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A scheme for comprehensive computational cost reduction in proper orthogonal decomposition

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This paper addresses the issue of offline and online computational cost reduction of the proper orthogonal decomposition (POD) which is a popular nonlinear model order reduction (MOR) technique. Online computational cost is reduced by using the discrete empirical interpolation method (DEIM), which reduces the complexity of evaluating the nonlinear term of the reduced model to a cost proportional to the number of reduced variables obtained by POD: this is the POD-DEIM approach. Offline computational cost is reduced by generating an approximate snapshot-ensemble of the nonlinear dynamical system, consequently, completely avoiding the need to simulate the full-order system. Two snapshot ensembles: one of the states and the other of the nonlinear function are obtained by simulating the successive linearization of the original nonlinear system. The proposed technique is applied to two benchmark large-scale nonlinear dynamical systems and clearly demonstrates comprehensive savings in computational cost and time with insignificant or no deterioration in performance.

K e y w o r d s: proper orthogonal decomposition, reduced order model, discrete empirical interpolation, approximate snapshot ensemble

1 Introduction

The aim of POD is to obtain a compact system by projecting a high-dimensional system into a low-dimensional subspace while retaining the dominant features of state evolution dynamics. The low dimensional subspace is obtained from state snapshots in response to certain inputs to which the high-dimensional system, *ie* a full order model (FOM) is subjected [1]. However, it is well known that this conventional method of generating a reduced-order model has an associated high computational cost related to the projected high-dimensional nonlinear function. The computational difficulties associated with nonlinear function were recognized early by the model order reduction (MOR) community, and a number of approaches were proposed to overcome these difficulties. These approaches include the missing point estimation (MPE) [2], "best points" method, empirical interpolation method (EIM) [3], and the gappy POD method [4–7]. The MPE method computes the Galerkin projection over a restricted subset of the spatial domain; the gappy POD is a used in the case of sparse measurements. The applications of these methods are closely related to the number of spatial grid points. For a small number of grid points, MPE fails to converge whereas, for the same small number of grid points, gappy POD, EIM and DEIM may converge [8]. EIM was proposed to avoid the complete evaluation of the nonlinear function and in the Jacobian matrix to work iteratively, whereas DEIM [9] is a discrete variant of EIM and represents a well-received effort towards a solution of the nonlinear function.

In [10], which is related to this work, attention of the MOR community has been drawn to the offline computational cost of the POD. In [11], a method was suggested to reduce the procedural-cost for obtaining the reduced-order model, which is offline, so that the process of generating and simulating a reduced-order model leads to overall savings in computational resources. This was done by eliminating the need for computationally heavy, prior simulations of the high-dimensional problem to generate state snapshot-ensembles by proposing to generate an approximate snapshot ensemble obtained from simulations of successive linearization of the nonlinear system.

This paper is an effort to extend the idea of approximate snapshots to the POD-DEIM approach. The aim is to reduce both the online and offline computational cost of the POD procedure. This is done by creating and using approximate snapshot ensembles for the states as well as the nonlinear term of the original high-dimensional system.

We review POD and DEIM, followed by sections on the generation of approximate snapshot ensembles and their subsequent application in DEIM for creating the reduced-order model. Calculation of computational savings are presented and, the proposed approach is validated on two benchmark models, showing improved offline and online computational performance with little to no loss of accuracy. Pseudo-codes are reproduced wherever necessary.

2 Review

2.1 POD

This method produces a low-order approximate description of a higher-order system. For an input func-

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tion or an initial condition applied to a dynamical system whose state-trajectory evolves in R^n, the objective is to approximate it by a trajectory in R^r with $r < n$, [11]. The problem can be stated as follows, Given a set of snapshots $(x^1, x^2, \dots, x^{n_s}) \in R^n$, let $\chi = \text{span}(x^1, x^2, \dots, x^{n_s}) \subset R^n$, and $r = \text{rank}(\chi)$. Find an orthonormal basis vector set $(\phi_1, \phi_2, \dots, \phi_k)$ whose span best approximates χ for given $k < r$. This can be rewritten as a matrix approximation problem: Let $\chi = (x^1, x^2, \dots, x^{n_s}) \subset R^n$, and find $\widetilde{X}$ with $\text{rank}(\widetilde{X}) = k$ such that the error $E = \|\chi - \widetilde{X}\|_2^F$ is minimized. The solution to this $\widetilde{X}$ is given by the Schmidt-Mirsky result [1, p. 37]

