall some notions on wavelets, see e.g. [27] for further details. For any function \(f \in L^2(\mathbb{R})\) and a starting resolution level \(J_0\), representation in the wavelet basis is given by the reconstruction formula:

\[
f(y) = \sum_{k=-\infty}^{\infty} \tilde{J}_{J_0,k} \phi_{J,k}(y) + \sum_{j=J_0}^{\infty} \sum_{k=-\infty}^{\infty} \tilde{f}_{J_0,k} \psi_{J,k}(y) \tag{3.10}
\]

where

\[
\phi_{J,k}(y) = 2^{j/2} \phi(2^j y - k),
\psi_{J,k}(y) = 2^{j/2} \psi(2^j y - k),
\tag{3.11}
\]

are scaled and translated versions of the father wavelet (or scaling function) \(\phi(y)\) and the mother wavelet \(\psi(y)\). We will assume that \(\psi\) has zero average and compact support, and that the wavelet family \((\psi_{j,k}(y))_{j \in \mathbb{N}, k \in \mathbb{Z}}\) is an orthonormal family. One can show existence of the scaling function \(\phi\), defined such that the orthogonal complement in \(L^2(\mathbb{R})\) of the linear space spanned by the wavelets is itself orthogonally spanned by the translates of the function \(\phi\).

The coefficients \(\tilde{f}_{j,k} = \langle f | \psi_{j,k} \rangle = \int_{\mathbb{R}} f \psi_{j,k}\) of a function \(f\) in this wavelet family, called detail coefficients, describe fluctuations of the function \(f\) at scale \(2^{-j}\) around the position \(k/2^j\). Large values of \(j\) correspond to fine scales, small values to coarse scales. The coefficients \(\tilde{J}_{j,k} = \langle f | \phi_{j,k} \rangle\) are called the scaling coefficients. The first sum on the right-hand side of formula (3.10) forms a smooth approximation of \(f\) at the coarse scale \(2^{-J_0}\), and the second sum represents a correction formed by the addition of details at successively finer scales.
When the scaling coefficients $f_{J,k}$ are known at a certain scale $J$, all the wavelet coefficients at coarse scales ($0 \leq j \leq J$) can be computed using the fast discrete wavelet transform (DWT) algorithm [28].

In this work, we employ the basic Haar wavelet as well as the commonly used Daubechies 6 wavelet family, defined by having six vanishing moments:

$$\int_{\mathbb{R}} y^m \psi(y) = 0, \quad 0 \leq m < 6.$$  

This implies that the first six moments of the distribution function depend only on its scaling coefficients, and not on the detail coefficients.

**Remark 3.5.** The reconstruction formula (3.10) involves an infinite sum over the position index $k$. In practice we are interested only in functions defined over a bounded domain, and the commonly used alternative is to periodize the wavelet transform over this domain [28]. Throughout the paper we will consider only periodic wavelets.

### 3.3.2. Coarse time-stepper

Let us now describe in detail the proposed method. As in the EFREE method presented in Sec. 3.2, we assume that the electrons are adiabatic and that their distribution function is well approximated by a shifted Maxwellian. However, we lift the requirements of quasi-neutrality and, most importantly, the assumption of Maxwellian-distributed ions.

Let $V_{\text{max}} > 0$ be an appropriately chosen upper bound for the ion velocities. We also choose a fine resolution $J_m$ and a coarse resolution $J_0$ to define the fine and coarse scales in the velocity discretization. For a given resolution $j_0 \leq J \leq J_m$, the ion distribution function $f^i(x,v)$ is approximated by a truncated wavelet expansion in the velocity coordinate $v \in [-V_{\text{max}},V_{\text{max}}]$, parameterized by the space coordinate $x$:

$$f^i(x,v) \approx \sum_{k=-\infty}^{\infty} f_{J,i,k}(x) \phi_{j,k}(v). \quad (3.12)$$

Note that in practice, Eq. (3.12) is not exactly the representation that is used. Instead, we assimilate the fine-scale coefficients $\overline{f}_{J,i,k}(x)$ with the rescaled values of a histogram of the ion distribution function constructed over a grid of size $2^{j_0}$ in the velocity direction and parameterized by $x$. This greatly simplifies the computation: indeed, the exact computation of the true fine scaling coefficients $\overline{f}_{J,i,k} = (f^i|_{\phi_{j,k}})_v$ from the empirical distribution function (2.4) is difficult since the values of the function $\psi_{j,k}$ are not known analytically. Furthermore, the construction of the conditional inverse cumulative distribution functions needed for the quiet start procedure functions is not straightforwardly obtained from (3.12).

The scaling coefficients $\overline{f}_{J,i,k}(x)$ at the coarse resolution $J_0$ are chosen as the ’active’ variables. In particular, the coarse representation of the data is defined as the values at the nodes of the coarse grid in space, as we use the same two-scale grid structure as discussed in Sec. 3.2.

