Model Order Reduction of Electromagnetic Particle-in-Cell Kinetic Plasma Simulations via Proper Orthogonal Decomposition

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Abstract—The Proper Orthogonal Decomposition technique is applied to a finite-element time-domain particle-in-cell algorithm for the simulation of kinetic plasmas, resulting in a reduced-order system. The reduced model is tested with representative examples involving an accelerated electron beam and a plasma ball expansion, and compared with full-order simulations. The strengths and weakness of this type of model order reduction when applied to particle-in-cell algorithms are discussed through the analysis of the results. In particular, the method allows for a major reduction in the field degrees of freedom necessary to capture the relevant physics, but it can also lead to spurious results if proper care is not taken when assembling the reduced order system.

Index Terms—Maxwell-Vlasov equations, model order reduction, particle-in-cell algorithm, plasma.

I. INTRODUCTION

Particle-in-Cell (PIC) algorithms have been widely used over the years for problems involving kinetic plasmas, see e.g [1]–[5] for general overviews and [6]–[14] for a more comprehensive list of references. However, PIC algorithms are computationally very demanding. Model Order Reduction (MOR) is a set of useful techniques aimed at reducing resource costs in computational simulations by lowering the order (dimension) of the state space associated with the numerical model, i.e., the number of degrees of freedom necessary to compute the solution to the problem at a desired accuracy level. One such MOR technique is the Proper Orthogonal Decomposition (POD), alternatively called Karhunen-Loève Decomposition (KLD), Principal Component Analysis (PCA), or Singular Value Decomposition (SVD) depending on application and mathematical interpretation [15]–[18]. The POD has been successfully employed in fluid dynamics applications [19]–[22] among other areas [23] including electromagnetic (EM) simulations [24]–[26], though it has not been applied to PIC-based EM simulations involving charged particles. In this work the POD is applied to a finite-element time-domain (FETD) PIC algorithm for consistently solving the Maxwell-Vlasov equations governing the interaction of EM fields and collisionless charged particle (plasma) systems. Two important applications of MOR are to extrapolate data from a “short” training period to future states or to provide a low-cost interpolation over a parametric input space (parameter sweep). In this work, the focus is given to the former application. The remainder of this work is organized as follows. Section II presents an overview of the FETD-PIC algorithm. Section III introduces the POD method and applies it to the algorithm presented in the previous section. Section IV provides numerical experiments to verify the applicability of the reduced-order model. Section V provides concluding remarks.

II. FETD-PIC ALGORITHM

The present FETD-PIC algorithm consists of using an irregular (unstructured) computational mesh to capture field dynamics and using computational particles or “super-particles” within the computational domain to simulate the Maxwell-Vlasov equations [13], [27]. The combined field-particle system is evolved in time through repetition of four update steps at each time-step: field update, field gather, particle update and particle scatter. In the field update step, the discrete representations degrees of freedom of the EM field are updated on the mesh. In the gather step, ambient field values are calculated at each particle location via a Whitney-form-based interpolation from the discrete field degrees of freedom [27]–[32]. In the particle update step, positions and velocities of all superparticles in the domain are accelerated (“pushed”) according to the fields acting on them via the Lorentz force law. Finally, in the particle scatter step the electric currents due to the particles’ movement and charges due to their new positions are transferred back to edges and nodes, respectively, of the mesh. One key feature of the present FETD-PIC algorithm is that it yields charge and energy conservation from first principles [13], [27]. This feature has eluded most prior FE-based PIC algorithms on irregular meshes, with some notable exceptions [10], [11]. Each of the steps is briefly outlined next.

A. Field Update

Using the exterior calculus of differential forms, the time-dependent Maxwell’s curl equations can be consistently discretized on simplicial (triangular or tetrahedral) meshes [27]–[39]. The fundamentals to obtain the FETD field update...
scheme are briefly described here. In the language of differential forms, and using the same notation as [27], Maxwell’s curl equations are written as

\[ \frac{\partial}{\partial t} \mathcal{B} = -d \mathcal{E}, \]  

\[ \frac{\partial}{\partial t} (*\mathcal{E}) = d (*_{\mu-1} \mathcal{B}) - \mathcal{J}, \]  

where \( \mathcal{E} \) is the electric field intensity 1-form, \( \mathcal{B} \) is the magnetic flux density 2-form, \( \mathcal{J} \) is the electric current density 2-form, \( d \) is the exterior derivative and \( * \) and \( *_{\mu-1} \) are Hodge operators that incorporate the permittivity and permeability of the medium, respectively. Explicit expressions for the matrices that discretize \( * \) and \( *_{\mu-1} \) are provided in (4) below.

