Standardized Non-Intrusive Reduced Order Modeling Using Different Regression Models With Application to Complex Flow Problems

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Abstract

We present a non-intrusive reduced basis method (RBM) for unsteady non-linear parametrized partial differential equations (PDEs) based on proper orthogonal decomposition (POD) with regression. Three different regression models are compared, including radial basis function (RBF) regression, Gaussian process regression (GPR) and artificial neural networks (ANNs). The established method is extended with additional preprocessing steps, including centering before POD standardization by singular values before regression and a standardized error measure. These steps benefit the interpretability and allow to reuse the presented framework on different problems. Furthermore, we propose to treat time not as a parameter but rather as a discretized coordinate similar to space. The approach is first validated on steady as well as time-dependent driven cavity viscous flows. Additionally, we study the flow of plastic melt inside a cross-section of a co-rotating twin-screw extruder. This is characterized by a time- and temperature-dependent flow of a generalized Newtonian fluid on a moving domain. The achieved standardized errors are less than 3\% for the predicted velocity, pressure and temperature distributions. We find that GPR can offer several advantages over an ANN, constituting a viable and computationally inexpensive non-intrusive RBM.

Keywords: non-intrusive reduced order modeling, proper orthogonal decomposition, artificial neural networks, Gaussian process regression, radial basis function regression, non-Newtonian flow

1. Introduction

Many problems in engineering and science are modeled as \textsuperscript{PDEs} that may be parametrized in material properties, initial and boundary conditions or geometry. Numerical methods, such as the finite element method (FEM), have been widely adopted to solve these problems. However, obtaining a high-fidelity solution for complex problems is demanding in terms of the required computational resources. Especially in many-query contexts, such as uncertainty-quantification, design or optimization, where the \textsuperscript{PDE} is repeatedly solved for different parameters, the computational burden becomes impractical. Similarly, in time-critical applications, e.g. control, the real-time evaluation of a complex model requires prohibitive amounts of computational power and storage.

Reduced order modeling (ROM) is an umbrella term for methods aiming to alleviate this computational cost by replacing the full-order system by one with a significantly smaller dimension and paying a price of a controlled loss in accuracy \textsuperscript{[1]}. ROM methods have been developed simultaneously in different fields of research, notably control, structural mechanics and fluid dynamics \textsuperscript{[2–4]}. As a result, a multitude of ROM methods and classifications thereof have developed. Antoulas et al. \textsuperscript{[2]} classify ROM in \textit{truncation} based methods, which focus on preserving key characteristics of the system rather than reproducing the solution, and \textit{projection} based methods, which replace the high dimensional...
solution space with a reduced space of much smaller dimension. Eldred and Dunlavy [5] and Benner et al. [4] use three categories instead—projection-based, data-fit and hierarchical reduced models. The latter include a range of physics-based approaches, although other authors exclude simplified-physics methods from ROM [3, 6]. Data-fit models use interpolation or regression methods to map system inputs to outputs, i.e., parameters to solutions. Finally, according to this classification, in projection-based methods the full-order operators are projected onto a reduced basis (RB) space allowing to solve a small reduced model quickly.

In other communities, including computational fluid dynamics (CFD), RBMs are so widely adopted, that they are almost synonymous to ROM [3, 7]. These are further divided into intrusive RBMs which correspond to the previous definition of projection based methods, and non-intrusive RBMs in which instead the solutions are projected onto the RB. This yields a compact representation of a solution in the RB as a vector of reduced coefficients. Regression or interpolation can then be applied to rapidly determine the reduced coefficients at a new parameter instance making the non-intrusive RBMs fall into the previously defined data-fit ROM class. Both intrusive and non-intrusive RBMs are characterized by an offline-online paradigm. The offline phase is associated with some computational investment due to generating a collection of solutions, extracting the RB, and setting up the ROM. However, this allows to rapidly evaluate the ROM during the online stage. Ideally, the complexity of the online evaluation is independent of the full-order model.

A central question of how to determine the RB remains. A multitude of methods have been proposed in literature such as greedy algorithms, dynamic mode decomposition, autoencoders and others [4, 7]. However, the arguably most popular method is POD which constructs a set of orthonormal basis vectors representing common modes in a collection of solutions [7].

Within the intrusive RBM framework, mostly the Galerkin procedure is used [7, 9, 12]. However, a naive approach of projecting the operators onto the RB space has a crucial flaw for non-linear problems, namely, the parameter dependent full-order operators still have to be reassembled during the online computation severely limiting rapid evaluation of new reduced solutions. Affine expansion mitigates this problem under the assumption of affine decomposability of the operators in the weak form. However, this assumption is violated for general non-affine problems [12]. Approaches like empirical interpolation method (EIM) [13], discrete EIM [14] and trajectory piece-wise linear (TPWL) method [15] have been introduced to recover the advantage of an affine decomposition by another approximation [4, 7], but they are problem-dependent and often impractical for general non-linear problems [9].

An alternative approach is offered by non-intrusive methods which enable a purely data-driven approach, as the solution set for the offline phase can originate either from an unmodified solver or experimental data. By projecting a solution onto the RB typically acquired via POD, the solution is compactly represented as a vector of reduced coefficients. The key step in the non-intrusive framework is fitting a regression model that maps the parameters to reduced coefficients. In principle, any interpolation or regression method can be used with POD such as, least squares regression [16] or cubic spline interpolation [17], but more common methods in the literature are RBF interpolation [3, 16, 18–21], GPR [9, 10, 22] and recently ANNs [8, 23–25].

In the CFD context, non-intrusive RBMs have been applied to a variety of problems. Examples of POD/GPR applications include time-dependent one-dimensional Burgers’ equation [10], incompressible fluid flow around a cylinder [10] and moving shock in a transonic turbulent flow [22]. POD ANN has been used for quasi-one dimensional unsteady flows in continuously variable resonance combustors [23], steady incompressible lid-driven skewed cavity problem [8], convection dominated flows with application to Rayleigh-Taylor instability [24], transient flows described by one-dimensional Burgers and two-dimensional Boussinesq equations [26] and aerostructural optimization [25]. Numerous examples of POD/RBF also exist [3, 16, 13, 20]. For a more complete overview on ROM in CFD we refer to existing reviews [3, 7].

To authors’ best knowledge these are all examples for Newtonian fluids. In contrast, only a few works utilizing any ROM for general Newtonian fluids exist. Examples include the TPWL method for transient elastohydrodynamic contact problems [27]. POD/Galerkin method for a steady incompressible flow of a pseudo-plastic fluid in a circular runner [28] and ROM based on residual minimization for generic power-law fluids [29]. However, all these works use intrusive methods. In [30] a non-intrusive ROM based on ANN has been applied to viscoplastic flow modeling. In this work, we construct a non-intrusive RBM framework using POD with regression and apply it to a range of complex flow problems. Three different models, namely, RBF regression, GPR and ANNs are used and assessed. We emphasize several adjustments to the established non-intrusive RBM—centering before POD standardization by singular values before regression and the use of a standardized error measure. These steps intend to increase the
We refer to VA commonly used tool to compute the RB is POD (see Section 2.1), which generates a set of orthonormal RB vectors reduced coe...

This work is structured as follows: Section 2 more formally introduces the non-intrusive RBM and the proposed adjustments. Section 3 describes the used RBF, GPR and ANN regression models. Section 4 outlines the governing equations and numerical method used to compute the datasets. In Section 5 our non-intrusive RBM is first validated against existing results on the skewed lid-driven cavity problem. Afterwards, the framework is transferred to the oscillating lid-driven cavity problem and, finally, the twin-screw extruder.

2. Non-intrusive reduced-basis method

After providing a high-level overview on ROM in Section 1, the non-intrusive RBM using POD and regression is described more formally in the following. First we describe the method as it is commonly reported [7–9, 12] and propose adjustments afterwards. Although the data for the non-intrusive RBM can originate from any numerical scheme or even experimental measurements, we illustrate the purpose of a basis using FEM. The high-fidelity solution to a parametrized PDE provided by an FEM solver is typically of the form

\[ s(x; \mu) = s^T(\mu)\phi(x) = \sum_{i=1}^{N_h} s_i(\mu)\phi_i(x) , \]  

where \( \phi = [\phi_1(x) \cdots |\phi_{N_h}(x)]^T \in \mathbb{R}^{N_h} \) is a collection of the (e.g. Lagrange) basis functions and the solution vector \( s(\mu) \in \mathbb{R}^{N_h} \) fixes the coefficient values for all \( N_h \) degrees of freedom (DOFs). The vector \( \mu \in \mathbb{R}^{N_d} \) collects all \( N_d \) input parameters. Given a training set with \( N_r \) different parameter samples \( P_r = \{ \mu_l \}_{l=1}^{N_r} \), and corresponding high-fidelity solution coefficients \( S_r = \{ s(\mu_l) \}_{l=1}^{N_r} \), the key idea in RBM is to construct a set of \( L \) reduced basis vectors \( V = [v_1^T] \cdots [v_L^T] \in \mathbb{R}^{N_h \times L} \) such that for any solution vector \( s(\mu) \) an approximation \( s_L(\mu) \) can be constructed as a linear combination of a small number of RB vectors \( L \ll N_h \):

\[ s(\mu) \approx s_L(\mu) = \sum_{i=1}^{L} y_i(\mu)v_i^T = Vy(\mu) , \]  

with the corresponding reduced coefficients \( y(\mu) = [y_1|\cdots|y_L]^T \in \mathbb{R}^L \). Inserting Equation [2] in Equation [1] gives the spatially interpolated approximation:

\[ s(x; \mu) \approx s_L(x; \mu) = y^T(\mu)V^T \phi(x) . \]  

