

Article

Real-Time Models for Manufacturing Processes: How to Build Predictive Reduced Models

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Abstract: New data science and real-time modeling techniques facilitate better monitoring and control of manufacturing processes. By using real-time data models, industries can improve their processes and identify areas where resources are being wasted. Despite the challenges associated with implementing these data models in transient and multi-physical processes, they can significantly optimize operations, reduce trial and error, and minimize the overall environmental footprint. Implementing real-time data analytics allows industries to make quicker, informed decisions and immediate corrections to material processes. This ensures that manufacturing sustainability targets are regularly met and product quality is maintained. New concepts such as digital twins and digital shadows have been developed to bridge the gap between physical manufacturing processes and their virtual counterparts. These virtual models can be continuously updated with data from their physical counterparts, enabling real-time monitoring, control, and optimization of manufacturing processes. This paper demonstrates the predictive power of real-time reduced models within the digital twin framework to optimize process parameters using data-driven and hybrid techniques. Various reduced and real-time model-building techniques are investigated, with brief descriptions of their mathematical and analytical foundations. The role of machine learning (ML) and ML-assisted data schemes in enhancing predictions and corrections is also explored. Real-world applications of these reduced techniques for extrusion and additive manufacturing (AM) processes are presented as case studies.



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1. Introduction

Digital twin and shadowing concepts enable material-based industries to evaluate the performance of their processes and products quickly and efficiently. The framework includes defining process objectives, gathering process data (e.g., live sensor, experimental, mining, and simulation data), building digital models (including predictive and corrective models), and creating data interfaces and filters. These concepts help reduce costs and improve the entire production chain by offering prediction and correction routines that optimize performance [1–7]. Some successful applications of digital twin or shadow frameworks for manufacturing processes have already been reported in the literature [4–7]. Real-time modeling and its applications within the digital twin framework for manufacturing processes have been developed to incorporate fast and reliable prediction techniques within the industrial digitalization framework [8–11].

The use of data-driven techniques, along with the training and learning of manufacturing data, is a new trend in the design and optimization of industrial production chains. This might include predictive analytics, data learning (i.e., supervised, unsupervised, reinforced, hybrid, etc.), and data training using simulation results. Although many advanced numerical simulation technologies have been employed to design and optimize material processes within the manufacturing chain (e.g., offline optimizations), the digitalization drive has generated a strong demand for quick and real-time predictive models where live data can be interpreted and used as training data for fast responsive models [12,13]. While both offline and real-time optimization approaches have been employed for manufacturing processes, the difficulties with adapting to process variations, environmental conditions, and process constraint complexities can limit the use of offline optimization techniques.

With the advancement of data science schemes, including techniques like ML technologies, industrial digitalization concepts have driven the development of greener and more efficient manufacturing processes. Specifically, ML techniques can notably enhance the optimization of real-world manufacturing processes by improving product quality control, predictive maintenance, process automation, and energy consumption management [14,15]. Model order reduction (MOR) techniques are an integral part of digital twin and shadowing schemes, which help create digital counterparts for real-time monitoring, controlling, and optimization. These schemes can combine data-driven reduced models and ML modules to create fast and accurate predictive models. MOR technology trends have promoted many new ideas for process optimization and monitoring, leading to more efficient processes and achieving cheaper, higher-quality productions and parts [16–19].

Lassila et al. [20] have investigated the application of MOR technology for fluid dynamics, while Schilders et al. [21] have studied the more general theoretical and practical applicability of these techniques for engineering applications. Antoulas [22] has explored MOR applications for large-scale dynamical systems, while Silva et al. [23] have examined challenges related to applying these techniques in electrical engineering. Choi [24] discussed the spatial and temporal decomposition of dynamical engineering systems, investigating the block structure of space–time reduced bases. Benner et al. [25] have investigated MOR techniques based on data projection for parametric dynamical systems, providing a comparative discussion that highlights the advantages and disadvantages of various methods.

One of the main challenges in applying reduced predictive models to industrial processes is the creation and verification of these models. Numerous data-driven and hybrid techniques are available for reduced modeling in general engineering applications (e.g., physics-based, eigen-based, regression, etc.), but their suitability, accuracy, and efficiency for steady-state and time-transient process modeling have not been fully verified [26–28]. Some techniques have specific features that limit their applicability to general process modeling (e.g., rate dependency, data fitting), while others may not be accurate enough for modeling transient changing conditions during real-world industrial processes.