The continuum quantities can be projected onto the discrete degrees of freedom (DoFs) in the primal mesh (i.e. the finite element mesh) by using a Whitney form expansion viz. [13], [27], [37]

\[ \mathcal{E}(t, \vec{r}) = \sum_{j=1}^{N_1} e_j(t) \, w_j^{(1)}(\vec{r}), \]  

\[ \mathcal{B}(t, \vec{r}) = \sum_{k=1}^{N_2} b_k(t) \, w_k^{(2)}(\vec{r}), \]  

\[ *\mathcal{J}(t, \vec{r}) = \sum_{j=1}^{N_1} i_j(t) \, w_j^{(1)}(\vec{r}), \]

where \( N_1 \) is the number of 1-dimensional simplices (edges) and \( N_2 \) is the number of 2-dimensional simplices (faces) on the mesh. \( w_j^{(1)} \) represents a Whitney 1-form, \( w_k^{(2)} \) represents a Whitney 2-form, \( e_j(t) \), \( b_k(t) \) and \( i_j(t) \) are the discrete degrees of freedom for the electric field, magnetic flux and Hodge dual of the current density respectively. The time and space dependencies are left explicit to clearly indicate that the spatial interpolation is accomplished by the Whitney forms and the DoFs are time-dependent expansion coefficients.

Applying the discretization (2) into (1) and using a leapfrog time integration scheme, a finite-dimensional system projection can be written as [13], [27], [37]

\[ b^{n+\frac{1}{2}} = b^{n-\frac{1}{2}} - \Delta t \, [C] \cdot e^n, \]  

\[ [\star_e] \cdot e^{n+1} = [\star_e] \cdot e^n + \Delta t \left( [\star_{\mu-1}] \cdot b^{n+\frac{1}{2}} - i^{n+\frac{1}{2}} \right), \]

where \( e = [e_1, e_2, ..., e_{N_1}]^T \), \( b = [b_1, b_2, ..., b_{N_2}]^T \), \( i = [i_1, i_2, ..., i_{N_1}]^T \). The superscripts denote the time-step at which quantities are evaluated, \( \Delta t \) is the time-step interval, \( [C] \) and its transpose \( [C]^T \) are metric-free incidence matrices that encode the discrete representation of the curl operator in the primal and dual meshes [13], [32], respectively, and \( [\star_e] \) and \( [\star_{\mu-1}] \) are matrix representations of the Hodge operators

\[ * \] and \( *_{\mu-1} \), respectively, obtained by Galerkin projection as [13], [27], [37]

\[ [\star_e]_{j,j} = \int_{\Omega} \frac{w_j^{(1)} \wedge (\star_e w_j^{(1)})}{\epsilon} = \int_{\Omega} \Omega \frac{w_j^{(1)} \wedge (\star w_j^{(1)})}{\epsilon}, \]  

\[ [\star_{\mu-1}]_{K,k} = \int_{\Omega} \frac{w_k^{(2)} \wedge (\star_{\mu-1} w_k^{(2)})}{\mu} = \int_{\Omega} \Omega \frac{w_k^{(2)} \wedge (\star w_k^{(2)})}{\mu}, \]

where \( \Omega \) is the domain problem. Because Whitney \( p \)-forms have compact support, the integrals above need to be carried only on the intersection of their support.

The linear solve in (3b) can be obviated by application of a sparse approximate inverse (SPAD) [37], [38], which yields an approximate inverse of \( [\star_e] \) denoted by \( [\star_e]^{-1}_{\text{SPAD}} \) with an enforced sparsity pattern \( \text{SP} \left( [\star_e]^{-1}_{\text{SPAD}} \right) = \text{SP} \left( [\star_e]^{-1} \right) \), where \( \text{SP} ([A]) \) denotes the sparsity pattern of \([A]\). This approximation allows for explicit time-stepping with a tradeoff between sparsity and accuracy that is tunable by the choice of exponent \( k \) [37].

B. Field Gather

The field gather step consists of evaluating the electric field intensity \( \mathcal{E} \) and magnetic flux density \( \mathcal{B} \) at each super-particle position. Interpolated Maxwell fields at the individual particle location are given by evaluation of (2a) and (2b). The vector proxies for these quantities can be written as

\[ \tilde{E}^n_p = \tilde{E} (n \Delta t, r^n_p), \]

\[ \tilde{B}^{n+\frac{1}{2}}_p = \tilde{B} \left( (n+\frac{1}{2}) \Delta t, r^{n+\frac{1}{2}}_p \right), \]

where \( r^n_p \) is the position of the \( p \)-th particle at the \( n \)-th time step.

