

A Computationally Optimal Randomized Proper Orthogonal Decomposition Technique

Dan Yu,

Suman Chakravorty

Abstract—In this paper, we consider the model reduction problem of large-scale systems, such as systems obtained through the discretization of partial differential equations. We propose a computationally optimal randomized proper orthogonal decomposition (RPOD^{*}) technique to obtain the reduced order model by perturbing the primal and adjoint system using Gaussian white noise. We show that the computations required by the RPOD^{*} algorithm is orders of magnitude cheaper when compared to the balanced proper orthogonal decomposition (BPOD) algorithm while the performance of the RPOD^{*} algorithm is better than BPOD. It is optimal in the sense that a minimal number of snapshots is needed. We also relate the RPOD^{*} algorithm to random projection algorithms. One numerical example is given to illustrate the procedure.

I. INTRODUCTION

In this paper, we are interested in the model reduction of large scale systems, such as those governed by partial differential equations (PDE). The dimension of the system is large due to the discretization of the PDEs. For instance, consider the atmospheric dispersion of air pollutants [1]. The emission of the contaminants on the ground level is shown in Fig. 1 with four point sources labeled from S1 to S4.

This is a three dimensional problem, and after discretizing the PDE, the dimension of the system is 10^6 . Therefore, we are interested in constructing a reduced order model (ROM) that can capture the input/output characteristics of the large model such that this ROM can be used by a filtering algorithm for updating the states of the field, such as the Kalman filter. Also, the actuators and sensors could be placed anywhere in this field, which leads to a model reduction problem of a large-scale system with a large number of inputs/outputs.

There are two popular contemporary model reduction techniques that have been studied in the past few decades: Principal component analysis (PCA) and randomization algorithms. Among the PCA algorithms, Balanced POD [2], [3] based on the balanced truncation [4] and eigensystem realization algorithm (ERA) [5] have been widely used, and BPOD is equivalent to ERA procedure [6]. BPOD algorithm collects the impulse responses of the primal and adjoint systems, and forms the Hankel matrix using the primal and adjoint system simulations as opposed to the input-output data as in ERA. For both BPOD and ERA, collecting the primal and adjoint simulation datasets and solving the singular value decomposition (SVD) problem for the resulting

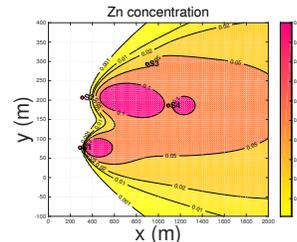


Fig. 1. Air pollutant problem

Hankel matrix are computationally expensive for a large scale system with a large number of inputs/outputs. To reduce the computational cost of BPOD, [3] proposed an output projection method while the algorithm still faces a high computational burden when both the numbers of the inputs and outputs are large, and the method cannot make any claim regarding the closeness of the solution to one that is obtained from the full Hankel matrix.

There are two major classes of randomization algorithms used for low-rank matrix approximations: random sampling algorithms and random projection algorithms. Denote $\|H\|_F$ as the Frobenius norm of H , and $\|H\|$ as the spectral 2-norm of H . For the random sampling algorithm, a rank k approximation matrix \hat{H} is constructed by choosing and rescaling some columns of H according to certain sampling probabilities [7], [8], so the error satisfies $\|H - \hat{H}\|_F \leq (1 + \epsilon)\|H - H_{(k)}\|_F$, with high probability, where $H_{(k)}$ is a best rank k approximation of H , ϵ is a specified tolerance. In random projection method [9], the large matrix H is projected on to an orthonormal basis Q such that the error satisfies $\|H - QQ^*H\| \leq (1 + \epsilon)\|H - H_{(k)}\|$ with high probability. A Gaussian test matrix Ω is generated, and the orthonormal basis Q is constructed by performing a QR factorization of the matrix product $H\Omega$. A direct application of both algorithms would require the full Hankel matrix to be constructed, which is prohibitively expensive.

We had introduced an RPOD algorithm in [10] that randomly chooses a subset of the input/output trajectories. A sub-Hankel matrix is constructed using the sampled trajectories, and then forms a ROM in the usual BPOD fashion. The Markov parameters of the ROM constructed using the sub-Hankel matrix were shown to be close to the Markov parameters of the full order system with high probability. We proved that a lower bound exists for the number of the input/output trajectories that need to be sampled. The major problem associated with this algorithm is that different choices of the sampling algorithms would lead to different

D. Yu is a Graduate Student Researcher, Department of Aerospace Engineering, Texas A&M University, College Station

S. Chakravorty is an Associate Professor of Aerospace Engineering, Texas A&M University, College Station

lower bounds, and the choice of a good sampling algorithm other than the uniform distribution is unclear.

