Reduced order modelling of nonlinear cross-diffusion systems

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Abstract

In this work, we present a reduced-order model for a nonlinear cross-diffusion problem from population dynamics, for the Shigesada-Kawasaki-Teramoto (SKT) equation with Lotka-Volterra kinetics. The finite-difference discretization of the SKT equation in space results in a system of linear–quadratic ordinary differential equations (ODEs). The reduced order model (ROM) has the same linear-quadratic structure as the full order model (FOM). Using the linear-quadratic structure of the ROM, the reduced-order solutions are computed independent of the full solutions with the proper orthogonal decomposition (POD). The computation of the reduced solutions is further accelerated by applying tensorial POD. The formation of the patterns of the SKT equation consists of a fast transient phase and a long steady-state phase. Reduced order solutions are computed by separating the time into two-time intervals. In numerical experiments, we show for one-and two-dimensional SKT equations with pattern formation, the reduced-order solutions obtained in the time-windowed form, i.e., principal decomposition framework (P-POD), are more accurate than the global POD solutions (G-POD) obtained in the whole time interval. Furthermore, we show the decrease of the entropy numerically by the reduced solutions, which is important for the global existence of nonlinear cross-diffusion equations such as the SKT equation.

Keywords: Pattern formation, finite differences, entropy, proper orthogonal decomposition, principal interval decomposition, tensor algebra.

1 Introduction

The interaction between species has been widely studied with reaction–diffusion models. Cross-diffusion systems are quasilinear parabolic equations in which the gradient of one variable induces a flux of another variable. They arise in multi-component systems from physics, chemistry, and biology. The correlation between diffusion and cross-diffusion terms may cause an unstable steady-state,
called Turing instability or diffusion-driven instability, leads to formation of patterns [16, 17]. In this paper we consider a well-known cross-diffusion system from population dynamics, the Shigesada-Kawasaki-Teramoto (SKT) with Lotka-Volterra kinetics [32]. Reaction-diffusion systems as SKT equation have to be computed for many parameters to predict the patterns. Therefore the numerical simulations are computationally costly. Reduced-order models (ROMs) have emerged as a powerful approach to reduce the cost of evaluating large systems of partial differential equations (PDEs) in multi-query scenario for different parameters. The proper orthogonal decomposition (POD) has been widely used and is a computationally efficient reduced-order modeling technique in large-scale numerical simulations of nonlinear PDEs. Applying POD Galerkin projection, dominant modes of the PDEs are extracted from the snapshots of the full-order solutions and the reduced-order solutions are computed in a linear reduced space. During the offline stage, a set of reduced basis is extracted from a collection of high-fidelity solutions of the full-order model (FOM). In the online stage, the reduced-order solutions are computed in low-order reduced space, spanned by a set of basis functions.

The SKT equation has linear and quadratic nonlinear terms, both in the cross-diffusion and in the Lokta-Volterra parts. Consequently, the semi-discretization of the SKT equation by second order finite difference results in a system of linear-quadratic ordinary differential equations (ODEs). For time discretization, we use second-order linearly implicit Kahan’s method [23, 12], which is designed for ODEs with quadratic nonlinear terms, as the SKT equation. In contrast to the fully implicit schemes, such as the Crank-Nicolson scheme, Kahan’s method requires only one step Newton iteration at each time step. When nonlinear PDEs like the SKT equation have polynomial structure, projecting the FOM onto the reduced space yields low-dimensional matrix operators that preserve the polynomial structure of the FOMs, such that the offline and online phases are separated. This enables construction of computationally efficient ROMs without using hyper-reduction techniques like discrete empirical interpolation (DEIM) [13]. Online computation of the ROMs are further accelerated by matricizations of tensors [6, 8, 24]. Applying tensorial POD (T-POD) to the SKT equation recovers an efficient offline-online decomposition. Here we make use of the sparse matrix technique MULTIPROD [26] to speed up the tensor calculations.

For smooth systems where the systems energetics can be characterized by using few modes, the global POD (G-POD) method in the whole time interval provides a very efficient way to generate reduced-order systems. However, its applicability to complex, nonlinear PDEs is often limited by the errors associated with the finite truncation in POD modes and unsteadiness of the problem. An alternative (and complementary) approach is the principal interval decomposition (PID) [31, 2, 3], which optimizes the length of time windows over which to perform the POD procedure in such systems. The cross-diffusion systems with pattern formation as the SKT equation have a rapidly changing short transient phase and long stationary phase. This two phases provide as natural decomposition of the whole time domain into two sub-intervals in the principal decomposition framework (P-POD). We show for one- and two dimensional SKT equations, the patterns can be more efficiently and accurately computed with P-POD than with the G-POD. Moreover, cross-diffusion systems have an entropy structure. We show that dissipation of reduced entropy is well preserved
for the SKT equation.

The organization of this paper is as follows. In Section 2, we briefly describe the SKT equation. The fully discrete model in space and time is derived in Section 3. The three reduced order methods, G-POD, P-POD and T-POD are described in Section 4. Numerical experiments for one- and two-dimensional SKT equations are presented in Section 5. Finally, we provide brief conclusions and directions for future work.