C. Particle Update

In the non-relativistic regime, with the ambient field values obtained from the previous step, the particles themselves are updated by solving the Lorentz force and Newton’s law of motion

\[ \frac{\partial}{\partial t} \tilde{v}_p = \frac{q_p}{m_p} \left( \tilde{E}(t, \vec{r}_p) + \vec{v}_p \tilde{B}(t, \vec{r}_p) \right), \]

\[ \frac{\partial}{\partial t} \vec{r}_p = \vec{v}_p, \]

where \( q_p \), \( m_p \), and \( \vec{v}_p \) are charge, mass, and velocity, respectively, for the \( p \)-th particle.

The discretized equations for the particle update can be written, after some algebraic manipulations, as [27]

\[ r^{*}_{n+1} = r^n_p + \Delta t \vec{v}_p^{n+\frac{1}{2}}, \]

\[ \vec{v}_p^{n+\frac{1}{2}} = [N]^{-1} \cdot [N]^T \cdot \vec{v}_p^{n-\frac{1}{2}} + \frac{q_p \Delta t}{m_p} \tilde{E}^n_p, \]

where

\[ [N] = \left[ \begin{array}{cc} 1 & -\frac{q_p \Delta t}{2m_p} B_{p,z}^n \\frac{q_p \Delta t}{2m_p} B_{p,z}^n \end{array} \right], \]

\[ \tilde{B}_p^{\frac{1}{2}} = \frac{1}{2} \left( \tilde{B}_p^{n+\frac{1}{2}} + \tilde{B}_p^{n-\frac{1}{2}} \right). \]
D. Particle Scatter

In the scatter step, the motion of each charged-particle during the time-interval $\Delta t$ is converted back to the electric current density on the mesh for use in the subsequent field-update step. Discrete representation of the scatter current at the $j$th term is defined by [27],

$$i_j = \sum_{p=1}^{N_p} q_p \Delta L_p \int u^{(1)}_p \cdot \vec{d}L_p, \quad (9)$$

where the first integral is written in the language of differential forms and the second integral is its vector proxy representation. Here, $\vec{d}L_p = \vec{r}^{(1)}_p - \vec{r}^{(0)}_p$ is the $p$th particle’s trajectory and $\hat{W}^{(1)}$ is the vector proxy of the Whitney 1-form.

III. POD APPLIED TO THE FETD-PIC SCHEME

POD-based methods require sampled data-points from the quantity of interest [15], [17], which can be obtained from a regular FETD-PIC simulation through the construction of a “snapshot” matrix that encodes the spatial and temporal variations of said quantity. For the FETD-PIC scheme, both electric field intensity and magnetic flux density are quantities of interest and have separate numerical DoFs, so two snapshot matrices are required for application of POD, one for $E$ and another for $B$. Let $u$ denote either 1-D array of DoFs, i.e., $u^n = e^n$ or $b^{n-\frac{1}{2}}$. The snapshot matrix for $u$ with $l$ entries is constructed by harvesting the values of all DoFs of the transient solution at specific sampling points $n_i, i \in \{1, 2, ..., l\}$ and arranging them side-by-side so that $[A_u]_{ij} = u^n_i$, i.e.,

$$[A_u] = \begin{bmatrix} u^{n_1}_1 & u^{n_2}_1 & \cdots & u^{n_l}_1 \\ u^{n_1}_2 & u^{n_2}_2 & \cdots & u^{n_l}_2 \\ \vdots & \vdots & \ddots & \vdots \\ u^{n_1}_{N_{DoF}}, & u^{n_2}_{N_{DoF}}, & \cdots & u^{n_l}_{N_{DoF}} \end{bmatrix}, \quad (10)$$

where $N_{DoF}$ is the size of the array of DoFs for $u$ ($N_{DoF,E} = N_1$ and $N_{DoF,B} = N_2$). For simplicity, the sampling points are chosen to be equidistant in this work.

