01 Jan 2011

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Recommended Citation

J. R. Singler, "Balanced Pod for Model Reduction of Linear PDE Systems: Convergence Theory," *Numerische Mathematik*, Springer Verlag, Jan 2011.
The definitive version is available at https://doi.org/10.1007/s00211-011-0424-x

Balanced POD for Model Reduction of Linear PDE Systems: Convergence Theory

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Abstract

We consider convergence analysis for a model reduction algorithm for a class of linear infinite dimensional systems. The algorithm computes an approximate balanced truncation of the system using solution snapshots of specific linear infinite dimensional differential equations. The algorithm is related to the proper orthogonal decomposition, and it was first proposed for systems of ordinary differential equations by Rowley (Internat. J. Bifur. Chaos Appl. Sci. Engrg., 15(3), 997–1013). For the convergence analysis, we consider the algorithm in terms of the Hankel operator of the system, rather than the product of the system Gramians as originally proposed by Rowley. For exponentially stable systems with bounded finite rank input and output operators, we prove that the balanced realization can be expressed in terms of balancing modes, which are related to the Hankel operator. The balancing modes are required to be smooth, and this can cause computational difficulties for PDE systems. We show how this smoothness requirement can be lessened for parabolic systems, and we also propose a variation of the algorithm that avoids the smoothness requirement for general systems. We prove entrywise convergence of the matrices in the approximate reduced order models in both cases, and present numerical results for two example PDE systems.

1 Introduction

In an earlier work [33], we proposed an algorithm for approximate balanced model reduction of an linear infinite dimensional system using a variation of the proper orthogonal decomposition (POD). The algorithm was an extension of the balanced POD algorithm given by Rowley [30] for finite dimensional systems. In this work, we provide convergence theory for two variations of the algorithm for a class of linear infinite dimensional systems.

Balanced truncation is a standard model reduction procedure originally introduced by Moore [28] for linear systems of ordinary differential equations [11, 36]. For large-scale systems, such as those arising from a discretization of a partial differential equation system, standard algorithms are no longer applicable. Much recent research has focused on the development and analysis of algorithms for such systems [2, 6]. Rowley's approximation of the balanced truncation of a large-scale system is constructed using a variation of the proper orthogonal decomposition with data composed of solution snapshots of certain linear differential equations. For recent applications of balanced POD to model reduction of fluid systems, see [24, 3, 4, 1]. As is often done, one can apply Rowley's algorithm to the discretization of an infinite dimensional system, however we showed in our earlier work that this can lead to incorrect results if one does not properly take into account the underlying infinite dimensional system.

Preprint; published in: Numer. Math. 121 (2012), no. 1, 127-164.

There are many potential advantages in developing the algorithm at the infinite dimensional level, as we do in this work. First, we do not require matrix approximations of the infinite dimensional operators. These matrices can be difficult to obtain for certain problems (such as linearized fluid flow systems), or they may not inherit properties of the infinite dimensional operators. It is possible that losing such properties may slow or destroy convergence of the resulting approximations. Second, computing the solutions of the linear infinite dimensional differential equations arising in the algorithm can be performed with existing simulation code, and one can take advantage of special techniques for accuracy and efficiency improvement. In particular, adaptive refinement techniques can be used to ensure accuracy in the computations. Also, the convergence theory in this work gives easily verifiable conditions guaranteeing the convergence of the approximating reduced order models to the exact balanced truncation.

The development of the algorithm here is slightly different than the derivation of the algorithm given in our earlier work, or Rowley's original paper. Specifically, instead of relating the balancing modes (or balancing transformation, see below) to the product of the Gramians of the system, we relate the balancing modes directly to the Hankel operator of the system. To approximate the balancing modes (or balanced POD) of the system, we use variations of the method of snapshots and the quadrature approach for standard POD. Although the balanced POD procedure differs therefore from the earlier works, the resulting approximations are similar and in some cases identical. However, looking at the algorithm in terms of the Hankel operator results in a clearer convergence analysis.

We now provide a brief background on balanced truncation and give an outline of our approach.

1.1 Background and Approach

Balanced model reduction finds a low order system

$$\dot{a}(t) = A_r a(t) + B_r u(t), \quad y_r(t) = C_r a(t),$$

that is an approximation to the system

$$\dot{x}(t) = Ax(t) + Bu(t), \quad y(t) = Cx(t),$$

in the sense that the input-to-output error is small. Specifically, let $G(s) = C(sI - A)^{-1}B$ and $G_r(s) = C_r(sI_r - A_r)^{-1}B_r$ be the transfer functions of the original and reduced systems. Then the balanced truncation satisfies the error bound

$$\|G - G_r\|_\infty \leq 2 \sum_{k>r} \sigma_k, \tag{1}$$

where $\{\sigma_k\}$ are the ordered Hankel singular values of the system (see Section 2), and the $\mathcal{H}^\infty$ norm is the largest singular value of the function along the imaginary axis. Therefore, if the Hankel singular values decay rapidly, then the approximation error can be made small for a small value of r.

Balanced truncation is a well known technique for systems of ordinary differential equations. One can find a different system realization (A^b, B^b, C^b), called the balanced realization, which has the same transfer function G as the original system; furthermore, the controllability and observability Gramians Z_B^b and Z_C^b of the balanced system are equal and diagonal. The Gramians are the solutions of the Lyapunov equations

$$A^b Z_B^b + Z_B^b (A^b)^* + B^b (B^b)^* = 0, \quad (A^b)^* Z_C^b + Z_C^b A^b + (C^b)^* C^b = 0,$$

and the diagonal entries of the Gramians are the Hankel singular values of the system. The balanced truncated model can be computed by first finding a transformation to balance the system, and then truncating the balanced realization according to the size of the Hankel singular values.

For infinite dimensional systems, the balancing theory can be found in [8, 14]; see also the review in [7]. The balanced realization exists when the Hankel operator is trace class (or nuclear), i.e., when the (infinite) sum of the Hankel singular values is finite – note that this condition is necessary for the balancing error bound (1) to be finite. The balanced realization holds over ℓ^2, the Hilbert space of square summable sequences, and the Gramians are equal to infinite diagonal matrices with the Hankel singular values again along the diagonals.

If we follow the above procedure to compute the balanced truncation in the finite dimensional case, we would first apply a transformation to the infinite dimensional system (A, B, C) to arrive at the infinite dimensional balanced system (A^b, B^b, C^b), and then truncate. However, it is not clear that such a transformation would be well defined. For exponentially stable infinite dimensional systems with bounded, finite rank input and output operators, we show that we may indeed write the balanced realization (A^b, B^b, C^b) in terms of the original system operators (A, B, C) and the balancing modes. This result is presented in Section 2, and the proof is given in Section 5.

Once we have this representation of the balanced realization, in Section 3 we present an overview of the snapshot balanced truncation algorithm in general form. The balancing modes are required to be smooth, and this can cause computational difficulties for PDE systems. We show how this smoothness requirement can be weakened for parabolic systems, and we also propose a variation of the algorithm that avoids the smoothness requirement for general systems. The approximation of the balancing modes (or balanced proper orthogonal decomposition) is considered in detail in Section 4. The proofs of convergence for balanced POD and the balanced POD model reduction algorithm in both cases are given in Section 6. We follow with numerical results for two example PDE systems, and then discuss open questions.

Before we present the balancing modes and the balanced realization in Section 2, we give our assumptions on the infinite dimensional system (A, B, C) and define notation used throughout this work.

1.2 Assumptions and Notation

Unless otherwise indicated, let X be a separable infinite dimensional Hilbert space with inner product $(\cdot, \cdot)$ and corresponding norm $\|\cdot\| = (\cdot, \cdot)^{1/2}$. For simplicity, we assume the inner product is real valued. We consider infinite dimensional systems with operators A, B, and C having the following properties. The operator $A : D(A) \subset X \to X$ generates an exponentially stable[1] C_0-semigroup e^{At} over X, and the operators $B : \mathbb{R}^m \to X$ and $C : X \to \mathbb{R}^m$ are both finite rank and bounded. This assumption implies that B and C must take the form

$$Bu = \sum_{j=1}^{m} b_j u_j, \quad Cx = [\,(x, c_1), \ldots, (x, c_p)\,]^T$$

where each b_j and c_j are in X and $u = [\,u_1, \ldots, u_m\,]^T \in \mathbb{R}^m$ (see [35, Theorem 6.1]).

Although we focus on the infinite dimensional case in this work, the algorithms are also applicable to finite dimensional systems. In this case, X is taken to be $\mathbb{R}^n$ and the inner product can be taken as the standard dot product, $(a, b) = a^T b$, or a weighted dot product, $(a, b) = a^T M b$, where $M \in \mathbb{R}^{n \times n}$ is symmetric positive definite. The matrix $A \in \mathbb{R}^{n \times n}$ is exponentially stable,

[1] that is, there are constants $M \geq 1$ and $\omega > 0$ such that $\|e^{At}x\| \leq Me^{-\omega t}\|x\|$ for all $x \in X$

$B \in \mathbb{R}^{n \times m}$, and $C \in \mathbb{R}^{p \times n}$. The above representations of the operators B and C also hold for the matrix problem; in this case, b_j is the jth column of B and c_j is the transpose of the jth row of C.

We require the following spaces of time varying functions taking values in a Banach space X. For $1 \leq p < \infty$, let $L^p(0, \infty; X)$ be the Banach space of all functions x such that $x(t) \in X$ for all $t > 0$ with finite norm

$$\|x\|_{L^p(0,\infty;X)} = \left(\int_0^\infty \|x(t)\|^p \, dt \right)^{1/p}.$$

A sequence of functions $\{x_k\} \subset L^p(0, \infty; X)$ converges to $x \in L^p(0, \infty; X)$ if $\|x_k - x\|_{L^p(0,\infty;X)} \to 0$ as $k \to \infty$. When $p = 2$ and X is a Hilbert space, $L^2(0, \infty; X)$ is a Hilbert space with inner product

$$(x, y)_{L^2(0,\infty;X)} = \int_0^\infty (x(t), y(t)) \, dt.$$

When the space is understood from the context, we will not use subscripts to denote the space on norms or inner products.

2 Balancing Modes and the Balanced Realization

In our earlier work [33], we followed Rowley [30] and used alternate representations of the controllability and observability Gramians of the system (A, B, C) to derive a snapshot balancing algorithm. Here, as indicated above, we take a slightly different approach and use an alternate representation of the Hankel operator of the system to derive the algorithm and study its convergence.

The Hankel operator $\mathcal{H} : L^2(0, \infty; \mathbb{R}^m) \to L^2(0, \infty; \mathbb{R}^p)$ of the linear system (A, B, C) is defined by

$$[\mathcal{H}u](t) = [\mathcal{C}\mathcal{B}u](t) = \int_0^\infty Ce^{A(t+s)}Bu(s) \, ds,$$

where the controllability operator $\mathcal{C} : X \to L^2(0, \infty; \mathbb{R}^p)$ and the observability operator $\mathcal{B} : L^2(0, \infty; \mathbb{R}^m) \to X$ are defined by

$$[\mathcal{C}x](t) = Ce^{At}x, \quad \mathcal{B}u = \int_0^\infty e^{As}Bu(s) \, ds.$$

The adjoint operators $\mathcal{C}^* : L^2(0, \infty; \mathbb{R}^p) \to X$ and $\mathcal{B}^* : X \to L^2(0, \infty; \mathbb{R}^m)$ are given by

$$\mathcal{C}^*y = \int_0^\infty e^{A^*s}C^*y(s) \, ds, \quad [\mathcal{B}^*x](t) = B^*e^{A^*t}x$$

In our earlier work [33], we provided alternate forms for these operators; we repeat the short proof here for completeness.

Proposition 1. *Under the above assumptions, the operators $\mathcal{C}$, $\mathcal{C}^*$, $\mathcal{B}$, and $\mathcal{B}^*$ defined above are also given by*

$$[\mathcal{C}x](t) = [\, (x, z_1(t)), \, \ldots \, , (x, z_p(t)) \,]^T, \quad \mathcal{C}^*y = \int_0^\infty \sum_{j=1}^p y_j(s)z_j(s) \, ds, \tag{2}$$

$$\mathcal{B}u = \int_0^\infty \sum_{j=1}^m u_j(s)w_j(s) \, ds, \quad [\mathcal{B}^*x](t) = [\, (x, w_1(t)), \, \ldots \, , (x, w_m(t)) \,]^T, \tag{3}$$

where $z_i(t) = e^{A^* t} c_i$ *and* $w_j(t) = e^{At} b_j$ *are in* $L^2(0, \infty; X)$ *and are the unique solutions of the linear evolution equations*

$$\dot{z}_i(t) = A^* z_i(t), \qquad z_i(0) = c_i, \tag{4}$$

$$\dot{w}_j(t) = A w_j(t), \qquad w_j(0) = b_j, \tag{5}$$

for $i = 1, \ldots, p$ *and* $j = 1, \ldots, m$.

Proof. Given the above assumptions on B, the operator must have the form $Bu = \sum_{j=1}^{m} b_j u_j$, where $u = [\, u_1, \, \ldots \, , u_m \,]^T \in \mathbb{R}^m$, and each b_j is in X. Then we have

$$\mathcal{B}u = \int_0^\infty e^{As} B u(s)\, ds = \int_0^\infty \sum_{j=1}^{m} u_j(s) w_j(s)\, ds,$$

where $w_j(t) = e^{At} b_j$ is the solution of the linear evolution equation (5) for $j = 1, \ldots, m$. Since e^{At} is exponentially stable, there are constants $M \geq 1$ and $\omega > 0$ so that $\|e^{At} x\| \leq M e^{-\omega t} \|x\|$ for any $x \in X$; therefore, each w_j is in $L^2(0, \infty; X)$. Computing the adjoint of this representation of $\mathcal{B}$ shows that $\mathcal{B}^*$ takes the above form.

The expressions for $\mathcal{C}^*$ and $\mathcal{C}$ are proved in a similar fashion. □ □

Remark 1. If c_i is not in $D(A^*)$, then $z_i(t) = e^{A^* t} c_i$ is not necessarily a classical solution of the differential equation (4). Also, if $b_j \notin D(A)$, then $w_j(t) = e^{At} b_j$ may not be a classical solution of (5). However, $z_i(t)$ and $w_j(t)$ are the unique solutions of (4) and (5) in a generalized or weak sense; see, e.g., [10, Example A.5.29] or [29, page 105]. Throughout this work, a solution of an infinite dimensional differential equation is always understood in a generalized or weak sense.

