Multi-scale simulation for plasma science

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Abstract. In order to perform a computer simulation of a large time and spatial scale system, such as a fusion plasma device and solar-terrestrial plasma, macro simulation model, where micro physics is modeled analytically or empirically, is usually used. However, kinetic effects such as wave-particle interaction play important roles in most of nonlinear plasma phenomena and result in anomalous behavior. This limits the applicability of macro simulation models. In a past few years several attempts have been performed to overcome this difficulty. Two types of multi-scale simulation method for nonlinear plasma science are presented. First one is the Micro-Macro Interconnected Simulation Method (MMIS), where micro model and macro model are connected dynamically through an interface [1]. Second one is the Equation Free Projective Integration Method (EFPI), where macro space and time scale simulation is performed by using only a micro simulator [2]. MMIS is useful for phenomena where a small scale event is concentrated in the small region. This is successfully applied to multi-scale simulations of magnetic reconnection [3], shock [4] and aurora formation [5]. MMIS needs a reliable macro simulation model. However, it is difficult to prove a reliability of macro model because of the so-called “closure problem”. EFPI does not use macro equation or model. 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. The EFPI was first

1. Introduction  
Currently, development of self-consistent simulation which covers large space and time scales is being performed in variety of fields. Full torus Magneto-hydrodynamic (MHD) simulation of a large scale fusion device became realistic. Here, micro physical quantity such as transport coefficient is modeled analytically or empirically. However, micro-scale kinetic effects such as wave-particle interaction play important roles in most of nonlinear plasma phenomena limiting the applicability of macro simulation models. Therefore the macro model cannot fully explain physical mechanisms and experimentally observed results. We have to develop new methods to describe observed plasma phenomena. In this paper we present two typical methodologies which try to perform multi-scale self-consistent simulation. First one is the Micro-Macro Interconnected Simulation Method (MMIS), where micro model and macro model are connected dynamically through an interface [1]. Second one is the Equation Free Projective Integration Method (EFPI), where macro space and time scale simulations are performed by using only a micro simulator [2]. MMIS is useful for phenomena where a small scale event is concentrated in the small region. This is successfully applied to multi-scale simulations of magnetic reconnection [3], shock [4] and aurora formation [5]. MMIS needs a reliable macro simulation model. However, it is difficult to prove a reliability of macro model because of the so-called “closure problem”. EFPI does not use macro equation or model. 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. The EFPI was first
time applied to the plasma phenomenon by Shay [6] who investigated the nonlinear ion acoustic wave propagation and steepening applying a Particle-in-cell (PIC) code as a micro simulator. First, to initialize the PIC, the macro 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 space. The time derivatives are estimated by numerical extrapolation, and coarse variables are projected in large steps. The process is repeated. 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, although important differences arise as a consequence of the assumptions proposed in the lifting procedure (from macro to micro scale). In particular, it was assumed that the ion PDF is Maxwellian, and that electrons are adiabatic. In this paper, we would like to explain the concept of EFPI and a primal-EFPI plasma simulation scheme to simulate the ion acoustic wave paradigm, which includes nonlinear wave steeping and kinetic effects in a plasma.

2. Micro-macro interconnected simulation method

Micro-macro interconnected simulation method (MMIS) has been proposed as a method for a variety of multi-scale problems. Here, we would like to present an application to magnetic reconnection. Magnetic reconnection is a typical multi-hierarchy phenomenon. When magnetic reconnection occurs, the field topology changes on a macroscopic scale and global plasma transport takes place. On the other hand, an electric resistivity controlled by a microscopic process is necessary as a trigger. Therefore, for complete understanding of magnetic reconnection, multi-hierarchy simulation model, which calculates both microscopic and macroscopic physics consistently and simultaneously, should be developed.

![Figure 1. Time flow of Micro-Macro Interconnected Simulation Model.](image)

In the multi-hierarchy structure of magnetic reconnection, the characteristic space-time scale changes with distance from the neutral sheet. Reconnection dynamics is controlled by the particle kinetic effects within the ion-meandering orbit scale \( l_{mi} \) while it can be expressed by an one-fluid model far from the neutral sheet.

Based on the above features, the domain decomposition method is employed. The domains differ in algorithm. Physics in the domain where microscopic kinetic effects play a crucial role is solved by particle-in-cell simulation method. This domain is called the PIC domain. On the other hand, dynamics on the periphery of the PIC domain is expressed by magneto hydrodynamics simulation method. We shall refer to this domain as the MHD domain. Between the PIC and MHD domains, an Interface domain with a finite width is inserted. The physics in the Interface domain is calculated by both the PIC and MHD algorithms. Macroscopic physical quantities in the Interface domain (for
instance, magnetic field and fluid velocities) are obtained by a hand-shake scheme, $Q_{\text{interface}} = aQ_{\text{MHD}} + (1-a)Q_{\text{PIC}}$, where $Q_{\text{MHD}}$ and $Q_{\text{PIC}}$ indicate the values of $Q$ calculated by the MHD and PIC algorithms, respectively. The parameter $a$ is a function of the coordinates. Individual particle velocities in the Interface domain are newly determined so as to satisfy the (shifted) Maxwellian using the obtained macroscopic quantities at every time step. The PIC and MHD domains can be smoothly interlocked via the Interface domain.