This paper briefly summarizes the performance of available MOR techniques for manufacturing processes, scrutinizing issues of accuracy, speed, and reliability of model predictions. As case studies, the application of MOR techniques for extrusion and AM processes is concisely presented, where time-transient temperature histories are predicted using tailored MOR techniques. In the first part of the paper, various MOR techniques and their applications for dynamic material processes were presented. In the second part, real-time models were developed for two real-world case studies of extrusion and AM processes. Both their effectiveness and the challenges related to accuracy, heat rate dependency, and thermal initial boundary conditions were examined.

2. MOR Techniques for Material Processes

The application of model order reduction (MOR) and hybrid modeling for manufacturing processes and their sub-processes (such as cooling and heating) has been widely debated to determine the most effective modeling approaches. Various reduced modeling techniques have been developed for general engineering applications, utilizing different data science methods to simplify complex simulations. Techniques such as eigen-based reduction, two-stage reduction, conventional and symbolic regression, support vector machines, clustering, and other popular data science methods have been employed to achieve this dimensionality reduction in engineering simulations.

Eigen-based reduction techniques, such as Principal Component Analysis (PCA), aim to transform the original data structure into a new set of uncorrelated variables called principal components. In contrast, regression-based reduction techniques focus on predicting one variable based on others, effectively reducing the number of variables needed. Other techniques, such as proper generalized decomposition (PGD), Krylov subspace methods (KSMs), balanced truncation (BT), and reduced basis methods (RBMs), have also been employed to create lower-dimensional representations of processes. The KSMs create a sequence of vectors that form a subspace, known as the Krylov subspace. This subspace is constructed from the initial vector and the matrix representing the process data.

In particular, the application of PGD methods for processes with a large number of input parameters has been investigated due to their efficient separation of variables. Additionally, KSM reduction techniques (e.g., PRIMA, SPRIM) can project data related to complex processes with many parameters onto a lower-dimension space with reduced computational demands [29]. RBM and BT techniques can also be employed to reduce the data dimensionality of engineering processes by truncation and the utilization of basis functions corresponding to the original data structure.

2.1. Eigen-Base Model Builders

Proper Orthogonal Decomposition (POD), Singular Value Decomposition (SVD), and Proper Generalized Decomposition (PGD) are among the most popular eigen-based reduced modeling techniques for process simulations [18,19]. These techniques can be defined as decomposition schemes (both spatial and temporal) where algebraic approximations of system responses are created to allow for fast reconstruction of system characteristics. In eigen-based techniques, dimensionality reduction is achieved by approximating essential data information using mathematical eigenvalue analyses. The initial data for these reduced models can originate from experimental work, verified numerical simulations, hybrid analytical simulations, and/or mined data, where variations of predefined system parameters are considered to fill the so-called snapshot matrix. For POD and SVD, the factorization of the system response can be mathematically expressed as [27]:

$$Ax = F(x, t) \rightarrow F(x, t) = U\Sigma V^T \quad (1)$$

where x is the eigenvector of A ; the decomposed matrices U and V^T are orthogonal matrices related to spatial and temporal decomposition, respectively; and Σ is the eigenvalue matrix. These reduced model builders are popular for manufacturing processes because they can easily characterize processes using an appropriate number of data eigenmodes.

For multi-physical material processes involving thermal and mechanical evolutions (e.g., heating, cooling, warping), generating reduced versions of the full process models is more challenging due to the transient nature of these processes. The integration of these reduced models into digital twin or shadow frameworks is also limited by the high volume of data required for modeling. Therefore, proper data modeling techniques that employ a balanced combination of MOR and ML techniques are essential to achieving accurate

real-time predictions. If the same mathematical basis as in Equation (1) is employed for predicting temperature (and stress) responses during a material process, it can be written as [11]:

$$[Y(x, t)] = U \sum V^T \rightarrow T_k(x, y, z, t) = U_k \sum_k V_k^T \quad \sigma_k(x, y, z, t) = U_{k\sigma} \sum_{k\sigma} V_{k\sigma}^T \quad (2)$$

where T_k and σ_k are temperatures and stresses at process time t . Hence, stress, deformation, and temperature at any nodal point can be predicted during the material process (e.g., AM, extrusion) using a proper data interpolation scheme. An application of eigen-based reduction techniques for transient casting processes is discussed in [26], where the validation of these techniques is provided.

