รายงานวิจัยฉบับสมบูรณ์

โครงการ **การพัฒนาวิธีลดรูปโมเดลไม่เชิงเส้นที่รักษาลักษณะโครงสร้างและสมดุลของระบบ**

โดย **ดร.สายฝน จาตุรันตบุตร**

กรกฎาคม พ.ศ. 2560

สัญญาเลขที่ TRG5880216

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ผู้วิจัย **ดร.สายฝน จาตุรันตบุตร**
สังกัด มหาวิทยาลัยธรรมศาสตร์

สนับสนุนโดยสำนักงานกองทุนสนับสนุนการวิจัยและต้นสังกัด มหาวิทยาลัยธรรมศาสตร์

รายงานวิจัยฉบับสมบูรณ์

ประกอบด้วย

- ส่วนที่ 1: บทคัดย่อภาษาไทย และภาษาอังกฤษ
- ส่วนที่ 2: เนื้อหา และสรุปผล
- ส่วนที่ 3: ภาคผนวก

1) Proceeding:

   Chaturantabut, S., Reduced-Order Modeling with Monotonicity Property, *AIP Conference Proceeding of the 2nd International Conference "Numerical Computations: Theory and Algorithms,"* pp. 090019: 1-4, 2016.

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2) Preprint (อยู่ในระหว่างรอผลการตอบรับ *Journal of Computational and Applied Mathematics, (Elsevier)*

   ภายใต้หัวข้อเรื่อง

   "Stabilized Nonlinear Complexity Reduction through Contractivity-Preserving Framework"

ส่วนที่ 1

บทคัดย่อภาษาไทย และภาษาอังกฤษ

Abstract

Project Code: TRG5880216

Project Title: Development of Structure-Preserving Nonlinear Model Reduction

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Project Period: 2 years

Numerical simulations of many natural phenomena described by nonlinear differential equations can lead to dynamical systems with very large spatial dimension when a standard discretization scheme is applied. To reduce the computational cost for solving each of these large-scale systems, model reduction methods can be used to produce relatively low dimensional model that still provides accurate solution of the original system. In general, the accuracy of a given model reduction technique is evaluated through certain error measurements when compared with some known reference solutions. Besides considering these approximation errors, this work aims to preserve fundamental behavior of the original system, which will be done through contraction analysis.

This work develops a nonlinear model reduction approach that not only reduces the computational complexity or substantially decreases the simulation time, but also preserves monotonicity and contractivity properties of the original full-order model to ensure the stability as well as the existence and uniqueness of the solution. The proposed technique is based on using basis sets from proper orthogonal decomposition method and modifying an interpolatory projection approach, called discrete empirical interpolation method, by enforcing a symmetric structure of the approximation. The efficiency and accuracy of the proposed method are illustrated through the numerical tests on a nonlinear model describing reaction diffusion problems.

Keywords: Model order reductions, Contractivity, Ordinary differential equations (ODEs), Partial differential equations (PDEs), Proper orthogonal decomposition (POD), Discrete empirical interpolation method (DEIM)

เอกสารแนบหมายเลข 2

บทคัดย่อ

รหัสโครงการ: TRG5880216

ชื่อโครงการ: การพัฒนาวิธีลดรูปโมเดลไม่เชิงเส้นที่รักษาลักษณะโครงสร้างและสมดุลของระบบ

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ระยะเวลาโครงการ: 2 ปี

ในปัจจุบัน มีการศึกษาปรากฏการณ์ต่าง ๆ ในธรรมชาติหรือการทดลองทางวิทยาศาสตร์ ที่อาศัยการใช้แบบจำลอง ร่วมกับการใช้ระเบียบวิธีเชิงตัวเลข เพิ่มมากขึ้น โดยทั่วไปเมื่อปรากฏการณ์ที่เราสนใจสอดคล้องกับสมการเชิงอนุพันธ์ย่อยไม่เชิงเส้น (nonlinear differential equations) การจำลองนั้นจะมีความยุ่งยากซับซ้อน และมีความจำเป็นที่จะต้องเพิ่มความละเอียดของ Discretization หรือเพิ่มจำนวนตัวแปรเพื่อให้ค่าประมาณจากผลเฉลยเชิงตัวเลขมีความแม่นยำมากขึ้น ซึ่งการเพิ่มความละเอียดนี้จะส่งผลให้ขนาดของระบบสมการเชิงอนุพันธ์ที่เกิดขึ้นมีขนาดใหญ่ส่งผลให้เวลาที่ใช้ในการคำนวณแบบจำลองมากขึ้นตามไปด้วย ดังนั้นการจำลองเชิงตัวเลขนี้อาจจะยังมีประสิทธิภาพไม่เพียงพอสำหรับนำไปใช้เพื่อพยากรณ์หรือคาดการณ์ผลลัพธ์ที่จะเกิดขึ้นจริงหรือจากการทดลอง โครงการวิจัยนี้มีเป้าหมายเพื่อแก้ไขข้อจำกัดในเรื่องของเวลาที่ใช้คำนวณและขนาดของระบบที่ใช้เก็บข้อมูลตามที่กล่าวมาข้างต้น สำหรับการทำแบบจำลองสำหรับปัญหาไม่เชิงเส้น

โครงการวิจัยนี้ได้พัฒนาแบบจำลองลดรูป (reduced-order modeling) ที่ลดความซับซ้อนในการคำนวณเชิงตัวเลข และยังคงมีความถูกต้องแม่นยำและรักษาคุณสมบัติเดิมของระบบตั้งต้นไว้ได้ โดยใช้การวิเคราะห์คุณสมบัติการหดตัว (contractivity analysis) ของฟังก์ชันไม่เชิงเส้นที่ปรากฏอยู่ในสมการเชิงอนุพันธ์ งานวิจัยนี้ได้พิสูจน์ว่าคุณสมบัติการหดตัว (contractivity) สามารถนำมาใช้เพื่อยืนยันว่าระบบลดรูปที่สร้างขึ้น รักษาเสถียรภาพของระบบตั้งต้นได้ หลักการที่ใช้ในงานวิจัยนี้ มีแนวคิดมาจากการใช้วิธี proper orthogonal decomposition เพื่อสร้าง basis set ที่สามารถดึงลักษณะสำคัญของระบบออกมาได้อย่างแม่นยำ ร่วมกับแนวคิดของวิธี discrete empirical interpolation method ซึ่งสามารถลดความซับซ้อนในการคำนวณเชิงตัวเลขได้อย่างมีประสิทธิภาพ รูปแบบของโมเดลลดรูปที่ได้จะรักษาโครงสร้างที่มีผลต่อคุณสมบัติการหดตัว โดยเมื่อนำไปทดสอบกับสมการเชิงอนุพันธ์ที่สอดคล้องกับปัญหา nonlinear diffusion-reaction ผลลัพธ์ที่ได้แสดงถึงประสิทธิภาพและความแม่นยำของโมเดลลดรูปที่พัฒนาขึ้น

ส่วนที่ 2

เนื้อหา และสรุปผล

FINAL REPORT

(2 YEARS)

TRF GRANT FOR NEW RESEARCHER: 2015-2017

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Title: **Development of Structure-Preserving Nonlinear Model Reduction**

by

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July, 2017

Abstract

Development of Structure-Preserving Nonlinear Model Reduction

by

Saifon Chaturantabut

This work develops a nonlinear model reduction approach that not only reduces the computational complexity or substantially decreases the simulation time, but also preserves monotonicity and contractivity properties of the original full-order model to ensure the stability as well as the existence and uniqueness of the solution. The proposed technique is based on using basis sets from proper orthogonal decomposition method and modifying an interpolatory projection approach, called discrete empirical interpolation method, by enforcing a symmetric structure of the approximation. The efficiency and accuracy of the proposed method are illustrated through the numerical tests on a nonlinear model describing reaction diffusion problems.

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Chapter 1

Introduction

Introduction to the research problem and its significance

In many practical applications, the simulation of complex physical phenomena often involves nonlinear differential equations, which upon spatial discretization, lead to dynamical models with very large spatial dimension. This creates a need for *model reduction* methods that can produce relatively low dimensional models but can still provide accurate behavior of the original systems.

For a number of physical systems, including a large class of mechanical systems and network models, it is crucial to preserve certain structures and properties, such as stability, through the corresponding reduced-order systems. For linear dynamical systems, various structure-preserving model reduction frameworks have been proposed [61, 11, 45, 46]. For nonlinear systems, projection-based model reduction approaches with basis from proper orthogonal decomposition (POD) or Karhunen-Loeve expansion [38, 37, 10] have been successful in substantially reducing the number of state variables, as well as preserve the system structures. However, these approaches fail to reduce the computational complexity involved with evaluating nonlinear terms. Unless there is a special structure, such as a bi-linear form, the evaluation of nonlinear terms has the same order of complexity as the full order system. Hence, developing efficient model reduction approaches that preserve system properties is still a challenging research issue.

Literature review

A common model reduction approach is based on applying the Galerkin projection onto a *low dimensional* subspace, which is expected to contain dominant characteristics of the corresponding solution space [2]. This subspace can be represented by a set of *reduced basis* vectors with global support which are *"learned"* ; they are constructed from high fidelity classical discretization schemes. These reduced basis functions are hence problem dependent. Fine scale detail is *encoded* in these global basis functions and this makes it possible to obtain good approximation with relatively few basis functions.

The basis that is commonly used with Galerkin projection is constructed from proper orthogonal decomposition (POD). POD has been successfully used with a Galerkin projection to provide reduced-order models in numerous applications such as compressible flow [53], computational fluid dynamics [35, 52], aerodynamics [14], and optimal control [34].

Although the Galerkin projection-based methods with POD basis have been successful in substantially reducing the number of state variables, they typically fail to reduce the computational complexity used for evaluating nonlinear terms. This inefficiency of the POD-Galerkin approach arises from the high computational complexity in repeatedly calculating the inner products required to evaluate the projected nonlinearities. Several approaches have been proposed to address this fundamental issue.

In [4], Missing Point Estimation (MPE) was proposed to improve the complexity of the POD-Galerkin reduced system in finite volume discretization, essentially, by solving only a subset of equations of the original model. A reduced system is obtained by first extracting certain equations corresponding to specially chosen spatial grid points and then projecting the extracted system onto the space spanned by the restricted POD with components/rows corresponding to only these selected grid points. This procedure can be viewed as performing the Galerkin projection onto the truncated POD basis via a specially constructed inner product as defined in [7] that evaluates only at selected grid points instead of computing the usual $\mathcal{L}^2$ inner product. Two heuristic methods for selecting these spatial grid points are introduced in [4, 3, 6, 5] by aiming to minimize aliasing effects in using only partial spatial points. This was shown to be equivalent to a criterion for preserving the orthogonality of the restricted POD basis vectors, which is further translated into a criterion for controlling condition number growth. These grid point selection procedures were later improved by incorporating a greedy algorithm from [60]. The applications of the MPE method are primarily in the context of a linear time varying system arising from finite volume discretization of a nonlinear computational fluid dynamic model for a glass melting furnace [4, 3, 6, 5]. It has also been used in modeling heat transfer in electrical circuits [58] and in subsurface flow simulation [16].

Alternatively, techniques for approximating a nonlinear function can be used in conjunction with the POD-Galerkin projection method to overcome this computational inefficiency. There are a number of examples that use model reduction approaches with nonlinear approximation based on pre-computation of coefficients defining multi-linear forms of polynomial nonlinearities followed by POD-Galerkin projection [22, 23, 42, 8, 26, 15]. One of these approaches is found in the trajectory piecewise-linear (TPWL) approximation proposed by Rewienski and White [51, 50], which is based on approximating a nonlinear function by a weighted sum of linearized models at selected points along a state trajectory. These linearization points are selected using prior knowledge from a training trajectory of the full-order nonlinear system [49]. The TPWL approach was successfully applied to several practical nonlinear systems, especially in circuit simulations [48, 49, 50, 58, 12]. However, there are still many nonlinear functions that may not be approximated well by using low degree piecewise polynomials unless there are very many constituent polynomials.

In order to handle general form of nonlinearity, empirical interpolation method (EIM) was proposed by Barrault, Maday, Nguyen and Patera in [9] in the finite element setting. Discrete empirical interpolation (DEIM) [18] was then introduced for general nonlinear ordinary differential equations. A considerable reduction in complexity is achieved by DEIM because evaluating the approximate nonlinear term does not require a prolongation of the reduced state variables back to the original high dimensional state approximation required to evaluate the nonlinearity in the POD approximation. DEIM therefore improves the efficiency of the POD approximation and achieves a complexity reduction of the nonlinear term with a complexity proportional to the number of reduced variables. An error bound for the DEIM approximation is given in [18] which shows it is nearly as accurate as the optimal POD approximation. Recently, DEIM has been successfully used for model reduction in many applications such as in neural modeling of full Hodgkin-Huxley models for realistic spiking neurons [33], in shallow water equations [57], coupled circuit-device systems [31], and reduced order quadrature algorithm [1].

However, these *efficient* nonlinear model reduction approaches based on interpolatory projection, e.g. gappy-POD, EIM and DEIM, may not preserve the structure of the original systems as required in the application of port-based systems or mechanical models. The existing works on structure preserving for nonlinear systems [38, 37, 10] are based on special modifications of POD-Galerkin projection extended from the approaches for linear systems [61, 43, 29, 44, 11]. Hence, the resulting reduced systems still always have complexity proportional to the full-order dimension in the case of *general nonlinear* functions. That is, these reduced systems may not be able to achieve a significant reduction in actual computation time. This project will employ a concept of interpolatory projection-based nonlinear model reduction approach, particularly DEIM, and enforce the structured form of the approximated nonlinear term to derive a structure-preserving nonlinear model reduction approach that can be computed with low computational complexity.

Chapter 2

PRELIMINARY: Monotonicity and Contractivity

This chapter presents some theoretical background required for deriving a structure-preserving model reduction for dynamical systems. The desired form of system structure to be preserved will be discussed together with the significance of this structure.

2.1 Problem Formulation

Consider the system of nonlinear ordinary differential equations (ODEs) of the form:

$$\frac{d\mathbf{y}}{dt} = \mathbf{F}(\mathbf{y}), \qquad \mathbf{y}(0) = \mathbf{y}_0, \tag{2.1}$$

where $\mathbf{y} = \mathbf{y}(t)$ is an n dimensional state variable at certain time $t \geq 0$ and $\mathbf{F}$ is a differentiable nonlinear vector field in $\mathbf{y}$ with Jacobian of $\mathbf{F}$ given by $J_F(\mathbf{y}, t) = \frac{\partial f}{\partial \mathbf{y}}(\mathbf{y}, t)$. The goal is to construct a reduced system that can provide approximate solutions that preserve the behavior of the original system. In particular, we are interested in the property called **monotonicity** of the vector field, which can be used to guarantee the contractivity of the flow in the solutions of dynamical systems. The contractivity is an important tool for deriving the conditions for stability, as well as the existence and uniqueness of equilibrium solutions.

2.2 Monotonicity & Contractivity

We first consider the **logarithmic norm**, introduced independently by Germund Dahlquist and Sergei Lozinskii in 1959 [40, 25] defined next in a special case of Euclidean space.

Definition 2.2.1 *Let* $\mathbf{A} \in \mathbb{R}^{n\times n}$ *be a constant matrix. the associated matrix measure, called* **logarithmic norm** *is defined as*

$$\mu[\mathbf{A}] = \lim_{h\to 0^+} \frac{\|I + h\mathbf{A}\| - 1}{h}, \tag{2.2}$$

where $\|\cdot\|$ *is the standard Euclidean norm.*

The logarithmic norm can be used to measure the distance between matrices. Note that $\|\cdot\|$ can be any norm and when it is the Euclidean 2-norm, $\mu(\mathbf{A})$ is the maximum eigenvalue of the symmetric part of $\mathbf{A}$. In particular, it can be shown that [55], for the Euclidean 2-norm $\|\cdot\|$

$$\mu[\mathbf{A}] = \lambda_{\max}\left(\frac{\mathbf{A}+\mathbf{A}^T}{2}\right), \tag{2.3}$$

where $\lambda_{\max}(\cdot)$ gives the maximum eigenvalue of the input quantity. Equivalently, it can also be shown that, for any induced norm in Hilbert space, for $\mathbf{u}, \mathbf{v} \in \mathbb{R}^n$

$$\mu[\mathbf{A}] = \sup_{\mathbf{u}\neq\mathbf{v}} \frac{\operatorname{Re}\langle \mathbf{u}-\mathbf{v}, \mathbf{A}\mathbf{u}-\mathbf{A}\mathbf{v}\rangle}{\langle \mathbf{u}-\mathbf{v}, \mathbf{u}-\mathbf{v}\rangle}, \tag{2.4}$$

where $\|\mathbf{x}\|^2 = \langle \mathbf{x}, \mathbf{x}\rangle$, $\mathbf{x} \in \mathbb{R}^n$. Consider the system (2.1) is a linear problem of the form $\mathbf{F}(\mathbf{y}) = \mathbf{A}\mathbf{y} + \mathbf{r}(t)$, i.e.

$$\dot{\mathbf{y}} = \mathbf{A}\mathbf{y} + \mathbf{r}(t), \qquad \mathbf{y}(0) = \mathbf{y}_0.$$

Using the identity (2.4) for the Euclidean 2-norm and $\|\mathbf{y}\|\frac{d}{dt}\|\mathbf{y}\| = \frac{1}{2}\|\mathbf{y}\|^2 = \mathbf{y}^T\dot{\mathbf{y}} = \langle \mathbf{y}, \dot{\mathbf{y}}\rangle$, we have

$$\begin{aligned}
\frac{d}{dt}\|\mathbf{y}\| &= \frac{1}{\|\mathbf{y}\|}\langle \mathbf{y}, \dot{\mathbf{y}}\rangle \\
&= \frac{1}{\|\mathbf{y}\|}\langle \mathbf{y}, \mathbf{A}\mathbf{y} + \mathbf{r}(t)\rangle \\
&= \frac{1}{\|\mathbf{y}\|^2}\langle \mathbf{y}, \mathbf{A}\mathbf{y}\rangle\|\mathbf{y}\| + \frac{1}{\|\mathbf{y}\|}\langle \mathbf{y}, \mathbf{r}(t)\rangle \\
&\leq \mu[\mathbf{A}]\|\mathbf{y}\| + \|\mathbf{r}(t)\|.
\end{aligned}$$

Integrating the above differential inequality gives

$$\|\mathbf{y}(t)\| \leq \|\mathbf{y}(0)\|\ e^{\mu[\mathbf{A}]t} + \int_0^t \|r(\tau)\|\ e^{(t-\tau)\mu[\mathbf{A}]} d\tau. \tag{2.5}$$

The above bound illustrates the application of **logarithmic norm** on certain system's properties, such as stability and perturbation. The logarithmic norms can also be used to show contractivity of differential equations, as well as the general form of differential inequalities, which can further extend to the convergence analysis for numerical schemes used in solving differential equations.

The notion of logarithmic norm can be extended to the nonlinear operator in Banach spaces as shown next [55].

2.2.1 Logarithmic Lipschitz constants

We now define and state elementary properties of logarithmic Lipschitz constants, which can be used in the applications to ODEs.