In this paper, we propose the RPOD* algorithm which is closely related to random projection algorithms. In RPOD* algorithm, we perturb the primal and adjoint system with Gaussian white noise. We prove that similar to the BPOD algorithm, the controllable and observable modes are retained in the ROM. The Markov parameters of the ROM constructed using RPOD* are shown to be close to the Markov parameters of the full order system, while the error is bounded. The RPOD* algorithm can be viewed as applying the random projection on the full Hankel matrix H twice without constructing the full Hankel matrix H , i.e., $\hat{H} = \Omega_2' Z' X \Omega_1 = \Omega_2' H \Omega_1$, where $(\cdot)'$ denotes the transpose of (\cdot) , Ω_1, Ω_2 are two random projection matrices, and Z, X are the usual impulse response matrices of the adjoint and primal system. However, we actually only generate $Z\Omega_2$ and $X\Omega_1$ which can be constructed from a single white noise perturbed trajectory each of the adjoint and primal system respectively, and thus, are orders of magnitude smaller in size than the impulse responses Z and X . Thus, the computational cost to generate the Hankel matrix and to solve the SVD problem is saved by orders of magnitude. We believe that it is the most computational efficient POD algorithm. In practice, the RPOD* algorithm can be solved in real-time.

The rest of the paper is organized as follows. In Section II, the problem is formulated, and in Section III, we review the BPOD algorithm and illustrate in a simplified fashion how to relate the BPOD ROM to the controllable and observable modes of the system. The RPOD* algorithm is proposed in Section IV, and the formal proofs and results are shown. Also, we discuss the relationship between RPOD* algorithm and the BPOD algorithm, and some implementation problems in this section. In Section V, we provide computational results comparing the RPOD* with the BPOD for a three dimensional atmospheric dispersion problem.

II. PROBLEM FORMULATION

Consider a stable linear input-output system:

$$\begin{aligned} x_k &= Ax_{k-1} + Bu_k, \\ y_k &= Cx_k, \end{aligned} \quad (1)$$

where $x_k \in \mathbb{R}^N$, $u_k \in \mathbb{R}^p$, $y_k \in \mathbb{R}^q$ are the states, inputs, and outputs at discrete time instant t_k respectively. The Markov parameters of the system is defined as $CA^iB, i = 1, \dots$.

The adjoint system is defined as:

$$z_k = A'z_{k-1} + C'v_k, w_k = B'z_k, \quad (2)$$

where $z_k \in \mathbb{R}^N$, $w_k \in \mathbb{R}^p$ is the state and output of the adjoint system at time t_k respectively, $v_k \in \mathbb{R}^q$.

Suppose A is diagonalizable, and let $A = V\Lambda U'$, where Λ are the eigenvalues, (V, U) are the corresponding right and left eigenvectors.

A mode (Λ_i, U_i, V_i) is not controllable if $U_i' B = 0$, and is not observable if $C V_i = 0$, where (Λ_i, V_i, U_i) is the i^{th} eigenvalue-eigenvector pair. Therefore, we partition the

eigenvalues and eigenvectors (Λ, V, U) into four parts:

$$A = \begin{pmatrix} V_{co}' \\ V_{c\bar{o}}' \\ V_{\bar{c}o}' \\ V_{\bar{c}\bar{o}}' \end{pmatrix}' \begin{pmatrix} \Lambda_{co} & & & \\ & \Lambda_{c\bar{o}} & & \\ & & \Lambda_{\bar{c}o} & \\ & & & \Lambda_{\bar{c}\bar{o}} \end{pmatrix} \begin{pmatrix} U_{co}' \\ U_{c\bar{o}}' \\ U_{\bar{c}o}' \\ U_{\bar{c}\bar{o}}' \end{pmatrix}, \quad (3)$$

where $(\Lambda_{co}, V_{co}, U_{co})$ are the controllable and observable modes, $(\Lambda_{c\bar{o}}, V_{c\bar{o}}, U_{c\bar{o}})$ are the controllable but not observable modes, $(\Lambda_{\bar{c}o}, V_{\bar{c}o}, U_{\bar{c}o})$ are the not controllable but observable modes, and $(\Lambda_{\bar{c}\bar{o}}, V_{\bar{c}\bar{o}}, U_{\bar{c}\bar{o}})$ are the not controllable and not observable modes.

In this paper, we consider the model reduction problem for large scale systems with a large number of inputs/outputs. The goal is to construct a ROM such that the outputs of the ROM y_r are close to the outputs of the full order system y , i.e., $|y - y_r|$ is bounded and all the controllable and observable modes of system (A, B, C) are preserved in the ROM.