To complete the description of the system, we determine the electron ’passive’ variables $n^e$, $V^e$ and $T^e$ by first computing the ion density and velocity $n^i$ and $V^i$ by integrating numerically (3.12) along the velocity coordinate. Using the assumption of adiabatic electrons (3.3), we solve self-consistently for the electrostatic potential the nonlinear Poisson-Boltzmann equation:

$$-\Delta \phi = \frac{e}{\varepsilon_0} \left( n^i - n_0 \exp \left( \frac{e\psi}{k_B T_0^i} \right) \right), \quad (3.13)$$

Equivalently, we look for the rescaled potential $\tilde{\phi} = e\phi/(k_B T_0^i)$ such that

$$-\lambda^2 \Delta \tilde{\phi} + \exp(\tilde{\phi}) = n^i/n_0. \quad (3.14)$$

In practice, this equation is discretized on the coarse grid and solved iteratively using a Newton method. Then, the values for the electron variables are recovered from Eqs. (3.2), (3.3) and (3.6):

$$n^e = n_0 \exp(\tilde{\phi}), \quad V^e = V^i, \quad T^e = T_0^e. \quad (3.15)$$
Lifting operator. The lifting step consists of three important stages:

- Increasing the phase space resolution of the data using the linear interpolation (3.7) and the inverse DWT in (3.12);
- Reconstructing the inverse conditional cumulative ion distribution functions (inverse CCDF) for the velocity at each fine grid point in space;
- Loading the particles using the quiet start procedure.

Let us detail some aspects of this procedure. Indeed, the loading scheme is particularly important as it controls the initial level of the noise.

Once the scaling coefficients data has been lifted to the fine grid, we recover at each node $x_f^j$ of the fine grid with $1 \leq j \leq x_m^m$ the approximated histogram of the ion distribution function. We then compute the value of the ion density $n^i(x_f^j)$ and, by summation, the values of the normalized conditional cumulative distribution function $F_v$:

$$F_v(v_k | x = x_f^j) \approx \frac{1}{n^i(x_f^j)} \int_{v_k}^{\infty} f^i(x_f^j,v) dv,$$

at points $v_k = V_{max} \cdot (2^{1-j_m}k - 1), 0 \leq k \leq 2^j_m$. Due to the extrapolation process or the properties of the wavelets, some values of the approximate histogram may be negative. This results in a non-monotone CCDF, which is nonphysical and must be corrected. We propose here a simple reconstruction method, presented in Fig. 2, and which is found to give good results in practice. Let $g = (g_k)_{0 \leq k \leq 2^j_m}$ be an array such that $g_0 = 0, g_{2^j_m} = 1$. Suppose that $g$ is not monotone. Then there exists a smallest $k_0$ such that $g_{k_0} > g_{k_0+1}$. In this case, we define $k_M$ as the smallest index such that $g_{k_M} \geq \min(g_{k_0},1)$ and $k_m$ is the largest index such that $g_{k_m} \leq \max(g_{k_0},0)$ for all $k = k_0, \ldots, k_M$. Then define

$$\tilde{g}_k = \begin{cases} g_k & \text{if } k \leq k_m \text{ or } k \geq k_M, \\
\frac{g_{k_0} + k_m - k}{M-m} (g_{k_M} - g_{k_m}) & \text{else.}
\end{cases}$$

Now $\tilde{g}$ is monotone up to $k = k_M > k_0$. Proceeding recursively, we obtain in all cases a corrected monotone array $g^+$ where the + denotes that the correction is computed from the lower to the upper indexes. To ensure symmetry of the reconstruction, it is necessary to compute another corrected array $g^-$, computed in similar fashion but starting from the higher indexes. Finally, we define the reconstructed array $Rg$ as:

$$Rg = (g^+ + g^-)/2.$$
Once all the reconstructed arrays \( (RF_v(x|x=x_i^j))_{0 \leq k \leq 2^j} \) have been computed, the quiet loading of the ion particles proceeds as follows.

Recall that each particle is parameterized by its position \( X_i^j \), velocity \( V_i^j \) and weight \( \omega_i^j \). Let \( (a_j,b_j) \in \mathbb{N} \subset [0,1)^2 \) be a low discrepancy sequence (e.g. the Hammersley sequence), which yields numbers that are more evenly distributed than a random number numbers. Then, we set the initial particle parameters as

\[
\begin{align*}
X_i^j &= L \cdot a_i, \\
V_i^j &= (RF_v)^{-1}(b_i | x = X_i^j), \\
\omega_i^j &= n' (X_i^j),
\end{align*}
\]

(3.19)

where all values are linearly interpolated between the two closest points of the fine grid. The inverse mapping \((RF_v)^{-1}(\cdot | x = X_i^j)\) is evaluated by lookup and linear interpolation. To finish initializing the PIC code, the electrons are loaded using the normal quiet start procedure for a shifted Maxwellian function.