$$\widetilde{X} = V_k \Sigma_k W_k^\top \tag{1}$$

where $\chi = V \Sigma W^\top$ is the singular value decomposition (SVD) of χ with the columns of V and W consisting of left and right singular vectors respectively, $\Sigma \in R^{n \times n_s}$ has singular-values $\sigma_1 \geq \sigma_2 \cdots \geq \sigma_r$ on the main-diagonal and other elements are zero. It can be expressed as follows, $\Sigma_k = \text{diag}(\sigma_1, \sigma_2, \dots, \sigma_r) \in R^{k \times k}$, $V_k \in R^{n \times k}$ consists of the first k columns of V and $W_k^\top \in R^{k \times n}$ consists of the top k rows of $W^\top$. The error in the approximation of (1) is

$$\|\chi - \widetilde{X}\| = \sum_{i=k+1}^{r} \sigma_i^2 . \tag{2}$$

Hence the optimal orthonormal basis of rank k which can approximate the state-trajectory evolving in R^n can be written as

$$\{\phi_i\}_{i=1}^k = \{v_i\}_{i=1}^k . \tag{3}$$

The approximation is optimal in the 2-induced norm with the error given by

$$\|\chi - \widetilde{X}\|_2 = \sigma_{k+1} . \tag{4}$$

In reduced order modelling, the POD is used in conjunction with the Galerkin projection [12]. The projection matrix V_k for forming the ROM is the basis obtained from the SVD of the snapshot-ensemble χ and is given by

$$V_k = \{v_i\}_{i=1}^k . \tag{5}$$

In particular, consider the following nonlinear system with input $u(t)$, state vector $x(t)$ and nonlinear function $f\big(x(t)\big)$ where the state trajectory, $x(t)$ evolves in R^n

$$\dot{x}(t) = f\big(x(t)\big) + Bu(t) . \tag{6}$$

B is the input matrix [13]. The reduced order model (ROM) of order $k \ll n$, which approximates the original system from a subspace spanned by a reduced basis of dimension k in R^n is obtained by using Galerkin projection. Using the projection matrix obtained in (5) and projecting the system in (6) onto subspace V_k, the reduced system takes the following form

$$\dot{\widetilde{x}}(t) = V_k^\top f\big(V_k \widetilde{x}(t)\big) + V_k^\top u(t). \tag{7}$$

Here $\widetilde{x}(t) \in R^k$ and $x(t) \approx V_k \widetilde{x}(t)$ with $x(t) \in R^n$. The model in (7) is reduced in state variables, but the evaluation complexity of the nonlinear term still persists, $f\big(V_k \widetilde{x}(t)\big) \in R^n$ as in the original model. To discuss the complexity, consider the low order evolution of the nonlinear term $V_k^\top f\big(V_k \tilde{x}(t)\big)$. For instance, consider the nonlinear function $f = x^3$ and take two modes [14] as follows

$$x^3 = \widetilde{x}_1^3 v_1^3 + 3\widetilde{x}_1^2 \widetilde{x}_2 v_1^2 v_2 + 3\widetilde{x}_1 \widetilde{x}_2^2 v_1 {v_2}^2 + \widetilde{x}_2^3 v_2^3 . \tag{8}$$

The dynamics $\widetilde{x}_1(t)$, $\widetilde{x}_2(t)$ are computed in reduced subspace with respect to basis vector $v_1(s)$ and $v_2(s)$, where s is the space variable. Equation (8) needs double computations for the inner product of order $O(k^3)$.

