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Model order reduction for the cross-diffusive Brusselator Equation

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Abstract

The cross-diffusive Brusselator equation is a reaction-diffusive system that models complex chemical and biological process with both self-diffusion and cross-diffusion effects. These equations exhibit rich spatiotemporal dynamics, including Turing patterns and instability-driven pattern formations. Despite its significance, the computational cost of solving high-dimensional discretized versions of the cross-diffusive Brusselator equation can be prohibitive, particularly in parameter-dependent or long-time simulations. This study presents a model order reduction (MOR) framework tailored to the Brusselator equation, leveraging Proper Orthogonal Decomposition (POD) combined with Galerkin projection along with the Discrete Empirical Interpolation Method (DEIM) and the Dynamic Mode Decomposition Method (DMD) to efficiently approximate nonlinear dynamics. The reduced models are constructed to preserve key features of the original system, including stability and accuracy, while achieving substantial computational savings. Numerical experiments validate the proposed approach, demonstrating its effectiveness in capturing the essential dynamics of the Brusselator equation under various parameter settings. These findings provide a robust pathway for efficient simulation and analysis of reaction-diffusion systems in scientific and engineering applications.

Keywords: Model Order Reduction; Cross-Diffusive Brusselator Equation; Proper Orthogonal Decomposition; Discrete Empirical Interpolation Method; Dynamic Mode Decomposition; Reaction-Diffusion Systems; Computational Efficiency

1. Introduction

Reaction-diffusion systems are central to modeling various physical, chemical, and biological processes, from chemical oscillations to pattern formation in biological systems. Among these, the Brusselator equation stands out as a paradigmatic model for studying oscillatory chemical reactions and nonlinear dynamics [12]. Originally introduced to capture the essence of autocatalytic reactions, the Brusselator has become a benchmark system for exploring spatiotemporal phenomena and the onset of complex patterns under varying parameter regimes. However, classical Brusselator models assume that the species diffuse independently of each other, neglecting interactions between the diffusion process of different species.

In many real-world applications, such as in ecological models, chemical process, or biological systems, the diffusion of one species may be influenced by the concentration gradients of others. This interaction is captured by cross-diffusion, where the diffusion of each species is coupled with the concentration gradient of the other species. The cross-diffusive Brusselator equation extends the classical model by incorporating these cross-diffusion effects, providing a more realistic representation of coupled reaction-diffusion systems. Despite its theoretical and practical significance, solving the high-dimensional discretized cross-diffusive Brusselator equation remains computationally expensive, particularly when dealing with large spatial domains, fine resolutions, or parametric studies. These challenges are exacerbated in scenarios requiring real-time simulations or repeated evaluations, such as optimization, uncertainty quantification, or control problems.

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Model Order Reduction (MOR) techniques offer a powerful solution to the computational challenges posed by high-dimensional systems [6, 8]. These methods construct low-dimensional surrogate models that approximate the full-order system with minimal loss of accuracy, enabling significant acceleration of simulations while maintaining the essential dynamics of the system. Techniques such as Proper Orthogonal Decomposition (POD) [7, 8, 9], Discrete Empirical Interpolation Method (DEIM) [2, 4, 5, 11], and Dynamic Mode Decomposition (DMD) [1] have proven particularly effective in addressing the nonlinearities and stiffness inherent in reaction-diffusion equations. POD is widely used to extract the dominant modes of a system from time-dependent data, making it an efficient method for model reduction. DEIM complements POD by approximating the nonlinear terms in a reduced space, thus helping to reduce the computational burden associated with nonlinear dynamics. Additionally, DMD provides a data-driven approach to capture the dynamic behavior of the system by identifying the dominant temporal and spatial modes, making it especially useful for systems where explicit equations may not be available. Together, these methods offer complementary strategies for tackling the challenges of reducing the complexity of reaction-diffusion systems while preserving their key characteristics.

In this paper, we propose a tailored MOR framework for the cross-diffusive Brusselator equation, leveraging these techniques to construct efficient and reliable reduced models. Our approach ensures the preservation of critical features, such as stability and pattern formation dynamics, while achieving substantial computational gains. Through a series of numerical experiments, we demonstrate the efficacy of the proposed method across different parameter regimes, highlighting its potential for broader applications in reaction-diffusion systems.

