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Wavelet Techniques for Coarse Projective Integration in Multiscale Plasma Dynamics

G. Stantchev[1], A. Maluckov[2,3], M. Shay[4,1], J. Drake[1], W.Dorland[1], S.Ishiguro[2], M.Skoric[2]

[1] *Center for Multi-scale Plasma Dynamics, University of Maryland, USA*

[2] *National Institute for Fusion Science, Toki, Japan*

[3] *Faculty of Science, University of Nis, Serbia and Montenegro*

[4] *Department of Physics and Astronomy, University of Delaware, USA*

Introduction

Multi-scale problems such as magnetic reconnection and turbulence are notoriously hard to simulate because the physics of micro and macroscales are strongly linked. Over the past few years, a simulation framework called Equation-Free Projective Integration (EFPI) has been applied to a variety of multi-scale phenomena in engineering problems in which coarse-scale behavior can be obtained through short-time simulations within the fine-scale models (microscopic, stochastic etc) [1]. Recently, the first application of EFPI to a plasma system has been developed and implemented by Shay ([2]). He studies the propagation and steepening of a 1D ion acoustic wave using both a kinetic particle in cell (PIC) code as well as an EFPI code. He finds that the EFPI code reproduces the PIC code well, however differences arise due to physics assumptions made in the lifting part of the algorithm, specifically that the ion velocity probability density functions (PDF) remain Maxwellian and that the plasma remains quasineutral.

This paper discusses a generalization of Shay's projective integration scheme that removes the assumption on the velocity PDF. In particular, we propose a scheme that estimates the joint x-v phase space PDF using non-linear wavelet approximation. We use a small number of wavelet coefficients, which represent the coarse grained structure of the joint PDF, as the macroscopic observables of the evolving system. An alternative method for tracking of an arbitrary PDF has been proposed by Zou ([3]). They use projection of the inverse Cumulative Distribution Function onto an orthogonal polynomial basis (shifted Legendre polynomials) to obtain relevant EFPI quantities. We believe that wavelets, with their inherent multiresolution structure, and localized behaviour, are better suited for representing arbitrary PDF's in the context of EFPI for plasma dynamics simulations.

Wavelet Approximation Basics

Wavelets have been used in a vast number of application area but it was not until recent years that they have been applied statistics, in particular for density estimation (see for instance the

excellent monograph by Vidakovic ([4]). The basic idea is that for a function $f \in L_2(\mathbb{R})$, and a wavelet basis defined through generating functions ϕ and ψ, one writes an expansion:

$$f = \sum_{k\in\mathbb{Z}} c_{J_0,k}\phi_{J_0,k} + \sum_{j=J_0}^{\infty}\sum_{k\in\mathbb{Z}} d_{J_0,k}\psi_{j,k}$$

where the basis $\{\phi_{J_0,k}, \psi_{j,k}\}$ is obtained via translations and dilations of ϕ and ψ:

$$\phi_{J_0,k}(t) = 2^{J_0/2}\phi(2_0^J t - k), \quad \psi_{j,k}(t) = 2^{j/2}\psi(2^j t - k)$$

The sets $\{c_{J_0,k}\}$ and $\{d_{j,k}\}$ are known as *approximation* and *detail* coefficients respectively. When wavelet basis is orthonormal and f is a probability density function the wavelet coefficients are moments of basis functions:

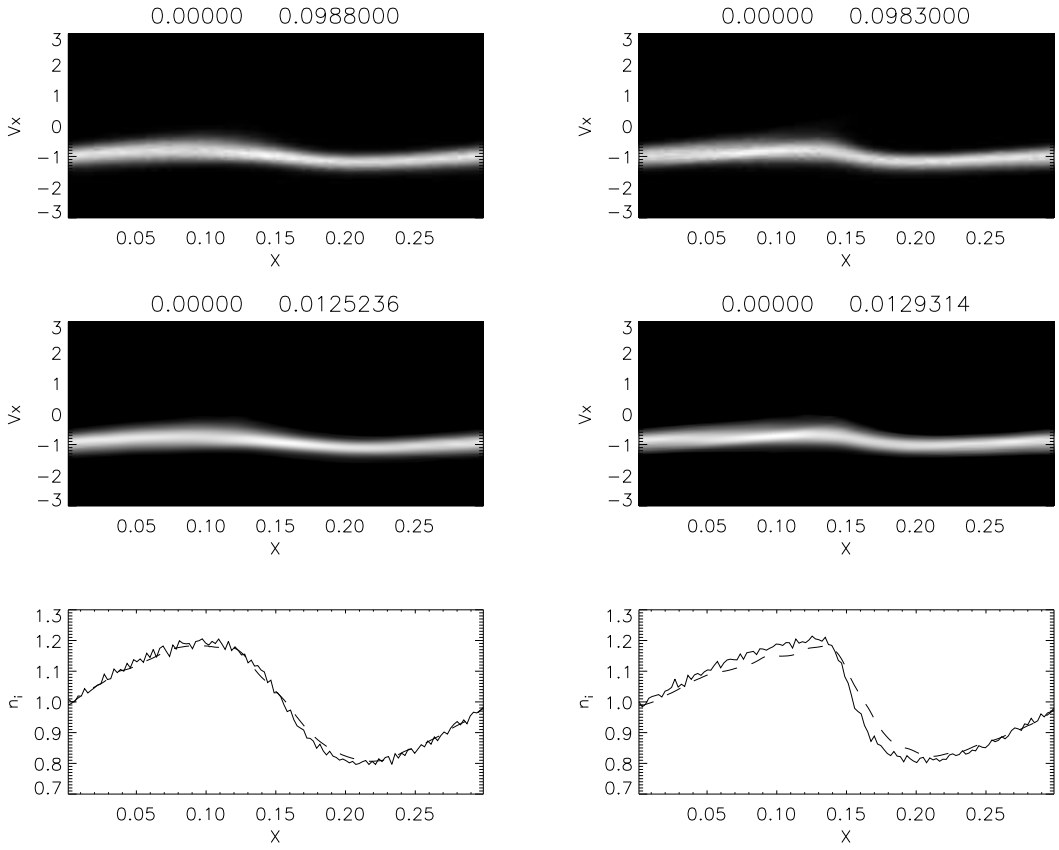
$$\begin{aligned} c_{J_0,k} &= \langle f, \phi_{J_0,k}\rangle = \int f\phi_{J_0,k} = \quad E[\phi_{J_0,k}] \\ d_{j,k} &= \langle f, \psi_{j,k}\rangle = \int f\phi_{j,k} = \quad\ E[\phi_{j,k}] \end{aligned} \tag{1}$$

