Primal Macro-Projective Integration Method for Multi-Scale Plasma Simulation

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We discuss a simulation framework, called Equation-Free Projective Integration (EFPI), which can perform macro-simulations while still taking the effects of micro-scale physics into account. In particular, we propose a *primal*-EFPI scheme to simulate the ion sound wave paradigm, which includes nonlinear wave steepening and kinetic effects in a plasma.

Keywords: nonlinear plasmas, multi-scale simulation, equation free projective integration

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Multi-scale problems, such as magnetic reconnection and turbulence, are difficult to simulate because of the strongly interconnected physics of micro- and macro-scales, which basically defy direct computational schemes. In recent years, a novel simulation framework, Equation-Free Projective Integration (EFPI), has been proposed and applied to a variety of multi-scale phenomena in different fields, in which coarse-scale (macro) behavior can be realized through short-time simulations within fine-scale models (microscopic, stochastic, etc.) [1]. In EFPI, the simulation acts on both the scales. The macro-scale dynamics is determined by repeated forward extrapolation of coarse-scale estimates obtained from short micro-scale simulations.

Recently, Shay *et al.* made the first application of EFPI to plasmas [2]. This application studies the propagation and steepening of 1D ion sound waves using a particle-in-cell (PIC) code as a microscopic simulator. First, to initialize the PIC, the macro (coarse) variables are "lifted" to a fine microscopic representation. The PIC code is stepped forward for a short time, and kinetic results are restricted—smoothed back to macro (coarse) space. The time derivatives are estimated by numerical extrapolation, and coarse variables are projected in large steps. The process is then repeated. Originally in [2], the macro-step forward in time was performed using only the first three moments of the ion velocity probability density function (PDF). It is claimed that EFPI can reproduce PIC results, but large differences arise due to the physics assumptions made in the lifting algorithm (macro to micro). In particular, it was assumed that the ion PDF is Maxwellian, and that electrons are adiabatic. A recent suggestion [3] has been to generalize Shay's projective integration scheme [2] to remove the restriction on the velocity PDF. It was proposed to estimate the joint (x-v) phase space PDF with a non-linear wavelet approximation [3]. A limited number of wavelet coefficients, which represent the coarse grained structure of the joint PDF, are introduced as the macroscopic observables.

More recently, these authors proposed a new EFPI method, based on the marginal and conditional cumulative PDFs as macro-scale (coarse) observables, with the potential of representing nonlinear and kinetic plasmas, tested on the ion sound paradigm [4].

Here, as a complementary effort aimed at exploring the feasibility of the EFPI method, we implement an original scheme, called, *primal*-EFPI to account for nonlinear and kinetic plasma effects [5]. The basic platform for micro-simulation is a standard 1D Electrostatic PIC [6]. The working hypothesis is that the separation of scales allows us to assume that the ion dynamics is inherently coarse grained, or macroscopic, compared to electron micro-scale motion. Hence, individual ion orbits are tracked and extrapolated in time to make the projection. In contrast to the original EFPI [2], here, ions are not restricted via three PDF moments. Rather, ions are kept as they are, i.e., theoretically preserving nonlinear kinetic effects fully.

Indeed, by inspecting ion orbits for an ensemble of test particles, we found that most projected individual orbits agree well with the original PIC prediction. We also note that a typical coarse projection time step ($\Delta t_{\rm p}$) of, e.g., 100 times the micro-step (Δt), is still close to the intrinsic ion time step [2]. Further, we can find a non-uniform ion density from the projected ion orbits, and to lift ions, we actually just restart the ion motion. Next, we track the electric potential and coarse grain, i.e., the average over the electron plasma period ($2\pi/\omega_{\rm pe}$) to smooth micro-scale