We refer to \( V^T \phi(x) \) as the RB functions. However, throughout this work we mostly operate on the discrete entities \( V \) and \( s(\mu) \) and refer to them simply as RB and solution, respectively. A commonly used tool to compute the RB is POD (see Section 2.1), which generates a set of orthonormal RB vectors such that \( V^TV = I \). As a result, the reduced coefficients can be computed by projecting the high-fidelity solutions onto the RB:

\[ y(\mu) = V^Ts(\mu) . \]  

The final step of the offline stage is to recover the unknown underlying mapping from parameters to the reduced coefficients \( \pi: \mu \mapsto y(\mu) \). This is done by fitting a regression model \( \pi \) on the training data consisting of the input set of parameter samples \( P_r \), and the output set of the corresponding reduced coefficients \( y = (y(\mu))_{\mu \in P_r} \). Several choices
for regression models are described in Section 5. During the online stage the fitted regression model can be evaluated rapidly for new parameter samples to obtain the predicted reduced coefficients ̂y. These can be transformed back to the full space to reconstruct the predicted solution ̂s:

\[ ̂s_L(µ) = V_δ(µ) = V_δ(µ) . \]

(5)

Note that the online evaluation is completely independent of the solver used during the offline phase. In this work we reconstruct the full solutions at all \( N_f \) DOFs. The recovery \( V_δ(µ) \) involves \( O(N_f L) \) operations due to the matrix-vector multiplication, which still involves the number of DOFs in the full-order problem \( N_f \). However, this is not a fundamental drawback of the proposed method which focuses on the prediction of the reduced coefficients. Additionally, we do not necessarily have to use the same DOFs as the high-fidelity solver– the solution fields can also be subsampled.

2.1. Proper orthogonal decomposition

Given a snapshot matrix \( S = [s(µ_1), \ldots, s(µ_{N_s})] \in \mathbb{R}^{N_s \times N_f} \) in which the high-fidelity solutions are arranged columnwise, [POD] makes use of the singular value decomposition (SVD) to decompose the normalized snapshot matrix \( S/ \sqrt{N_f} \) into two orthonormal matrices \( W \in \mathbb{R}^{N_s \times N_f} \), \( Z \in \mathbb{R}^{N_f \times N_f} \) and a diagonal matrix \( Σ \in \mathbb{R}^{N_f \times N_f} \) such that

\[ S/ \sqrt{N_f} = W Σ Z^T . \]

(6)

Columns of \( W = [w_1| \cdots |w_{N_f}] \) and \( Z = [z_1| \cdots |z_{N_f}] \) are the left and right singular vectors of both \( S \) and \( S/ \sqrt{N_f} \). The entries in the rectangular diagonal matrix \( Σ = \text{diag}(σ_1, \ldots, σ_{N_f}) \) are the singular values of \( S/ \sqrt{N_f} \) and are ordered decreasingly \( σ_1 \geq σ_2 \geq \cdots \geq σ_{N_f} \geq 0 \). The closeness between a snapshot \( s(µ) \) and its rank \( L \) approximation \( s_L(µ) \) in the basis \( V \) can be quantified as their Euclidean distance using Equations (3) and (4):

\[ δ_{POD}(µ; V) = ||s(µ) - s_L(µ)||_2 = ||s(µ) - V V^T s(µ)||_2 . \]

(7)

The Schimdt-Eckart-Young (SEY) [32, 33] theorem states that the first \( L \) left singular vectors of \( S \), i.e., \([w_1| \cdots |w_{L}]\) are the optimal choice among all orthonormal bases \( V \in \mathbb{R}^{N_f \times L} \)

\[ V = [w_1| \cdots |w_{L}] = \text{argmin}_V δ_{POD}(P_{N_f}; V) \]

(8)

with respect to minimizing the root-mean-square of the projection error over all training snapshots

\[ δ_{POD}(P_{N_f}; V) = \sqrt{\frac{1}{N_f} \sum_{µ \in \mathcal{P}_{N_f}} δ_{POD}(µ; V)^2} = \frac{1}{\sqrt{N_f}} ||S - VV^T S||_F , \]

(9)

where \( ||.||_F \) denotes the Frobenius matrix norm. The notation \( δ_{POD}(P_{N_f}) \) is a generalization of \( δ_{POD}(µ) = δ_{POD}(µ) \), where we simply drop the brackets of the singleton set for ease of notation. The SEY theorem also states that the minimal associated projection error can be expressed as the root-squared sum of the left out singular values

\[ δ_{POD}(P_{N_f}; V) = \sqrt{\sum_{l=L+1}^{N_f} σ_l^2} . \]

(10)

In practice, computing \( \text{SVD} \) directly is prohibitively expensive, so the more efficient method of snapshots is used [34]. The idea is to first compute the eigenvalue decomposition of either \( SS^T/ N_f \in \mathbb{R}^{N_f \times N_f} \) or \( S^T S/ N_f \in \mathbb{R}^{N_f \times N_f} \), depending on which one is smaller. This limits the computational complexity of [POD] to be at worse cubic in the minimum of these dimensions \( O(\min\{N_f, N_f\}^3) \) [35]. Typically, the number of nodes \( N_b \) is much larger than number of snapshots \( N_s \), so the eigendecomposition works out as \( S^T S/ N_f = ZΛZ^T \), with \( Z \in \mathbb{R}^{N_f \times N_f} \) collecting the orthonormal eigenvectors and \( Λ = \text{diag}(λ_1, \cdots, λ_{N_f}) \) containing the real and positive eigenvalues of \( S^T S/ N_f \). With the above definition of [SVD] it follows that \( Σ = Λ^{1/2} \) and \( W = SZΣ^{-1}/ \sqrt{N_f} \).
2.2. Preprocessing

2.2.1. Snapshot centering

Within the ROM community, there is no clear consensus on whether to perform POD on non-centered data as described in Section 2.1 or on centered data. The centered snapshot matrix $S' = [s'(μ^1), \ldots, s'(μ^N)]$, where the mean over all columns $\bar{s} = 1/N_{tr} \sum_{μ \in \mathcal{P}_{tr}} s(μ)$ has been subtracted from each snapshot:

$$s'(μ) = s(μ) - \bar{s}. \quad (11)$$

Some authors suggest that centering before POD is ‘customary’ in ROM [11, 19, 36], but many counterexamples to this can also be found [17, 19, 37]. In [36] it is even argued for and in [17] against centering based on empirical evidence from specific applications. We prefer centering based on the following motivation.

According to the SEY theorem, the optimal reduced basis for centered data $c$ helps illustrate the described transformation steps.

Standardization allows to set tight bounds on the search-space or even reuse hyperparameters (see Section 3). Fig. 1 must be found using tedious trial-and-error or an extensive and computationally expensive hyperparameter-tuning.

2.2.2. Coefficient standardization

The standardized reduced coefficients are obtained by scaling the coefficients by the corresponding standard deviations:

$$\hat{y}'(μ) = (Σ^{-1})y'(μ). \quad (15)$$

$y'(μ)$ have a zero mean and unit variance for each of its $L$ components and can thus be viewed as a multi-variate Z-score of the centered reduced coefficients. This standardizes datasets across different problems and allows to reuse similar regression model architectures and learning processes, which are controlled by their hyperparameters. Normally, these must be found using tedious trial-and-error or an extensive and computationally expensive hyperparameter-tuning. Standardization allows to set tight bounds on the search-space or even reuse hyperparameters (see Section 3). Fig. 1 helps illustrate the described transformation steps.