2 Shigesada-Kawasaki-Teramoto equation

The interaction between species has been widely studied with reaction-diffusion models. The most prominent example is the Lotka-Volterra competition diffusion system which has been extensively investigated in population ecology. When the diffusion of one of the species depends not only on the density of these species but also on the density of the other species, then cross-diffusion occurs, which may rise to formation of patterns. The species with high densities diffuse faster than predicted by the usual linear diffusion towards lower density areas, that leads to the coexistence of two spatial segregated competing species, known as cross-diffusion induced instability. When cross- and self-diffusion are absent, for linear diffusion in a convex domain, the only stable equilibrium solutions are spatially homogenous. In reaction-diffusion with cross-diffusion, the destabilization of a constant steady-state, is followed by the transition to a non-homogeneous steady-state, i.e., formation of patterns. The linear stability analysis shows that the cross-diffusion is the key mechanism for the formation of spatial patterns through Turing instability [34]. In this paper, we consider the strongly coupled reaction-diffusion system with nonlinear self-and cross-diffusion terms. One of the most popular model in population ecology with pattern formation is the SKT cross-diffusion system [32] with the Lotka-Volterra reaction terms

\[
\frac{\partial u_1}{\partial t} = \Delta (c_1 + a_1 u_1 + b_1 u_2) u_1 + \Gamma (r_1 - \gamma_{11} u_1 - \gamma_{12} u_2) u_1
\]

\[
\frac{\partial u_2}{\partial t} = \Delta (c_2 + a_2 u_2 + b_2 u_1) u_2 + \Gamma (r_2 - \gamma_{21} u_1 - \gamma_{22} u_1) u_2
\]

in a convex bounded domain \(\Omega \subset \mathbb{R}^d\), \((d = 1, 2)\) with a smooth boundary \(\partial \Omega\) on the time interval \(t \in [0, T] \subset \mathbb{R}\) with \(T > 0\). In Eq (1), \(u_1(x, t)\) and \(u_2(x, t)\) with \(x \in \Omega \subset \mathbb{R}^d\) denote population densities of two competing species and \(\Delta\) is the Laplace operator. The initial and boundary conditions are

\[
u_1(x, 0) = u_1^0(x), \quad u_2(x, 0) = u_2^0(x), \quad \text{in } \Omega, \quad \frac{\partial u}{\partial n} = \frac{\partial v}{\partial n} = 0 \text{ on } \partial \Omega \times (0, T)
\]

where \(n\) is the unit outward normal vector to the boundary \(\partial \Omega\). The homogeneous Neumann (zero-flux) boundary conditions impose the weakest constraint on formation of self-organizing patterns [15] [17].

The parameters \(a_i\) and \(c_i\) are self-diffusion and linear diffusion coefficients, respectively, while the parameters \(b_i\) are the cross-diffusion coefficients. The parameters \(a_i, b_i, c_i, \gamma_{ij}\), \((i, j = 1, 2)\) are assumed to be non-negative. The parameters \(r_i\) denote the intrinsic growth rates, \(\gamma_{ii}\) the intra-specific competition coefficients, and \(\gamma_{ij}, (i \neq j)\) are inter-specific competition rates. The parameter \(\Gamma\) represents the relative strength of reaction terms.
Pattern formation in the SKT system \((1)\) was investigated using linear and weakly nonlinear stability analysis in \([16, 17]\). Cross-diffusion destabilizes the uniform equilibrium leading to traveling fonts \([16]\) in the one-dimensional SKT equation \((1)\) and formation of patterns in the two-dimensional SKT equation \((1)\) \([17]\). In both papers, it was shown, for parameter values \(b_1 > b_c^1\), patterns start to emerge, from an initial condition with a random periodic perturbation of the equilibrium \((u_1^*, u_2^*)\).

\[
(u_1^*, u_2^*) = \left( \frac{r_1 \gamma_{12} - r_2 \gamma_{11}}{\gamma_{11} \gamma_{22} - \gamma_{12} \gamma_{21}}, \frac{r_2 \gamma_{11} - r_1 \gamma_{21}}{\gamma_{11} \gamma_{22} - \gamma_{12} \gamma_{21}} \right).
\]

The critical value of bifurcation parameter \(b_c^1\) is calculated using the Turing instability analysis for one- and two-dimensional SKT equations \((1)\) in \([16, 17]\).