III. BALANCED PROPER ORTHOGONAL DECOMPOSITION

In this section, first we briefly review the BPOD algorithm. Then we give an informal proof to illustrate in a simplified fashion how the transformation bases and the Markov parameters of the ROM constructed using the BPOD algorithm can be related to the controllable and observable modes $(\Lambda_{co}, V_{co}, U_{co})$ of the system matrix A . The simplified analysis is critical to understand the fundamentals of the proposed RPOD* algorithm in Section IV.

A. Simplified Analysis of BPOD

The BPOD algorithm can be found in [3], [10], and is briefly summarized here.

Step 1. Collect the impulse responses X_b, Z_b of the primal and adjoint system (1)-(2).

Step 2. Construct the Hankel matrix H_b and solve the SVD problem of the Hankel matrix.

$$H_b = Z_b' X_b = \begin{pmatrix} U_b & U_1 \end{pmatrix} \begin{pmatrix} \Sigma_b & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} V_b' \\ V_1' \end{pmatrix}, \quad (4)$$

where Σ_b contains the first l non-zero singular values, and (U_b, V_b) are the corresponding left and right singular vectors.

Step 3. The BPOD bases are:

$$T_b = X_b V_b \Sigma_b^{-1/2}, S_b = \Sigma_b^{-1/2} U_b' Z_b', \quad (5)$$

Step 4. The ROM is:

$$A_b = S_b A T_b, B_b = S_b B, C_b = C T_b. \quad (6)$$

In the following, we provide a simplified analysis of the BPOD algorithm.

The snapshot ensemble X_b can be written as:

$$X_b = \begin{pmatrix} A^{t_1-1} B & A^{t_2-1} B & \dots & A^{t_m-1} B \end{pmatrix}, \quad (7)$$

where t_1, \dots, t_m are the time steps we take the snapshots.

Assume A is diagonalizable, then from (3), we have:

$$A^{t_k-1} B = \begin{pmatrix} V_{co} & V_{c\bar{o}} \end{pmatrix} \begin{pmatrix} \Lambda_{co} & \\ & \Lambda_{c\bar{o}} \end{pmatrix}^{t_k-1} \begin{pmatrix} U_{co}' \\ U_{c\bar{o}}' \end{pmatrix} B. \quad (8)$$

Thus, X_b can be written as:

$$X_b = (V_{co} \quad V_{\bar{c}o}) \begin{pmatrix} \alpha_{co}^b \\ \alpha_{\bar{c}o}^b \end{pmatrix}, \quad (9)$$

where $\alpha_{co}^b, \alpha_{\bar{c}o}^b$ the coefficient matrices. Similarly, $Z_b = (U_{co} \quad U_{\bar{c}o}) \begin{pmatrix} \beta_{co}^b \\ \beta_{\bar{c}o}^b \end{pmatrix}$, where $\beta_{co}^b, \beta_{\bar{c}o}^b$ are coefficient matrices.

In the following, to simplify the analysis, we assume there are only controllable and observable eigenvectors present in the snapshot ensembles, i.e., $\alpha_{\bar{c}o}^b = 0, \beta_{\bar{c}o}^b = 0$. Thus,

$$X_b = V_{co}\alpha_{co}^b, Z_b = U_{co}\beta_{co}^b. \quad (10)$$

Note that this assumption may not hold in practice, and is relaxed in the formal proof of our main result, Proposition 1, in Section IV.

Suppose there are l controllable and observable modes,

$$Z_b' X_b = (\beta_{co}^b)' \alpha_{co}^b = U_b \Sigma_b V_b', \quad (11)$$

where $\Sigma_b \in \mathbb{R}^{l \times l}$ are the l non-zero singular values and (U_b, V_b) are the corresponding left and right singular vectors.

Consider the ROM:

$$\begin{aligned} A_b &= S_b A T_b = \Sigma_b^{-1/2} U_b' (Z_b' A X_b) V_b \Sigma_b^{-1/2} \\ &= \underbrace{\Sigma_b^{-1/2} U_b' (\beta_{co}^b)'}_{P_b} \Lambda_{co} \underbrace{\alpha_{co}^b V_b \Sigma_b^{-1/2}}_{\hat{P}_b}. \end{aligned} \quad (12)$$

It can be proved that Λ_{co} are the eigenvalues of A_b , and P_b are the eigenvectors, i.e.,

$$\Lambda_{co} = (P_b^{-1} S_b) A (T_b P_b). \quad (13)$$

The proof is shown in the technical report [11], and is omitted here due to the page limit.