2.2 DEIM

The discrete empirical interpolation method (DEIM) was introduced to address the computational inefficiency that occurs in solving the reduced-order model derived above. Equation (7) has the nonlinear term

$$N\big(\widetilde{x}(t)\big) = V_k^\top f\big(V_k \widetilde{x}(t)\big). \tag{9}$$

$N\big(\widetilde{x}(t)\big)$ has a computational complexity that depends on n, the dimension of the full-order system [15]. DEIM [9] is an effective way to overcome this difficulty. The function in (7) is approximated by projecting it onto a subspace that approximates the space generated by the nonlinear function and is of dimension, $m \ll n$. From [9], the nonlinear function in (7) can be approximated as

$$\widetilde{f}\big(V_k \widetilde{x}(t)\big) \approx U_m \big(P^\top U_m\big)^{-1} P^\top f\big(V_k \widetilde{x}(t)\big), \tag{10}$$

where the nonlinear function is first projected onto the subspace spanned by the columns of and then U_m distinguished rows are selected by pre-multiplying the whole system with $P^\top$, where $P = [e_{\wp_1}, e_{\wp_2}, \dots, e_{\wp_m}] \in R^{n \times m}$ and $e_{\wp_i}$ is the $\wp_i^{\text{th}}$ column of $I_n \in R^{n \times n}$. The Projection basis $U_m = [v_1, v_2, \cdots\cdots, v_m]$ for the nonlinear function $f(V_k \tilde{x}(t))$ is constructed by applying POD on the nonlinear function snapshots $F = [f(x_1(t)), f(x_2(t)), \dots, f(x_{n_s}(t))]$ obtained from the original system in (6). The interpolation indices $\wp_1, \dots, \wp_m$ are selected from the basis $U_m = [v_1, v_2, \dots, v_m]$ by the DEIM algorithm. Substituting (10) in (9), the nonlinear term can be written as

$$\tilde{N}(\tilde{x}(t)) = V_k^\top U_m (P^\top U_m)^{-1} P^\top f(V_k \tilde{x}(t)) \tag{11}$$

where $P^\top f\big(V_k \widetilde{x}(t)\big)$ in (10) has been replaced by $f\big(P^\top V_k \widetilde{x}(t)\big)$ in (11) if the function f evaluates component-wise at $x(t)$ (see [2]). Further the part $\psi = V_k^\top U_m (P^\top U_m)^{-1}$ can be precomputed [16]. From (7), (9) and (11) the final reduced order model can be written as

$$\dot{\widetilde{x}}(t) = \psi f\big(P^\top V_k \widetilde{x}(t)\big) + V_k^\top Bu(t) . \tag{12}$$

This model in (12) has reduced the complexity of the order from $O(k^3)$ to $O(k)$.

3 Generation of approximate snapshot ensembles of $x(t)$ and $f\big(x(t)\big)$

In [10], It had been shown that an acceptable basis to find V_k can be extracted from an approximate snapshot ensemble of the states $x(t)$. An algorithm to generate such an ensemble was given. To generate approximate snapshots, it was proposed that instead of simulating the nonlinear system, successive linearized systems are simulated. [10] had shown that depending on the evaluation cost of the nonlinear function and its Jacobian as compared to the Gaussian elimination process, substantial savings in computational cost and resources can be obtained. In this paper, we extend the idea of approximate ensemble generation to evaluate U_m from estimates of $f\big(x(t)\big)$ obtained from the approximate trajectory.

To generate the approximate snapshot ensemble for the states, given a training input $u(t)$ and an initial state x_0, the nonlinear system is linearized at x_0. This linear system is simulated till its state vector x reaches a threshold δ from x_0, *ie* , till $\|x-x_0\| < \delta$. At this point another linearization is done, and the new linear system is now simulated. The process continues, with new linearization done wherever the distance between the linear system being simulated from all previous linearization points is greater than δ. The result is that an approximate trajectory of the nonlinear system is traced, and if the state vectors are stacked at each time step (or after some time steps) an approximate snapshot ensemble is obtained. Similarly, $f(x)$ can be estimated from $f(x) \approx \widetilde{f}(x) = A_i x + f(x_i) - A_i x_i$ along the approximate trajectory. The approximate snapshot ensemble for $f(x)$ is thus obtained by stacking the estimates $\widetilde{f}(x)$ at each time step. The pseudo-code for the proposed method is given in Algorithm 1.