A simple estimator of the expectation $E[X]$ of a random variable is the mean value of a set of observations $\{X_i\}$: $\hat{c}_{J_0,k} = (1/n)\sum_{i=1}^{n}\phi_{J_0,k}(X_i)$ and $\hat{d}_{j,k} = (1/n)\sum_{i=1}^{n}\psi_{j,k}(X_i)$. In practice, however, evaluating basis functions can be computationally expensive thus estimates for the wavelet coefficients are typically obtained through a Discrete Wavelet Transform (DWT) of a histogram of f sampled on an appropriate grid.

In order to eliminate noise and irrelevant small scale structures detail coefficient estimates are further thresholded and shrunk by a quantity that can be chosen adaptively for each level j of the wavelet decomposition. This reduces the number of non-zero estimation coefficients to about 98% of the original number. Thus after wavelet decomposition and thresholding the estimate $\hat{f}$ of the function f is associated with a vector of coefficients $\overrightarrow{C}_{\hat{f}} = \{\hat{c}_{J_0,k}, \hat{d}_{j,k}\}$.

Wavelet Based EFPI

The above approach is easily extended to functions defined over multidimensional domains. In particular in the case of the 1-d ion acoustic wave problem we track the *x*-*v* phase space dynamics via 2-d wavelet decomposition. The approximations coefficients along with the detail coefficients that remain after thresholding provide the set of macroscopic observables that are stepped forward during the projective integration step. These coefficients are responsible of the coarse (global) features of the density functions and they coherent structures that persist on the slower time scale. Currently we use simple linear least square fit to estimate the time derivative of each coefficient and then use the resulting set of linear polynomials to extrapolate further in time. At the end of a projection step we perform an inverse DWT to recover the predicted histogram of the density function which is then used to reload particles in the PIC simulator. Figure 1 shows the results of a EFPI simulation compared to those from the PIC code.



(a) after 1400 micro-time steps

(b) after 2800 micro-time steps

Figure 1: Top two rows: ion density distribution in *x*-*v* phase space from PIC and EFREE respectively. Bottom row: comparison plots of ion spatial density; PIC and EFREE results shown in solid and dashed line respectively

Double Layer Acoustic Problem

As a complementary effort we report on the ongoing activity aimed at exploring the feasibility of a different EFPI scheme, which we call “primal EFREE” (p-EFREE). The basic platform for micro-simulation is a standard version of 1D ES PIC code. The working hypothesis is that the ion motion is inherently coarse grained, as compared to electrons, to represent the macro-scale dynamics sufficiently well. Accordingly, we track individual ion orbits in time and simply extrapolate to project. In contrast to the original EFREE scheme, ions are not restricted via PDF or the corresponding moments; rather, we keep ions “as they are”, i.e., in theory, preserving kinetic ion effects. By inspecting ion orbits for an ensemble of test particles, we find that most of projected individual orbits agree reasonably well with the original PIC prediction. We note that, a typical coarse projection step. e.g. 100 times the micro-step is still close to the intrinsic ion-time step. We simply find a non-uniform ion density from projected ion orbits, and to lift

ions, we actually just restart ion motion. Further, we track electric potential and coarse grained average over ω_{pe} (which removes micro-scale electron dynamics) to extrapolate and project. Also, we do not use simplifying adiabatic approximation for electrons; instead, self-consistently calculate projected non-uniform electron density from the Poisson equation, using projected values of the potential and ion-density. By sampling electron phase space we find standard electron PDF in the velocity space; being rather smooth, it is easy to extrapolate and project. Finally, we lift electrons by using above two projected "marginal" PDF's in velocity and real space, respectively. While this work is in an early stage, some preliminary results are already motivating. While the projection step was modest (20) the actual agreement with full PIC is reasonable. We further point out that while in p-EFREE the total energy fluctuates close to the initial level, PIC simulations show standard numerical heating proportional to a number of time steps; perhaps, an inherent potential of such methods in large-scale plasma simulations.

References

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