2.2. Kriging and Regression Model Builders

The combination of two-stage Kriging and principal component analysis (PCA) model-building schemes is among the most powerful dimensional-reduction techniques. These methods maintain primary data characteristics and their dimensions while eliminating less important dimensions using correlation methods. In these techniques, the spatial correlations between sample data are used to create a new coordinate system where maximum data variances are aligned. Although these techniques are popular for reduced model building in manufacturing processes, their rate dependencies limit their applicability for processes with rapidly changing parameters (e.g., high gradient time-transient data). The Kriging interpolator can estimate values for new entries (e.g., temperature) based on the existing database as follows:

$$\hat{T}(x) = \sum_{i=1}^n \lambda_i T(x_i)$$

where $\hat{T}(x)$, λ_i , and $T(x_i)$ are the estimated temperature value at location x , the Kriging weights assigned to each known temperature value, and the known temperature values in the database, respectively. The variogram values between locations can be calculated based on the spatial distances between data points and the Lagrange multiplier [27]. Since the interpolation technique guarantees that the Kriging weights sum to one and that the estimation is unbiased, it can be employed for moderate data rate-dependent process applications.

Conventional and symbolic regression techniques are among the oldest reduction methods, where data variables can be sorted based on their impacts. Variables can be ranked by their importance indexes, allowing less important data to be ignored to reduce data dimensions. Symbolic regression (SR) and genetic algorithm symbolic regression (GASR) are more sophisticated regression techniques, where regression analysis is performed within a multi-dimensional search space for mathematical expressions and operators to find the most suitable model. Although these regression techniques have been extensively applied to reduce the data dimensionality of steady-state processes, their applications for transient processes are limited due to higher error margins for data with high gradient changes.

2.3. Clustering and SVM Model Builders

Clustering-based reduced model building is a well-known technique among various data science methods, involving the grouping and clustering of data points with common features. It can be defined as an unsupervised learning scheme used to identify patterns in available data for better insights. Recently developed clustering techniques include density-based spatial clustering, expectation-maximization clustering, mean-shift clustering, K-means clustering, and hierarchical clustering. For applications in industrial process

simulations, clustering techniques, along with interpolation methods (e.g., Kriging, radial basis functions, inverse distance), can be employed to predict real-time responses.

Support vector machine (SVM) is another ML scheme (supervised learning) that can represent spatio-temporal data for both steady-state and transient processes, mapping data into different categories based on existing gaps in time and coordinate space. Various kernel functions, including linear, polynomial, radial basis functions, and Fourier kernel functions, can be used in SVM to classify process-related data. The powerful classification and regression features of SVM can be employed to predict real-time process responses, facilitating the control and optimization of transient industrial processes while avoiding data overfitting. While clustering and SVM techniques are effective for identifying and grouping process data in high-dimensional spaces, eigen-based techniques excel in data representation and uncovering important process data patterns.

3. Case Study—Process Applications

The introduction of data-driven and real-time accurate models for industrial processes has begun to transform the control and optimization of these processes. The traditional numerical simulations are often unable to provide real-time process control and optimization due to computational complexities, computational resources, and lack of flexibility and adaptivity. Data real-time models for processes like industrial extrusion and AM are rapidly evolving to generate faster and more reliable prediction models. In the case of the extrusion process, the large thermo-mechanical deformation of the material requires frequent updates to the material state. This demands significant computational resources, including data mapping, data preparation, and solver launching, to maintain the accuracy and stability of the process simulation. For AM processes, with their frequently changing demands due to more complex geometries, innovative power sources, and new materials, the need for fast and accurate models has been emphasized [30].

Although numerical simulations of these processes using finite element and computational fluid dynamics (CFD) techniques have been extensively used in industries, real-time control and optimization require much faster models. To investigate the application of fast reduced models for extrusion and AM processes, comprehensive frameworks have been established to evaluate the performance of these real-time predictive tools.