Since the Hankel operator $\mathcal{H}$ is given by $\mathcal{H} = \mathcal{C}\mathcal{B}$, the above representations of the controllability and observability operators immediately give the following alternate expression for the Hankel operator.

Corollary 1. *Under the above assumptions, the Hankel operator* $\mathcal{H} : L^2(0, \infty; \mathbb{R}^m) \to L^2(0, \infty; \mathbb{R}^p)$ *of the system* (A, B, C) *is given by*

$$[\mathcal{H}u](t) = \int_0^\infty k(t, s) u(s)\, ds, \tag{6}$$

where the $p \times m$ *kernel function* $k(t, s)$ *has* ij *entries*

$$k_{ij}(t, s) = (z_i(t), w_j(s)),$$

and $z_i(t) = e^{A^* t} c_i$ *and* $w_j(t) = e^{At} b_j$ *are the unique solutions of the linear evolution equations (4) and (5), for* $i = 1, \ldots, p$ *and* $j = 1, \ldots, m$.

For the class of systems (A, B, C) considered here, the Hankel operator is known to be trace class (or nuclear), and therefore compact [9, Theorem 4]. Therefore, there exist singular values $\sigma_1 \geq \sigma_2 \geq \cdots \geq 0$ (with repetitions according to multiplicity) and corresponding singular vectors $\{f_k(\cdot)\} \subset L^2(0, \infty; R^m)$ and $\{g_k(\cdot)\} \subset L^2(0, \infty; R^p)$ satisfying

$$\mathcal{H} f_k = \sigma_k g_k, \quad \mathcal{H}^* g_k = \sigma_k f_k.$$

The singular vectors are also orthonormal with respect to the L^2 inner product:

$$(f_j, f_k)_{L^2(0,\infty;R^m)} = \int_0^\infty f_j^T(t) f_k(t)\, dt = \delta_{jk},$$
$$(g_j, g_k)_{L^2(0,\infty;R^p)} = \int_0^\infty g_j^T(t) g_k(t)\, dt = \delta_{jk},$$

where δ_{jk} is the Kronecker delta. If σ_j is nonzero define the jth balancing modes φ_j and ψ_j in X by

$$\varphi_j = \sigma_j^{-1/2} \mathcal{B} f_j = \sigma_j^{-1/2} \int_0^\infty \sum_{k=1}^{m} f_{j,k}(t) w_k(t)\, dt, \tag{7}$$

$$\psi_j = \sigma_j^{-1/2} \mathcal{C}^* g_j = \sigma_j^{-1/2} \int_0^\infty \sum_{k=1}^{p} g_{j,k}(t) z_k(t)\, dt, \tag{8}$$

where $f_{j,k}$ and $g_{j,k}$ are the kth components of f_j and g_j.

With this background, we present how the balanced realization (A^b, B^b, C^b) of the infinite dimensional system (A, B, C) can be obtained using the balancing modes. Our proof, which is found in Section 5, relies on the exact representation of the balanced realization in terms of the Hankel singular values and singular vectors given by Curtain and Glover [8]. As in that work, we assume the Hankel singular values are distinct throughout.

Theorem 1. *Let X be a separable infinite dimensional Hilbert space with real-valued inner product $(\cdot,\cdot)$. Suppose the operator $A : D(A) \subset X \to X$ generates an exponentially stable C_0-semigroup over X, and the operators $B : X \to \mathbb{R}^m$ and $C : X \to \mathbb{R}^p$ are bounded. If the Hankel singular values of the system (A, B, C) are distinct, then the following hold:*

1. *The balancing modes defined in (7) and (8) satisfy $\varphi_i \in D(A)$ and $\psi_i \in D(A^*)$ for each i, and*
$$A\varphi_i = -\sigma_i^{-1/2}\Big(\mathcal{B}\dot{f}_i + Bf_i(0)\Big), \quad A^*\psi_i = -\sigma_i^{-1/2}\Big(\mathcal{C}^*\dot{g}_i + C^* g_i(0)\Big). \tag{9}$$

2. *A balanced realization (A^b, B^b, C^b) over ℓ^2 of the system (A, B, C) is given by*
$$A^b_{ij} = (A\varphi_j, \psi_i) = (\varphi_j, A^*\psi_i), \tag{10}$$
$$B^b_{ij} = (b_j, \psi_i), \tag{11}$$
$$C^b_{ij} = (\varphi_j, c_i), \tag{12}$$
where $Bu = \sum_{j=1}^m u_j b_j$ and $Cx = [(x, c_1), \ldots, (x, c_p)]^T$, with each b_j and c_j in X.

The assumptions of the theorem guarantee that all of the Hankel singular values are nonzero and therefore the balancing modes are well defined.

3 Balanced POD Model Reduction Algorithm

We now describe implementation of the balanced POD algorithm for approximate balanced truncation of the class of infinite dimensional systems considered above. The algorithms are also valid for the finite dimensional case; however, we focus on the infinite dimensional case. Convergence theory is found in Section 6.

We begin by describing a basic balanced POD algorithm. We approximate the above representation of the Hankel operator by approximating the solutions of the differential equations (4) and (5). We then use these solution snapshots to approximate the Hankel singular values and singular vectors and use these to construct the balancing modes and the balanced truncated system.

Basic Balanced POD Algorithm for Balanced Truncation Model Reduction:

1. For $i = 1, \ldots, p$, compute an approximation $z_i^N(t)$ to the solution $z_i(t) = e^{A^* t} c_i$ of the linear differential equation (4).

2. For $j = 1, \ldots, m$, compute an approximation $w_j^N(t)$ to the solution $w_j(t) = e^{At} b_j$ of the linear differential equation (5).

3. Compute approximations $\{\sigma_k^N\}$, $\{f_k^N(\cdot)\}$, and $\{g_k^N(\cdot)\}$ of the Hankel singular values and singular vectors, e.g., by the balanced POD method of snapshots or quadrature method presented in Section 4.1.

4. Choose r and form the first r approximate balancing modes given by

$$\varphi_j^N = (\sigma_j^N)^{-1/2} \int_0^\infty \sum_{k=1}^m f_{j,k}^N(t) w_k^N(t)\, dt, \tag{13}$$

$$\psi_i^N = (\sigma_i^N)^{-1/2} \int_0^\infty \sum_{k=1}^p g_{i,k}^N(t) z_k^N(t)\, dt, \tag{14}$$

   where $f_{j,k}^N$ and $g_{i,k}^N$ are the kth components of f_j^N and g_i^N.

5. Use the modes to approximate the matrices in the balanced truncated model (A_r, B_r, C_r):

$$\begin{aligned} A_r^N &= [\,(A\varphi_j^N, \psi_i^N)\,] = [\,(\varphi_j^N, A^*\psi_i^N)\,] \in \mathbb{R}^{r\times r}, \\ B_r^N &= [\,(b_j, \psi_i^N)\,] \in \mathbb{R}^{r\times m}, \\ C_r^N &= [\,(\varphi_j^N, c_i)\,] \in \mathbb{R}^{p\times r}, \end{aligned} \tag{15}$$

Remark 2. Above we dropped the superscript b on the operators of the balanced truncated realization. We follow this convention in the remainder of this work.

A difficulty in constructing the approximate reduced model in this way is computing the matrix A_r. Specifically, the approximate balancing modes $\{\varphi_j^N\}$ must be in the domain of A (or $\{\psi_i^N\}$ must be in the domain of A^*) for the computation to even make sense. By definition (13)-(14), the approximate balancing modes automatically inherit the smoothness of the approximate solution data $\{z_i^N, w_j^N\}$. Certain numerical methods for partial differential equations (e.g., finite elements, discontinuous Galerkin methods, etc.) produce approximate solution data with less smoothness than the domain of A (or A^*), and therefore the approximate balancing modes may not have the required smoothness to directly form A_r.

We focus on two ways to circumvent this difficulty. First, we consider parabolic systems arising from a continuous sesquilinear form, and we use properties of these systems to directly approximate the entries of the matrix A_r by lessening the smoothness requirement on the balancing modes. Second, we consider general systems and compute the entries of the matrix A_r^N by directly approximating $A\varphi$ or $A^*\psi$ using expression (9) of Theorem 1.

3.1 Parabolic Systems

First, consider parabolic systems arising from a continuous sesquilinear form. Assume there is another Hilbert space V with inner product $(\cdot,\cdot)_V$ and corresponding norm $\|\cdot\|_V = (\cdot,\cdot)_V^{1/2}$ that is continuously embedded in X, i.e., V is a dense subspace of X and there is a positive constant C so that $\|v\| \leq C\|v\|_V$ for all $v \in V$. An operator $A : D(A) \subset X \to X$ can be derived from a continuous sesquilinear form $a : V \times V \to \mathbb{R}$ (which we assume is real valued for simplicity) as follows:

$$Ax = y \quad \text{if there is a } y \in X \text{ so that} \quad (y, v) = -a(x, v) \quad \text{for all } v \in V. \tag{16}$$

The set $D(A)$ consists of all functions x in V where there is a y (which must be unique) such that the above holds. We assume the sesquilinear form is bounded and coercive, i.e.,

$$a(u, v) \leq C\|u\|_V \|v\|_V, \quad a(v, v) + \lambda\|v\|^2 \geq \alpha\|v\|_V^2, \tag{17}$$

for some constants $C > 0$, $\lambda \geq 0$, and $\alpha > 0$, and all vectors u and v in V. Then the operator A generates an analytic C_0-semigroup (see, e.g., [27, Section 4.5]), which we assume is exponentially stable. The adjoint operator $A^* : D(A^*) \subset X \to X$ can also be derived from the sesquilinear form: $x \in D(A^*)$ and $A^*x = y$ if there is a $y \in X$ so that $(y, v) = -a(v, x)$ for all $v \in V$.

Using the above representation (16) of A, the approximation of the reduced model (A_r, B_r, C_r) takes the form

$$A_r^N = [\, -a(\varphi_j^N, \psi_i^N)\,], \quad B_r^N = [\,(b_j, \psi_i^N)\,], \quad C_r^N = [\,(\varphi_j^N, c_i)\,]. \tag{18}$$

To form A_r^N, the approximate balancing modes are now only required to be in the space V. Elements of the space V are "smoother" than elements of X, but not as smooth as elements of $D(A)$ and $D(A^*)$. Therefore, we relax the smoothness requirements of the approximate balancing modes. Many numerical schemes for parabolic equations construct approximations in V; we may use such methods to construct approximate balancing modes with the required smoothness.

Therefore, the basic balanced POD algorithm above remains the same except (i) the approximate solutions $z_i^N(t)$ and $w_j^N(t)$ of the differential equations must take values in the space V, and (ii) the reduced order model is formed using equation (18) above.

3.2 General Systems

Next, we describe a modification of the basic balanced POD algorithm that is valid for general systems (A, B, C).

As mentioned above, in forming the entries of the matrix A_r it may be difficult to construct smooth approximate balancing modes φ_j^N and ψ_i^N so that $A\varphi_j^N$ and $A^*\psi_i^N$ are well defined. An alternative approach is to approximate $A\varphi_j$ or $A^*\psi_i$ directly using the representations (9) of Theorem 1, which we rewrite in terms of the data $z_i(t) = e^{A^*t}c_i$ and $w_j(t) = e^{At}b_j$ as follows:

$$\begin{aligned} A\varphi_i &= -\sigma_i^{-1/2}\Big(\int_0^\infty \sum_{j=1}^m w_j(t)\, \dot{f}_{i,j}(t)\, dt + \sum_{j=1}^m w_j(0)\, f_{i,j}(0)\Big), \\ A^*\psi_i &= -\sigma_i^{-1/2}\Big(\int_0^\infty \sum_{j=1}^p z_j(t)\, \dot{g}_{i,j}(t)\, dt + \sum_{j=1}^m z_j(0)\, g_{i,j}(0)\Big), \end{aligned}$$

where, as before, $f_{i,j}$ and $g_{i,j}$ are the jth components of f_i and g_i.

Therefore, the basic balanced POD algorithm is modified as follows. In addition to computing approximations $\{\sigma_k^N, f_k^N, g_k^N, \varphi_k^N, \psi_k^N\}$ to the Hankel singular values, singular vectors, and balancing modes, we require approximations $\{\xi_k^N, \eta_k^N\}$ to the derivatives $\{\dot{f}_k, \dot{g}_k\}$ and approximations $\{f_k^N(0), g_k^N(0)\}$ of the values $\{f_k(0), g_k(0)\}$. Then form either of the approximations $\Phi_i^N \approx A\varphi_i$ or $\Psi_i^N \approx A^*\psi_i$ by

$$\begin{aligned}\Phi_i^N &= -(\sigma_i^N)^{-1/2}\Big(\int_0^\infty \sum_{j=1}^m w_j^N(t)\, \xi_{i,j}^N(t)\, dt + \sum_{j=1}^m w_j^N(0)\, f_{i,j}^N(0)\Big),\\ \Psi_i^N &= -(\sigma_i^N)^{-1/2}\Big(\int_0^\infty \sum_{j=1}^p z_j^N(t)\, \eta_{i,j}^N(t)\, dt + \sum_{j=1}^m z_j^N(0)\, g_{i,j}^N(0)\Big),\end{aligned}$$

The matrices B_r and C_r in the reduced model are computed as before, but the entries of the matrix A_r are computed as

$$A_{r,ij}^N = [\,(\Phi_j^N, \psi_i^N)\,], \quad \text{or} \quad A_{r,ij}^N = [\,(\varphi_j^N, \Psi_i^N)\,].$$

Approximating the derivatives of the singular vectors is discussed below in Section 4.1.3.

4 Balanced Proper Orthogonal Decomposition

We now define the (continuous time) balanced proper orthogonal decomposition of two datasets $\{z_i\}_{i=1}^p \subset L^2(0,\infty;X)$ and $\{w_j\}_{j=1}^m \subset L^2(0,\infty;X)$ and discuss its properties. When the data $\{z_i, w_j\}$ is given by $z_i(t) = e^{A^*t}c_i$ and $w_j(t) = e^{At}b_j$, i.e., the unique solutions of the linear evolution equations (4) and (5), then the balanced POD of $\{z_i, w_j\}$ consists of the Hankel singular values, Hankel singular vectors, and balancing modes for the system (A, B, C).