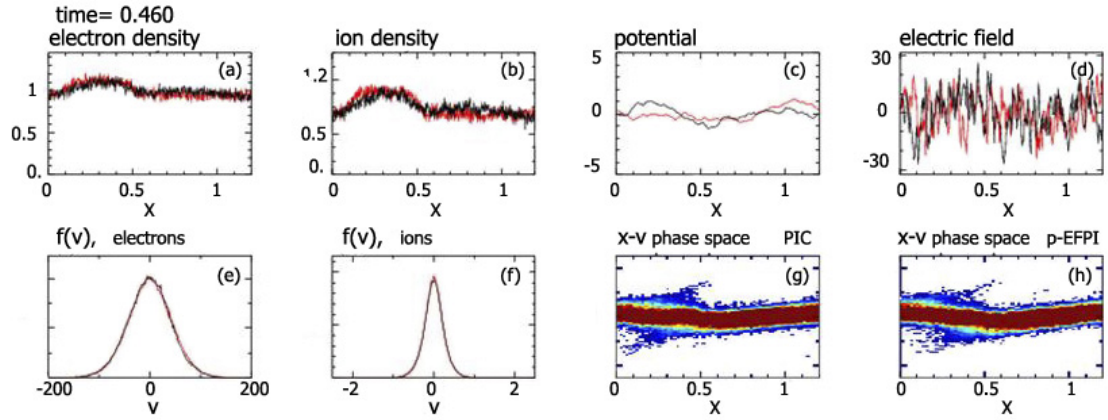

Fig. 1 Snapshots of (a) electron and (b) ion density, (c) potential, (d) electric field and (e) electron, (f) ion PDF, for PIC (red) and p-EFPI (black) at, $t = 0.46$; and ion phase space (g) PIC vs. (h) p-EFPI.

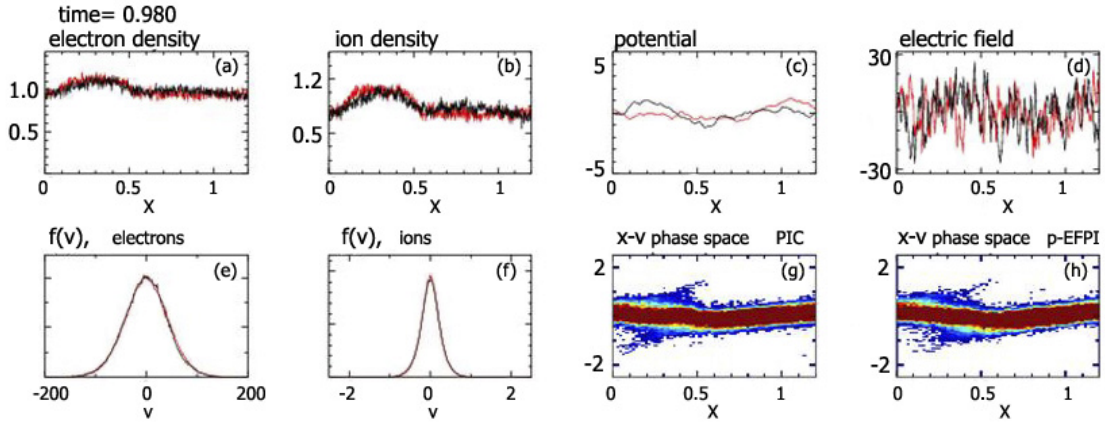

Fig. 2 Same snapshots as in Fig. 1, however, at time $t = 0.98$.

fluctuation to extrapolate and project. However, a simplifying (adiabatic) approximation for electrons is not used. Instead, we self-consistently solve for non-uniform electron density from the Poisson equation, and use corresponding projected values for potential and ion density. By sampling the electron phase space, we find the standard electron velocity PDF, which appears rather smooth and easy to interpolate and project. Finally, to lift electrons, we use two projected PDFs, called marginal DFs, representing the velocity and real space distributions (number density).