Definition 2.2.2 *Let $(X, \|\cdot\|_X)$ be a normed space and $f : Y \to X$ be a function where $Y \subseteq X$. The* **least upper bound (lub)** *and the* **greatest lower bound (glb) Lipschitz constants** *of f induced by the norm $\|\cdot\|_X$ on Y are defined, respectively, by*

$$L_{Y,X}[f] = \sup_{u \neq v \in Y} \frac{\|f(u) - f(v)\|_X}{\|u - v\|_X}, \qquad \text{and} \qquad \ell_{Y,X}[f] = \inf_{u \neq v \in Y} \frac{\|f(u) - f(v)\|_X}{\|u - v\|_X}.$$

The **least upper bound (lub)** *and the* **greatest lower bound (glb) logarithmic Lipschitz constants** *of f induced by the norm $\|\cdot\|_X$ on Y are defined by*

$$M_{Y,X}[f] = \lim_{h\to 0^+} \frac{L_{Y,X}[I+hf]-1}{h}, \qquad and \qquad m_{Y,X}[f] = \lim_{h\to 0^-} \frac{L_{Y,X}[I+hf]-1}{h}.$$

Note that, this work considers the setting for systems of ODEs with $X = Y \subseteq \mathbb{R}^n$ and we will use the notation $L_{Y,X}[\cdot] = L[\cdot]$, $\ell_{Y,X}[\cdot] = \ell[\cdot]$ and $M_{Y,X}[\cdot] = M[\cdot]$, $m_{Y,X}[\cdot] = m[\cdot]$ in this case. Moreover, we will use the Euclidean 2- norm for $\|\cdot\|_X$, which will be simply denoted as $\|\cdot\|$, and from [55], it can be shown that $M[\cdot] = m[\cdot]$ and for $\mathbf{u}, \mathbf{v} \in \mathbb{R}^n$,

$$M[\mathbf{F}] = \sup_{\mathbf{u}\neq\mathbf{v}} \frac{\langle \mathbf{u}-\mathbf{v}, \mathbf{F}(\mathbf{u})-\mathbf{F}(\mathbf{v})\rangle}{\|\mathbf{u}-\mathbf{v}\|^2} = \sup_{\mathbf{u}\neq\mathbf{v}} \frac{(\mathbf{u}-\mathbf{v})^T(\mathbf{F}(\mathbf{u})-\mathbf{F}(\mathbf{v}))}{\|\mathbf{u}-\mathbf{v}\|^2}. \tag{2.6}$$

We will next consider the notion the *motonicity* of a vector field, which can further imply the *contractivity* for the flow of the vector field.

Definition 2.2.3 *A map $\mathbf{F}$ defined from X to Y, where $Y \subseteq X \subseteq \mathbb{R}^n$ is said to be uniformly negative monotone if $M[\mathbf{F}] < 0$. For the differential equation: $\dot{\mathbf{y}} = \mathbf{F}(\mathbf{y})$, the map $e^{t\mathbf{F}} : \mathbf{y}(0) \to \mathbf{y}(t)$ is a contractive flow if $L[e^{t\mathbf{F}}] < 1$.*

<u>**Remarks**</u>

- If $\mathbf{F}$ is a *uniform negative monotone* vector field, i.e. $M[\mathbf{F}] < 1$, then the corresponding flow $e^{t\mathbf{F}}$ is contractive. This follow from the fact that $L[e^{t\mathbf{F}}] \leq e^{t\ M[\mathbf{F}]}$ as given in [55].

- Contractive property of the flow is often used to guarantee the existence and uniqueness of (2.1), as well as the exponential stability.

- Suppose $\mathbf{y}^*$ is the zero equilibrium solution, i.e. it satisfies $\mathbf{F}(\mathbf{y}^*) = 0$. The existence of $\mathbf{y}^*$ can be guaranteed when $\mathbf{F}$ is *uniformly negative monotone* or $M[\mathbf{F}] < 0$. It can be shown that $M[\mathbf{F}] < 0$ implies $L[\mathbf{F}^{-1}] \leq -\frac{1}{M[\mathbf{F}]} < \infty$ [55]. That is, there exists an inverse function $\mathbf{F}^{-1}$ so that $\mathbf{y}^* = \mathbf{F}^{-1}(0)$.

- The monotonicity is generally used for deriving a bound for perturbation at the equilibrium of (2.1). In particular, suppose $\mathbf{y}$ is the solution of the perturbed system $\mathbf{F}(\mathbf{y}) = \mathbf{p}$ for $\mathbf{p} \in \mathbb{R}^n$ with small $\|\mathbf{p}\|$. Then $\|\mathbf{y}^* - \mathbf{y}\| \leq \frac{\|\mathbf{p}\|}{M[\mathbf{F}]}(e^{tM[\mathbf{F}]} - 1)$. When $\mathbf{F}$ is *uniformly negative monotone*, i.e. $M[\mathbf{F}] < 0$, we have

$$\|\mathbf{y}^* - \mathbf{y}\| \leq -\frac{\|\mathbf{p}\|}{M[\mathbf{F}]},$$

  which implies that there exists a unique stable equilibrium since $\|\mathbf{y}^* - \mathbf{y}\| \to 0$ as $\|\mathbf{p}\| \to 0$.

Next, we will use these notions to derive a form of model reduction that can preserve the negative monotonicity, and hence provide solutions with contractive flow as well as the stability [55].

Chapter 3

PRELIMINARY: Model Reduction Techniques

This chapter presents two model reduction techniques for nonlinear ordinary differential equations (ODEs). First note that, model order reduction aims to reduce the number of unknowns and not to reduce the order of the derivatives. A common technique used in dimension reduction is Proper Orthogonal Decomposition (POD) combined with Galerkin projection. For nonlinear problems, this technique can reduced only dimensions of linear term, because POD cannot reduce the complexity of nonlinear term. Therefore, we combine POD approximation with Discrete Empirical Interpolation Method (DEIM), which can reduce the complexity of nonlinear term so that it does not depend on the large dimension of full-order system.

3.1 Model reduction techniques

The goal of model reduction techniques used in this work is to decrease the dimension of the discretized systems from nonlinear partial differential equations (PDEs). The discretization is generally in the form of system of nonlinear ordinary differential equations (ODEs):

$$\frac{d}{dt}\mathbf{y}(t) = \mathbf{A}\mathbf{y}(t) + \mathbf{F}(\mathbf{y}(t)), \tag{3.1}$$

where $\mathbf{y}(t) = [\mathbf{y}_1(t), \ldots, \mathbf{y}_n(t)]^T \in \mathbb{R}^n$ is the state variable with initial condition $\mathbf{y}(0) = \mathbf{y}_0 \in \mathbb{R}^n$, t is time, $\mathbf{A} \in \mathbb{R}^{n\times n}$ is a constant matrix, and $\mathbf{F}$ is a nonlinear vector-valued function evaluated at $\mathbf{y}(t)$ componentwise. This type of system often arises from the discretization of nonlinear PDEs. The dimension n, which is the number of unknowns of this system, is generally required to be very large to obtain accurate numerical solution. In this work, we will call (3.1) as original full-order system or full-order system of dimension n, which will be costly to compute in practice. We can reduce the computational complexity and simulation time by using the following methods.

3.2 Projection-based model order reduction

Projection-based method can construct a reduced-order system by projecting (3.1) onto a low dimensional subspace. Let $\mathbf{V}_k \in \mathbb{R}^{n\times k}$ be a matrix whose columns form a set of an orthonormal basis of dimension k, where $k < n$. Then, we can approximate the state variable $\mathbf{y}(t)$ in the space spanned by the columns of $\mathbf{V}_k$, i.e.

$$\mathbf{y}(t) \approx \mathbf{V}_k\tilde{\mathbf{y}}(t), \tag{3.2}$$

where $\tilde{\mathbf{y}}(t) \in \mathbb{R}^k$. By substituting (3.2) into (3.1), we obtain the following reduced system with k unknows in $\tilde{\mathbf{y}}(t)$.

$$\frac{d}{dt}\mathbf{V}_k\tilde{\mathbf{y}}(t) = \mathbf{A}\mathbf{V}_k\tilde{\mathbf{y}}(t) + \mathbf{F}(\mathbf{V}_k\tilde{\mathbf{y}}(t)), \tag{3.3}$$

with initial condition

$$\mathbf{V}_k\tilde{\mathbf{y}}(0) = \mathbf{y}_0. \tag{3.4}$$

Then, applying the Galerkin projection which will give the smallest error of the residual in the direction of $span\{\mathbf{V}_k\}$. The POD reduced system is of the form:

$$\mathbf{V}_k^T\frac{d}{dt}\mathbf{V}_k\tilde{\mathbf{y}}(t) = \mathbf{V}_k^T\mathbf{A}\mathbf{V}_k\tilde{\mathbf{y}}(t) + \mathbf{V}_k^T\mathbf{F}(\mathbf{V}_k\tilde{\mathbf{y}}(t)), \tag{3.5}$$

and the initial condition (3.4) of the POD reduced system becomes

$$\mathbf{V}_k^T\mathbf{V}_k\tilde{\mathbf{y}}(0) = \mathbf{V}_k^T\mathbf{y}_0. \tag{3.6}$$

Since $\mathbf{V}_k^T \mathbf{V}_k = \mathbf{I}_k$, (3.3) and (3.4) can be written as

$$\frac{d}{dt}\tilde{\mathbf{y}}(t) = \underbrace{\mathbf{V}_k^T \mathbf{A} \mathbf{V}_k}_{\tilde{\mathbf{A}}} \tilde{\mathbf{y}}(t) + \mathbf{V}_k^T \mathbf{F}(\mathbf{V}_k \tilde{\mathbf{y}}(t)), \tag{3.7}$$

$$\tilde{\mathbf{y}}(0) = \mathbf{V}_k^T \mathbf{y}_0, \tag{3.8}$$

where $\tilde{\mathbf{A}} = \mathbf{V}_k^T \mathbf{A} \mathbf{V}_k \in \mathbb{R}^{k \times k}$ can be precomputed because it does not depend on time and (3.7) is called POD reduced system. In this setting, $\mathbf{V}_k$ can be obtained from any orthogonal basis. However, to get a good approximation from this reduced system, we will consider the basis constructed by Proper Orthogonal Decomposition (POD) which will be described in Section 3.3.

3.3 Proper Orthogonal Decomposition (POD)

This section considers the procedure of POD. In 1937, John Lumley initially proposed POD in the context of inhomogeneous structure turbulent flows[**?**] and stochastic tools in turbulence (1970)[41]. POD is also known by other names, for example, Karhunen-Love decomposition (KLD), Principal Component Analysis (PCA), or Singular Value Decomposition (SVD). POD has been used in many applications, e.g. [13, 39, 36, 54, 30]. We will next consider construct a low dimensional by using POD with the Galerkin projection.

3.3.1 POD basis

The aim of POD is to construct a set of global basis functions by extracting basis that describes the main dynamics from the system of interest, which can be obtained by the singular value decomposition (SVD) of solutions or snapshots:$\mathbf{Y} \in \mathbb{R}^{n \times n_s}$. The singular value decomposition of a rectangular matrix $\mathbf{Y} \in \mathbb{R}^{n \times n_s}$ is given by the following theorem.

Theorem 3.3.1 (Singular value decomposition,[28]) *Let $\mathbf{Y} = [\mathbf{y}_1, \ldots, \mathbf{y}_{n_s}] \in \mathbb{R}^{n \times n_s}$ be a snapshot matrix of rank r with $\mathbf{y}_i \cong y(t_i), t_i \in \mathcal{I}, i = 1, \ldots, n_s$. Then there exists a decomposition of the form*

$$\mathbf{Y} = \hat{\mathbf{U}} \begin{bmatrix} \sigma_1 & & 0 \\ & \ddots & \\ 0 & & \sigma_r \end{bmatrix} \mathbf{Z}^T = \hat{\mathbf{U}} \Sigma \mathbf{Z}^T \tag{3.9}$$

where $\hat{\mathbf{U}} \in \mathbb{R}^{n \times r}$ and $\mathbf{Z} \in \mathbb{R}^{n_s \times r}$ are orthogonal matrices and $\Sigma = diag(\sigma_1, \ldots, \sigma_r) \in \mathbb{R}^{r \times r}$. The columns in $\hat{\mathbf{U}} = [\mathbf{u}_1, \ldots, \mathbf{u}_n]$ are called the (left) singular vectors of $\mathbf{Y}$ and for the singular values σ_i it holds: $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_r > 0$.

Proof: The formal derivation can, for example, be found in [28]. □

Notice that, for the SVD of $\mathbf{Y} = \hat{\mathbf{U}} \Sigma \mathbf{Z}^T$, the following diagonalization holds

$$\mathbf{Y}\mathbf{Y}^T = (\hat{\mathbf{U}} \Sigma \mathbf{Z}^T)(\hat{\mathbf{U}} \Sigma \mathbf{Z}^T)^T = \hat{\mathbf{U}} \Sigma^2 \hat{\mathbf{U}}^T, \tag{3.10}$$

and therfore, the columns of $\hat{\mathbf{U}}$ are eigenvectors of the matrix $\mathbf{Y}\mathbf{Y}^T$ with corresponding eigenvalues $\lambda_i = \sigma_i^2 > 0, i = 1, \ldots, r$.

Next, the calculation of POD basis can be done by using the following steps in Algorithm 1.

Algorithm 1 Algorithm to create POD basis

INPUT: $\{\mathbf{y}_j\}_{j=1}^{n_s}$ is the snapshots.
OUTPUT: $\mathbf{V}_k$ is POD basis.

1: Create snapshots: $\mathbf{Y} = [\mathbf{y}_1, \ldots, \mathbf{y}_{n_s}] \in \mathbb{R}^{n \times n_s}$and Let $r = rank(\mathbf{Y})$
2: Compute by using SVD: $\mathbf{Y} = \hat{\mathbf{U}}\Sigma\mathbf{Z}^T$
3: POD basis: $\mathbf{V}_k = [\mathbf{v}_1, \ldots, \mathbf{v}_k] = \hat{\mathbf{U}}(:, 1 : k)$

From POD basis Algorithm 1, we create first the snapshots which are the solutions in the different time steps. Then, we find POD basis $\mathbf{V}_k$ from the snapshots by using SVD or POD. Likewise, in the case of nonlinear term, we find POD basis from Algorithm 2.

Algorithm 2 Algorithm to create POD basis for varying parameters

INPUT: $\{\mathbf{F}(\mathbf{y}(t_j))\}_{j=1}^{n_t}$ is the snapshots.
OUTPUT: $\mathbf{U}_m$ is POD basis.

1: Create snapshots: $\{\mathbf{F}(\mathbf{y}(t_j))\}_{j=1}^{n_t}$, and Let $r = rank(\{\mathbf{F}(\mathbf{y}(t_j))\}_{j=1}^{n_t})$ where $\mathbf{y}(t) = [\mathbf{y}_1(t), \ldots, \mathbf{y}_{n_s}(t)]^T \in \mathbb{R}^{n_s}$
2: Compute by using SVD: $\{\mathbf{F}(\mathbf{y}(t_j))\}_{j=1}^{n_t} = \hat{\mathbf{U}}\Sigma\mathbf{Z}^T$
3: POD basis: $\mathbf{U}_m = [\mathbf{u}_1, \ldots, \mathbf{u}_m] = \hat{\mathbf{U}}(:, 1 : m)$

One of the most important properties of POD is that it can construct an approximation that minimizes the error in 2−norm for a given fixed basis rank. More details on this will be discussed next in Section 3.3.2.

3.3.2 POD error

We have presented the computation for a POD basis by using SVD. Alternately, it can be shown that the POD basis matrix $\mathbf{V}_k$ is the solution to the following optimization problem (3.12)

Theorem 3.3.2 (POD basis,[59]) *Let* $\mathbf{Y} \in \mathbb{R}^{n \times n_s}$ *be a snapshot matrix* $\mathbf{Y} = [\mathbf{y}_1, \ldots, \mathbf{y}_{n_s}]$ *with rank* $r \leq min\{n, n_s\}$. *Further, let* $\mathbf{Y} = \hat{\mathbf{U}}\Sigma\mathbf{Z}^T$ *be the singular value decomposition of* $\mathbf{Y}$ *with orthogonal matrices* $\hat{\mathbf{U}} = [\mathbf{u}_1, \ldots, \mathbf{u}_n]$ *and* $\hat{\mathbf{Z}} = [\mathbf{z}_1, \ldots, \mathbf{z}_{n_s}]$ *as in* (3.9). *Then, for any* $\ell \in \{1, \ldots, r\}$ *the solution to the optimization problem*

$$\max_{\varphi_i,\ldots,\varphi_\ell} \sum_{i=1}^{\ell} \sum_{j=1}^{n_s} \|\langle \mathbf{y}_j, \varphi_i \rangle\|^2 \quad s.t. \quad \langle \varphi_i, \varphi_j \rangle = \varphi_i^T, \varphi_j = \delta_{i,j} \quad for \quad 1 \leq i, j \leq \ell \quad (3.11)$$

is given by the left singular vectors $\{\mathbf{u}_i\}_{i=1}^{\ell}$. *The set of vectors* $\varphi_1, \ldots, \varphi_\ell$ *are called the POD basis of rank* ℓ. *Here,* $\delta_{i,j} = \begin{cases} 1, & if \quad i \neq j \\ 0, & if \quad i = j \end{cases}$, $for \quad 1 \leq i, j \leq \ell$ *denotes the Kronecker delta.*

Proof: The proof is given in [[59], p. 5-6] □

Moreover, the optimization problem (3.12) will have minimum error when the POD basis approximation $\mathbf{y}_j \cong \mathbf{V}_k \mathbf{V}_k^T \mathbf{y}_j$ is used for $j = 1, \ldots, n_s$. This error is given by

$$\sum_{j=1}^{n_s} \|\mathbf{y}_j - \mathbf{V}_k \mathbf{V}_k^T \mathbf{y}_j\|_2^2 = \sum_{\ell=k+1}^{r} \sigma_\ell^2, \tag{3.12}$$

which is the sum of the neglected singular values $\sigma_{k+1}, \ldots, \sigma_r$ from SVD of $\mathbf{Y} = [\mathbf{y}_1, \ldots, \mathbf{y}_{n_s}]$. We can proof by the method of low-rank approximation which can be found in [59].

Although we use POD to reduced the number of unknowns of the full-order system and POD can reduce the large dimension of linear term, it cannot reduce computational complexity for nonlinear term, which may still depend on the full dimension for $\mathbf{V}_k^T \mathbf{F}(\mathbf{V}_k \tilde{\mathbf{y}}(t))$ from (3.7). For this reason, we will combine POD aprroximation with Discrete Empirical Interpolation Method (DEIM), which will be described in Section 3.4.

3.4 Discrete Empirical Interpolation Method (DEIM)

This section considers the nonlinear term $\mathbf{V}_k^T \mathbf{F}(\mathbf{V}_k \tilde{\mathbf{y}}(t))$ in (3.7). Notice that the computational complexity for evaluating this term still depends on the full dimension n. To eliminate this dependence, we combine POD approximation with the Discrete Empirical Interpolation method (DEIM), which is recently proposed in [9, 21]. DEIM has been used in many applications such as 1-D FitzHugh-Nagumo equations with morphological structure spiking neurons [33], non-linear miscible viscous fingering in a 2-D porous medium [20], 2-D shallow-water equations [24], four-dimensional variational data assimilation [56], three-dimensional nonlinear aeroelasticity model [27], and some extension to DEIM such as electrical, thermal, and microelectromechanical Systems [32]. We first consider $\mathbf{V}_k^T\mathbf{F}(\mathbf{V}_k\tilde{\mathbf{y}}(t))$ in the form

$$\mathbf{F}(\mathbf{V}_k\tilde{\mathbf{y}}(t)) = \mathbf{f}(t) \tag{3.13}$$

and

$$\mathbf{N}(t) = \mathbf{V}_k^T\mathbf{F}(\mathbf{V}_k\tilde{\mathbf{y}}(t)). \tag{3.14}$$

Estimate (3.13) by projecting $\mathbf{f}(t)$ onto subspace $span\{\mathbf{U}\}$ of the form

$$\mathbf{f}(t) \approx \mathbf{U}\mathbf{c}(t) \tag{3.15}$$

where $\mathbf{U} = [\mathbf{u}_1, \ldots, \mathbf{u}_m] \in \mathbb{R}^{n\times m}$ is the projection basis with $m \ll n$. The basis matrix $\mathbf{U}$ can be found by using SVD of $[\mathbf{F}(\mathbf{y}_1), \ldots, \mathbf{F}(\mathbf{y}_{n_s})], \mathbf{y}_i \cong \mathbf{y}(t_i)$. Then we can calculate $\mathbf{c}(t)$ from the following interpolation method. First, consider matrix

$$\mathbf{P} = [\mathbf{e}_{\wp_1}, \ldots, \mathbf{e}_{\wp_m}] \in \mathbb{R}^{n\times m} \tag{3.16}$$

where $\mathbf{e}_{\wp_i} = [0, \ldots, 0, 1, 0, \ldots, 0]^T \in \mathbb{R}^n$ is the $\wp_i$-th column of the identity matrix $\mathbf{I}_n \in \mathbb{R}^{n\times n}$, for $i = 1, \ldots, m$, for selecting m rows of $\mathbf{U}$. Then assume that $\mathbf{P}^T\mathbf{U}$ is nonsingular and solve for $\mathbf{c}(t)$ from

$$\mathbf{P}^T\mathbf{f}(t) = (\mathbf{P}^T\mathbf{U})\mathbf{c}(t) \tag{3.17}$$

so,

$$\mathbf{c}(t) = (\mathbf{P}^T\mathbf{U})^{-1}\mathbf{P}^T\mathbf{f}(t). \tag{3.18}$$

Finally, the approximation is given by

$$\mathbf{F}(\mathbf{V}_k\tilde{\mathbf{Y}}(t)) = \mathbf{f}(t) \approx \mathbf{U}\mathbf{c}(t) = \mathbf{U}(\mathbf{P}^T\mathbf{U})^{-1}\underbrace{\mathbf{P}^T\mathbf{F}(\mathbf{V}_k\tilde{\mathbf{y}}(t))}_{m\times 1}. \tag{3.19}$$

In the case when the nonlinear function $\mathbf{F}$ is componentwise, we have

$$\mathbf{F}(\mathbf{V}_k\tilde{\mathbf{Y}}(t)) = \mathbf{f}(t) \approx \mathbf{U}\mathbf{c}(t) = \mathbf{U}(\mathbf{P}^T\mathbf{U})^{-1}\underbrace{\mathbf{F}(\mathbf{P}^T\mathbf{V}_k\tilde{\mathbf{y}}(t))}_{m\times 1}. \tag{3.20}$$

Note that, multiplying $\mathbf{P}^T$ in (3.17) is equivalent to extracting the m rows corresponding to the interpolation indices $\wp_1, \ldots, \wp_m$, which are used in (3.16). The procedure for selecting these indices is shown next.