Algorithm 1 Approximate snapshot-ensemble generation for x and $f(x)$ and extraction of projection matrices

1. $i \leftarrow 0, j \leftarrow 0, X = [x_j], F = []$, x_o: Initial state, T: Number of simulation time-steps, δ: is an appropriate selected constant
2. Linearize the nonlinear system at x_i, $i = 1, \cdots\cdots, n$.

$$\begin{aligned} \dot{x} &= A_i x + f(x_i) - A_i x_i + Bu(t) \\ y &= Cx(t) \end{aligned} \tag{13}$$

3. $F \leftarrow [F, f(x_i)]$ ▷ Store the $f(x)$ snapshots
4. Simulate equation (12) with initial condition $x = x_j$, for one step
5. $X \leftarrow [X, x_{j+1}]$ ▷ Store the state $x(t)$ snapshot
6. $\tilde{f}(x_{j+1}) = A_i x_{j+1} + f(x_i) - A_i x_i$
7. $\boldsymbol{F} \leftarrow [F \tilde{f}(x_{j+1})]$ ▷ Store the $f(x)$ snapshots
8. $\min_{(0\le k\le i)} \frac{\|x_{j+1}-x_k\|}{\|x_k\|} > \delta$, then
9. $i \leftarrow i+1, j \leftarrow j+1$. Go to step 2
10. Else
11. $j \leftarrow j+1$. Go to step 4
12. End if
13. Snapshot matrix of state vectors (χ), find SVD of it, $\chi = V \Sigma W^\top$
14. Retain columns of V corresponding to singular values larger than some ε_1
15. The projection matrix is $V_k = \{v_i\}_{i=1}^k$
16. F=Snapshot matrix of $f(x)$, find SVD of F, $F = U \Lambda Q^\top$
17. Retain columns of U corresponding to singular values larger than some ε_2
18. The projection matrix is $U_m = \{\upsilon\}_{i=1}^m$

4 DEIM using approximate snapshot ensemble and simulation of the nonlinear system

In this section we describe the algorithm for our proposed method, DEIM using Approximate Snapshot Ensemble ($\mathrm{DEIM_{ae}}$). The inputs to the algorithm are the two projection matrices V_k, U_m obtained using Algorithm-1. The projection basis U_m uniquely determines the interpolation indices and consequently the matrix P. The matrices V_k, U_m, and P are finally used to construct the reduced order model, which gives savings in both online and offline computational cost. The pseudo-code is given in Algorithm 2.

Algorithm 2 Reduced order model using $\mathrm{DEIM_{ae}}$ algorithm

1. Input $U_m = \{\upsilon\}_{i=1}^m$ and $V_k = \{v_i\}_{i=1}^k$ from Algorithm 1.
2. Output sampling matrix, P
3. $[|p|, \rho_1] = \max |\upsilon_1|$,
4. $U_m = [\upsilon_1]$, $P = [e_{\rho_1}]$, $\rho = [\rho_1]$
5. For $l = 2$ to m do
6. Solve $(P^\top U_m)c = P^\top \upsilon_l$ for c
7. $r = \upsilon_l - U_m c$
8. $[|p|, \rho_l] = \max |r|$
9. $U_m \leftarrow [U_m, \upsilon_l]$, $P \leftarrow [P, e_{\rho_l}]$
10. End for
11. Pre-compute offline, $\psi = V_k^\top U_m \big(P^\top U_m\big)^{-1}$
12. Reduced model, $\dot{\tilde{x}}(t) = \psi f\big(P^\top V_k \widetilde{x}(t)\big) + V_k^\top Bu(t)$

5 Computational savings

MOR minimizes computational cost drastically while preserving the physical behavior of the FOM. The computational cost is associated with the number of modes in operators for both linear and nonlinear terms. The number of modes come from orthogonal projection or Galerkin projection (V) and interpolatory projection