The snapshot matrices can be decomposed via singular value decomposition (SVD), viz. [15]

$$[A_u] = [U_u] \cdot [\Sigma_u] \cdot [V_u]^T, \quad (11)$$

where $[U_u]$ and $[V_u]$ are unitary matrices with sizes $N_{DoF,u} \times N_{DoF,u}$ and $l \times l$, respectively, and $[\Sigma_u]$ is a rectangular diagonal matrix with main diagonal elements containing the singular values $\sigma_{u,i}$ of $[A_u]$ in descending order. The columns of $[U_u]$ form a set of orthonormal vectors $\{\psi_{u,1}, \psi_{u,2}, \cdots, \psi_{u,N_{DoF,u}}\}$ that can be regarded as a basis for the spatial dynamics (note that these are not necessarily the eigenmodes of the problem), while the columns of $[V_u]$ form a set of orthonormal vectors $\{\phi_{u,1}, \phi_{u,2}, \cdots, \phi_{u,l}\}$ that can be regarded as a basis for the temporal dynamics [18], [40]. Generally speaking, the original transient simulation can be reconstructed under acceptable accuracy by using only a small number of modes associated with the dominant singular values. The number of such dominant modes $d_u$ can be determined through an appropriate error measure [25], [26].

In this work, the error measure used is as follows: let $\sigma_{u}$ be the vector of singular values and $\sigma_{u}^{*}$ be the vector of singular values up to the chosen number of reduced modes $d_u \leq r_u$. Then the associated normalized $p$-norm error between the original system captured by the snapshots and the reduced system with $d_u$ modes is

$$\epsilon_p (d_u) = \left\| \frac{\sigma_{u}^{*}}{\|\sigma_{u}\|_p} \right\|_p = \left( \sum_{i=d_u+1}^{l} \left( \frac{\sigma_{u,i}}{\sum_{j}^{p} (\sigma_{u,j})^{p}} \right)^{1/p} \right)^{1/p}, \quad (12)$$

which can then be evaluated with respect to some criterion or specification. Then, the resulting POD basis vectors for the shrunk dimension $d_u$ is the set $\{\Psi_{u,i}\}_{i=1}^{d_u}$ or, in matrix form, $[\Psi_{u}]$ with size $N_{DoF,u} \times d_u$. The field update based on the reduced POD basis set can now be obtained via Galerkin projection. Replacing the original DoFs $e^n$ and $b^{n-\frac{1}{2}}$ by

$$e^n \approx [\Psi_{e}] \cdot \alpha_{e}^n, \quad (13a)$$

$$b^{n-\frac{1}{2}} \approx [\Psi_{b}] \cdot \alpha_{b}^{n-\frac{1}{2}}, \quad (13b)$$

with new unknown arrays $\alpha_{u} = [\alpha_{u,1}, \alpha_{u,2}, \cdots, \alpha_{u,d_u}]$ that can be thought of as a time-varying weighting factor for each POD basis vector. Substituting (13) into (3) and pre-multiplying the equation for the electric field DoFs by $[\Psi_{e}]^T$, the POD update equations can be found after some algebraic manipulations as

$$\alpha_{b}^{n+\frac{1}{2}} = \alpha_{b}^{n-\frac{1}{2}} - \Delta t \left([\Psi_{b}]^T \cdot [C] \cdot [\Psi_{e}] \cdot \alpha_{e}^n \right), \quad (14a)$$

$$\alpha_{e}^{n+1} = \alpha_{e}^n + \Delta t \left( [\Psi_{e}]^T \cdot [s] \cdot [\Psi_{e}] \right)^{-1} \left( [\Psi_{e}]^T \cdot [C]^T \cdot \left[\Psi_{b}\right] \cdot \alpha_{b}^{n+\frac{1}{2}} - [\Psi_{e}]^T \cdot [s] \cdot [\Psi_{e}] \right), \quad (14b)$$

In the presence of sources, the DoFs of the source can also be directly projected onto each POD basis and the projected terms added to above POD-FETD scheme.

Major benefits in using POD-FETD scheme are: (1) the size of original DoFs is significantly reduced and (2) the need for the large mass matrix linear solver or SPAI strategy is obviated since the size of the POD mass matrix $[\Psi_{e}]^T \cdot [s] \cdot [\Psi_{e}]$ is much smaller such that its inverse calculation becomes simpler and less resource intensive. It should be noted that the POD mass matrix is a full matrix; hence, significant dimension reduction with respect to the original mass matrix needs to be guaranteed so that the gains surpass the cost of performing a full matrix inversion.

The steps to obtain the POD-FETD scheme can be summarized as follows:

1. Construction of field snapshot matrices based on FETD simulation data.
2. Decomposition of the snapshot matrices into spatial and temporal modes through SVD.
3. Truncation of the singular values (mode selection).
4. Replacement of the original DoFs in the FETD scheme by the fewer number of unknown POD DoFs.
IV. Numerical Results

To validate and study the application of the POD-based MOR to the FETD-PIC algorithm, some representative problems are analyzed in this section. In IV-A the problem of an electron beam within a cavity is used to investigate the POD method's capabilities of extrapolating results in time. In IV-B the electron beam experiment is repeated, but now with an external oscillating magnetic flux that causes the particles to have more complicated dynamics. In IV-C the electron beam experiment is tuned such that the formation of a virtual cathode occurs, and the capability of the POD method to extrapolate results in parameter space is explored. In IV-D the problem of a plasma ball expansion is analyzed.