We performed a number of simulation runs within the same plasma variable ranges as in [2], by varying the other p-EFPI scheme parameters. Comparative snapshots at an earlier time $t = 0.46$ (in ion periods) are given in Fig. 1, to present the PIC data and the p-EFPI code results (red curve). Snapshots of the electron (1) and ion (2) density and PDFs, electric potential, and electric field at $t = 0.46$ are provided along with ion phase space plots, PIC versus p-EFPI (bottom right). As expected, a discrepancy appears in the potential and electric field (non-coarse, both macro- and micro-scale) as a phase mismatch, due to the interruptive nature of the p-EFPI simulation cycle. This stems from a difficulty in accurately reconstructing the phase relation in coherent particle dynamics, in particular, with intrinsically noisy PIC data. Our very recent optimization of the numerical scheme has improved the phase space matching. However, the smoothed variables, similar to particle density, PDFs, and even the ion phase space, compare well. Snapshots repeated at a later time, $t = 0.98$, shown in Fig. 2, show less agreement in the nonlinear kinetic regime. We also note that a difference in particle density defies simple electron adiabaticity. Finally, to check the important energy conservation of the scheme, Fig. 3 shows a plot of the comparative time evolution of the ES field energy, electron and ion kinetic and drift energies, and the total energy for PIC and p-EFPI, in total energy units. A phase-mismatch time lead in the ion wave kinetics compared to PIC is typically observed. While the p-EFPI projection step was modest (20-30Δt), the actual agreement with full PIC is reasonable, which gives a speedup factor of 2 in the 1D case, or

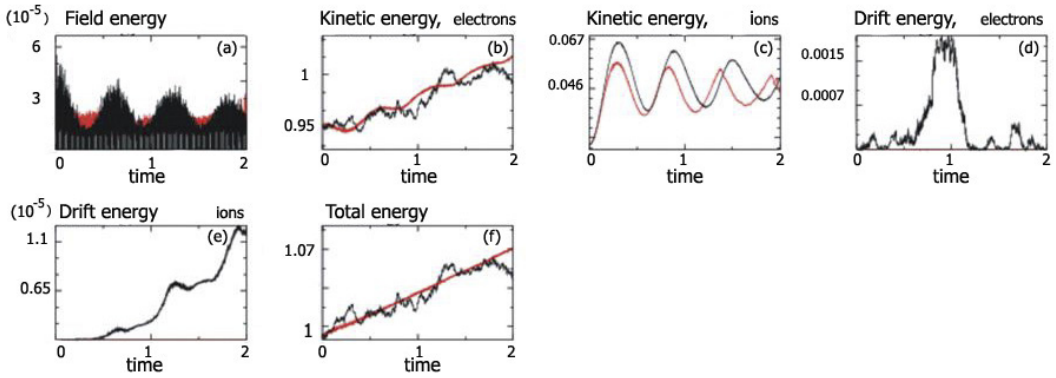

Fig. 3 Time evolution of field, particle, and total energies for PIC (red) and p-EFPI (black).

theoretically scales as 2^3 in a 3D problem.

For EFPI feasibility as a multi-scale code, the speedup depends on the smallest number of micro-steps (PIC) combined with the largest projection step possible. However, fundamental stability, as stated by the Courant condition, requires that $\Delta x/\Delta t > c_s$ for both micro- (PIC) and macro-projection grids, where c_s is the characteristic speed in a problem (here, the ion sound). Unexpectedly, it appears as a physical effect, even if no explicit macro-scale equation was solved [2, 4, 5]. For a large projection time step, it is necessary to change the fine (micro) to a coarse (macro) spatial grid. However, with p-EFPI, we maintained the original PIC fine resolution (512 points in space).

Although we are in an early stage, the preliminary results seem promising. We point out that, as opposed to PIC with standard numerical heating proportional to a number of time steps, in p-EFPI, the total energy fluctuated around the initial level. Some of the above ideas and methods concerning EFPI, in particular, those relating to reconstructing and interlinking between macro- and micro-scale dynamic models, could be relevant to other attempts to make efficient multi-scale plasma simulations.

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