2.2.3. Parameter standardization

Similar to the standardized reduced coefficients, we also introduce the standardized parameters as

$$\mu' = (μ - \hat{μ})/\hat{μ} \quad \text{with the mean } \hat{μ} = 1/N_{tr} \sum_{μ \in \mathcal{P}_{tr}} μ \text{ and the standard deviation } \hat{μ} = \sqrt{1/N_{tr} \sum_{μ \in \mathcal{P}_{tr}} (μ - \hat{μ})^2}. \quad (16)$$

These again have zero mean and unit variance on any dataset following the same distribution as the training dataset. This standardization step is beneficial for regression tasks in problems, where different parameters are on different scales (see e.g. Section 5.3). Both RBF and GPR rely on distances in parameter space and would otherwise neglect the smaller parameters (see Section 3.3 and Section 3.2). Similarly, ANNs show faster convergence with standardized inputs [39].
presented approach allows to estimate the true and predicted solutions to the naive approach via computing $\tilde{\delta}$ and $\delta$:

$$\tilde{\delta}(\mu; V^s) = \|s(\mu) - s_L(\mu)\|_2 = \|s^c(\mu) - VV^T s^c(\mu)\|_2.$$  (17)

Similarly, the absolute regression error $\delta_{\text{REG}}$ between the prediction $\hat{s}_L(\mu)$ and the projection $s_L(\mu)$ is introduced to describe how close the learned regression map $\hat{\pi}'$ approximates the observed regression map $\pi': \mu \mapsto y'$:

$$\delta_{\text{REG}}(\mu; V^s, \hat{\pi}') = \|\hat{s}_L(\mu) - s_L(\mu)\|_2 = \|\hat{s}_L^c(\mu) - s_L^c(\mu)\|_2 = \|V^s y'(\mu) - s_L^c\|_2 = \|\Sigma^c (\hat{\pi}'(\mu) - \pi'(\mu))\|_2.$$  (18)

Lastly, the absolute total error $\delta_{\text{POD-REG}}$ is introduced as the distance between the true and predicted solutions to quantify the performance of the whole non-intrusive RBM:

$$\delta_{\text{POD-REG}}(\mu; V^s, \hat{\pi}') = \|s(\mu) - \hat{s}_L(\mu)\|_2 = \|s^c(\mu) - \hat{s}_L^c(\mu)\|_2.$$  (19)

Fig. 2 illustrates these three types of errors. Additionally, it can be seen that the total error is composed of two orthogonal components, namely the regression and projection errors:

$$\delta_{\text{POD-REG}}(\mu)^2 = \delta_{\text{POD}}(\mu)^2 + \delta_{\text{REG}}(\mu)^2.$$  (20)

This can also be shown formally using the definition of the Euclidean vector norm $\|a\|_2^2 = a^T a$ and the fact that the predictions already belong to the linear span of the RBV $VV^T \hat{s}_L^c = \hat{s}_L^c$:

$$\|s^c - VV^T s^c\|^2 + \|VV^T s^c - \hat{s}_L^c\|^2 = s^c - s^c + s^c - \hat{s}_L^c = s^c - \hat{s}_L^c = \|s^c - \hat{s}_L^c\|^2.$$  (21)

Lastly, we note that the equivalence in Equation 18, paired with Equation 20, allows to compute both $\delta_{\text{REG}}$ and $\delta_{\text{POD-REG}}$ in $O(L)$ operations given that $\delta_{\text{POD}}$ is regression independent and can be pre-computed once. In contrast to the naive approach via computing $\hat{s}_L^c = V^T \hat{s}$ requiring $O(N h L)$ operations due to matrix-vector multiplication, the presented approach allows to efficiently use and monitor all errors during the training of the regression models.

2.3. Errors

2.3.1. Absolute errors

The absolute projection error $\delta_{\text{POD}}$ has already been introduced in Equation 7 as the Euclidean distance between the snapshot and its projection onto the reduced basis. The same holds with centering:

$$\delta_{\text{POD}}(\mu; V^s) = \|s(\mu) - s_L(\mu)\|_2 = \|s^c(\mu) - VV^T s^c(\mu)\|_2.$$  (17)

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$$\|s^c - VV^T s^c\|^2 + \|VV^T s^c - \hat{s}_L^c\|^2 = s^c - s^c + s^c - \hat{s}_L^c = s^c - \hat{s}_L^c = \|s^c - \hat{s}_L^c\|^2.$$  (21)

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The total error $\delta_{\text{POD-REG}}$ can be decomposed into two orthogonal components – the projection error $\delta_{\text{POD}}$ perpendicular to the span of centered basis $V^c$ and the regression error $\delta_{\text{REG}}$ belonging to the span. Illustration uses three degrees of freedom $N_b = 3$ and two reduced basis vectors $L = 2$.

Figure 2: The total error $\delta_{\text{POD-REG}}$ can be decomposed into two orthogonal components – the projection error $\delta_{\text{POD}}$ perpendicular to the span of centered basis $V^c$ and the regression error $\delta_{\text{REG}}$ belonging to the span. Illustration uses three degrees of freedom $N_b = 3$ and two reduced basis vectors $L = 2$.

The corresponding aggregate projection, regression and total errors $\delta_*(P)$, $* \in \{\text{POD, REG, POD-REG}\}$ on any dataset $P$ of cardinality $N$ are defined via the root-mean-square error (RMSE):

$$\delta_*(P) := \sqrt{\frac{1}{N} \sum_{\mu \in P} \delta_*(\mu)^2}.$$  

This choice is motivated by the form of the SEY theorem and treats both physical and parameter dimensions equally. Hence, Equation (20) holds for both individual and aggregate errors. From a statistical perspective, RMSE weights outliers more heavily than mean aggregation.

2.3.2. Standardized errors

The use of absolute errors makes it difficult to assess and interpret the performance of RBM especially across different datasets. The corresponding standardized projection, regression and total errors are defined in the following way:

$$\varepsilon_*(P) := \frac{\delta_*(P)}{\sqrt{\frac{1}{N_{tr}} \sum_{\mu \in P_{tr}} \|s(\mu) - \bar{s}\|^2}}.$$  

The choice of the denominator is motivated by its relation to the standard deviation of the training set. Hence, $\varepsilon$ can be interpreted as a multivariate extension of Z-score and describes the ratio between the Euclidian distance of two vectors and the standard deviation of the particular dataset. Always naively predicting the mean vector $\bar{s}$ leads to 100% aggregated total error $\varepsilon_{\text{POD-REG}}(P_{tr}) = 1$. Furthermore, the denominator can be related to POD since $1/N_{tr} \sum_{\mu \in P_{tr}} \|s(\mu) - \bar{s}\|^2 = 1/N_{tr} \text{Tr}(S^c S^c) = \sum_{n=1}^{N_b} (\sigma_n^c)^2$. Consequentially, it is easy to relate the relative projection error to SEY and Equation (10):

$$\varepsilon_{\text{POD}}(P_{tr}, V^c_L) = \frac{\sum_{n=L+1}^{N_b} (\sigma_n^c)^2}{\sum_{n=1}^{N_b} (\sigma_n^c)^2}.$$  

This corresponds to a commonly used measure known as relative information loss, which can be used to guide the choice of number of bases $L$. Furthermore, $\varepsilon$ is invariant to scaling and translation of snapshots and thus independent of the choice of units. This alleviates the need for designing dimensionless or normalized problems in order to interpret the errors and altogether allows for a more data-driven approach to non-intrusive RBM. Finally, within the broader classification of existing error measures, our definition of $\varepsilon$ can be viewed as a multivariate extension of the root-relative-squared error, option 2 as classified by Botchkarev [40].
2.4. Time-resolved problems

To our best knowledge, authors within the non-intrusive RBM framework, the trained regression model is used to predict the reduced coefficients at a new parameter location using \( \tilde{\pi} : \mu \mapsto \tilde{y} \). Note, that we standardize both inputs and outputs (see Section 2.2). As described in Section 1, any regression method can in principle be used. However, RBF regression is commonly used due to its simplicity, but lately the more flexible GPR and ANN methods have been adopted in the ROM community [3, 7]. In the following, these three models are described in more detail. Since a complete description of GPR and ANN including implementation details, is beyond the scope of this work, the reader is encouraged to consult the corresponding literature for more detail.

3. Regression models

Within the non-intrusive RBM framework, the trained regression model is used to predict the reduced coefficients at a new parameter location using \( \tilde{\pi} : \mu \mapsto \tilde{y} \). Note, that we standardize both inputs and outputs (see Section 2.2). As described in Section 1, any regression method can in principle be used. However, RBF regression is commonly used due to its simplicity, but lately the more flexible GPR and ANN methods have been adopted in the ROM community [3, 7]. In the following, these three models are described in more detail. Since a complete description of GPR and ANN including implementation details, is beyond the scope of this work, the reader is encouraged to consult the corresponding literature for more detail.

3.1. Radial basis function regression

RBF regression is a widely used tool in multivariate scattered data approximation. A radial function \( \Phi : \mathbb{R}^{N_r} \mapsto \mathbb{R} \) is multivariate, but can be reduced to a univariate function in some norm \( ||\cdot|| \) of its argument: \( \Phi(\mu^s) = \phi(\mu||\nu) \forall \mu^s \in \mathbb{R}^{N_r} \). Typically the Euclidean norm \( ||\cdot|| \) is used. RBF is radial in the sense that the norm of the argument can be interpreted as a radius from the origin or the center, i.e., \( r = ||\mu||_2 \). In this work the multiquadric RBF \( \phi(r) = \sqrt{1 + (r/r_0)^2} \) is used. The hyperparameter \( r_0 \) controlling the scale is chosen as the mean distance between the training points in parameter space.