**Restriction: Wavelet-based density estimation in a co-evolving frame.** The process for restricting the PIC data to the coarse level is quite simple: the histogram of the empirical ion distribution function (2.4) is reconstructed at each grid point by projecting each particle using the PIC weighting scheme in space and in the correct bin according to its velocity. For \( 1 \leq j \leq N_p \) this is expressed

\[
\begin{align*}
\left\{ \begin{array}{l}
n x = \left[ \frac{n_m \cdot X_j^i}{L} \right] + 1, \\
\theta_x = \frac{n_m \cdot X_j^i}{L} - \left[ \frac{n_m \cdot X_j^i}{L} \right], \\
v_{j} = \left[ 2^{J_m-1}, \frac{V_{j}^{i} + V_{max}}{V_{max}} \right] + 1,
\end{array} \right.
\end{align*}
\]

\[
\begin{align*}
&\left( \mathcal{T}_{J_m,nv}^{(i)} \right)_{n x} \left( \mathcal{T}_{J_m,nv}^{(i)} \right)_{n x} + (1 - \theta_x) \cdot \omega_i^j, \\
&\left( \mathcal{T}_{J_m,nv}^{(i)} \right)_{n x + 1} \left( \mathcal{T}_{J_m,nv}^{(i)} \right)_{n x + 1} + \theta_x \cdot \omega_i^j.
\end{align*}
\]

(3.20)

where \([ \cdot ]\) denotes the nearest smaller integer. Then, the linear smoothing scheme (3.8) and the discrete Fourier transform are used to coarsen the phase space resolution of the data. In particular, the detail coefficients from level \( J_m \) to \( J_0 \) are discarded.

In practice, the scheme described above suffers in some cases from the numerical noise due to the PIC method. To further reduce the error associated with the projective integration, it is known that one can take advantage of an appropriate choice of "co-evolving frame" associated with the solution [4]. Typically, the error is reduced due to a smaller time derivative in the new spatial frame. In the case of a strongly hyperbolic problem such as the Vlasov-Poisson problem, traveling with an approximate flow can result in big improvements in terms of noise and accuracy as we will show further on.

Here, the motivation is that the self-consistent potential \( \phi \) computed at the lifting step by solving equation (3.13) is typically slow-moving and quite smooth. As a consequence, a good approximation to the flow characteristics can be recovered and will naturally take into account the "transport component" of the equation. The idea is then to weigh each particle at a projected location instead of its actual location, which amounts to transporting backwards along approximated characteristics the grid on which the histogram is computed. The deposition scheme is then as follows:

Let \( E_x^0 = -\nabla_x \phi \) be the electrical field computed at initialization of the microscopic PIC time stepper, e.g. at time 0. Let \( \delta t \) be the microscopic time step, and \( \Delta t \) the macroscopic time step. At the \( n \)-th microscopic time step, we set for each particle

\[
\begin{align*}
\tilde{X}_j^i &= X_j^i + (\Delta t - n \delta t) \cdot V_j^i, \\
\tilde{V}_j^i &= V_j^i + \frac{e}{m_i} (\Delta t - n \delta t) \cdot E_x (X_j^i).
\end{align*}
\]

(3.21)
The deposition scheme then is

\[
\begin{align*}
    n_x &= \left\lfloor \frac{n_m \cdot \bar{X}^j}{L} \right\rfloor + 1, \quad \theta_x = \frac{n_m \cdot \bar{X}^j}{L} - \left\lfloor \frac{n_m \cdot \bar{X}^j}{L} \right\rfloor, \quad n_v = 2^{j_m-1} \cdot \left\lfloor \frac{V^j + V_{\text{max}}}{V_{\text{max}}} \right\rfloor + 1, \\
    (\mathcal{T}_{j_m,n_v}^{(l)})_{n_x} &= (\mathcal{T}_{j_m,n_v}^{(l)})_{n_x} + (1 - \theta_x) \cdot \omega^j, \\
    (\mathcal{T}_{j_m,n_v}^{(l)})_{n_x+1} &= (\mathcal{T}_{j_m,n_v}^{(l)})_{n_x+1} + \theta_x \cdot \omega^j.
\end{align*}
\]

(3.22)

Finally, the linear smoothing scheme (3.8) and the discrete Fourier transform is used to coarsen the phase space resolution of the data.

3.3.3. Denoising and multiresolution in phase space

We finally present a simple denoising algorithm which is used to post-process the data obtained from the proposed wavelet-based equation free approach. Based on the 'PURE-shrink' estimator, proposed in [30], this algorithm adaptively selects a threshold for each wavelet resolution level, hence allowing the selection of the relevant wavelet detail coefficients. Particularly adapted to the Poisson-type noise observed in particle-based histograms, it is based on the use of the Haar basis. Note that this results in blocking artifacts, and more sophisticated algorithms should be investigated for use with higher order wavelets, see e.g. [29].

The algorithm is based on the Poisson Unbiased Risk Estimate [30]. We recall that \( m \) is a Poisson random variable of intensity \( \mu > 0 \) if and only if for every \( k \in \mathbb{N} \):

\[
\text{Probability}(m = k) = e^{-\mu} \frac{\mu^k}{k!}.
\]

Let us consider the vector of fine-scale scaling coefficients \( \mathbf{f}_{j_m,k}^{(l)} \), \( 1 \leq k \leq 2^{j_m} \) at a given grid point, obtained by computing the histogram of the ion particles at the maximum resolution \( J_m \). We assume that this vector is a noisy realization \( \mathbf{m} \) of \( 2^{J_m} \) of independent scaled Poisson processes of intensity of the true signal \( \mu \). We denote by \( \mathbf{d}_j = (d_{j,k}), \mathbf{s}_j = (s_{j,k}), \) \( 1 \leq k \leq 2^j \), respectively the detail and scaling coefficients of the noisy signal at resolution \( j \leq J_m \) and \( \mathbf{\delta}_j = (\delta_{j,k}), \mathbf{\sigma}_j = (\sigma_{j,k}) \) respectively the detail and scaling coefficients of the original noise-free signal. Given a resolution level \( j \leq J_m \), we define \( (e_{j,k}) \) to be the canonical basis of \( \mathbb{R}^{2^j} \). Then, the following result, proven in [30], is