3.4.1 DEIM: algorithm for interpolation indices

Discrete Empirical Interpolation Method (DEIM) estimates nonlinear term by finding projection basis from POD and selecting the interpolation indices by a greedy algorithm. The interpolated indices $\wp_1, \ldots, \wp_m$, can be obtained form the following

DEIM algorithm [21].

Algorithm 3 Algorithm to create for Interpolation Indices DEIM

INPUT: $\{\mathbf{u}_\ell\}_{\ell=1}^m \subset \mathbb{R}^n$ linearly independent

OUTPUT: $\vec{\wp} = [\wp_1, \ldots, \wp_m]^T \in \mathbb{R}^m$

1: $[|\rho|, \wp_1] = \max\{|\mathbf{u}_1|\}$
2: $\mathbf{U} = [\mathbf{u}_1], \mathbf{P} = [\mathbf{e}_{\wp_1}], \vec{\wp} = [\wp_1]$;
3: **for** $\ell \leftarrow 2$ to m **do**
4: Solve $(\mathbf{P}^T\mathbf{U})\mathbf{c} = \mathbf{P}^T\mathbf{u}_\ell$;
5: $\mathbf{r} = \mathbf{u}_\ell - \mathbf{U}\mathbf{c}$ $[|\rho|, \wp_\ell] = \max\{|\mathbf{r}|\}$
6: $\mathbf{U} \leftarrow [\mathbf{U} \quad \mathbf{u}_\ell], \mathbf{P} \leftarrow [\mathbf{P} \quad \mathbf{e}_{\wp_\ell}], \vec{\wp} \leftarrow \begin{bmatrix} \vec{\wp} \\ \wp_\ell \end{bmatrix}$
7: **end**

The aim of DEIM algorithm is to select the interpolation indices so that the approximation has smallest error $\mathbf{r} = \mathbf{u}_\ell - \mathbf{U}\mathbf{c}$ in each interation ℓ. The procedure of DEIM algorithm 3 is as follows: First, we start with a basis of rank m, which can be obtained by using POD of nonlinear term. Then, select the index of a component in the first basis vector $\mathbf{u}_1$ with the largest absolute value. Next, we select the other indices so that we have minimum residual error $\mathbf{r} = \mathbf{u}_\ell - \mathbf{U}\mathbf{c}$ in each step.

3.4.2 DEIM error

The corresponding error of DEIM approximation defined formally in Definition 3.4.1 was proposed in [21] as shown in Theorem 3.4.2. The extension of this error bound of to the state-space error estimate can be found in [17].

Definition 3.4.1 (DEIM approximation) *Let $\mathbf{f} : \mathcal{D} \mapsto \mathbb{R}^n$ be a nonlinear vector-valued function with $\mathcal{D} \subset \mathbb{R}^d$ for some positive integer d. Let $\{\mathbf{u}_\ell\}_{\ell=1}^m \subset \mathbb{R}^n$ be a* *linearly independent set for* $\ell \in \{1, \ldots, m\}$. *For* $t \in \mathcal{D}$, *the DEIM approximation of order* m *for* $\mathbf{f}(t)$ *in the space spanned by* $\{\mathbf{u}_\ell\}_{\ell=1}^m$ *is given by*

$$\hat{\mathbf{f}}(t) = \mathbf{U}(\mathbf{P}^T\mathbf{U})^{-1}\mathbf{P}^T\mathbf{f}(t), \tag{3.21}$$

where $\mathbf{U} = [\mathbf{u}_1, \ldots, \mathbf{u}_m] \in \mathbb{R}^{n\times m}$ *and* $\mathbf{P} = [\mathbf{e}_{\wp_1}, \ldots, \mathbf{e}_{\wp_m}] \in \mathbb{R}^{n\times m}$, *with* $\{\wp_1, \ldots, \wp_m\}$ *being the output from Algorithm 3 with the input basis* $\{\mathbf{u}_i\}_{i=1}^m$.

Theorem 3.4.2 (Error bound of DEIM approximation, [21]) *Let* $\mathbf{f} \in \mathbb{R}^n$ *be arbitrary vector. Let* $\{\mathbf{u}_\ell\}_{\ell=1}^m \subset \mathbb{R}^n$ *be a given orthonormal set of vectors. From Definition 3.1, the DEIM approximation of order* $m \leq n$ *for* $\mathbf{f}$ *in the space spanned by* $\{\mathbf{u}_\ell\}_{\ell=1}^m$ *is* $\hat{\mathbf{f}} = \mathbf{U}(\mathbf{P}^T\mathbf{U})^{-1}\mathbf{P}^T\mathbf{f}$, *where* $\mathbf{U} = [\mathbf{u}_1, \ldots, \mathbf{u}_m] \in \mathbb{R}^{n\times m}$ *and* $\mathbf{P} = [\mathbf{e}_{\wp_1}, \ldots, \mathbf{e}_{\wp_m}] \in \mathbb{R}^{n\times m}$, *with* $\{\wp_1, \ldots, \wp_m\}$ *being the output from Algorithm 2.3 with the input basis* $\{\mathbf{u}_i\}_{i=1}^m$. *An error bound for* $\hat{\mathbf{f}}$ *is then given by*

$$\|\mathbf{f} - \hat{\mathbf{f}}\|_2 \leq \mathcal{C}\mathcal{E}_*(\mathbf{f}), \tag{3.22}$$

where

$$\mathcal{C} = \|(\mathbf{P}^T\mathbf{U})^{-1}\|_2 \quad \textit{and} \quad \mathcal{E}_*(\mathbf{f}) = \|(\mathbf{I} - \mathbf{U}\mathbf{U}^T)\mathbf{f}\|_2 \tag{3.23}$$

is the error of the best 2-norm approximation for $\mathbf{F}$ *from the space Range*$(\mathbf{U})$.

Next chapter will use the concept of POD-DEIM approach discussed here to obtain a reduced model that preserves monotonicity and contractivity properties.

Chapter 4

STRUCTURE -PRESERVING MODEL REDUCTION

Model reduction techniques with certain structure that can preserve the monotonicity and contractivity of the original system will be derived. As stated earlier, the monotonicity and contractivity can be used to guaranteed the stability, as well as the existence and uniqueness of the equilibrium solution for each dynamical system. It can also be used to derive an error bound of the perturbed solution. We will next provide the conditions in which the reduced systems from POD and POD-DEIM approaches preserve the monotonicity property of the original system. It will be shown that while POD reduced systems always preserve the monotonicity of the original system, this may not be true for POD-DEIM reduced systems. We therefore derive some modifications for POD-DEIM reduced systems that preserve the monotonicity.

4.1 Proposed General Form

Recall that a dynamical system in a general form, with state variable $\mathbf{y} \in \mathbb{R}^n$,

$$\frac{d\mathbf{y}}{dt} = \mathbf{F}(\mathbf{y}) \tag{4.1}$$

is contractive if the vector field $\mathbf{F}$ is uniformly negative monotone, i.e. the logarithmic Lipschitz constant of $\mathbf{F}$ is negative, $M[\mathbf{F}] < 0$. An equivalent definition of logarithmic Lipschitz constant in Euclidean space [55], which will be used in the derivation, is given by: for $\mathbf{u}, \mathbf{v} \in \mathbb{R}^n$,

$$M[\mathbf{F}] = \sup_{\mathbf{u}\neq\mathbf{v}} \frac{\langle \mathbf{u}-\mathbf{v}, \mathbf{F}(\mathbf{u}) - \mathbf{F}(\mathbf{v})\rangle}{\|\mathbf{u}-\mathbf{v}\|^2} = \sup_{\mathbf{u}\neq\mathbf{v}} \frac{(\mathbf{u}-\mathbf{v})^T(\mathbf{F}(\mathbf{u}) - \mathbf{F}(\mathbf{v}))}{\|\mathbf{u}-\mathbf{v}\|^2}. \tag{4.2}$$

We propose the following general form of reduced systems that can preserve the monotonicity and contractivity of the original system (4.1):

$$\dot{\tilde{\mathbf{y}}} = \widetilde{\mathbf{F}}(\tilde{\mathbf{y}}), \qquad \text{with} \quad \widetilde{\mathbf{F}}(\tilde{\mathbf{y}}) = \mathbf{V}^T\mathbf{W}\mathbf{F}(\mathbf{W}^T\mathbf{V}\tilde{\mathbf{y}}) \tag{4.3}$$

where $\tilde{\mathbf{y}} = \tilde{\mathbf{y}}(t) \in \mathbb{R}^k$, $\mathbf{W} \in \mathbf{R}^{n\times n}$ and $\mathbf{V} \in \mathbf{R}^{n\times k}$, for $k \ll n$, $t \geq 0$ and the solution $\mathbf{y}$ of the original full-order system is approximated by $\mathbf{V}\tilde{\mathbf{y}}$.

Note that the matrix $\mathbf{W}$ is introduced to allow the reduced system to cooperate additional efficient nonlinear complexity reduction as explained later in the next section.

Lemma 4.1.1 *Suppose the nonlinear vector field* $\mathbf{F}$ *in (4.1) is uniformly negative monotone. Then the nonlinear vector field* $\widetilde{\mathbf{F}}(\hat{\mathbf{y}})$ *given in (4.3) is also uniformly negative monotone if* $\widetilde{\mathbf{W}}^T\widetilde{\mathbf{W}} = \mathbf{I}$ *where* $\widetilde{\mathbf{W}} = \mathbf{W}^T\mathbf{V}$ *and* $\mathbf{I}$ *is a k-by-k identity matrix.*

Proof: Let $M[\mathbf{F}]$ and $M[\widetilde{\mathbf{F}}]$ be the logarithmic Lipschitz constants of $\mathbf{F}$ and $\widetilde{\mathbf{F}}$, respectively. For $\tilde{\mathbf{u}}, \tilde{\mathbf{v}} \in \mathbb{R}^k$ and $\mathbf{u}, \mathbf{v} \in \mathbb{R}^n$, since $\mathbf{F}$ in system (1) is uniformly negative monotone, i.e. $M[\mathbf{F}] < 0$, then

$$\begin{aligned}
M[\widetilde{\mathbf{F}}] &= \sup_{\tilde{\mathbf{u}} \neq \tilde{\mathbf{v}}} \frac{(\tilde{\mathbf{u}} - \tilde{\mathbf{v}})^T(\widetilde{\mathbf{F}}(\tilde{\mathbf{u}}) - \widetilde{\mathbf{F}}(\tilde{\mathbf{v}}))}{\|\tilde{\mathbf{u}} - \tilde{\mathbf{v}}\|^2} \\
&= \sup_{\tilde{\mathbf{u}} \neq \tilde{\mathbf{v}}} \frac{(\tilde{\mathbf{u}} - \tilde{\mathbf{v}})^T(\widetilde{\mathbf{W}}^T\mathbf{F}(\widetilde{\mathbf{W}}\tilde{\mathbf{u}}) - \widetilde{\mathbf{W}}^T\mathbf{F}(\widetilde{\mathbf{W}}\tilde{\mathbf{v}}))}{\|\tilde{\mathbf{u}} - \tilde{\mathbf{v}}\|^2} \\
&= \sup_{\tilde{\mathbf{u}} \neq \tilde{\mathbf{v}}} \frac{(\widetilde{\mathbf{W}}\tilde{\mathbf{u}} - \widetilde{\mathbf{W}}\tilde{\mathbf{v}})^T(\mathbf{F}(\widetilde{\mathbf{W}}\tilde{\mathbf{u}}) - \mathbf{F}(\widetilde{\mathbf{W}}\tilde{\mathbf{v}}))}{\|\widetilde{\mathbf{W}}\tilde{\mathbf{u}} - \widetilde{\mathbf{W}}\tilde{\mathbf{v}}\|^2} \\
&\leq \sup_{\mathbf{u} \neq \mathbf{v}} \frac{(\mathbf{u} - \mathbf{v})^T(\mathbf{F}(\mathbf{u}) - \mathbf{F}(\mathbf{v}))}{\|\mathbf{u} - \mathbf{v}\|^2} \\
&= M[\mathbf{F}] < 0,
\end{aligned}$$

where $\widetilde{\mathbf{W}} = \mathbf{W}^T\mathbf{V}$. That is, $M[\widetilde{\mathbf{F}}] < 0$ and $\widetilde{\mathbf{F}}$ is uniformly negative monotone. ■

4.2 Structure-Preserving POD reduced system

In order to derive a reduced-order modeling in the form (4.3) that is useful in practice, we will first consider a well-known method called proper orthogonal decomposition (POD) as a starting point. In particular, the POD reduced system for the original system (2.1) is given by

$$\dot{\tilde{\mathbf{y}}} = \mathbf{V}^T\mathbf{F}(\mathbf{V}\tilde{\mathbf{y}}), \qquad \tilde{\mathbf{y}}(0) = \mathbf{V}^T\mathbf{y}_0, \tag{4.4}$$

where the basis matrix $\mathbf{V} \in \mathbb{R}^{n\times k}$, called POD basis, can generally capture the main characteristic of the solutions [47]. This basis can be computed via the singular value decomposition (SVD) of the snapshots, which are the sampled solutions at certain time steps or parameter values. The POD reduced system can be written in the form of (4.3) by setting $\mathbf{W} = \mathbf{I}$. As a result, POD reduced system preserves the monotonicity of the original system. In addition, we can obtain the following result.

Corollary 4.2.1 *Suppose the nonlinear vector field* $\mathbf{F}$ *in system (4.1) is uniformly negative monotone. Then the reduced systems in the form (4.3) has the following properties.*

(i) The reduced system (4.3) preserves the exponential stability of (4.1) .

(ii) The reduced system (4.3) has a unique equilibrium $\tilde{\mathbf{y}}_e$*, i.e.* $\widetilde{\mathbf{F}}(\tilde{\mathbf{y}}_e) = 0$*. Moreover, if* $\mathbf{y}_e$ *is the unique equilibrium solution of (4.1), then* $\mathbf{y}_e$ *can be approximated by* $\mathbf{V}\tilde{\mathbf{y}}_e$ *with the error bound*

$$\|\mathbf{y}_e - \mathbf{V}\tilde{\mathbf{y}}_e\| \le \frac{-\|\mathbf{p}\|}{M[\mathbf{F}]}, \qquad \textit{where} \qquad \mathbf{p} = \mathbf{F}(\mathbf{V}\tilde{\mathbf{y}}_e).$$

Proof: (i) Since, from [55], the solution of the reduced system satisfies $\|\tilde{\mathbf{y}}\| \le e^{M[\widetilde{\mathbf{F}}]t}\|\tilde{\mathbf{y}}(0)\|$ and $M[\widetilde{\mathbf{F}}] < 0$ for $t \ge 0$.

(ii) First note that , from [55], $M[\mathbf{F}] < 0$ implies that the map $\mathbf{F}$ is bijective and there must be a unique solution $\mathbf{y}_e$ such that $\mathbf{F}(\mathbf{y}_e) = 0$. Similarly, from Lemma 4.1.1, $M[\mathbf{F}] < 0$ implies $M[\widetilde{\mathbf{F}}] < 0$, which also further gives the existence of the unique solution $\tilde{\mathbf{y}}_e$ such that $\widetilde{\mathbf{F}}(\tilde{\mathbf{y}}_e) = 0$. To derive the bound, let $\mathbf{p} := \mathbf{F}(\mathbf{V}\tilde{\mathbf{y}}_e)$ and consider $\frac{\langle \mathbf{V}\tilde{\mathbf{y}}_e - \mathbf{y}_e, \mathbf{F}(\mathbf{V}\tilde{\mathbf{y}}_e) - \mathbf{F}(\mathbf{y}_e)\rangle}{\|\mathbf{V}\tilde{\mathbf{y}}_e - \mathbf{y}_e\|^2} \leq M[\mathbf{F}]$. Since $M[\mathbf{F}] < 0$,

$$\begin{aligned}
\|\mathbf{V}\tilde{\mathbf{y}}_e - \mathbf{y}_e\|^2 &\leq \frac{1}{M[\mathbf{F}]} \langle \mathbf{V}\tilde{\mathbf{y}}_e - \mathbf{y}_e, \mathbf{p}\rangle \\
&\leq \left| \frac{1}{M[\mathbf{F}]} \right| \|\mathbf{V}\tilde{\mathbf{y}}_e - \mathbf{y}_e\| \, \|\mathbf{p}\| \\
&= \frac{-\|\mathbf{p}\|}{M[\mathbf{F}]} \|\mathbf{V}\tilde{\mathbf{y}}_e - \mathbf{y}_e\| \\
\|\mathbf{V}\tilde{\mathbf{y}}_e - \mathbf{y}_e\| &\leq \frac{-\|\mathbf{p}\|}{M[\mathbf{F}]}.
\end{aligned}$$

■

Although the number of unknowns is reduced to k, the complexity for computing $\mathbf{V}^T F(\mathbf{V}\hat{\mathbf{y}})$ for each t still depends on the original dimension n. That is, POD may not truly reduce the complexity of nonlinear dynamical system as explained in [19]. An efficient way to overcome this problem is to further apply the discrete empirical interpolation (DEIM).

4.3 Structure-Preserving POD-DEIM reduced system

Recall that the POD-DEIM reduced system can be written in the following form:

$$\dot{\tilde{\mathbf{y}}} \;=\; \mathbf{V}^T\mathbf{U}(\mathbf{P}^T\mathbf{U})^{-1}\mathbf{P}^T\mathbf{F}(\mathbf{V}\tilde{\mathbf{y}}), \qquad \tilde{\mathbf{y}}(0) = \mathbf{V}^T\mathbf{y}_0, \tag{4.5}$$

where $\mathbf{V} \in \mathbb{R}^{n\times k}$ is the POD basis matrix of rank k obtained from the solution snapshots, $\mathbf{U} \in \mathbb{R}^{n\times m}$ is the POD basis matrix of rank m, $m \ll n$, obtained from the nonlinear snapshots of $\mathbf{F}$, and $\mathbf{P} \in \mathbb{R}^{n\times m}$ is the matrix corresponding to the interpolated indices in the nonlinear approximation as described in [19]. The term $\mathbf{V}^T\mathbf{U}(\mathbf{P}^T\mathbf{U})^{-1}$ can be precomputed in advance and multiplying by $\mathbf{P}^T$ is equivalent to selecting the m components. Hence, in the actual computation for solving the POD-DEIM reduced system, the complexity depends only on small dimensions k and m. Notice that, although the POD-DEIM reduced system can decrease the computational time for nonlinear problem, it may not always preserve some important properties of the original system.

