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Reduced Order Modelling of Shigesada-Kawasaki-Teramoto Cross-Diffusion Systems

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Abstract

Shigesada-Kawasaki-Teramoto (SKT) is the most known equation in population ecology for nonlinear cross-diffusion systems. The full order model (FOM) of the SKT system is constructed using symmetric interior penalty discontinuous Galerkin method (SIPG) in space and the semi-implicit Euler method in time. The reduced order models (ROMs) are solved using proper orthogonal decomposition (POD) Galerkin projection. Discrete empirical interpolation method (DEIM) is used to solve the nonlinearities of the SKT system. Numerical simulations show the accuracy and efficiency of the POD and POD-DEIM reduced solutions for the SKT system.

1. Introduction

The nonlinear cross-diffusion systems has a general form which is given by $z=(z_1,...,z_M):\Omega\times[0,T)\to\mathbb{R}^M$ such that

$$\begin{aligned}\frac{\partial \mathbf{z}}{\partial t} &= \Delta\beta(\mathbf{z})+f(\mathbf{z}) \quad \text{in} \quad \Omega\times([0,T] \\ \frac{\partial \beta(\mathbf{z})}{\partial n} &= 0 \quad \text{on} \quad \partial\Omega\times(0,T) \\ \mathbf{z}(\cdot,0) &= \mathbf{z}^0 \quad \text{in} \quad \Omega,\end{aligned} \tag{1.1}$$

where $\Omega\subset\mathbb{R}^d;(d=1,2)$ is a bounded domain, $\partial\Omega$ is a smooth boundary, T is a positive constant, $z^0=(z_1^0,...,z_M^0):\Omega\to\mathbb{R}^M$ are population densities, $\beta=(\beta_1,...,\beta_M)$, $f=(f_1,...,f_M):\mathbb{R}^M\to\mathbb{R}^M$ are nonlinear functions of population densities, and n is the unit outward normal vector to the boundary $\partial\Omega$ [1].
The most known and popular nonlinear cross-diffusion system is the Shigeseda-Kawasaki-Teramato (SKT) equation with Lotka-Volterra kinetics [2] in population ecology. The SKT system represents the spatial and temporal behavior of two species under population pressure due to intra and interspecific interference. The interaction of two species may cause different diffusion rates. This leads to destabilization of the constant steady-state and occurs a pattern formation like labyrinth, spot and stripe. The SKT system with Lotka-Volterra kinetics is defined as [3]

$$\frac{\partial z_1}{\partial t} = \Delta\underbrace{(a_1+b_1z_1+c_1z_2)z_1}_{\beta_1}+\underbrace{\Gamma(\mu_1-\gamma_{11}z_1-\gamma_{12}z_2)z_1}_{f_1}, \tag{1.2}$$

$$\frac{\partial z_2}{\partial t} = \Delta\underbrace{(a_2+b_2z_2+c_2z_1)z_1}_{\beta_2}+\underbrace{\Gamma(\mu_2-\gamma_{21}z_1-\gamma_{22}z_2)z_2}_{f_2} \tag{1.3}$$

where β_1,β_2 are the nonlinear cross-diffusion and f_1,f_2 are the Lotka-Volterra kinetics, and a_i, b_i, c_i, $\gamma_{ij}(i,j=1,2)$ are nonnegative constants. The constants μ_i denote the intrinsic growth rates, γ_{ii} the intraspecific competition coefficients, and $\gamma_{ij},(i\neq j)$ the interspecific