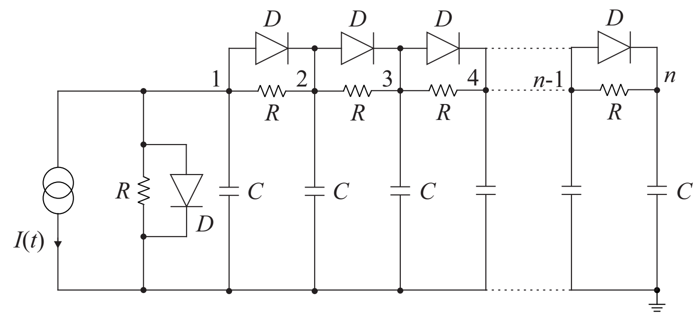

Fig. 1. Nonlinear transmission line model

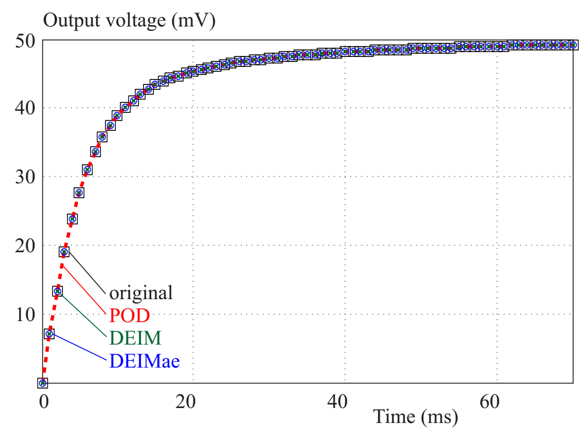

Fig. 2. Output voltage for step input in nonlinear transmission line model

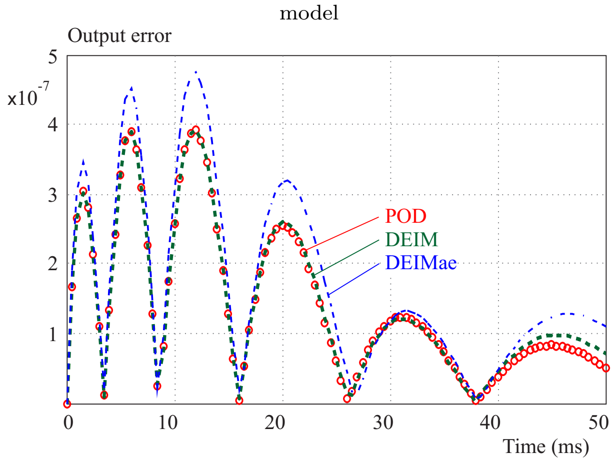

Fig. 3. Output error for step input in nonlinear transmission line model

$\big(U\big(P^\top U^{-1}P^\top\big)$ of linear and nonlinear terms respectively [9]. The computation of $P^\top f\big(V_k\widetilde{x}(t)\big)$ is cheaper than $f\big(V\widetilde{x}(t)\big)$.

The theoretical and approximation errors in orthogonal projection are computed by $E = \big\|\chi - \widetilde{X}\big\|_2^F$ and $\frac{\|x(t)-\widetilde{x}(t)\|}{\|x(t)\|}$ respectively, where $\widetilde{x}(t)$ has been extracted from algorithm 1.

The theoretical error associated with U in DEIM approximation $\widetilde{f}$ and original function f is given as

$$\|f - \widetilde{f}\| \leq \big\|\big(P^\top U_m\big)^{-1}\big\|_2 \big\|\big(I - UU^\top\big)f\big\|_2 . \qquad (14)$$

The value of $\big\|(I - UU^\top f\big\|_2$ should be decreased and $\big\|\big(P^\top U_m^{-1}\big\|_2$ must be bounded, minimal for increasing the accuracy of approximation [16–17]. The approximation error is $\frac{\|f(t)-\widetilde{f}(t)\|}{\|f(t)\|}$, where $\widetilde{f}$ has been extracted from algorithm 1.

In our study, for nonlinear term, two different sets of basis are extracted, one from DEIM approximation and other from the approximate snapshot ensemble, DEIM_{ae}. The extracted basis of the approximate snapshot ensemble completely eliminates residual computation and results in local basis extraction, furthermore, system order is again reduced. The computer memory requirement for basis vector in the online phase drastically goes down using interpolatory matrix instead of orthogonal projection. It was possible due to reduction in size of nonlinearity. As a result the cumulative number of basis vectors is minimal and does not increase drastically for bounded norm-2 error.

6 Numerical Validation

The proposed algorithms are validated on two nonlinear transmission line models shown in Figs. 1 and 6, which serve as benchmark examples for MOR [19–20]. The mathematical equations [21] of the models are formulated as given in (12).