We consider the following system, namely cross-diffusive Brusselator equation

$$\begin{aligned} u_t &= d_{11} \Delta u + d_{12} \Delta v + f(u, v) \\ v_t &= d_{21} \Delta u + d_{22} \Delta v + g(u, v) \end{aligned}$$

where Δu and Δv represent the Laplacian operators; $d_{11}, d_{12}, d_{21}, d_{22}$ are diffusion coefficients for species u and v . $f(u, v)$ and $g(u, v)$ are the nonlinear reaction terms: $f(u, v) = -(\beta + 1)u + u^2v + \alpha$ and $g(u, v) = \beta u - u^2v$.

2. Full order model

This section outlines the DG discretization of the semi-discrete (continuous in time) form of the cross-diffusive Brusselator equation with homogeneous Neumann (zero-flux) boundary conditions [3]. We begin by describing the classical (continuous) weak solution of the equation, which satisfies the variational formulation for $t \in (0, T]$,

$$\begin{aligned} (u_t, w_1) + a(d_{11}; u, w_1) + a(d_{12}; v, w_1) - (f(u, v), w_1) &= 0, \forall w_1, \\ (v_t, w_2) + a(d_{21}; u, w_2) + a(d_{22}; v, w_2) - (g(u, v), w_2) &= 0, \forall w_2 \end{aligned}$$

With the initial conditions satisfying

$$(u(0), w_1) = (u_0, w_1), (v(0), w_2) = (v_0, w_2).$$

The expression $(\cdot, \cdot) := (\cdot, \cdot)_\Omega$ represents the L_2 inner product over the domain Ω , where the inner product is defined as the integral of the product of two functions over Ω . The test functions w_1 and w_2 are used to approximate the solution in the weak formulation. Additionally, the bilinear form $a(d; u, w) = (d \nabla u, \nabla w)_\Omega$ refers to the classical bilinear form.

Let ϵ_h be the disjoint partition of the domain Ω with disjoint elements (triangles) $\{E_i\}_{i=1}^{N_{el}} \in \epsilon_h$, where N_{el} denotes the number of elements in the partition. On ϵ_h , we set the discrete solution and test function space is defined as:

$D_k = D_k(\epsilon_h) := \{w \in L^2(\Omega): w_E \in P_k(E) \forall E \in \epsilon_h\}$ where $P_k(E)$ is the space of polynomials of degree at most k defined on each element $E \in \epsilon_h$.

Next, by multiplying equation by the test functions w_1 and w_2 and applying Green's theorem to each element of the mesh, we obtain the semi-discrete variational formulation, where for all $t \in (0, T]$, we seek $u_{h(t)}$ and $v_{h(t)}$ in D_k that satisfy the following system:

$$\left(\frac{\partial u_h}{\partial t}, w_1\right) + a_h(d_{11}; u_h, w_1) + a_h(d_{12}; v_h, w_1) - (f(u_h, v_h), w_1) = 0, \forall w_1 \in D_k,$$

$$\left(\frac{\partial v_h}{\partial t}, w_2\right) + a_h(d_{21}; v_h, w_2) + a_h(d_{22}; v_h, w_2) - (g(u_h, v_h), w_2) = 0, \forall w_2 \in D_k,$$

here the SIPG bilinear form $a_h(d; u, w)$ is expressed as follows:

$$a_h(d; u, w) = \int_{\Omega} d \nabla u \cdot \nabla w \, dx + \sum_{\partial\Omega} (\text{boundary terms})$$

This bilinear form involves the integral of the product of the gradients of the solution u and test function w over the domain Ω , with an additional contribution from the boundary terms, which are handled using the Symmetric Interior Penalty Galerkin (SIPG) method [10]. The boundary terms are designed to ensure stability and conformity at the domain boundaries, particularly when dealing with non-matching meshes or discontinuities at the element interfaces.

The SIPG method is widely used in solving PDEs in finite element analysis, especially for reaction-diffusion equations and cross-diffusion systems, as it allows for higher-order accuracy and flexibility when dealing with complex boundary conditions and discontinuous coefficients.