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competition rates. The i^{th} species keeps away from high-density areas of the j^{th} species due to cross-diffusion terms. The parameter Γ represents the relative strength of the reaction terms. SKT systems are not a simple nonlinear problem when it comes to dealing with the cross-diffusivities. Therefore, it is more useful fo the analysis of SKT systems to remove the cross-diffsuion component. Murakawa [1, 4] proposed an approximation to the SKT system (1.2) by a semilinear reaction-diffusion system. In this approximation, the system has a simple reaction and linear diffusion terms. Nonlinear problems are difficult to solve compared to semilinear problems. Various methods can be considered for discretizing semilinear systems, such as the finite element approximation [5], the finite difference method [6], and the finite volume approximation [7].
In this paper, symmetric interior penalty discontinuous Galerkin finite elements (SIPG) method [8] for spatial discretization and semi-implicit Euler method for temporal discretization [1, 3, 9] are considered. The SIPG approximation uses discontinuous polynomials and captures singularities locally. Even though fully implicit methods provide better accuracy and stability, they are not easy to implement when dealing with semilinear reaction-diffusion systems. The semi-implicit Euler method is easy to implement and is a stable numerical method. Recently, model order reduction techniques are developed for the dimension reduction of large dynamic systems in engineering and science. The main idea of reduced order modelling is to construct basis functions in a low-dimensional reduced space and then project the full order model equation onto the reduced space to obtain a reduced order system. The most known and most commonly used technique is proper orthogonal decomposition (POD) [10, 11]. In POD method, the Galerkin projection is used to approximate reduced solutions. POD is a useful method for linear problems, but for nonlinear problems, the dimension of the solutions of the reduced order model (ROM) has the same dimension as the solutions of the full order model (FOM) [12]. To reduce the computational cost of the nonlinear terms in the reduced order model, some methods have been developed. The empirical interpolation method(EIM) [13] and the discrete empirical interpolation method(DEIM) [14] are the most commonly used methods. The DEIM method is introduced for nonlinear functions. The nonlinear kinetics depends on single variables in the finite difference method while it depends on the mesh and the degree of the polynomial in the finite element methods. Therefore, the POD-DEIM is developed for efficiency [15, 16]. The reduced basis functions in POD-DEIM are computed in the offline phase by applying singular value decomposition (SVD) to large snapshot matrices. Randomized singular value decomposition (rSVD) [17, 18] is used as a fast and accurate method. By using rSVD in the offline phase, the computational cost is reduced. This paper is divided into the following sections: In Section 2, the full discrete solution of the SKT system in space and time discretization is obtained. The model order reduction methods POD and DEIM are described in Section 3. Numerical simulations are presented for the SKT equation in two-dimensional case in Section 4.

2. Full Order Model

The SKT system (1.2- 1.3) has a nonlinear diffusion part. To remove the nonlinear diffusion part, a semi-linear reaction-diffusion system is proposed to approximate (1.2- 1.3) [9]:

$$\begin{aligned}
\frac{\partial \mathbf{u}}{\partial t} &= \frac{1}{\nu}\Delta \mathbf{u} - \frac{1}{\varepsilon}(\mathbf{u} - \beta(\nu \mathbf{u} + \mathbf{v})) + \frac{1}{\varepsilon} f(\nu \mathbf{u} + \mathbf{v}) \quad \text{in} \quad \Omega \times (0,T], \\
\frac{\partial \mathbf{v}}{\partial t} &= \frac{\nu}{\varepsilon}\mathbf{u} - \beta(\nu \mathbf{u} + \mathbf{v}), \quad \text{in} \quad \Omega \times (0,T], \\
\frac{\partial \mathbf{u}}{\partial n} &= 0, \quad \text{on} \quad \partial\Omega \times (0,T], \\
\mathbf{u}(\cdot,0) &= \mathbf{u}^{0,\varepsilon}, \quad \mathbf{v}(\cdot,0) = \mathbf{v}^{0,\varepsilon} \quad \text{in} \quad \Omega.
\end{aligned} \tag{2.1}$$

where u and v are the population densities and $z = u + v$ is taken in equation (1.2). Then, the weak solutions $\mathbf{u}^{\varepsilon}$ and $\mathbf{v}^{\varepsilon}$ are approximations to $\beta(\mathbf{z})$ and $(\mathbf{z} - \nu\beta(\mathbf{z}))$, where ν and ε are positive parameters. The initial conditions are approximated as $\mathbf{u}^{0,\varepsilon} \approx \beta(\mathbf{z}^0)$ and $\mathbf{v}^{0,\varepsilon} \approx (\mathbf{z}^0 - \nu\beta(\mathbf{z}^0))$. In (2.1), the system (1.1) is approximated by a system of M semilinear PDEs coupled with M ordinary differential equations (ODEs), which has the advantage of solving semi-linear problems instead of nonlinear systems.
The semi-discrete systems (2.1) is discretized by semi-implicit Euler method in time [1]:

$$\begin{aligned}
\frac{U_i^n - U_i^{n-1}}{\tau} &= \frac{1}{\mu}\Delta U_i^n - \frac{1}{\varepsilon}(U_i^{n-1} - \beta(\mu U_i^{n-1} + V_i^{n-1})) + \frac{1}{\mu} f(\mu U_i^{n-1} + V_i^{n-1}) \quad \text{in} \quad \Omega \\
\frac{\partial U_i^n}{\partial \nu} &= 0 \quad \text{on} \quad \partial\Omega \\
\frac{V_i^n - V_i^{n-1}}{\tau} &= \frac{\mu}{\varepsilon}(U_i^{n-1} - \beta(\mu U_i^{n-1} + V_i^{n-1})) \quad \text{in} \quad \Omega
\end{aligned}$$

where the time step size τ is given by $\frac{T}{N_T}$ and $n = 1, 2, ..., N_T, \quad i = 1, 2$. The scheme can be rewritten by setting $Z_i^n = \mu U_i^n + V_i^n$, choosing $\varepsilon = \tau$ and adding μU_i^n on both sides to the third relation, then the following semi-linear scheme is obtained

$$\begin{aligned}
U_i^n - \frac{\tau}{\mu}\Delta U_i^n &= \beta(Z_i^{n-1}) + \frac{\tau}{\mu} f(Z_i^{n-1}) \quad \text{in} \quad \Omega, \\
\frac{\partial U_i^n}{\partial \nu} &= 0 \quad \text{on} \quad \partial\Omega, \\
Z_i^n &= Z_i^{n-1} + \mu(U_i^n - \beta(Z_i^{n-1})) \quad \text{in} \quad \Omega,
\end{aligned} \tag{2.2}$$

where Z_i^n and U_i^n solutions are approximations to $z(\cdot, n\tau)$ and $\beta(z(\cdot, n\tau))$, respectively. A simple system of equations is obtained to solve. Here M independent linear equations is solved in U_i^n and then Z_i^n is calculated.

Symmetric interior penalty Galerkin(SIPG) method is used to obtain a fully discrete system to (1.2) in space discretization. The continuous weak solutions (2.2) solve the variational formulation

$$(U_i^n, w_i) + a(\frac{\tau}{\mu}; U_i^n, w_i) = (\beta(Z_i^{n-1}), w_i) + (\frac{\tau}{\mu}; Z_i^{n-1}, w_i)$$

where the L^2 inner product is defined as $(\cdot,\cdot) = (\cdot,\cdot)_\Omega$ on the domain Ω, and $a(\frac{\tau}{\mu}; U_i^n, w_i) = (d\nabla u, \nabla w)$ is the bilinear form.

$\{\mathscr{D}_h\}$ is a disjoint partition of the domain Ω with triangles $\{T_i\}_{i=1}^{N_{el}} \in \mathscr{D}_h$ where N_{el} is the number of elements in the partition. The space of discrete solution and test functions is defined as

$$D_h = \{w \in L^2(\Omega) : w_K \in \mathbb{P}_d(K), \quad \forall K \in \mathscr{T}_h\},$$

where $\mathbb{P}_d(K)$ is the set of polynomials defined on $K \in \mathscr{D}_h$ of degree at most d. (2.2) is multiplied by test functions w_i, integrated over each mesh element, Green's theorem is used and the variational formulation is obtained:

$$(U_{ih}^n, w_i) + a_h(\frac{\tau}{\mu}; U_{ih}^n, w_i) = (\beta(Z_{ih}^{n-1}), w_i) + (\frac{\tau}{\mu}; Z_{ih}^{n-1}, w_i) \tag{2.3}$$

with the SIPG bilinear form as follows

$$\begin{aligned} a_h(\frac{\tau}{\mu}; U^n, w) \quad &= \textstyle\sum_{K\in\mathscr{D}} \int \frac{\tau}{\mu}\nabla U \cdot \nabla w dx - \sum_{E\in\varepsilon_h^0\cup\varepsilon_h^D} \int_E \{\frac{\tau}{\mu}\nabla U\}\cdot[w] ds + \\ &\textstyle\sum_{E\in\varepsilon_h^0\cup\varepsilon_h^D} \int_E \{\frac{\tau}{\mu}\nabla w\}\cdot[U] + \sum_{E\in\varepsilon_h^0\cup\varepsilon_h^D} \frac{\sigma}{h}\frac{\tau}{\mu}\int_E [u]\cdot[w] ds \end{aligned}$$

