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# On the Choice of Basis in Proper Orthogonal Decomposition-Based Surrogate Models

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**Abstract.** To reduce scrap in metal forming processes, one should aim for robustness by means of optimization, control or a combination of both. Due to the high computational costs, a Finite Element (FE) model of a metal forming process cannot be used in optimization routines or control algorithms directly. Alternatively, a surrogate model of the process response to certain variables can be created that enables efficient control or optimization algorithms. When the process response is more than a scalar function only, reduction methods such as Proper Orthogonal Decomposition (POD) can be applied to obtain a surrogate model. In this work, the results of a set of FE analyses are decomposed using a single and separated snapshot matrices using different preprocessing methods. Additionally, a new method for projecting in different parts of the snapshot matrix is proposed. The bases obtained using different preprocessing methods are compared. Thereafter, the surrogate models of the process are built by interpolating the amplitudes obtained in different bases. The accuracy of all surrogate models is assessed by comparing the reduced results with the results from the FE analyses.

## INTRODUCTION

To reduce scrap in metal forming processes, one should aim for robustness by means of optimization, control or a combination of both. An efficient optimization or control algorithm requires an accurate description of the process. The Finite Element (FE) method is a powerful tool to model metal forming processes. However, due to the high computational costs, the finite element method cannot be used in optimization routines or control algorithms directly. An alternative approach is to create a surrogate model of the process response. When this response is more than a scalar function only, for example a measured force curve [1, 2], a displacement field [3] and/or a stress field [4]; all time steps, nodal or integration point data must be included in the surrogate model. To analyze such data sets efficiently, reduction techniques such as Proper Orthogonal Decomposition (POD) in combination with interpolation methods such as Kriging can be used.

To obtain a surrogate model that best describes the original data, the so-called snapshot matrix can be accomplished in different ways before applying POD. For instance, to model the displacement field, one can place the displacement in $x$- and $y$-direction [3] in separate snapshot matrices, or all nodal displacements can be placed in one single snapshot matrix [1]. A similar controversy is found when different data types need to be modelled. For example, separate snapshot matrices are used to model stress components, plastic strain, damage indicator and temperature in [4], while one single snapshot matrix is used to model the equivalent plastic strain, thickness and a damage criterion in [5]. Besides this controversy in handling the snapshot matrices separately or not, many different preprocessing methods can be found in literature [6, 7, 8].

In this work, the results of FE analyses are decomposed using one single and separated snapshot matrices using different preprocessing methods. Additionally, a new method for projecting in different parts of the snapshot matrix is proposed. The quality of the bases acquired using different preprocessing methods is assessed. Thereafter, surrogate models of the process are built using the obtained bases and the accuracy of all surrogate models is assessed.

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## PREPROCESSING THE SNAPSHOT MATRIX

Consider that the result of an FE analysis can be placed in an $M$-by-1 column vector $\mathbf{y}_n$, where $M$ denotes (the sum of) the nodal degrees of freedom and the number of integration points. As an example, we consider a snapshot matrix $\mathbf{Y}$ that collects all $N$ result vectors of a Design Of Experiments (DOE). This snapshot matrix consists of three parts corresponding to the $M_u$-by-$N$ displacement field matrix $\mathbf{Y}_u$, the $M_\varepsilon$-by-$N$ equivalent plastic strain $\mathbf{Y}_\varepsilon$ and the $M_\sigma$-by-$N$ stress tensor matrix $\mathbf{Y}_\sigma$. Hence, the $M$-by-$N$ snapshot matrix $\mathbf{Y}$ collects the elements $y_{mn}$ corresponding to different fields.

$$\mathbf{Y} = \left[\mathbf{y}_1 \dots \mathbf{y}_N\right] = \begin{bmatrix} [\mathbf{Y}_u] \\ [\mathbf{Y}_\varepsilon] \\ [\mathbf{Y}_\sigma] \end{bmatrix} \tag{1}$$

In the remainder of this article it is assumed that the snapshot matrix is in row-variate form and that $N \ll M$. This *Unprocessed* snapshot matrix can already be used to construct a reduced basis. However, in the following sections different preprocessing methods will be introduced. All different preprocessing methods will be indicated using *Italic* script and correspond to the names used in Fig. 2 and Fig. 3 in which the different bases and surrogate models using the lowest $K$ basis vectors are compared, respectively.