**Lemma 3.6.** Let \( \theta_j(d_j, s_j) \) be an estimate of the noise-free wavelet coefficients \( \delta_j \). Define \( \theta_j^+(d_j, s_j) \) and \( \theta_j^-(d_j, s_j) \) as:

\[
\begin{align*}
    \theta_j^+(d_j, s_j) &= \theta_j(k, d_j + e_k, s_j - e_k), \\
    \theta_j^-(d_j, s_j) &= \theta_j(k, d_j - e_k, s_j - e_k).
\end{align*}
\]

(3.23)

Then the random variable:

\[
\varepsilon_j = 2^{-j} (\|\theta_j(d_j, s_j)\|^2 + \|d_j\|^2 - 1 \cdot s_j) - d_j \cdot (\theta_j^-(d_j, s_j) + \theta_j^+(d_j, s_j)) - s_j \cdot (\theta_j^+(d_j, s_j) - \theta_j^-(d_j, s_j))
\]

(3.24)

is an unbiased estimate of the mean-square error \( 2^{-j}\|\theta_j(d_j, s_j) - \delta_j\|^2 \), i.e. both variables have the same expected value.

This result can be used to serve as a data-dependent measure which can be minimized to estimate the underlying Poisson intensity of the signal. It is based on the fact that the Haar wavelet decomposition preserves the Poisson properties (because the sum of two Poisson variables is a Poisson variable), allowing to process each resolution level separately.
We apply the robust PURE-shrink algorithm [30] to denoise the wavelet data describing the velocity distribution at each coarse space grid point. The following estimator is adopted:

\[ \hat{\theta}_{j,k}^{\text{PUREshrink}}(d_{j,k}, s_j) = \max \left( d_{j,k} - a_j \sqrt{|s_{j,n}|} \right), \]  

(3.25)

where \( a_j \) is an adjustable parameter. The algorithm follows the three main steps:

- Rescale the data by empirically measuring the local variance and mean,
- Determine adaptively a threshold for each level of wavelet decomposition by setting the parameter \( a_j \) to the value that minimizes the PURE estimate (3.24),
- Compute the new detail coefficients for the denoised signal using (3.25).

We stress that this algorithm is currently used as a post-processing tool only and not directly implemented. Nevertheless, it is an important step to demonstrate the effectiveness of the nonlinear thresholding wavelet techniques at handling the PIC-generated noise for the future application to projective integration algorithms.

**Remark 3.7.** Future implementations of wavelet-based projective algorithms could use such algorithms to adaptively select the relevant wavelet coefficients as a sparse description of the distribution at the coarse scale. In particular, the development of projective integration approaches in higher dimensions would benefit greatly from this approach to reduce the number of active degrees of freedom.

4. Test cases

We now illustrate the performance of the proposed approach for solving the Vlasov-Poisson system by modeling two different test cases, and seek to compare the results obtained with the classical PIC scheme and with the proposed coarse time-stepping algorithm. Simulations with the original EFPI algorithm proposed by Shay et al. [20] are also considered in the first test case, comprising an ion acoustic wave, for a comparison.

The second test case is a plasma expansion in a vacuum.

4.1. Ion acoustic wave test-case

The first test case is the propagation and nonlinear steepening of an ion acoustic wave in a Maxwellian two-species plasma. In previous studies [20, 21], other versions of EFPI-accelerated PIC-based codes were applied to this test case and we refer in particular to [20] for a detailed account of the theory and initial setup of the wave. We initialize the Vlasov-Poisson system with

\[ f^{i,e}(x,v,t=0) = C^{i,e}(1 + \delta \cos(2\pi k \cdot x/L)) \exp \left( -\frac{1}{2} \left( \frac{v - \delta \cos(2\pi k \cdot x/L)}{v_{ti,e}} \right)^2 \right), \]  

(4.1)

where \( C^{i,e} \) are renormalization constants, \( \delta = 0.2 \) is the initial amplitude of the perturbation and \( k > 0 \) is the perturbation mode. The initial thermal velocities are chosen as \( v_{ti} = 0.22 \) and \( v_{te} = 42.5 \), since the condition \( T_e \gg T_i \) is necessary to minimize Landau damping of the wave.

The set of numerical parameters normalized for the XES1-based PIC code [6] are \( \epsilon_0 = 1, N^e = N^i = N_p = 512236, \omega_p^e = 5091, q_e/m_e = -1.0, \omega_p^i = 120, q_i/m_i = 5.55592 \cdot 10^{-4}. \) The time step is chosen as \( \delta t = 10^{-4} \). The number of mesh cells \( nx \) is adjusted depending on the system length \( L \), taking respectively the values 512, 1024 respectively for \( L = 4.8, 9.6 \), for a constant grid step \( dx \approx 10^{-2} \). These parameters correspond to the same case as in [20, 21]. Under these conditions, both the fast space and time scales (the Debye length and the electron plasma period) are resolved, and the PIC method is stable.