where h denotes the length of edge e, ε_h^0 denotes the set of interior faces (edges), [], and $\{\}$ denotes the jump and the average, respectively. The semi-discrete solutions are given as

$$U_{ih} = \sum_{k=1}^{n_e}\sum_{m=1}^{n_l} u_m^k(t)\varphi_m^k(x), \quad i = 1,2,$$

where u_m^k is the unknown vectors, φ_m^k are the basis functions in D_h, for $k = 1,2,...,n_e$, and $m = 1,2,...,n_l$. The number n_e is the number of triangles in $\mathscr{D}_h$, and n_l is the local dimension on each element given by $n_l = (d+1)(d+2)/2$, where d is the degree of polynomial order. Then the SIPG system (2.3) leads to a full order solution (FOM):

$$\begin{aligned} M U + \frac{\tau}{\mu} A U &= \beta_1(Z_1^{n-1}) + \frac{\tau}{\mu} f(Z_1^{n-1}) && (2.4)\\ M Z_1^n &= M Z_1^{n-1} + \mu(M U^n - \beta_1(Z_1^{n-1})) && (2.5)\\ M V + \frac{\tau}{\mu} A V &= \beta_2(Z_2^{n-1}) + \frac{\tau}{\mu} g(Z_2^{n-1}) && (2.6)\\ M Z_2^n &= M Z_2^{n-1} + \mu(M V^n - \beta_2(Z_2^{n-1})), \end{aligned}$$

where $M \in \mathbb{R}^{N\times N}$ is the mass matrix, and $A \in \mathbb{R}^{N\times N}$ is the stiffness matrix. The number $N = N_{loc} \times N_{el}$ indicates the degree of freedom in the DG method, where N_{loc} is the number of local dimensions in each triangle and N_{el} represents the number of elements. Moreover, $F(Z) = \beta_1(Z^{n-1}) + \frac{\tau}{\mu} f(Z^{n-1})$ and $G(Z) = \beta_2(Z^{n-1}) + \frac{\tau}{\mu} g(Z^{n-1}) \in \mathbb{R}^N$ are nonlinear forms. Then the solutions of 2.4 and 2.6 have the following form:

$$U(t) = \sum_{i=1}^N u_i(t)\varphi_i(x) = \varphi \mathbf{u}(\mathbf{t}), \quad V(t) = \sum_{i=1}^N v_i(t)\varphi_i(x) = \varphi \mathbf{v}(\mathbf{t}) \tag{2.7}$$

where $u_i(t), v_i(t)$ are the unknown coefficients and φ_i are the DG basis functions.

3. Reduced Order Model

In this section, the reduced order model (ROM) is introduced for nonlinear cross-diffusion systems. Proper orthogonal decomposition (POD) method with Galerkin projection [12] and the discrete empirical interpolation method (DEIM) for nonlinear reaction terms are considered for the SKT system.

3.1. Proper orthogonal decomposition

The FOM solutions $U(t)$ and $V(t)$ (2.4) approximate the ROM solutions of dimension $k \ll N$ onto subspaces spanned by a set of L^2 -orthogonal basis functions $\{\psi_u\}_{i=1}^k$ and $\{\psi_v\}_{i=1}^k$

$$U(t) = \sum_{i=1}^N \tilde{U}(t)\psi_u, \quad V(t) = \sum_{i=1}^N \tilde{V}(t)\psi_v \tag{3.1}$$

where $\tilde{U}(t) = (\tilde{U}_1(t), \cdots, \tilde{U}_k(t))$ and $\tilde{V}(t) = (\tilde{V}_1(t), \cdots, \tilde{V}_k(t))$ are the coefficient vectors of the ROM solutions. The reduced basis functions $\{\psi_u\}_{i=1}^k$ and $\{\psi_v\}_{i=1}^k$ are in the form of linear combination of the DG basis functions $\{\varphi_i\}_{i=1}^N$

$$\psi_{u,i} = \sum_{j=1}^{N} \Psi_{u,j,i}\varphi_j(x), \quad \psi_{v,i} = \sum_{j=1}^{N} \Psi_{v,j,i}\varphi_j(x) \tag{3.2}$$