### Preprocessing methods

The first and most common preprocessing method is subtracting the mean $\bar{y}_m$ of each row. The elements of the *Mean subtracted* snapshot matrix are:

$$y^0_{mn} = y_{mn} - \bar{y}_m \quad \text{where: } \bar{y}_m = \frac{1}{N}\sum_{n=1}^{N} y_{mn} \tag{2}$$

Another preprocessing method, commonly used when applying Principal Component Analysis (PCA), a special type of POD, is scaling the snapshot matrix by the number of experiments $N$ after subtracting the mean [8]. This procedure will only scale the obtained amplitudes and will not change the shape, and therefore the quality, of the basis vectors. This preprocessing methods is therefore left out of consideration. However, when different parts of the snapshot matrix are scaled to the same order, this will change the shape of the basis vectors. In the *Scaled* snapshot matrix all different fields are scaled to 1 order of magnitude, hence:

$$[\mathbf{Y}_u]\cdot 10^2, \quad [\mathbf{Y}_\varepsilon]\cdot 10^1 \quad \text{and} \quad [\mathbf{Y}_\sigma]\cdot 10^{-2}. \tag{3}$$

Data that has been mean subtracted can also be divided by the standard deviation $s_m$ of each row to obtain the $Z$-scores [6]. The elements of the snapshot matrix with *Z-scores* are:

$$y^Z_{mn} = \frac{1}{s_m} y^0_{mn} \quad \text{where: } s_m = \sqrt{\frac{1}{N-1}\sum_{n=1}^{N}(y_{mn} - \bar{y}_m)^2} \tag{4}$$

### Method for projecting in a subspace

As an example, the full, single snapshot matrix will be projected into the the displacement field matrix $\mathbf{Y}_u$. Projecting in other parts of the snapshot matrix will follow the same procedure, one can simply replace the subscript. Note that when the full snapshot matrix is used to project in, the subscript $u$ can be omitted and the method below describes a classical POD. The $i$-th displacement field based basis vector $\boldsymbol{\varphi}_i$ can be be calculated as follows:

$$\boldsymbol{\varphi}_i = \mathbf{Y}\cdot\mathbf{v}_i\cdot\lambda_i^{-1/2} \tag{5}$$

Where $\mathbf{v}_i$ and $\lambda_i$ are the eigenvectors and eigenvalues of the $N$-by-$N$ matrix $\mathbf{D}_u = \mathbf{Y}_u^T\mathbf{Y}_u$. Due to the multiplication with the full snapshot matrix, the basis vectors are not orthonormal any more. To normalize the basis vectors, they are divided by their norm. The full displacement field based basis $\mathbf{\Phi}_u$ is constructed by sorting the basis vectors by descending order of eigenvalues. As the obtained basis is not orthogonal, the amplitudes must be obtained using:

$$\mathbf{A}_u = (\mathbf{\Phi}_u^T\mathbf{\Phi}_u)^{-1}\mathbf{\Phi}_u^T\mathbf{Y} \tag{6}$$

When the full snapshot matrix is used, the basis vectors are orthonormal and equation (6) reduces to $\mathbf{A} = \mathbf{\Phi}^T\mathbf{Y}$. The snapshot matrix *Based on the displacement field* is:

$$\mathbf{Y} = \mathbf{\Phi}_u\mathbf{A}_u \tag{7}$$

## DEMONSTRATOR PROCESS

A demonstrator process is used to generate FE results and analyse the different preprocessing methods of the snapshot matrix. The metal forming process under investigation is a simple bending step modelled in 2D using the FE analysis software MSC Marc/Mentat. A graphical interpretation of the bending step can be found in Figure 1. A Latin Hypercube Sampling is used to generate a DOE of $N = 21$ sample points with maximized minimum distance in the design space $\mathbf{x}$ [5]. This set of sample points is used to obtain the different bases and to train the surrogate models. The design space is 2 dimensional and consists of the design parameters thickness ($x_1$) and punch depth ($x_2$). The sheet metal is modelled with an elastic-plastic isotropic material model with Von Mises Yield criterion and a tabular equivalent plastic strain. The sheet metal is meshed using 1200 quadrilateral elements ($N_{elem}$) and 1296 nodes ($N_{nod}$). Hence, with two degrees of freedom per node this leads to $M_u = 2 \cdot N_{nod} = 2592$ nodal displacements. The elements are fully integrated using four integration points per element. Hence, the equivalent plastic strain consists of $M_\varepsilon = 4 \cdot N_{elem} = 4800$ integration points and the stress tensor consist of $M_\sigma = 4 \cdot 4 \cdot N_{elem} = 19200$ integration points. Overall this results in a total snapshot matrix size of $M = M_u + M_\varepsilon + M_\sigma = 26592$ by $N = 21$.