A. Electron Beam

Consider a square two-dimensional cavity with size $h \times h$, initially with zero net electromagnetic fields and no charged particles. At simulation start particles are injected randomly into the cavity near the center of the bottom wall at the region $[h/2-b, h/2+b]$, where $b$ is a set (half) beamwidth parameter. The particles possess a given initial velocity $v_0$ in the $y$ direction. An external voltage $V_b$ is applied between the top and bottom walls. The particles are absorbed upon hitting the upper wall. The cavity walls are assumed to be perfect electric conductors (i.e. zero tangential electric field component). With $h = 1$ [m] assumed, the domain is discretized via an irregular mesh with $N_0 = 1633$ nodes, $N_1 = 4768$ edges and $N_2 = 3136$ faces. The beam width is chosen as 0.2 [m], so that $b = 0.1$ [m]. Particles are injected with velocity $v_0 = 5 \times 10^6$ [m/s] and the external bias is set to $V_b = 1 \times 10^3$ [V]. Each computational particle represents 500,000 physical electrons, and five particles are injected every time-step according to a uniform random distribution at $0.4 < x < 0.6$ with $y = 0$. The time-step interval is $\Delta t = 10$ [ps]. A full FETD-PIC simulation is run to provide the harvested values for the snapshot matrix constructions and for comparison purposes. The snapshot matrices are constructed by harvesting $l = 40$ instances of the DoF values from the full simulation at every 500 time-steps. Singular value distributions for the snapshot matrices are shown in Fig. 1. The distribution showcases that the number of relevant modes required to capture the problem dynamics is less than the full number of decomposed modes as some singular values are much larger than others (i.e. there is more energy contained within their associated modes). The number of modes used in the reduced order system is chosen to be 7 for the electric field and 3 for the magnetic flux. According to (12), this indicates an expected 2-norm error of $\epsilon_2(7) = 0.0141$ for the electric field values. Fig. 2 shows superparticle positions (yellow dots) and electric field distribution (green arrows) at the end of the simulation for both the full and reduced models. It is clear that the reduced model is able to reproduce the particle dynamics, including the widening of the beam due to self-field effects, even deep into the extrapolation region.

Fig. 3 (left) shows the calculated error between the electric fields obtained in the POD simulation and the full simulation,

$$\delta_n = \frac{\|E_{\text{pod}} - E_{\text{full}}\|_2}{\|E_{\text{full}}\|_2},$$  \hspace{1cm} (15)$$

which is smaller than the predicted value at all points in the harvesting region (indicated in green color)\(^2\) and Fig. 3 (right) shows the particle number density and $y$ component of the average electron velocity as a function of the vertical position along the cavity. Fig. 4 shows the distribution of the first four POD electric field modes.

\(^2\)The error measure assumes high values at the start of the simulation because the field values (denominator of eq. (15)) are then small, rather than because of large differences between the models.
Fig. 3. Left: Evolution of the two-norm error between the electric field of the reduced and full models, as a function of the time step in the electron beam simulation. The green shaded region represents the interval from which samples were extracted. Right: Particle number density and average particle velocity in the $y$ direction as a function of the vertical position along the beam in steady state, for the reduced and full models.

Fig. 4. Normalized electric field distribution and vector map for the six first POD modes.

Fig. 5. Singular value distributions for the case with external oscillating magnetic flux. The singular values have been normalized by their largest value, and those associated with the retained modes in the reduced model are shown in red.

Fig. 6. Superparticle positions (yellow dots) and electric field distribution (green arrows) of the electron beam at the end of the simulation, taken from the full simulation (right) and the reduced simulation (left), for the external oscillating magnetic flux case.

Notice that the error comparison extends beyond the interval from which the snapshot entries were harvested. This indicates the ability of the reduced model to simulate the correct dynamics even when extrapolating the results from the full simulation. In other words, a costly simulation can be run for a short time to build the POD model and then the rest of the simulation can be completed using the reduced order system having only 7 degrees of freedom for the electric field and 3 for the magnetic field. In the results shown here the original simulation also runs for the entire duration only for comparison purposes. This of course wouldn’t be necessary when using the model to reduce the complexity of a simulation of interest. Notice also that the error shows a gradual increase in the extrapolation region. However, these effects remain small in relation to the bulk behavior, which is still captured as seen in the particle positions in Fig. 2 and the particle density and velocity distributions in Fig. 3.