The coefficient vectors of the reduced basis function $\psi_{u,i}$ and $\psi_{v,i}$ are in the columns of the matrices $\Psi_u = [\Psi_{u,\cdot,1}, \cdots, \Psi_{u,\cdot,k}]$ and $\Psi_v = [\Psi_{v,\cdot,1}, \cdots, \Psi_{v,\cdot,k}]$.
The reduced basis functions are calculated by applying randomized singular value decomposition (rSVD) to the snapshot matrix

$$S_1 = [U_1, \cdots, U_N], \quad S_2 = [V_1, \cdots, V_N]$$

where each component of S_1 and S_2 corresponds to the coefficient vectors of the discrete solutions of the FOM (2.4). The FOM and the ROM coefficient vectors have a relation using the expansion (2.7),(3.1),(3.2)

$$\mathbf{U} = \Psi_u\tilde{\mathbf{U}}, \quad \mathbf{V} = \Psi_v\tilde{\mathbf{V}} \tag{3.3}$$

$k-$dimensional ROM is constructed by substituting (3.3) and projected onto the reduced subspace leading to the system

$$\begin{aligned}
\tilde{M}_u\mathbf{U}^n + \frac{\tau}{\mu}\tilde{A}_u\mathbf{U}^n &= \Psi_u^T(\beta_1(\mathbf{z_1}^{n-1}) + \frac{\tau}{\mu}f_1(\mathbf{z_1}^{n-1})) \\
\tilde{M}_{z_1}\mathbf{z_1}^n &= \tilde{M}_{z_1}\mathbf{z_1}^{n-1} + \mu(\mathbf{U}^n - \Psi_u^T\beta_1(\mathbf{z_1}^{n-1})) \\
\tilde{M}_v\mathbf{V}^n + \frac{\tau}{\mu}\tilde{A}_v\mathbf{V}^n &= \Psi_v^T(\beta_2(\mathbf{z_2}^{n-1}) + \frac{\tau}{\mu}f_2(\mathbf{z_2}^{n-1})) \\
\tilde{M}_{z_2}\mathbf{z_2}^n &= \tilde{M}_{z_2}\mathbf{z_2}^{n-1} + \mu(\mathbf{V}^n - \Psi_v^T\beta_2(\mathbf{z_2}^{n-1}))
\end{aligned}$$

with the reduced matrices

$$\begin{aligned}
\tilde{M}_u &= \Psi_u^T M\Psi_u, \quad \tilde{A}_u = \Psi_u^T A\Psi_u, \quad \tilde{M}_{z_1} = \Psi_{z_1}^T M\Psi_{z_1}, \\
\tilde{M}_v &= \Psi_v^T M\Psi_v, \quad \tilde{A}_v = \Psi_v^T A\Psi_v, \quad \tilde{M}_{z_2} = \Psi_{z_2}^T M\Psi_{z_2},
\end{aligned}$$

3.2. Discrete empirical interpolation method

Though the reduced system has a smaller dimension than the full system, the dimension of the nonlinear vectors is the same as the dimension of the full system. DEIM is used to approximate the nonlinear vectors $f(z(t)) = \Psi^T f(\Psi Z^{n-1}))$ and $\beta(z(t)) = \Psi^T\beta(\Psi Z^{n-1}))$ from a subspace generated by the nonlinear functions. $\mathscr{F} = [f_1, f_2, ..., f_j] \in \mathbb{R}^{N\times J}$ and $\mathscr{B} = [\beta_1, \beta_2, ..., \beta_j] \in \mathbb{R}^{n\times J}$ represent the snapshot matrices of the nonlinear functions. rSVD is applied to the matrices $\mathscr{F}$ and $\mathscr{B}$, and find $m \ll N$ orthogonal basis functions $\{Q_i\}_{i=1}^m$. Then the approximation of the nonlinear functions is given by $Q = [Q_1, Q_2, ..., Q_m] \in \mathscr{R}^{N\times m}$

$$f(\Psi Z(t)) \approx Qh(t), \quad \beta(\Psi Z(t)) \approx Qh(t) \tag{3.4}$$

with the coefficient vector $h(t)$. The system (3.4) is overdetermined. m distinguished rows is taken from the system $Qh(t)$ for the computation of $h(t)$ through the projection matrix $P = [e_{\wp_1}, \ldots, e_{\wp_m}] \in \mathbb{R}^{N\times m}$ with $e_{\wp_i} = [0, ..., 0, \underbrace{1}_{\wp_i}, 0, ..., 0] \in \mathbb{R}^N$. Since P^TQ is nonsingular, the coefficient vector $h(t)$ can be written as with the projection:

$$h(t) = (P^TQ)^{-1}P^T f(\Psi_u Z(t)), \quad h(t) = (P^TQ)^{-1}P^T\beta(\Psi_u Z(t)) \tag{3.5}$$