In practice, we will not have the exact data $\{z_i, w_j\}$, but we will have approximate data $\{z_i^N, w_j^N\}$. In Section 4.1 below, we discuss snapshot and quadrature approaches for approximating the balanced POD of $\{z_i, w_j\}$ given approximate data. We also discuss approximating the derivatives of the singular vectors for the exact data $z_i(t) = e^{A^*t}c_i$ and $w_j(t) = e^{At}b_j$ in Section 4.1.3.

The approach to balanced POD considered here relies on concepts from both Rowley's original algorithm [30], and standard (continuous time) POD for data in a Hilbert space as found in the recent works of Kunisch and Volkwein [25, 26] and Henri and Yvon [18, 19, 20]. We note that balanced POD provides an optimal reconstruction of two general datasets [32] in an analogous way that standard POD optimally reconstructs a single dataset, e.g., [22].

We now define the balanced POD operator, which is the analogue of the Hankel operator. The singular value decomposition of this operator allows us to define analogues of the Hankel singular values, Hankel singular vectors, and balancing modes for any two collections of functions $\{z_i\}$ and $\{w_j\}$ in $L^2(0,\infty;X)$.

Definition 1. *The balanced POD operator $\mathcal{H} : L^2(0,\infty;\mathbb{R}^m) \to L^2(0,\infty;\mathbb{R}^p)$ for two datasets $\{z_i\}_{i=1}^p \subset L^2(0,\infty;X)$ and $\{w_j\}_{j=1}^m \subset L^2(0,\infty;X)$ is defined by*

$$[\mathcal{H}u](t) = \int_0^\infty k(t,s)u(s)\, ds, \tag{19}$$

where the $p \times m$ kernel function $k(t,s)$ has ij entries $k_{ij}(t,s) = (z_i(t), w_j(s))$.

In Proposition 4 below, we prove that the balanced POD operator for any two datasets $\{z_i\}_{i=1}^p \subset L^2(0,\infty;X)$ and $\{w_j\}_{j=1}^m \subset L^2(0,\infty;X)$ is trace class and therefore compact. Therefore, there exist singular values $\sigma_1 \geq \sigma_2 \geq \cdots \geq 0$ (with repetitions according to multiplicity) and corresponding singular vectors $\{f_k(\cdot)\} \subset L^2(0,\infty;R^m)$ and $\{g_k(\cdot)\} \subset L^2(0,\infty;R^p)$ satisfying $\mathcal{H} f_k = \sigma_k g_k$, and $\mathcal{H}^* g_k = \sigma_k f_k$. The singular vectors are also orthonormal with respect to the L^2 inner product, i.e., $(f_j, f_k)_{L^2(0,\infty;R^m)} = \delta_{jk}$ and $(g_j, g_k)_{L^2(0,\infty;R^p)} = \delta_{jk}$. We call these quantities the balanced POD singular values and singular vectors, or the balancing singular values and singular vectors, for the data $\{z_i, w_j\}$. We define the balanced POD modes, or balancing modes, for $\{z_i, w_j\}$ by

$$\varphi_j = \sigma_j^{-1/2} \int_0^\infty \sum_{k=1}^m f_{j,k}(t) w_k(t)\, dt, \quad \psi_i = \sigma_i^{-1/2} \int_0^\infty \sum_{k=1}^p g_{i,k}(t) z_k(t)\, dt, \tag{20}$$

where $f_{j,k}$ and $g_{i,k}$ are the kth components of f_j and g_i. We refer to the balancing singular values and balancing modes as the balanced POD of the two datasets $\{z_i\}$ and $\{w_j\}$.

4.1 Approximating the Balanced Proper Orthogonal Decomposition

As with the standard continuous time proper orthogonal decomposition, the balanced POD of two datasets can be approximated using many methods. We provide variations on the method of snapshots and the quadrature approach for standard POD to balanced POD. In the method of snapshots, the main idea is to approximate the time-varying data with functions whose balanced POD singular values and modes are easily computable. In the quadrature approach, the balanced POD integral operator is approximated using quadrature leading to easily computable approximate balanced POD singular values and modes. For standard POD, there are algorithms to compute the POD of very large datasets [5, 13]. We are not aware of any similar algorithms for balanced POD; we leave this for future work.

4.1.1 Snapshot Approach

We begin with the method of snapshots for balanced POD. This method is a variation on the method of snapshots for standard POD introduced by Sirovich in [34]. A popular approach to the method of snapshots is to use piecewise constant functions (in time) to approximate the time varying data. It is possible to generalize this algorithm if more variation in time is desired.

We focus on the case of a single function in each dataset. The case of multiple functions is similar and can be treated by "stacking" the data as in the original quadrature approach (see [30, 33]). Let z and w in $L^2(0,\infty;X)$ be piecewise constant functions defined by

$$z(t) = \sum_{i=1}^{N_z} a_i^z \chi_i^z(t), \quad w(t) = \sum_{i=1}^{N_w} a_i^w \chi_i^w(t), \tag{21}$$

where each a_i^z and a_i^w are in X, and the weighted characteristic functions χ_i^z and χ_i^w are defined by

$$\chi_i^z(t) = \begin{cases} \delta_i^z, & t_{i-1}^z < t < t_i^z \\ 0, & \text{otherwise} \end{cases}, \quad \chi_i^w(t) = \begin{cases} \delta_i^w, & t_{i-1}^w < t < t_i^w \\ 0, & \text{otherwise} \end{cases}, \tag{22}$$

for $i = 1, \ldots, N_z$ and $i = 1, \ldots, N_w$. The weights δ_i^z and δ_i^w are given by $\delta_i^z = (t_i^z - t_{i-1}^z)^{-1/2}$ and $\delta_i^w = (t_i^w - t_{i-1}^w)^{-1/2}$ for given time grids $\{t_i^z\}_{i=0}^{N_z}$ and $\{t_i^w\}_{i=0}^{N_w}$. The characteristic functions are weighted in this way so that they are orthonormal with respect to the $L^2(0,\infty)$ inner product, i.e.,

$$\int_0^\infty \chi_i^z(t) \chi_j^z(t)\, dt = \delta_{ij}, \quad \int_0^\infty \chi_i^w(t) \chi_j^w(t)\, dt = \delta_{ij}.$$

This is not necessary, but it simplifies the resulting formulas.

The coefficients in the piecewise constant expansions can be taken as approximate weighted averages of the functions $z(t)$ and $w(t)$. Specifically, suppose we have approximations $\{z_i\}$ and $\{w_i\}$ of the functions $z(t)$ and $w(t)$ at the time values $\{t_i^z\}$ and $\{t_i^w\}$. Then the coefficients $\{a_i^z\}$ and $\{a_i^w\}$ can be chosen as

$$a_i^z = \frac{(1-\theta^z) z_i - \theta^z z_{i-1}}{2\delta_i^z}, \quad a_i^w = \frac{(1-\theta^w) w_i - \theta^w w_{i-1}}{2\delta_i^w}, \tag{23}$$

where $0 \leq \theta^z, \theta^w \leq 1$.

With such piecewise constant data, the balancing computations can be reduced to the singular value decomposition of a matrix of coefficient inner products. In the following result, we generalize slightly to allow any $\{\chi_i^z\}$ and $\{\chi_i^w\}$ to be any orthonormal sets in $L^2(0,\infty)$. This result can be further generalized to allow these sets of functions to be any (nonorthogonal) linearly independent sets in $L^2(0,\infty)$ if desired.

Proposition 2. *Let z and w in $L^2(0,\infty;X)$ be defined by the expansions (21) above, where $\{a_i^z\}_{i=1}^{N_z}$ and $\{a_i^w\}_{i=1}^{N_w}$ are any subsets of X, and $\{\chi_i^z\}$ and $\{\chi_i^w\}$ are any orthonormal sets in $L^2(0,\infty)$. Define the $N_z \times N_w$ matrix Γ of coefficient inner products by its ij entries $\Gamma_{ij} = (a_i^z, a_j^w)$. Let $\{\sigma_k, u_k, v_k\}$ be the singular values and singular vectors of Γ, i.e., $\Gamma u_k = \sigma_k v_k$ and $\Gamma^T v_k = \sigma_k u_k$, with orthonormal scaling $u_j^T u_k = v_j^T v_k = \delta_{jk}$.*

Then the nonzero singular values $\sigma_1 \geq \sigma_2 \geq \cdots > 0$ of the matrix Γ are equal to the nonzero balanced POD singular values of $\{z,w\}$. The balanced POD singular vectors $f_k(t)$ and $g_k(t)$ of $\{z,w\}$ are given by

$$f_k(t) = \sum_{i=1}^{N_w} u_{k,i} \chi_i^w(t), \quad g_k(t) = \sum_{i=1}^{N_z} v_{k,i} \chi_i^z(t), \tag{24}$$

where $u_{k,i}$ and $v_{k,i}$ are the ith components of u_k and v_k. Furthermore, if $\sigma_k \neq 0$, then the balanced POD modes φ_k and ψ_k of $\{z,w\}$ are given by

$$\varphi_k = \sigma_k^{-1/2} \sum_{i=1}^{N_w} u_{k,i} a_i^w, \quad \psi_k = \sigma_k^{-1/2} \sum_{i=1}^{N_z} v_{k,i} a_i^z. \tag{25}$$

Proof. The balanced POD operator $\mathcal{H} : L^2(0,\infty) \to L^2(0,\infty)$ for $\{z,w\}$ is given by

$$[\mathcal{H}f](t) = \int_0^\infty (z(t), w(s))\, f(s)\, ds = \sum_{i=1}^{N_z} \sum_{j=1}^{N_w} \Gamma_{ij} \left(\int_0^\infty \chi_j^w(s) f(s)\, ds \right) \chi_i^z(t).$$

Similarly, the adjoint operator $\mathcal{H}^* : L^2(0,\infty) \to L^2(0,\infty)$ is given by

$$[\mathcal{H}^* g](t) = \int_0^\infty (w(t), z(s))\, g(s)\, ds = \sum_{i=1}^{N_w} \sum_{j=1}^{N_z} \Gamma_{ij}^T \left(\int_0^\infty \chi_j^z(s) g(s)\, ds \right) \chi_i^w(t).$$

Consider the equations for the singular value decomposition: $\mathcal{H} f_k = \sigma_k g_k$ and $\mathcal{H}^* g_k = \sigma_k f_k$. Substituting in the above expressions for $\mathcal{H} f$ and $\mathcal{H}^* g$ shows that there must exist vectors u_k and v_k such that each f_k and g_k must be of the form (24).

Substituting these expressions for f_k and g_k into the singular value decomposition equations for $\mathcal{H}$ yields the singular value decomposition equations for the matrix Γ, i.e., $\Gamma u_k = \sigma_k v_k$, and

$\Gamma^T v_k = \sigma_k u_k$. Here, we used the orthonormality of the functions $\{\chi_i^z\}$ and $\{\chi_i^w\}$. This shows that the nonzero singular vectors of Γ and $\mathcal{H}$ are equal, and that f_k and g_k are singular vectors of $\mathcal{H}$. The singular vectors f_k and g_k are also scaled so that they are orthonormal:

$$\int_0^\infty f_j(t) f_k(t)\,dt = \sum_{i=1}^{N_w} u_{j,i} u_{k,i} = u_j^T u_k = \delta_{jk},$$

where we have again used that $\{\chi_i^w\}$ is an orthonormal set. A similar argument shows $\int_0^\infty g_j(t) g_k(t)\,dt = \delta_{jk}$.

Equation (25) for the balancing modes follows directly from the definition of the balanced POD modes (20) and the orthonormality of the functions $\{\chi_i^z\}$ and $\{\chi_i^w\}$. □ □

4.1.2 Quadrature Approach

Next, we describe approximating the balanced POD using a quadrature approach. We derive the approximation procedure by applying quadrature to the balanced POD operator (or Hankel operator) directly. This is a different approach than was taken in earlier works [30, 33], however the resulting algorithm is the same. Again, we treat the case of a single function in each dataset; the case of multiple functions is similar.

Let $\{\alpha_i^z, \tau_i^z\}_{i=1}^{N_z}$ and $\{\alpha_i^w, \tau_i^w\}_{i=1}^{N_w}$ be the weights and nodes for two quadrature rules. Apply the quadrature rules to the equations $\mathcal{H} f = \sigma g$ and $\mathcal{H}^* g = \sigma f$ and evaluate at the quadrature nodes to obtain the approximate equations

$$[\mathcal{H} f](\tau_i^z) \approx \sum_{j=1}^{N_w} \alpha_j^w \left(z(\tau_i^z), w(\tau_j^w) \right) f(\tau_j^w) \approx \sigma g(\tau_i^z),$$

$$[\mathcal{H}^* g](\tau_i^w) \approx \sum_{j=1}^{N_w} \alpha_j^z \left(w(\tau_i^w), z(\tau_j^z) \right) g(\tau_j^z) \approx \sigma f(\tau_i^w).$$

Replace the above approximate equations by equalities and scale the resulting equations by $(\alpha_i^z)^{1/2}$ and $(\alpha_i^w)^{1/2}$, respectively. Define the scaled quantities

$$a_i^z = (\alpha_i^z)^{1/2} z(\tau_i^z), \qquad a_j^w = (\alpha_j^w)^{1/2} w(\tau_j^w), \tag{26}$$

$$u_j = (\alpha_j^w)^{1/2} f(\tau_j^w), \qquad v_i = (\alpha_i^z)^{1/2} g(\tau_i^z), \tag{27}$$

and let Γ be the $N_z \times N_w$ matrix with ij entries $\Gamma_{ij} = (a_i^z, a_j^w)$. We have

$$\Gamma u = \sigma v, \quad \Gamma^T v = \sigma u.$$

Therefore, the singular value decomposition of Γ gives approximations to the nonzero singular values of $\mathcal{H}$ and the balancing singular vectors evaluated at the quadrature points. The balancing modes (20) are approximated using quadrature on the integrals:

$$\varphi_k \approx \sigma_k^{-1/2} \sum_{j=1}^{N_w} \alpha_j^w f(\tau_j^w) w(\tau_j^w) = \sigma_k^{-1/2} \sum_{j=1}^{N_w} u_{k,j} a_j^w,$$

$$\psi_k \approx \sigma_k^{-1/2} \sum_{i=1}^{N_z} \alpha_i^z g(\tau_i^z) z(\tau_i^z) = \sigma_k^{-1/2} \sum_{i=1}^{N_z} v_{k,i} a_i^z.$$

It is possible to relate the quadrature approach to the snapshot approach by defining piecewise constant approximations to the data $z(t)$ and $w(t)$ as follows. Let the time grid $\{t_i^z\}_{i=0}^{N_z}$ satisfy

$$0 = t_0^z \leq \tau_1^z, \quad \tau_i^z < t_i^z < \tau_{i+1}^z, \quad \text{for } i = 1, \ldots, N_z - 1, \text{ and } \quad \tau_{N_z}^z \leq t_{N_z}^z.$$

Here we place a time node in between successive quadrature nodes (with possible equality at the endpoints). Let the time grid $\{t_j^w\}_{j=0}^{N_w}$ satisfy similar requirements with $\{\tau_j^w\}$. Also let χ_i^z and χ_i^w be the weighted piecewise constant functions defined in (22) above. Define the following approximations:

$$z(t) = \sum_{i=1}^{N_z} d_i^z \chi_i^z(t), \quad w(t) = \sum_{i=1}^{N_w} d_i^w \chi_i^w(t),$$

where $d_i^z = (\delta_i^z)^{-1} a_i^z$ and $d_i^w = (\delta_i^w)^{-1} a_i^w$, and a_i^z and a_i^w are the scaled variables defined in (26). Using these approximations in the snapshot algorithm yields the same balanced POD quantities as the quadrature approach.