Let (Ψ_b, Φ_b) denote the new POD bases constructed by projecting (T_b, S_b) onto the ROM eigenspace, then

$$\begin{aligned} \Psi_b &= T_b P_b = X_b V_b \Sigma_b^{-1/2} \Sigma_b^{-1/2} U_b' (\beta_{co}^b)' \\ &= V_{co} \alpha_{co}^b V_b \Sigma_b^{-1} U_b' \beta_{co}^b = V_{co}, \end{aligned} \quad (14)$$

and similarly, $\Phi_b = P_b^{-1} S_b = U_{co}'$, i.e., under the approximation of exactly l controllable and observable modes being present in the snapshots, the modal coordinates of the BPOD ROM are precisely these l modes. Thus, the modal BPOD ROM constructed using (Ψ_b, Φ_b) is:

$$\hat{A}_b = \Lambda_{co}, \hat{B}_b = U_{co}' B, \hat{C}_b = C V_{co}. \quad (15)$$

Remark 1: From the analysis above, we see that the modal BPOD ROM consists of the controllable and observable modes, and is invariant to the data X_b and Z_b . Thus, we make the following observation.

As long as the snapshot ensembles are:

$$X = V_{co} \alpha, Z = U_{co} \beta, \quad (16)$$

the modal ROM consists of the controllable and observable modes, and the ROM is given by (15).

Remark 2: Now, consider the impulse response snapshot

ensembles collected in the BPOD:

$$X_b = \underbrace{V_{co}}_{N \times l} \underbrace{\alpha_{co}^b}_{l \times pm}, Z_b = \underbrace{U_{co}}_{N \times l} \underbrace{\beta_{co}^b}_{l \times qn}, \quad (17)$$

and the Hankel matrix: $H_b = Z_b' X_b \in \mathbb{R}^{qn \times pm}$.

There are two main parts to the computation:

- 1) The primal and adjoint snapshot ensembles $X_b \in \mathbb{R}^{N \times pm}, Z_b \in \mathbb{R}^{N \times qn}$, and hence, the construction of H_b takes time $O(pqmnN)$.
- 2) The computational cost to solve the SVD of H_b is $O(\min\{p^2 m^2 qn, pmq^2 n^2\})$.

However, H_b is only rank “ l ”, where $l \ll N, pm, qn$. Therefore, if we can generate optimal snapshot ensembles,

$$X^* = V_{co} \underbrace{\alpha^*}_{l \times l}, Z^* = U_{co} \underbrace{\beta^*}_{l \times l}, \quad (18)$$

where $l \ll pm, qn$, then the BPOD result still holds for the optimal snapshot ensembles X^*, Z^* while solving the SVD of $H^* = (Z^*)' X^*$ would be reduced by orders of magnitude.

The snapshot ensembles X^*, Z^* are considered to be optimal because the rank of X^*, Z^* is l , and only l snapshots are needed to guarantee all the controllable and observable modes V_{co}, U_{co} would be preserved in X^*, Z^* .

Furthermore, given that only l snapshots are needed, the construction time of X^*, Z^* is also reduced by orders of magnitude from $N \times qn, pm$ to $N \times l$ since $l \ll pm, qn$. Bearing this observation in mind, in the next section, we introduce RPOD* algorithm which generates snapshot ensembles using white noise perturbations, such that (18) holds.

IV. COMPUTATIONALLY OPTIMAL RANDOMIZED PROPER ORTHOGONAL DECOMPOSITION (RPOD*)

In this section, first, we give the reader the fundamental insight into the derivation of the RPOD* algorithm. The RPOD* algorithm is then formalized and treated rigorously in Section IV-B. We discuss implementation issues of the algorithm in Section IV-C, and compare the RPOD* algorithm with random projection and BPOD in Section IV-D.

A. Derivation of the RPOD*

Consider the system (1-2), since A is stable, there exists a finite number t_{ss} , such that $\|A^{t_{ss}}\| \approx 0$.

A Gaussian matrix $\Omega_1 \in \mathbb{R}^{n \times m}$ is defined as:

$$\Omega_1 = \begin{pmatrix} \omega_{11} & \omega_{12} & \cdots & \omega_{1m} \\ \vdots & \vdots & \cdots & \vdots \\ \omega_{n1} & \omega_{n2} & \cdots & \omega_{nm} \end{pmatrix} \quad (19)$$

where each element ω_{ij} of Ω_1 is an independent, identically distributed (i.i.d) variable with Gaussian distribution $N(0, 1)$. Suppose $m \leq n$, in [9], it is shown that the columns of a Gaussian matrix Ω_1 are almost surely in general position, so Ω_1 has full column rank with probability one. The primal snapshot ensemble collected in the BPOD are: $X_b = (B, AB, \dots, A^{t_{ss}-1} B) \in \mathbb{R}^{N \times pt_{ss}}$, and we project X_b onto a Gaussian matrix $\Omega_1 \in \mathbb{R}^{pt_{ss} \times l}$:

$$\underbrace{X^*}_{N \times l} = (X_1^* \quad X_2^* \quad \cdots \quad X_l^*)$$

$$= \underbrace{(B \quad \cdots \quad A^{t_{ss}-1}B)}_{X_b = V_{co}\alpha_{co}^b} \underbrace{\begin{pmatrix} \omega_{1,1} & \cdots & \omega_{1,l} \\ \vdots & \cdots & \vdots \\ \omega_{t_{ss},1} & \cdots & \omega_{t_{ss},l} \end{pmatrix}}_{\Omega_1} \quad (20)$$

where $\omega_{i,j} \in \mathbb{R}^{p \times 1}$, $i = 1, \dots, t_{ss}$, $j = 1, \dots, l$. Suppose that the same assumption is made as in the heuristic analysis, i.e., only “I” controllable and observable modes are present in the snapshot ensemble X_b . The snapshot X_j^* in X^* is:

$$X_j^* = \sum_{i=1}^{t_{ss}} A^{i-1} B \omega_{i,j}, j = 1, \dots, l. \quad (21)$$

Since Ω_1 is a Gaussian matrix, each element of Ω_1 is an i.i.d Gaussian variable with distribution $N(0,1)$, and thus, $\omega_{i,j}$ is a Gaussian random vector with zero mean and covariance $I_{p \times p}$. Therefore, X_j^* is merely the snapshot of the primal system with a unit intensity white noise perturbation in each input channel, and given that we have waited long enough such that $\|A^{t_{ss}}\| \approx 0$. Consequently,

$$X^* = V_{co}\alpha_{co}^b \Omega_1 = V_{co} \underbrace{\alpha^*}_{l \times l}, \quad (22)$$

and similarly, we may generate the adjoint snapshot ensembles Z^* by projecting Z_b onto the Gaussian matrix $\Omega_2 \in \mathbb{R}^{q \times l}$, $Z^* = U_{co}\beta_{co}^b \Omega_2 = U_{co}\beta^*$.

We know that X_b, Z_b are linear combinations of V_{co}, U_{co} respectively, thus, by projecting X_b, Z_b onto the Gaussian matrices, at least “ l ” of the state snapshots in X^*, Z^* are still linearly independent, and X^*, Z^* are still linear combinations of V_{co}, U_{co} , since Ω_1 and Ω_2 are rank l with probability 1. Therefore, due to Remark 2, the SVD of $H^* = (Z^*)' X^*$ would still result in obtaining the l controllable and observable modes while drastically reducing the computation in both computing the snapshots as well as the SVD.

From the analysis above, we see that the optimal snapshot ensembles (18) can be generated by collecting the white noise perturbation responses of system (1)-(2). We generate the snapshots as follows.

We perturb the primal system (1) with unit intensity white noise, i.e., $u_k \sim N(0, I)$, and zero initial condition, then collect the snapshots at discrete time $0 \leq t_1 < t_2 < \cdots < t_m$, where $t_m \geq t_{ss}$, and $\|A^{t_{ss}}\| \approx 0$. The primal snapshot ensemble is:

$$X^* = [x(t_1), x(t_2), \dots, x(t_m)]. \quad (23)$$

The adjoint snapshot ensemble Z^* is generated by collecting the white noise perturbation responses of the adjoint system through all the output channels in a similar fashion. The details regarding how to choose the snapshots are discussed in the subsection IV-C. In the following, the RPOD* algorithm is proposed and the formal proof follows.

Algorithm 1 RPOD* Algorithm

- 1) Perturb the primal system (1) with white noise u_k , collect m snapshots at time step t_1, t_2, \dots, t_m , and denote the snapshot ensemble X_r as:

$$X_r = (x_1 \quad x_2 \quad \cdots \quad x_m). \quad (24)$$

- 2) Perturb the adjoint system (2) with white noise v_k , collect n snapshots at time step $\hat{t}_1, \hat{t}_2, \dots, \hat{t}_n$, and denote the adjoint snapshot ensemble Z_r as:

$$Z_r = (z_1 \quad z_2 \quad \cdots \quad z_n). \quad (25)$$

- 3) Solve the SVD problem:

$$Z_r' X_r = \begin{pmatrix} U_r & U_o \end{pmatrix} \begin{pmatrix} \Sigma_r & 0 \\ 0 & \Sigma_o \end{pmatrix} \begin{pmatrix} V_r' \\ V_o' \end{pmatrix}, \quad (26)$$

and truncate at σ_l , where l is the number of controllable and observable modes present in the snapshot ensembles. Σ_r contains the first l non-zero singular values $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_l > 0$, (U_r, V_r) are the corresponding right and left singular vectors.

