
Model Reduction via Proper Orthogonal Decomposition

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1 Introduction

In many fields of science and engineering, like fluid or structural mechanics and electric circuit design, large-scale dynamical systems need to be simulated, optimized or controlled. They are often given by discretizations of systems of non-linear partial differential equations yielding high-dimensional discrete phase spaces. For this reason during the last decades research was mainly focused on the development of sophisticated analytical and numerical tools to understand the overall system behavior. Not surprisingly, the number of degrees of freedom for simulations kept pace with the increasing computing power. But when it comes to optimal design or control the problems are in general too large to be tackled with standard techniques. Hence, there is a strong need for *model reduction techniques* to reduce the computational costs and storage requirements. They should yield low-dimensional approximations for the full high-dimensional dynamical system, which reproduce the characteristic dynamics of the system.

In this work, we present a method known as *proper orthogonal decomposition* (POD), which is widely discussed in literature during the last decades. The original concept goes back to Pearson [28]. The method is also known as Karhunen–Loève decomposition [15, 22] or principal component analysis [13]. Further names are factor analysis or total least-squares estimation. It provides an optimally ordered, orthonormal basis in the least-squares sense for a given set of theoretical, experimental or computational data [2]. Reduced order models or surrogate models are then obtained by truncating this optimal basis. Clearly, the choice of the data set plays a crucial role and relies either on guesswork, intuition or simulations. Most prominent is the *method of snapshots* introduced by Sirovich [36]. Here, the data set is chosen as time snapshots containing the spatial distribution of a numerical simulation at certain time instances reflecting the system dynamics.

As an a posteriori, data dependent method it does not need a priori knowledge of the system behavior and can also be used to analyze patterns in data. Due to this fact, it was intensively used to study turbulence phenomena and coherent structures

in fluid dynamics [4, 14, 32, 35, 36] as well as in signal analysis and pattern recognition [9, 33]. More recently, it has been used in optimal control of partial differential equations [1, 8, 10, 12, 16–19, 31], inverse problems in structural dynamics [6] and controller design for real-time control [3, 27, 37].

POD falls into the general category of projection methods where the dynamical system is projected onto a subspace of the original phase space. In combination with Galerkin projection [12, 17, 18] it provides a powerful tool to derive surrogate models for high-dimensional or even infinite dimensional dynamical systems, since the subspace is composed of basis functions inheriting already special characteristics of the overall solution. This is in contrast to standard finite element discretizations where the choice of the basis functions is in general independent of the system dynamics.

The main advantage of POD lies in the fact that it requires only standard matrix computations, despite of its application to nonlinear problems. Although projecting only onto linear or affine subspaces the overall nonlinear dynamics is preserved, since the surrogate model will still be nonlinear. Nevertheless, it is computationally more convenient than to reduce the dynamics onto a curved manifold [30], like it is done in the methods of intrinsic lower-dimensional manifolds (ILDM) for reducing chemical kinetics [23].

In Section 2 we present the construction of the POD basis which is either based on data sets or on the method of snapshots. Further, we use Galerkin projections to reduce the system dimensionality and discuss the connection of POD and singular value decomposition. Section 3 is dedicated to an numerical test of the POD method in radiative heat transfer. Finally, we give in Section 4 some conclusions and future research perspectives.

2 Proper Orthogonal Decomposition

POD can be seen as a model reduction technique or as a method for data representation. Being a projection method the latter point of view can be translated into the question [29, 30]:

Find a subspace approximating a given set of data in an optimal least-squares sense.

This is related to model reduction of dynamical systems by the choice of the data points, which are either given by samplings from experiments or by trajectories of the physical system extracted from simulations of the full model.

2.1 Construction of the POD Basis

To put all this into a mathematical framework (see also [30] for a more detailed discussion) we start with a vector space V of finite or infinite dimension and a given set of data in V . Considering a dynamical system described by partial differential equations this resembles the phase space of an ordinary differential system, which one gets after a spatial discretization via a method of lines, or to the infinite dimensional

state space in which the solution lies. In the following we will restrict ourself to finite dimensions and set $V = \mathbb{R}^n$. Then, a set of sampled data $Y = \{y_1(t), \dots, y_m(t)\}$ is given by trajectories $y_i(t) \in \mathbb{R}^n$, $i = 1, \dots, m$ and $t \in [0, T]$.