4.1.3 Approximating the Derivatives of the Singular Vectors

In the balanced POD algorithm variation for general systems in Section 3.2, we require approximations of the derivatives $\{\dot{f}_k\}$ and $\{\dot{g}_k\}$ of the Hankel singular vectors. Approximating the derivatives is not necessarily straightforward since the approximate singular vectors f_k^N and g_k^N may not even be differentiable. For example, if the data $\{z_i^N(t)\}$ and $\{w_j^N(t)\}$ is piecewise constant in time or arises from a discontinuous Galerkin time stepping method for the approximation of the differential equations (4) and (5), then the approximate singular vectors f_k^N and g_k^N can be discontinuous in time. However, even if the approximate singular vectors are not differentiable, we propose a convergent approach to approximating the derivatives of the exact singular vectors. Again, for simplicity we consider only one function in each dataset.

If the data $\{z(t), w(t)\}$ is differentiable in time, then it is not difficult to approximate the derivatives. For the quadrature approach, one may simply approximate the derivatives of the balanced POD singular vectors pointwise with second order differences, or some related approach. For the snapshot approach, let the data be given by (21), i.e., $z(t) = \sum_{i=1}^{N_z} a_i^z \chi_i^z(t)$ and $w(t) = \sum_{i=1}^{N_w} a_i^w \chi_i^w(t)$. If each set $\{\chi_i^z\}$ and $\{\chi_i^w\}$ of the time varying functions is linearly independent (and not necessarily orthonormal), an extension of Proposition 2 gives that the balanced POD singular vectors can be expanded in terms of the same χ functions (although the coefficients in the expansions (24) are different). Therefore, if the χ functions are differentiable in time, then the derivatives of the singular vectors can be computed directly. We do not consider convergence of the derivatives for approximate data for these approaches here.

When the data is not differentiable in time, we only consider the specific exact data $z(t) = e^{A^* t} c$ and $w(t) = e^{At} b$, i.e., the solutions to the differential equations (4)-(5), and approximate data $\{z^N(t), w^N(t)\}$. If $c \notin D(A^*)$ and $b \notin D(A)$, then the exact data may not be differentiable in time, and the approximate data also may not be differentiable in time.

In this case, we approximate the derivatives of the exact balanced POD singular vectors (i.e., the Hankel singular vectors) by solving the following system of linear equations

$$\begin{aligned} \sigma_k^N \xi_k^N + \mathcal{H}_N^* \eta_k^N - \vartheta_k^N f_k^N &= -\mathcal{B}_N^* \sum_{j=1}^{p} z_j^N(0)\, g_{k,j}^N(0), \\ \mathcal{H}_N \xi_k^N + \sigma_k^N \eta_k^N + \vartheta_k^N g_k^N &= -\mathcal{C}_N \sum_{j=1}^{m} w_j^N(0)\, f_{k,j}^N(0), \end{aligned} \tag{28}$$

$$-(f_k^N, \xi_k^N) + (g_k^N, \eta_k^N) + \vartheta_k^N \, \sigma_k^N \;\; = \;\; 0,$$

where for any $x \in X$, $\mathcal{B}_N^* x \in L^2(0,\infty;\mathbb{R}^m)$ and $\mathcal{C}_N x \in L^2(0,\infty;\mathbb{R}^p)$ are defined by

$$\begin{aligned}
[\mathcal{B}_N^* x](t) &= [\,(x, w_1^N(t)), \, \ldots \, , (x, w_m^N(t))\,]^T, \\
[\mathcal{C}_N x](t) &= [\,(x, z_1^N(t)), \, \ldots \, , (x, z_p^N(t))\,]^T.
\end{aligned}$$

Also, $[\mathcal{H}_N^* \eta](t) = \int_0^\infty \ell(t,s)\, \eta(s)\, ds$, where $\ell_{ij} = (w_i^N(t), z_j^N(s))$. We show in Section 6.2 that $\xi_k^N \to \dot{f}_k$ and $\eta_k^N \to \dot{g}_k$ as the data converges.

We briefly outline a snapshot approach for computing ξ_k^N and η_k^N using (28). Suppose the approximate data is given by

$$z^N(t) = \sum_{i=1}^{N_z} a_i^z \chi_i^z(t), \quad w^N(t) = \sum_{i=1}^{N_w} a_i^w \chi_i^w(t).$$

(Here, the terms in the sums can all depend on N, but we suppress this dependence for ease of notation.) For simplicity, assume each set of time varying functions $\{\chi_i^z\}$ and $\{\chi_i^w\}$ are orthonormal (e.g., weighted piecewise constant functions); this can be generalized if desired. Assume $\{\sigma_k^N, f_k^N, g_k^N\}$ are the balanced POD singular values and vectors of the approximate data as in Proposition 2. As before, let Γ be the $N_z \times N_w$ matrix with ij entries $\Gamma_{ij} = (a_i^z, a_j^w)$. Let $\{\sigma_k^N, u_k^N, v_k^N\}$ be the singular values and orthonormal singular vectors of Γ, i.e., $\Gamma u_k^N = \sigma_k^N v_k^N$ and $\Gamma^T v_k^N = \sigma_k^N u_k^N$.

It can be checked that the solution $\{\xi_k^N, \eta_k^N, \vartheta_k^N\}$ of the system (28) above is given by

$$\xi_k^N = \sum_{\ell=1}^{N_w} \theta_\ell^w \chi_\ell^w(t), \quad \eta_k^N = \sum_{\ell=1}^{N_z} \theta_\ell^z \chi_\ell^z(t),$$

where θ_ℓ^w and θ_ℓ^z are the ℓth entries of the vectors $\theta^w \in \mathbb{R}^{N_w}$ and $\theta^z \in \mathbb{R}^{N_z}$, and $\{\theta^w, \theta^z, \vartheta_k^N\}$ solve the linear system

$$\begin{pmatrix} \sigma_k^N I & \Gamma^T & -u_k^N \\ \Gamma & \sigma_k^N I & v_k^N \\ -(u_k^N)^T & (v_k^N)^T & \sigma_k^N \end{pmatrix} \begin{pmatrix} \theta^w \\ \theta^z \\ \vartheta_k^N \end{pmatrix} = \begin{pmatrix} -\sum_{i=1}^{N_w} (z^N(0) g_k^N(0), a_i^w) \\ -\sum_{i=1}^{N_z} (w^N(0) f_k^N(0), a_i^z) \\ 0 \end{pmatrix}.$$

5 Proof of the Balanced Realization in Theorem 1

We now prove Theorem 1 and show that the balancing modes $\{\varphi_j\} \subset X$ and $\{\psi_i\} \subset X$ defined in (7) and (8) can be used to construct the balanced realization of the system (A, B, C). We also give a lemma concerning the derivatives of the singular vectors that we use later to prove convergence of the procedure given above in Section 4.1.3 for approximating the derivatives of the Hankel singular vectors.

We begin with a lemma that allows us to show below that the balancing modes satisfy the smoothness properties $\{\varphi_j\} \subset D(A)$ and $\{\psi_i\} \subset D(A^*)$.

Let $C^1(0,\infty)$ be the space of real-valued functions $u(t)$ that are continuous for $0 \le t \le \infty$ whose derivatives exist in $L^1(0,\infty)$. Note that continuity at $t = \infty$ requires $\lim_{t\to\infty} u(t) = u(\infty)$.

Lemma 1. *Let X be a Banach space and suppose $A : D(A) \subset X \to X$ generates an exponentially stable C_0-semigroup e^{At}. Also let $x \in X$ and $u \in C^1(0,\infty)$, as defined above, with $u(\infty) = 0$. If $y \in X$ is defined by $y = \int_0^\infty u(t) e^{At} x \, dt$, then $y \in D(A)$ and*

$$Ay = -u(0)x - \int_0^\infty \dot{u}(t) e^{At} x \, dt.$$

Proof. First, let $u \in C^1(0,\infty)$. Our proof follows a similar argument used by Miklavčič [27, Theorem 4.3.1 (7)]. Let $z(t) = \int_0^t e^{As} x \, ds$ so that $\dot{z}(t) = e^{At}x$. We first prove that we can integrate by parts to obtain

$$y = \int_0^\infty u(t)\dot{z}(t)\,dt = u(t)z(t)\Big|_{t=0}^{t=\infty} - \int_0^\infty \dot{u}(t)z(t)\,dt = -\int_0^\infty \dot{u}(t)z(t)\,dt, \tag{29}$$

since $u(\infty) = 0$ and $z(0) = 0$. This is done as follows. Let ℓ be any element of X^*. The Bochner integral satisfies (see, e.g., [27, Theorem 4.2.3])

$$\ell(y) = \int_0^\infty \ell(u(t)\dot{z}(t))\,dt = \int_0^\infty u(t)\ell(\dot{z}(t))\,dt.$$

We have $\ell(\dot{z}(t)) = (d/dt)\ell(z(t))$ since $\dot{z}(t) = e^{At}x$ and

$$\frac{d}{dt}\ell(z(t)) = \frac{d}{dt}\int_0^t \ell(e^{As}x)\,ds = \ell(e^{At}x) = \ell(\dot{z}(t)).$$

We now use scalar-valued integration by parts:

$$\ell(y) = \int_0^\infty u(t)\ell(\dot{z}(t))\,dt = \int_0^\infty u(t)\frac{d}{dt}\ell(z(t))\,dt = -\int_0^\infty \dot{u}(t)\ell(z(t))\,dt,$$

where we have again used $u(\infty) = 0$ and $z(0) = 0$. The integral on the right hand side is well defined since $\dot{u} \in L^1(0,\infty)$ and since $\ell(z(t))$ is finite for $0 \le t \le \infty$ (because e^{At} is exponentially stable). Since $\ell \in X^*$ is arbitrary, this proves the integration by parts in equation (29) is valid.

We compute Ay by proving that we can pass the closed operator A through the integral. First, we know $z(t) \in D(A)$ for all t, and $Az(t) = e^{At}x - x$ (see, e.g., [10, Theorem 2.1.10 e], [27, Theorem 4.3.1 (3)]). This implies $\dot{u}(t)z(t) \in D(A)$ for all t. Since e^{At} is exponentially stable, both $\|z(t)\|$ and $\|Az(t)\|$ are finite for $0 \le t \le \infty$. Therefore, $\dot{u} \in L^1(0,\infty)$ implies both $\dot{u}z$ and $\dot{u}Az$ are in $L^1(0,\infty;X)$.

The operator A is closed, and thus the above properties imply (see, e.g., [21, Theorem 3.7.12], [27, Theorem 4.2.10]) that $y \in D(A)$ and

$$\begin{aligned} Ay &= -\int_0^\infty \dot{u}(t)Az(t)\,dt = -\int_0^\infty \dot{u}(t)e^{At}x\,dt + \int_0^\infty \dot{u}(t)x\,dt \\ &= -\int_0^\infty \dot{u}(t)e^{At}x\,dt - u(0)x. \end{aligned}$$

□ □

The following result concerning the balanced POD modes of arbitrary data $\{z_i, w_j\} \subset L^2(0,\infty;X)$ can be found in [32, Propostion 2]. Here, we only need the result for the data $z_i = e^{A^*t}c_i$ and $w_j = e^{At}b_j$, for which the balanced POD modes equal the balancing modes.

Proposition 3 ([32]). *The balancing modes $\varphi_j = \sigma_j^{-1}\mathcal{B}f_j$ and $\psi_i = \sigma_j^{-1}\mathcal{C}^*g_j$ defined in (7) and (8) corresponding to nonzero singular values have the following properties:*

1. *The balancing modes are biorthogonal, i.e., $(\varphi_j, \psi_i) = \delta_{ij}$, where δ_{ij} is the Kronecker delta.*

2. *The balancing modes are the eigenvectors of the product of the Gramians $Z_C = \mathcal{C}^*\mathcal{C}$ and $Z_B = \mathcal{B}\mathcal{B}^*$ with corresponding eigenvalues $\{\sigma_i^2\}$, i.e.,*

$$Z_C Z_B \psi_i = \sigma_i^2 \psi_i, \quad Z_B Z_C \varphi_i = \sigma_i^2 \varphi_i.$$

3. The Hankel singular vectors can be expressed in terms of the balancing modes:

$$f_i = \sigma_i^{-1/2} \mathcal{B}^* \psi_i, \quad g_i = \sigma_i^{-1/2} \mathcal{C} \varphi_i. \tag{30}$$

We now prove that the balanced realization can be expressed in terms of the balancing modes as in Theorem 1.

Theorem 1. First, we prove part 1 of the theorem that the balancing modes satisfy $\varphi_i \in D(A)$ and $\psi_i \in D(A^*)$, and that $A\varphi_i = -\sigma_i^{-1/2}(\mathcal{B}\dot{f}_i + Bf_i(0))$ and $A^*\psi_i = -\sigma_i^{-1/2}(\mathcal{C}^*\dot{g}_i + C^*g_i(0))$.