- 4) Construct the POD bases:

$$T_r = X_r V_r \Sigma_r^{-1/2}, S_r = \Sigma_r^{-1/2} U_r' Z_r'. \quad (27)$$

- 5) Construct the ROM \tilde{A} , find the eigenvalues Λ_r and eigenvectors P_r of \tilde{A} .

$$\tilde{A} = S_r A T_r = P_r \Lambda_r P_r^{-1}, \quad (28)$$

- 6) Construct new POD bases:

$$\Phi_r = P_r^{-1} S_r, \Psi_r = T_r P_r. \quad (29)$$

- 7) The ROM is:

$$A_r = \Phi_r A \Psi_r, B_r = \Phi_r B, C_r = C \Psi_r \quad (30)$$

B. RPOD* Algorithm

The RPOD* algorithm is summarized in Algorithm 1.

Given a stable linear system, the following result holds.

Proposition 1: Denote (A_r, B_r, C_r) as the ROM constructed using RPOD* following Algorithm 1. Suppose there are l controllable and observable modes present in the snapshot ensembles X_r, Z_r collected using (24-25). Assume that the contribution of the not controllable modes in X_r and the contribution of the not observable modes in Z_r are relative small comparing to the other modes, i.e., $U_{\bar{c}o}' B = \epsilon C_1, U_{\bar{c}o}' B = \epsilon C_2, C V_{\bar{c}o} = \epsilon C_3, C V_{\bar{c}o} = \epsilon C_4$, where C_1, C_2, C_3, C_4 are some coefficient matrices, and ϵ is a small number. If we keep the first l non-zero singular values, then $\|C_r A_r^i B_r - C A^i B\| \propto O(\epsilon), i = 1, \dots$.

Proof: From the assumption made in the Proposition 1, the snapshot ensembles are expressed as follows.

$$X_r = V_{co}\alpha_{co} + V_{c\bar{o}}\alpha_{c\bar{o}} + V_{\bar{c}o}\epsilon\alpha_{\bar{c}o} + V_{\bar{c}\bar{o}}\epsilon\alpha_{\bar{c}\bar{o}}, \quad (31)$$

$$Z_r = U_{co}\beta_{co} + U_{c\bar{o}}\epsilon\beta_{c\bar{o}} + U_{\bar{c}o}\beta_{\bar{c}o} + U_{\bar{c}\bar{o}}\epsilon\beta_{\bar{c}\bar{o}}. \quad (32)$$

Therefore,

$$\begin{aligned} Z_r' X_r &= \beta_{co}' \alpha_{co} + \epsilon \beta_{c\bar{o}}' \alpha_{c\bar{o}} + \beta_{\bar{c}o}' \epsilon \alpha_{\bar{c}o} + \epsilon \beta_{\bar{c}\bar{o}}' \epsilon \alpha_{\bar{c}\bar{o}} \\ &= \beta_{co}' \alpha_{co} + \epsilon \underbrace{(\beta_{c\bar{o}}' \alpha_{c\bar{o}} + \beta_{\bar{c}o}' \alpha_{\bar{c}o})}_{E_1} + O(\epsilon^2), \\ &= \beta_{co}' \alpha_{co} + \epsilon E_1 + O(\epsilon^2). \end{aligned} \quad (33)$$

From the perturbation theory [12]–[14], and following the same proof in Section III-A, the ROM Markov parameters:

$$\|C_r A_r^i B_r - C A^i B\| \propto O(\epsilon). \quad (34)$$

The proof is shown in the technical report [11] and is omitted here due to the page limit. ■

C. Implementation Issues

Here we discuss some implementation problems in the RPOD* algorithm.

Snapshot selection From the analysis in Section IV-B, we only need to collect $m = l_1$ snapshots from the primal simulations, where l_1 is the number of the controllable modes. However, l_1 is not known a priori, thus, in practice, we start with a random guess $m \ll N$, where N is the dimension of the system, or we can choose m from experience. For instance, in a fluid system with 10^6 degrees of freedom, m is $O(10) \sim O(10^2)$. Similarly, we guess n , and then we check the rank of $Z_r' X_r$. If $Z_r' X_r$ has full rank, i.e., $\text{rank}(Z_r' X_r) = \min(m, n)$, then it is possible that we did not take enough snapshots, and hence, we increase m, n , until $\text{rank}(Z_r' X_r) < \min(m, n)$.

We take m snapshots for the primal simulation, and we assume that the snapshots are taken at $\Delta T, 2\Delta T, \dots, m\Delta T$, WLOG. Here, ΔT is a small constant, and we require that $m\Delta T \geq t_{ss}$, where $\|A^{t_{ss}}\| \approx 0$. As ΔT increases, each column in Ω_1 is well separated, and hence, the ROM is more accurate, while it takes longer time to generate the snapshots. Thus, this is a trade-off between the accuracy and the computational efficiency.