Next, we use a *principal component analysis* of this data to find a d -dimensional subspace $V_d \subset V$ approximating the data in some optimal least-squares sense, i.e. we seek an orthogonal projection $\Pi_d : V \rightarrow V_d$ of fixed rank d that minimizes the total least-squares distance

$$\|Y - \Pi_d Y\|^2 := \sum_{i=1}^m \int_0^T \|y_i(t) - \Pi_d y_i(t)\|^2 dt.$$

The solution of this problem relies on the introduction of the *correlation matrix* $K \in \mathbb{R}^{n \times n}$ defined by

$$K = \sum_{i=1}^m \int_0^T y_i(t) y_i(t)^* dt, \quad (1)$$

where the star stands for the transpose (with additional complex conjugation in case of $V = \mathbb{C}^n$) of a vector or a matrix. By definition, K is a symmetric positive semi-definite matrix with real, nonnegative ordered eigenvalues $\lambda_1 \geq \dots \geq \lambda_n \geq 0$. Let u_j denote the corresponding eigenvectors given by

$$K u_j = \lambda_j u_j, \quad j = 1, \dots, n.$$

Due to the special structure of the matrix K we can choose them in fact as an orthonormal basis of V .

The main result of POD is that the optimal subspace V_d of dimension d representing the data is given by $V_d = \text{span}\{u_1, \dots, u_d\}$. The vectors u_j , $j = 1, \dots, d$ are then called *POD modes*. More precisely, we have the following result [20]:

Theorem 1. *Let K be the correlation matrix of the data defined by :=correlation and let $\lambda_1 \geq \dots \geq \lambda_n \geq 0$ be the ordered eigenvalues of K . Then it holds*

$$\min_{V_d} \|Y - \Pi_d Y\| = \sum_{j=n-d+1}^n \lambda_j,$$

where the minimum is taken over all subspaces V_d of dimension d . Further, the optimal orthogonal projection $\Pi_d : V \rightarrow V_d$, with $\Pi_d \Pi_d^* = I$, is given by

$$\Pi_d = \sum_{j=1}^d u_j u_j^*.$$

Each data vector $y_i(t) \in V$ can be written as

$$y_i(t) = \sum_{j=1}^n y_{ij}(t) u_j,$$

where $y_{ij}(t) = \langle y_i(t), u_j \rangle$. Then it holds

$$\Pi_d y_i(t) = \sum_{j=1}^d u_j u_j^* \left(\sum_{l=1}^n y_{il}(t) u_l \right) = \sum_{j=1}^d y_{ij}(t) u_j,$$

since $\langle u_i, u_j \rangle = \delta_{ij}$.

Remark 1. Often, one is interested in finding rather an approximating affine subspace than a linear subspace [30]. Consider for example the flow around a cylinder, where one can observe Karman's vortex street [12]. Physically speaking, we have then the superposition of the mean flow, in which we are not interested, and the vortex structures on which our main focus lies. So, we construct first the mean value of the data given by

$$\bar{y} := \frac{1}{mT} \sum_{i=1}^m \int_0^T y_i(t) dt$$

and then build-up the *covariance matrix* \bar{K} defined by

$$\bar{K} := \sum_{i=1}^m \int_0^T (y_i(t) - \bar{y})(y_i(t) - \bar{y})^* dt.$$

Now, we can proceed in analogy. Let $\lambda_1 \geq \dots \geq \lambda_n \geq 0$ be the ordered eigenvalues of \bar{K} and u_j the corresponding eigenvectors. We define $V_d = \text{span}\{u_1, \dots, u_d\}$. Then the optimal affine subspace fixed in \bar{y} is given by $V_{d,\bar{y}} = \bar{y} + V_d$ and the optimal orthogonal projection is given by