The entropy structure is crucial to understand various theoretical properties of cross-diffusion systems, such as existence, regularity and long time asymptotic weak solutions of the SKT equation \((1)\). The SKT equation \((1)\) can be written alternatively as \([20, 21, 14]\)

\[
\frac{\partial u}{\partial t} = \text{div}(A(u) \nabla u) + f(u) \tag{3}
\]

with the diffusion matrix

\[
A(u) = \begin{pmatrix}
c_1 + 2a_1 u_1 + b_1 u_2 & b_1 u_1 \\
b_2 u_2 & c_2 + b_2 u_1 + 2a_2 u_2
\end{pmatrix},
\]

where \(u = (u_1, u_2)^T\) and \(f(u) = (f_1(u), f_2(u))^T\) with \(f_i(u)\) representing the Lotka-Volterra reaction terms, \(i = 1, 2\). A characteristic feature of the cross-diffusion is that the diffusion matrix is generally neither symmetric nor positive definite which complicates the mathematical analysis. However, using a transformation of variables (called entropy variable), the transformed diffusion matrix becomes positive definite and sometimes even symmetric. Hence the existence of global solutions can be established. The entropy for the SKT equation \((3)\) is given without the reaction terms \(f(u)\) \([20, 21, 14]\) as

\[
\mathcal{H}(u) = \int_{\Omega} h(u) \, dx, \quad h(u) = \pi_1 u_1 (\log u_1 - 1) + \pi_2 u_2 (\log u_2 - 1), \tag{4}
\]

when two constants \(\pi_1\) and \(\pi_2\) exist satisfying \(\pi_1 b_1 = \pi_2 b_2\). The entropy decreases in time \(\frac{d\mathcal{H}}{dt} \leq 0\).

### 3 Full order model

The SKT system \((1)\) has been solved by various numerical methods: fully implicit finite volume method \([1]\), semi-implicit finite difference method \([15]\), semi-implicit spectral method \([17]\), explicit Euler and finite difference method \([16]\). In \([29, 28]\), the SKT system \((1)\) is transformed to a semi-linear PDE through replacing the nonlinear self and cross-diffusion terms by linear reaction-diffusion terms. The resulting semi-linear equations with Lotka-Volterra reaction terms and linear diffusion terms are solved by explicit Euler method with finite difference or finite volume discretization in space.
Here we discretize the SKT equation in space by finite differences, which leads to a system of ODEs of the form

\[
\begin{align*}
\frac{du_1}{dt} &= A(c_1 u_1 + a_1 u_1^2 + b_1 u_1 \circ u_2) + \Gamma(r_1 u_1 - \gamma_{11} u_1^2 - \gamma_{12} u_1 \circ u_2), \\
\frac{du_2}{dt} &= A(c_2 u_2 + a_2 u_2^2 + b_2 u_1 \circ u_2) + \Gamma(r_2 u_2 - \gamma_{22} u_2^2 - \gamma_{21} u_1 \circ u_2),
\end{align*}
\]

where \( u_1(t), u_2(t) : [0, T] \to \mathbb{R}^n \) are semi-discrete approximations to the exact solutions \( u_1(x, t) \) and \( u_2(x, t) \) at \( N \) spatial grid nodes, and the powers together with the multiplication operator \( \circ \) are driven element-wise. The number \( N \) of spatial grid nodes differ for one- and two-dimensional regions. The components of the semi-discrete solution vectors \( u_i(t) \) \( (i = 1, 2) \) in the case of one- and two-dimensional regions are given respectively by

\[
\begin{align*}
u_i(t) &= (u_i(x_1, t), \ldots, u_i(x_{nx}, t))^T, \\
u_i(t) &= (u_i(x_1, y_1, t), \ldots, u_i(x_{nx}, y_1, t), u_i(x_2, y_1, t), \ldots, u_i(x_{nx}, y_{ny}, t))^T,
\end{align*}
\]

with \( N = nx \) on one-dimensional regions and \( N = nx \times ny \) on two-dimensional regions, where \( nx \) and \( ny \) are the number of partition in \( x \) and \( y \)-directions, respectively.

In the ODE system, the matrix \( A \) represents the finite difference matrix related to the second order centered finite differences approximation to the Laplace operator \( \Delta \) under homogeneous Neumann boundary conditions. More clearly, let \( I_n \in \mathbb{R}^{n \times n} \) denotes the \( n \)-dimensional identity matrix, and let the matrix \( B_n \in \mathbb{R}^{n \times n} \) given by

\[
B_n = \begin{pmatrix}
-2 & 2 \\
1 & -2 & 1 \\
& \ddots & \ddots & \ddots \\
& & 1 & -2 & 1 \\
& & & 2 & 1
\end{pmatrix},
\]

corresponds to the centered finite differences approximation to the Laplace operator under homogeneous Neumann boundary conditions with \( n + 1 \) grid nodes. Then, we have on the one-dimensional regions

\[
A = \frac{1}{\Delta x^2} B_{nx} \in \mathbb{R}^{nx \times nx},
\]

whereas on the two-dimensional regions we get that

\[
A = \frac{1}{\Delta x^2} (B_{nx} \otimes I_{ny}) + \frac{1}{\Delta y^2} (I_{nx} \otimes B_{ny}) \in \mathbb{R}^{nx \times nx \times ny},
\]

where \( \Delta x \) and \( \Delta y \) are the mesh sizes in \( x \) and \( y \)-directions, respectively, and \( \otimes \) denotes the Kronecker product.