B. Electron Beam with Oscillating External Magnetic Flux

To explore different particle dynamics, we consider next an electron beam in the presence of an external oscillating magnetic flux given by $\mathbf{B} = A_b \sin(\omega_b n) \hat{z}$, with $A_b = 4 \times 10^{-4}$.

and \(\omega_b = \frac{2\pi}{2000}\), which causes the particles to oscillate in the transverse direction as they travel through the cavity. All other parameters remain the same, as does the snapshot matrix construction and the number of modes retained. Fig. 5 shows the singular value distribution for both electric field and magnetic flux for this case. Fig. 6 shows a comparison of the particle position and field distribution at the end of the simulation. Notice that the beam still widens as it travels through the cavity due to self-field effects, but the particle dynamics are dominated by the external magnetic flux. Fig. 7 shows the error between full and reduced simulation as time progresses and a comparison of the particle density and velocity distributions in steady state. The error for this case is has negligible growth in the extrapolation region since particle paths are primarily determined by the external flux instead of by self-field effects, and the former is very well captured in the harvesting stage. Fig. 8 shows the distribution of the first six electric field modes. Notice how the higher-order modes capture the self-fields generated by the electron distribution.

C. Electron Beam with Virtual Cathode Formation

We next consider an electron beam with an increased injection current such that formation of a virtual cathode occurs. In this case, we are interested in evaluating the capabilities of POD for parameter extrapolation, the parameter here being the injection current. Higher current values in this case are obtained by setting each computational particle to represent \(10^7\) physical electrons and then varying the number of computational particles in the domain. The time-step interval is set to \(\Delta t = 20\) [ps] and all other parameters remain unchanged. The external electric field is turned off and the external magnetic field is given by \(\mathbf{B} = B_y \hat{y}\), with \(B_y = 10^2\) [A/m]. This strong focusing magnetic field confines the beam and offsets (in the transverse direction) the stronger self-field interactions due to the higher current magnitude. A base case is considered in which the injected current is given by \(I_b = 320, 435\) [A], which corresponds to roughly two times the over-injection current for this geometry. Due to the more complicated dynamics of this case, the snapshot matrices are constructed by harvesting \(l = 2000\) instances of the DoF values every 10 time-steps until \(n = 20,000\). Eight modes are retained both for the electric field and the magnetic flux.

Fig. 9 shows a comparison of the particle position and field distribution at the end of the simulation. The electron bunching and sideways streaming characteristic of 2D virtual cathodes can be clearly seen in both full and reduced models. For this case and all others in this section, there is no extrapolation in time as we will focus on parameter extrapolation. Fig. 10 shows the error between full and reduced simulation as time progresses and a comparison of the particle density and velocity distributions in steady state. Fig. 11 shows the distribution of the first four electric field modes, clearly showcasing the virtual cathode modes from the second mode.
onward. These base case results already indicate the ability of the reduced order model to properly reproduce the nonlinear virtual cathode formation.

To investigate the extrapolation capabilities of the POD method in parameter space, full simulations are run for select values of injected current \( I \in [0.1 \, 2 I_b] \), and reduced order models are created for each of these cases. Then each of the ROMs is run for cases spanning the same interval \( I \in [0.1 \, 2 I_b] \), and compared to a full simulation run at that parameter point.

First, it is important to verify the point where the problem transitions from a normal beam case to the virtual cathode formation. This transition happens when the current is increased from \( I = 0.5 I_b \) to \( I = 0.7 I_b \), as shown in Fig. 12. Fig. 13 shows the phase-space plot for simulations run at the parameter points \( I = 0.1 I_b \), \( I = I_b \) and \( I = 2 I_b \) with the model constructed from the \( I = I_b \) case. The \( 0.1 I_b \) and \( 2 I_b \) cases correspond therefore to parameter extrapolations, and it can be seen from the figure that the reduced order model manages to reproduce the bulk of the behavior.