By introducing the degrees of freedom $N := N_{loc} \times N_{el}$, where N_{loc} is the local dimension of each element, dependent on the polynomial order k , the semi-discrete DG solutions of equation can be written as:

$$u_h(t) = \sum_{i=1}^N u_{i(t)} \phi_i, v_h(t) = \sum_{i=1}^N v_{i(t)} \phi_i.$$

Here, $u(t) = (u_{1(t)}, \dots, u_{N(t)})^T$ and $v(t) = (v_{1(t)}, \dots, v_{N(t)})^T$ represents vectors of time-dependent unknown coefficients for u_h and v_h , respectively, and $\phi = (\phi_1, \dots, \phi_N)^T$ is the vector of basis functions. Substituting these expressions into the scheme (6) and choosing $w_1 = w_2 = \phi_i$ for $i = 1, \dots, N$, we obtain a system of $2 \times N$ dimensional ordinary differential equations (ODEs) for the unknown vectors u and v as

$$M u_t + S_u u + S_{uv} v - F(u, v) = 0,$$

$$M v_t + S_v v + S_{vu} u - G(u, v) = 0.$$

Here $M, S_u, S_v, S_{uv}, S_{vu} \in R^{N \times N}$ denote the mass matrix and the stiffness matrices for the diffusion and cross-diffusion terms, while the remaining terms represent vectors in R^N associated with the unknown coefficients u and v .

This obtained semi-discretized form is discretized in time by implicit Euler method. We split the time interval $[0, T]$ into J equally-length subintervals $(t_{k-1}, t_k]$ with $0 = t_0 < t_1 < \dots < t_J = T$ with the uniform step-size $\Delta t = t_k - t_{k-1}, k = 1, 2, \dots, J$. Using the implicit Euler scheme, we replace the time derivatives in the semi-discrete form with finite differences

$$(M + \Delta t \cdot S_u) u^{k+1} + \Delta t \cdot S_{uv} v^{k+1} - M u^k - \Delta t \cdot F(u^{k+1}, v^{k+1}) = 0,$$

$$(M + \Delta t \cdot S_v) v^{k+1} + \Delta t \cdot S_{vu} u^{k+1} - M v^k - \Delta t \cdot G(u^{k+1}, v^{k+1}) = 0.$$

This obtained fully-discrete system of nonlinear equations is solved by Newton's method on each time interval $(t_{k-1}, t_k]$ with $0 = t_0 < t_1 < \dots < t_J = T$.

3. Reduced order model

The cross-diffusive Brusselator equation, a classical reaction-diffusion model, is widely used to study oscillatory chemical reactions and complex spatial-temporal patterns. While its theoretical importance is well-established, solving high-dimensional discretized versions of this model can become computationally expensive, especially for real-time

simulations, parametric studies, or optimization tasks. This motivates the use of model reduction techniques to simplify the problem while retaining its essential dynamics.

Several reduction methods have proven effective for reaction-diffusion systems like the Brusselator, including POD, DEIM, and DMD. Each of these approaches offers unique advantages in capturing the dominant features of the system. POD reduces the complexity of a system by constructing a low-dimensional subspace from high-fidelity simulation data, typically using snapshot-based analysis. For the Brusselator Equation, POD identifies the most energy-dominant modes of the reaction-diffusion dynamics, enabling efficient approximation of the state variables with minimal loss of accuracy. DEIM is often combined with POD to handle nonlinearities efficiently. In the Brusselator model, where nonlinear reaction terms play a crucial role in generating complex behaviors, DEIM approximates these terms in a reduced-dimensional space, significantly accelerating computations without compromising precision. DMD focuses on extracting spatiotemporal modes from data, offering a purely data-driven approach to model reduction. For the Brusselator equation, DMD can capture dominant oscillatory patterns and uncover coherent structures, making it particularly useful for analyzing dynamic behaviors and predicting future states.

These methods, individually or in combination, provide a robust framework for reducing the computational burden of solving the Brusselator equation. In this study, we explore their application to the Brusselator model, evaluating their effectiveness in preserving key features such as pattern formation and oscillatory dynamics, while achieving significant computational gains. The insights derived can extend to other reaction-diffusion systems, broadening the utility of these reduction techniques in scientific and engineering problems.