Parameters for the simulation runs used for this study are shown in Table 1.
Table 1: Simulation runs presented for this test case. $L$ is the domain length, $k$ the initial perturbation mode, $n_m$ and $n_c$ respectively the number of fine and coarse space grid points, $J_m$ and $J_0$ respectively the fine and coarse wavelet resolution, $\Delta t$ and $\delta t$ respectively the fine and coarse time steps.

<table>
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<th>Type</th>
<th>$L$</th>
<th>$k$</th>
<th>$n_m$</th>
<th>$n_c$</th>
<th>$J_m$</th>
<th>$J_0$</th>
<th>$\Delta t/\delta t$</th>
</tr>
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<td>4.8</td>
<td>2</td>
<td>512</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>2</td>
<td>EFPI</td>
<td>4.8</td>
<td>2</td>
<td>512</td>
<td>128</td>
<td>9</td>
<td>9</td>
<td>200</td>
</tr>
<tr>
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<td>4.8</td>
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<td>1024</td>
<td>-</td>
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</tbody>
</table>

4.1.1. Choice of EFPI numerical parameters

The EFPI algorithm presents two main parameters, both of which require some tuning to obtain optimal results: the coarse time step $\Delta t$ and the number of microscopic time steps needed during each projective integration cycle $N_e$. As noted in [20], in the first case $\Delta t$ is controlled by a Courant-type condition which is well understood.

However, the choice of $N_e$ is more delicate, and as we show here, problem-dependent. In [20], various choices ranging from $N_e = 10$ to $N_e = 20$ are analyzed numerically showing a strong effect on the error, with the simulation diverging quickly for $N_e \leq 14$ and almost indistinguishable results for $N_e \geq 16$. In addition, they observed that the minimum value of $N_e$ for which the EFPI run remains stable does not depend on the size of the system, $L_e$, nor on the number of particles.

Figure 3 shows the relative $L^2$ error in the ion density function obtained with the proposed wavelet-based method depending on the choice of $N_e$ and over a total of 10 or 20 macro time steps, using the parameters for run 2. One may expect the error to decrease uniformly with the number of samples per cycle $N_e$, but another interesting pattern emerges.

Note that the electron plasma period is approximately $0.0012 \approx 12 \delta t$ with the chosen numerical parameters. In this case, we observe that the error is minimized by averaging over 1.5, 2.5 or 3.5 periods of the fast electron plasma wave. This curve is consistent with the least-squares computation of the zero average slope of a regularly sampled harmonic wave. This suggests that the dominant error is caused by a resonance with the electron plasma waves. Hence, the electron plasma period supplies a first indication as to the correct
choice for $N_c$ for a given $\delta t$.

4.1.2. Numerical results

Figures 4 and 5 show results for runs 1, 2 and 3, respectively, at times $t = 1$ and $t = 2$. We show the unnormalized ion distribution function for the PIC scheme (run 1), our proposed wavelet-based method with no thresholding ($J_m = J_0$, run 2) and with thresholding (run 3). A fourth distribution is obtained by post-processing data from run 2 using the denoising algorithm discussed in Sec. 3.3.3. The PIC simulation is taken as the reference. We can see that as the wave propagates, it deforms and steepens as a shock develops. At time $t = 1$, the ion distribution function is very smooth. The different schemes are in good agreement with each other and all main features are well represented. The upper velocity tail around the shock starts to deviate from the Maxwellian distribution. The propagation speed of the ion wave is very well matched by the proposed method, as was the case for the original EFREE [20]. A large amount of noise can be observed in the distribution from run 2 which simply extrapolates the values of the raw velocity histogram without using the wavelet framework. It is remarkable that, thanks to the reconstruction operator (3.18), the method remains stable. However, this noise will degrade the accuracy of the method. On the other hand, the distribution from run 3 shows no such corruption by noise and stays very smooth. Note also that the number of coarse variables is divided by 8, compared to run 2, with no loss in accuracy. This result shows that the (linear) thresholding of the wavelet coefficients is very efficient and already very well adapted to use in the EFPI algorithm. Thirdly, the post-processed distribution is also very smooth, despite suffering from blocking artifacts (due to the use of the Haar basis). In particular, this shows that the noise present in the data from run 2 can be almost completely removed by the use of the nonlinear thresholding algorithm. At time $t = 2$, shocks have fully developed. There is a noticeable difference between the reference PIC simulation and results from our proposed approach presented in Figure 5. While the ion wave propagates at the correct speed, the shock is only marginally resolved by the coarse resolution of the equation-free approach. The discontinuities in ion density and velocity are severely smoothed. Large-scale structures are, however, well reproduced, in particular the presence of an asymmetric upper speed tail. Thus, increasing the resolution is sufficient for increasing the accuracy, as we show next. Finally, noise is still clearly present in the raw histogram data from run 2. It is also very non-homogeneous in space: its variance is especially strong at the shock position where the nonlinear denoising algorithm is challenged to extract useful data, e.g. at $x \approx 1$.

Next, Figures 6 and 7 show results for run 4 and 5 at times $t = 4$ and $t = 7$. In addition to the ion distribution, we plot the ion density and pressure. Although the pressure begins to deviate from the reference solution at $t = 7$, due to the lack of resolution around the shock, we obtain reasonably accurate results and the correct anharmonic shape is obtained. Note that fast oscillations at the timescale of the electron plasma waves appear around the shock in the PIC reference solutions, but are damped out by the coarse integration scheme. This is because the plasma oscillations are not resolved at all in this case. Also, note that the solution obtained by projective integration exhibits much less noise than the PIC data.