The parameter extrapolation capabilities of the reduced order model are summarized in the error plot provided in Fig. 14. In this plot, the rows indicate the point in parameter space where the full order models were run to harvest data for the reduced order models, and the columns indicate the point in parameter space where the reduced order model is subsequently being run at. For example, the row labeled “1.0” corresponds to runs of a same reduced order model using different injection currents wherein the modes of the given reduced order model were obtained based on data extracted from a full order simulation with \( I = 1.0 I_b \). The color in each entry indicates the two-norm error between the electric fields at the end of the simulation obtained by the full order model (“ground truth”) and the extrapolated (in parameter space) reduced order model. The diagonal values exhibit less error as expected because they do not entail any extrapolation; they simply correspond to the error between the reduced and full order models.
order models for a given \( I_b \). The first three rows (i.e., the models constructed from data harvested from the \( I = 0.1 I_6 \), \( I = 0.3 I_6 \) and \( I = 0.5 I_6 \) cases) show relatively high errors when run at cases with \( I \geq 0.7 I_b \), which is also expected since those modes were extracted from cases without any virtual cathode formation. Additionally, as the parameter at which the reduced model is being run is chosen farther apart from the parameter where the modes thereof were extracted from, the quality of the reconstruction degrades as seen in the elements which are far off from the diagonal.

### D. Plasma Ball Expansion

A plasma ball expanding into a vacuum is an important problem in many scenarios including e.g. laser ignition applications. Consider a vacuum-filled square domain of size \( h \times h \) with a plasma ball of diameter \( D_{pb} \) located at the center, with \( h = 10 \) [m] and \( D_{pb} = 1 \) [m]. The domain is discretized by an irregular mesh with \( N_0 = 8,030 \) nodes, \( N_1 = 23,829 \) edges, \( N_2 = 15,800 \) faces, and the cavity has perfect magnetic conductor (PMC) walls, i.e., the normal component of the electric field is set to zero. The time-step interval is \( \Delta t = 50 \) [ps]. The plasma ball is initially assumed to be perfectly neutral, i.e., the same number of electrons and ions are uniformly distributed within the circular disk of radius \( D_{pb} \). Each electron-ion pair is initially located at exactly the same position for zero net initial field conditions. The number density of actual electrons and ions, \( n_e \) and \( n_i \), is set to be \( n_e = n_i = 6.37 \times 10^{10} \) [m\(^{-2}\)]. In the simulation, only the motion of electrons is tracked since ions are much heavier and hence can be assumed stationary. A Maxwellian distribution is used for the electron velocities, with the thermal velocity

\[
v_{th} = 0.01c,
\]

see Fig. 15. With these conditions the Debye length of the plasma ball is

\[
\lambda_D = (\epsilon_0 k T / n_e q_e)^{1/2} = 0.21 \text{ [m]}.
\]

The average edge length in the mesh is chosen as \( \ell_{ave} = 0.141 \) [m] to mitigate self-grid-heating effects [41]. The number of electron super-particles is \( N_{sp,e} = 2 \times 10^5 \) and each super-particle represents \( 2.5 \times 10^5 \) actual electrons. Table I shows all parameters associated with the plasma ball simulation.

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3Here, thermal velocity, \( |v_{th}| \), is defined as the root mean square of the velocity in any one dimension, then \( |v_{th}| = (k_B T/m)^{1/2} \).
Fig. 14. Table representing the logarithm of the 2-norm error between the electric field of the reduced and full simulations at the last time-step of simulation. See the main text for more details.

(a) Initial velocity distribution. (b) Initial speed distribution.

Fig. 15. Realization of a Maxwellian velocity distribution describing the initial electron velocities in the plasma ball.

A full FETD-PIC simulation is run for the plasma ball expansion up to \( N_t = 80,000 \). The DoFs from the full simulation are sampled at evenly separated time-steps to construct the snapshot matrices. In order to study the effects of \( \Delta n_s \) (time-step spacing for the field sampling) and \( N_{t,s} \) (last time-step for the field sampling) on the results, three cases are considered to construct the snapshot matrix while keeping the total number of harvested instances fixed as \( l = 40 \), as shown in Table II.

Table I

<table>
<thead>
<tr>
<th>Simulation Setup for the Plasma Ball Expansion</th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>( n_e = n_i ) [m(^{-2})]</td>
<td>6.37 \times 10^{10}</td>
<td>0.01c</td>
</tr>
<tr>
<td>( D_{ph} ) [m]</td>
<td>( 1 )</td>
<td>( \sigma_x = \sigma_y )</td>
</tr>
<tr>
<td>( \lambda_0 ) [m]</td>
<td>0.2</td>
<td>( \omega_{pe} ) [m]</td>
</tr>
<tr>
<td>( C_{sp,e} )</td>
<td>2.5 \times 10^5</td>
<td>( N_{p,e} )</td>
</tr>
<tr>
<td>( N_0 )</td>
<td>8,030</td>
<td>( N_f )</td>
</tr>
<tr>
<td>( N_2 )</td>
<td>15,800</td>
<td>( \Delta t ) [ps]</td>
</tr>
</tbody>
</table>

\( \sigma_x \) or \( \sigma_y \) denote a standard deviation for \( x \) or \( y \) direction, respectively, in a normal distribution of each component of velocity.