In a regression task, multiple translated radial functions \( \{\phi(||\mu^s - \epsilon^{(m)}||)\}_{1 \leq m \leq M} \) are used to form a basis. The most natural and widely used choice is to use as many basis functions as there are data-samples \( M = N_t \), and to use the data locations as \( \epsilon^{(m)} = \mu^{(m)} \). The approximating regression function \( \tilde{\pi}_l^j : \mathbb{R}^{N_r} \mapsto \mathbb{R} \), \( \tilde{\pi}_l^j(\mu) = \tilde{y}_l^j \) for a single output component \( l \in [1, L] \) is expressed as a linear combination of the RBFs

\[
\tilde{\pi}_l^j(\mu; w) = \sum_{m=1}^M w_l^{(m)} \phi \left( ||\mu^s - (\mu^s)^{(m)}|| \right).
\]  

The weights \( w_l \) can be determined by enforcing the exact interpolation condition on the training data \( \tilde{\pi}_l^j((\mu^s)^{(n)}) = (\tilde{y}_l^j)^{(n)} \forall n \in [1, N_t] \). This leads to a linear system \( \mathbf{A}w_l = \tilde{y}_l^j \) with \( \mathbf{A} = (\phi(||\mu^s - (\mu^s)^{(m)}||))_{1 \leq m \leq N_t} \) being the coefficient matrix.

Note, that \( \tilde{\pi}_l^j \) is a scalar function. For \( L \) number of outputs, a different and independent function is constructed for each output dimension. However, solving multiple linear systems \( \mathbf{A}w_l = \tilde{y}_l^j \) for \( 1 \leq l \leq L \) is efficient, since they share the same coefficient matrix \( \mathbf{A} \), which must be ‘inverted’ or, in practice, decomposed only once. All the scalar interpolation functions can finally be gathered as components in the vector function \( \tilde{\pi} = [\tilde{\pi}_1^j \cdots \tilde{\pi}_L^j]^T \).

For more detailed information the interested reader is referred to [44]. The RBF implementation used in our work is based on the SciPy module for Python [45].
3.2. Gaussian process regression

In Gaussian process regression (GPR), a scalar regression function \( \tilde{f}_i^* : \mathbb{R}^N \rightarrow \mathbb{R} \), \( \tilde{f}_i^*(\mu^t) = y_i^* \) is constructed. However, instead of assuming a particular parametric form of the function and determining the parameters from the data, a non-parametric approach is pursued, in which the probability distribution over all functions consistent with the observed data is determined. This distribution can then be used to predict the expected output at some unseen input.

A central assumption in GPR is that any finite set of outputs, gathered in the vector \( y_i^* \), follows a multivariate Gaussian distribution \( y_i^* \sim \mathcal{N}(m, K) \) with the mean vector \( m \) and covariance matrix \( K \). This informs the notion that the regression function is itself an ‘infinite-dimensional’ or ‘continuous’ multivariate distribution or, formally, a Gaussian process (GP):

\[
\tilde{f}_i^*(\mu^t) \sim \mathcal{GP}(m(\mu^t), k(\mu^t, \mu^*_t)).
\]

Here, \((\mu^t, \mu^*_t)\) are all possible pairs in the input domain and \( k(\mu^t, \mu^*_t) = \mathbb{E}[f(\mu^t) - m(\mu^t)](\tilde{f}_i^*(\mu^*_t) - m(\mu^*_t)) \) are the mean and covariance functions, respectively. The mean vector \( m \) and the covariance matrix \( K \) are thus just particular realizations of these functions at the \( N \) corresponding input samples \( P = [\mu^t(1) \cdots \mu^t(N)] \in \mathbb{R}^{N \times N} \):

\[
m = m(P) := [m(\mu^t(0))]_{1 \leq i \leq N} \in \mathbb{R}^N
\]
\[
K = k(P, P) := [k(\mu^t(i), \mu^t(j))]_{1 \leq i, j \leq N} \in \mathbb{R}^{N \times N}.
\]

The central issue in GPR is determining a prior on these functions, represented by the best belief on the function’s behaviour (e.g. smoothness) before any evidence is taken into account. The prior is updated using training data to form a posterior on the mean and covariance functions. For the mean function, we adopt a widely used assumption of zero-mean \( m(\mu) = 0 \) [7, 46, 47]. This corresponds to the actual prior belief since data centering is used [46] as described in Section 2.2.1.

Determining the covariance function requires making stronger assumptions. The most widely adopted assumption is stationarity of the inputs, expressing that the covariance between outputs only depends on the Euclidian distance between them in the input space. A common example is the squared exponential function:

\[
k(\mu^t, \mu^*_t; \sigma_f, d) = \sigma_f^2 \exp \left( -\frac{1}{2d} \| \mu^t - \mu^*_t \|^2 \right)
\]

with \( \sigma_f \) being the prior covariance describing the level of uncertainty for predictions far away from training data and \( d \) being the correlation lengthscale. In this work, the more general anisotropic squared exponential kernel is used, which prescribes unique correlation lengthscale \( d_i \) for each input dimension and assumes additional observational noise \( \varepsilon \) for numerical stabilization [7, 46]:

\[
k(\mu^t, \mu^*_t; \sigma_f, d, \varepsilon) = \sigma_f^2 \exp \left( -\sum_{i=1}^{N} \left( \frac{\mu^t_i - \mu^*_t_i}{2d_i} \right)^2 \right) + \delta, \quad \text{where} \quad \delta = \begin{cases} \varepsilon & \text{if } \mu^t_i = \mu^*_i, \\ 0 & \text{else.} \end{cases}
\]

The hyperparameters \( \mathbb{H} = [\sigma_f, d, \varepsilon] \) are determined from the training input-output pairs \( \{P, y_i^*\} \) via maximum likelihood estimation:

\[
\mathbb{H} = \arg\max_{\mathbb{H}} \log p(y_i^*|K_0(\mathbb{H})) = \arg\max_{\mathbb{H}} \left\{ -\frac{1}{2} y_i^\top K_0^{-1}(\mathbb{H}) y_i - \frac{1}{2} \log |K_0^{-1}(\mathbb{H})| - \frac{N}{2} \log(2\pi) \right\},
\]

with \( K_0(\mathbb{H}) = k(P, P; \mathbb{H}) \) being the prior covariance matrix on training data and \( |\cdot| \) denoting the matrix determinant. To this end, the box-constrained limited-memory Broyden-Fletcher-Goldfarb-Shanno (L-BFGS) optimizer with 10 random initialization restarts is used. Due to standardizing outputs to unit variance (see Section 2.2.2), we can specify relatively tight bounds on the prior covariance \( \sigma_f \in [10^{-2}, 10^2] \) as we expect values within few orders of magnitude around 1.

Similarly, input standardization (see Section 2.2.3) allows us to set meaningful bounds for correlation lengthscales as \( d_i \in [10^{-2}, 10^2] \) for any problem. The lower bound \( 10^{-2} \) is chosen much smaller than the average distance between the
3.3. Artificial neural networks

ANNs are a computational paradigm within the field of machine learning (ML) that is loosely inspired by biological neural networks. With the theoretical property of being universal function approximators they have been used in a range of applications requiring non-linear function approximations. Different types or architectures of ANNs have proven to be particularly suitable in different domains, such as convolutional neural networks in image processing or recurrent neural networks in natural language processing [49]. In function regression tasks, the comparatively simple feedforward neural network (FNN) architecture has found a lot of success [50] and is used throughout this work. As the name suggests, ANNs is a network of simple computational units called neurons. Depending on the architecture these are arranged in different ways. In a FNN the neurons are organized in several layers and each neuron is connected to all neurons in both adjacent layers. These connections are directed and information flows from the lowest to the highest layer, called input layer \( \nu' \) and output layer \( \nu'' \), respectively. In between are multiple hidden layers \( \{\nu^h\}_{j \in [J]} \). This establishes an input-output mapping \( \tilde{\pi}^t : \mu' \mapsto \tilde{y}^t \). \( \pi^{t'}(\mu'; \Theta) = \tilde{y}^t \), which is parametrized by the strength of the connections between neurons, described formally by the weights \( \Theta_W \) and biases \( \Theta_b \). Additionally, non-linear activation functions \( g \) enable non-linear behavior of the ANN. Altogether an FNN can be modeled as

\[
\pi^{t'}(\mu'; \Theta) = \begin{cases} 
\nu' = \mu' \\
\nu^h = g^{h_i}(\Theta_W^{h_i} \nu^h + \Theta_b^{h_i}) \\
\nu^o = g^{o}(\Theta_W^{o} \nu^h + \Theta_b^{o}) \\
\tilde{y}^t = \nu'' 
\end{cases}
\]  

(33)

In a supervised learning paradigm, the ANN learns the weights and biases from the presented training data. Although learning differs from pure optimization because ultimately the performance on unseen test data or the generalization ability matters [49], the training process is posed as a non-convex optimization problem minimizing some loss function on the training data. We use the standardized regression error \( e_{\text{ANN}} \) with \( \text{RMSE} \) aggregation as introduced in Section 2.3

\[
\Theta = \arg\min_{\Theta} \sqrt{\frac{1}{\sum_{t \in T'} N_{t'}} \sum_{t \in T'} e^2_{\text{ANN}}(\mu; \pi^t(\mu'; \Theta))} = \arg\min_{\Theta} e_{\text{ANN}}(\nu''; \Theta) .
\]  