3.1. Reduced Models for Extrusion Process

Extrusion processes are adaptable manufacturing methods used to produce various profiles with different shapes, sizes, and complex cross-sections using pre-designed dies. Numerical simulations and fast real-time models can help optimize these processes and provide insights into the large thermo-mechanical deformations of materials during the process. To build accurate and reliable real-time models for these processes, the following steps can be followed:

- Any real-time data model needs a properly sized initial database that provides enough data points with the right balance of data density within its multi-dimensional search spaces. To generate such a database, parallel numerical simulation and experimental frameworks need to be set up.
- After conducting limited experimental trials, the data need to be compared to numerical simulation runs that resemble these experiments. Calibrations and further verifications are then performed to confirm the accuracy and reliability of offline numerical simulations of the process.
- In the next step, the most influential process parameters are defined and selected, and a proper sampling technique (e.g., Sobol, LHS) is employed to form a snapshot matrix.

- Using the process scenarios in the snapshot matrix, real-time models based on appropriate mathematical and data science schemes are generated. These models need to be agile enough to cover the entire data within the search space (e.g., within the limits of process parameters).
- To validate the accuracy and reliability of these models, further design of experiments (DOEs) process scenarios is carried out to provide benchmark results for model validations.
- Model validations are carried out using DOEs data at three levels: normal conditions, near boundary conditions, and extrapolation stages. Data from within, near the limits, and outside of the search space are used to perform the full validation exercise.

Nevertheless, there are challenges in integrating data-reduced models with existing extrusion control systems, such as model accuracy, reliability, data availability, data quality, and model validation. To address these challenges, a combination of appropriate data solver–interpolators, balanced and appropriately sized data spaces, efficient data sampling and snapshotting, and continuous validation and testing are required to ensure successful implementation.

For the numerical simulations of extrusion processes in this research work, the thermo-mechanical solver HyperXtrude (HX) is used, which employs the arbitrary Lagrangian–Eulerian (ALE) hybrid approach to calculate large material deformations [31]. Both the ram speed and initial billet temperature are defined as major process parameters, with their variations based on the billet material (aluminum 6060) and the limits of the extrusion machine. These variations are defined as initial billet temperatures ranging from 440 °C to 550 °C and ram speeds ranging from 1 to 10 mm/s for the cylindrical aluminum billet (with a 50 mm diameter). The numerical domain is discretized using 172,000 volumetric elements, and only a quarter of the model is simulated due to double symmetric conditions. Figure 1 shows the geometry and the finite element (FE) mesh for the extrusion process, along with the snapshot matrix for the model-building exercise.

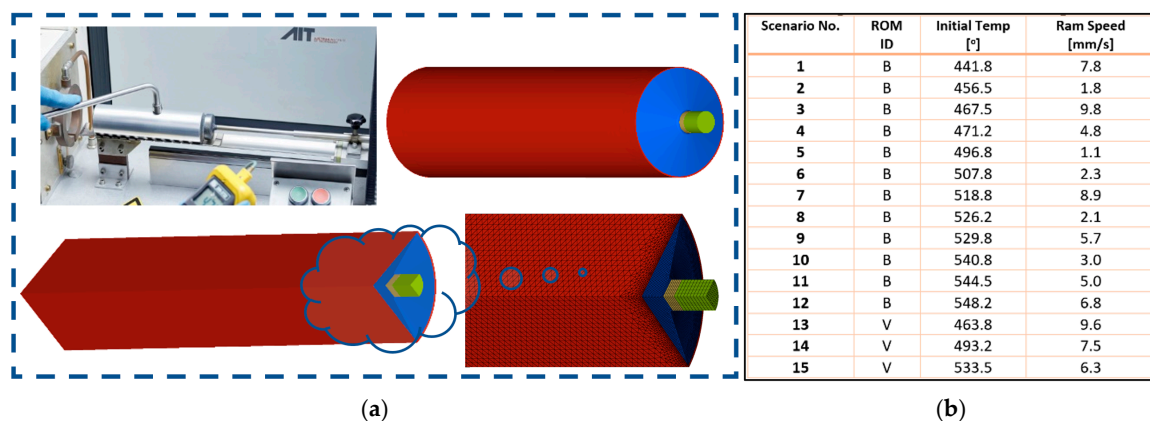


Figure 1. (a) Experimental setup, geometry model, FE mesh, and (b) snapshot matrices for the extrusion process.