Collecting linear and quadratic parts, the system can be written as the following linear-quadratic ODE system

\[
\begin{align*}
du_1 &= L_1 u_1 + Q_{11} u_1^2 + Q_{12} (u_1 \circ u_2), \\
du_2 &= L_2 u_2 + Q_{22} u_2^2 + Q_{21} (u_1 \circ u_2),
\end{align*}
\]
where we set

\[ L_1 = c_1 A + \Gamma_1, \quad Q_{11} = a_1 A - \Gamma_{11}, \quad Q_{12} = b_1 A - \Gamma_{12}, \]
\[ L_2 = c_2 A + \Gamma_2, \quad Q_{21} = b_2 A - \Gamma_{21}, \quad Q_{22} = a_2 A - \Gamma_{22}. \]

In compact form, we can also write as

\[
\frac{du}{dt} = F(u) = Lu + R_1(u) + R_2(u),
\]

where \( u = (u_1, u_2) \in \mathbb{R}^{2N} \) is the state vector, \( L \in \mathbb{R}^{2N \times 2N} \) represents the matrix of linear terms, and \( R_i \in \mathbb{R}^{2N} \) \((i = 1, 2)\) includes the quadratic terms given by

\[
L = \begin{pmatrix} L_1 & 0 \\ 0 & L_2 \end{pmatrix},
R_1 = \begin{pmatrix} Q_{11} & 0 \\ 0 & Q_{22} \end{pmatrix} \begin{pmatrix} H(u_1 \otimes u_1) \\ H(u_2 \otimes u_2) \end{pmatrix},
R_2 = \begin{pmatrix} 0 & Q_{12} \\ Q_{21} & 0 \end{pmatrix} \begin{pmatrix} H(u_1 \otimes u_2) \\ H(u_1 \otimes u_2) \end{pmatrix}.
\]

In (7), \( H \in \mathbb{R}^{N \times N^2} \) stands for the matricized tensor so that it satisfies the identity \( H(w \otimes v) = w \circ v \) for any vector \( w, v \in \mathbb{R}^N \).

The ODE system (6) can be solved in time using explicit or implicit methods. Explicit methods require small time steps and can produce unstable solutions. The implicit integrators require at each time step solution of nonlinear equations iteratively. We solve the semi-discrete linear-quadratic ODE system (6) in time by linearly implicit Kahan’s method \([22, 23]\):

\[
\frac{u^{n+1} - u^n}{\Delta t} = \frac{1}{2} L(u^n + u^{n+1}) + \tilde{R}_1(u^n, u^{n+1}) + \tilde{R}_2(u^n, u^{n+1})
\]

where \( \tilde{R}_i(u^n, u^{n+1}) \) are the symmetric bilinear forms obtained by the polarization of the quadratic vector fields \( R_i \) \([11]\):

\[
\tilde{R}_i(u^n, u^{n+1}) = \frac{1}{2} R_i(u^n + u^{n+1}) - R_i(u^n) - R_i(u^{n+1}), \quad i = 1, 2.
\]

and \( \Delta t \) is the time step size, and \( u^n \) is the full discrete solution vector at time \( t_n \). Kahan’s method is time-reversal, symmetric and linearly implicit, i.e., \( u^{n+1} \) can be computed by solving a single linear system

\[
\left( I_{2N} - \frac{\Delta t}{2} F_j(u^n) \right) \tilde{u} = \Delta t F(u^n), \quad u^{n+1} = u^n + \tilde{u},
\]

where \( F_j(u^n) \) is the Jacobian matrix of \( F(u) \) evaluated at \( u^n \).

Kahan’s method can also be written as a second order convergent Runge-Kutta method of the form \([12]\):

\[
\frac{u^{n+1} - u^n}{\Delta t} = -\frac{1}{2} F(u^n) + 2 F \left( \frac{u^{n+1} + u^n}{2} \right) - \frac{1}{2} F(u^{n+1}).
\]

When fully implicit time integrators are used, at each time step nonlinear equations have to be solved iteratively by Newton’s method or by fixed-point iteration. The linearly implicit Kahan’s methods is much faster than the fully implicit time integrators like the implicit Euler and mid-point rule.
4 Reduced order model

In this section, we introduce three different types of ROMs. The standard way of constructing ROMs is the use of POD with Galerkin projection on the whole time interval, Global-POD (G-POD). The solutions of the SKT equation (1) converge quickly to steady-state after a short transient phase. We have constructed partitioned-POD (P-POD) in two sub-intervals respecting different behavior of the average densities of the FOM solutions in the transient and steady-state phase. The computation of the quadratic terms scale in the reduced order model with $N^2$. We have constructed an efficient tensorial-POD (T-POD) exploiting the quadratic form of the semi-discrete SKT equation (6).