The following proposition provides the condition that guarantee the uniform negative monotonicity, and hence the contractivity as well as stability, of the resulting POD-DEIM reduced system.

Proposition 4.3.1 *The nonlinear vector field of the POD-DEIM reduced system (4.5) is uniformly negative monotone if* $M[\mathbb{P}\mathbf{F}] < 0$*, where* $\mathbb{P} = \mathbf{U}(\mathbf{P}^T\mathbf{U})^{-1}\mathbf{P}^T$ *and* $\mathbf{F}$

is defined in (4.1) .

<u>Proof:</u> Consider the POD-DEIM reduced system (4.5) in the form $\dot{\tilde{\mathbf{y}}} = \widehat{\mathbf{F}}(\tilde{\mathbf{y}})$ where $\widehat{\mathbf{F}}(\tilde{\mathbf{y}}) := \mathbf{V}^T \mathbb{P}\mathbf{F}(\mathbf{V}\tilde{\mathbf{y}})$,

$$\begin{aligned} M[\widehat{\mathbf{F}}] &= \sup_{\widehat{\mathbf{u}} \neq \widehat{\mathbf{v}}} \frac{(\widehat{\mathbf{u}} - \widehat{\mathbf{v}})^T (\mathbf{V}^T \mathbb{P}\mathbf{F}(\mathbf{V}\widehat{\mathbf{u}}) - \mathbf{V}^T \mathbb{P}\mathbf{F}(\mathbf{V}^T \widehat{\mathbf{v}}))}{\|\widehat{\mathbf{u}} - \widehat{\mathbf{v}}\|^2} \\ &= \sup_{\widehat{\mathbf{u}} \neq \widehat{\mathbf{v}}} \frac{(\mathbf{V}\widehat{\mathbf{u}} - \mathbf{V}\widehat{\mathbf{v}})^T \mathbb{P}(\mathbf{F}(\mathbf{V}\widehat{\mathbf{u}}) - \mathbf{F}(\mathbf{V}\widehat{\mathbf{v}}))}{\|\mathbf{V}\widehat{\mathbf{u}} - \mathbf{V}\widehat{\mathbf{v}}\|^2} \\ &\leq M[\mathbb{P}\mathbf{F}]. \end{aligned}$$

That is, $M[\mathbb{P}\mathbf{F}] < 0$ implies $M[\widehat{\mathbf{F}}] < 0$. ■

Next, this work proposes a specific form for constructing a reduced-order model with the structure given in (4.3), which can efficiently reduce the computational complexity of the nonlinear term. This form is based on the form of POD-DEIM reduced system: $\dot{\tilde{\mathbf{y}}} = \mathbf{V}^T \mathbb{P}\mathbf{F}(\mathbf{V}\tilde{\mathbf{y}})$, where $\mathbb{P} = \mathbf{U}(\mathbf{P}^T\mathbf{U})^{-1}\mathbf{P}^T$. We can obtain the form (4.3) by setting $\mathbf{W} = \mathbb{P}$ so that the reduced system becomes

$$\dot{\tilde{\mathbf{y}}} = \mathbf{V}^T \mathbb{P}\mathbf{F}(\mathbb{P}^T \mathbf{V}\tilde{\mathbf{y}}), \qquad \tilde{\mathbf{y}}(0) = \mathbf{V}^T \mathbf{y}_0. \tag{4.6}$$

It is possible to use other variations that fit the general form given in (4.3), e.g. using $\mathbf{W} = \mathbf{P}\mathbf{P}^T$ where $\mathbf{P}$ is the selection matrix obtained from the DEIM procedure. That is, let $\mathbf{V}_\wp = \mathbf{P}\mathbf{P}^T\mathbf{V}$, the reduced system is in the form:

$$\dot{\tilde{\mathbf{y}}} = \mathbf{V}_\wp^T \mathbf{F}(\mathbf{V}_\wp \tilde{\mathbf{y}}), \qquad \tilde{\mathbf{y}}(0) = \mathbf{V}^T \mathbf{y}_0 \tag{4.7}$$

We next illustrate the accuracy and efficiency of the proposed reduced model (4.6) through a nonlinear differential equations that describes a diffusion-reaction problem. To improve the accuracy, the linear and the nonlinear terms will be separated in actual computation. In particular, for $\mathbf{F}(\mathbf{y}) = \mathbf{A}\mathbf{y} + \mathbf{f}(\mathbf{y})$, where $\mathbf{A} \in \mathbb{R}^{n \times n}$, the POD approach will be applied to the linear term $\mathbf{A}\mathbf{y}$ and reduced system of the form (4.8) will be used for the nonlinear term $\mathbf{f}(\mathbf{y})$, i.e.

$$\dot{\tilde{\mathbf{y}}} = \widetilde{\mathbf{A}}\tilde{\mathbf{y}} + \mathbb{P}\mathbf{f}(\mathbb{P}\mathbf{V}\tilde{\mathbf{y}}), \tag{4.8}$$

where $\widetilde{\mathbf{A}} = \mathbf{V}^T\mathbf{A}\mathbf{V} \in \mathbb{R}^{k \times k}$ can be precomputed in advance.

Chapter 5

Numerical Results

In this work, we consider two numerical tests on a nonlinear diffusion reaction model. The first numerical test considers only one fixed parameter value. The second one considers the case of varying parameter values.

5.1 Reaction-Diffusion Model

Consider the nonlinear reaction-diffusion initial boundary value problem:

$$\frac{\partial u}{\partial t} = \epsilon \frac{\partial^2 u}{\partial x^2} + u - u^3, \quad x \in \Omega = [0, 2\pi], \qquad t \geq 0, \tag{5.1}$$

with initial condition : $u(x, 0) = 0.25 \sin(x)$, and homogeneous boundary conditions : $u(0, t) = 0, \quad u(2\pi, t) = 0, \quad$ for $t \geq 0$. In the following numerical tests, we use finite different discretizaion with spatial point $n = 600$ on $[0, 2\pi]$, time steps $= n_t = 700$

on $[0, 5]$ and $\epsilon = 0.01$. Figure 5.1 compares the solutions obtained from the original full-order system of the form (2.1) with the ones from the two reduced models: (i) the POD reduced system (4.4), and (ii) the POD-DEIM reduced system that preserves the monotonicity (4.8), which are indistinguishable. The absolute error and the CPU time (normalized with the simulation time of the original full-order system) of these 2 reduced models (4.4) and (4.8) that preserve monotonicity are given in Table 5.1. Notice that, although the POD give more accurate approximations, the proposed model can accurately approximate the solution with much less simulation time, e.g. POD-DEIM reduce system with $k = 30$, $m = 30$ has CPU time reduced to $0.0024 \approx 1/400$ of the simulation time used for the original system, while CPU time for POD with $k = 30$ is only reduced to $0.4781 \approx 1/2$ of the time used in the original system.

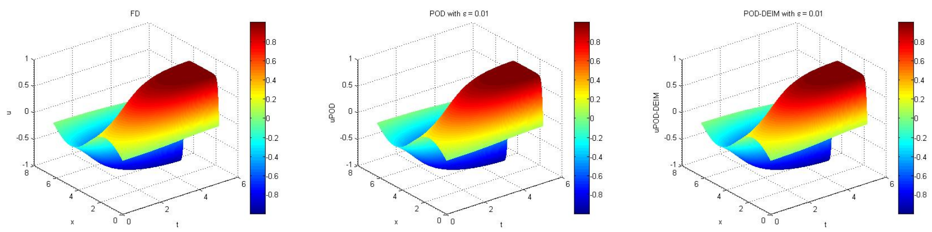

Figure 5.1: Solutions of (5.1) from the full-order system (2.1), the POD system (4.4) with $k = 30$, and the POD-DEIM system that preserves monotonicity (4.8) with $k = m = 30$.

POD basis (k)	Relative Error	Runtime (scaled)	DEIM (m) POD $k = 30$	Relative Error	Runtime (scaled)
Full: $n = 600$	-	1	Full: $n = 600$	-	1
$k = 10$	2.4601e-06	0.4433	$m = 10$	4.1170e-02	0.0021
$k = 20$	3.7046e-07	0.4569	$m = 20$	6.2412e-03	0.0022
$k = 30$	1.7271e-07	0.4781	$m = 30$	4.1483e-03	0.0024
$k = 40$	1.0819e-07	0.4896	$m = 40$	5.4461e-04	0.0029
$k = 50$	3.3184e-08	0.4931	$m = 50$	1.4553e-04	0.0031

Table 5.1: Runtime and relative error of the POD reduced system (left) the POD-DEIM reduced system with monotonicity preserved (right). Each runtime is normalized with the CPU time of the original full-order system (dimension $n = 600$).

5.2 Numerical Example: Varying parameters

This section considers an application for the same nonlinear reaction-diffusion equation with different initial conditions and using various different values of ϵ:

$$\frac{\partial u}{\partial t} = \epsilon \frac{\partial^2 u}{\partial x^2} + u - u^3, \quad x \in \Omega = [0, 1], \qquad t \geq 0, \tag{5.2}$$

The initial condition is $u(x, 0) = \sin(5\pi x)$, the homogeneous boundary conditions are $u(0, t) = 0, \quad u(1, t) = 0, \quad$ for $t \geq 0$. The finite difference discretization is used with spatial point $n = 1000$ on $[0, 1]$ and the number of time steps is $= n_t = 100$ on $[0, 2]$.

The three plots in Figure 5.3 illustrate, respectively, the full-order solutions with the parameter values $\epsilon = 0.001$ and $\epsilon = 0.1$ and the singular values, which are corresponding to the POD basis of the solution snapshots from these two parameters.

The POD basis sets for projecting the solution and for the DEIM nonlinear approximation are constructed from the solution snapshots shown in Figures 5.3, which

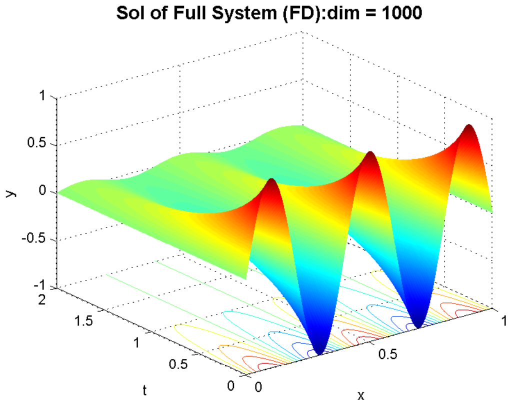

Figure 5.2: Solutions of (5.2) from the full-order system ($n = 1000$, $\epsilon = 0.01$)

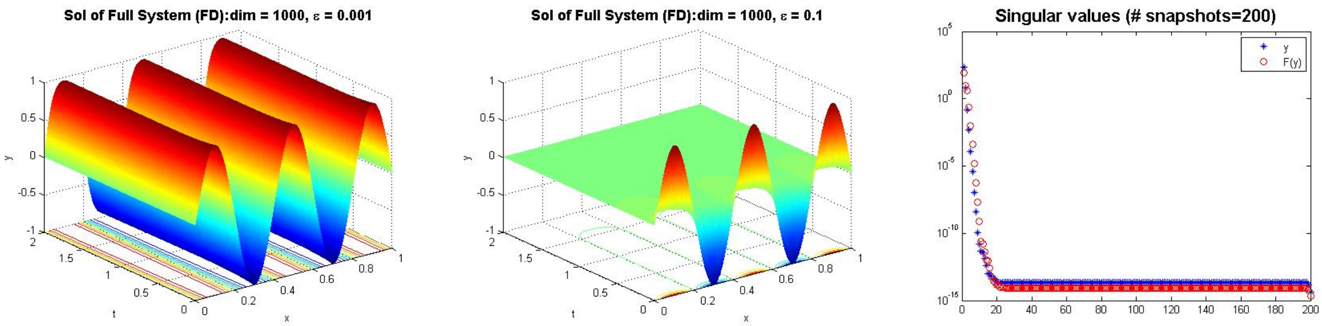

Figure 5.3: Solution Snapshots of (5.2) ($n = 1000$) with $\epsilon = 0.001$ and $\epsilon = 0.1$.

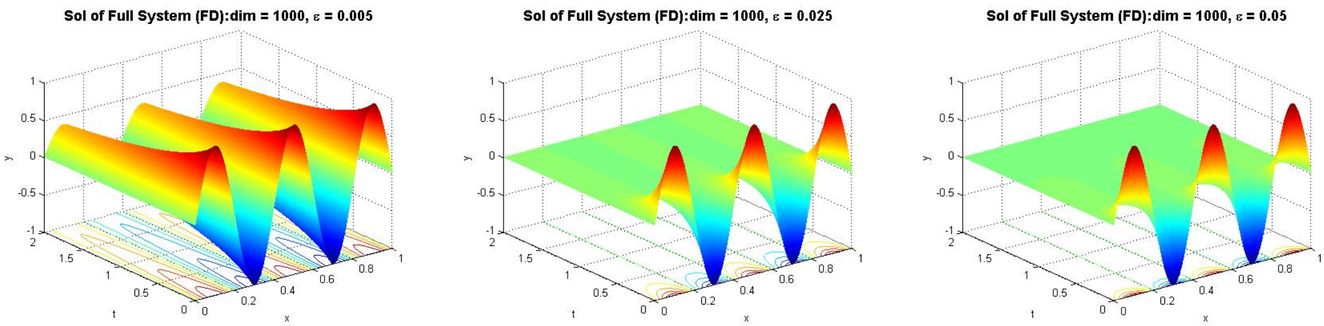

Figure 5.4: Solutions of (5.2) from the full-order system ($n = 1000$) with parameter $\epsilon = 0.0025, 0.005, 0.0250.05$.

are corresponding to 2 parameter values $\epsilon = 0.001$ and $\epsilon = 0.1$. This numerical test considers the solutions corresponding to different parameter values. Figures 5.4, 5.5, 5.6 demonstrate, respectively, the solutions from the full-order system, the POD

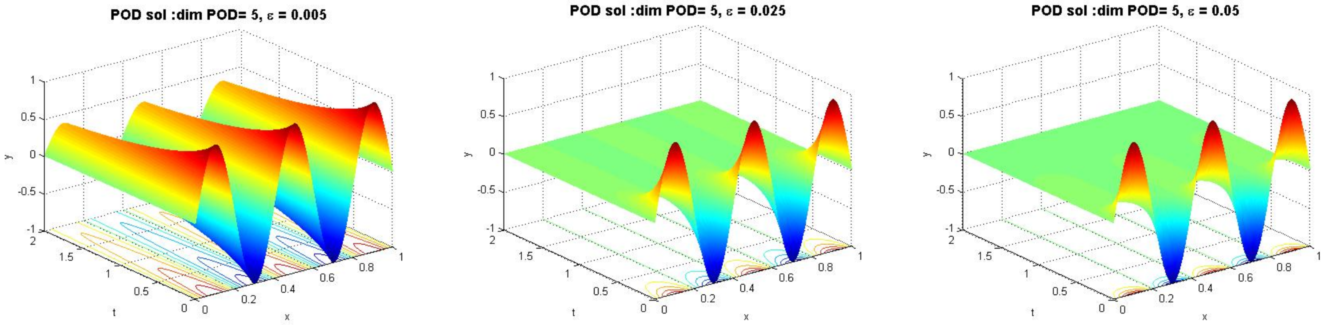

Figure 5.5: Solutions of (5.2) from the POD reduced system ($n = 1000$) with parameter $\epsilon = 0.0025, 0.005, 0.0250.05$.

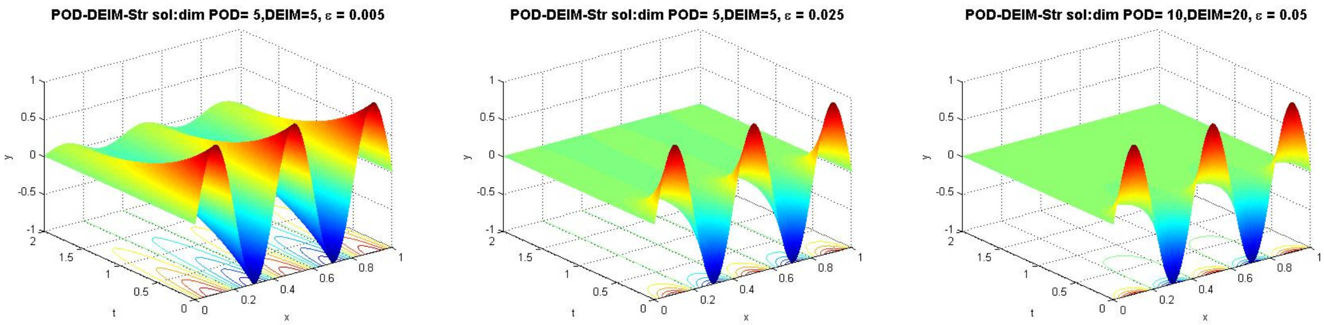

Figure 5.6: Solutions of (5.2) from the structure-preserving POD-DEIM reduced system ($n = 1000$) with parameter $\epsilon = 0.0025, 0.005, 0.0250.05$.

reduced system, and the structure-preserving POD-DEIM reduced system with parameter $\epsilon = 0.0025, 0.005, 0.0250.05$. The solutions from the POD reduced system in Figure 5.5 are shown to accurately capture the dynamics of the original systems although the projection basis sets employ snapshots from different parameter values. Similar observations can be obtained from the solutions from the structure-preserving POD-DEIM reduced system in Figure 5.6. Note however, that the simulation time of the POD reduced systems is roughly a factor of 1/30 less than the simulation time used for the original full-order system while the structure-preserving POD-DEIM reduced system can further the simulation time approximately to a factor of 1/200.

Chapter 6

Conclusions

This work proposes a general form of nonlinear reduced-order modeling that preserves the contractivity and monotonicity properties of the original systems, which can be used for guaranteeing the existence, uniqueness of the solution, and stability of the dynamical system. A specific formulation presented and used in this work is based on proper orthogonal decomposition (POD) and discrete empirical interpolation method (DEIM) approaches with some modification. Other specific forms are still possible and left for future research. An error bound for the approximate equilibrium solution from the proposed reduced system is also derived. This work investigates the monotonicity and contractivity of the existing POD and POD-DEIM techniques. It can be shown that POD reduced systems always preserve the monotonicity and contractivity of the original system, but POD-DEIM systems do not. The conditions under which the POD-DEIM approach preserves monotonicity and contractivity properties are provided.

The numerical tests on the nonlinear reaction diffusion problem demonstrate that, while preserving negative monotonicity, the proposed model can accurately approximate the solutions with much less simulation time.

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ส่วนที่ 3

ภาคผนวก

1) Proceeding:

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   ภายใต้หัวข้อเรื่อง

   "Stabilized Nonlinear Complexity Reduction through Contractivity-Preserving Framework"

<u>เอกสารแนบหมายเลข 3</u>

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Nonlinear reduced-order modeling with monotonicity property

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Nonlinear Reduced-Order Modeling with Monotonicity Property

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Abstract. This work proposes a general form of nonlinear model reduction approach that preserves the monotonicity property of the original full-order model, which can be used to guarantee the existence and uniqueness of the solution. The derivation of the proposed methodology is based on using basis from proper orthogonal decomposition method and modifying an interpolatory projection approach, called discrete empirical interpolation method, by enforcing a symmetric structure of the approximation. The efficiency and accuracy of the proposed method are illustrated through the numerical tests on a nonlinear model describing reaction diffusion problems.