The reduced-order model (ROM) for our equation, with a dimension $k \ll N$, is constructed by approximating the full-order model (FOM) solutions $u(t)$ and $v(t)$ within a subspace spanned by a set of M-orthogonal basis functions $\{\psi_{u,i}\}_{i=1}^k$ and $\{\psi_{v,i}\}_{i=1}^k$ where k represents the reduced dimension in R^N . The ROM solutions are then obtained by projecting the system onto this subspace. The approximate ROM solutions take the form:

$$u(t) \approx \sum_{i=1}^k \tilde{u}_i(t)\psi_{u,i}, \quad v(t) \approx \sum_{i=1}^k \tilde{v}_i(t)\psi_{v,i}$$

where $\tilde{u}(t) = (\tilde{u}_1(t), \dots, \tilde{u}_k(t))^T$ and $\tilde{v}(t) = (\tilde{v}_1(t), \dots, \tilde{v}_k(t))^T$ are the coefficients vectors for the ROM solutions. The reduced basis functions $\{\psi_{u,i}\}$ and $\{\psi_{v,i}\}$ are in the form of linear combination of the DG basis functions

$$\psi_{u,i} \approx \sum_{j=1}^N \Psi_{u,j,i} \phi_j(x) = \phi \Psi_u, \quad \psi_{v,i} \approx \sum_{j=1}^N \Psi_{v,j,i} \phi_j(x) = \phi \Psi_v,$$

where the coefficient vectors of the reduced basis function $\psi_{u,i}$ and $\psi_{v,i}$ are in the columns of the matrices $\Psi_u = [\psi_{u,,1}, \dots, \psi_{u,,k}] \in R^{N \times k}$ and $\Psi_v = [\psi_{v,,1}, \dots, \psi_{v,,k}] \in R^{N \times k}$.

The M-orthogonal reduced basis functions $\psi_{u,i}$ and $\psi_{v,i}$ for $i=1,2,\dots,k$, are derived using the POD method [9]. This process starts by constructing snapshot matrices $U = [\mathbf{u}^1, \dots, \mathbf{u}^J]$ and $V = [\mathbf{v}^1, \dots, \mathbf{v}^J] \in R^{N \times J}$, where each column represents the coefficient vector corresponding to the discrete solutions $\{u^i\}_{i=1}^J$ and $\{v^i\}_{i=1}^J$ of the full-order model (FOM) for equation (25) at specific time instances Here, $u_i \approx u(t_i)$ and $v_i \approx v(t_i)$.

For $w \in \{u, v\}$, the M-orthogonal reduced basis functions $\{\psi_{w,i}\}_{i=1}^k$ are obtained by solving an optimization problem that minimizes the error between the original snapshot data and its projection onto a k-dimensional subspace in the M-orthogonal sense.

$$\min_{\psi_{w,1}, \dots, \psi_{w,k}} \frac{1}{J} \sum_{j=1}^J \left\| w^j - \sum_{i=1}^k (w^j, \psi_{w,i})_{L^2(\Omega)} \psi_{w,i} \right\|_{L^2(\Omega)}^2$$

subjected to $(\psi_{w,i}, \psi_{w,j})_{L^2(\Omega)} = \Psi_{w,,i}^T M \Psi_{w,,j} = \delta_{ij}, 1 \leq i, j \leq k$, with kronecker delta δ_{ij} .

Using the above equations, we obtain $\mathbf{u} = \Psi_u \tilde{\mathbf{u}}, \mathbf{v} = \Psi_v \tilde{\mathbf{v}}$.

When we substitute this into the FOM, we obtain the following ROM:

$$\mathbf{M}\tilde{\mathbf{u}}_t + \mathbf{S}_u\tilde{\mathbf{u}} + \mathbf{S}_{uv}\tilde{\mathbf{v}} - F(\Psi_u\tilde{\mathbf{u}}, \Psi_u\tilde{\mathbf{v}}) = 0,$$

$$\mathbf{M}\tilde{\mathbf{v}}_t + \mathbf{S}_v\tilde{\mathbf{v}} + \mathbf{S}_{vu}\tilde{\mathbf{u}} - G(\Psi_v\tilde{\mathbf{u}}, \Psi_v\tilde{\mathbf{v}}) = 0,$$

with the reduced matrices $\mathbf{M} = \Psi_u^T \mathbf{M} \Psi_u$, $\mathbf{S}_u = \Psi_u^T \mathbf{S} \Psi_u$, $\mathbf{S}_{uv} = \Psi_u^T \mathbf{S} \Psi_v$, $\mathbf{S}_v = \Psi_v^T \mathbf{S} \Psi_v$, $\mathbf{S}_{vu} = \Psi_v^T \mathbf{S} \Psi_u$.

