Dynamic Mode Decomposition Reduced-Order Models for Multiscale Kinetic Plasma Analysis

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***Abstract*—We demonstrate the efficacy of dynamic mode decomposition (DMD) based reduced-order model (ROM) in characterizing the transient behavior of full-order kinetic plasma simulation. The full-order kinetic plasma model makes use of the finite-element time-domain (FETD) based electromagnetic particle-in-cell (EM-PIC) algorithm. We apply the suggested reduced-order method for the case of an expanding plasma ball and study the effect of DMD reconstructed self fields on the particle dynamics in transient region. Such analysis is highly desirable for understanding underlying physics of complex plasmas as well as for reducing computation cost of high-fidelity plasma simulations.**

I. Introduction

The nonlinear nature of existing fluid-based and kinetic plasma models not only makes it difficult to comprehend the underlying multiscale physics, but also act as bottleneck for model based control techniques such as model predictive control (MPC) [1]. In recent years several studies have revealed that for a vast majority of scenarios involving plasma simulations, the total energy can be modelled using few (less than ten) spatio-temporal coherent features [2], [3]. This showcases the need for reduced order methods able to extract the key underlying spatio-temporal features from high fidelity plasma simulations. Dynamic Mode Decomposition (DMD) is a data-driven reduced order method which became popular since its introduction [4] for its “equation-free” nature. References [5], [6] have demonstrated DMD’s effectiveness in extracting low dimensional features from magnetohydrodynamics (MHD) simulations. Our preliminary work [7] shows promise of such method for collisionless kinetic plasma models based on electromagnetic particle-in-cell (EM-PIC) simulations. However, the effect of DMD predicted fields on particle (electron) behavior in the transient region for PIC algorithms is yet to be explored. Transient plasma analysis can be useful for several physical scenarios of interest [8], [9]. In this paper we take a simple case of expanding plasma ball and observe the effect of DMD reconstructed self fields on particle dynamics in the transient state.

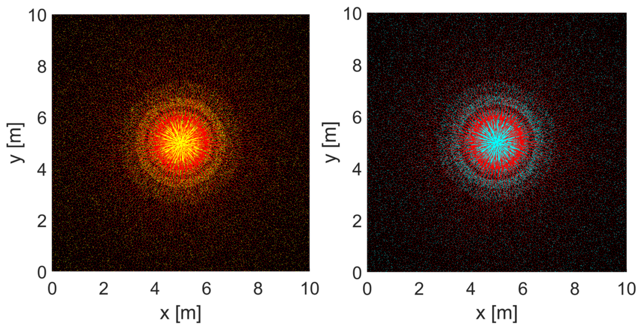
II. Theoretical Background

The EM-PIC algorithm updates the self electric and magnetic fields on a discrete spatial grid via Maxwell’s equations and implements the plasma particle kinetics through four cyclic stages, 1) field-update, 2) gather, 3) particle-pusher, 4) scatter [10], [11].

Using the harvested data from the EM-PIC simulation, DMD produces a set of DMD modes ($\Phi_k,\ k = 1, 2,\ \ldots,\ r$) and corresponding DMD frequencies (ω_k) to capture the spatio-temporal variation of the system [12], [13]. We will give a brief overview of the standard DMD algorithm [13] using the degree of freedom (DoF) [10] of self electric field (e) as the quantity of interest. The first step is the data harvesting step where we collect $(m + 1)$ snapshots of $\mathbf{e}$ at different time instants inside a specified time window, which we refer to as the harvesting region/window or the DMD window. We form the snapshot matrix ($X = [\mathbf{e}^{(n_0)}\ \mathbf{e}^{(n_0+\Delta n)}\ \ldots\ \mathbf{e}^{(n_0+(m-1)\Delta n)}]$) and the shifted snapshot matrix ($X' = [\mathbf{e}^{(n_0+\Delta n)}\ \mathbf{e}^{(n_0+2\Delta n)}\ \ldots\ \mathbf{e}^{(n_0+m\Delta n)}]$), where $\mathbf{e}^{(n)} = [e_1^{(n)}\ e_2^{(n)}\ \ldots\ e_{N_1}^{(n)}]^T$, $e_j^{(n)}$ being the DoF of self electric field at j^{th} edge at n^{th} time step. N_1 is the number of mesh edges in the discrete spatial mesh and Δn is the number of time steps between two consecutive snapshots. DMD assumes $X' \approx AX$. Next we perform singular value decomposition (SVD) of X producing $X = U\Sigma V^*$. Performing order reduction, we choose only the first r significant columns of U, r rows and columns for Σ and r columns for V, giving us U_r, Σ_r and V_r respectively. The low-dimensional projection of A is given by $\tilde{A} = U_r^* X' V_r \Sigma_r^{-1}$, the eigendecomposition of which generates $\tilde{A}W = W\Lambda$. The DMD modes are essentially the columns of $\mathbf{\Phi}$, where $\mathbf{\Phi} = X' V_r \Sigma_r^{-1} W$. The corresponding DMD frequencies are given as $\omega_k = ln(\lambda_k)/(\Delta n \Delta_t)$, where λ_k are the elements of the diagonal matrix Λ and Δ_t is the time step interval. The final reconstruction is given by $\mathbf{e}(t) = \sum_{k=1}^{r} \vartheta_k \Phi_k e^{\omega_k (t-t_0)}$, where $t_0 = n_0 \Delta_t$ and ϑ_k are the scaling factors which are calculated by solving an optimization problem [14]. For better accuracy we use stacked snapshot matrices. Further details can be found in [12].