ROM size selection In Proposition 1, we assume that there are l controllable and observable modes, and we keep exactly l non-zero singular values. However, l is not known a priori. In practice, we decide l by trial and error. We start with $k = \text{rank}(Z_r' X_r)$, and check the eigenvalues of $\tilde{A} = S_r A T_r$. We keep decreasing the value of k until \tilde{A} is stable. From the development in [11], we know there is a region $[l, l + a]$, where a is a small number, such that most of the eigenvalues of \tilde{A} remain the same for different value of k (l controllable and observable modes with $k - l$ perturbations of the zero eigenvalues), then we stop, and pick the number l as the number of non-zero eigenvalues of \tilde{A} .

D. Comparison with Random Projection and BPOD

From the analysis in Section IV-A, we see that the snapshot ensembles collected in RPOD* can be written as:

$$X_r = X_b \Omega_1, Z_r = Z_b \Omega_2, \quad (35)$$

where $X_b \in \mathfrak{R}^{N \times p t_{ss}}, Z_b \in \mathfrak{R}^{N \times q t_{ss}}$ are the impulse response snapshot ensembles that need to be collected in the

BPOD algorithm from time step $(1, \dots, t_{ss})$, and $\|A^{t_{ss}}\| \approx 0$. $\Omega_1 \in \mathfrak{R}^{p t_{ss} \times m}$ and $\Omega_2 \in \mathfrak{R}^{q t_{ss} \times n}$ are Gaussian random matrices. We have:

$$\underbrace{H_r}_{\text{rank } l} = Z_r' X_r = \Omega_2' Z_b' X_b \Omega_1 = \Omega_2' \underbrace{H_b}_{\text{rank } l} \Omega_1, \quad (36)$$

There is a significant difference between the proposed algorithm and a direct application of the random projection algorithm on BPOD. A direct application of the random projection would require to generate the Hankel matrix H_b (and X_b, Z_b) first. However, in practice, the construction and the storage of the Hankel matrix is computationally prohibitive when N is large and the number of inputs/outputs is large. Also, the bottleneck of the random projection algorithm is the projection of X_b, Z_b onto the Gaussian test matrices. In the proposed algorithm, the snapshot ensembles are constructed directly from the primal and adjoint simulations, and hence, the computational cost to generate the Hankel matrix and to project it onto the Gaussian test matrices is saved.

From the analysis in Section IV-C, we know that only $m = l_1$ and $n = l_2$ snapshots needs to be collected in RPOD*, where l_1, l_2 are the number of controllable modes and the number of observable modes respectively. For BPOD, the snapshots are collected from time step $(1, 2, \dots, t_{ss})$, where $\|A^{t_{ss}}\| \approx 0$. In practice, $m, n \propto O(10) \sim O(10^2)$, and $m, n \ll t_{ss}$. As mentioned before, N is the dimension of the system, p, q are the number of inputs and outputs respectively, and WLOG, we assume $p \leq q, m \leq n$.

For constructing $Z' X$ matrix, the computational time using RPOD* is $O(mnN)$, while using BPOD is $O(pqt_{ss}^2 N)$. For solving the SVD problem, the computation time using RPOD* is $O(m^2 n)$, and using BPOD is $O(p^2 qt_{ss}^3)$, where $m, n \ll t_{ss}$. This is a significant saving when the dimension of the system is large, or the number of inputs/ outputs is moderate to large.

V. COMPUTATIONAL RESULTS

The three-dimensional advection-diffusion equation describing the contaminant transport in the atmosphere is:

$$\frac{\partial c}{\partial t} + \nabla \cdot (c\vec{u}) = \nabla \cdot (K(\vec{X})\nabla c) + Q\delta(\vec{X} - \vec{X}_s), \quad (37)$$

where $c(\vec{X}, t)$ denotes mass concentration at location $\vec{X} = (x, y, z)$. $\vec{X}_s = (x_s, y_s, z_s)$ is the location of the point source. $\vec{u} = (4m/s, 0, 0)$ is the wind velocity. Q denotes contaminant emitted rate, ∇ is the gradient operator. $K(\vec{X}) = \text{diag}(K_x(x), K_y(x), K_z(x))$ is a diagonal matrix whose entries are the turbulent eddy diffusivities. In general $K(\vec{X})$ is a function of the downwind distance x only. Define $\sigma_y^2(x) = \frac{2}{u} \int_0^x K_y(\eta) d\eta$, $\sigma_z^2(x) = \frac{2}{u} \int_0^x K_z(\eta) d\eta$, where $\sigma_y(x) = a_y x(1 + b_y x)^{0.5}$, $\sigma_z(x) = a_z x(1 + b_z x)^{0.5}$, and $a_y = 0.008, b_y = 0.00001, a_z = 0.006, b_z = 0.00015$.