$$\Pi_d y := \Pi_d(y - \bar{y}) + \bar{y}.$$

2.2 Choosing the Dimension

Finally, we have to answer the question how to choose the dimension d of the subspace V_d such that we get a *good* approximation of our data set. Here, Theorem 1 can guide us, since it provides the overall least-squares error. Hence, we only have to study the eigenvalues of K . In terms of a dynamical system, large eigenvalues correspond to main characteristics of the system, while small eigenvalues give only small perturbations of the overall dynamics. The goal is to choose d small enough while the *relative information content* [1] of the basis for V_d , defined by

$$I(d) = \frac{\sum_{j=1}^d \lambda_j}{\sum_{j=1}^n \lambda_j},$$

is near to one. I.e. if the subspace V_d should contain a percentage p of the information in V , then one should choose d such that

$$d = \text{argmin} \left\{ I(d) : \quad I(d) \geq \frac{p}{100} \right\}.$$

Remark 2. If one wants to significantly reduce the dimension of the problem, i.e. $d \ll n$, one needs clearly that the eigenvalues decrease sufficiently fast. In many applications like fluid dynamics or heat transfer one observes an exponential decrease of the eigenvalues, such that one has indeed a good chance to derive low-order approximate models (see also Section 3).

Remark 3. Note, that the POD modes are optimally approximating a given data set in the least-squares sense, but they are not constructed to be the modes approximating the dynamics generating the given the data set. For example, consider a low Mach number flow where acoustic effects play a crucial role [34]. Due to their small energy compared to the high energy hydrodynamic pressure fluctuations, they would be neglected in our reduced model, although being a relevant feature of the full dynamical system. Further, although an increase of the number of POD modes leads to a decrease of the least squares error, it might happen that more POD modes lead to a worse approximation of the full dynamics. New approaches exploiting the relation between POD and balanced truncation [21, 34, 37] or dual techniques [24, 25] yield a way out of this problem.

2.3 POD and Galerkin Projection

To get reduced order models for dynamical systems one uses a *Galerkin projection* onto the subspace V_d . This is the standard technique to reduce partial differential equations with a method of lines to a system of ordinary differential equations. Standard finite element approaches for the spatial discretization are using basis functions which are in general not correlated with the overall system dynamics [12, 17]. This approach holds for any subspace V_d , but having now the POD modes at hand one can use naturally this optimal approximating subspace. So, let $f : V \rightarrow V$ be a vector field and consider the solution $y(t) : [0, T] \rightarrow V$ of the dynamical system

$$\dot{y}(t) = f(y(t)),$$

which we e.g. get from a discretization of a partial differential equation via finite elements or finite differences. Further, we construct an approximating d -dimensional subspace $V_d = \text{span}\{u_1, \dots, u_d\}$ via POD. The reduced order model is then given by

$$\dot{y}_d(t) = \Pi_d f(y_d(t)) \quad (2)$$

with solution $y_d(t) : [0, T] \rightarrow V_d$. Here, $\Pi_d f(y_d(t))$ is just the projection of the original vector field f onto the subspace V_d . To rewrite :=reduced component wise we use

$$y_d(t) = \sum_{j=1}^d \chi_j(t) u_j$$

and substitute this into :=reduced. Then, a multiplication with u_j^* yields

$$\dot{\chi}_j(t) = u_j^* f(y_d(t)) = u_j^* f \left(\sum_{j=1}^d \chi_j(t) u_j \right), \quad j = 1, \dots, k,$$

i.e. we are left with a coupled system of d ordinary differential equations for the evolution of $y_d(t)$. Clearly, also the initial condition has to be projected, i.e.

$$y_d(0) = \Pi_d y(0).$$

Remark 4. For an affine subspace $V_{d,\bar{y}}$ the reduced model for the dynamics of $y_d : [0, T] \rightarrow V_{d,\bar{y}}$ can be derived in analogy.

2.4 POD and Snapshots

Concerning real world applications like flow problems, one has to encounter many degrees of freedom, such that the dimension n of the phase space might be very large. In practical computations this can lead to a phase space with dimension $n = 10^6 - 10^{10}$. Hence, the calculation of the POD modes would require the solution of a large eigenvalue problem for a full matrix $K \in \mathbb{R}^{n \times n}$, which might be infeasible. To overcome this problem Sirovich [36] proposed the *method of snapshots*, which proves to a powerful tool for the computation of the eigenfunctions. Instead of solving the eigensystem for the matrix $K \in \mathbb{R}^{n \times n}$ one only needs to consider a matrix in $\mathbb{R}^{m \times m}$, where m is the number of snapshots considered (for a more detailed discussion we refer to [12, 17] and the references therein).