INTRODUCTION

A number of physical phenomena can be described by nonlinear partial differential equations (PDEs), which may not be solved analytically in general, and it is therefore unavoidable to use approximate solutions instead. These solutions are often obtained from numerical methods that require certain spatial discretization. Increasing the accuracy of the resulting numerical solutions normally leads to a discretized system with a very large state-space dimension. An efficient approach for decreasing the computational cost in solving these large-scale systems is based on the *model reduction* concept, which can generate a comparatively low dimensional problem with accurate approximations. Model reduction approaches have been recently proposed to substantially decrease the computational complexity of many large-scale discretized PDEs. However, most existing efficient approaches for nonlinear systems may not directly preserve the important properties of the original systems.

This work focuses on projection-based model reduction approaches, called proper orthogonal decomposition (POD) and discrete empirical interpolation method (DEIM). POD is a well-known method and has been successfully used in a large number of previous works, e.g. [1, 2, 3], to reduce the dimension of the original systems. However, computing the projected nonlinear term in the POD reduced system generally still depends on the large dimension of original system. To overcome this difficulty, DEIM approach [4] can be used to further reduced the computational complexity of the nonlinear term by selecting the interpolation indices through a greedy algorithm.

Although the approach that combines POD and DEIM has been efficiently applied in various applications, e.g. [5, 6], it may not preserve the important properties of the original system. This work proposes a nonlinear reduced-order modeling that preserves the monotonicity, which can be used to guarantee the existence and uniqueness of the reduced-order solution, as well as provide certain conditions that preserve the stability of the original system. The derivation of the proposed methodology is based on modifying the POD-DEIM approach by enforcing a symmetric structure of the system. A nonlinear reaction diffusion problem is used to test the efficiency of this new approach.

BACKGROUND AND PROBLEM FORMULATION

Consider the system of nonlinear ordinary differential equations (ODEs) of the form:

$$\frac{d\mathbf{y}}{dt} = \mathbf{F}(\mathbf{y}), \qquad \mathbf{y}(0) = \mathbf{y}_0, \tag{1}$$

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where $\mathbf{y} = \mathbf{y}(t)$ is an n dimensional vector at certain time $t \geq 0$ and $\mathbf{F}$ is a differentiable nonlinear vector field in $\mathbf{y}$ variable with Jacobian of $\mathbf{F}$ given by $J_F(\mathbf{y}) = \frac{\partial \mathbf{F}}{\partial \mathbf{y}}(\mathbf{y})$. The goal is to construct a reduced system that can provide approximate solutions that preserve the behavior of the original system.

This section first considers the *logarithmic norm*, introduced independently by Germund Dahlquist and Sergei Lozinskii in 1959 [7, 8] defined as $\mu(\mathbf{A}) = \lim_{h\to 0^+} \frac{\|I+h\mathbf{A}\|-1}{h}$, which can be used to measure the distance between matrices. Note that $\|\cdot\|$ can be any norm and when it is the Euclidean 2-norm, $\mu(\mathbf{A})$ is the maximum eigenvalue of the symmetric part of $\mathbf{A}$. This notion can be extended to the nonlinear operator in Banach spaces as shown next [9].

Definition 1 *Let $(X, \|\cdot\|_X)$ be a normed space and $f : Y \to X$ be a function where $Y \subseteq X$. The least upper bound (lub) and the greatest lower bound (glb) Lipschitz constants of f induced by the norm $\|\cdot\|_X$ on Y are defined, respectively, by $L_{Y,X}[f] = \sup_{u\neq v\in Y} \frac{\|f(u)-f(v)\|_X}{\|u-v\|_X}$, and $\ell_{Y,X}[f] = \inf_{u\neq v\in Y} \frac{\|f(u)-f(v)\|_X}{\|u-v\|_X}$.*

The least upper bound (lub) and the greatest lower bound (glb) logarithmic Lipschitz constants of f induced by the norm $\|\cdot\|_X$ on Y are defined by

$$M_{Y,X}[f] = \lim_{h\to 0^+} \frac{L_{Y,X}[I + hf] - 1}{h}, \qquad \textit{and} \qquad m_{Y,X}[f] = \lim_{h\to 0^-} \frac{L_{Y,X}[I + hf] - 1}{h}.$$

Note that, this work considers the setting for systems of ODEs with $X = Y \subseteq \mathbb{R}^n$ and we will use the notation $L_{Y,X}[\cdot] = L[\cdot]$, $\ell_{Y,X}[\cdot] = \ell[\cdot]$ and $M_{Y,X}[\cdot] = M[\cdot]$, $m_{Y,X}[\cdot] = m[\cdot]$. Moreover, we will use the Euclidean 2- norm for $\|\cdot\|_X$, which will be simply denoted as $\|\cdot\|$, and from [9], it can be shown that $M[\cdot] = m[\cdot]$. In this case,

$$M[\mathbf{F}] = \sup_{\mathbf{u}\neq\mathbf{v}} \frac{\langle \mathbf{u}-\mathbf{v}, \mathbf{F}(\mathbf{u}) - \mathbf{F}(\mathbf{v})\rangle}{\|\mathbf{u}-\mathbf{v}\|^2} = \sup_{\mathbf{u}\neq\mathbf{v}} \frac{(\mathbf{u}-\mathbf{v})^T(\mathbf{F}(\mathbf{u}) - \mathbf{F}(\mathbf{v}))}{\|\mathbf{u}-\mathbf{v}\|^2} \tag{2}$$

for $\mathbf{u}, \mathbf{v} \in \mathbb{R}^n$. We will next consider the notion of the *motonicity* of a vector field, which can further imply the *contractivity* for the flow of the vector field.

Definition 2 *A map $\mathbf{F}$ defined from X to Y, where $Y \subseteq X \subseteq \mathbb{R}^n$ is said to be uniformly negative monotone if $M[\mathbf{F}] < 0$. For the differential equation: $\dot{\mathbf{y}} = \mathbf{F}(\mathbf{y})$, the map $e^{t\mathbf{F}} : \mathbf{y}(0) \to \mathbf{y}(t)$ is a contractive flow if $L[e^{t\mathbf{F}}] < 1$.*

In the next section, we will use these notions to derive a form of model reduction that can preserve the negative monotonicity, and hence provide solutions with contractive flow as well as the stability [9].

PROPOSED MODEL REDUCTION FORMULATION

We consider the following general form of reduced systems that can preserve the monotonicity and contractivity of the original system (1).

$$\dot{\tilde{\mathbf{y}}} = \widetilde{\mathbf{F}}(\tilde{\mathbf{y}}), \qquad \text{with} \quad \widetilde{\mathbf{F}}(\tilde{\mathbf{y}}) = \mathbf{V}^T\mathbf{W}\mathbf{F}(\mathbf{W}^T\mathbf{V}\tilde{\mathbf{y}}) \tag{3}$$

where $\tilde{\mathbf{y}} = \tilde{\mathbf{y}}(t) \in \mathbb{R}^k$, $\mathbf{W} \in \mathbb{R}^{n\times n}$ and $\mathbf{V} \in \mathbb{R}^{n\times k}$, for $k \ll n$, $t \geq 0$ and the solution $\mathbf{y}$ of the original full-order system is approximated by $\mathbf{V}\tilde{\mathbf{y}}$.

Suppose the nonlinear vector field $\mathbf{F}$ in (1) is uniformly negative monotone, i.e. $M[\mathbf{F}] < 0$. It can be shown using the definitions given earlier that the logarithmic Lipschitz constants $M[\widetilde{\mathbf{F}}] < 0$ where $\widetilde{\mathbf{F}}$ is the vector field in (3). For $\tilde{\mathbf{u}}, \tilde{\mathbf{v}} \in \mathbb{R}^k$, since $M[\mathbf{F}] < 0$, then

$$M[\widetilde{\mathbf{F}}] \quad = \quad \sup_{\tilde{\mathbf{u}}\neq\tilde{\mathbf{v}}} \frac{(\tilde{\mathbf{u}}-\tilde{\mathbf{v}})^T(\widetilde{\mathbf{W}}^T\mathbf{F}(\widetilde{\mathbf{W}}\tilde{\mathbf{u}}) - \widetilde{\mathbf{W}}^T\mathbf{F}(\widetilde{\mathbf{W}}\tilde{\mathbf{v}}))}{\|\tilde{\mathbf{u}}-\tilde{\mathbf{v}}\|^2} = \sup_{\tilde{\mathbf{u}}\neq\tilde{\mathbf{v}}} \frac{(\widetilde{\mathbf{W}}\tilde{\mathbf{u}} - \widetilde{\mathbf{W}}\tilde{\mathbf{v}})^T(\mathbf{F}(\widetilde{\mathbf{W}}\tilde{\mathbf{u}}) - \mathbf{F}(\widetilde{\mathbf{W}}\tilde{\mathbf{v}}))}{\|\widetilde{\mathbf{W}}\tilde{\mathbf{u}} - \widetilde{\mathbf{W}}\tilde{\mathbf{v}}\|^2} \leq M[\mathbf{F}] < 0$$

where $\widetilde{\mathbf{W}} = \mathbf{W}^T\mathbf{V}$. That is, $M[\widetilde{\mathbf{F}}] < 0$. This observation is summarized in the next lemma.

Lemma 1 *If the nonlinear vector field $\mathbf{F}$ in (1) is uniformly negative monotone, then so is the nonlinear vector field $\widetilde{\mathbf{F}}(\hat{\mathbf{y}})$ given in (3).*

Note that when $\mathbf{F}$ in (1) is uniformly negative monotone, using the standard analysis for differential equations [9] with the definitions of monotonicity and contractivity gives the following implications.
(i) The reduced system (3) preserves the exponential stability of (1).
(ii) The reduced system (3) has a unique equilibrium.

In order to derive a reduced-order modeling in the form (3) that is useful in practice, we will first consider a well-known method called proper orthogonal decomposition (POD) as a starting point. In particular, the POD reduced system for the original system (1) is given by

$$\dot{\tilde{\mathbf{y}}} = \mathbf{V}^T\mathbf{F}(\mathbf{V}\tilde{\mathbf{y}}), \qquad \tilde{\mathbf{y}}(0) = \mathbf{V}^T\mathbf{y}_0, \tag{4}$$

where the basis matrix $\mathbf{V} \in \mathbb{R}^{n\times k}$, called POD basis, can generally capture the main characteristic of the solutions [10]. This basis can be computed via the singular value decomposition (SVD) of the snapshots, which are the sampled solutions at certain time steps or parameter values. The POD reduced system can be written in the form of (3) by setting $\mathbf{W} = \mathbf{I}$. As a result, POD reduced system preserves the monotonicity of the original system. However, although the number of unknowns is reduced to k, the complexity for computing $\mathbf{V}^T\mathbf{F}(\mathbf{V}\hat{\mathbf{y}})$ for each t still depends on the original dimension n. That is, POD may not truly reduce the complexity of nonlinear dynamical system as explained in [4]. An efficient way to overcome this problem is to further apply the discrete empirical interpolation (DEIM). The POD-DEIM reduced system can be written in the following form:

$$\dot{\tilde{\mathbf{y}}} \;=\; \mathbf{V}^T\mathbf{U}(\mathbf{P}^T\mathbf{U})^{-1}\mathbf{P}^T\mathbf{F}(\mathbf{V}\tilde{\mathbf{y}}), \qquad \tilde{\mathbf{y}}(0) = \mathbf{V}^T\mathbf{y}_0, \tag{5}$$

where $\mathbf{V} \in \mathbb{R}^{n\times k}$ is the POD basis matrix of rank k obtained from the solution snapshots, $\mathbf{U} \in \mathbb{R}^{n\times m}$ is the POD basis matrix of rank m, $m \ll n$, obtained from the nonlinear snapshots of $\mathbf{F}$, and $\mathbf{P} \in \mathbb{R}^{n\times m}$ is the matrix corresponding to the interpolated indices in the nonlinear approximation as described in [4]. The term $\mathbf{V}^T\mathbf{U}(\mathbf{P}^T\mathbf{U})^{-1}$ can be precomputed in advance and multiplying by $\mathbf{P}^T$ is equivalent to selecting the m components. Hence, in the actual computation for solving the POD-DEIM reduced system, the complexity depends only on small dimensions k and m. Notice that, although the POD-DEIM reduced system can decrease the computational time for nonlinear problem, it may not always preserve some important properties of the original system. Besides proposing a general form (3) for the model reduction that preserves the monotonicity and the contractivity of the original system, we also introduce a specific form for a practical use as shown below.

$$\dot{\tilde{\mathbf{y}}} = \mathbf{V}^T\mathbb{P}\mathbf{F}(\mathbb{P}^T\mathbf{V}\tilde{\mathbf{y}}), \tag{6}$$

where $\mathbb{P} = \mathbf{U}(\mathbf{P}^T\mathbf{U})^{-1}\mathbf{P}^T$. It is clear that setting $\mathbf{W} = \mathbb{P}$ in (3) will give the above reduced system. To improve the accuracy, the linear and the nonlinear terms will be separated in actual computation. In particular, for $\mathbf{F}(\mathbf{y}) = \mathbf{A}\mathbf{y}+\mathbf{f}(\mathbf{y})$, where $\mathbf{A} \in \mathbb{R}^{n\times n}$, the POD approach will be applied to the linear term $\mathbf{A}\mathbf{y}$ and reduced system of the form (6) will be used for the nonlinear term $\mathbf{f}(\mathbf{y})$, i.e.

$$\dot{\tilde{\mathbf{y}}} = \widetilde{\mathbf{A}}\tilde{\mathbf{y}} + \mathbf{V}^T\mathbb{P}\mathbf{f}(\mathbb{P}^T\mathbf{V}\tilde{\mathbf{y}}), \tag{7}$$

where $\widetilde{\mathbf{A}} = \mathbf{V}^T\mathbf{A}\mathbf{V} \in \mathbb{R}^{k\times k}$ can be precomputed in advance. We next illustrate the efficiency of this model reduction form on a nonlinear reaction-diffusion problem.

NUMERICAL RESULTS

Consider the nonlinear reaction-diffusion initial boundary value problem:

$$\frac{\partial u}{\partial t} = \epsilon\frac{\partial^2 u}{\partial x^2} + u - u^3, \quad x \in \Omega = [0, 2\pi], \qquad t \geq 0, \tag{8}$$

with initial condition : $u(x, 0) = 0.25\sin(x)$, and homogeneous boundary conditions : $u(0, t) = 0$, $u(2\pi, t) = 0$, for $t \geq 0$. In the following numerical tests, we use finite different discretization with spatial point $n = 600$ on $[0, 2\pi]$, time steps $= n_t = 700$ on $[0, 5]$ and $\epsilon = 0.01$. Figure 1 compares the solutions obtained from the original full-order system of the form (1) with the ones from the two reduced models: (i) the POD reduced system (4), and (ii) the POD-DEIM reduced system that preserves the monotonicity (7), which are indistinguishable. The absolute error and the CPU time (normalized with the simulation time of the original full-order system) of these 2 reduced models (4) and (7) that

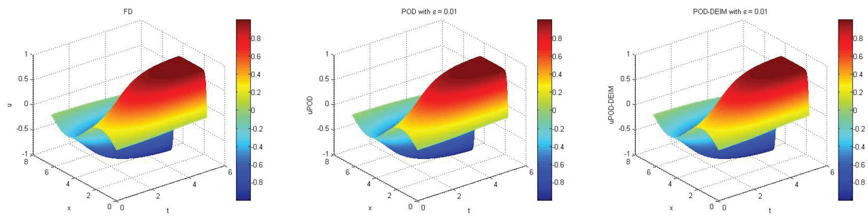

FIGURE 1. Solutions of (8) from the full-order system (1), the POD system (4) with $k = 30$, and the POD-DEIM system that preserves monotonicity (7) with $k = m = 30$.

TABLE 1. Runtime and relative error of the POD reduced system (left) the POD-DEIM reduced system with monotonicity preserved (right). Each runtime is normalized with the CPU time of the original system (dimension $n = 600$).

POD basis (k)	Error	Runtime	DEIM basis (m), with POD $k = 30$	Error	Runtime
10	2.4601e-06	0.4433	10	4.1170e-02	0.0021
20	3.7046e-07	0.4569	20	6.2412e-03	0.0022
30	1.7271e-07	0.4781	30	4.1483e-03	0.0024
40	1.0819e-07	0.4896	40	5.4461e-04	0.0029
50	3.3184e-08	0.4931	50	1.4553e-04	0.0031

preserve monotonicity are given in Table 1. Notice that, although the POD give more accurate approximations, the proposed model can accurately approximate the solution with much less simulation time, e.g. POD-DEIM reduce system with $k = 30$, $m = 30$ has CPU time reduced to $0.0024 \approx 1/400$ of the simulation time used for the original system, while CPU time for POD with $k = 30$ is only reduced to $0.4781 \approx 1/2$ of the time used in the original system.

CONCLUSION

This work proposes a general form of nonlinear reduced-order modeling that preserves the contractivity and monotonicity properties of the original systems, which can be used for guaranteeing the existence, uniqueness of the solution, and stability of the dynamical system. This formulation is based on POD and DEIM approaches with a minor modification. The numerical tests on the nonlinear reaction diffusion problem demonstrate that, while preserving negative monotonicity, the proposed model can accurately approximate the solutions with much less simulation time.

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Stabilized Nonlinear Complexity Reduction through Contractivity-Preserving Framework ☆

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Abstract

This work develops a technique for constructing a reduced-order system that not only has low computational complexity, but also maintains stability of the original nonlinear dynamical system. The proposed framework is designed to maintain the contractivity of the vector field in the original system, which can further guarantee stability preservation, as well as provide error bound for the approximated equilibrium solution of the resulting reduced system. This technique employs low-dimensional basis from proper orthogonal decomposition to optimally capture the dominant dynamics of the original system, and modifies the discrete empirical interpolation method by enforcing certain structure for the nonlinear approximation. The efficiency and accuracy of the proposed method are illustrated through the numerical tests on a nonlinear model describing reaction diffusion problems.

Keywords: Model order reductions, Contractivity, Ordinary differential equations (ODEs), Partial differential equations (PDEs), Proper orthogonal decomposition (POD), Discrete empirical interpolation method (DEIM)

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1. Introduction

Numerical simulations of many natural phenomena described by nonlinear differential equations can lead to dynamical systems with very large spatial dimension when a standard discretization scheme is applied. To reduce the computational cost for solving each of these large-scale systems, *model reduction* methods can be used to produce relatively low dimensional model that still provides accurate solution of the original system. In general, the accuracy of a given model reduction technique is evaluated through certain error measurements when compared with some known reference solutions. Besides considering these approximation errors, this work aims to preserve fundamental behavior of the original system, which will be done through contraction analysis. The contraction property can ensure not only the stability of the systems, but also the existence and uniqueness of the solution from the reduced system, as well as provide error bound for the approximated equilibrium solution.

One of the most popular model reduction methods that preserve contraction property is a projection-based approach using proper orthogonal decomposition (POD) with the Galerkin projection, i.e. POD-Galerkin or POD method. This method is successful in substantially reducing the number of state variables and has been used in numerous applications, e.g. [1, 2, 3, 4, 5]. However, for nonlinear systems, the computational complexity of this approach generally still depends on the high dimension of the original full-order system since it requires to compute orthogonal projection of nonlinear terms.

To avoid this inefficiency, new approaches have been proposed to improve the POD-Galerkin method for nonlinear systems. These approaches include trajectory piecewise-linear (TPWL) method [6, 7], Missing Point Estimation (MPE) [8], Discrete empirical interpolation (DEIM) [9]. TPWL approach is based on estimating a nonlinear function by using linearized approximation constructed from existing information of the original full-order system. It has been used in many applications, especially in circuit simulations [10, 11, 7, 12, 13]. However, not all nonlinear functions can be accurately estimated by linearized approximations. MPE can reduce the complexity of the POD-Galerkin reduced system by considering certain selected equations in the discretized system. This approach was further extended in the form of special inner product [14]. DEIM can be viewed as an improvement of MPE by combining oblique projection with interpolatory approximation. The interpolated indices are selected based on a greedy algorithm proposed in [15] for the empirical interpolation method (EIM), which was introduced in function space setting for finite element framework with projection basis obtained directly from snapshot solutions. An error bound for the DEIM approximation shown in [9] implies that it is nearly as accurate as the optimal POD approximation. DEIM has been successfully used with POD method for constructing reduced systems in many recent works, such as in neural modeling of full Hodgkin-Huxley models for realistic spiking neurons [16], subsurface flows [17, 18], coupled circuit-device systems [19], and reduced order quadrature algorithm [20].