The boundary conditions are:

$$\begin{aligned} c(0, y, z) &= 0, c(\infty, y, z) = 0, c(x, \pm\infty, z) = 0, \\ c(x, y, \infty) &= 0, K_z \frac{\partial c}{\partial z}(x, y, 0) = 0. \end{aligned} \quad (38)$$

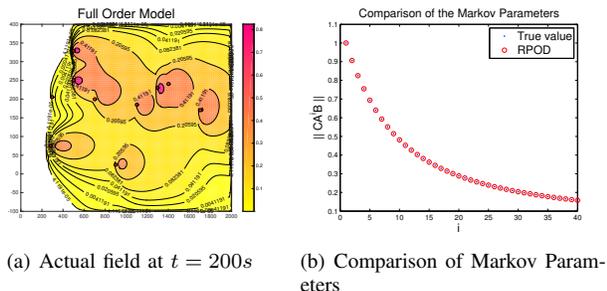


Fig. 2. Atmospheric Dispersion Problem

The system is discretized using finite difference method, and there are $100 \times 100 \times 10$ grids which are equally spaced. We take full field measurements (except the nodes on $x = 0, \infty$ and $y = \pm\infty$). In Fig. 2(a), we show the actual concentration of the full field at time $t = 200s$ with 10 point sources. We take 200 snapshots from $t \in [0, 300]s$ for both primal and adjoint simulations, which leads to a 200×200 SVD problem. We take the first 120 non-zero singular values to construct the ROM. In Fig. 2(b), we compare the Markov parameters of the ROM with the full order system.

It can be seen that the Markov parameters of the full order system and the ROM constructed using RPOD* are approximately the same. Since the system dimension is $N = 10^5$, constructing the ROM with the full field measurements using BPOD is computationally impossible, and thus, for comparison the RPOD* algorithm with BPOD algorithm, we discretize the system into $10 \times 10 \times 10$ grids, and take full field measurements.

For RPOD*, the system is perturbed by white noise with distribution $N(0, I_{10 \times 10})$. We take 200 snapshots which are equispaced from primal/adjoint simulations during time $t \in [0, 2000]s$, where at time $t_{ss} = 2000s$, $\|A^{t_{ss}}\| \approx 0$, and extract 180 modes. For BPOD, we collect 200 impulse responses snapshots which are equispaced from primal/adjoint simulations respectively during time $t \in [0, 2000]s$, and exact 180 modes. In Fig. 3(a), we compare the Markov parameters of the ROM constructed using RPOD* and BPOD with the full order system. Also, we perturb the system with random Gaussian noise, and compare the output relative errors in Fig. 3(b).

For RPOD*, the size of $Z'X$ is 200×200 , the construction of $Z'X$ takes time 2.58(s), and solving the SVD problem takes 0.086(s). For BPOD, the size of $Z'X$ is 162000×2000 , the construction of $Z'X$ takes time 1146.7(s), and solving SVD problem takes time 2357.8(s).

From the examples above, we can see that for a large scale system with even a moderate number of inputs/outputs, BPOD is computational prohibitive. For both examples showed in this paper, the RPOD* algorithm outperforms the BPOD algorithm by orders of magnitude in terms of the accuracy as well as the computation time.

VI. CONCLUSION

In this paper, we have introduced a computationally optimal randomized POD procedure for the extraction of

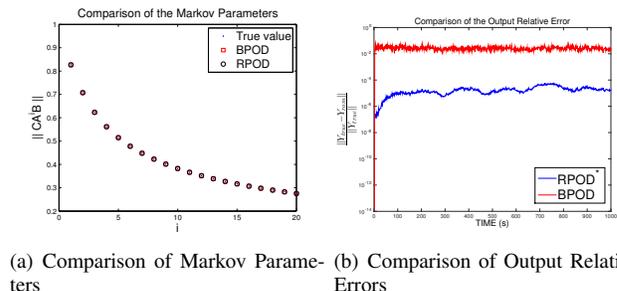


Fig. 3. Comparison between BPOD and RPOD*

ROMs for large scale systems such as those governed by PDEs. The ROM is constructed by perturbing the primal and adjoint system with Gaussian white noise, where the computational cost to construct the snapshot ensembles is saved when compared to perturbing the primal and adjoint system with impulses in BPOD. Also, it leads to a much smaller SVD problem, and an orders of magnitude reduction in the computation required for constructing ROMs over the BPOD procedure. The computational results show that for a large-scale system where BPOD is computationally impermissible, the RPOD* algorithm is still able to solve the problem in real-time.

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