Consider a test source, $u(t) = MH(t)$, where $H(t)$ is the unit-step input starting at $t = 0$ with magnitude $M = 7\,\text{V}$. In our case the input is a current source entering node-1, $u(t) = i(t)$, and the output is chosen to be the voltage at node-1 , $y(t) = x_1(t)$. The order of the larger system is $n = 1000$, and theoretical reduced-order model is truncated at $k = 25$ (POD modes) and $m = 24$ (DEIM modes). The basis coming from the approximate snapshot ensemble are truncated at $k = 18$ (POD modes) and $m = 19$ (DEIM modes) to obtain more cheap lower order model. The results with selected constant $\delta = 5 \times 10^{-4}$ are demonstrated on two benchmark models under different operational scenarios.

Case 1: For Model shown in Fig.1

Using the proposed algorithm 1 for an approximate ensemble generation with the given δ creates 359 linearizations. However, the time taken to simulate successive lin-

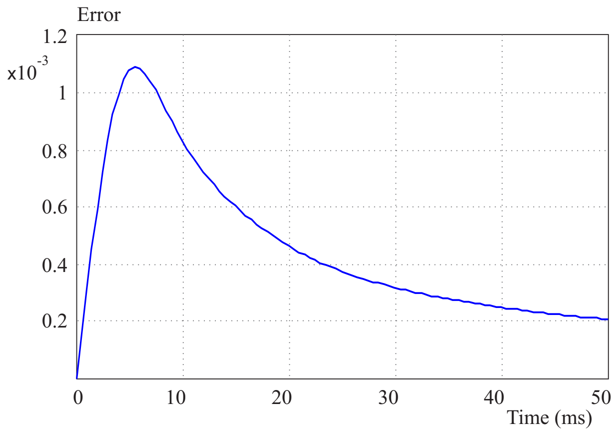

Fig. 4. Error between exact and approximate state for step input in nonlinear transmission line model

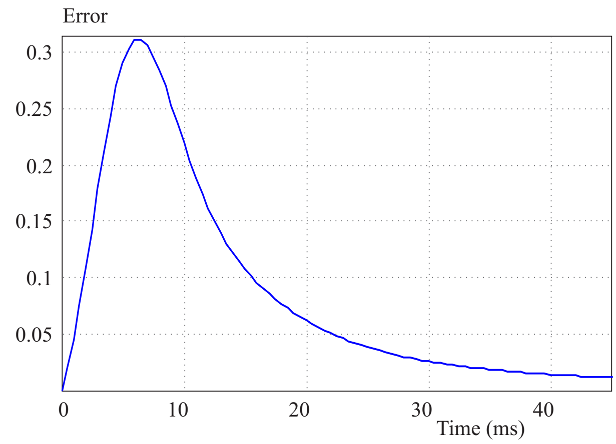

Fig. 5. Error between the exact and approximate nonlinear term in nonlinear transmission line model

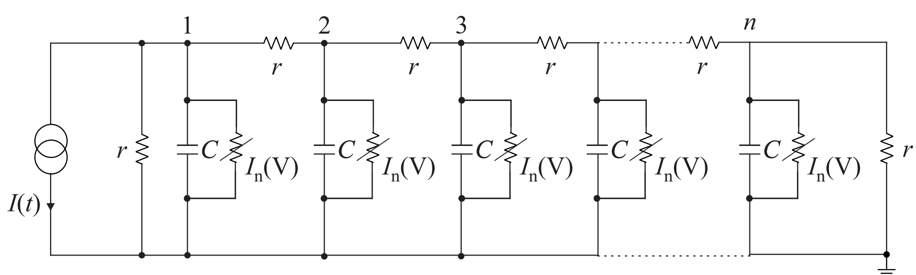

Fig. 6. RC ladder network

Table 1. Comparison of simulation time to find the exact and approximate ensemble basis for $u(t) = 7H(t)$

	Ensemble	
	Exact	Approximate
Time (s)	413.07	32.31

Table 2. Quantitative comparison of errors for the input $u(t) = 7H(t)$

Model	% Error in states	% Error in Output
POD	0.0722	2.88×10^{-4}
DEIM	0.0705	2.89×10^{-4}
DEIM_{ae}	0.0740	3.43×10^{-4}

Table 3. Comparison of simulation time to find the exact and approximate ensemble basis for $u(t) = 7H(t)$

	Ensemble	
	Exact	Approximate
Time (s)	441.65	31.23

Table 4. Quantitative comparison of errors for the input $u(t) = 7H(t)$

Model	% Error in states	% Error in Output
POD	0.1033	5.365×10^{-4}
DEIM	0.1032	5.680×10^{-4}
DEIM_{ae}	0.1587	2.424×10^{-4}

earization is much less as compared to the time required for the full-order simulation, as enumerated in Tab. 1.