The Hankel singular vectors are known to be C^1 as defined above [14]. Also, since the Hankel singular vectors are L^2 and continuous at $t = \infty$, they must decay to zero at $t = \infty$. Thus, part 1 follows directly from Lemma 1 and the alternate expressions for $\mathcal{B}$ and $\mathcal{C}^*$ given in Proposition 1.

Next, we prove part 2 of the theorem giving that the balanced realization is given by (10)-(12). Due to the assumptions on (A, B, C), the Hankel operator for the system is trace class (or nuclear) [9, Theorem 4]. Since the Hankel singular values are distinct, the Hankel operator is trace class, and the Hilbert space is infinite dimensional, all of the Hankel singular values are nonzero and the balanced realization over ℓ^2 is given by [8]

$$\begin{aligned} A^b_{ij} &= \left(\frac{\sigma_j}{\sigma_i}\right)^{1/2} \int_0^\infty g_i^T(t)\dot{g}_j(t)\, dt, && (31)\\ B^b &= [\sigma_1^{1/2} f_1(0), \sigma_2^{1/2} f_2(0), \ldots]^T, && (32)\\ C^b &= [\sigma_1^{1/2} g_1(0), \sigma_2^{1/2} g_2(0), \ldots], && (33) \end{aligned}$$

where $\{\sigma_k, f_k(\cdot), g_k(\cdot)\}$ are the Hankel singular values and vectors. To prove the result, use property 3 of Proposition 3 and express the Hankel singular vectors in terms of the balancing modes: $f_i = \sigma_i^{-1/2}\mathcal{B}^*\psi_i$ and $g_i = \sigma_i^{-1/2}\mathcal{C}\varphi_i$.

First, for B^b,

$$\begin{aligned} f_i(0) &= \sigma_i^{-1/2}[\mathcal{B}^*\psi_i](0) = \sigma_i^{-1/2}[(\psi_i, w_1(0)), \ldots, (\psi_i, w_m(0))]^T \\ &= \sigma_i^{-1/2}[(\psi_i, b_1), \ldots, (\psi_i, b_m)]^T. \end{aligned}$$

Substituting this expression into the form of B^b above gives the expression (11) for B^b in terms of the balancing modes. The expression (12) for C^b is obtained in a similar fashion.

For A^b, first note

$$\dot{g}_j(t) = \frac{d}{dt}\sigma_j^{-1/2}[\mathcal{C}\varphi_j](t) = \frac{d}{dt}\sigma_j^{-1/2} Ce^{At}\varphi_j = \sigma_j^{-1/2}[\mathcal{C}A\varphi_j](t).$$

This is true since φ_j is in $D(A)$ and so $(d/dt)e^{At}\varphi_j = e^{At}A\varphi_j$. Now compute:

$$\begin{aligned} A^b_{ij} &= \left(\frac{\sigma_j}{\sigma_i}\right)^{1/2} \int_0^\infty g_i^T(t)\dot{g}_j(t)\, dt \\ &= \left(\frac{\sigma_j}{\sigma_i}\right)^{1/2} \int_0^\infty \Big(\sigma_i^{-1}\mathcal{H}f_i\Big)^T(t)\Big(\sigma_j^{-1/2}\mathcal{C}A\varphi_j\Big)(t)\, dt \\ &= \sigma_i^{-3/2} \int_0^\infty \Big(\mathcal{H}\Big[\sigma_i^{-1/2}\mathcal{B}^*\psi_i\Big]\Big)^T(t)\Big(\mathcal{C}A\varphi_j\Big)(t)\, dt \\ &= \sigma_i^{-2}\Big(\mathcal{H}\mathcal{B}^*\psi_i, \mathcal{C}A\varphi_j\Big)_{L^2(0,\infty;\mathbb{R}^p)} \end{aligned}$$

$$
\begin{aligned}
&= \sigma_i^{-2}\Big(\mathcal{C}^*\mathcal{C}\mathcal{B}\mathcal{B}^*\psi_i, A\varphi_j\Big)_X \\
&= \sigma_i^{-2}\Big(Z_C Z_B \psi_i, A\varphi_j\Big)_X \\
&= (\psi_i, A\varphi_j)_X = (A^*\psi_i, \varphi_j)_X.
\end{aligned}
$$

Above, we used $\mathcal{H} f_i = \sigma_i g_i$, $\mathcal{H} = \mathcal{C}\mathcal{B}$, and $Z_C Z_B \psi_i = \sigma_i^2 \psi_i$ (property 2 of Proposition 3).

It is interesting to note that is also possible to prove part part 2 of this theorem using only part 1. □ □

We use the following lemma to prove Proposition 6 below.

Lemma 2. *Under the assumptions of Theorem 1:*

1. *The derivatives of the Hankel singular vectors satisfy $\dot f_k \in L^2(0,\infty;\mathbb{R}^m)$ and $\dot g_k \in L^2(0,\infty;\mathbb{R}^p)$ for each k.*

2. *For each k, the linear equations*

$$
\begin{aligned}
\sigma_k\, \xi_k + \mathcal{H}^*\, \eta_k - \vartheta_k\, f_k &= -\mathcal{B}^* C^* g_k(0), \\
\mathcal{H}\, \xi_k + \sigma_k\, \eta_k + \vartheta_k\, g_k &= -\mathcal{C}\, B\, f_k(0), \\
-(f_k, \xi_k) + (g_k, \eta_k) + \vartheta_k\, \sigma_k &= 0,
\end{aligned}
\tag{34}
$$

have a unique solution $\{\xi_k, \eta_k, \vartheta_k\} \subset L^2(0,\infty;\mathbb{R}^m) \times L^2(0,\infty;\mathbb{R}^p) \times \mathbb{R}$; furthermore, $\xi_k = \dot f_k$, $\eta_k = \dot g_k$, and $\vartheta_k = 0$.

Proof. The same proof for part 1 of Theorem 1 gives

$$
A\mathcal{B} f_k = -\mathcal{B}\dot f_k - B f_k(0), \quad A^*\mathcal{C}^* g_k = -\mathcal{C}^*\dot g_k - C^* g_k(0). \tag{35}
$$

Differentiate $\sigma_k g_k = \mathcal{H} f_k$ and use $\mathcal{C} = C e^{At}$ to obtain $\sigma_k \dot g_k = (d/dt)\mathcal{C}\mathcal{B} f_k = \mathcal{C} A \mathcal{B} f_k$. Similarly, we have $\sigma_k \dot f_k = \mathcal{B}^* A^* \mathcal{C}^* g_k$. Then (35) gives

$$
-\mathcal{H}\dot f_k - \mathcal{C} B f_k(0) = \sigma_k \dot g_k, \quad -\mathcal{H}^*\dot g_k - \mathcal{B}^* C^* g_k(0) = \sigma_k \dot f_k. \tag{36}
$$

These equations hold in L^1 since $\dot f_k$ and $\dot g_k$ are C^1 as defined in the beginning of this section.

Now, $\mathcal{H}\dot f_k$ is in $L^2(0,\infty;\mathbb{R}^p)$ since $\mathcal{H} = \mathcal{C}\mathcal{B}$ and $\mathcal{B}$ maps $L^1(0,\infty;\mathbb{R}^p)$ into X. Similarly, $\mathcal{H}^*\dot g_k \in L^2(0,\infty;\mathbb{R}^m)$. Thus, the left hand side of each of these equations is in L^2; therefore, $\dot f_k$ and $\dot g_k$ are in L^2 for each k.

The two equations (36) also show that $\xi_k = \dot f_k$, $\eta_k = \dot g_k$, and $\vartheta_k = 0$ satisfy the first two equations of (34). A property of the exact balanced realization is $(\dot f_k, f_k) = (\dot g_k, g_k)$ [8]. Therefore, the third equation of (34) is also satisfied by $\xi_k = \dot f_k$, $\eta_k = \dot g_k$, and $\vartheta_k = 0$.

To show the linear equations (34) are uniquely solvable, rewrite (34) as $(\sigma_k I - Q)\ell = F$, where

$$
Q = \begin{pmatrix} 0 & -\mathcal{H}^* & f_k \\ -\mathcal{H} & 0 & -g_k \\ (f_k)^* & -(g_k)^* & 0 \end{pmatrix}, \quad \ell = \begin{pmatrix} \xi_k \\ \eta_k \\ \vartheta_k \end{pmatrix}, \quad F = \begin{pmatrix} -\mathcal{B}^* C^* g_k(0) \\ -\mathcal{C}\, B\, f_k(0) \\ 0 \end{pmatrix}. \tag{37}
$$

Here, the operator $(f_k)^*$ is defined by $(f_k)^*\xi = (f_k, \xi)$, and $(g_k)^*$ is defined similarly. The operator Q mapping the space $L^2(0,\infty;\mathbb{R}^m) \times L^2(0,\infty;\mathbb{R}^p) \times \mathbb{R}$ into itself is compact, and it can be checked that σ_k is not an eigenvalue of Q. Therefore, since $\sigma_k > 0$ the operator $\sigma_k I - Q$ is invertible, and the equations (34) have a unique solution in $L^2(0,\infty;\mathbb{R}^m) \times L^2(0,\infty;\mathbb{R}^p) \times \mathbb{R}$. □ □

Note: Given $f_k(0)$ and $g_k(0)$, equations (36) in the proof above are not enough to uniquely determine $\dot f_k$ and $\dot g_k$ since σ_k is a singular value of $\mathcal{H}$. Therefore, the technique of [17, Section 4.8.5] was used to construct the augmented equations (34).

6 Proof of the Convergence Results

In this section, we prove the convergence results for balanced POD and the balanced POD balanced truncation algorithm.

We briefly introduce some operator norms we use below. Let K be a compact linear operator from a Hilbert space X_1 to a Hilbert space X_2 with ordered singular values $\sigma_1 \geq \sigma_2 \geq \cdots \geq 0$. The operator norm of K is given by

$$\|K\| = \sup_{x \in X_1, x \neq 0} \frac{\|Kx\|}{\|x\|} = \sigma_1.$$

The operator K is Hilbert-Schmidt (HS) if the following Hilbert-Schmidt norm of K is finite:

$$\|K\|_{HS} = \Big(\sum_{k \geq 1} \sigma_k^2 \Big)^{1/2} = \Big(\sum_{j \geq 1} \|K\varphi_j\|^2 \Big)^{1/2},$$

for any orthonormal basis $\{\varphi_j\} \subset X_1$. The operator K is trace class (or nuclear) if the sum of all of the singular values of K is finite; in this case, the trace norm of K is given by the sum:

$$\|K\|_{\mathrm{tr}} = \sum_{k \geq 1} \sigma_k.$$

If two operators $K : X_1 \to X_2$ and $L : X_2 \to X_3$ are HS, then the product $KL : X_1 \to X_3$ is trace class and $\|KL\|_{\mathrm{tr}} \leq \|K\|_{HS} \|L\|_{HS}$. Also, $\|K\| = \|K^*\|$ for any of the above norms and $\|K\| \leq \|K\|_{HS} \leq \|K\|_{\mathrm{tr}}$.

6.1 Balanced POD

We begin by considering the convergence of the balanced proper orthogonal decomposition. Let $\{z_i\}_{i=1}^p$, $\{z_i^N\}_{i=1}^p$, $\{w_j\}_{j=1}^m$, and $\{w_j^N\}_{j=1}^m$ be any collections of functions in $L^2(0,\infty;X)$. We show in Theorem 2 below that if each z_i^N and w_j^N converges to z_i and w_j in $L^2(0,\infty;X)$, then the balanced POD singular values converge and the balanced POD singular vectors and modes corresponding to distinct singular values converge. Furthermore, if the data converges in another Banach space, then the balancing modes also converge in this Banach space.

To begin, we introduce analogues of the controllability and observability operators $\mathcal{C}$ and $\mathcal{B}$ discussed in Section 2; specifically, the operators will take the forms in Proposition 1 above. Define $\mathcal{C} : X \to L^2(0,\infty;\mathbb{R}^p)$ and $\mathcal{B} : L^2(0,\infty;\mathbb{R}^m) \to X$ by

$$[\mathcal{C}x](t) = [\, (x, z_1(t)), \, \ldots \, , (x, z_p(t)) \,]^T, \quad \mathcal{B}u = \int_0^\infty \sum_{j=1}^m u_j(s) w_j(s) \, ds.$$

The operators $\mathcal{C}_N$ and $\mathcal{B}_N$ are defined similarly with the data $\{z_i^N, w_j^N\}$ replacing the data $\{z_i, w_j\}$.

As with the Hankel operator, it is straightforward to check that the balanced POD operator in Definition 1 can be factored in terms of the above operators.

Lemma 3. *The balanced POD operator $\mathcal{H} : L^2(0,\infty;\mathbb{R}^m) \to L^2(0,\infty;\mathbb{R}^p)$ for any two datasets $\{z_i\}_{i=1}^p \subset L^2(0,\infty;X)$ and $\{w_j\}_{j=1}^m \subset L^2(0,\infty;X)$ can be factored as $\mathcal{H} = \mathcal{C}\mathcal{B}$, where the operators $\mathcal{C}$ and $\mathcal{B}$ are defined above.*

We use properties of the above operators to study the convergence properties of the balanced POD. The following Hilbert-Schmidt properties of $\mathcal{C}$ and $\mathcal{B}$ can be found in [31, Lemma 4.4].

Lemma 4. *For any two datasets $\{z_i\}_{i=1}^p$ and $\{w_j\}_{j=1}^m$ in $L^2(0,\infty;X)$, the operators $\mathcal{C}$ and $\mathcal{B}$ are Hilbert-Schmidt, and the Hilbert-Schmidt norms are given by*

$$\|\mathcal{C}\|_{HS} = \left(\int_0^\infty \sum_{i=1}^p \|z_i(t)\|^2 \, dt \right)^{1/2}, \quad \|\mathcal{B}\|_{HS} = \left(\int_0^\infty \sum_{j=1}^m \|w_j(t)\|^2 \, dt \right)^{1/2}.$$

The above factorization of the balanced POD operator immediately gives that the balanced POD operator is trace class, and therefore compact.