4.1 Global-POD

The POD basis vectors are computed using the method of snapshots. The POD basis for the semi-discrete SKT system (5) can be obtained by stacking all $u_1$ and $u_2$ in one vector $u$ and to determine the common subspace $V$ by taking the singular value decomposition (SVD) of that data. But this may produce unstable ROMs such that the resulting ROMs do not preserve the coupling structure of the PDE [6, 30]. In order to maintain the coupling structure in ROMs of the coupled SKT equation, we compute the snapshot matrices and the POD basis vectors separately for the state components $u_1$ and $u_2$. Consider the discrete state vectors $u_1$ and $u_2$ of (5). The snapshot matrix $S_i$ corresponding to the state $u_i$ is defined as

$$S_i := [u_{1i}^1, \ldots, u_{Ni}^N] \in \mathbb{R}^{N \times N_t}, \quad i = 1, 2,$$

where each column vector $u_n^i \in \mathbb{R}^N$ is the full discrete solution vector at the time instance $t_n$, $n = 1, \ldots, N_t$. Assuming $N > N_t$, we then expand the SVD of the snapshot matrix

$$S_i = V_i \Sigma_i U_i^T,$$

where the columns of $V_i \in \mathbb{R}^{N \times N_t}$ and $U_i \in \mathbb{R}^{N_t \times N_t}$ are the left and right singular vectors of $S_i$, respectively, and $\Sigma_i \in \mathbb{R}^{N_t \times N_t}$ is the diagonal matrix whose diagonal elements are the singular values $\sigma_{i,1} \geq \sigma_{i,2} \geq \cdots \geq \sigma_{i,N_t} \geq 0$.

The $k$-POD basis matrix $V_{i,k} \in \mathbb{R}^{N \times k}$ minimizes the least squares error of the snapshot reconstruction

$$\min_{V_{i,k} \in \mathbb{R}^{N \times k}} ||S_i - V_{i,k} V_{i,k}^T S_i||_F^2 = \min_{V_{i,k} \in \mathbb{R}^{N \times k}} \sum_{n=1}^{N_t} ||u_n^i - V_{i,k} V_{i,k}^T u_n^i||_2^2 = \sum_{n=k+1}^{N_t} \sigma_{i,n}^2,$$

where $|| \cdot ||_2$ denotes the Euclidean 2-norm and $|| \cdot ||_F$ denotes the Frobenius norm. The optimal solution of basis matrix $V_{i,k}$ to this problem is given by the $k$ left singular vectors of $S_i$ corresponding to the $k$ largest singular values. The POD state approximation is then $u_i \approx V_{i,k} \hat{u}_i$, where $\hat{u}_i \in \mathbb{R}^k$ is the reduced state vector. Throughout the paper, we omit the subscript $k$ for easy notation and we denote by simply $V_i$ the $k$-POD basis matrix corresponding to the state $u_i$. Moreover, we may choose different number of POD modes $k_1$ and $k_2$ related to each state component $u_1$ and $u_2$, respectively.
Once the POD basis matrices $V_i$ are found, the ROM for the SKT system is obtained as a linear-quadratic ODE as the FOM\(^6\):

$$\frac{d}{dt} \hat{u} = \hat{L}\hat{u} + \hat{R}_1(\hat{u}) + \hat{R}_2(\hat{u}),$$

(9)

where $\hat{u} = (\hat{u}_1, \hat{u}_2)$, $\hat{L} = V^T LV$, $\hat{R}_i(\hat{u}) = V^T R_i(V\hat{u})$, and

$$V = \begin{pmatrix} V_1 & 0 \\ 0 & V_2 \end{pmatrix} \in \mathbb{R}^{2N \times (k_1+k_2)}.$$

The number of POD modes $k_i$ for each component $u_i$ ($i = 1, 2$) is determined usually by the relative information content (RIC) defined by

$$\frac{\sum_{n=1}^{k_i} \sigma_{i,n}^2}{\sum_{n=1}^{N} \sigma_{i,n}^2} < \text{tol}_{\text{RIC}}$$

(10)

with a tolerance $\text{tol}_{\text{RIC}}$.

### 4.2 Partitioned POD

POD depends on a global approximation of the snapshot data, which can result in overall deformation of the obtained modes for systems with fast variations in state and the constructed POD cannot capture any dominant structure at all. The PID approach is developed\(^{[19, 9, 31, 1, 2, 3]}\) as an alternative approach which preserves the optimality of POD respecting local characteristics of the solutions. In PID, the time domain is divided into non-overlapping intervals, each characterizing a specific stage in the systems dynamics and evolution. The same POD algorithm is applied within each subinterval to generate a set of basis functions that best fit the respective partition locally. In short, the PID approach can be viewed as decomposing the G-POD subspace into a few of locally optimal subspaces to obtain accurate partitioned ROMs with smaller sizes in each individual sub-interval. The PID was first studied in\(^{[19]}\) and then is applied successfully to nonlinear convective fluid problems: Burgers equation, Boussinesq equation and Navier-Stokes equation\(^{[9, 31, 1, 2]}\) and two-dimensional turbulence flow\(^{[3]}\). Adaptive partitioning and clustering techniques can be used to construct the sub-intervals of different size, but also the time domain may be decomposed into equidistant sub-intervals.