Using the equations (3.4),(3.5) the nonlinear vectors can be approximated as follows

$$f(z(t)) \approx WF, \quad \beta(z(t)) \approx WB$$

where the matrix $W = \Psi_u^T Q(P^TQ)^{-1} \in \mathbb{R}^{k\times m}$ is precomputable and $F = P^T f(\Psi_u Z(t)) \in \mathbb{R}^m$ and $B = P^T\beta(\Psi_u Z(t)) \in \mathbb{R}^m$ are the m-dimensional nonlinear vectors.

4. Numerical results

In this section, the numerical results for two-dimensional SKT system (1.2- 1.3) are presented. The solutions of FOM and ROM are compared with the results of POD and POD-DEIM.
The initial conditions are taken as a random perturbation around the stationary solutions $(u_0, v_0) = (1.67, 0.92)$ given by using MATLAB function rand, uniformly distributed pseudo-random numbers. The parameters are set as follows

$$\begin{aligned} a_1 &= 0.01, \quad a_2 = 0.001, \quad b = 7.264, \quad b_2 = 1.1, \quad c_1 = 0.1, \quad c_2 = 0.2 \\ \mu_1 &= 1.2, \quad \gamma_{11} = 0.5, \quad \gamma_{12} = 0.4, \quad \mu_2 = 1, \quad \gamma_{21} = 0.38, \quad \gamma_{22} = 0.4, \quad \Gamma = 28.05. \end{aligned}$$

The spatial interval is set to $\Omega = [0, \sqrt{2}\pi] \times [0, 2\pi]$. The time step size is taken as $dt = 0.01$.
In Figure 4.1, the FOM solutions of components Z_1 and Z_2 are plotted which are very close to those in [19]. In Figure 4.2, normalized singular values are plotted for each component and the nonlinear components. The singular values decrease very fast at the beginning. In Figure 4.3, the ROM solutions are obtained by using 3-POD and 24 and 21 DEIM basis functions for each components, respectively. The ROM solutions are almost the same as the FOM solutions. In Table 4.1, the L^2- relative errors for the POD and POD-DEIM solutions are presented. The results are acceptable since POD-DEIM is applied to the nonlinear part. CPU time and speed-up factors C_{POD} and C_{DEIM} are calculated for POD and POD-DEIM. The results show the increasing of the speed-up factors which represents the efficiency of POD-DEIM.

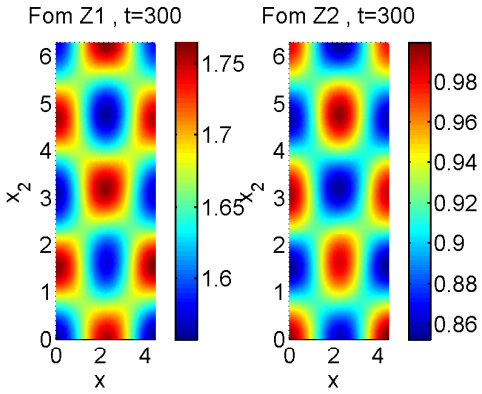

Figure 4.1: FOM solutions for the component Z_1 and Z_2.

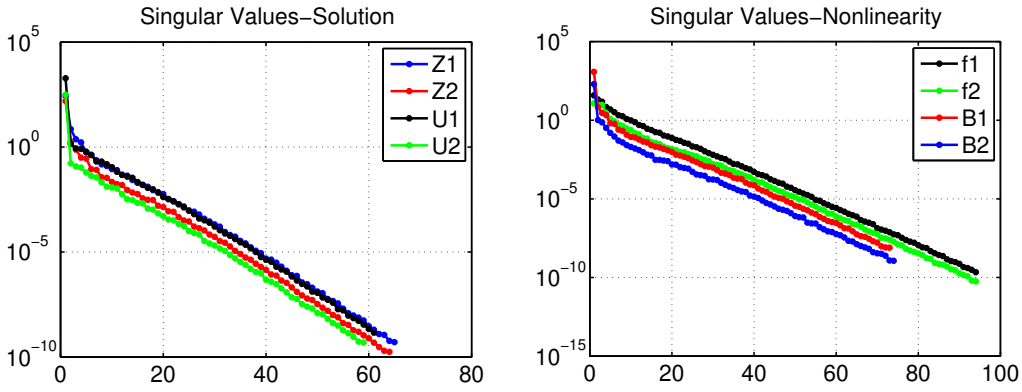

Figure 4.2: Decay of normalized singular values for the state components Z_1, Z_2, U_1 and U_2