Despite the success of POD-DEIM approach in various applications, it still cannot be proved theoretically to preserve stability and other fundamental properties of the original systems. In fact, it will guarantee stability in contractivity analysis only under certain conditions, as shown later in this work. Existing model reduction methods aimed to preserve the system properties for only some special classes of nonlinear dynamical systems, for example, the framework for preserving Lagrangian structure of the nonlinear mechanical systems was introduced in [21], and the approach for preserving nonlinear port-Hamiltonian structure was proposed in [22]. For general cases, only stability for linearized systems has been considered in [23]. This work focuses on preserving stability for general nonlinear systems without requiring linearization. In particular, this work derives a contractivity-preserving framework for nonlinear vector fields, which will be shown to maintain important behaviors of the dynamical systems, such as exponential stability, existence and uniqueness of the solution, and convergence of perturbed equilibrium. The proposed framework applies the concept of interpolatory projection-based nonlinear model reduction approach using DEIM with certain structured form of the approximated nonlinear term.

This work is organized as follows. First, the general form of nonlinear differential equation and the fundamental notions of contractivity are introduced in Section 2 . Two projection-based model reduction methods: POD and POD-DEIM approaches are reviewed in Section 3. Based on these approaches, Section 4 presents the derivation of a model reduction framework that preserves contractivity of vector field from the original dynamical system. The contractivity is shown to further imply the stability of the solution, as well as can be used to obtain an error bound for a perturbed equilibrium solution. This section also investigates the contractivity property of the existing POD and POD-DEIM techniques. It can be shown that POD reduced systems always preserve the contractivity of the original system, but POD-DEIM systems do not. The conditions under which the POD-DEIM approach preserves contractivity property are discussed at the end of Section 4. In Section 5, two numerical tests are performed on a nonlinear reaction-diffusion problem to demonstrate the efficiency of the proposed framework. The summary of this work and some final remarks are discussed in Section 6.

2. Problem Formulation and Contractivity

This section provides some theoretical background required for deriving a model reduction scheme that preserves contractivity of nonlinear dynamical systems. The desired form of system structure to be preserved will be discussed together with its significance.

Consider the system of nonlinear ordinary differential equations (ODEs) of the form:

$$\frac{d\mathbf{y}}{dt} = \mathbf{F}(t, \mathbf{y}), \qquad \mathbf{y}(0) = \mathbf{y}_0, \tag{1}$$

where $\mathbf{y} = \mathbf{y}(t)$ is an n dimensional state variable at certain time $t \geq 0$ and $\mathbf{F} : [0, \infty) \times Y \to \mathbb{R}^n$ is a differentiable nonlinear vector-valued function, $Y \subseteq \mathbb{R}^n$ with the Jacobian given by $J_{\mathbf{F}}(t, \mathbf{y}) = \frac{\partial \mathbf{F}}{\partial \mathbf{y}}(t, \mathbf{y})$.

We are interested in constructing model reduction that preserves stability properties of the original system. The standard stability properties are generally analyzed through Lyapunov-based approach. However, a main difficulty for this standard analysis often arises as it requires equilibrium points to be specified in advance. In this work, we consider an alternative stability criterion using *contraction* analysis, which is generally easier to analyze but stronger than the standard one. In particular, while standard nonlinear stability has to be analyzed with respect to an equilibrium solution, contraction is concerned with the behavior of system trajectories with respect to each other and do not require the prior knowledge of steady-state solution. Contraction analysis considers mainly a property of the vector field defining the dynamical system.

2.1. Logarithmic norm and Logarithmic Lipschitz constants

We first consider the **logarithmic norm**, introduced independently by Germund Dahlquist and Sergei Lozinskii in 1959 [24, 25]. The definition of logarithmic norm is given next in a special case of Euclidean space.

Definition 2.1. *Let* $\mathbf{A} \in \mathbb{R}^{n\times n}$ *be a constant matrix. The associated matrix measure, called* **logarithmic norm** *is defined as*

$$\mu[\mathbf{A}] = \lim_{h\to 0^+} \frac{\|I + h\mathbf{A}\| - 1}{h}, \tag{2}$$

where $\|\cdot\|$ *is the standard Euclidean norm.*

In the above definition, $\|\cdot\|$ can be any norm. When $\|\cdot\|$ is the Euclidean norm, it can be shown that [26], $\mu[\mathbf{A}]$ is the maximum eigenvalue of the symmetric part of $\mathbf{A}$, i.e.

$$\mu[\mathbf{A}] = \lambda_{\max}\left(\frac{\mathbf{A}+\mathbf{A}^T}{2}\right), \tag{3}$$

where $\lambda_{\max}(\cdot)$ gives the maximum eigenvalue of the input quantity. Equivalently, it can also be shown that, for any induced norm in Hilbert space, for $\mathbf{u}, \mathbf{v} \in \mathbb{R}^n$

$$\mu[\mathbf{A}] = \sup_{\mathbf{u}\neq\mathbf{v}} \frac{\mathrm{Re}\,\langle \mathbf{u}-\mathbf{v}, \mathbf{A}\mathbf{u}-\mathbf{A}\mathbf{v}\rangle}{\langle \mathbf{u}-\mathbf{v}, \mathbf{u}-\mathbf{v}\rangle}, \tag{4}$$

where $\|\mathbf{x}\|^2 = \langle \mathbf{x}, \mathbf{x}\rangle$, $\mathbf{x} \in \mathbb{R}^n$.

The notion of logarithmic norm has been extended to generalize nonlinear operator in Banach space by introducing the notion of *logarithmic Lipschitz constants* [26]. The definition and some elementary properties of logarithmic Lipschitz constants are given below.

Definition 2.2. *Let $(X, \|\cdot\|_X)$ be a normed space and $F : Y \to X$ be a function where $Y \subseteq X$. The* **least upper bound (lub)** *and the* **greatest lower bound (glb) Lipschitz constants** *of F induced by the norm $\|\cdot\|_X$ on Y are defined, respectively, by*

$$L_{Y,X}[F] = \sup_{u \neq v \in Y} \frac{\|F(u) - F(v)\|_X}{\|u - v\|_X}, \quad \textit{and} \quad \ell_{Y,X}[F] = \inf_{u \neq v \in Y} \frac{\|F(u) - F(v)\|_X}{\|u - v\|_X}.$$

The **least upper bound (lub)** *and the* **greatest lower bound (glb) logarithmic Lipschitz constants** *of F induced by the norm $\|\cdot\|_X$ on Y are defined by*

$$M_{Y,X}[F] = \lim_{h \to 0^+} \frac{L_{Y,X}[I + hF] - 1}{h}, \quad \textit{and} \quad m_{Y,X}[F] = \lim_{h \to 0^-} \frac{L_{Y,X}[I + hF] - 1}{h}.$$

Note that, this work considers the setting for systems of ODEs with $X = Y \subseteq \mathbb{R}^n$ and will use the notation $L_{X,X}[\cdot] = L[\cdot]$, $\ell_{X,X}[\cdot] = \ell[\cdot]$ and $M_{X,X}[\cdot] = M[\cdot]$, $m_{X,X}[\cdot] = m[\cdot]$. Moreover, we will use the Euclidean norm for $\|\cdot\|_X$, which will be simply denoted as $\|\cdot\|$. In this case, it can be shown [26] that $M[\cdot] = m[\cdot]$ and for any $\mathbf{u}, \mathbf{v} \in \mathbb{R}^n$,

$$M[F] = \sup_{\mathbf{u} \neq \mathbf{v}} \frac{\langle \mathbf{u} - \mathbf{v}, F(\mathbf{u}) - F(\mathbf{v}) \rangle}{\|\mathbf{u} - \mathbf{v}\|^2} = \sup_{\mathbf{u} \neq \mathbf{v}} \frac{(\mathbf{u} - \mathbf{v})^T (F(\mathbf{u}) - F(\mathbf{v}))}{\|\mathbf{u} - \mathbf{v}\|^2}. \tag{5}$$

Note that, when $F = \mathbf{A} \in \mathbb{R}^{n \times n}$, $\mu[\mathbf{A}] = M[\mathbf{A}]$.

Lemma 2.3. *[27, 28] Let M be the (lub) logarithmic Lipschitz constant induced by the Euclidean norm on $\mathbb{R}^n$ and $Y \subseteq \mathbb{R}^n$ be a connected set. Then for any Lipschitz and continuously differentiable function $F : Y \to \mathbb{R}^n$, with Jacobian J_F,*

$$\sup_{\mathbf{y} \in Y} M[J_F(\mathbf{y})] \leq M[F]. \tag{6}$$

In addition, if Y is convex, then

$$\sup_{\mathbf{y}\in Y} M[J_F(\mathbf{y})] = M[F]. \tag{7}$$

This lemma is useful in practice for estimating or computing $M[F]$ when the Jacobian J_F is known.

2.2. Contractivity

The definition and related properties of *contractivity* will be presented next for the vector field $\mathbf{F}$ of the system of differential equations in (1).

Definition 2.4. *[27, 29] The time-dependent vector field $\mathbf{F} : [0,\infty) \times Y \to \mathbb{R}^n$, $Y \subseteq \mathbb{R}^n$, in the system (1), is said to be* **infinitesimally contracting** *on a set $Y \subseteq \mathbb{R}^n$ with respect to the Euclidean norm if, for some constant $c > 0$,*

$$\mu[J_{\mathbf{F}}(t, \mathbf{y})] \leq -c, \qquad \forall \mathbf{y} \in Y, \quad \forall t \geq 0. \tag{8}$$

where $J_{\mathbf{F}}(t, \mathbf{y}) \in \mathbb{R}^{n\times n}$ is the Jacobian of $\mathbf{F}((t, \mathbf{y})$. The constant c is called **contraction rate**.

<u>Remark:</u> For $\mathbf{F} : [0,\infty) \times Y \to \mathbb{R}^n$, $Y \subseteq \mathbb{R}^n$, recall from Lemma 2.3 that

$$\sup_{\mathbf{y}\in Y} \mu\left[J_{\mathbf{F}}(t, \mathbf{y})\right] \leq M[\mathbf{F}_t], \qquad \forall t \geq 0,$$

where $\mathbf{F}_t(\mathbf{y}) = \mathbf{F}(t, \mathbf{y})$. That is, the function $\mathbf{F}$ is **infinitesimally contracting** if the following condition holds true:

$$\sup_{t\in[0,\infty)} M[\mathbf{F}_t] < 0. \tag{9}$$

In this work, the above stronger condition of being *infinitesimally contracting* given in (9) will be used instead of (8) to make it more convenient for applying on general nonlinear functions when deriving contractivity-preserving model reduction approach. For the time-independent function $\mathbf{F}$, i.e. $\mathbf{F}(t, \mathbf{y}) = \mathbf{F}(\mathbf{y}), \forall t \in [0,\infty)$, which will be considered mainly in this work, the condition (9) becomes simply $M[\mathbf{F}] < 0$. It can be further shown that [30], *infinitesimal contractivity* implies *global contractivity.*

Theorem 2.5. *[30, 27] Let* $\|\cdot\|$ *be the Euclidean norm and* $\mathbf{F} : [0,\infty)\times Y \to X]$ *be (globally) Lipschitz and continuously differentiable function, where* $Y \subseteq X = \mathbb{R}^n$*. Suppose* $\mathbf{y}$ *and* $\hat{\mathbf{y}}$ *are the solutions of* $\frac{d\mathbf{y}}{dt} = \mathbf{F}(t,\mathbf{y})$*, with initial conditions* $\mathbf{y}(0) = \mathbf{y}_0$ *and* $\mathbf{y}(0) = \hat{\mathbf{y}}_0$*, respectively. Define* $\mathbf{F}_t(\mathbf{y}) = \mathbf{F}(t,\mathbf{y})$*. Then, for*

$$k \quad := \quad \sup_{t\in[0,\infty)} M[\mathbf{F}_t], \tag{10}$$

$$\|\mathbf{y}(t) - \hat{\mathbf{y}}(t)\| \quad \leq \quad e^{kt}\|\mathbf{y}_0 - \hat{\mathbf{y}}_0\|, \qquad \forall t \geq 0. \tag{11}$$

From Theorem 2.5, when $\mathbf{F}$ is infinitesimally contracting, i.e. $k < 0$, the trajectories globally and exponentially converge to each other. In the remaining parts of this paper, the *contractivity* of a function will refer to the condition (9), which will imply both *infinitesimal contractivity* and *global contractivity.*

To see some effects of contractivitiy on the behaviors of dynamical systems with nonlinear vector field $\mathbf{F}$, consider a simple mathematical explanation. Without loss of generality, the system of differential equations (1) is assumed to be autonomous for notational convenience. Consider the two systems of differential equations:

$$\frac{d\mathbf{y}}{dt} \quad = \quad \mathbf{F}(\mathbf{y}), \qquad \mathbf{y}(0) = \mathbf{y}_0, \tag{12}$$

$$\frac{d\hat{\mathbf{y}}}{dt} \quad = \quad \mathbf{F}(\hat{\mathbf{y}}) + \mathbf{p}(t) \qquad \hat{\mathbf{y}}(0) = \hat{\mathbf{y}}_0. \tag{13}$$

The system (13) can be viewed as perturbed system of the system (12). Let $\mathbf{E}(t) = \hat{\mathbf{y}}(t) - \mathbf{y}(t)$ be the difference of the solutions from these two systems. Then $\dot{\mathbf{E}}(t) = \dot{\hat{\mathbf{y}}}(t) - \dot{\mathbf{y}}(t) = \mathbf{F}(t,\hat{\mathbf{y}}) - \mathbf{F}(t,\mathbf{y}) + \mathbf{p}(t)$. By using the identity (5) and $\|\mathbf{E}\|\frac{d}{dt}\|\mathbf{E}\| = \frac{1}{2}\|\mathbf{E}\|^2 = \mathbf{E}^T\dot{\mathbf{E}} = \langle \mathbf{E}, \dot{\mathbf{E}}\rangle$, we have

$$\begin{aligned}
\frac{d}{dt}\|\mathbf{E}\| &= \frac{1}{\|\mathbf{E}\|}\langle \mathbf{E}, \dot{\mathbf{E}}\rangle = \frac{1}{\|\mathbf{E}\|}\langle \mathbf{E}, \mathbf{F}(t,\hat{\mathbf{y}}) - \mathbf{F}(t,\mathbf{y}) + \mathbf{p}(t)\rangle \\
&= \frac{1}{\|\mathbf{E}\|}\langle \mathbf{E}, \mathbf{F}(t,\hat{\mathbf{y}}) - \mathbf{F}(t,\mathbf{y})\rangle + \frac{1}{\|\mathbf{E}\|}\langle \mathbf{E}, \mathbf{p}(t)\rangle \\
\frac{d}{dt}\|\hat{\mathbf{y}} - \mathbf{y}\| &= \frac{1}{\|\hat{\mathbf{y}} - \mathbf{y}\|}\langle \hat{\mathbf{y}} - \mathbf{y}, \mathbf{F}(t,\hat{\mathbf{y}}) - \mathbf{F}(t,\mathbf{y})\rangle + \frac{1}{\|\mathbf{E}\|}\langle \mathbf{E}, \mathbf{p}(t)\rangle \\
&\leq M[\mathbf{F}]\|\hat{\mathbf{y}} - \mathbf{y}\| + \|\mathbf{p}(t)\| \\
\frac{d}{dt}\|\mathbf{E}\| &\leq M[\mathbf{F}]\|\mathbf{E}\| + \|\mathbf{p}(t)\|.
\end{aligned}$$

Integrating the above differential inequality gives

$$\|\mathbf{E}(t)\| \leq \|\mathbf{E}(0)\|\ e^{M[\mathbf{F}]t} + \int_0^t \|\mathbf{p}(\tau)\|\ e^{(t-\tau)M[\mathbf{F}]} d\tau. \tag{14}$$

The above bound illustrates the effects of *logarithmic Lipschitz constant* on certain system's properties, such as stability and perturbation. As shown in [26], two fundamental cases should be considered for the error $\|\mathbf{E}(t)\| = \|\hat{\mathbf{y}}(t) - \mathbf{y}(t)\|$ using (14).

Case 1: When $\mathbf{p}(t) = 0$, the bound in (14) gives

$$\|\hat{\mathbf{y}}(t) - \mathbf{y}(t)\| \leq e^{M[\mathbf{F}]t} \|\hat{\mathbf{y}}(0) - \mathbf{y}(0).\|$$

When $\mathbf{F}$ is infinitesimally contracting, i.e. $M[\mathbf{F}] < 0$, the solution is exponentially stable.

Case 2: When $\mathbf{E}(0) = 0$, i.e. the initial conditions $\mathbf{y}_0$ and $\hat{\mathbf{y}}_0$ are the same, the bound in (14) gives

$$\|\hat{\mathbf{y}}(t) - \mathbf{y}(t)\| \leq \frac{e^{tM[\mathbf{F}]} - 1}{M[\mathbf{F}]} \max_{t \in [0,\infty)} \|\mathbf{p}(t)\|,$$

by using straightforward integration. Notice that when $\mathbf{F}$ is infinitesimally contracting, i.e. $M[\mathbf{F}] < 0$, we have $e^{tM[\mathbf{F}]} \in (0,1)$ and the bound becomes $\|\hat{\mathbf{y}}(t) - \mathbf{y}(t)\| \leq \frac{-1}{M[\mathbf{F}]} \max_{t\in[0,\infty)} \|\mathbf{p}(t)\|$, which implies that $\hat{\mathbf{y}}(t) \to \mathbf{y}(t)$ as $\max_{t\in[0,\infty)} \|\mathbf{p}(t)\| \to 0$.

From the discussion above, it is essential to maintain the contractivity of the vector field when constructing the approximate low-dimensional system, so that the fundamental behaviors of the original system are preserved.

3. Model order reduction

In order to derive a contractivity-preserving reduced-order modeling, this section will first consider a well-known method called proper orthogonal decomposition (POD) and its combination with discrete empirical interpolation method (DEIM).

Recall the nonlinear differential equation (1) in the form of autonomous system:

$$\frac{d\mathbf{y}}{dt} = \mathbf{F}(\mathbf{y}), \qquad \mathbf{y}(0) = \mathbf{y}_0, \tag{15}$$

where $\mathbf{y} : [0, \infty) \rightarrow \mathbb{R}^n$ is the state variable and $\mathbf{F} : Y \subseteq \mathbb{R}^n \rightarrow \mathbb{R}^n$ is the nonlinear vector field. Projection-based model reduction method can construct a reduced-order system by projecting (15) onto a low dimensional subspace. Let $\mathbf{V} \in \mathbb{R}^{n \times k}$ be a matrix whose columns form a set of an orthonormal basis of dimension k, where $k \leq n$. Then, we can approximate the state variable $\mathbf{y}(t)$ in the space spanned by the columns of $\mathbf{V}$ in the form $\mathbf{y}(t) \approx \mathbf{V}\tilde{\mathbf{y}}(t)$, where $\tilde{\mathbf{y}}(t) \in \mathbb{R}^k$. By substituting this approximation into (1), and applying the Galerkin projection which will give the smallest error of the residual in the direction of $span\{\mathbf{V}\}$, i.e. $\mathbf{V}^T \left(\frac{d}{dt}\mathbf{V}\tilde{\mathbf{y}}(t) - \left[\mathbf{V}^T\mathbf{F}(\mathbf{V}\tilde{\mathbf{y}}(t))\right]\right) = 0$. When the columns of $\mathbf{V}$ are orthonormal, the POD reduced system is of the form:

$$\frac{d}{dt}\tilde{\mathbf{y}}(t) = \mathbf{V}^T\mathbf{F}(\mathbf{V}\tilde{\mathbf{y}}(t)), \quad \tilde{\mathbf{y}}(0) = \mathbf{V}_k^T\mathbf{y}_0, \tag{16}$$

The system (16) is called POD reduced system. In this setting, $\mathbf{V}$ can be constructed from any orthogonal basis. However, to get an accurate approximation from this reduced system, we will consider the basis constructed by Proper Orthogonal Decomposition (POD), which can optimally extract the dominant characteristics from any given system of interest.