Although the dimension of this reduced system is small, the computation of the nonlinear terms still relies on the full-system dimension. To address this, we employ the DEIM [11] to approximate the nonlinear functions F and G using a lower-dimensional subspace. This subspace is constructed from a set of snapshots of the nonlinear function values in a similar way with POD [6].

As an alternative to DEIM, DMD, data-driven post-processing technique used to extract dynamic and spatially relevant information from numerical or experimental datasets, is also used. This method is particularly useful for analyzing complex systems without needing explicit knowledge of the governing equations. The DMD algorithm identifies eigenvalues, eigenmodes, and spatial structures associated with each mode, offering insights into the underlying dynamics [1]. In this context, we compare the effectiveness of DMD with the DEIM for approximating nonlinear terms in state equations. While both methods serve to reduce the computational complexity, DMD focuses on capturing dynamic behavior and system modes from data, while DEIM optimizes the approximation of nonlinear functions in reduced-order models, providing complementary approaches to model reduction and system analysis.

4. Numerical results

We consider the cross-diffusive Brusselator model on the spatial time domain $Q = \Omega \times [0, T] = [0, 20]^2 \times [0, 100]$ with the following spatial and temporal mesh sizes $\Delta x = \Delta y = 0.3125$, $\Delta t = 0.05$. For the time discretization, we use implicit Euler method.

We consider zero flux boundary conditions with the following initial conditions

$$u(x, y, 0) = 5.8 + \frac{1}{3} \cdot rand(x), \quad v(x, y, 0) = 0.13 + \frac{1}{10} \cdot rand(x).$$

The parameters are chosen as

$$(d_{11}, d_{12}, d_{21}, d_{22}, \alpha, \beta) = (0.4, 32, 0.02, 2, 6, 1).$$

For $d_{12} = 24$, the resulting patterns is spots; for $d_{12} = 32$, it is labyrinthic-like patterns.

The POD basis functions are determined according to the relative information content (RIC)

$$\epsilon(k) = \frac{\sum_{i=1}^k \sigma_i^2}{\sum_{i=1}^s \sigma_i^2}$$

which represents the energy captured by the first k POD modes over all s POD modes, s is the rank of snapshot matrix, and σ_i is the corresponding singular value of i -th mode. In the following results, k is chosen as $\min_k \epsilon(k) \geq 99.99\%$.

In the following results, we use 26 POD, 90 DEIM, and 90 DMD basis functions. In Figure 1, the FOM solutions for the cross-diffusive Brusselator equation are shown. In Figure 2, the decay of the singular values related to \mathbf{u} and \mathbf{v} are given. ROM solutions and the corresponding errors are given in Figure 3 and Figure 4, resp. In Figure 5 and Table 1, we also see relative L_2 errors between FOM and ROMs. In these graphs, it is evident that the reduced models successfully capture key dynamics, such as Turing patterns and other spatiotemporal structures, when compared to the full system solution. The POD-based reduced model achieves a high level of accuracy with significantly fewer degrees of freedom, and as the number of POD modes increases, the reduced model solution converges more closely to the full solution. Even with a relatively low number of modes, the reduced model effectively captures the essential dynamics of the system. In terms of computational efficiency, the reduced models show a considerable reduction in simulation time, highlighting their advantage in long-time simulations or parameter-dependent studies. These results clearly demonstrate how POD, DEIM, and DMD methods can be effectively used to solve complex reaction-diffusion systems like the Brusselator, while preserving the key dynamic behaviors and significantly reducing computational costs.