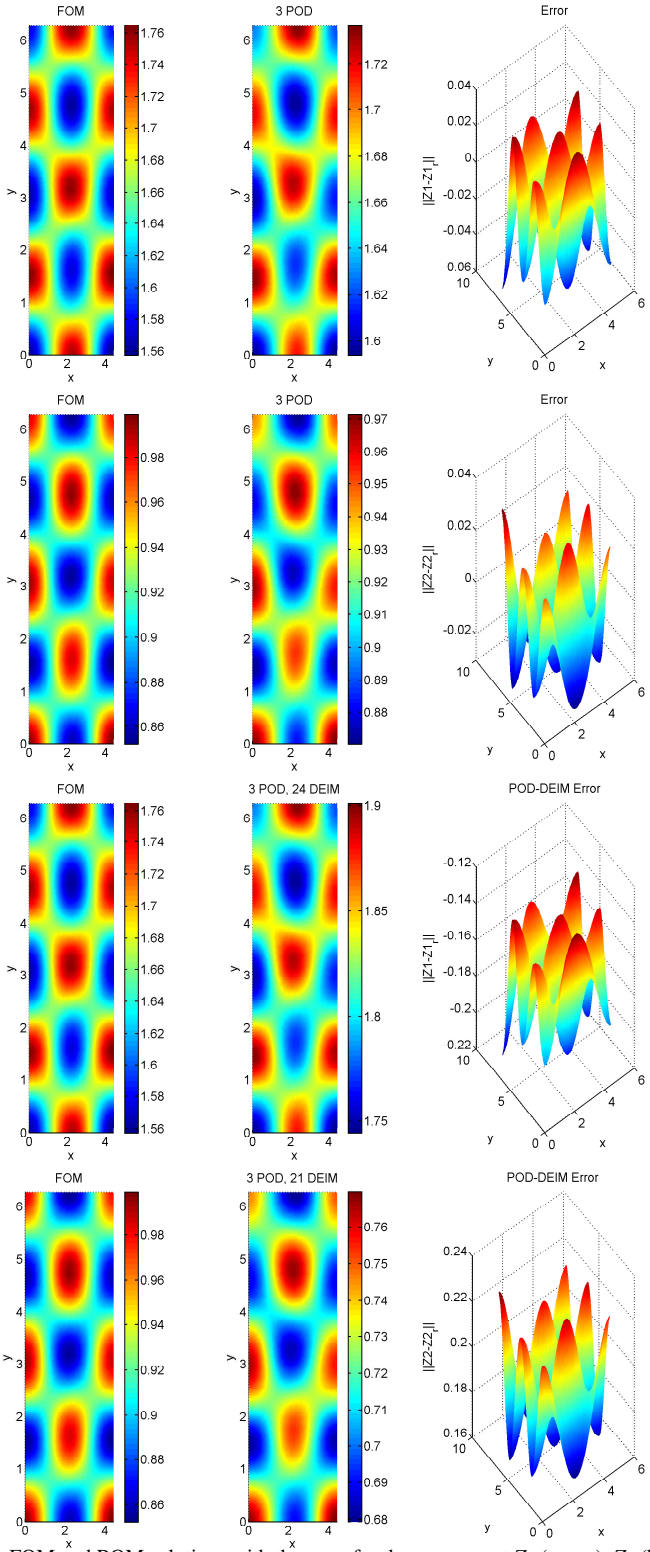

Figure 4.3: FOM and ROM solutions with the error for the component Z_1 (upper), Z_2 (bottom).

	Error Z_1	*Error* Z_2	*CPU Time*	*Speed-up*
FOM	-	-	2382.09	-
POD	1.16e-02	1.37e-02	329.55	7.23
POD-DEIM	4.72e-02	1.04e-01	135.60	17.57

Table 4.1: Relative errors and speed up factors.

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