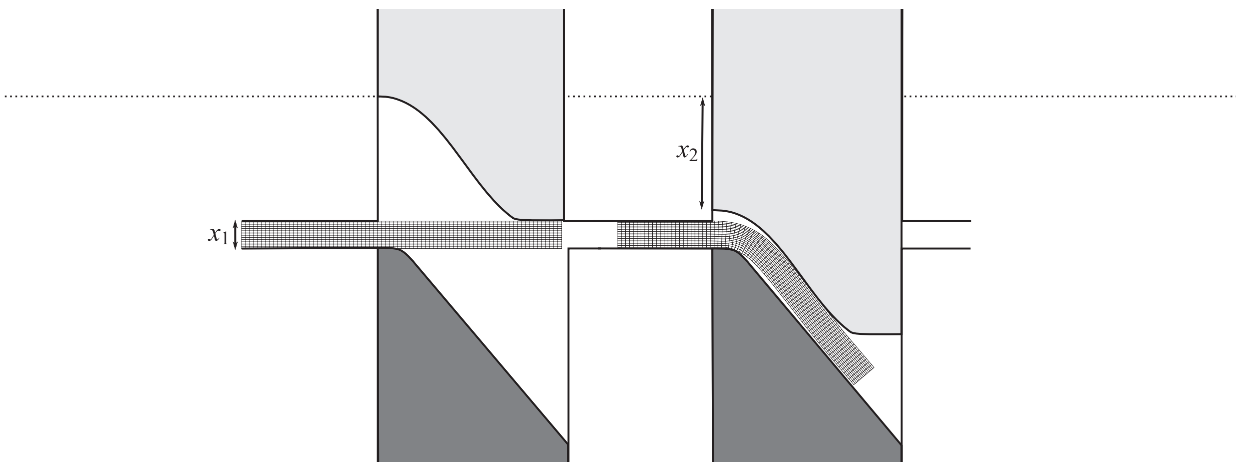



**FIGURE 1.** FE model with design parameters thickness ($x_1$) and punch depth ($x_2$) before bending (left) and after bending (right).

### Bases obtained using different preprocessing methods

A modified version of the mean relative reconstruction error $\epsilon_{rc}$ as proposed in [3] is used to compare the quality of the surrogate models obtained using different bases:

$$\epsilon_{rc} = \sqrt{\frac{1}{N}\sum_{n=1}^{N}\frac{||\hat{\mathbf{y}}_n - \mathbf{y}_n||^2}{||\mathbf{y}_n||^2}} \tag{8}$$

where $\hat{\mathbf{y}}_n$ is the result vector of experiment $n$ reconstructed in the different bases using the $K$ lowest basis vectors and $|| \, ||^2$ is the squared Euclidean norm.

In Fig. 2 it can be seen that overall the unprocessed snapshot matrix, the snapshot matrix with $Z$-scores and a basis based on the displacement field are less accurate. The relative construction errors using a basis based on the displacement field, strain field or stress field are the same as the errors using separate bases of that specific part because their $\mathbf{D}_u$, $\mathbf{D}_\varepsilon$ and $\mathbf{D}_\sigma$ matrices are the same respectively. Note that the bases obtain from all the snapshot matrices from which the mean is subtracted have one basis vector less than the unprocessed snapshot matrix as their rank is 1 lower.