(34)
The training is typically done using gradient-based iterative optimizers in conjuncture with backpropagation for efficient gradient computation \[^{51}\]. In this work, the weight update in each iteration \(i\) is computed using a mini-batch \(\mathbb{P}_b \subset \mathbb{P}_{tr}\) consisting of \(N_b\) elements from the training set:

\[
\Theta^{i+1} = \Theta^i - \alpha G \left( \frac{\partial \text{ANN}(\mathbb{P}_b; \Theta^i)}{\partial \Theta} \right) .
\] (35)

We use \(N_b = 10\) and train for 5000 epochs or 5000\(N_{tr}/N_b\) iterations, since an epoch consists of presenting each training sample once. \(\alpha\) is the learning rate and the function \(G\) depends on the specific optimizer. The choice of optimizer is not straight forward, since its performance can strongly depend on the choice of training hyperparameters and the problem itself \[^{52}\]. In preliminary testing, the Adam optimizer \[^{53}\] is found to perform more consistently on different problems and to converge in fewer steps than competing optimizers, such as stochastic gradient descent (SGD) with Nesterov accelerated gradient (NAG) \[^{54}\] and L-BFGS. Even though other optimizers perform better in specific settings, we select Adam and note, that choosing the right optimizer is an active area of research in and of itself \[^{55}\].

The Adam hyperparameter values for stabilization and momentum decay \(\epsilon = 10^{-8}, \beta_1 = 0.9, \beta_2 = 0.999\) are chosen as suggested by Kingma and Ba \[^{53}\]. Similarly to Hesthaven and Ubbiali \[^{8}\], we restrict ourselves to shallow ANNs with two hidden layers \(N^l = 2\) each consisting of \(N_v\) neurons. We also use the hyperbolic tangent activation function \(g(x) = \tanh(x) = (e^x - e^{-x})/(e^x + e^{-x})\). Although in theory the Adam optimizer computes an adaptive learning rate for each trainable parameter, we find it beneficial to use a learning rate decay \(\alpha(e) = \alpha_0/(1 + 0.005 * e)\), where \(\alpha_0\) is the initial learning rate and \(e\) is the current epoch. It is observed that the choice of \(\alpha_0\) has a significant impact on the training process, so hyperparameter-tuning is performed for the initial learning rate \(\alpha_0\) and number of neurons per hidden layer \(N_v\). This is implemented as a grid-search over the hyperparameter space \((\alpha_0 \times N_v) \in [10^{-4}, 1] \times [10, 50]\) using the Tune module for Python \[^{56}\]. The best initial learning rate is expected to be a few orders of magnitude below that of the data, which is \(O(1)\) due to the standardization (see Section 2.2.2). For an appropriate ANN size we use the heuristic, that the number of learnable degrees of freedom should be similar to the number of outputs in the training dataset \(L N_v\). Using \(L = 20\) and \(N_{tr} = 100\) (see Section 5) we expect the optimal \(N_v\) to not be much larger than 35. A much smaller ANN could generalize well, but might not have the flexibility to approximate the function dynamics, while a much larger ANN might overfit. The ANN is implemented in PyTorch \[^{57}\].

4. Governing equations and numerical methods

In this work, we consider the fluid flow of a viscous, incompressible fluid on a time-dependent, deforming computational domain \(\Omega(t) \subset \mathbb{R}^{n_{u,t}}\), where \(t \in [0, t_{max}]\) is an instant of time and \(n_{u,t}\) is the spatial dimension. It is enclosed by its boundary \(\Gamma(t)\). The parameter dependent quantities as the velocity \(u = u(x, t; \mu)\), pressure \(p = p(x, t; \mu)\) and temperature \(T = T(x, t; \mu)\) are governed by incompressible Navier-Stokes and heat equations with viscous dissipation:

\[
\nabla \cdot u = 0 \quad \text{on} \quad \Omega(t) ,
\] (36a)

\[
\varrho \left( \frac{\partial u}{\partial t} + u \cdot \nabla u \right) - \nabla \cdot \sigma = 0 \quad \text{on} \quad \Omega(t) ,
\] (36b)

\[
\varrho c_p \left( \frac{\partial T}{\partial t} + u \cdot \nabla T \right) - \kappa \Delta T - 2\eta \nabla u : \varepsilon = 0 \quad \text{on} \quad \Omega(t) .
\] (36c)

The fluid density \(\varrho\), heat conductivity \(\kappa\) and specific heat capacity \(c_p\) are material specific parameters. The set of equations is closed by defining the Cauchy stress tensor \(\sigma\)

\[
\sigma(u, p) = -pI + 2\eta\dot{\gamma} + T\varepsilon(u) ,
\] (37)

where \(\varepsilon\) is the rate of strain tensor

\[
\varepsilon(u) = \frac{1}{2} \left( \nabla u + \nabla u^\top \right) .
\] (38)
The dynamic viscosity $\eta$ is a material constant for Newtonian fluids. Within this work we also consider generalized Newtonian fluids to model shear-thinning effects in flows of plastic melts. In this case, the dynamic viscosity also depends on the temperature $T$ and the shear rate $\dot{\gamma} = \sqrt{2} \gamma \langle \dot{\mathbf{u}} : \dot{\mathbf{e}}(\mathbf{u}) \rangle$. We use the Cross-William-Landel-Ferry (WLF) material model to describe this relation [58]:

$$
\eta(\dot{\gamma}, T) = \frac{\eta_0(T)}{1 + (\eta_0(T) \dot{\gamma}/\tau^*)^{1-n}}, 
$$

(39a)

$$
\eta_0(T) = D_1 \exp \left( \frac{A_1 (T - T_{ref})}{A_2 + (T - T_{ref})} \right),
$$

(39b)

$\tau^*$ is the critical shear stress at the transition from the Newtonian plateau, $D_1$ is the viscosity at a reference temperature $T_{ref}$ and $A_1$ and $A_2$ are parameters that describe the temperature dependency.

The Dirichlet and Neumann boundary conditions for temperature and flow are defined as:

$$u = g^f \text{ on } \Gamma_g^f(t),$$

(40a)

$$n \cdot \sigma = h^f \text{ on } \Gamma_g^f(t),$$

(40b)

$$T = g^T \text{ on } \Gamma_g^T(t),$$

(40c)

$$n \cdot \kappa \nabla T = h^T \text{ on } \Gamma_g^T(t).$$

(40d)

$\Gamma_g^f(t)$ and $\Gamma_g^T(t)$ are complementary portions of $\Gamma_g(t)$, with $i = f$ (Fluid), $T$ (Temperature).

As solution method, we use a deforming spatial domain (DSD) stabilized space-time (SST) finite element formulation [59], which constructs the weak formulation of the governing equations for the space-time domain. This solution method naturally takes deforming domains into account. The time interval $[0, T]$ is divided into subintervals $I_n = [t_n, t_{n+1}]$, where $n$ defines the time level. A space-time slab $Q_n$ is defined as the volume enclosed by the two surfaces $\Omega(t_n), \Omega(t_{n+1})$ and the lateral surface $P_n$, which is described by $\Gamma(t_n)$ as it traverses $I_n$. The individual space-time slabs are coupled weakly in time. First-order interpolation is used for all degrees of freedom. Thus, a streamline-upwind/Petrov-Galerkin (SUPG)/pressure-stabilizing/Petrov-Galerkin (PSPG) stabilization technique is used to fulfill the Ladyzhenskaya-Babuška-Brezzi (LBB) condition [60]. For a more detailed description of the solution method the interested reader is referred to [31, 59, 61].

For the selection of snapshots for the ROM we have to take into account that two spatial solution fields exist at a discrete time instance $t_{n+1}$: the upper field of the space-time slabs at $I_n$ and the lower field of the space-time slabs at $I_{n+1}$. These fields do not necessarily match exactly since they are only coupled weakly. However, we are only interested in the solution at the discrete time level. Thus, we only use the upper solution field of $I_n$. As described in Section 2 data for the non-intrusive ROM can stem from any discretization method or even experimental observations.

5. Numerical results

5.1. Skewed lid-driven cavity

The described method and implementation are validated on the skewed lid-driven cavity problem as described by Hesthaven and Ubbiali [8]. They investigate this problem using both POD-Galerkin and POD-ANN methods. We use the latter as a reference for our results. The lid-driven cavity is a well-known benchmark problem for two-dimensional viscous incompressible flows. The concerned problem setup is shown in Fig. 3. The computational domain consists of a parallelogram-shaped cavity with the no-slip condition on the base and the slanted walls, whereas the lid is driven horizontally with unit flow. The parameter space for the ROM is spanned by three geometrical parameters: horizontal length $\mu_1 \in [1, 2]$, wall length $\mu_2 \in [1, 2]$ and slanting angle $\mu_3 \in [\pi/6, 5\pi/6]$. We are interested in the steady velocity and pressure distributions, so any temperature and time effects in Equation (56) are neglected. The pressure is fixed at zero at the lower left corner. A Newtonian fluid model is used with unit density. The constant dynamic viscosity is computed depending on the geometry such that Reynolds number is always 400 according to the dimensionless equation $Re = \max(\mu_1, \mu_2)/\eta$. 