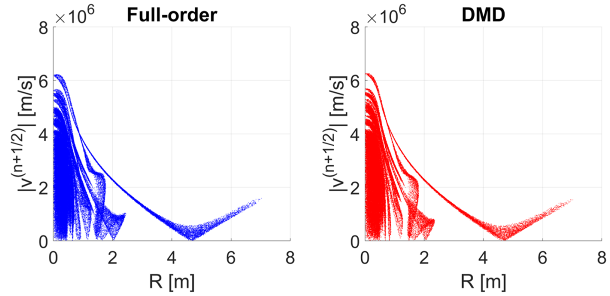
III. Numerical Experiment and Discussion

We consider a two dimensional (2-D) expanding plasma ball in a square cavity surrounded by perfect magnetic conductor (PMC) walls. The solution domain with dimension $L \times L$ with $L = 10$ m (see Fig. 1a), is discretized by an unstructured grid having $N_0 = 8037$ nodes, $N_1 = 23797$ edges and $N_2 = 15761$ triangular cells. Superparticles are initially placed within a circle of radius 0.5 m at the center of the cavity. Initially the

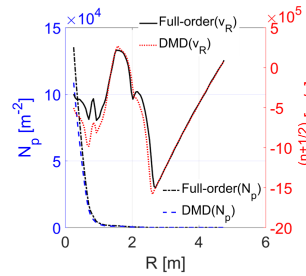


(a) Full-order (b) With DMD predicted self fields

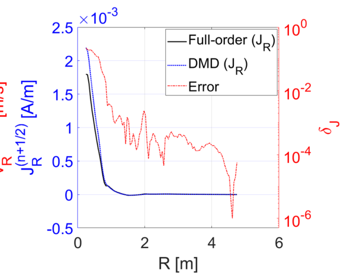
Fig. 1. Snapshot of the plasma ball expansion at $n = 25000$. Yellow (full-order) and cyan (DMD) dots represent the superparticles. Red arrows for both cases show the self electric field lines.



(a)



(b)



(c)

Fig. 2. Particle dynamics comparison between full-order EM-PIC and DMD at $n = 25000$. (a) Phase-space plot comparison wrt. absolute velocity. (b) Comparison of radial particle density and average radial velocity. (c) Average radial current density comparison. The relative error $\delta_J = |J^{(n+1/2)}_{R,DMD}(R) - J^{(n+1/2)}_{R,full}(R)|/\max_R |J^{(n+1/2)}_{R,full}|$.

plasma ball is assumed to be neutral, with each electron-ion pair located at the exact same position. Superparticles representing electrons are then provided with initial radial velocity following a Maxwellian distribution and they are absorbed after they hit the outer boundary. Each superparticle represents 2×10^5 electrons. The time step interval $\Delta_t = 0.1$ ns. We sample the data at every 500^{th} time step until $n = 500000$.

The plasma ball initially expands and then contracts due to the self-field interaction, causing oscillations which eventually dies down and the superparticles attain equilibrium producing a steady state self-field configuration. We are interested in observing the effect of DMD predicted self-fields on the particle behavior, namely the phase-space plot, average radial velocity (v_R), radial particle density (N_p) and average current density (J_R) during this transient regime. The DMD window spans from $n = 500(n_0)$ to $n = 50000$ with $\Delta n = 1000$. We perform DMD on both DoF of self electric field (e) and self magnetic field (b). We choose $r = 19$ and 1 leading to 11 and 1 DMD modes for $\mathbf{e}$ and $\mathbf{b}$ respectively. We replace the self field values in the field update stage with DMD-reconstructed ones $\mathbf{e}, \mathbf{b}$ and carry out the gather and particle-pusher stage to observe the effect on superparticles. Fig. 2a shows similarity between full-order and DMD predicted phase-space plot. This is also reflected in the radial (R) variation of N_p, v_R (Fig. 2b) and J_R (Fig. 2c), (calculated on $[R-\epsilon, R+\epsilon]$). Overall, the particle behavior predicted by DMD reconstructed self-fields shows good agreement with full-order EM-PIC simulation.

ACKNOWLEDGEMENT

This work was supported in part by DTRA grant HDTRA 1-18-1-0050 and OSC grant PAS-0110.

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