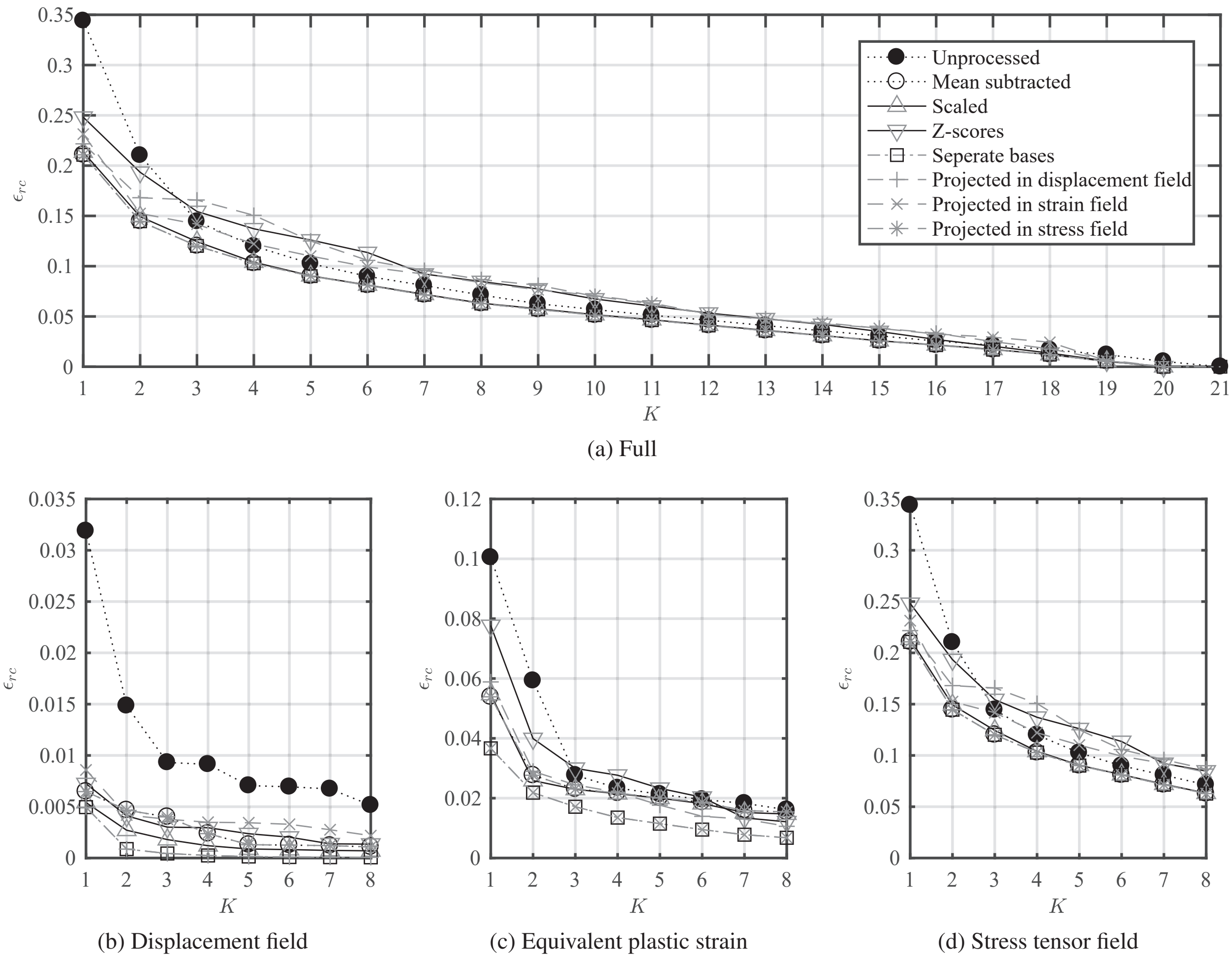
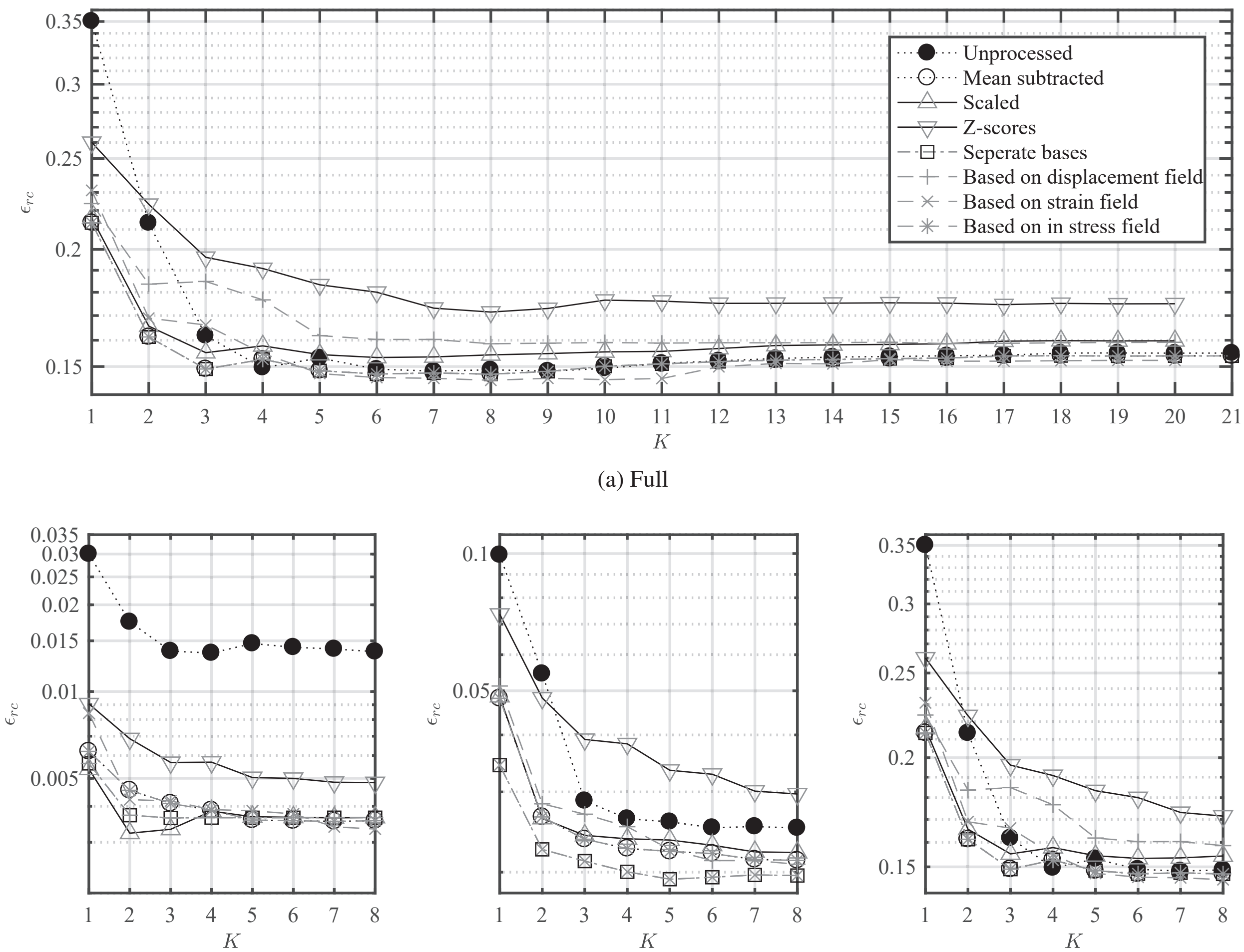