12
\[ \mu_3 \]

\[ \mu_1 \]

\[ \mu_2 \]

Figure 3: Parametrized geometry of the domain (left) and boundary conditions (right) of the skewed lid-driven cavity problem.

A regular structured computational mesh with 100 \times 100 nodes and space-time elements with 8-nodes is used. Training \( P_{tr} \), validation \( P_{va} \) and test \( P_{te} \) sets of sizes \( N_{tr} = 100 \), \( N_{va} = 50 \) and \( N_{te} = 50 \), are sampled from the parameter-space using randomized Latin-hypercube-sampling (LHS). A typical solution is shown in Fig. 4. Two separate RBs are constructed— one for the velocity \( u \) and one for the pressure \( p \). Both utilize \( L_u = L_p = 20 \) basis vectors. In each case, the three regression models described in Section 3 are trained to approximate the mapping from the standardized parameters to the standardized reduced coefficients \( \tilde{\pi}_s \): \( \mu_s \mapsto \gamma_s \). The training set is used to determine the parameters of RBF and ANN and the hyperparameters of the GPR. The validation set is used only for tuning the ANN’s hyperparameters. Finally, the test set is used to quantify how the models perform on unseen data.

Figure 4: An exemplary solution of the skewed lid-driven cavity for \( \mu = (1.90, 1.50, 1.60) \).

In order to compare the models, we first need to find an appropriate initial learning rate \( \alpha_0 \) and the number of neurons in both hidden layers \( N_{\nu} \) for the ANN. As described in Section 3.3, this is implemented as a grid-search over these two hyperparameters. The results are illustrated in Fig. 5. In both cases the performance is less sensitive to the size of the ANN— for any given \( N_{\nu} \) an appropriate \( \alpha_0 \) with the performance close to the optimum can be found. This suggests that perhaps tuning only over \( \alpha_0 \) is a viable alternative. In both cases, very large or very small initial learning rates lead to poor results. Lastly, larger ANNs tend to train better with smaller learning rates.

Fig. 6 compares the best identified ANN configurations (marked in Fig. 5) to RBF and GPR in terms of the total error on the test set \( \varepsilon_{POD-REG}(P_{te}) \). The models rank as one might expect— more flexible models perform better, i.e., ANN outperforms GPR which in turn outperforms RBF. The stagnation beyond a certain number of basis vectors \( L \) is consistent with observations by other authors [8, 62].
Figure 5: ANN hyperparameter tuning results for the skewed lid-driven cavity. Depicted are response surfaces of aggregated standardized regression errors on the validation set $\epsilon_{\text{ANN}}(\mathcal{P}_{\text{te}})$ over the initial learning rate $\alpha_0$ and number of hidden neurons $N_\nu$. The respective best configurations are marked.

Figure 6: Error analysis of different regression models for the skewed lid-driven cavity problem. The best identified ANN configurations marked in Fig. 5 are used.
To compare our findings with results published by Hesthaven and Ubbiali [8] the model performance is plotted again in Fig. 7 using their error definitions:

\[
\rho_{\text{POD}}(P_{te}) := \frac{1}{N_{te}} \sum_{\mu \in P_{te}} \frac{||s(\mu) - s_L(\mu)||_2}{||s(\mu)||_2} ,
\]

\[
\rho_{\text{POD-REG}}(P_{te}) := \frac{1}{N_{te}} \sum_{\mu \in P_{te}} \frac{||s(\mu) - \tilde{s}_L(\mu)||_2}{||s(\mu)||_2} ,
\]

For the specific result they use a similar ANN with \(N_{\nu} = 20\) and \(N_{p\nu} = 15\) neurons in both hidden layers, trained with the Levenberg-Marquardt algorithm on 100 training snapshots. As shown in Table 1 most relative errors are in close agreement suggesting our approach and implementation is valid. Interestingly, our relative projection error for \(p\) is much larger. This could potentially be attributed to differences in computational meshes and element types, but we do not investigate this further.

|       | \(u\)      | \(p\)      | \(\rho_{\text{POD}}\) | \(\rho_{\text{POD-ANN}}\) | \(\rho_{\text{POD}}\) | \(\rho_{\text{POD-ANN}}\) |
|-------|------------|------------|----------------------|----------------------|----------------------|----------------------|
| This work | 0.016      | 0.022      | 0.014                | 0.029                |                      |                      |
| Hesthaven and Ubbiali [8] | 0.010      | 0.020      | 0.004                | 0.030                |                      |                      |

Table 1: The achieved relative errors are in close agreement with the results reported by Hesthaven and Ubbiali [8] serving as validation to our approach.

Note, that the behaviour of the relative error is similar to the standardized error, including the qualitative behaviour, order that the models rank in and even the order of magnitude of errors. This is largely due to all quantities of the benchmark problem being normalized to \(O(1)\) per construction. However, in terms of the relative error for pressure, the ANN performs noticeably better than the GPR. This is likely explained by our aggregation of standardized errors relying upon RMSE, which weights outliers more heavily than the mean aggregation used for the relative error. This in turn suggests that the GPR deals better with more extreme solutions in pressure than ANN. However, the relative errors for \(L = 0\) are around 50% due to snapshot centering. In contrast, the standardized error is constructed such that naively predicting the mean of snapshots results in 100% error.

![Figure 7](image-url) ROM performance over number of basis functions in terms of the total relative error as defined by Hesthaven and Ubbiali [8].

Lastly, Fig. 8 shows streamlines at the same parameters as Hesthaven and Ubbiali [8], who argue that streamlines can visually uncover minor differences in the solutions. In all projections and predictions (using POD-ANN with \(L = 20\)) the main circulation zone corresponds closely to the high-fidelity snapshots. On the other hand, streamlines in areas of low-velocity, in particular recirculation zones are reconstructed only partially even in projections and even less in predictions. Especially in the left-most case, the predicted recirculation zone is very poor. This is also evident in
the relative error, which is twice as high as the mean on the test set. Note, that the projections can be made almost arbitrarily close to the truths by increasing the number of bases $L$, but beyond a certain point this does not benefit the prediction as illustrated in Fig. 6 and Fig. 7.

$$\mu = (1.12, 1.70, 1.08)$$

$$\mu = (1.90, 1.50, 1.60)$$

$$\mu = (1.78, 1.99, 2.29)$$

$$\varepsilon_{\text{POD}} = 2.3 \times 10^{-2}$$

$$\varepsilon_{\text{POD}} = 3.6 \times 10^{-2}$$

$$\varepsilon_{\text{POD}} = 1.7 \times 10^{-2}$$

$$\rho_{\text{POD}} = 1.3 \times 10^{-2}$$

$$\rho_{\text{POD}} = 1.4 \times 10^{-3}$$

$$\rho_{\text{POD}} = 7.6 \times 10^{-3}$$

$$\varepsilon_{\text{POD-ANN}} = 6.8 \times 10^{-2}$$

$$\varepsilon_{\text{POD-ANN}} = 3.8 \times 10^{-2}$$

$$\varepsilon_{\text{POD-ANN}} = 5.2 \times 10^{-2}$$

$$\rho_{\text{POD-ANN}} = 3.8 \times 10^{-2}$$

$$\rho_{\text{POD-ANN}} = 1.5 \times 10^{-2}$$

$$\rho_{\text{POD-ANN}} = 2.3 \times 10^{-2}$$

Figure 8: Streamlines for the skewed lid-driven cavity at three different parameter values. $L = 20$ bases and the ANN regression model are used. The corresponding errors illustrate that streamlines can uncover minor differences in flows, especially in the stagnating regions.

5.2. Oscillating lid-driven cavity

Having successfully validated our method and implementation, we aim to construct an intermediate problem with several characteristics found in the twin-screw extruder problem (see Section 5.3), namely, time dependency, parametrization of material properties and temperature distribution as output. Similar to the first problem, the unsteady lid-driven cavity problem is a common benchmark for time dependent flows. However, in ROM literature often either only the output velocity is examined or the problem is parametrized only in time [1, 62–66]. Since the literature does not offer a suitable benchmark, we define the oscillating lid-driven cavity problem as illustrated in Fig. 9.

The top of a unit square domain is driven horizontally with oscillating velocity $10 \sin(2\pi t)$ and has a constant temperature of 10. The initial fluid and all other walls are stationary and have zero temperature. 100 time steps of 0.01 each are considered in total corresponding to a single full oscillation of the sinusoidal lid velocity. Due to circulation, the warm top fluid is transported into the interior forming distinct temperature traces whose characteristic
depends on the heat conductivity and viscosity of the Newtonian fluid, parametrized as $\kappa = \mu_1 \in [0.001, 0.01]$ and $\eta = \mu_2 \in [0.01, 0.1]$. The fluid density and heat-capacity are fixed at $\varrho = 1$ and $c_p = 1$, respectively, and again a spatial mesh of $100 \times 100$ nodes is used. An exemplary solution is shown in Fig. 10 and in the top row of Fig. 13. The temperature fields have richer features, since the advective terms are more dominant than the diffusive terms compared to the flow problem.