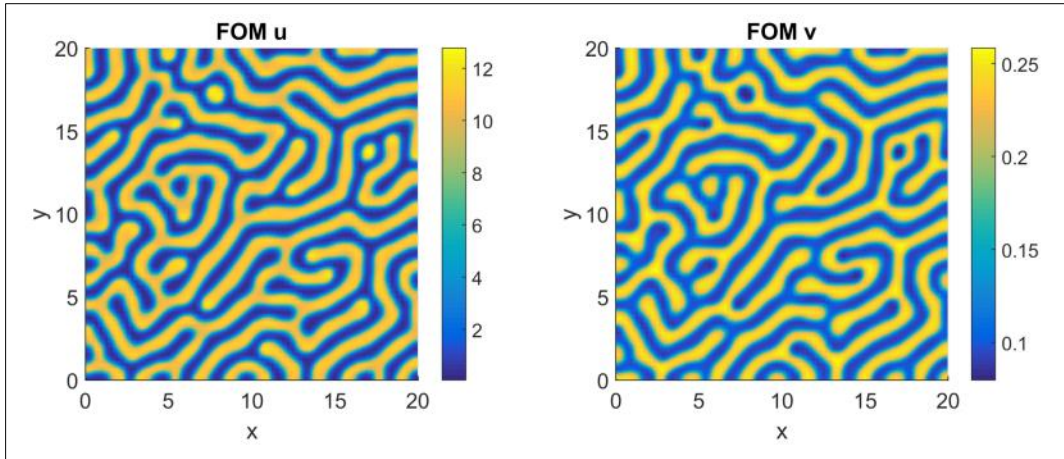


Figure 1 FOM solutions for the component u (left), v(right)

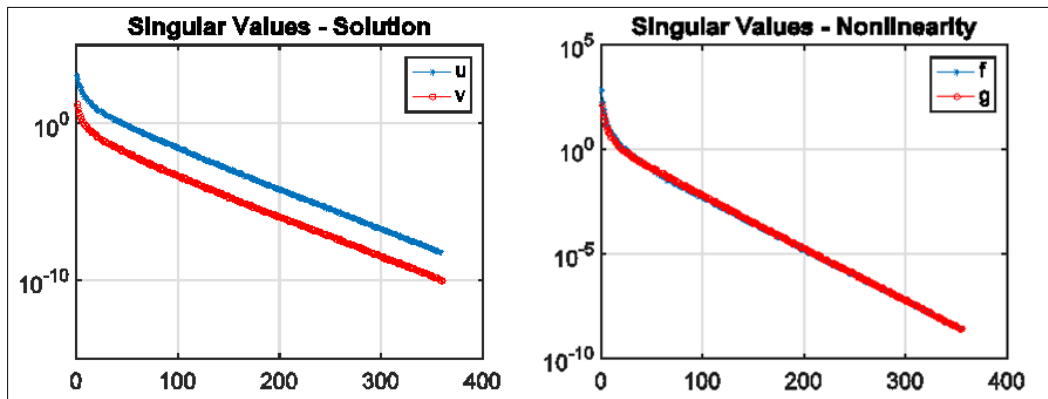


Figure 2 Decay of the singular values for u, v (left) and the nonlinearity f, g (right)