**FIGURE 2.** Relative construction error ($\epsilon_{rc}$) between the data from the FE model and the reconstructed result vector obtained using different preprocessing methods as a function of the number of POD-directions included in the basis ($K$) of the full snapshot matrix (a) and different parts of the snapshot matrix (b)-(d).

## SURROGATE MODEL RESULTS

To construct surrogate models of the process results, second order Kriging is used to interpolate the $N$ amplitudes obtained from the training set using different preprocessing methods. Using Latin Hypercube Sampling an additional set of $P = 21$ validation points in constructed to test the surrogate model. Again the mean relative reconstruction error as proposed in equation (8) is used to assess the quality of the obtained surrogate models relative to the FE results. Note that in this case $n$ and $N$ are replaced with $p$ and $P$ respectively. In that case $\hat{\mathbf{y}}_p$ is the result vector obtained using a surrogate model evaluated at validation point $\mathbf{x}_p$.

In Fig. 3 it can be seen that overall the unprocessed snapshot matrix and the snapshot matrix with $Z$-scores are less accurate. Again, as it should, the relative construction errors using a basis based on the displacement field, strain field or stress field are the same as the errors using separate bases of that specific part. Scaling the different parts to the same order improves the approximation of the displacement field, while slightly deteriorating the approximation of the stress field. This can be explained by the emphasis on the displacement field and the disregard on the stress field introduced by the scaling method as proposed in equation (3). The majority of the surrogate models reaches a steady state when 5 basis vectors are included in the surrogate model. From that point, including more basis vectors does not increase the quality of the surrogate model any further because the approximation error by the surrogate model




(a) Full

(b) Displacement field (c) Equivalent plastic strain (d) Stress tensor field

**FIGURE 3.** Relative construction error ($\epsilon_{rc}$) between the validation data from the FE model and the surrogate model as a function of the number of POD-directions included in the basis ($K$) of the full snapshot matrix (a) and different parts of the snapshot matrix (b)-(d).

outweighs the truncation error of the reduced basis. Using separate bases gives the best approximation of the strain field. For the displacement and stress field this improvement is less apparent.

## CONCLUSION, RECOMMENDATION & OUTLOOK

Subtracting the mean of the snapshot matrix is beneficial for the quality of the surrogate models. Although the division by the standard deviation makes the snapshot matrix dimensionless, the use of $Z$-scores is not beneficial for the quality of the surrogate model. The usage of separate snapshot matrices gives the best surrogate model, however the added computational time is a disadvantage. In future work, the surrogate model results will be propagated to an FE model of a subsequent process stage to address the assumption that all parts of the snapshot matrix are equally important.

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