4.1.3. Discussion

Strongly non-Maxwellian effects appear progressively during the ion acoustic wave propagation. In particular one observes reflected particles and a double-peaked ion distribution function at the shock. The simple system representation by shifted Maxwellians in the original EFREE implementation [20] lead to noticeable differences with the reference simulation. In particular, the ion pressure diverges quickly and does not develop the correct strongly anharmonic shape. We have illustrated here how the wavelet-based equation free method substantially improves on these results. Our projective integration scheme gives reasonably accurate results even in the strongly nonlinear regime, after the creation of the shock, while using a large macroscopic time step. This shows that the EFPI framework can be effective in a kinetic setting, provided a non-parametric representation of the general non-maxwellian ion distribution function is used.

Two kinds of fluctuations appear important to take into account when using the PIC kinetic micro-solver. First, fast plasma waves give rise to periodic fluctuations which one must average out by carefully choosing the duration of the micro integration stage during the EFPI cycle. Here, the electron plasma period is
Figure 4: Comparison between unnormalized ion distribution function plots obtained with a reference brute-force particle simulation (Run 1) and EFPI-accelerated results (Runs 2 and 3 in Table 1), $t = 1$.

Figure 5: Comparison between unnormalized ion distribution function plots obtained with a reference brute-force particle simulation (Run 1) and EFPI-accelerated results (Runs 2 and 3 in Table 1), $t = 2$.

identified as an appropriate choice of $N_e$ and $\delta t$ to minimize the EFPI error. In other cases, oversampling or more advanced techniques may be necessary to reduce the resonance error.
Figure 6: Comparison between full particle (Run 4) and EFPI (Run 5 in Table 1) results at $t = 4$. Top left: ion distribution function with PIC scheme. Bottom left: ion distribution function with wavelet-based EFPI scheme. Top right: ion density with PIC and EFPI schemes. Bottom right: ion pressure with PIC and EFPI schemes.

Figure 7: Full particle (Run 4) and EFPI (Run 5 in Table 1) results at $t = 7$. Top left: ion distribution function with PIC scheme. Bottom left: ion distribution function with wavelet-based EFPI scheme. Top right: ion density with PIC and EFPI schemes. Bottom right: ion pressure with PIC and EFPI schemes.
Second, random-like fluctuations due to the PIC codes necessitate a careful treatment. As we have shown, the level of fluctuations in the active (ion) variables has been successfully reduced by our proposed wavelet-based approach due to (a) linear smoothing from fine to coarse grid, (b) denoising by linear or nonlinear thresholding of wavelet coefficients, (c) projection in a co-evolving frame, (d) quiet start. This last factor appears particularly efficient since the micro-integration is only realized for a small number of timesteps, enabling the PIC error to scale as $\log(N_p)/N_p$ instead of $1/\sqrt{N_p}$ [24]. Note that both issues will be especially important in more general multiscale cases where electron variables must be projectively integrated directly as ‘active’ variables, as they experience much higher levels of fluctuations.

4.2. One-dimensional plasma expansion test-case

As a second test case, we consider a one-dimensional expansion problem, described in [31, 32, 16]. The ions initially uniformly occupy a thin slab of thickness $a \gg L$, while the electrons are initialized as the adiabatic Maxwell-Boltzmann equilibrium in a self-consistent potential. The test problem requires the observation of the expansion of the ion slab, initialized with:

$$f^i(x, v, t = 0) = \begin{cases} C^i \exp \left(-\frac{1}{2} (v/v_i)^2 \right) & \text{if } |x| \leq a/2, \\ f^i(x, v, t = 0) = 0 & \text{else,} \end{cases} \tag{4.2}$$

where $C^i$ is a renormalization constant, and the electron distribution function is deduced by solving the nonlinear Poisson-Boltzmann equation (3.14) and hypothesis (3.15). Note that this is the same procedure used when lifting the coarse ion data in the approach developed in this paper.

The initial electron temperature is 1000 times higher than the initial ion temperature: the thermal velocities are set as $v_i^e = 0.0316$, $v_i^e = 42.84857$. As in the previous test case, the electron motion is much faster than the ion motion and we can exploit this separation of scales with EFPI, since the expansion occurs roughly at the speed of the ion acoustic wave [16]. The set of numerical parameters normalized for the PIC code are, in code units, $\epsilon_0 = 1$, $\omega_p^e = 42.8486$, $q_i/m_e = -1.0$, $\omega_p^i = 1$, $q_i/m_i = 5.5447 \times 10^{-4}$. The time step is chosen as $\delta t = 10^{-3}$. Note that because of the discontinuous initial condition, stability constraints impose a much smaller time step compared to the electron plasma period as $\omega_p^e \delta t \approx 0.05$ (whereas $\omega_p^i \delta t \approx 0.5$ in the ion acoustic wave case). The number of mesh cells is $n_x = nm = 8192$ for a system length $L = 2000$, and the initial ion slab occupies a fraction of 2% of the domain with $a = 40$. These parameters are summarized in Table 2.