Time flow in the multi-hierarchy model is shown in Fig. 1. We employ multi-time scale scheme, where MHD and PIC domains have different time steps. Large time steps are for MHD model, and small ones are for PIC model. For advancing time from $t_1$ to $t_2$, PIC model receives interpolation values of data at $t_1$ and at $t_2$ from MHD model at every step. On the other hand, at $t_1$, MHD model gets PIC data averaged over several steps around $t_1$.

The following procedure indicates how time advances from $t_1$ to $t_2$. (1) At $t = t_1$, physical quantities of MHD and PIC exist. (2) MHD model sends MHD information at $t_1$, to PIC model. (3) PIC model advances to $t = t_1 + \delta t$, where $\delta t$ is time which correspond to several PIC steps. (4) PIC information averaged over the period form $t_1-\delta t$ to $t_1+\delta t$ is sent to MHD model. (5) MHD model goes ahead one step and reaches $t_2$. (6) PIC model receives MHD data at $t_1$ and at $t_2$. (7) PIC information from $t_1$ to $t_1 + \delta t$ which were obtained at (3) is removed. (8) PIC model advances to $t_2$. Figure 2 shows a schematic diagram of the multi-hierarchy model. The PIC domain covers the central region close to the neutral sheet, and the MHD domains are outside the PIC domain. The Interface domain is located between the PIC and MHD domains.

Before demonstrating MMIS of magnetic reconnection, some test problems are performed. The first test is the propagation of a linear Alfvén wave. Smooth wave propagation was observed [7, 8]. The second test is the plasma injection from the MHD domain to the PIC domain. A smooth and continuous plasma flow propagation is observed, as shown in Fig. 3[9].
Here, we present a multi-hierarchy simulation of magnetic reconnection [3]. The initial condition is given by an one-dimensional Harris-type equilibrium as $B_x(y) = B_0 \tanh(y/L)$ for the magnetic field, where $B_0$ is a constant and $L$ is the scale height along the $y$ axis. The system is periodic in the $x$ and $z$ directions and is free in the $y$ direction. An external electric field $E_{zd}(t)$ is applied at the entire outside boundary of the MHD domain. Plasmas are injected inward in the $y$ direction. The electric field $E_{zd}(t)$ in the MHD domain is programmed to evolve from zero to a constant value $E_0$. Figure 4 displays the magnetic lines of force (left panel) and fluid velocity vectors (right panel) in the $(x,y)$ plane in the whole multi-hierarchy simulation domain at $\omega_{ce} t = 1323$. The lines of force and the fluid velocity are smoothly connected between the MHD and PIC domains via the Interface domain. An X point exists at the center. We can see that inflows come inward from the MHD domain and drive magnetic reconnection at the center of the PIC domain.

**Figure 3.** Time evolution of plasma density profile. Plasmas are injected from the MHD domains to the PIC domain.
3. Equation-free projective integration method