Fig. 16 shows singular values obtained for each case. The number of modes used in the reduced order system is chosen to be 10 for the electric field and 2 for the magnetic flux in all cases. Fig. 17 illustrates snapshots for the evolution of the plasma ball and Fig. 18 the corresponding phase-space plots, for the full model and the reduced model (case 1). It can be observed that the plasma ball is initially expanding into vacuum but then cools down due to the strong electric fields created by ions that attract the electrons back to the center of the plasma ball. The results of the three different reduced order simulations are compared to the full case. Fig. 19 illustrates the calculated error given by

\[
\delta_n^e = \frac{\left\| E_{n,f}^{f} - E_{n,p}^{p} \right\|_2}{\left\| \frac{1}{N_f} \sum_{n} E_{n,f}^{p} \right\|_2},
\]

for all cases. This error is different from the one adopted before to suppress the large relative errors seen in the early stages of the simulation and make the difference between the relative errors seen at the later stages more salient. Over the interpolation (harvesting) intervals, case 1 shows the best performance since it is constructed from the snapshot matrix with shortest \( \Delta n_s \). However, in the extrapolated intervals, case 3 has the least errors due to having the largest \( N_{t,s} \) and therefore having sampled the dynamics for longer. This can also be seen in Fig. 18, where the phase plot of the reduced simulation in case 1 diverges from the full simulation at late times due to poor sampling of the problem’s late-time dynamics.

Next, the (macroscopic) radial current from the plasma ball...
Fig. 17. Simulation results for the plasma ball expansion from the full model (in red, left) and the reduced case 1 model (in blue, right). Except for the $n = 10,000$ case, all figures from the reduced model were taken at the extrapolated region, after field harvesting was done.

Fig. 18. Simulation results for the electron phase-space plots at different time-steps on the plasma ball expansion from the full model (in red, left) and the reduced case 1 model (in blue, right). Except for the $n = 10,000$ case, all figures from the POD simulation were taken at the extrapolated region, after field harvesting was done.

The radial current is calculated as

$$I_r^{n+rac{1}{2}} = \int_{\phi=0}^{2\pi} \int_{r=r_0-\epsilon}^{r_0+\epsilon} \left[ \sum_{p=1}^{N_p} \rho_p v_p^{n+rac{1}{2}} \cdot \hat{r} \right] rdrd\phi$$

$$= 2\pi r_0 \sum_{p} N_p \rho_p v_p^{n+rac{1}{2}} \cdot \hat{r} [A],$$

where $\hat{r}$ is the unit vector along the radial direction and $\epsilon$ denotes a small radial width around each $r_0$. Fig. 20 depicts the radial current averaged over five realizations versus the plasma ball radius at different time-steps. The poor performance of case 1 outside of the interpolated region showcases the necessity of considering a harvesting interval spanning the problem’s dynamics in order to properly reproduce the correct...
behavior. In order to further explore this requirement, the plasma ball experiment is repeated with sampling parameters given by Table III. In this case, the sampling interval $\Delta n_s$ is kept fixed but the last time-step $N_{t,s}$ changes for each case, which affects consequently the number of modes harvested $l$. In the reduced model, only 10 modes are kept for the electric field and 2 for the magnetic flux again. Fig. 21 shows the error comparison for these cases, clearly showing that the cases with longer harvesting yield better results.

A POD-based model order reduction was applied to the field update step of the FETD-PIC algorithm, yielding a reduced system that can be effectively used in particle simulations of collisionless plasma problems. The reduced-order model capabilities to extrapolate in time and in the parameter space were confirmed, with the reduced model providing accurate results in either case. However, care must be taken to ensure that the samples used to construct the snapshot matrices span the dynamics that need to be reproduced, otherwise late-time errors can emerge, in the case of extrapolation in time, as the dynamics of the reduced order model diverge from the actual dynamics of the problem. In the case of extrapolation in parameter, the same problem arises if the characteristics of the problem being run are fundamentally different from those from where the model was extracted from. This might happen if the parameter used for the reduced order (online) simulation...
is too distant from the parameter used in the offline model to extract the reduced order modes or if there was is a marked transition between the two points. If the proper care is taken, then the POD technique successfully reproduces field and particle behaviors with acceptable accuracy while enabling a reduction of degrees of freedom of several orders of magnitude.

REFERENCES