Proposition 4. *For any two datasets $\{z_i\}_{i=1}^p \subset L^2(0,\infty;X)$ and $\{w_j\}_{j=1}^m \subset L^2(0,\infty;X)$, the balanced POD operator $\mathcal{H}$ for $\{z_i, w_j\}$ is trace class.*

We now prove that the balanced POD operator $\mathcal{H}_N = \mathcal{C}_N \mathcal{B}_N$ for the data $\{z_i^N, w_j^N\}$ converges in trace norm to the balanced POD operator $\mathcal{H} = \mathcal{C}\mathcal{B}$ for $\{z_i, w_j\}$ when the data converges in $L^2(0,\infty;X)$.

Proposition 5. *The trace norm error between $\mathcal{H}$ and $\mathcal{H}_N$ can be bounded as follows:*

$$\begin{aligned} \|\mathcal{H} - \mathcal{H}_N\|_{\mathrm{tr}} \leq & \left(\int_0^\infty \sum_{i=1}^p \|z_i(t)\|^2 \, dt \right)^{1/2} \left(\int_0^\infty \sum_{j=1}^m \|w_j(t) - w_j^N(t)\|^2 \, dt \right)^{1/2} \\ & + \left(\int_0^\infty \sum_{j=1}^m \|w_j^N(t)\|^2 \, dt \right)^{1/2} \left(\int_0^\infty \sum_{i=1}^p \|z_i(t) - z_i^N(t)\|^2 \, dt \right)^{1/2}. \end{aligned}$$

Therefore, if each $z_i^N \to z_i$ and each $w_j^N \to w_j$ in $L^2(0,\infty;X)$, then $\mathcal{H}_N \to \mathcal{H}$ in the trace norm.

Proof. First, since $\{w_j - w_j^N\}_{j=1}^m$ is a subset of $L^2(0,\infty;X)$ and

$$(\mathcal{B} - \mathcal{B}_N)u = \int_0^\infty \sum_{j=1}^m u_j(t) \Big(w_j(t) - w_j^N(t) \Big) \, ds,$$

Lemma 4 implies that $\mathcal{B} - \mathcal{B}^N$ is Hilbert-Schmidt with HS norm

$$\|\mathcal{B} - \mathcal{B}_N\|_{HS} = \left(\int_0^\infty \sum_{j=1}^m \|w_j(t) - w_j^N(t)\|^2 \, ds \right)^{1/2}. \tag{38}$$

A similar result holds for the operator $\mathcal{C} - \mathcal{C}^N$.

We use the factorizations $\mathcal{H} = \mathcal{C}\mathcal{B}$ and $\mathcal{H}_N = \mathcal{C}_N \mathcal{B}_N$ to bound the error as follows:

$$\begin{aligned} \|\mathcal{H} - \mathcal{H}_N\|_{\mathrm{tr}} & \leq \|\mathcal{H} - \mathcal{C}\mathcal{B}_N\|_{\mathrm{tr}} + \|\mathcal{C}\mathcal{B}_N - \mathcal{H}_N\|_{\mathrm{tr}} \\ & \leq \|\mathcal{C}\|_{HS} \|\mathcal{B} - \mathcal{B}_N\|_{HS} + \|\mathcal{C} - \mathcal{C}_N\|_{HS} \|\mathcal{B}_N\|_{HS}. \end{aligned}$$

The result follows from the above observation and Lemma 4. □ □

With this result, we prove that convergence of the data gives convergence of the balanced POD.

Theorem 2. *Let $\{z_i\}_{i=1}^p$ and $\{w_j\}_{j=1}^m$ be two collections of functions in $L^2(0,\infty;X)$ with balanced POD singular values, singular vectors, and modes denoted by $\{\sigma_k\}$, $\{f_k, g_k\}$, and $\{\varphi_k, \psi_k\}$. Let $\{z_i^N\}_{i=1}^p$ and $\{w_j^N\}_{j=1}^m$ be two other datasets in $L^2(0,\infty;X)$ with corresponding balanced POD quantities denoted by $\{\sigma_k^N\}$, $\{f_k^N, g_k^N\}$, and $\{\varphi_k^N, \psi_k^N\}$.*

If each $z_i^N \to z_i$ and each $w_j^N \to w_j$ in $L^2(0,\infty;X)$ as $N \to \infty$, then the following statements hold:

1. *The individual balanced POD singular values converge as* $N \to \infty$*, i.e., for each* k*,*

$$\lim_{N\to\infty} |\sigma_k^N - \sigma_k| = 0.$$

2. *The sum of the balanced POD singular values converge as* $N \to \infty$*, i.e.,*

$$\lim_{N\to\infty} \sum_{k\geq 1} \sigma_k^N = \sum_{k\geq 1} \sigma_k.$$

3. *If the* k*th balanced POD singular value* σ_k *is distinct, then the* k*th balanced POD singular vectors (suitably normalized) converge in* L^2*, and the* k*th balanced POD modes converge in* X*, i.e.,*

$$\lim_{N\to\infty} \|f_k^N - f_k\|_{L^2(0,\infty;\mathbb{R}^m)} = 0, \qquad \lim_{N\to\infty} \|g_k^N - g_k\|_{L^2(0,\infty;\mathbb{R}^p)} = 0,$$
$$\lim_{N\to\infty} \|\varphi_k^N - \varphi_k\|_X = 0, \qquad \lim_{N\to\infty} \|\psi_k^N - \psi_k\|_X = 0.$$

Furthermore, let W *and* Z *be Banach spaces. Suppose each* $z_i^N \to z_i$ *in* $L^2(0,\infty;Z)$ *and each* $w_j^N \to w_j$ *in* $L^2(0,\infty;W)$*. If the* k*th balanced POD singular value* σ_k *is distinct, then* $\|\varphi_k^N - \varphi_k\|_W \to 0$ *and* $\|\psi_k^N - \psi_k\|_Z \to 0$*.*

Proof. Let $\mathcal{H}$ and $\mathcal{H}^N$ denote the balanced POD operators for the datasets $\{z_i, w_j\}$ and $\{z_i^N, w_j^N\}$, respectively. As each $z_i^N \to z_i$ and each $w_j^N \to w_j$ in $L^2(0,\infty;X)$, the above result gives that $\mathcal{H}^N$ converges to $\mathcal{H}$ in the trace norm and therefore also in the (weaker) operator norm. Convergence in the trace norm implies the sum of the singular values converge. Convergence in the operator norm implies the individual singular values converge since $|\sigma_k - \sigma_k^N| \leq \|\mathcal{H} - \mathcal{H}_N\|$ (see, e.g., [15, Corollary 2.3]). Since $\mathcal{H}^N$ and $\mathcal{H}$ are compact and $\mathcal{H}^N$ converges to $\mathcal{H}$ in norm, [14, Appendix 2] gives the convergence in L^2 of the singular vectors corresponding to distinct singular values.

Convergence of the balancing modes in X is established as follows. We have $\varphi_k = \sigma_k^{-1/2}\mathcal{B}^* f_k$ and $\varphi_k^N = (\sigma_k^N)^{-1/2}\mathcal{B}_N f_k^N$. Equation (38) above shows $\mathcal{B}_N$ converges to $\mathcal{B}$ in the Hilbert-Schmidt norm and therefore also in the (weaker) operator norm; therefore, the convergence of the balanced POD singular values and singular vectors established above gives φ_k^N converges to φ_k in X. A similar argument shows ψ_k^N converges to ψ_k.

Assume each w_j^N converges to w_j in $L^2(0,\infty;W)$. We consider convergence of φ_k^N to φ_k in W. This follows the same argument above once we show (1) $\mathcal{B}$ and $\mathcal{B}_N$ are bounded as operators from $L^2(0,\infty;\mathbb{R}^m)$ into W, and (2) $\|\mathcal{B} - \mathcal{B}_N\| \to 0$, where the norm is the operator norm from $L^2(0,\infty;\mathbb{R}^m)$ into W. First,

$$\begin{aligned}
\|\mathcal{B}u\|_W &\leq \int_0^\infty \sum_{j=1}^m |u_j(s)|\, \|w_j(s)\|_W \, ds \\
&\leq \Big(\int_0^\infty \sum_{j=1}^m |u_j(s)|^2 \, ds \Big)^{1/2} \Big(\int_0^\infty \sum_{j=1}^m \|w_j(s)\|_W^2 \, ds \Big)^{1/2} \\
&= \|u\|_{L^2(0,\infty;\mathbb{R}^m)} \Big(\sum_{j=1}^m \|w_j\|_{L^2(0,\infty;W)}^2 \Big)^{1/2}.
\end{aligned}$$

Therefore, the operator $\mathcal{B} : L^2(0,\infty;\mathbb{R}^m) \to W$ is bounded and the operator norm is bounded as follows

$$\|\mathcal{B}\|_{\mathcal{L}(L^2,W)} \leq \Big(\sum_{j=1}^m \|w_j\|_{L^2(0,\infty;W)}^2 \Big)^{1/2}.$$

A similar result holds for $\mathcal{B}_N$. The same argument shows

$$\|\mathcal{B}-\mathcal{B}_N\|_{\mathcal{L}(L^2,W)} \leq \Big(\sum_{j=1}^{m} \|w_j - w_j^N\|^2_{L^2(0,\infty;W)} \Big)^{1/2}.$$

Therefore, the operator norm tends to zero as each w_j^N converges to w_j in $L^2(0,\infty;W)$. This proves the convergence of φ_k^N to φ_k in W; a similar argument proves $\psi_k^N \to \psi_k$ in Z. □ □

6.2 Convergence of the Hankel Singular Values and Singular Vectors

The following basic convergence result for the Hankel singular values, singular vectors, and balancing modes follows directly from Theorem 2 above.

Corollary 2. *Let the assumptions of Theorem 1 hold. Let $\{z_i^N\}_{i=1}^p$ and $\{w_j^N\}_{j=1}^m$ be two collections of functions in $L^2(0,\infty;X)$ with balanced POD singular values, singular vectors, and modes denoted by $\{\sigma_k^N\}$, $\{f_k^N, g_k^N\}$, and $\{\varphi_k^N, \psi_k^N\}$. For $z_i(t) = e^{A^*t}c_i$ and $w_j(t) = e^{At}b_j$, if*

$$\int_0^\infty \|z_i^N(t) - z_i(t)\|_X^2\, dt \to 0, \quad \int_0^\infty \|w_j^N(t) - w_j(t)\|_X^2\, dt \to 0, \tag{39}$$

for $i = 1,\dots,p$ and $j = 1,\dots,m$, then

1. *the Hankel singular values converge, i.e., $|\sigma_k^N - \sigma_k| \to 0$ for each k;*
2. *the balancing error bound (1) converges, i.e.,*
$$\lim_{N\to\infty} 2\sum_{k>r} \sigma_k^N = 2\sum_{k>r}\sigma_k;$$
3. *the Hankel singular vectors converge in L^2, i.e., $\|f_k^N - f_k\|_{L^2(0,\infty;\mathbb{R}^m)} \to 0$ and $\|g_k^N - g_k\|_{L^2(0,\infty;\mathbb{R}^p)} \to 0$ for each k;*
4. *the balancing modes converge in X, i.e., $\|\varphi_k^N - \varphi_k\|_X \to 0$ and $\|\psi_k^N - \psi_k\|_X \to 0$ for each k.*

Next, we consider stronger convergence of the Hankel singular vectors required for the balanced POD algorithm for general systems in Section 3.2.

We showed in Lemma 2 that the derivatives of the Hankel singular values are uniquely determined by the equations (34), which can be written as $(\sigma_k I - Q)\ell = F$, where Q, ℓ, and F are defined in (37). In Section 4.1.3, we proposed approximating the derivatives of the Hankel singular vectors by computing the solution of the linear equations (28), which are repeated here for convenience:

$$\begin{aligned} \sigma_k^N\, \xi_k^N + \mathcal{H}_N^*\, \eta_k^N - \vartheta_k^N\, f_k^N &= -\mathcal{B}_N^* \sum_{j=1}^p z_j^N(0)\, g_{k,j}^N(0), \\ \mathcal{H}_N\, \xi_k^N + \sigma_k^N\, \eta_k^N + \vartheta_k^N\, g_k^N &= -\mathcal{C}_N \sum_{j=1}^m w_j^N(0)\, f_{k,j}^N(0), \\ -(f_k^N, \xi_k^N) + (g_k^N, \eta_k^N) + \vartheta_k^N\, \sigma_k^N &= 0, \end{aligned} \tag{40}$$

These equations can be written as $(\sigma_k^N I - Q_N)\ell_N = F_N$, where Q_N, ℓ_N, and F_N are defined analogously to Q, ℓ, and F in Lemma 2. The following result gives convergence of the derivatives of the Hankel singular values when approximated using this procedure.

Proposition 6. *Let the assumptions of Theorem 1 and Corollary 2 hold. Assume the data* $\{z_i^N(t)\}$ *and* $\{w_j^N(t)\}$ *is continuous at* $t=0$. *If* $z_i^N \to z_i$ *and* $w_j^N \to w_j$ *in* $L^2(0,\infty;X)$ *and also each* $z_i^N(0) \to z_i(0)$ *and* $w_j^N(0) \to w_j(0)$ *weakly in* X *as* $N \to \infty$, *then the following hold.*

1. *The approximate singular vectors* $\{f_k^N\}$ *and* $\{g_k^N\}$ *are continuous at* $t=0$, *and* $f_k^N(0) \to f_k(0)$ *and* $g_k^N(0) \to g_k(0)$ *as* $N \to \infty$.

2. *For each* k, *the linear equations (40) have a unique solution* $\{\xi_k^N, \eta_k^N, \vartheta_k^N\} \subset L^2(0,\infty;\mathbb{R}^m) \times L^2(0,\infty;\mathbb{R}^p) \times \mathbb{R}$ *for* N *large enough; also,*

$$\|\xi_k^N - \dot{f}_k\|_{L^2(0,\infty;\mathbb{R}^m)} \to 0, \quad \|\eta_k^N - \dot{g}_k\|_{L^2(0,\infty;\mathbb{R}^p)} \to 0,$$

and $\vartheta_k^N \to 0$ *as* $N \to \infty$.

Proof. For item 1, consider $\sigma_k^N g_k^N = \mathcal{H}_N f_k^N = \mathcal{C}_N x_N$, where $x_N = \mathcal{B}_N f_k^N$. Since $[\mathcal{C}_N x_N]_j(t) = (x_N, z_j^N(t))$ and z_j^N is continuous at $t=0$, it follows that g_k^N is also continuous at $t=0$. A similar argument proves the same for f_k^N.