The so-called Equation-free-projective integration (EFPI) method has been proposed and applied to a variety of multi-scale phenomena in engineering problems in which coarse-scale behaviour can be obtained through short-time simulations within the fine-scale models [2]. In EFPI, the simulation acts on two scales. The macro scale dynamics is determined by repeatedly extrapolating forward coarse scale estimates obtained from the short micro scale simulations. In the EFPI framework, the main tool that allows the performance of numerical tasks at the macroscopic level using the microscopic simulation codes is the so-called coarse time-stepper. It consists of three parts: lifting (mapping from coarse-macroscopic to fine-microscopic level), short time micro calculations around which the macroscopic calculations are wrapped and restriction (mapping from fine-micro scale to macroscopic level). The coarse time stepper is combined with time projection at macroscopic level, i.e. time projection of the coarse observables on the macroscopic scale. This structure is schematically presented in Fig. 5.
First attempt to apply EFPI to plasma physics was performed by Shay et al., in the context of the ion acoustic wave paradigm [6]. In their EFPI scheme the electrons are assumed to be adiabatic, both the electron and ion velocity distributions are assumed to be the shifted Maxwellian and quasi-neutrality is proposed. The results of EFPI calculations are discussed with respect to the full micro-PIC simulations. At the first step the coarse observables are determined. First three moments: ion density, ion velocity and pressure are taken as the ‘active’ coarse observables, i.e. those macro variables which are directly computed forward in time. On the other hand, the electron density, electron velocity and electric field are taken as the ‘passive’ coarse variables, i.e. variables which are not calculated directly but from active macro observables. These observables are defined on the coarse mesh by the linear interpolation procedure. The micro quantities, the ion and electron positions are obtained through the lifting from corresponding densities and the ion and electron velocities are lifted from corresponding velocity distributions (approximated by the shifted Maxwellian). The PIC solver is then applied for the short time in order to ensure the system to stay near the so-called slow manifold. In other words, the implementation of the micro solver has to ensure the reconstruction of the values of the macro quantities which would be obtained under the same conditions but using only the micro solver. The coarse-macro observables are generated by the reversed operation – restriction. After the linear interpolation they are projected in time. Approximately time interval for the micro calculation is around 20 micro time steps and the macro time step is two order of magnitude larger than the micro time step. However, above procedure basically neglects kinetic effects in a plasma. The problems which appear in the reconstruction of the ion acoustic wave when the wave steepening is noticed were related to the particle trapping, non-Maxwellian features are violating quasi-neutrality. Instead of the moments, the wavelet technique for reconstructing the particle probability distribution function was indicated as a possible solution [10]. Furthermore, schemes to test an applicability of the EFPI framework, attempting to include the correlation effects in the nonlinear ion acoustic wave paradigm was undertaken by some of these authors [11]. That approach uses the marginal and conditional cumulative particle distribution functions in the ion phase space as the macro scale observables, which results in a better agreement with a fully kinetic electrostatic PIC solver.

Figure 5. Structure of Equation Free Projective Integration (EFPI) method [13].
Here, as an illustration 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 [12, 13]. The basic platform for micro-simulation is the standard electrostatic PIC. Still, 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, 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 (\(\Delta t_p\)) of, e.g., 100 times the micro-step (\(\Delta t\)), is still close to the intrinsic ion time step. Further, we find a non-uniform ion density from the projected ion orbits, while 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 (\(2\pi/\omega_{pe}\)) to smooth micro-scale fluctuations in order to extrapolate and project. Moreover, a simplifying (adiabatic) approximation for

![Figure 6. Structure of primal Equation Free Projective Integration Plasma Simulation [13].](image)

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![Figure 7. Snapshots of (a) electron, (b) ion density, (c) electric potential, (d) electric field and (e) electron PDF, for PIC (red) and p-EFPI (black) at \(t = 0.46\); and ion phase space, PIC (g) versus p-EFPI[12].](image)

**Figure 7.** Snapshots of (a) electron, (b) ion density, (c) electric potential, (d) electric field and (e) electron PDF, for PIC (red) and p-EFPI (black) at \(t = 0.46\); and ion phase space, PIC (g) versus p-EFPI[12].
electrons is not used. Instead, we self-consistently solve for non-uniform electron density from the Poisson equation, and user 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 [6], by varying the other p-EFPI scheme parameters. Comparative snapshots at an earlier time $t = 0.46$ (in ion periods) are given in Fig. 7, 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. 8, show less agreement in the nonlinear kinetic region. We also note that a difference in particle density defies simple electron adiabaticity.

Finally, to check the important energy conservation of the scheme, Figure 9 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 (20-30 $\Delta t$), the actual agreement with full PIC is reasonable, which gives a speed-up factor of 2 in the 1D case. For EFPI feasibility as a multi-scale code, the speed-up 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 acoustic wave). Unexpectedly, this was found to appear as a physical effect, even if no explicit macro-scale equation was solved. Accordingly, 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 grid points in space). Although we are in an early stage, the preliminary results seem to be promising.
4. Summary

Development of multi-scale simulation methods is presently among hot topics in a variety of fields. In this paper, we show two typical methodologies, i.e. Micro-Macro Interlocked Simulation Method (MMIS) and Equation Free Projective Integration Method (EFPI). These methods are under construction and we hope that these activity bridge to future holistic self-consistent simulation of fusion plasma device.

Acknowledgements

Stimulated discussions with T. Sato, K. Kusano, T. Sugiyama, and G. Stantchev are gratefully acknowledged. This study was performed under the auspices of and with the support of the National Institute of Natural Science (NINS) – National Institute for Fusion Science (NIFS) Collaborative Research Project (NIFS05KEIN0041, NIFS06KEIN0041, NIFS08KTAL015, NIFS09KNXN174, NIFS10KEIN1201) and NIFS Collaborative Program (NIFS04KDAT007, NIFS05KDAT007, NIFS07KDAN001). Partial support under the Ministry for Science and Technology of Serbia, Project No. 141034 is acknowledged.

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Figure 9. Time evolution of electric field, particle, and total energies for PIC (red) and p-EFPI (black) [12].