The cross-diffusion with pattern formation like SKT equation\(^{[1]}\) is characterized by short transient phase and long stationary phase. This leads to a natural decomposition of the whole time domain into two sub-intervals in the PID approach, one for the transient phase and the other for the stationary phase. The transition from transient phase to stationary phase can be determined by using average densities

$$\langle u_1(x, y, t) \rangle = \frac{1}{|\Omega|} \int_{\Omega} u_1(x, y, t) dx dy, \quad \langle u_2(x, y, t) \rangle = \frac{1}{|\Omega|} \int_{\Omega} u_2(x, y, t) dx dy,$$

(11)

When the difference of the both average densities at two consecutive time instances are lower than a prespecified tolerance $\text{tol}_{\text{PID}}$, the stationary phase occur. This transition point is then used as the interface of two sub-intervals.
in the PID approach. More clearly, let \( t_p \) denotes the transition point, i.e., the
index \( 1 < p < N_t \) is the minimum integer such that

\[
|(u_i(x, y, t_p)) - (u_i(x, y, t_{p-1}))| < \text{tol}_{\text{PID}}, \quad i = 1, 2,
\]

for a given tolerance \( \text{tol}_{\text{PID}} \). Then, we decompose the whole time-interval
\([t_0, t_{N_t}]\) into two sub-intervals \( I_1 = [t_0, t_p] \) and \( I_2 = [t_p, t_{N_t}] \) with the
common interface \( t_p \). According to the PID approach, we set different POD basis
matrices \( V^{(1)}_i \) and \( V^{(2)}_i \) through the snapshot matrices composed of the full
solution vectors on either intervals \( I_1 \) and \( I_2 \), respectively. Finally, we should
enforce the interface constraint that the full discrete solution vectors
\( V_u \) on the second interval
\( I_2 \) can be recovered from the reduced solution vector at the interface \( t_p \) on the interval
\( I_1 \) as

\[
\hat{V}_i^{(2)}(t_p) = (V_i^{(1)})^T V_i^{(1)} \hat{V}_i^{(1)}(t_p), \quad i = 1, 2.
\]

### 4.3 Tensorial POD

Although the dimension of the ROM [9] is small compared to the dimension
of the FOM [5], the computation of the quadratic nonlinearities still scale with
the dimension of FOM. T-POD approach can handle this computational ineffi-
ciency utilizing the matricized tensor together with the properties of Kronecker
product.

The explicit form of the reduced quadratic terms in the SKT equation [9] are given by

\[
\hat{R}_1(\hat{u}) = V^T R_1(V \hat{u}) = \begin{pmatrix}
V_i^T Q_{11} H((V_i \hat{u}_1) \otimes (V_i \hat{u}_1)) \\
V_i^T Q_{22} H((V_i \hat{u}_2) \otimes (V_i \hat{u}_2))
\end{pmatrix}
\]

\[
\hat{R}_2(\hat{u}) = V^T R_2(V \hat{u}) = \begin{pmatrix}
V_i^T Q_{12} H((V_i \hat{u}_1) \otimes (V_i \hat{u}_2)) \\
V_i^T Q_{21} H((V_i \hat{u}_2) \otimes (V_i \hat{u}_1))
\end{pmatrix}
\]

It is clear that all the terms above are of the form

\[
V_i^T Q_{ij} H((V_i \hat{u}_i) \otimes (V_j \hat{u}_j)), \quad i, j = 1, 2.
\]

The terms with tensor \( H \) in [12] are computed using the properties of
Kronecker product, which depends on the computation of the reduced tensor
\( \tilde{H} = H(V_i \otimes V_j) \in \mathbb{R}^{N \times k_i k_j} \) so that we get

\[
V_i^T Q_{ij} H((V_i \hat{u}_i) \otimes (V_j \hat{u}_j)) = V_i^T Q_{ij} \tilde{H}(\hat{u}_i \otimes \hat{u}_j),
\]

where the small matrix \( V_i^T Q_{ij} \tilde{H} \in \mathbb{R}^{k_i \times k_i k_j} \) can be precomputed in the offline
stage. Although \( \tilde{H} \) is computed offline, the explicit computation of \( V_i \otimes V_j \) may
be inefficient since it depends on the full dimension $N$. In order to avoid from this computational burden, $V_i \otimes V_j$ is computed in an efficient way using $\mu$-mode matricizations of tensors [5].