Next, we show $g_k^N(0) \to g_k(0)$. We have $\sigma_k^N g_k^N(0) = [\mathcal{C}_N x_N]_j(0)$ and $\sigma_k g_k(0) = [\mathcal{C}x]_j(0)$, where $x = \mathcal{B} f_k$. Subtracting gives

$$\sigma_k^N (g_k(0) - g_k^N(0)) = [(\mathcal{C} - \mathcal{C}_N)x](0) + [\mathcal{C}_N(x - x_N)](0) + (\sigma_k^N - \sigma_k) g_k(0).$$

Since $[(\mathcal{C} - \mathcal{C}_N)x]_j(0) = (x, z_j(0) - z_j^N(0))$, the first term tends to zero since $z_j^N(0) \to z_j(0)$ weakly. The second term tends to zero since $x_N \to x$ and $\|z_j^N(0)\|$ is bounded (because $z_j^N(0) \to z_j(0)$ weakly). The last term tends to zero since $\sigma_k^N \to \sigma_k$. This proves $g_k^N(0) \to g_k(0)$, and $f_k^N(0) \to f_k(0)$ follows similarly.

For item 2, write the equations (40) as $(\sigma_k^N I - Q_N)\ell_N = F_N$, as discussed above. From Lemma 2, we know $\ell = [\dot{f}_k, \dot{g}_k, \vartheta_k]^T$ satisfies $(\sigma_k I - Q)\ell = F$. The operators $\mathcal{B}_N^*$, $\mathcal{B}^*$, $\mathcal{C}_N$, and $\mathcal{C}$ are all compact and $\mathcal{B}_N^* \to \mathcal{B}^*$ and $\mathcal{C}_N \to \mathcal{C}$ in the operator norm; therefore, the convergence of the singular vectors at $t=0$ and the weak convergence of the data at $t=0$ gives $F_N \to F$ strongly in X. Since $\sigma_k^N \to \sigma_k$ and $Q_N \to Q$ in the operator norm, we have $\sigma_k^N I - Q_N$ is invertible for N large enough and also $\ell_N \to \ell$. □ □

6.3 Balancing

Next, consider the convergence of the balanced truncation in the parabolic case described in Section 3.1. Below, we use Theorem 2 to prove convergence of the balancing modes in V; therefore, we need convergence of the data in $L^2(0,\infty;V)$. It is well known that the data z_i and w_j must be in $L^2(0,T;V)$ for any $T>0$; to be complete, we give a simple proof that we can take $T=\infty$ when e^{At} is exponentially stable (which implies the same is true for e^{A^*t}).

Proposition 7. *If the operator* A *satisfies assumptions (16) and (17) and* e^{At} *is exponentially stable, then* $e^{At}x$ *is in* $L^2(0,\infty;V)$ *for any* $x \in X$.

Proof. Let $x \in X$, and suppose e^{At} is exponentially stable. We use the bound (17) on the sesquilinear form $a(\cdot,\cdot)$ to estimate the V norm of $w(t) = e^{At}x$ as follows. First, $w(t)$ satisfies $\dot{w}(t) = Aw(t)$. Taking the inner product of this equation with $w(t)$ gives

$$\begin{aligned} & (\dot{w}(t), w(t)) = (Aw(t), w(t)) \\ \Longrightarrow \quad & \frac{d}{dt}\frac{1}{2}\|w(t)\|_X^2 + a(w(t), w(t)) = 0 \end{aligned}$$

$$\begin{aligned} &\Longrightarrow \quad \frac{d}{dt}\frac{1}{2}\|w(t)\|_X^2 - \lambda\|w(t)\|_X^2 + \alpha\|w(t)\|_V^2 \le 0 \\ &\Longrightarrow \quad \int_0^T \|w(t)\|_V^2\, dt \le \frac{\lambda}{\alpha}\int_0^T \|w(t)\|_X^2 + \frac{1}{2\alpha}\|w(0)\|_X^2 - \frac{1}{2\alpha}\|w(T)\|_X^2. \end{aligned}$$

Since e^{At} is exponentially stable, the right hand side is finite for $T = \infty$; therefore, $w(t) = e^{At}x$ is in $L^2(0,\infty;V)$. □ □

Theorem 3. *Let the assumptions of Theorem 1 hold. Let $\{z_i^N\}_{i=1}^p$ and $\{w_j^N\}_{j=1}^m$ be two collections of functions in $L^2(0,\infty;X)$ with balanced POD singular values, singular vectors, and modes denoted by $\{\sigma_k^N\}$, $\{f_k^N, g_k^N\}$, and $\{\varphi_k^N, \psi_k^N\}$. For $z_i(t) = e^{A^*t}c_i$ and $w_j(t) = e^{At}b_j$, if*

$$\int_0^\infty \|z_i^N(t) - z_i(t)\|_V^2\, dt \to 0, \qquad \int_0^\infty \|w_j^N(t) - w_j(t)\|_V^2\, dt \to 0, \tag{41}$$

for $i = 1,\dots,p$ and $j = 1,\dots,m$, then the results of Corollary 2 hold, the balancing modes converge in V, i.e., $\|\varphi_k^N - \varphi_k\|_V \to 0$ and $\|\psi_k^N - \psi_k\|_V \to 0$ for each k, and the approximate balanced truncation (A_r^N, B_r^N, C_r^N) converges entrywise to the exact balanced truncated system (A_r, B_r, C_r).

Proof. Let $z_i(t) = e^{A^*t}c_i$ and $w_j(t) = e^{At}b_j$. By proposition 7, each z_i and w_j are in $L^2(0,\infty;V)$. Since each $z_i^N \to z_i$ and each $w_j^N \to w_j$ in $L^2(0,\infty;V)$, they must also converge in $L^2(0,\infty;X)$. The convergence of the Hankel singular values, Hankel singular vectors, balancing modes in V, and balancing error bound follows directly from the balanced POD convergence theory given in Theorem 2 (with $W = Z = V$).

Convergence of the balanced truncation follows directly from the convergence of the balanced POD modes to the balancing modes in V (and therefore also in X) as well as the continuity of the inner product on $X \times X$ and the sesquilinear form $a(\cdot,\cdot)$ on $V \times V$. □ □

The above convergence result for the balanced truncation requires convergence of the data in V, which is stronger than convergence of the data in X. For many numerical methods for approximating solutions of parabolic partial differential equations, convergence in the V norm is often slower than convergence in the X norm. This situation can be remedied by using special numerical methods (e.g., mixed finite element methods). Such methods may be beneficial to use in the balanced POD algorithm; we leave the exploration of this topic for future work.

Next, consider the general case described in Section 3.2. Entrywise convergence of the balanced truncation follows directly from the convergence of the Hankel singular values, singular vectors, and balancing modes in Corollary 2, and the stronger convergence of the Hankel singular vectors in Proposition 6.

Theorem 4. *Let the assumptions of Theorem 1 hold. Let $\{z_i^N\}_{i=1}^p$ and $\{w_j^N\}_{j=1}^m$ be two collections of functions in $L^2(0,\infty;X)$ that are continuous at $t = 0$ with balanced POD singular values, singular vectors, and modes denoted by $\{\sigma_k^N\}$, $\{f_k^N, g_k^N\}$, and $\{\varphi_k^N, \psi_k^N\}$. Assume the approximate derivatives $\{\xi_k^N, \eta_k^N\}$ are computed using (28), and the approximate balanced truncation (A_r^N, B_r^N, C_r^N) is computed as described in Section 3.2.*

For $z_i(t) = e^{A^*t}c_i$ and $w_j(t) = e^{At}b_j$, if $z_i^N \to z_i$ and $w_j^N \to w_j$ in $L^2(0,\infty;X)$ and also $z_i^N(0) \to z_i(0)$ and $w_j^N(0) \to w_j(0)$ weakly in X as $N \to \infty$ for $i = 1,\dots,p$ and $j = 1,\dots,m$, then the approximate balanced truncation (A_r^N, B_r^N, C_r^N) converges entrywise to the exact balanced truncated system (A_r, B_r, C_r).

7 Numerical Results

In our earlier work [33], we gave numerical results for a one dimensional convection diffusion system for which we could compute the transfer function exactly for comparison. We also compared results with standard balancing computations using matrix approximations of the infinite dimensional operators. In this work, we apply the algorithm to two example PDE systems: (1) a two dimensional parabolic convection diffusion equation, and (2) a one dimensional hyperbolic PDE. We focus on verifying the convergence results.

7.1 Example 1 - a 2D Parabolic Convection Diffusion Equation

The parabolic partial differential equation is given by

$$w_t = \mu(w_{xx} + w_{yy}) - c_1(x,y)w_x - c_2(x,y)w_y + b(x,y)u(t),$$

over the spatial domain $\Omega = [0,1] \times [0,1]$, with Dirichlet boundary conditions on the bottom, right, and top walls:

$$w(t,x,0) = 0, \quad w(t,1,y) = 0, \quad w(t,x,1) = 0,$$

and a Neumann boundary condition on the left wall:

$$w_x(t,0,y) = 0.$$

System measurements are taken of the form

$$\eta(t) = \int_\Omega c(x,y)w(t,x,y)\,dx\,dy.$$

We assume μ is a positive constant, the convection coefficients $c_1(x,y)$ and $c_2(x,y)$ are bounded, and the functions $b(x,y)$ and $c(x,y)$ are square integrable over Ω.

For this problem, we take the Hilbert space X to be $L^2(\Omega)$, the space of square integrable functions defined over Ω, with standard inner product $(f,g) = \int_\Omega f(x,y)g(x,y)\,dx\,dy$. The operators $B : \mathbb{R}^1 \to X$ and $C : X \to \mathbb{R}^1$ are then given by $[Bu](x,y) = b(x,y)u$ and $Cw = (w,c)$. The sesquilinear form $a(\cdot,\cdot)$ is constructed by multiplying the convection diffusion operator by a test function and integrating by parts. Let $H^m(\Omega)$ be the Hilbert space of functions in $L^2(\Omega)$ with m distributional derivatives that are all square integrable, and also let Γ_0 be the portion of the boundary with the Dirichlet boundary conditions. Take V to be the Hilbert space

$$V = \left\{ v \in H^1(\Omega) : v = 0 \text{ on } \Gamma_0 \right\},$$

with inner product $(v,w)_V = (v_x,w_x) + (v_y,w_y)$. The bilinear form $a : V \times V \to \mathbb{R}$ is then given by

$$a(v,w) = \mu(v,w)_V + (c_1 v_x, w) + (c_2 v_y, w).$$

For our numerical experiments, we chose $\mu = 0.1$, convection coefficients

$$c_1(x,y) = -x\sin(2\pi x)\sin(\pi y), \quad c_2(x,y) = -y\sin(\pi x)\sin(2\pi y),$$

control input function $b(x,y) = 5\sin(\pi x)\sin(\pi y)$ if $x \geq 1/2$ and $b(x,y) = 0$ otherwise, and observation function $c(x,y) \equiv 5$. To approximate the solutions $z(t,x,y)$ and $w(t,x,y)$ of the partial differential equations (4) and (5), we used standard piecewise linear finite elements with equally spaced nodes for the spatial discretization. The resulting approximating ordinary differential equations were integrated until $t = 10$ using Matlab's adaptive solver `ode15s`. At $t = 10$, the norm of the approximate solutions was less than 10^{-2}. The method of snapshots was used for the balanced POD computations; the time nodes returned from `ode15s` were used for the time grid. We chose $\theta^z = \theta^w = 1/2$ in the definition of the piecewise constant coefficients (23).

We begin by considering the convergence of the approximate Hankel singular values in Figure 1. Here, the first 30 approximate singular values are shown for computations using 31, 63, and 95 equally spaced finite element nodes in each coordinate direction. The convergence is clear. Also, for each equally spaced finite element grid, we set $r = 4$ and computed the approximate balancing error bound in (1); the result for each grid was approximately 2.7×10^{-4}.

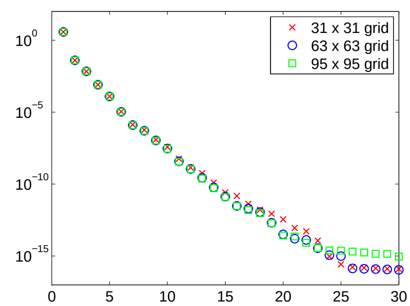

Figure 1: Approximate Hankel singular values computed using 31, 63, and 95 equally spaced finite element nodes in each coordinate direction.

Figure 2 shows approximate Hankel singular vectors $f_2(t)$ and $g_4(t)$. The function $f_2(t)$ is shown for $0 \le t \le 10$, and $g_4(t)$ is only shown for $0 \le t \le 1$. We see the approximations are converged, and also that the higher numbered Hankel singular vectors become more oscillatory, especially near $t = 0$. The latter phenomenon appears to be connected with the solutions of the partial differential equations, which undergo the most change in time near $t = 0$.

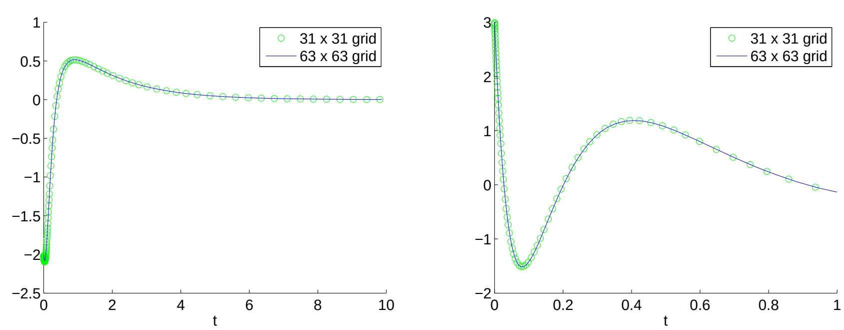

Figure 2: Approximate Hankel singular vector $f_2(t)$ for $0 \le t \le 10$ (left) and $g_4(t)$ for $0 \le t \le 1$ (right) computed using 31 and 63 equally spaced finite element nodes in each coordinate direction.