Snapshots are constructed from the trajectories of the dynamical system by evaluating them at certain discrete time instances $t_1, \dots, t_m \in [0, T]$, i.e. they are given by $y_i = y(t_i) \in \mathbb{R}^n$. Then, we get a new correlation matrix K defined by

$$K = \sum_{i=1}^m y(t_i)y(t_i)^*. \quad (3)$$

Remark 5. But how many snapshots should one choose? An educated guess would be to choose less than n , since we cannot expect to get more than n linearly independent vectors. On the other hand, snapshots should be always taken whenever the dynamics of the system is changing. Hence, it might happen that $m > n$. Be aware that the chosen snapshot vectors might be linearly dependent, such that it is not clear, if one can reconstruct a suitable basis. Further note that the snapshots depend clearly on the initial datum and on a given input.

We build the matrix $Y = (y(t_1), \dots, y(t_m)) \in \mathbb{R}^{n \times m}$ consisting in the columns of the snapshots. Hence, in each row we find the trajectories of the dynamical system at discrete time events. Then, the sum (3) can be written as $K = YY^*$. In the method of snapshots one considers now instead the matrix $Y^*Y \in \mathbb{R}^{m \times m}$ and solves the eigenvalue problem

$$Y^*Yv_j = \lambda_j v_j, \quad j = 1, \dots, m, \quad v_j \in \mathbb{R}^m.$$

In the following we will see that the eigenvalues are indeed the same. Again, we can choose an orthonormal basis of eigenvectors $\{v_1, \dots, v_m\}$ and the corresponding POD modes are given then given by

$$u_j = \frac{1}{\sqrt{\lambda_j}} Yv_j, \quad j = 1, \dots, m.$$

2.5 POD and SVD

The above discussion suggest that there is indeed a strong connection of POD and *singular value decomposition* (SVD) for rectangular matrices (for an excellent overview see [12, 16, 17]). Consider a matrix $Y \in \mathbb{R}^{n \times m}$ with rank d . From standard SVD we know that there exist real numbers $\sigma_1 \geq \dots \geq \sigma_d > 0$ and unitary matrices $U \in \mathbb{R}^{n \times n}$ and $V \in \mathbb{R}^{m \times m}$ such that

$$U^* Y V = \begin{pmatrix} \Sigma_d & 0 \\ 0 & 0 \end{pmatrix} = \Sigma \in \mathbb{R}^{n \times m}, \quad (4)$$

where $\Sigma_d = \text{diag}(\sigma_1, \dots, \sigma_d) \in \mathbb{R}^{d \times d}$.

The positive numbers σ_i are called singular values of Y . For $U = (u_1, \dots, u_n)$ and $V = (v_1, \dots, v_m)$ we call $u_i \in \mathbb{R}^n$ the left singular vectors and $v_i \in \mathbb{R}^m$ the right singular vectors, which satisfy

$$Y v_i = \sigma_i u_i \quad \text{and} \quad Y^* u_i = \sigma_i v_i, \quad i = 1, \dots, d.$$

These are eigenvectors of YY^* and Y^*Y with eigenvalues σ_i^2 , $i = 1, \dots, d$.

The link between POD and SVD lies in the fact that the approximating POD basis should contain as much information or energy as possible. Mathematically, we can write the problem of approximating the snapshot vectors y_i by a single vector u as the constrained optimization problem

$$\max \sum_{j=1}^m |\langle y_j, u \rangle|^2 \quad \text{s.t.} \quad |u| = 1. \quad (5)$$

Using the Lagrangian formalism we derive that a necessary condition for this problem is given by the eigenvalue problem

$$YY^*u = \sigma^2 u.$$

The singular value analysis yields that u_1 solves this eigenvalue problem and the functional value is indeed σ_1^2 . Now, we iterate this procedure and derive that u_i , $i = 1, \dots, d$ solves

$$\max \sum_{j=1}^m |\langle y_j, u \rangle|^2 \quad \text{s.t.} \quad |u| = 1 \text{ and } \langle u, u_j \rangle = 0, \quad j = 1, \dots, i-1 \quad (6)$$

and the value of the functional is given by σ_i^2 .