To deal with the introduced time dependency when performing POD and regression, time is treated similar to space as proposed in Section 2.4. In addition to the preprocessing steps, this allows to follow the same procedure as described in Section 5.1 to construct and assess the ROMs. The results of the ANN tuning are displayed in Fig. 11. The qualitative behaviour of the tuning on the same hyperparameter space closely resembles the skewed lid-driven cavity problem in Fig. 5. This illustrates the intended purpose of data preprocessing and is discussed in more detail in Section 5.3. Again the performance is much less sensitive to the size of the network and optimal learning rates are similar.

Fig. 12 depicts the errors resulting from the best ANN configurations together with the other two regression models. Interestingly, both projection and prediction errors for velocity and pressure are several orders of magnitude smaller than for the skewed lid-driven cavity problem. We hypothesize this is due to $u$ and $p$ effectively being parametrized only in viscosity $\nu = \mu_1$ because the temperature equation is decoupled from the flow equations for a Newtonian fluid (see Equations 36 to 39). Since the parameter space is sampled with LHS, no two training parameter samples have equal viscosities $\mu_1(i) = \mu_1(j)$ or $d_1 \neq j$ and the effectively one-dimensional parameter space is sampled more densely. Temperature on the other hand depends on both parameters and shows greater complexity and errors.

To our surprise, the GPR significantly outperforms the ANN, especially for $u$ and $p$ despite the computational investment associated with hyperparameter tuning. We argue this is due to our choice of GPR’s anisotropic kernel (see Equation (29)), which can learn a unique correlation length for each input dimension. For all bases of $u$ and $p$ the learned lengthscales are less than one for viscosity $d_1 < 1$ indicating the presence of local dynamics. However, for heat conductivity most learnt lengthscales are at the upper bound of the box-constrained search space $d_2 = 100$. This implies
Figure 11: ANN hyperparameter tuning results for the oscillating lid-driven cavity. Depicted are response surfaces of aggregated standardized regression error on the validation set $\varepsilon_{\text{ANN}}$ over the initial learning rate $\alpha_0$ and number of hidden neurons $N_{\nu}$. The respective best configurations are marked.

Figure 12: Error analysis of different regression models for the oscillating lid-driven cavity problem. The best identified ANN configurations marked in Fig. 11 are used.
that the anisotropic GPR successfully recognizes the stationarity with respect to the second parameter. Increasing the upper bound might even further improve the GPR’s performance. We can test the limit case by manually fixing $d_2$ at infinity, i.e., explicitly neglecting the heat-conductivity. The resulting decrease in the regression errors can be seen in Table 2. Note, that the achieved regression errors are smaller than the projection errors, suggesting a very good fit and indicating that $L$ can be increased to further reduce the total error. If instead the isotropic squared exponential kernel (see Equation (28)) is used, the GPR ranks between ANN and RBF ($\varepsilon_{GPR}^{POD} = 1.3 \times 10^{-2}$ and $4.3 \times 10^{-3}$ for $u$ and $p$ respectively). Despite the ANN also having the flexibility to represent the stationarity with respect to $\mu_2$, it is not as straightforward to investigate whether this behaviour is learnt due to the abstract role of ANN’s weights. Instead, we can explicitly enforce this behaviour prior to hyperparameter tuning by removing the second input neuron altogether. Even though the regression errors decrease roughly five-fold, the result is still a magnitude worse than the anisotropic GPR. However, this observed disadvantage of ANNs is consistent with results in the literature. Especially relative to their computational cost, ANNs reportedly tend to outperform ANNs on small and smooth, i.e., densely sampled datasets, whereas [ANNS] excel at generalizing non-local function dynamics [67, 68]. RBF regression benefits the most from ignoring the second parameter, since it is isotropic per construction. In the one-dimensional and densely-sampled setting, it performs almost as well as the GPR. However, this demonstrates how RBF might underperform in other problem settings with more subtle anisotropy. More exotic anisotropic RBF regression methods have been proposed [69], but to the authors’ best knowledge these have not seen widespread adoption, especially in the ROM community.

Table 2: Regression errors when using both input parameters versus ignoring the heat-conductivity, which the velocity and pressure do not depend on. Some regression errors are less than the respective projection errors $\varepsilon_{POD} = 7.8 \times 10^{-6}$ and $5.9 \times 10^{-5}$ for $u$ and $p$, suggesting a very good fit.

|       | $u$       | $p$       |
|-------|-----------|-----------|
| $\tilde{\pi}(\mu_1, \mu_2)$ | $\varepsilon_{RBF} = 3.8 \times 10^{-2}$ | $\varepsilon_{GPR} = 2.4 \times 10^{-5}$ | $\varepsilon_{ANN} = 1.6 \times 10^{-3}$ |
| $\tilde{\pi}(\mu_1)$       | $\varepsilon_{RBF} = 8.1 \times 10^{-6}$ | $\varepsilon_{GPR} = 5.3 \times 10^{-6}$ | $\varepsilon_{ANN} = 6.7 \times 10^{-4}$ |

Fig. 13 illustrates the true temperature distribution of a sample from the test set alongside the absolute error of the predicted solution made by the GPR over several time steps. As expected, the largest errors manifest in the most dynamic regions.

![Figure 13](image1.png)  

**Figure 13:** The high-fidelity solution $T(\mu = (0.055, 0.0069) \in \mathbb{P}_u)$ (top) and the error in prediction made by the best GPR (bottom) at several time steps. Over all investigated time steps the standardized total error in the prediction is $\varepsilon_{POD-GPR} = 3.9 \times 10^{-3}$. 

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Notice, that the error of the particular prediction $\varepsilon_{\text{POD-GPR}}(\mu = (0.055, 0.0069)) \in P_{te} = 3.9 \times 10^{-3}$ is an order of magnitude smaller than the aggregated error over the whole test set $\varepsilon_{\text{POD-GPR}}(P_{te}) = 3.2 \times 10^{-2}$. Due to RMSE aggregation, a few outliers can determine the magnitude of the aggregated error. In our case, this manifests by errors not being distributed evenly over the parameter space. This is best illustrated on the effectively one-dimensionally parametrized velocity $u$. Fig. 14 shows a few training samples of the underlying regression maps which tend to become more dynamic towards small viscosities. For the first bases this effect is negligible, but as $l$ increases towards $L$, this region becomes undersampled and has higher test errors. Bottom row of Fig. 14 illustrates this for $\varepsilon_{\text{POD-GPR}}(P_{te})$, but all other investigated models, as well as the projection error behave the same. This is an indication that adaptive sampling methods can offer a performance boost [70].

Figure 14: A few select standardized reduced coefficients of the training set $P_{tr}$ over the viscosity $\nu = \mu_1$ for the velocity $u$ for the oscillating lid-driven cavity problem (top). For small $\mu_1$ the higher regression maps are undersampled which leads to large prediction errors in this region (bottom).

5.3. Twin-Screw Extruder

For our main use-case, we consider the flow of plastic melt inside a cross-section of a twin-screw extruder. It is characterized by a time- and temperature-dependent flow of a generalized Newtonian fluid on a moving domain. In contrast to previous problems, the non-Newtonian Cross-WLF fluid model is used for which the viscosity $\eta(\dot{\gamma}, T)$ depends on both the shear rate and temperature (see Equation (39)). This constitutes a strongly coupled problem in which not only the flow influences the temperature distribution but also vice-versa. This problem has already been investigated in a non-parametrized and non-ROM context in [71]. As mentioned in Section 1, the moving domain and the small gap sizes make the problem numerically challenging. Thus, the computational burden in a many-query context is very high and the potential of non-intrusive [ROM] is promising. However, to reduce the computational cost of the offline phase, we restrict the investigation to a two-dimensional cross-section of the extruder. The problem setup in Fig. 15 depicts two screws rotating with unit frequency $f$ inside a barrel with the geometries and material properties used in [71]. All fluid boundaries are prescribed a no-slip condition. The screws are adiabatic whereas the barrel is subject to a Dirichlet boundary condition of a linear increase in temperature along the $x$ direction. The pressure is fixed at zero at the upper cusp point. We are interested in 100 time steps of 0.0125 each corresponding to $1\frac{1}{4}$ full revolutions. We use a structured spatial mesh with 2459 nodes. The mesh is adapted to the changing domain over time using a spline-based mesh update technique [71] based on the on snapping reference mesh update method (SRMUM) [31]. The initial fluid temperature is 473 and velocities are zero. We choose to provide dimensionless quantities despite this being an engineering problem. However, all quantities can be interpreted in their corresponding SI units. The constants in Equation (39) describing the Cross-WLF fluid are $A_1 = 28.315$, $A_2 = 51.6$, $T_{ref} = 263.14$, 20
\[ \tau^* = 25000 \text{ and } n = 0.2923. \] The specific heat capacity is \( c_p = 1000 \). The screw movement forces the fluid through the small gap between screws with a large velocity and creates a significant pressure drop. The gap region is subject to large shear rates and thus local differences in viscosity. Due to viscous dissipation the fluid heats up and is transported upwards with the left screw and downwards with the right. This can be seen in exemplary solutions in Fig. 16 and the left column of Fig. 20. To build the ROM we consider a parameter space spanned by thermal conductivity \( \kappa = \mu_1 \in [10^0, 10^1] \), reference viscosity \( D_1 = \mu_2 \in [10^{12}, 10^{13}] \) and density \( \varrho = \mu_3 \in [10^2, 10^3] \) and again generate 100, 50 and 50 high-fidelity solutions for training, validation and testing. \( L = 20 \) bases are used for velocity, pressure and temperature alike.  