Recently tensorial algorithms are developed by exploiting the particular structure of Kronecker product [8, 7]. The reduced matrix $\tilde{H}$ can be given in MATLAB notation as follows

$$\tilde{H} = \begin{pmatrix} V_i(1,:) \otimes V_j(1,:) \\ \vdots \\ V_i(N,:) \otimes V_j(N,:) \end{pmatrix},$$

which utilizes the structure of $H( V_i \otimes V_j)$ without constructing $H$ explicitly. In [8, 7] the CUR matrix approximation [27] of $H( V_i \otimes V_j)$ is used to increase computational efficiency. Instead, here we make use of the "MULTIPROD" [26] to increase computational efficiency. The MULTIPROD [26] handles multiple multiplications of the multi-dimensional arrays via virtual array expansion. It is a fast and memory efficient generalization for arrays of the MATLAB matrix multiplication operator. For any given two vectors $a$ and $b$, the Kronecker product satisfies

$$( \text{vec}(ba^\top))^\top = (a \otimes b)^\top = a^\top \otimes b^\top,$$

where vec $(\cdot)$ denotes the vectorization of a matrix. Using the identity in (14), the matrix $C = H( V_i \otimes V_j)$ can be constructed as

$$C(m,:) = (\text{vec}(V_i(m,:)^\top V_j(m,:))^\top, m \in \{1, 2, \ldots, N\}.$$  

Reshaping the matrix $V_i \in \mathbb{R}^{N \times k_i}$ as $\tilde{V}_i \in \mathbb{R}^{N \times 1 \times k_i}$ and computing MULTIPROD of $V_j$ and $\tilde{V}_i$ in 2 and 3 dimensions, we obtain

$$C = \text{MULTIPROD}(V_j, \tilde{V}_n) \in \mathbb{R}^{N \times k_j \times k_i}.$$  

5 Numerical results

In this section we present results of the numerical experiments for the one-and two dimensional SKT system (1). We compare the FOM and ROM solutions by G-POD and P-POD, computational gain by TPOD over POD, and show the decreasing structure of the entropy.

Initial conditions are taken as random periodic perturbation around the equilibrium $(u^*_1, u^*_2)$ given in (2). We stop the computation of the FOMs when the solutions are sufficiently close to the steady-states, e.g., when the termination condition

$$\frac{||u^n_i - u^{n-1}_i||_{L^2(\Omega)}}{||u^n||_{L^2(\Omega)}} \leq \text{tol}_{ST}, \quad i = 1, 2,$$

is satisfied for a prescribed tolerance $\text{tol}_{ST} > 0$, where $\cdot ||_{L^2(\Omega)}$ denotes the usual $L^2$-norm over the domain $\Omega$, and calculated by the trapezoidal quadrature. We take in all simulations $\text{tol}_{ST} = 10^{-6}$.

[1]https://www.mathworks.com/matlabcentral/fileexchange/8773-multiple-matrix-multiplications-with-array-expansion-enabled
The accuracy of the ROM solutions are measured using the time averaged relative $L^2$-errors defined by

$$\|u - \hat{u}\|_{rel} = \frac{1}{N_t} \sum_{n=1}^{N_t} \frac{\|u^n - \hat{u}^n\|_{L^2}}{\|u^n\|_{L^2}}.$$  \hspace{1cm} (15)

All the simulations are performed on a machine with Intel: CoreTM i7 2.5 GHz 64 bit CPU, 8 GB RAM, Windows 10, using 64 bit MatLab R2014. For the time-dependent problems with many time steps, such as the SKT system, the snapshot matrix is large, leading to an expensive SVD. We use randomized SVD (rSVD) algorithm \cite{18} which only needs to perform SVD of small matrices, to efficiently generate a reduced basis with large snapshot matrices. In the ROMs, T-POD framework is applied in both the G-POD and P-POD approaches.

5.1 One-dimensional SKT equation

Our first example is the one-dimensional SKT equation \cite{4} with the parameters are taken as in \cite{16}

$$a_1 = 0.0001, \quad a_2 = 0.1, \quad b_1 = 6.5, \quad b_2 = 0.3, \quad c_1 = 0.2, \quad c_2 = 0.2,$$

$$\Gamma = 49.75, \quad r_1 = 1.2, \quad r_2 = 1, \quad \gamma_{11} = 0.5, \quad \gamma_{12} = 0.4, \quad \gamma_{21} = 0.38, \quad \gamma_{22} = 0.41,$$

where, $b_1$ is taken larger than the critical value of the bifurcation parameter $b_c = 5.297$, so that pattern formation can occur. Spatial interval is set to $\Omega = [-\pi, \pi]$ with the mesh size $\Delta x = 2\pi/200$, and time step size is taken as $\Delta t = 0.001$. The steady-states are reached at $t = 11.219$.

In Figure 1 left, the patterns at the steady-state are shown, that are formed starting from an initial datum which is a random periodic perturbation of the equilibrium $\hat{u}$. The FOM solutions are very close to those in \cite{16}. In Figure 1 right, the densities start a plateau around $t = 5$. Accordingly, using the PID tolerance $ tol_{PID} = 10^{-8}$, we obtain the transition point $t_p = 4.023$, and the time interval is split into sub-intervals $I_1 = [0, 4.023]$ and $I_2 = [4.023, 11.219]$.