Note that these parameters are similar to those used in [16], but the setup differs in the boundary conditions as they simulate only a half-domain with a purely absorbing right boundary condition and an axis of symmetry on the left of the domain while we consider a periodic system. However, we assume that the simulation box is large enough so the choice of boundary conditions does not impact the simulation as long as the bulk of the plasma is far away from the boundary.

<table>
<thead>
<tr>
<th>Run</th>
<th>Type</th>
<th>$L$</th>
<th>$a$</th>
<th>$n_m$</th>
<th>$n_e$</th>
<th>$J_m$</th>
<th>$J_e$</th>
<th>$N_p$</th>
<th>$\Delta t/\delta t$</th>
</tr>
</thead>
<tbody>
<tr>
<td>6</td>
<td>PIC</td>
<td>2000</td>
<td>2</td>
<td>8192</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>7</td>
<td>EFPI</td>
<td>2000</td>
<td>2</td>
<td>8192</td>
<td>2048</td>
<td>9</td>
<td>6</td>
<td>2097152</td>
<td>500</td>
</tr>
</tbody>
</table>

Table 2: Simulation runs presented for this test case. $L$ is the domain length, $a$ the initial slab width, $n_m$ and $n_e$ respectively the number of fine and coarse space grid points, $J_m$ and $J_e$ respectively the fine and coarse wavelet resolution, $N_p$ the number of particles for each species, $\Delta t$ and $\delta t$ respectively the fine and coarse time steps.

4.2.1. Choice of EFPI numerical parameters

As in the ion acoustic wave test case, numerical experiments show that the coarse time step $\Delta t$ is controlled by a Courant-type condition. To choose the number $N_e$ of microscopic time steps computed for each projective integration cycle, we repeat the analysis from the previous test case by measuring empirically the relative $L^2$ error in the ion density function depending on $N_e$, using the parameters from run 7.

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Results are shown in Fig. 8. In contrast to the previous case, no clear pattern emerges but the choice of $N_e = 18$ seems to give the best results. For $N_e \leq 16$ the error is clearly driven by the particle noise and the simulations are unstable. The significant difference from the previous case is believed to be caused by $\delta t$ being much smaller than the electron plasma period, thus reducing the effect of the resonance error. Note that in our experiments, averaging over 1.5 electron plasma periods as previously ($N_e = 170$) did not yield more accurate results while being 10 times more expensive. This is likely a consequence of noise levels in the PIC simulations increasing over time after the quiet start [20].

4.2.2. Numerical results

Figures 9 and 10 show the results for runs 6 and 7, respectively, at times $t = 5$ and $t = 20$. We plot the unnormalized ion distribution function, the ion density and the mean velocity. As time advances, the ion slab expands from the initial interval $[-20, 20]$ roughly at the speed of the ion acoustic wave [33]. First, we observe that the proposed method gives a correct account of the speed of expansion of the ion acoustic wave, thus verifying that it correctly captures this wave as also seen earlier. Note that the expansion is noticeably slowed down with other methods (Direct-Implicit or Asymptotic-Preserving) as shown in [16], in contrary to the case here. Due to the very large time step and lower space resolution ($\Delta t$ is 500 times bigger than $\delta t$), there is a degradation in accuracy especially at the edges of the distribution. We note also that data is basically noise-free even though the simulation used 8 times less particles than the PIC run (see Table 2), at the cost of a noticeable smearing of the distribution in velocity space.

Nevertheless, our proposed wavelet-based method provides good results even in these highly under-resolved conditions. Note also that the assumptions on the electron distribution become progressively less valid as kinetic energy is transferred to the ions [33, 34]. It would be interesting to model the electron temperature as an ‘active’ time-dependent variable which could be projectively integrated directly. This should allow to go further in time as the expansion ‘freezes’ due to the progressive reduction in electron temperature.

4.3. Discussion: computational speedup

Finally, let us discuss the computational gains which have been realized in both test cases. The proposed equation-free method has been shown to remain accurate compared to a full-scale PIC simulation, even as
Figure 9: Comparison between full particle (Run 6) and EFPI (Run 7 in Table 2) results at $t = 5$. Top left: ion distribution function with PIC scheme. Bottom left: ion distribution function with wavelet-based EFPI scheme. Top right: ion density with PIC and EFPI schemes. Bottom right: mean ion velocity with PIC and EFPI schemes.

Figure 10: Full particle (Run 6) and EFPI (Run 7 in Table 2) results at $t = 20$. Top left: ion distribution function with PIC scheme. Bottom left: ion distribution function with wavelet-based EFPI scheme. Top right: ion density with PIC and EFPI schemes. Bottom right: mean ion velocity with PIC and EFPI schemes.
highly kinetic phenomena becomes important. To be considered an interesting candidate for multi-scale simulations, such a method must also provide an appreciable run time speedup compared over the classical PIC method.

As noted in [20], the majority of the computational time used to run the equation-free methods is used during the time-stepping of micro-scale PIC kinetic simulations. The remaining parts of the EFPI cycle (lifting, restricting, projecting) represents a small overhead, especially as the system grows bigger and needs a large numbers of particles. Then, the speedup mainly depends on the ability to keep the number of kinetic micro-time steps \( N_e \) small while using large projective time steps \( \Delta t \).