The exact and approximate snapshot ensembles of state and nonlinear term are used to find the basis using SVD, and the corresponding ROMs are simulated for the same input. The responses of ROM and FOM are in close agreement. The corresponding output voltage and output error profile are shown in Figs. 2 and 3.

The approximate snapshot-ensemble $\widetilde{x}(t)$ is very close to the exact ensemble $x(t)$. This is evident from the fact that the norm of the approximation error between $x(t)$ and $\widetilde{x}(t)$ evaluated over the complete simulation time is equal to $0.54\,\%$. This is close to the theoretical error of $0.52\,\%$. The error profile between exact and approximate ensemble is shown in Fig. 4.

Using algorithms 1 and 2, approximated nonlinear ensemble $\widetilde{f}(t)$ is very close to the exact nonlinear ensemble $f(t)$. This is evident from the fact that the norm of the approximation error between $f(t)$ and $\widetilde{f}(t)$ evaluated over the complete simulation time is equal to $1.23\,\%$. It is close to the theoretical error of $1.20\,\%$. The error profile in nonlinear term which is independent of input is shown in Fig. 5.

The comparisons of MOR techniques are enumerated in Tab. 2.

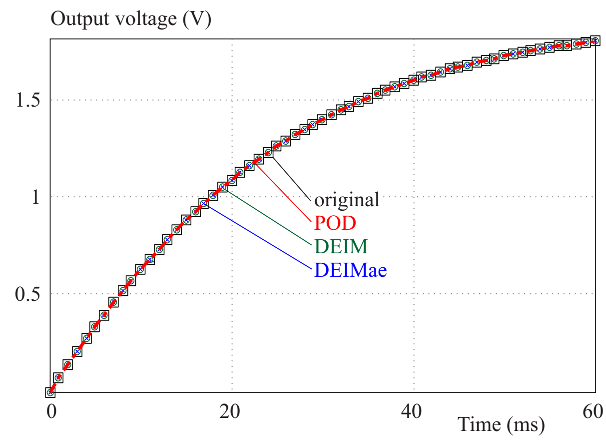

Fig. 7. Output voltage for step input in RC ladder network

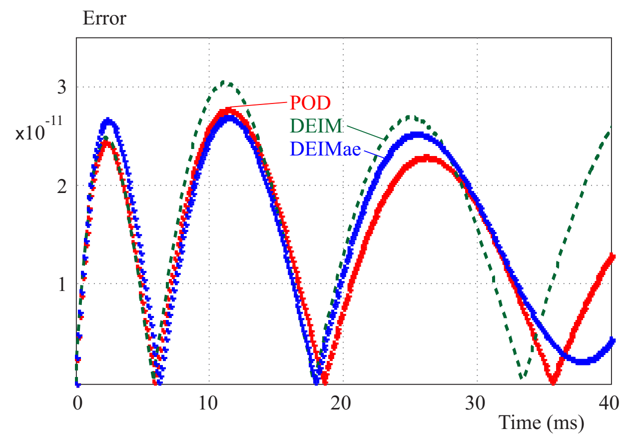

Fig. 8. Output voltage error for step input in RC ladder network

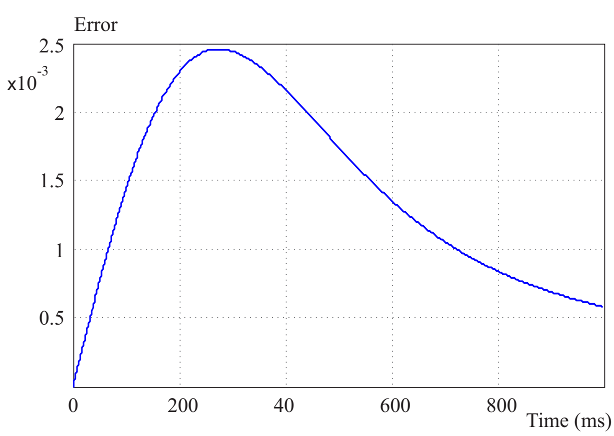

Fig. 9. Error between the exact and approximate state for step input in RC ladder network