![Figure 1: FOM solutions & densities for one-dimensional problem](image)

In Figure 2, singular values are plotted in the whole time interval, in the intervals $I_1$ of the transient and $I_2$ of the steady-state phases. The singular values decay at the same rate, slowly in the whole time interval and in the first interval $I_1$, whereas the decay is faster in the second interval $I_2$ of the steady-state phase.
The number of POD modes and the time averaged relative $L^2$-errors [15] between FOM and ROM approximations for different RIC tolerances $\text{tol}_{\text{RIC}}$ in (10) are listed in Table 1. For the same RIC tolerances, the P-POD requires fewer POD modes in the interval $I_2$ of the steady-states comparing with the ones required in the interval $I_1$ of the transition phase. The time averaged relative $L^2$-errors obtained by the P-POD are smaller than the errors obtained by the G-POD approach. The ROM solutions in Figure 3 computed using the RIC tolerance $\text{tol}_{\text{RIC}} = 10^{-4}$ are very close to the FOM solutions.

### 5.2 Two-dimensional SKT equation

Our second example is the two-dimensional SKT equation (1) with the parameters taken as in [17]

$$a_1 = 0.01, \quad a_2 = 0.001, \quad b_1 = 7.264, \quad b_2 = 1.1, \quad c_1 = 0.1, \quad c_2 = 0.2,$$

$$\Gamma = 28.05, \quad r_1 = 1.2, \quad r_2 = 1, \quad \gamma_{11} = 0.5, \quad \gamma_{12} = 0.4, \quad \gamma_{21} = 0.38, \quad \gamma_{22} = 0.4.$$  

Spatial domain is set to $\Omega = [0, \sqrt{2\pi}] \times [0, 2\pi]$. We take in both space directions the same number of partition $n_x = n_y = 100$, and time step size is set to $\Delta t = 0.001$. The steady-states are reached at $t = 2.938$.

In Figure 4, the densities start almost unchanged around $t = 0.5$. By the PID tolerance $\text{tol}_{\text{PID}} = 10^{-7}$, the time interval is split into sub-intervals $I_1 = [0, 0.484]$ and $I_2 = [0.484, 2.938]$. Decay of the singular values in Figure 5 is similar to the one-dimensional SKT equation in the previous example. The FOM and ROM solutions in Figure 6 computed with the RIC tolerance $\text{tol}_{\text{RIC}} = 10^{-6}$ agree well, and that the ones by the P-POD approach are almost the same as the FOM solutions.

The errors by G-POD and P-POD in Table 2 show the same behavior as the errors in Table 1 for the one-dimensional case.
Figure 3: FOM & ROM solutions for one-dimensional problem

Figure 4: FOM densities for two-dimensional problem

Table 2: Number of POD modes and errors for two-dimensional problem

| tolRIC | G-POD $u(v)$ | P-POD $u(v)$ |
|--------|--------------|--------------|
|        | #Modes | Error | #Modes | Error | #Modes-1 | #Modes-2 | Error |
| $10^{-4}$ | 4(3)   | 1.97e-03(2.18e-03) | 5(4)   | 1.26e-03(1.40e-03) |
| $10^{-5}$ | 6(5)   | 9.17e-04(1.02e-03) | 7(6)   | 3.53e-04(3.89e-04) |
| $10^{-6}$ | 9(8)   | 2.14e-04(2.30e-04) | 10(8)  | 2.20e-04(2.46e-04) |
| $10^{-7}$ | 12(11) | 6.73e-05(7.29e-05) | 11(10) | 5.76e-05(6.42e-05) |

5.3 Entropy preservation

The entropy (4) of the SKT equation is defined with the Lokta-Volterra kinetics terms $f_i(u) = 0$, $i = 1, 2$. The entropies are computed with the same diffusion coefficients for one and two dimensional SKT equation (1) setting the $f_1(u) = f_2(u) = 0$. Initial conditions are taken from [33] are given by

$$u_1(x) = e^{\frac{1}{2} \sin x}, \quad u_2(x) = e^{\frac{1}{2} \cos 2x},$$

$$u_1(x, y) = \frac{1}{2} (\sin(\pi(x + y))) + 1, \quad u_2(x, y) = \frac{1}{2} (\cos(\pi(x - y))) + 1,$$

for one and two dimensional problems, respectively. Since the SKT equation is solved without the reaction terms, the transient phase is absent. Therefore, the ROMs are computed only by the G-POD approach.
Figure 5: Decay of normalized singular values for two-dimensional problem

Figure 6: FOM & ROM solutions of $u$ (top) and $v$ (bottom) components for two-dimensional problem

In Figures 7-8, the FOM entropies decay with the time, and this structure is well preserved by the ROMs.

6 Conclusions

Exploiting the different behavior of transient and steady-state solutions of the SKT equation, reduced solutions are obtained in a computationally efficient way. The quadratic nonlinear terms of SKT equation are reflected in the semi-discrete linear-quadratic ODE system using finite-differences, which enables separation of the offline-online computation. The ROM solutions depend affinely on the parameters in both of the linear and quadratic parts. This allows the prediction of patterns for different parameter values without interpolation. We plan to investigate the bifurcation behavior of the SKT equation [25, 10] using ROM techniques.
Figure 7: Entropy decay for one-dimensional problem

Figure 8: Entropy decay for two-dimensional problem

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