Figure 3 shows approximate balancing modes $\varphi_1(x, y)$ and $\psi_3(x, y)$. The modes were each computed using 63 equally spaced nodes in each coordinate direction; refining the computational grid produced little change in the modes. The higher numbered balancing modes become more oscillatory, and this seems directly connected to the oscillatory behavior of the Hankel singular vectors.

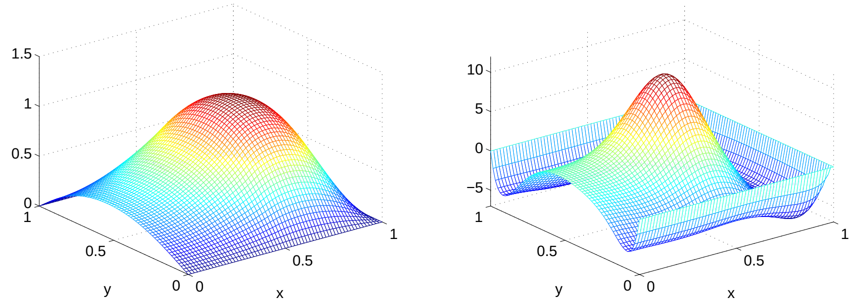

Figure 3: Approximate balancing modes $\varphi_1(x, y)$ (left) and $\psi_3(x, y)$ (right) computed using 63 equally spaced finite element nodes in each coordinate direction.

Now we consider the entrywise convergence of the matrices A_r^N, B_r^N, and C_r^N, as computed using (18) in the parabolic case. Recall that the balancing modes converge in V. As the higher numbered modes become more oscillatory, this convergence may become slower since the V norm measures the magnitudes of the partial derivatives with respect to x and y. Since the convergence of the entries of A_r^N depend on the convergence of the balancing modes in V, we may see slower convergence of the balanced truncation when we increase the size of the reduced model. We show below that this indeed occurs for this problem.

For $r = 4$, Table 1 shows that as the finite element mesh is refined, the maximum difference in the entries of each matrix is converging to zero. Thus, the balanced truncation is converging entrywise as in Theorem 3. Also, the entries of the matrices B_r^N and C_r^N are converging faster than the entries of A_r^N. This is not surprising since the convergence of the matrix A_r^N involves the convergence of the balancing modes in V, while the convergence of B_r^N and C_r^N only involves convergence of the balancing modes in X. As discussed earlier, standard finite element approximations of solutions of partial differential equations converge slower in V than in X. Since the approximate balancing modes are constructed using approximate solution data, we expect the convergence of the balancing modes to be slower in V than in X. Thus, the entries of A_r^N should converge slower than the entries of B_r^N and C_r^N. This observation shows that it may be beneficial to use special numerical methods where convergence in V is not slower than convergence in X.

Table 1: Maximum difference in entries for matrices in the reduced model (with $r = 4$) constructed using various finite element grids. The superscripts indicate the number of equally spaced finite element nodes used in each coordinate direction.

$A_4^{63} - A_4^{31}$	0.1287	$B_4^{63} - B_4^{31}$	2.2×10^{-3}	$C_4^{63} - C_4^{31}$	2.2×10^{-3}
$A_4^{95} - A_4^{63}$	0.0220	$B_4^{95} - B_4^{63}$	3.7×10^{-4}	$C_4^{95} - C_4^{63}$	3.9×10^{-4}

Furthermore, increasing the size of the reduced model to $r = 5$ further slows the convergence of A_r^N as seen in Table 2. (The convergence of the entries of B_r^N and C_r^N is nearly identical to the case $r = 4$ and is not shown.) This was predicted above since the higher numbered balancing modes become more oscillatory, and therefore the convergence of these modes in V should be slower. This in turn slows the convergence of A_r^N. Due to the algorithm comparison in our earlier work [33], we expect similar behavior in balancing computations using matrix approximations of the system operators.

Lastly, we consider the convergence of the transfer function in the $\mathcal{H}^\infty$ norm, which measures

Table 2: Maximum difference in entries for A_r^N (with $r = 5$) constructed using various finite element grids. The superscripts indicate the number of equally spaced finite element nodes used in each coordinate direction.

$A_5^{63} - A_5^{31}$	0.5402
$A_5^{95} - A_5^{63}$	0.0896

the maximum singular value of the function evaluated along the imaginary axis. Since the systems have only one input and one output, the $\mathcal{H}^\infty$ norm of a transfer function $G(s)$ is given by the largest value of $|G(i\omega)|$ for ω real. We chose $r = 4$, and approximated the $\mathcal{H}^\infty$ norm of the difference of transfer functions constructed using different finite element grids. (For the computations, we chose ω in the finite interval $10^{-4} \leq \omega \leq 10^4$.) The results in Table 3 show the convergence of the transfer functions as the finite element mesh is refined. It is interesting to note that the $\mathcal{H}^\infty$ norm error in the transfer functions converges to zero faster than the entries of the matrix A_r^N for $r = 4$.

Table 3: Approximate $\mathcal{H}^\infty$ norm error between transfer functions of the reduced systems (with $r = 4$) constructed using various finite element grids. The superscripts indicate the number of equally spaced finite element nodes used in each coordinate direction.

$\|G_4^{63} - G_4^{31}\|_\infty$	2.6×10^{-3}
$\|G_4^{95} - G_4^{63}\|_\infty$	4.6×10^{-4}

7.2 Example 2 - a 1D First Order Hyperbolic PDE

Next, we consider a 1D hyperbolic problem. We chose a simple problem for which the transfer function can be computed exactly for comparison.

The partial differential equation is given by

$$w_t = -a(x)w_x + b(x)u(t), \quad 0 < x < 1, \quad t > 0,$$

with boundary condition

$$w(t, 0) = 0.$$

System measurements are taken of the form

$$y(t) = \int_0^1 c(x)w(t, x)\, dx.$$

We take $a(x) = \beta - \alpha x$ with $\beta > \alpha > 0$, and $b(x)$ and $c(x)$ to be square integrable.

We take the Hilbert space X to be $L^2(0, 1)$ with standard inner product $(f, g) = \int_0^1 f(x)g(x)\, dx$. The operators $B : \mathbb{R}^1 \to X$ and $C : X \to \mathbb{R}^1$ are then given by $[Bu](x) = b(x)u$ and $Cw = (w, c)$. The operator $A : D(A) \subset X \to X$ is given by $[Aw](x) = -a(x)w_x(x)$, with $D(A) = H_L^1(0, 1)$. The space H_L^1 is the set of square integrable functions w with one square integrable distributional derivative that also satisfy the boundary condition $w(0) = 0$. It can be checked that the adjoint operator $A^* : D(A^*) \subset X \to X$ is given by $[A^*z](x) = (a(x)z(x))_x$, with $D(A^*) = H_R^1(0, 1)$. Functions in the space H_R^1 satisfy the boundary condition $z(1) = 0$.

For $a(x)$ given above, it can be checked that the exact transfer function $G(s) = C(sI - A)^{-1}B$ is given by

$$G(s) = \int_0^1 c(x)\,(\beta - \alpha x)^{s/\alpha} \int_0^x b(v)\,(\beta - \alpha v)^{-1-s/\alpha}\,dv\,dx.$$

In our numerical experiments, we chose $\beta = 0.5$, $\alpha = 0.4$, $b(x) = 1 - x$, and $c(x) = x$. In this case, these integrals can be computed exactly.

For these choices of $b(x) = 1 - x$ and $c(x) = x$, the solutions of the differential equations (4)-(5) required for the balanced POD algorithm are not classical solutions since $b \notin D(A)$ and $c \notin D(A^*)$. In fact, the solutions can be found exactly, and the solutions are discontinuous in the spatial variable x for $t < t_{\max} = \alpha^{-1} \ln(\beta/(\beta - \alpha))$. (The exact solutions are identically zero for all $t \geq t_{\max}$).

To test the balanced POD algorithm, we do not use the exact solutions of the differential equations (4)-(5). Instead, we approximate the solution with a simple first order accurate method: a discontinuous Galerkin method with piecewise constant basis functions (e.g., as in [12, Section 5.6] and [16, Section 4.8.2]), and forward Euler for the time stepping. We chose the constant time step $\Delta t = \beta \Delta x$, where Δx is the constant interval size of the piecewise constant basis functions. The equations were integrated until $t_f = t_{\max} + 1/2$. The method of snapshots was used for the balanced POD computations with $\theta^z = \theta^w = 1$ in the definition of the piecewise constant coefficients (23).

For this numerical method, the approximate solution data is $L^2(0,1)$ in space, and therefore the approximate balancing modes (13)-(14) are also only in $L^2(0,1)$. Therefore, the quantities $A\varphi_i^N$ and $A^*\psi_j^N$ are not well defined, and we approximate $A\varphi_i$ using the balanced POD algorithm variation of Section 3.2.

Figure 4 (left) shows the convergence of the Hankel singular values as Δx decreases. The convergence is clear, although it is slower than the parabolic example. Of course, the convergence speed could likely be increased by using a higher order numerical method for the approximate solutions of the PDEs. Figure 4 (right) shows approximations to $f_2(t)$ and $\dot{f}_2(t)$ with 500 spatial nodes. Increasing the number of nodes gave little change in the approximations.

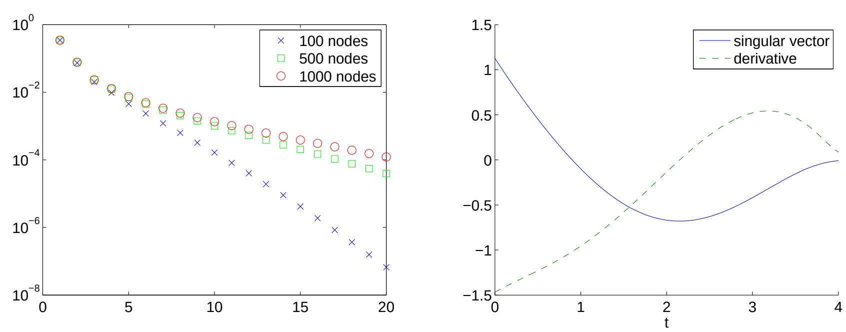

Figure 4: Approximate Hankel singular values (left) and approximations to $f_2(t)$ and $\dot{f}_2(t)$ for $0 \leq t \leq 4$ with 500 equally spaced spatial nodes (right).

Table 4 shows that as the grid is refined, the maximum difference in the entries of each matrix in the approximate reduced order model is converging to zero. Thus, the balanced truncation is converging entrywise as in Theorem 4. Again, we see that the entries of A_r converge more slowly than the entries of B_r and C_r.

Lastly, we consider the convergence of the transfer function in the $\mathcal{H}^\infty$ norm with $r = 5$ and $r = 10$ using different grids. (For the computations, we chose ω in the finite interval $10^{-3} \leq \omega \leq$

Table 4: Maximum difference in entries for matrices in the reduced model (with $r = 5$) constructed using various grids. The superscripts indicate the number of equally spaced spatial nodes.

$A_5^{500} - A_5^{100}$	0.1865	$B_5^{500} - B_5^{100}$	9.1×10^{-3}	$C_5^{500} - C_5^{100}$	9.1×10^{-3}
$A_5^{1000} - A_5^{500}$	0.0242	$B_5^{1000} - B_5^{500}$	6.1×10^{-4}	$C_5^{1000} - C_5^{500}$	6.1×10^{-4}

10^2.) Table 5 show the error between the exact and approximate transfer functions converges as the grid is refined.

Table 5: Approximate $\mathcal{H}^\infty$ norm error between the exact and approximate transfer functions of the reduced systems (with $r = 5$ and $r = 10$) constructed using various grids. The superscripts indicate the number of equally spaced spatial nodes.

$\|G - G_5^{100}\|_\infty$	0.0118	$\|G - G_{10}^{100}\|_\infty$	0.0091
$\|G - G_5^{500}\|_\infty$	0.0075	$\|G - G_{10}^{500}\|_\infty$	0.0027
$\|G - G_5^{1000}\|_\infty$	0.0075	$\|G - G_{10}^{1000}\|_\infty$	0.0020

8 Conclusion

In this work, we considered an algorithm for balanced truncation of exponentially stable linear infinite dimensional systems with bounded, finite rank input and output operators. The algorithm is an extension of Rowley's balanced POD algorithm for finite dimensional systems [30]. We developed the algorithm using the Hankel operator of the system, which is different from Rowley's original approach. We proved that the balanced realization of the system can be expressed in terms of balancing modes, which are related to the Hankel singular values and singular vectors of the system. We considered approximation techniques related to methods for the proper orthogonal decomposition to compute the balancing modes and the balanced realization. We proved convergence of the balanced POD model reduction approximations for parabolic systems, and also proved convergence of a modified algorithm for general systems. We also presented numerical results for two example PDE systems which demonstrated the convergence of the method, as predicted by the theory.

As discussed in the introduction, this method has the potential to be beneficial in situations where matrix approximations of system operators are not available, or may be undesirable to use. Another potential advantage of the algorithm is that the required simulations can be performed using existing code and special techniques, such as adaptive mesh refinement. It is important to note that even if another method is more computationally efficient, this algorithm is computationally tractable and therefore it may be preferable to use in many situations due to the advantages listed above.

In future work, we plan to explore the extension of this algorithm to systems with unbounded input and output operators. Furthermore, there are other questions raised in this work to be explored. First, the convergence analysis for the parabolic systems requires convergence of data in V, which is stronger than convergence in the underlying Hilbert space X. As mentioned above, convergence in V for many numerical methods for parabolic equations is often slower than convergence in X; therefore, it may be beneficial to use special numerical methods which give faster convergence in V. This approach needs to be tested.

Also, there are other approaches for approximating the balanced truncation that we intend to explore. First, we can directly approximate the exact representation (31)-(33) of the balanced realization given in terms of the Hankel singular values and singular vectors. Another approach is to use a formula similar to equation (4.9) in [14], which constructs the entries of A_r (for the output normal balanced realization) using the Hankel singular values and singular vectors evaluated at $t = 0$. The balanced POD algorithms here are able to produce convergent results for these exact representations. We plan to compare all of these approaches in future work.

If one of these other snapshot balanced POD approaches is superior to the algorithm considered here, the results of this work still have potential for model reduction of *nonlinear* systems. The balancing modes constructed for a linearized system can then be used to reduce the nonlinear system by a Petrov-Galerkin projection; see, e.g., [23]. The convergence of the balancing modes as established here would likely be important for such a procedure.

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