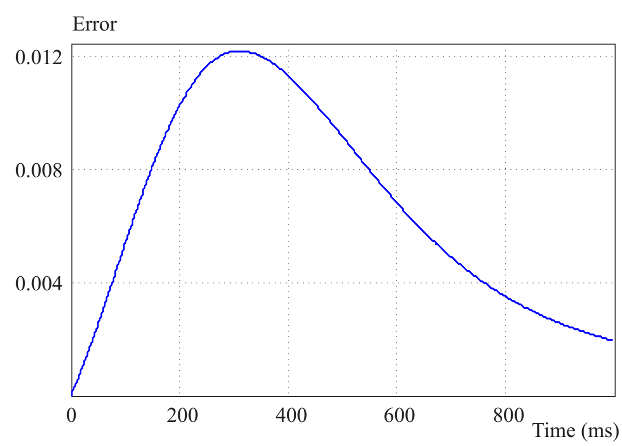

Fig. 10. Error between the exact and approximate nonlinear term in RC ladder network

Case 2: Model-2 as shown in Fig. 6

The proposed algorithm creates 179 linearizations and the time taken to simulate successive linearization is much less as compared to the time required for the full-order simulation, as enumerated in Tab. 3.

The error profile between the exact and approximate ensemble is shown in Fig. 9. The magnitude of approximation error is very less *ie* 0.24 % and is very close to the theoretical error of 0.21 %. The waveforms of the output voltage and output voltage error are shown in Figs. 7 and 8.

The error profile between the exact and approximate ensemble of states is shown in Fig. 9.

Moreover, the responses obtained from the algorithms 1 and 2 are in close agreement with the theoretical models. The norm of the approximation error between $f(t)$ and $\tilde{f}(t)$, evaluated over the complete simulation is equal to 2.1 %. It is close to the theoretical error of 1.99 %. The error profile of the nonlinear term is shown in Fig. 10.

The comparisons of MOR techniques are enumerated in Tab. 4.

Comparing Tabs. 1 and 3, it is observed that considerable improvement in simulation speed is obtained by simulating the reduced model. Tabs. 2 and 4 show that reduced models mimic the behavior of the original model. The sizes of the projection matrices are considerably reduced, which translates into a reduced memory requirement.

The comparison of FOM with ROM (DEIM and DEIM_{ae}) simulation under different scenarios (inputs) shows the transient behavior is accurately reproduced from ROM. Furthermore, for the simulation, no stability problems are observed under different scenarios. The pre-selected threshold values also affect the precision of ROM. Higher threshold values result in a loss of ROM precision. However, the number of basis limits the stability property. The basis selection plays the key role in MOR. Here, the basis is selected in such a way that the error decreases exponentially as given in Figs. 3, 4, 5 and 8, 9, 10 under different operational scenarios. It is clear that the basis extraction from approximate snapshot ensemble gives an acceptable DEIM model. Generally, this model has an error that is a bit more than the exact ensemble, but the overall magnitude is very small. The computational savings are remarkable and the reduction in basis extraction time is significantly improved.

7 Conclusion

In this paper, the idea of an approximate ensemble snapshot generation of basis extraction in POD has been extended to POD-DEIM. The proposed strategy reduces the online as well as offline computational efforts by minimizing the size of orthogonal and interpolatory projections. The reduced size projection matrices have been obtained in two stages truncation one from theoretical and other from the approximate snapshot ensemble. The techniques DEIM and $\mathrm{DEIM}_{\mathrm{ae}}$ had been compared to the performance with respect to each other and to the original FOM. Furthermore, it has been observed that the approximation error in both DEIM and $\mathrm{DEIM}_{\mathrm{ae}}$ is quite sharp and cheap. The numerical results presented in the paper clearly demonstrated saving for computational cost and time. The addressed approach can be extended to analog systems to improve the efficiency and accuracy of the corresponding ROM techniques.

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