By construction it is clear that for every $d \leq m$ the approximation of the columns $Y = (y_1, \dots, y_m)$ by the first d singular vectors $\{u_i\}_{i=1}^d$ is optimal in the least-squares sense among all rank d approximations to the columns of Y .

Altogether, this leads the way to the practical determination of a POD basis of rank d . If $m < n$ holds, then one can compute the m eigenvectors v_i corresponding to the largest eigenvalues of $Y^*Y \in \mathbb{R}^{n \times n}$. These relate to the POD basis as follows

$$u_i = \frac{1}{\sigma_i} Y v_i, \quad i = 1, \dots, d.$$

3 POD in Radiative Heat Transfer

In the following we want to test the POD approach for model reduction in a radiative heat transfer problem given by the so-called Rosseland model [26], which is given by the nonlinear parabolic partial differential equation

$$\partial_t y(x, t) = \operatorname{div} ((k_h + k_r y^3(x, t)) \nabla y(x, t)) \quad (7)$$

for the temperature distribution $y(x, t)$. Here, (x, t) is in the space-time cylinder $Q = \Omega \times (0, T)$, where Ω is a bounded domain in \mathbb{R}^2 . The coefficients k_h and k_r are positive constants related to the conductive and radiative heat transfer. This model has to be supplemented with boundary data

$$n \cdot \nabla y(x, t) = h(b(x, t) - y(x, t)) + \alpha (b^4(x, t) - y^4(x, t)) \quad (8)$$

for $(x, t) \in \partial\Omega \times (0, T)$ and an initial datum

$$y(x, 0) = y_0(x) \quad (9)$$

for $x \in \Omega$. Here, $y_0(x)$ is the initial temperature, $b(x, t)$ a specified boundary temperature, and h and α measure the conductive and radiative heat loss over the boundary, respectively. For the forthcoming simulations we choose

$$k_h = 1, k_r = 10^{-7}, h = 1, \alpha = 5 \cdot 10^{-7}, y_0(x) = 500, b(x, t) = 300.$$

Remark 6. Note, that this model has two nonlinearities: One in the heat conductivity which models volume radiation and one in the boundary condition which adds additional surface radiation to the standard Newton cooling law, where the temperature flux is proportional to the temperature difference. Hence, we can expect that boundary layers will appear in the solution such that the POD modes will significantly differ from the eigenfunctions of the Laplacian.

This nonlinear partial differential equation is solved using the finite element package FEMLAB. The computational domain $\Omega \subset \mathbb{R}^2$ is an ellipse depicted in Figure 1 with center zero and an aspect ratio of two. There, one also finds the triangular mesh consisting of 1769 degrees of freedom. For the discretization we use linear finite elements with the nodal basis $\{\varphi_i(x)\}_{i=1}^n$ and write the approximate solution as

$$y_h(x, t) = \sum_{i=1}^n y_i(t) \varphi_i(x).$$

The finite element ansatz for the equation :=RHT yields a dynamical system for $Y(t) = (y_1(t), \dots, y_n(t))$

$$\dot{Y}(t) = f(Y(t)),$$

where the right hand side is computed via the Galerkin projection onto the finite element space.