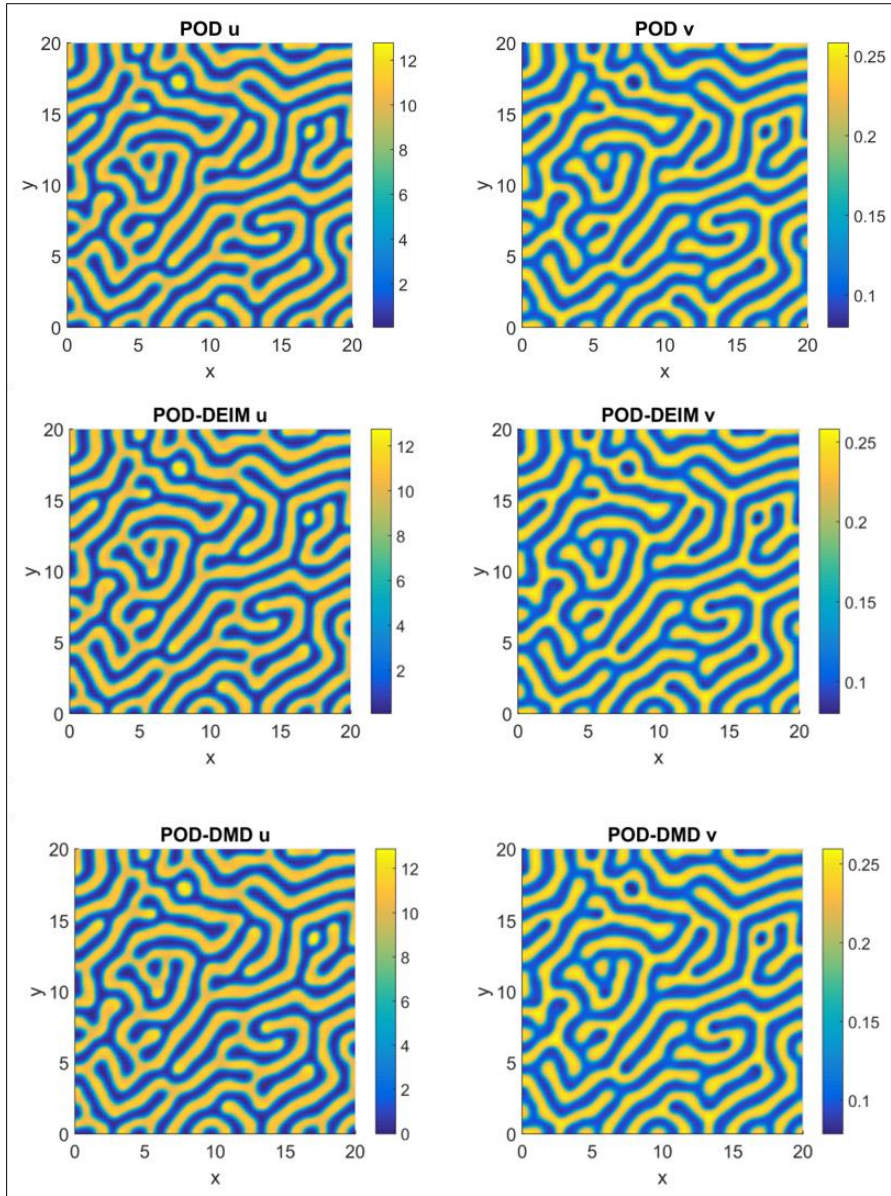


Figure 3 POD (top), POD-DEIM (middle), POD-DMD (bottom) solutions for the state components u_1 (left), u_2 (right)