Based on the numerical experiments presented here, we observe that, for both the original EFREE [20] and the wavelet-based method presented here, the macro time step is governed by the stability condition (3.9) i.e. a macro-scale physical effect. On the other hand, the number of necessary micro-time steps per cycle \( N_e \) has been shown to depend on micro-scale effects such as the shot noise and the electron plasma period. It is thus independent of macro-scale parameters, in particular the wavelength of the ion acoustic wave. This allows for substantial CPU time speedups, summarized in Table 3 for the simulation runs which we have presented.

<table>
<thead>
<tr>
<th>Type</th>
<th>Run</th>
<th>Speedup</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ion acoustic wave, ( L = 4.8 )</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>IAW, ( L = 9.6 )</td>
<td>2</td>
<td>6.2</td>
</tr>
<tr>
<td>Plasma expansion, ( L = 2000 )</td>
<td>3</td>
<td>5.4</td>
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<tr>
<td></td>
<td>4</td>
<td>1</td>
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<td></td>
<td>5</td>
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</tr>
<tr>
<td></td>
<td>6</td>
<td>1</td>
</tr>
<tr>
<td></td>
<td>7</td>
<td>88</td>
</tr>
</tbody>
</table>

Table 3: Observed speedup between identical EFPI and full PIC runs 1–7 in Tables 1 and 2. All simulations were performed on a single core of a 3.2GHz Intel Core i5.

As can be seen from runs 3 and 5, a linear scaling is achieved with the size of the system \( L \). The quiet start procedure implemented in the proposed method is probably an important factor for this result as the statistical particle noise scales as \( \log(N_{pc})/N_{pc} \) and not as \( 1/\sqrt{N_{pc}} \) for the very short PIC runs that are used during each EFPI cycle. Here \( N_{pc} \) is the number of particles per coarse grid cell. Reasoning as in [20], one estimates the signal-to-noise ratio of the least squares fit used to determine the time derivative as \( \xi = \sigma_f/M_t \), where \( \sigma_f \) the fitting error due to shot noise and \( M_t \) the time derivative. If we estimate the fitting error as \( \sigma_f \sim L/(N_{pc}\sqrt{N_e}) \sim \log(L)/(L\sqrt{N_e}) \) (from the least squares derivation) and assume \( M_t \sim 1/L \), this gives \( \xi \sim \log(L)/(N_e)^{1/2} \). As a consequence, a constant signal-to-noise ratio can be obtained with a very weak dependence of \( N_e \) on \( L \) or \( N_{pc} \). This is consistent with the numerical observations made above.

Finally, the noise reduction achieved in our proposed method allows the use of much lower number of particles than in corresponding full PIC simulations with no perceptible noise increase or accuracy loss. This was illustrated by the plasma expansion simulations where the number of particles is reduced by 8 using the projective integration approach. This is possibly also due to the better scaling achieved by the use of a quiet start for very short runs. In this case, it contributes to the high speedup demonstrated in run 7, with a gain of almost 2 orders of magnitude in runtime. This finding illustrates a promising aspect of the application of EFPI algorithms based on PIC micro-simulators.

5. Conclusions

In this paper we have presented a novel equation-free projective integration method for the Vlasov-Poisson equation. At the coarse level, the ion distribution function is represented on a non-parametric wavelet basis. At the fine level, a particle-in-cell description is implemented for both ions and electrons. A lifting operator and a restriction operator are used to go back and forth consistently between these descriptions, assuming that the electrons are adiabatic. During each macro time-step, an explicit PIC code is stepped forward for a small number of microscopic steps to determine the rate of change in the macroscopic variables, which are then projected forward. The effects of statistical shot noise are controlled using both wavelet-based techniques, such as linear thresholding of coefficients, and more usual techniques in the EFPI framework such as coarsening in space and integration with the flow.
To validate the method and investigate its potential for simulating plasma systems, we applied it to two test cases. The first, a well-known problem of the nonlinear propagation and steepening of an ion acoustic wave, was proposed in [20] to test the EFREE method as a first attempt at implementing the projective integration framework to model kinetic plasma phenomena. We also proposed a new second test case, the expansion of an ion slab in a vacuum. These tests have confirmed that the method is stable and allows the use of time and space steps which are much larger than for the standard PIC method. Large speedups have been demonstrated while lifting numerous restrictions of the original EFREE method, most notably the assumption of a Maxwellian ion distribution function.

To further increase the accuracy and speedup of the method, the next step is to implement a non-linear thresholding algorithm to adaptively select the relevant wavelet coefficients for the coarse description of the ion distribution function. This will allow the exploitation of the sparsity of the discretization of smooth ion distribution functions in a wavelet basis and reduce the size of the coarse discretization. This will be essential in higher dimensions. This approach should also be combined with a framework for adapting the coarse resolution in time and space. To realize this, new a posteriori error estimators should be developed to measure deviations between the coarse model and the underlying multiscale plasma system. The numerous algorithms which have been developed for applying wavelets to signal analysis and adaptive denoising offer many interesting possibilities for this new application. These various possible research directions show that the method still has a lot of potential for improvement.

Ultimately, the goal will be to apply the projective integration paradigm to more challenging plasma problems for which direct simulations by ordinary explicit, implicit or hybrid methods is out of reach due to the need to resolve micro-physics with a complex influence on the macroscopic behavior, such as transport driven by micro-turbulence.

Acknowledgment

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References