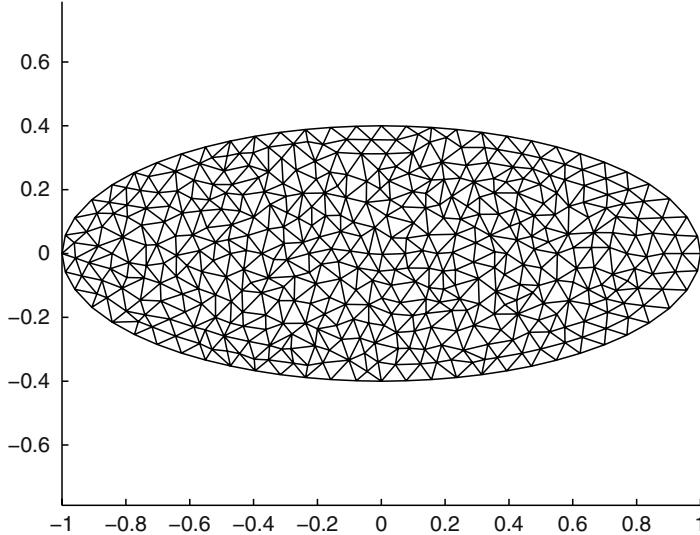


Fig. 1. Computational Domain and Mesh

For the POD analysis we take $m = 81$ equidistantly distributed snapshots $\{Y(t_j)\}_{j=1}^m$ in the interval $[0, T]$, build up the snapshot matrix

$$Y = \begin{pmatrix} y_1(t_1) & \cdots & y_1(t_m) \\ \vdots & & \vdots \\ y_n(t_1) & \cdots & y_n(t_m) \end{pmatrix} \in \mathbb{R}^{n \times m}$$

and introduce the correlation matrix $K = Y^*Y \in \mathbb{R}^{m \times m}$. Using the MATLAB routine `eigs.m` one can easily compute the eigenvalues λ_j and the eigenvectors u_j , $j = 1, \dots, m$. Despite of the high nonlinearity of our problem, we get exponential decay of the eigenvalues, which can be seen in Figure 2.

From the eigenvectors we can compute the POD basis $\{u_i\}_{i=1}^d$ of rank d as follows

$$u_i = \frac{1}{\sqrt{\lambda_i}} \sum_{j=1}^m v_i^j y_j, \quad i = 1, \dots, d,$$

where v_i^j is the j -th component of the eigenvector v_i . In the following we will use the normalized POD basis functions $\psi_i = u_i / \|u_i\|$. The first eight of these basis functions can be found in Figure 4. Computing the relative information content for the first mode yields already $I(1) = 99.96\%$.

To get a reduced POD model we use the POD basis $\{\psi_i\}_{i=1}^d$ in a Galerkin ansatz

$$y_d(x, t) = \sum_{i=1}^d \chi_i(t) \psi_i(x),$$

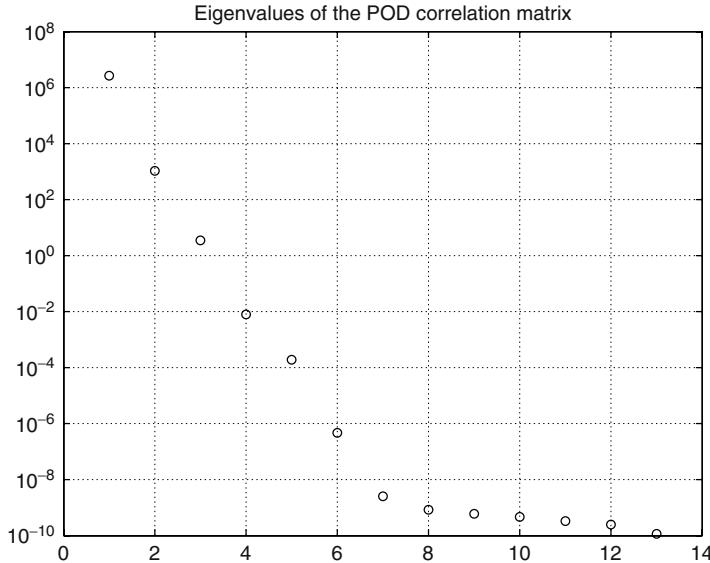


Fig. 2. Eigenvalues of the correlation matrix

plug this into the equation and test with χ_j , which yields

$$\begin{aligned} \partial_t \chi_i(t) &= - \int_{\Omega} \left(k_h + k_r \left(\sum_{k=1}^d \chi_k(t) \psi_k(x) \right)^3 \right) \sum_{i=1}^d \chi_i(t) \nabla \psi_i(x) \cdot \nabla \psi_j(x) \, dx \\ &\quad + \int_{\partial\Omega} \left(k_h + k_r \left(\sum_{k=1}^d \chi_k(t) \psi_k(x) \right)^3 \right) \sum_{i=1}^d \chi_i(t) n \cdot \nabla \psi_i(x) \psi_j \, ds \\ &=: g(\chi(t)), \quad i = 1, \dots, d, \quad \chi = (\chi_1, \dots, \chi_d). \end{aligned}$$

This gives the ordinary differential system $\dot{\chi}(t) = g(\chi(t))$ of size $d \times d$, which can be solved with an implicit Euler method for example.