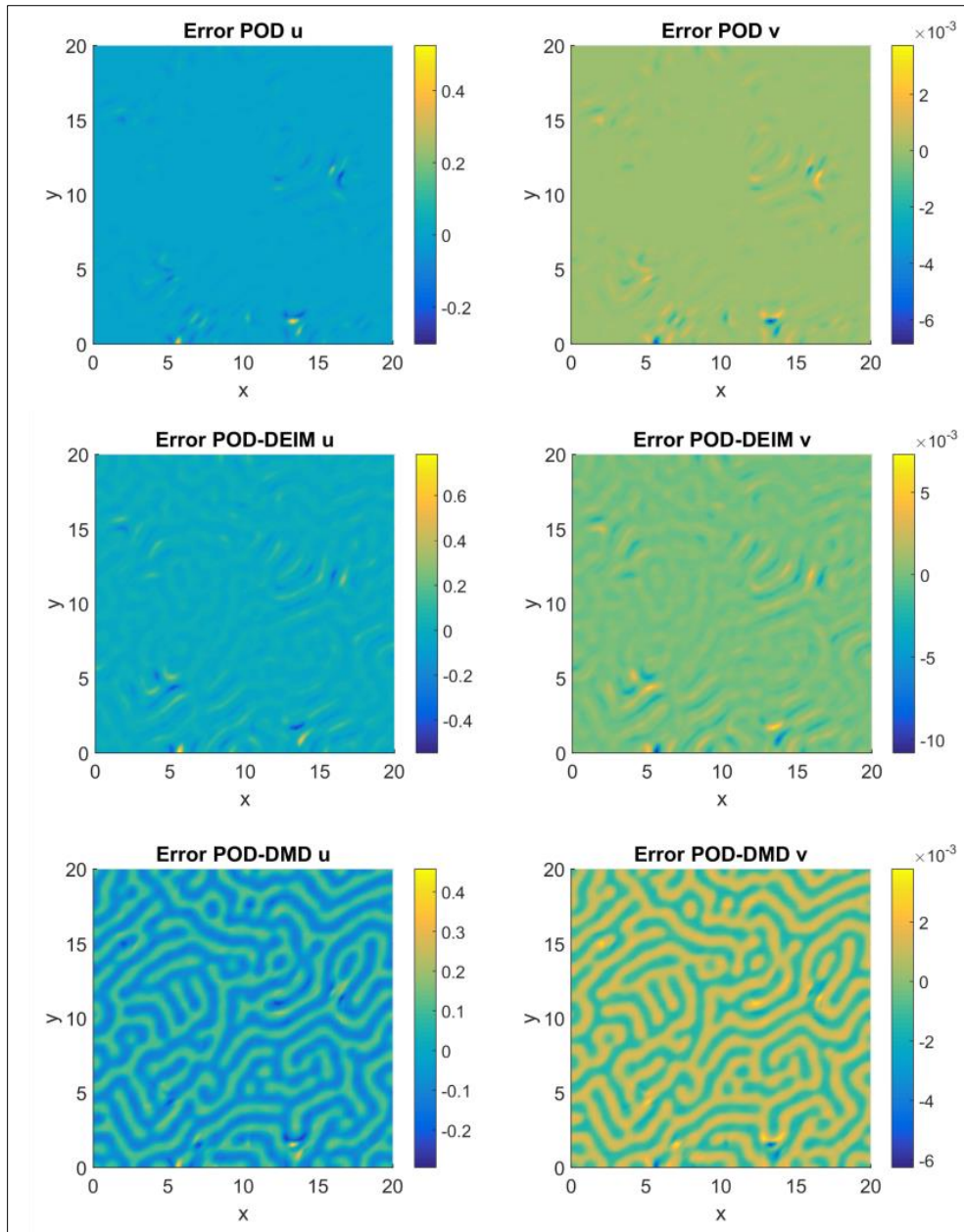


Figure 4 POD (top), POD-DEIM (middle), POD-DMD (bottom) errors for the state components u_1 (left), u_2 (right)

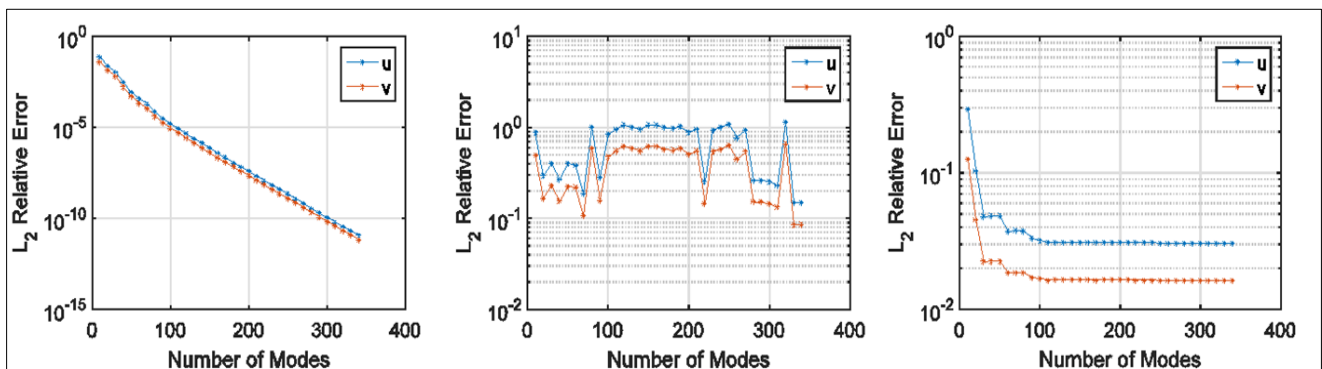


Figure 5 Relative L_2 errors with increasing number of modes: POD(left), POD-DEIM(right), POD-DMD(bottom)

Table 1 Results with POD, POD-DEIM and POD-DMD (from top to bottom)

	Relative L_2 Error u_1	Relative L_2 Error u_2	Speed-up
POD	$1.62e - 02$	$9.18e - 03$	3.30
POD-DEIM	$2.82e - 01$	$1.60e - 01$	15.67
POD-DMD	$3.32e - 02$	$1.71e - 02$	288

5. Conclusion

For nonlinear partial differential equations, using only POD as a model order reduction technique is not always sufficient in terms of computational efficiency. For approximating nonlinearities in a reduced-order model, DEIM is more effective, as it directly addresses the reduction of nonlinear terms. DMD, on the other hand, is useful for capturing the underlying dynamics and extracting dominant modes of the system, making it more suitable for dynamic analysis and prediction. Combining both methods could potentially leverage the strengths of each, with DEIM handling the nonlinear terms and DMD uncovering the system's dynamic behavior. Besides, DMD is faster than DEIM.

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