Proper Orthogonal Decomposition (POD) is also known by other names, for example, Karhunen-Love decomposition (KLD), Principal Component Analysis (PCA), or Singular Value Decomposition (SVD). POD has been used with the Galerkin projection in many applications to reduce number of variable of large-scaled discretized system, e.g. [1, 2, 3, 4, 5]. One of the most important properties of POD is that it can construct an approximation that minimizes the error in $2-$norm for a given fixed basis rank k. POD also can be obtained by using singular value decomposition (SVD) as discussed next.

Definition 3.1 (POD basis,[31]). *Let $\mathbf{Y} = [\mathbf{y}_1, \ldots, \mathbf{y}_{n_s}] \in \mathbb{R}^{n \times n_s}$ be a snapshot matrix with rank $r \leq min\{n, n_s\}$. POD basis of dimension k, where $k \leq r$, is the solution to the following optimization problem:*

$$\min_{\mathbf{\Phi}_k \in \mathbb{R}^{n \times k}} \sum_{j=1}^{n_s} \|\mathbf{y}_j - \mathbf{\Phi}_k\mathbf{\Phi}_k^T\mathbf{y}_j\|_2^2 \quad \textit{such that} \quad \mathbf{\Phi}_k^T\mathbf{\Phi}_k = \mathbf{I}_k \tag{17}$$

where $\mathbf{I}_k \in \mathbb{R}^{k\times k}$ *is the identity matrix.*

It can be shown [31] that POD basis defined above can be obtained from the left singular vector of the snapshot matrix $\mathbf{Y}$. Let $\mathbf{Y} = \hat{\mathbf{U}}\Sigma\mathbf{Z}^T$ be the singular value decomposition of $\mathbf{Y}$, where matrices $\hat{\mathbf{U}} = [\mathbf{u}_1, \ldots, \mathbf{u}_r] \in \mathbb{R}^{n\times r}$ and $\hat{\mathbf{Z}} = [\mathbf{z}_1, \ldots, \mathbf{z}_r] \in \mathbb{R}^{n_s\times r}$ are matrices with orthogonal columns and $\Sigma = diag(\sigma_1, \ldots, \sigma_r) \in \mathbb{R}^{r\times r}$ is a digonal matrix with $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_r > 0$. Then the POD basis of dimension k is $\mathbf{V} = [\mathbf{u}_1, \ldots, \mathbf{u}_k] \in \mathbb{R}^{n\times k}$, $k \leq r$ and it is well-known [31] that

$$\sum_{j=1}^{n_s} \|\mathbf{y}_j - \mathbf{V}\mathbf{V}^T\mathbf{y}_j\|_2^2 = \sum_{\ell=k+1}^{r} \sigma_\ell^2, \tag{18}$$

which is the sum of the neglected singular values $\sigma_{k+1}, \ldots, \sigma_r$ from the SVD of $\mathbf{Y}$.

Although POD-Galerkin can reduce the number of unknowns of the full-order system, it may not be able to reduce the complexity for computing the projected nonlinear term $\mathbf{V}^T\mathbf{F}(\mathbf{V}\tilde{\mathbf{y}}(t))$ from (16). To handle this complexity problem, POD will be used with the discrete empirical interpolation method (DEIM) [32], which derived from the continuous setting in [15].

DEIM approximates the nonlinear function $\mathbf{F}(\mathbf{y})$ by projecting it onto the space spanned by the columns of a basis matrix $\mathbf{U} \in \mathbb{R}^{n\times m}$ of rank $m \leq n$. The matrix $\mathbf{U}$ can be constructed from POD basis of nonlinear snapshot matrix $[\mathbf{F}(\mathbf{y}_1), \ldots, \mathbf{F}(\mathbf{y}_{n_s})]$, where $\mathbf{y}_i \cong \mathbf{y}(t_i)$. This DEIM approximation is therefore in the form of $\mathbf{U}\mathbf{c}(t)$, for some vector $\mathbf{c}(t)$ in $\mathbb{R}^m$. In order to specify $\mathbf{c}(t)$, a greedy selection procedure given in Algorithm1 is used to select m interpolated row indices of the interpolation approximation. That is, let $\wp_1, \ldots, \wp_m$ be interpolation indices from Algorithm1 corresponding to the input basis set from $\mathbf{U}$ and let $\mathbf{P} = [\mathbf{e}_{\wp_1}, \ldots, \mathbf{e}_{\wp_m}] \in \mathbb{R}^{n\times m}$ where $\mathbf{e}_{\wp_i} = [0, \ldots, 0, 1, 0, \ldots, 0]^T \in \mathbb{R}^n$ is the $\wp_i$-th column of the identity matrix $\mathbf{I}_n \in \mathbb{R}^{n\times n}$, for $i = 1, \ldots, m$. Since it has been shown in [32] that $\mathbf{P}^T\mathbf{U}$ is nonsingular, the vector $\mathbf{c}(t)$ can be uniquely solved from

$$\mathbf{P}^T\mathbf{F}(\mathbf{V}\tilde{\mathbf{y}}(t)) = (\mathbf{P}^T\mathbf{U})\mathbf{c}(t), \tag{19}$$

which gives a closed-form formula $\mathbf{c}(t) = (\mathbf{P}^T\mathbf{U})^{-1}\mathbf{P}^T\mathbf{F}(t)$. Therefore, the approximation is given by

$$\mathbf{F}(\mathbf{V}\tilde{\mathbf{y}}(t)) = \mathbf{U}(\mathbf{P}^T\mathbf{U})^{-1}\underbrace{\mathbf{P}^T\mathbf{F}(\mathbf{V}\tilde{\mathbf{y}}(t))}_{m\times 1}. \tag{20}$$

In the case when the nonlinear function $\mathbf{F}$ is componentwise, we have

$$\mathbf{F}(\mathbf{V}\tilde{\mathbf{y}}(t)) = \mathbf{U}(\mathbf{P}^T\mathbf{U})^{-1}\underbrace{\mathbf{F}(\mathbf{P}^T\mathbf{V}\tilde{\mathbf{y}}(t))}_{m\times 1}. \tag{21}$$

Note that, pre-multiplying $\mathbf{P}^T$ in (19) is equivalent to extracting the m rows corresponding to the interpolation indices $\wp_1, \dots, \wp_m$, and there is no actual matrix multiplication required. The procedure for selecting these indices is shown in Algorithm 1. It chooses each index by aiming to minimize the residual error $\mathbf{r} = \mathbf{u}_\ell - \mathbf{Uc}$ in each iteration ℓ. Finally, the POD-DEIM reduced system can be written in the following two equivalent forms:

$$\dot{\tilde{\mathbf{y}}} = \mathbf{V}^T\mathbf{U}(\mathbf{P}^T\mathbf{U})^{-1}\mathbf{P}^T\mathbf{F}(\mathbf{V}\tilde{\mathbf{y}}), \qquad \tilde{\mathbf{y}}(0) = \mathbf{V}^T\mathbf{y}_0, \tag{22}$$

$$\dot{\tilde{\mathbf{y}}} = \mathbf{V}^T\mathbb{P}\mathbf{F}(\mathbf{V}\tilde{\mathbf{y}}), \qquad \tilde{\mathbf{y}}(0) = \mathbf{V}^T\mathbf{y}_0, \tag{23}$$

where $\mathbb{P} := \mathbf{U}(\mathbf{P}^T\mathbf{U})^{-1}\mathbf{P}^T$ is an oblique projector.

Algorithm 1 Algorithm to create for Interpolation Indices DEIM

INPUT: $\{\mathbf{u}_\ell\}_{\ell=1}^m \subset \mathbb{R}^n$ linearly independent

OUTPUT: $\vec{\wp} = [\wp_1, \dots, \wp_m]^T \in \mathbb{R}^m$

$[|\rho|, \wp_1] = \max\{|\mathbf{u}_1|\}$

$\mathbf{U} = [\mathbf{u}_1], \mathbf{P} = [\mathbf{e}_{\wp_1}], \vec{\wp} = [\wp_1]$;

for $\ell \leftarrow 2$ to m **do**

Solve $(\mathbf{P}^T\mathbf{U})\mathbf{c} = \mathbf{P}^T\mathbf{u}_\ell$;

$\mathbf{r} = \mathbf{u}_\ell - \mathbf{Uc}$ $[|\rho|, \wp_\ell] = \max\{|\mathbf{r}|\}$

$\mathbf{U} \leftarrow [\mathbf{U} \quad \mathbf{u}_\ell], \mathbf{P} \leftarrow [\mathbf{P} \quad \mathbf{e}_{\wp_\ell}], \vec{\wp} \leftarrow \begin{bmatrix} \vec{\wp} \\ \wp_\ell \end{bmatrix}$

end

Although DEIM has been successfully used to obtain accurate low-complexity models in various applications, as can be seen in, e.g. [16, 33, 34, 35], it cannot be theoretically proved to preserve stability of original systems through contraction analysis. This work aims to derive a modified form of POD-DEIM reduced system to overcome this problem.

4. Contractivity-preserving model reduction

Motivated by projection-based model reduction approaches described in the previous section, this section will first propose a general form of model reduction scheme that preserves contractivity of nonlinear vector fields from original systems. The derivation is performed through the Euclidean norm. A specific form that preserves the contractivity will be considered at the end of this section by enforcing certain structure on the modified POD-DEIM reduced system. The contractivity of the existing POD and POD-DEIM approaches will be also investigated. It will be shown that while POD reduced systems always preserve the contractivity, this may not be true for POD-DEIM reduced systems. The conditions under which the POD-DEIM approach preserves these properties will be discussed.

4.1. Proposed General Form

Consider the autonomous differential equation of the form (15). This section will propose a general form of the projection-based model reduction that preserves the contractivity of the original system (15) with respect to the Euclidean norm.

Lemma 4.1. *Suppose the nonlinear vector field* $\mathbf{F}$ *in (15) is* **infinitesimally contracting**, *i.e.* $M[\mathbf{F}] < 0$. *Consider the reduced-order model in the form:*

$$\dot{\tilde{\mathbf{y}}} = \widetilde{\mathbf{F}}(\tilde{\mathbf{y}}), \qquad \textit{with} \quad \widetilde{\mathbf{F}}(\tilde{\mathbf{y}}) = \mathbf{V}^T\mathbf{W}\mathbf{F}(\mathbf{W}^T\mathbf{V}\tilde{\mathbf{y}}) \tag{24}$$

where $\tilde{\mathbf{y}} = \tilde{\mathbf{y}}(t) \in \mathbb{R}^k$, $\mathbf{W} \in \mathbf{R}^{n\times n}$ *and* $\mathbf{V} \in \mathbf{R}^{n\times k}$, *for* $k \leq n$, $t \geq 0$. *Suppose the solution* $\mathbf{y}$ *of the original full-order system (15) is approximated by* $\mathbf{V}\tilde{\mathbf{y}}$. *Then the nonlinear vector field* $\widetilde{\mathbf{F}}(\tilde{\mathbf{y}})$ *in (24) is also* **infinitesimally contracting** *if* $\mathbf{W}^T\mathbf{V} \in \mathbf{R}^{n\times k}$ *has full column rank, i.e.* $rank(\mathbf{W}^T\mathbf{V}) = k$.

Note that the matrix $\mathbf{W}$ is introduced in (24) for allowing the reduced system to cooperate additional efficient nonlinear complexity reduction, e.g. as explained in Section 3.

Proof: Let $M[\mathbf{F}]$ and $M[\widetilde{\mathbf{F}}]$ be the logarithmic Lipschitz constants of $\mathbf{F}$ and $\widetilde{\mathbf{F}}$, respectively. For $\tilde{\mathbf{u}}, \tilde{\mathbf{v}} \in \mathbb{R}^k$ and $\mathbf{u}, \mathbf{v} \in \mathbb{R}^n$, since $\mathbf{F}$ in system (1) is infinitesimally contracting, i.e. $M[\mathbf{F}] < 0$, then, for $\widetilde{\mathbf{W}} := \mathbf{W}^T\mathbf{V} \in \mathbf{R}^{n\times k}$,

$$\begin{aligned}
M[\widetilde{\mathbf{F}}] &= \sup_{\tilde{\mathbf{u}}\neq\tilde{\mathbf{v}}} \frac{(\tilde{\mathbf{u}}-\tilde{\mathbf{v}})^T(\widetilde{\mathbf{F}}(\tilde{\mathbf{u}})-\widetilde{\mathbf{F}}(\tilde{\mathbf{v}}))}{\|\tilde{\mathbf{u}}-\tilde{\mathbf{v}}\|^2} \\
&= \sup_{\tilde{\mathbf{u}}\neq\tilde{\mathbf{v}}} \frac{(\tilde{\mathbf{u}}-\tilde{\mathbf{v}})^T(\widetilde{\mathbf{W}}^T\mathbf{F}(\widetilde{\mathbf{W}}\tilde{\mathbf{u}})-\widetilde{\mathbf{W}}^T\mathbf{F}(\widetilde{\mathbf{W}}\tilde{\mathbf{v}}))}{\|\tilde{\mathbf{u}}-\tilde{\mathbf{v}}\|^2} \\
&= \frac{1}{K^2}\sup_{\tilde{\mathbf{u}}\neq\tilde{\mathbf{v}}} \frac{(\widetilde{\mathbf{W}}\tilde{\mathbf{u}}-\widetilde{\mathbf{W}}\tilde{\mathbf{v}})^T(\mathbf{F}(\widetilde{\mathbf{W}}\tilde{\mathbf{u}})-\mathbf{F}(\widetilde{\mathbf{W}}\tilde{\mathbf{v}}))}{\|\widetilde{\mathbf{W}}\tilde{\mathbf{u}}-\widetilde{\mathbf{W}}\tilde{\mathbf{v}}\|^2} \\
&\leq \frac{1}{K^2}\sup_{\mathbf{u}\neq\mathbf{v}} \frac{(\mathbf{u}-\mathbf{v})^T(\mathbf{F}(\mathbf{u})-\mathbf{F}(\mathbf{v}))}{\|\mathbf{u}-\mathbf{v}\|^2} \\
&= \frac{1}{K^2}M[\mathbf{F}] < 0,
\end{aligned}$$

where K is a positive constant such that $\|\tilde{\mathbf{u}}-\tilde{\mathbf{v}}\| = K\|\widetilde{\mathbf{W}}\tilde{\mathbf{u}}-\widetilde{\mathbf{W}}\tilde{\mathbf{v}}\|$. The assumption that $\widetilde{\mathbf{W}}$ has full column rank guarantees the existence of $K > 0$ and ensures that the denominator $\|\widetilde{\mathbf{W}}\tilde{\mathbf{u}}-\widetilde{\mathbf{W}}\tilde{\mathbf{v}}\|$ is nonzero. That is, $M[\widetilde{\mathbf{F}}] < 0$ and $\widetilde{\mathbf{F}}$ is infinitesimally contracting. ■

The above result can be extended to guarantee the stability and the existence of the equilibrium solution of the reduced system in the form (24) as discussed in Section 2.2.

Proposition 4.2. *Suppose the nonlinear vector field* $\mathbf{F}$ *in the full-order system (15) is infinitesimally contracting, i.e.* $M[\mathbf{F}] < 0$*. Then*
(i) the reduced system (24) preserves the exponential stability of (15) .
(ii) the reduced system (24) has a unique equilibrium $\tilde{\mathbf{y}}_e$*, i.e.* $\widetilde{\mathbf{F}}(\tilde{\mathbf{y}}_e) = 0$*. Moreover, if* $\mathbf{y}_e$ *is the unique equilibrium solution of (15), then* $\mathbf{y}_e$ *can be approximated by* $\mathbf{V}\tilde{\mathbf{y}}_e$ *with an error bound given by*

$$\|\mathbf{y}_e - \mathbf{V}\tilde{\mathbf{y}}_e\| \leq \frac{-\|\mathbf{p}\|}{M[\mathbf{F}]}, \qquad \text{where} \qquad \mathbf{p} = \mathbf{F}(\mathbf{V}\tilde{\mathbf{y}}_e). \tag{25}$$

Proof: (i) This part follows from [26] that the solution of the reduced system satisfies $\|\tilde{\mathbf{y}}\| \leq e^{M[\widetilde{\mathbf{F}}]t}\|\tilde{\mathbf{y}}(0)\|$ and that $\mathbf{F}$ in system (15) is infinitesimally contracting: $M[\widetilde{\mathbf{F}}] < 0$ for $t \geq 0$ from the previous lemma.

(ii) First note that , from [26], $M[\mathbf{F}] < 0$ implies that the map $\mathbf{F}$ is bijective and there must be a unique solution $\mathbf{y}_e$ such that $\mathbf{F}(\mathbf{y}_e) = 0$. Similarly, from Lemma 4.1, $M[\mathbf{F}] < 0$ implies $M[\widetilde{\mathbf{F}}] < 0$, which also further gives the existence of the unique solution $\tilde{\mathbf{y}}_e$ such that $\widetilde{\mathbf{F}}(\tilde{\mathbf{y}}_e) = 0$. To derive the bound, let $\mathbf{p} := \mathbf{F}(\mathbf{V}\tilde{\mathbf{y}}_e)$ and consider $\frac{\langle \mathbf{V}\tilde{\mathbf{y}}_e - \mathbf{y}_e, \mathbf{F}(\mathbf{V}\tilde{\mathbf{y}}_e) - \mathbf{F}(\mathbf{y}_e)\rangle}{\|\mathbf{V}\tilde{\mathbf{y}}_e - \mathbf{y}_e\|^2} \leq M[\mathbf{F}]$. Since $M[\mathbf{F}] < 0$,

$$
\begin{aligned}
\|\mathbf{V}\tilde{\mathbf{y}}_e - \mathbf{y}_e\|^2 &\leq \frac{1}{M[\mathbf{F}]} \langle \mathbf{V}\tilde{\mathbf{y}}_e - \mathbf{y}_e, \mathbf{p}\rangle \\
&\leq \left|\frac{1}{M[\mathbf{F}]}\right| \|\mathbf{V}\tilde{\mathbf{y}}_e - \mathbf{y}_e\| \, \|\mathbf{p}\| \\
&= \frac{-\|\mathbf{p}\|}{M[\mathbf{F}]} \|\mathbf{V}\tilde{\mathbf{y}}_e - \mathbf{y}_e\| \\
\|\mathbf{V}\tilde{\mathbf{y}}_e - \mathbf{y}_e\| &\leq \frac{-\|\mathbf{p}\|}{M[\mathbf{F}]}.
\end{aligned}
$$

■

Note that the bound given in (25) can be used to indicate the accuracy of the approximated equilibrium solution $\mathbf{V}\tilde{\mathbf{y}}_e$ from the reduced system (24), even though we do not know the exact value of $\mathbf{y}_e$. In addition, this bound guarantees the convergence of the approximate equilibrium, i.e. $\mathbf{V}\tilde{\mathbf{y}}_e \rightarrow \mathbf{y}_e$, as $\|\mathbf{p}\| \rightarrow 0$.

Corollary 4.3. *Suppose the nonlinear vector field* $\mathbf{F}$ *in the full-order system (15) is infinitesimally contracting. Then the nonlinear vector field of the POD reduced system (16) preserves the exponential stability of (15) and has a unique equilibrium* $\tilde{\mathbf{y}}_e^{POD}$*. If* $\mathbf{y}_e$ *is the unique equilibrium solution of (15), then* $\mathbf{y}_e$ *can be approximated by* $\mathbf{V}\tilde{\mathbf{y}}_e$ *with the error bound given in (25).*

Proof: This is a direct result from Lemma 4.1 and Proposition 4.2 when $\mathbf{W} = \mathbf{I}$.
■

While POD reduced system can be shown to be in the form of the reduce system (24), by setting $\mathbf{W} = \mathbf{I}$, DEIM reduced system cannot be rearranged in this form. Therefore, the POD reduced system preserves the contractivity of the vector field and other properties of the original full-order system as stated in Corollary 4.3, but POD-DEIM approach does not. The following corollary provides the condition that guarantees the contractivity as well as stability, of the resulting POD-DEIM reduced system.