Remark 7. Note that the ordinary differential system can be solved quite fast due to its small size. Nevertheless, one should be aware that building up the system might need some time since we have to compute the inner products for *global basis functions*, in contrast to the finite element basis which has compact support. Alternatively, one can compute the projections of the finite element matrices onto the reduced space.

To get an idea how well our reduced model approximates the full model, we measure the difference of $y_h(x, t)$ and $y_d(x, t)$ in the norm of the space $L^2(0, T; L^2(\Omega))$, i.e.

$$\|y_h - y_d\|_{L^2(0, T; L^2(\Omega))}^2 = \int_0^T \int_{\Omega} (y_h(x, t) - y_d(x, t))^2 \, dx \, dt.$$

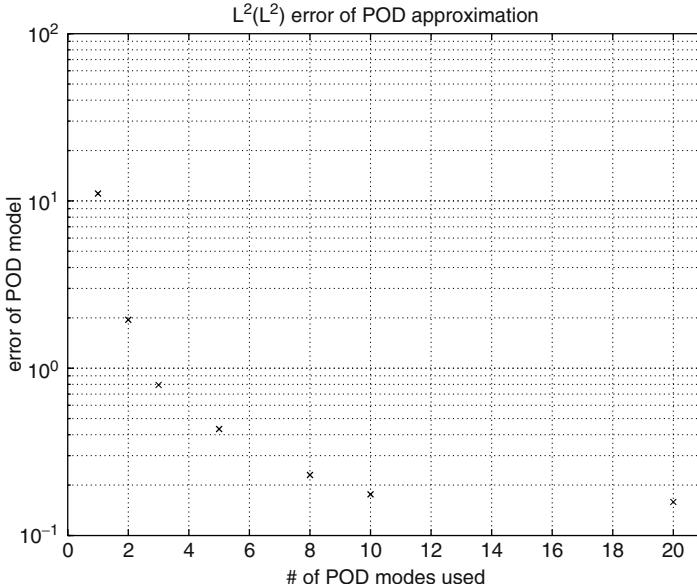


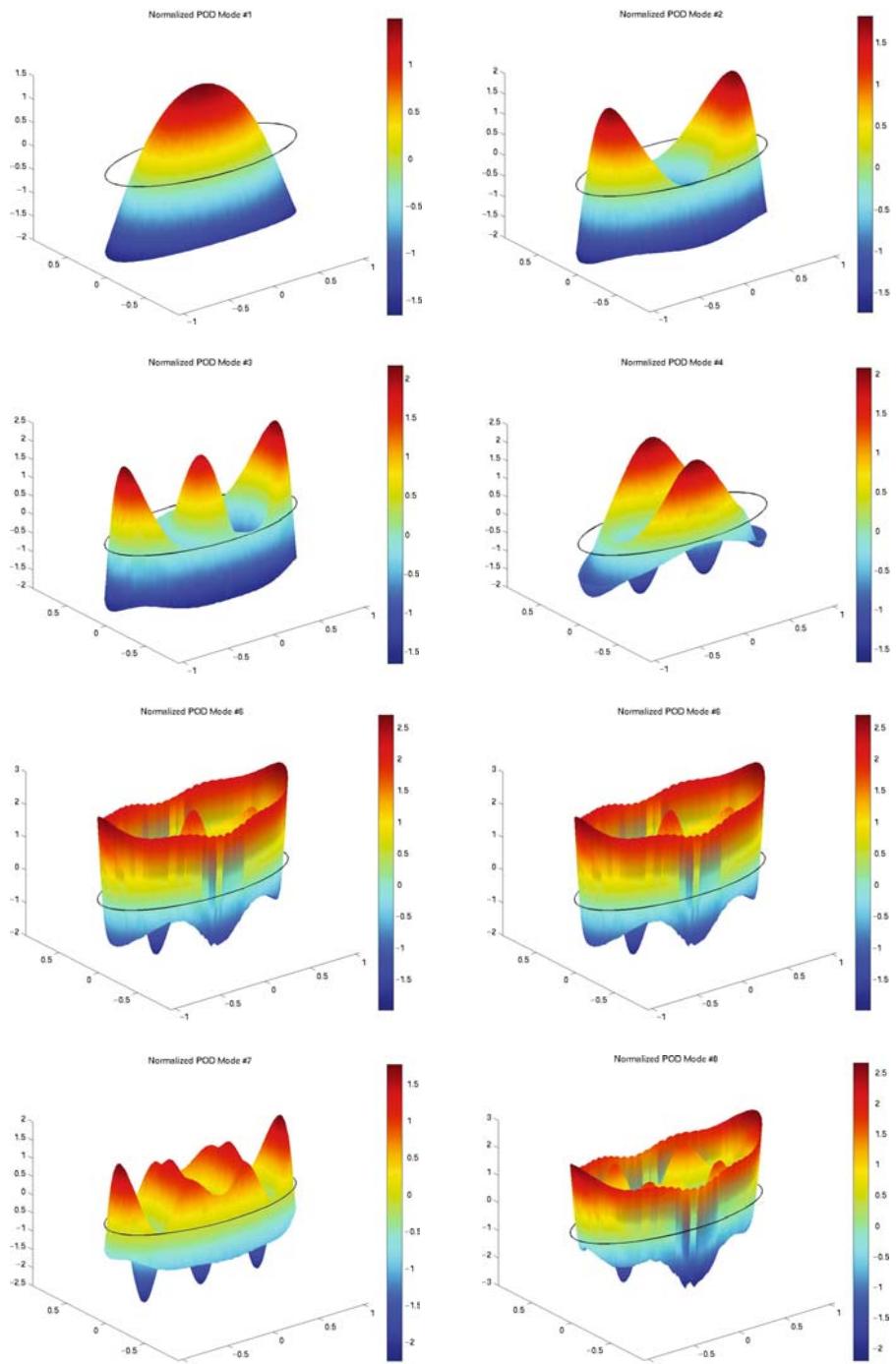
Fig. 3. Error between the full and the reduced model

This error is plotted in Figure 3 for different sizes d of the reduced model. Most remarkable is that already three POD modes yield a mean error of 1 in the temperature, which yields a relative mean error of less than 1%.

Remark 8. It is worth noting that in the context of partial differential equations, it is also possible to build up the correlation matrix using a different inner product, which is more related to the Galerkin ansatz, i.e. here one could also use the inner product of $H^1(\Omega)$. I.e. one replaces the correlation matrix by $K = YMY^*$, where $M \in \mathbb{R}^{n \times n}$ is a symmetric, problem dependent matrix. This yields a different POD basis which might give even better results (for the linear case see e.g. [11]). Further, it was pointed out that one may increase the accuracy of the reduced model by adding finite differences of the snapshots to the snapshot set, i.e. also considering time derivatives of the snapshots [12, 17]. Clearly, this does not change the space spanned by the snapshots since we are only adding linearly dependent vectors. Nevertheless, we get different weights in the correlation and thus again different modes.

4 Conclusions and Future Perspectives

Being a powerful tool for model reduction of large-scale dynamical systems, POD is acquiring increasing attention in the mathematics and engineering community. Presently, there is the tendency to test its performance in more and more fields of application, like fluid and structural dynamics, reducing models based on partial

**Fig. 4.** The first 8 POD modes

differential equations for devices in electric circuits, frequency averaging in radiative heat transfer, or even tire modeling. These different fields clearly will have different requirements on the POD method. Either, one wants to have structure preserving reduced models [5, 7, 20] or estimates on the quality of the surrogate model [11, 24, 25, 29, 30]. In particular, the derivation of error estimates for POD models is a field of intensive research which follows two lines: First, the combination of POD and balanced truncation (c.f. [34, 37] and the references therein) and second exploiting the special structure of Galerkin approximations to partial differential equations (c.f. [12, 17] and the references therein).

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