This more practical problem illustrates clearly, why input scaling (as introduced in Section 2.2.3) is necessary. Due to the vastly different parameter magnitudes, the RBF would otherwise effectively neglect \( \mu_1 \) and \( \mu_3 \) when computing the distance in parameter space. Although the anisotropic GPR has the ability to learn different lengthscales, this would require to manually specify problem dependent search bounds for each parameter. ANNs also show faster convergence with standardized inputs \([39]\). Similarly, the temperature distribution motivates the use of standardized errors and snapshot centering. If, for example, the relative error as in Equation (41) was used, naively predicting the mean flow or even a constant temperature of e.g. 473 would result in deceptively small relative errors due to the variation in temperature being much smaller than the offset. This could be remedied by re-stating the problem in a normalized manner. However, the standardized errors together with preprocessing steps not only achieve the same, but also are more in line with the 'data-driven' approach. This allows to easily apply the same presented workflow to any problem or data with the results being intuitive, comparable across problems and independent of choice of units. This can be seen in the results of the ANN hyperparameter tuning in Fig. 17 which are once again similar to both previous problems (see Fig. 5 and Fig. 11) despite the very different problem setting. As in all other cases, the optimal learning rate is between \( 10^{-3} \) and \( 10^{-2} \) and the number of hidden units is between 20 and 40. The results correspond well to the heuristic used in Section 3.3, even though the performance is less sensitive to the size.

Fig. 18 depicts the best ANN configurations together with the other two regression models. Again the tuned ANN does not outperform the GPR despite the computationally expensive hyperparameter tuning. Furthermore, the greater flexibility of the ANN also requires making several decisions about the fixed and tuned hyperparameters, which usually boils down to empirical and tedious trial-and-error.

On the one hand, our results suggest that these manual efforts can be avoided and an ANN can be trained with good success by following the described preprocessing steps, using the standardized error and automated hyperparameter search. On the other hand, in all the investigated settings GPR is at least as good as ANN despite it being easier to implement, train and interpret.

For this problem, the performance of the RBF is significantly worse than in the other two problems. Even so, since it can be implemented and trained in a fraction of time even compared to GPR, RBF regression can serve as a viable empirical upper-bound for the other models.
Figure 16: Exemplary solution of the twin-screw extruder for $\mu = (1.01, 6.52 \times 10^{12}, 504)$ at time step $t_{55}$.

Figure 17: ANN hyperparameter tuning results for twin-screw extruder. Depicted are response surfaces of aggregated standardized regression error on the validation set $\varepsilon_{\text{ANN}}(P_{\text{val}})$ over the initial learning rate $\alpha_0$ and number of hidden neurons $N_{\nu}$. The respective best configurations are marked.
Figure 18: Error analysis of different regression models for the twin-screw extruder problem using $N_{tr} = 100$ training samples. The best identified ANN configurations marked in Fig. 17 are used.

Figure 19: Error analysis for the twin-screw extruder problem using $N_{tr} = 400$ training samples. The best identified ANN configurations described in the text are used.
To investigate the nature of errors Fig. 20 illustrates the true temperature over several timesteps alongside the absolute error of the predicted solution computed using the POD-ANN. As expected, the errors are zero on the outer barrel, where the same Dirichlet boundary condition is prescribed to all high-fidelity solutions. Further away from the Dirichlet boundary the errors increase. The same cannot be observed on the adiabatic screws – particularly in regions where the warm melt sticks to the screw surface and is traced throughout the interior, the errors are the highest. Due to the fact that the right side is heated, errors in the right barrel tend to be smaller than in the left.

Even so, at no point the temperature is off by more than 0.7. The ratio of the typical range of errors to the typical range of temperature, i.e., $1.4/40$ happens to be close to the total standardized error for this sample at $e_{\text{POD-ANN}} = 0.034$, providing a good intuition behind the standardized error. Lastly, we illustrate the effect of increasing the number of training samples $N_{\text{tr}}$. This is an easy to implement although a computationally expensive approach to reduce the errors. Fig. 19 shows the errors over the number of bases $L$ using four times as many training samples $N_{\text{tr}} = 400$ and the same validation and test sets as before.

For tuning the hyperparameters of the ANNs, the upper bound for the search space of $N_{\text{tr}}$ is increased to 100 according to the heuristic discussed in Section 3.4. The regression errors for $u, p, T$ show the same qualitative behaviour as previously and the best identified $N_{\text{tr}}$ and $n_{\text{tr}}$ are 50, 70, 70 and $3 \times 10^{-3}, 1 \times 10^{-3}, 1 \times 10^{-3}$, respectively. Interestingly, increasing $N_{\text{tr}}$ beyond 100 has almost no effect on the projection error $e_{\text{POD}}$ suggesting that even less than 100 samples can be used for the POD with similar success. However, the regression models benefit significantly from more data as the total standardized errors $e_{\text{POD-REG}}$ decrease around two-fold for RBF and three-fold for ANN and four- to eight-fold for GPR. This speaks to another advantage of the GPR, however, this experiment also demonstrates the biggest drawback of GPR – its cubic complexity in data size $O(N_{\text{tr}}^3)$ due to the inversion of the covariance matrix (see Section 3.2). The RBF is also $O(N_{\text{tr}}^3)$ due to the inversion of the weight matrix (see Section 3.1). On the other hand, ANNs are known to scale very well with large datasets in practice, despite there not being a simple compact theoretical result for their time complexity [72, 74].

### 6. Conclusion

In this work, a non-intrusive RBM based on POD with regression is applied to unsteady non-linear parametrized PDEs. As regression models we use RBF, GPR, and ANNs. We extend the established method with preprocessing steps, including centering before POD and standardization by singular values before regression. This removes scale and translation effects from the data and allows to use similar regression model hyperparameters on different problems. Additionally, we use a standardized error measure which relates the error in the prediction to the variance in the dataset. This makes the error interpretable and relatable even across problems of different scales and complexities. We first validate the proposed framework on a steady skewed lid-driven cavity problem. The results are in close agreement with those reported in the literature. Next, we consider an unsteady oscillating lid-driven cavity problem. We propose to treat time as a spatial dimension to preserve the efficiency of POD and greatly simplify the regression maps. Finally, the same standard framework is applied to a twin-screw extruder, which is characterized by a time- and temperature-dependent flow of a generalized Newtonian fluid on a moving domain. We vary thermal conductivity, reference viscosity and density over an order of magnitude each. Despite the different problem setting and only 100 training samples, the aggregated errors are less than 3% for the predicted velocity, pressure and temperature distributions. Although this already is within engineering bounds, the errors can be reduced significantly by simply generating more data. Using 400 training samples we achieve errors below 0.5%.

The similarity in ANNs hypertuning results over all three problems suggests that preprocessing and standardized error can alleviate this computationally expensive procedure. In all results with 100 training samples, the optimal initial learning rate is between $10^{-3}$ and $10^{-2}$ and the width of the two hidden layers is between 20 and 40. Even so, the GPR is found to be a very competitive alternative to the ANN despite being easier to train, interpret and control. Especially in the strongly anisotropic and densely sampled oscillating lid-driven cavity problem, the GPR significantly outperforms the ANN. The RBF consistently performs worse, but due to its simplicity it can serve as an inexpensive reference for the other models. The biggest disadvantage of the GPR and RBF methods is their cubic time complexity in the number of training samples.

This work only studies specific architectures of the regression models and although we emphasize standardizing datasets to facilitate a data-driven approach, problem specific insights could still further boost the performance. Examples
Figure 20: The high-fidelity true solution $T(\mu = (1.01, 6.52 \times 10^{12}, 504) \in \mathbb{P}_\mu)$ (left) and the error in prediction made by the best ANN (right) at time steps $t_{60}, t_{65}, t_{70}, t_{75}$ and $t_{80}$. Over all investigated timesteps the standardized error of the prediction is $\varepsilon_{POD-ANN} = 0.034$. 

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The computations were conducted on computing clusters supplied by the IT Center of the RWTH Aachen University.

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