Corollary 4.4. *Let* $\mathbf{F}$ *be the nonlinear vector field of the full-order system (15). Suppose* $\mathbf{F}$ *is infinitesimally contracting. The corresponding nonlinear vector field* $\widehat{\mathbf{F}}(\tilde{\mathbf{y}}) := \mathbf{V}^T \mathbb{P} \mathbf{F}(\mathbf{V}\tilde{\mathbf{y}})$ *of the POD-DEIM reduced system (22) is infinitesimally contracting if* $M[\mathbb{P}\mathbf{F}] < 0$*, where* $\mathbb{P} = \mathbf{U}(\mathbf{P}^T\mathbf{U})^{-1}\mathbf{P}^T$.

<u>Proof:</u> Consider the POD-DEIM reduced system (22) in the form $\dot{\tilde{\mathbf{y}}} = \widehat{\mathbf{F}}(\tilde{\mathbf{y}})$ where $\widehat{\mathbf{F}}(\tilde{\mathbf{y}}) := \mathbf{V}^T \mathbb{P} \mathbf{F}(\mathbf{V}\tilde{\mathbf{y}})$,

$$\begin{aligned} M[\widehat{\mathbf{F}}] &= \sup_{\hat{\mathbf{u}} \neq \hat{\mathbf{v}}} \frac{(\hat{\mathbf{u}} - \hat{\mathbf{v}})^T (\mathbf{V}^T \mathbb{P} \mathbf{F}(\mathbf{V}\hat{\mathbf{u}}) - \mathbf{V}^T \mathbb{P} \mathbf{F}(\mathbf{V}^T \hat{\mathbf{v}}))}{\|\hat{\mathbf{u}} - \hat{\mathbf{v}}\|^2} \\ &= \sup_{\hat{\mathbf{u}} \neq \hat{\mathbf{v}}} \frac{(\mathbf{V}\hat{\mathbf{u}} - \mathbf{V}\hat{\mathbf{v}})^T \mathbb{P} (\mathbf{F}(\mathbf{V}\hat{\mathbf{u}}) - \mathbf{F}(\mathbf{V}\hat{\mathbf{v}}))}{\|\mathbf{V}\hat{\mathbf{u}} - \mathbf{V}\hat{\mathbf{v}}\|^2} \\ &\leq M[\mathbb{P}\mathbf{F}]. \end{aligned}$$

That is, $M[\mathbb{P}\mathbf{F}] < 0$ implies $M[\widehat{\mathbf{F}}] < 0$. ∎

It is desirable to have a model reduction that can both preserve important properties of the original systems and maintain low complexity in computing projected nonlinear term. One possible model reduction formulation in the proposed general form (24) is given by

$$\dot{\tilde{\mathbf{y}}} = \mathbf{V}^T \mathbb{P} \mathbf{F}(\mathbb{P}^T \mathbf{V} \tilde{\mathbf{y}}), \qquad \tilde{\mathbf{y}}(0) = \mathbf{V}^T \mathbf{y}_0. \tag{26}$$

When compared with the form (24), the matrix $\mathbf{W}$ in (24) is defined as $\mathbf{W} = \mathbf{U}(\mathbf{P}^T\mathbf{U})^{-1}\mathbf{P}^T$. This is obtained a modification of the POD-DEIM reduced system by enforcing a *symmetric* structure of the form (24). Other specific formulations are also possible.

In practical implementation, the vector field $\mathbf{F}$ will be separated into linear and nonlinear terms in actual computation to maintain the accuracy as much as possible through the linear part. In particular, $\mathbf{F}$ will be written as the sum of two terms: $\mathbf{F}(\mathbf{y}) = \mathbf{A}\mathbf{y} + \mathbf{f}(\mathbf{y})$, where $\mathbf{A} \in \mathbb{R}^{n \times n}$ and $\mathbf{f}(\mathbf{y}) = \mathbf{F}(\mathbf{y}) - \mathbf{A}\mathbf{y}$.

The POD approach will be applied to the linear term $\mathbf{Ay}$ and reduced system of the form (27) will be used for the nonlinear term $\mathbf{f}(\mathbf{y})$, i.e.

$$\dot{\tilde{\mathbf{y}}} = \widetilde{\mathbf{A}}\tilde{\mathbf{y}} + \mathbf{V}^T\mathbb{P}\mathbf{f}(\mathbb{P}^T\mathbf{V}\tilde{\mathbf{y}}), \tag{27}$$

where $\widetilde{\mathbf{A}} = \mathbf{V}^T\mathbf{AV} \in \mathbb{R}^{k\times k}$ can be precomputed in advance. The contractivity results for (27) discussed earlier can still be obtained in the same way, because logarithmic Lipschitz constants possess the subadditivity property, i.e. $M[\mathbf{F}] = M[\mathbf{A}+\mathbf{f}] \leq M[\mathbf{A}] + M[\mathbf{f}]$, where $M[\mathbf{A}] = \mu(\mathbf{A})$ for constant matrix $\mathbf{A} \in \mathbb{R}^{n\times n}$.

Numerical tests in the next section illustrate the efficiency of the proposed model reduction form given in (27) on a nonlinear reaction-diffusion problem.

5. Numerical Results

Consider the nonlinear reaction-diffusion initial boundary value problem:

$$\frac{\partial u}{\partial t} = \epsilon\frac{\partial^2 u}{\partial x^2} + u - u^3, \quad x \in \Omega = [x_0, x_f], \qquad t \geq 0, \tag{28}$$

with initial condition $u(x, 0)$, and homogeneous boundary conditions $u(x_0, t) = 0, \quad u(x_f, t) = 0, \quad \text{for } t \geq 0$. Before presenting the numerical results, consider the contractivity of the discretized system, which can be written in the form $\frac{d\mathbf{u}}{dt} = \mathbf{Au} + \mathbf{f}(\mathbf{u})$, where $\mathbf{A} = \frac{\epsilon}{h^2}\text{tridiag}[1 \quad -2 \quad 1] \in \mathbb{R}^{n\times n}$ is a symmetric tri-diagonal matrix, $\mathbf{f}(\mathbf{u}) = -\mathbf{u}^3 + \mathbf{u}$ a componentwise function, and $h = \frac{x_f - x_0}{n+1}$ is the spatial stepsize with $n+1$ spatial subintervals (i.e. there are $n+2$ grid points including the two points on the boundaries). Notice that $M[\mathbf{A}] = -\frac{4\epsilon}{h^2}\sin^2(\pi h/2) = -\epsilon\pi^2 + \epsilon h^2\pi^4/12 + \mathcal{O}(h^4)$ and $M[\mathbf{f}] = \max_{\mathbf{u}\in\mathbb{R}^n}\mu[J_f(\mathbf{u})] = 1$, where the Jacobian of $\mathbf{f}$: $J_f(\mathbf{u}) = \text{diag}(-3u_1^2 + 1, -3u_2^2 + 1, \ldots, -3u_n^2 + 1) \in \mathbb{R}^{n\times n}$. The contractivity of $\mathbf{f}$ can be checked through the logarithmic Lipschitz constant $M[\mathbf{A}+\mathbf{f}] \leq M[\mathbf{A}] + M[\mathbf{f}]$, by the subadditivity property.

5.1. Numerical Test 1: Fixed parameter value

This section considers the problem given in (28) with initial condition $u(x, 0) = 0.25\sin(x)$, $\Omega = [0, 2\pi]$ and homogeneous boundary conditions $u(0, t) = 0, \quad u(2\pi, t) = 0, \quad \text{for } t \geq 0$.

In the following numerical tests, we use finite different discretizaion with spatial point $n = 600$ on $[0, 2\pi]$, time steps $= n_t = 700$ on $[0, 5]$ and $\epsilon = 0.01$. Figure 1 compares the solutions obtained from the original full-order system of the form (1) with the solutions from the two reduced models: (i) the POD reduced system (16), and (ii) the POD-DEIM reduced system that preserves the monotonicity (27). The results seem to be indistinguishable when the dimension $k = 30$ for POD reduced system and when $k = m = 30$ for POD-DEIM reduced system. Note that k is the dimension of POD basis and m is the dimension of basis used in DEIM approximation. The absolute error and the CPU time (normalized with the simulation time of the original full-order system) of these 2 reduced models (16) and (27) that preserve monotonicity are given in Table 1. Notice that, although the POD give more accurate approximations, the proposed model can accurately approximate the solution with much less simulation time, e.g. POD-DEIM reduce system with $k = 30$, $m = 30$ has CPU time reduced to $0.0024 \approx 1/400$ of the simulation time used for the original system, while CPU time for POD with $k = 30$ is only reduced to $0.4781 \approx 1/2$ of the time used in the original system.

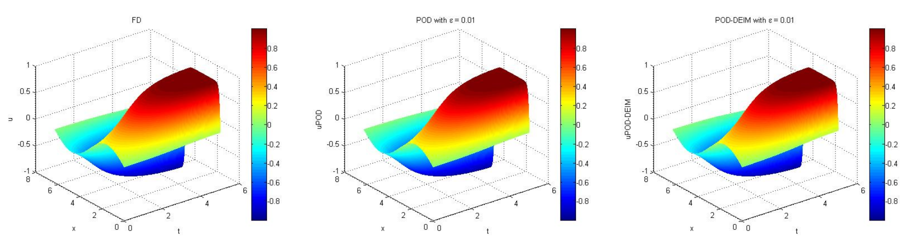

Figure 1: Solutions of (28) from the full-order system (1), the POD system (16) with $k = 30$, and the POD-DEIM system that preserves monotonicity (27) with $k = m = 30$.

5.2. Numerical Test 2: Varying parameter values

This section considers an application for the same nonlinear reaction-diffusion equation given in (28) with different initial conditions and using various different values of ϵ. The initial condition is $u(x, 0) = \sin(5\pi x)$, the homogeneous boundary conditions are $u(0, t) = 0, \quad u(1, t) = 0, \quad$ for $t \geq 0$. The finite differ-

POD basis (k)	Relative Error	Runtime (scaled)	DEIM (m) POD $k = 30$	Relative Error	Runtime (scaled)
Full: $n = 600$	-	1	Full: $n = 600$	-	1
$k = 10$	2.4601e-06	0.4433	$m = 10$	4.1170e-02	0.0021
$k = 20$	3.7046e-07	0.4569	$m = 20$	6.2412e-03	0.0022
$k = 30$	1.7271e-07	0.4781	$m = 30$	4.1483e-03	0.0024
$k = 40$	1.0819e-07	0.4896	$m = 40$	5.4461e-04	0.0029
$k = 50$	3.3184e-08	0.4931	$m = 50$	1.4553e-04	0.0031

Table 1: Runtime and relative error of the POD reduced system (left) the POD-DEIM reduced system with monotonicity preserved (right). Each runtime is normalized with the CPU time of the original full-order system (dimension $n = 600$).

ence discretization is used with spatial point $n = 1000$ on $[0, 1]$ and the number of time steps is $= n_t = 100$ on $[0, 2]$.

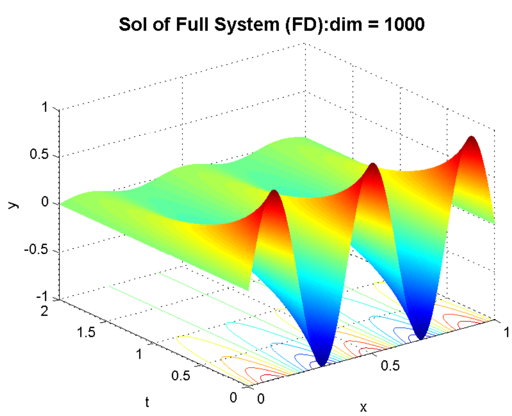

Figure 2: Solutions of (28) from the full-order system ($n = 1000$, $\epsilon = 0.01$)

The three plots in Figure 3 illustrate, respectively, the full-order solutions with the parameter values $\epsilon = 0.001$ and $\epsilon = 0.1$ and the singular values, which are corresponding to the POD basis of the solution snapshots from these two parameters.

The POD basis sets for projecting the solution and for the DEIM nonlinear

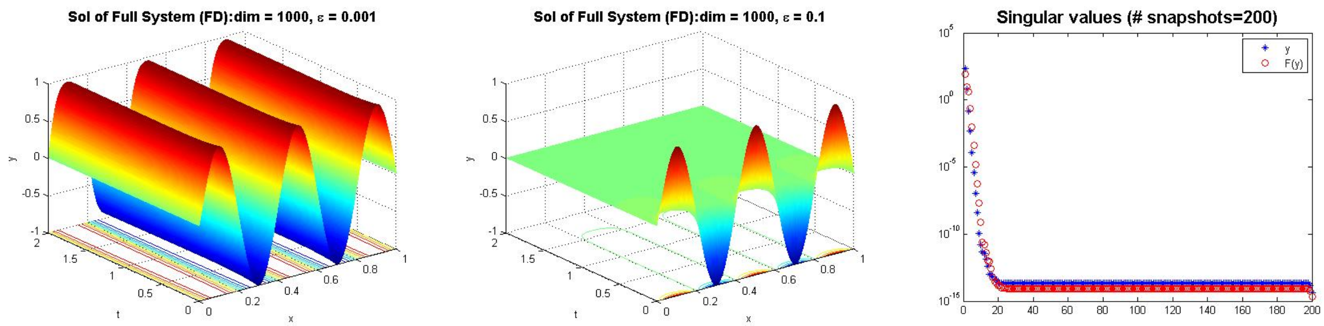

Figure 3: Solution Snapshots of (**??**) ($n = 1000$) with $\epsilon = 0.001$ and $\epsilon = 0.1$.

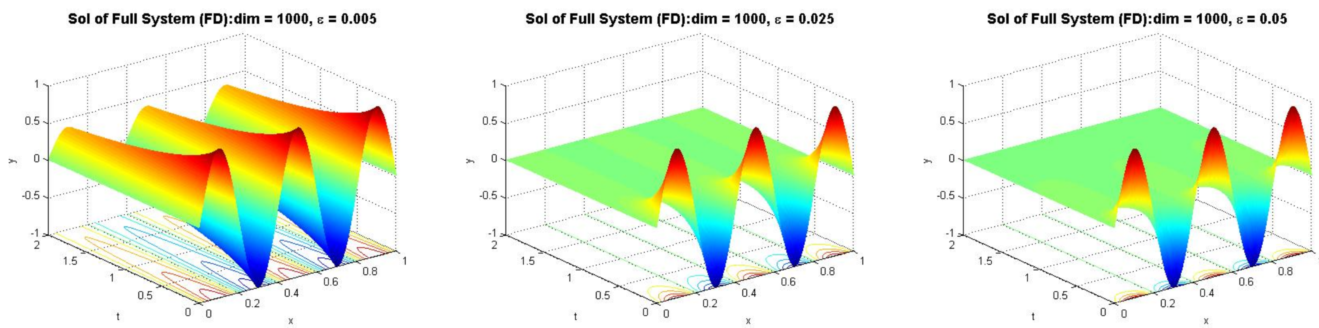

Figure 4: Solutions of (28) from the full-order system ($n = 1000$) with parameter $\epsilon = 0.0025, 0.005, 0.0250.05$.

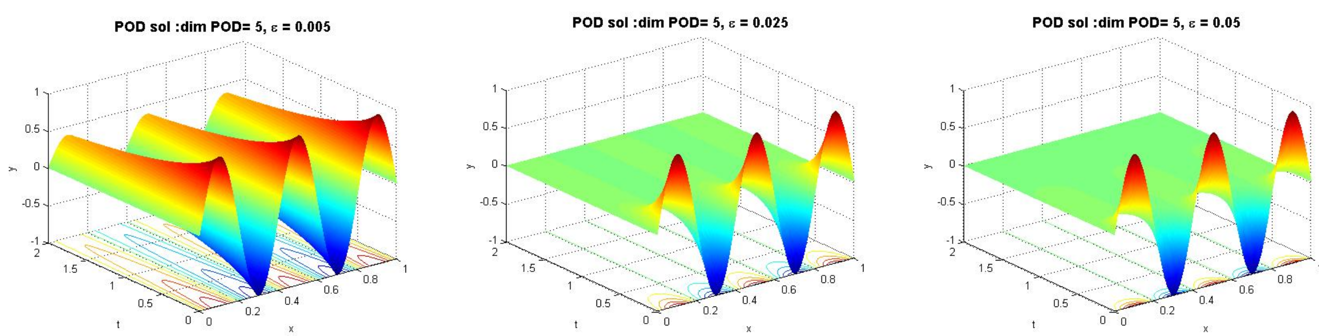

Figure 5: Solutions of (28) from the POD reduced system ($n = 1000$) with parameter $\epsilon = 0.0025, 0.005, 0.0250.05$.

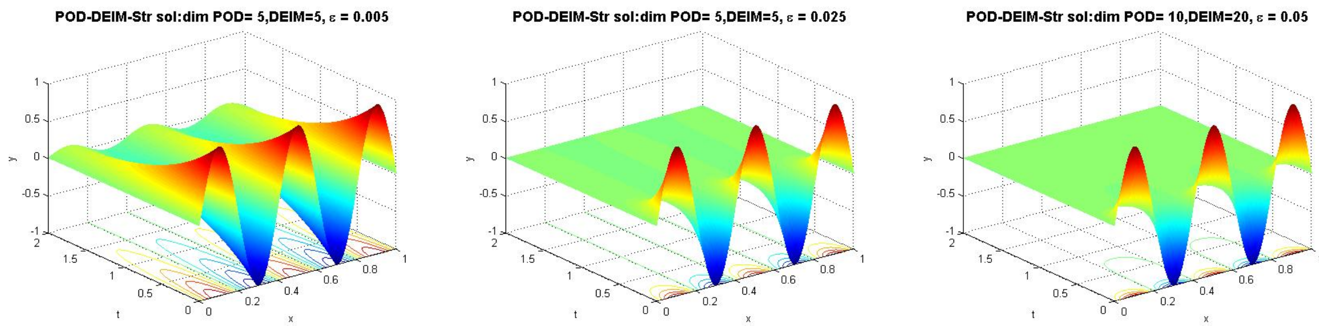

Figure 6: Solutions of (28) from the structure-preserving POD-DEIM reduced system ($n = 1000$) with parameter $\epsilon = 0.0025, 0.005, 0.0250.05$.

approximation are constructed from the solution snapshots shown in Figures 4, which are corresponding to 2 parameter values $\epsilon = 0.001$ and $\epsilon = 0.1$. This numerical test considers the solutions corresponding to different parameter values, i.e. $\epsilon = 0.0025, 0.005, 0.0250.05$. The resulting solutions from the full-order systems are shown in Figures 4. The solutions from the POD reduced system in Figure 5 shown to accurately capture the dynamics of the original systems although the basis sets employ snapshots from different parameter values. Similar observations can be obtained from the solutions from the structure-preserving POD-DEIM reduced system in Figure 6. Note however, that the simulation time of the POD reduced systems is roughly a factor of $1/30$ less than the simulation time used for the original full-order system while the structure-preserving POD-DEIM reduced system can further the simulation time approximately to a factor of $1/200$.

6. Conclusion

This work proposes a general form of nonlinear reduced-order modeling that preserves the contractivity property of the original systems, which can be used for guaranteeing the existence, uniqueness of the solution, and stability of the dynamical system. A specific formulation presented and used in this work is based on POD and DEIM approaches with some modification. Other specific forms are still possible and left for future research. The numerical tests on the nonlinear reaction diffusion problem demonstrate that, while preserving negative monotonicity, the proposed model can accurately approximate the solutions with much less simulation time.

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