3.2. Reduced Models for AM Process

For industrial wire arc AM processes, where the manufacturing of parts evolves over time, accurate and reliable reduced models are required to account for transient changes in material feeds, power, and thermal energy content. Although many different reduction techniques can be tailored and employed for real-time predictions, their generality and accuracy need to be scrutinized. Many of these models are either tailored for smooth data changes or are not suitable for transient data due to rate dependencies [32].

In the current research, various popular reduced model-building techniques were considered for the AM process, where available finite element (FE) and experimental data

could be processed to train the model. Following the previous extrusion process application, the procedure for reduced model building for AM processes can be summarized as follows:

- The initial verification of the FE model for the AM process was carefully conducted using experimental data (with Goldak heat source modeling [33]).
- A suitable snapshot matrix was defined to carry out detailed FE simulations with varying input parameters, including initial base temperature, torch power, and deposition speed.
- The snapshot results are used to create and train reduced models using different techniques.
- Further DOE scenarios were performed to create a validation matrix for the models.
- The performances of various models were investigated through an extensive comparative study between reduced and FE models for DOEs.
- The results of the comparative study were further post-processed to determine the most suitable techniques for AM-reduced models.

For the AM case study in this research work, a single-layer deposition process on top of a thermally pre-conditioned wall with dimensions of 100 mm × 50 mm × 6 mm was simulated. Aluminum 6061 wires were used for the deposition process, and welding was carried out using inert gas welding. For the initial validations, experimental trials were conducted to observe the thermal evolution and measure the temperature variations at selected locations. To build the reduced models, nine additional process simulation scenarios were performed with varying parameters such as torch power, deposition speed, and initial temperatures. Figure 2 shows the geometry and the FE mesh for the AM process, along with the snapshot matrix for the model-building exercise.

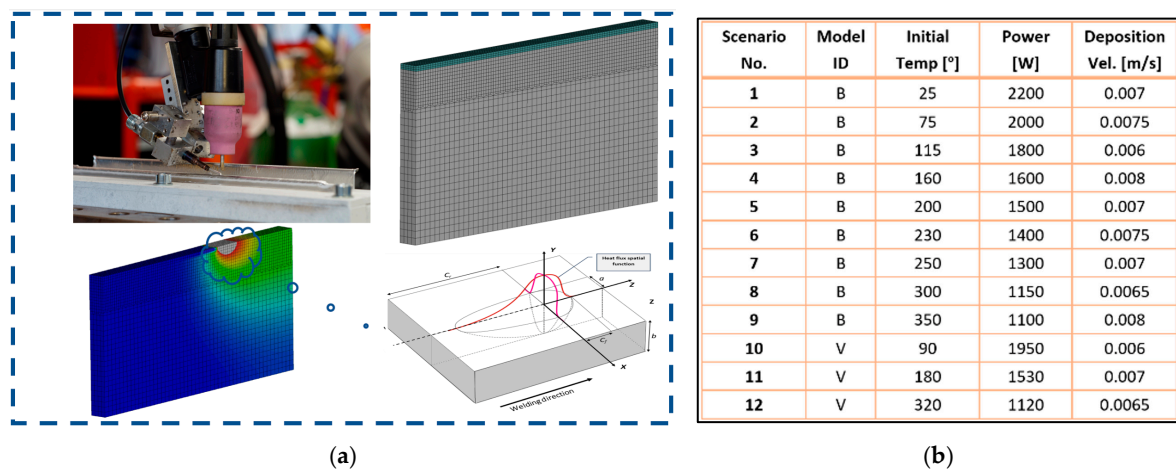


Figure 2. (a) Experimental setup, geometry model, FE mesh with Goldak heat sourcing schematic representation; (b) snapshot matrices for AM process.

4. Comparative Study

To evaluate the performance of real-time models and compare the outcomes of different reduced model-building techniques, comparative studies have been conducted for both industrial case studies. The aim is to investigate the accuracy and reliability of real-time models based on data provided by the verified FE results of DOEs. For the first case study on the extrusion process, popular eigen-based POD techniques and the more general SVD method, along with regression analyses, were employed for the model-building exercise. These two data techniques are more appropriate for the extrusion process due to the size and dimension of the process data space, the rate of changes in material temperature and deformations, and the availability of data. Figure 3 shows the comparisons of temperature time histories for SVD and regression techniques using DOE results. The data weight-

ing feature of the inverse distance (InvD) technique is used for the SVD solver as a data interpolator [27].

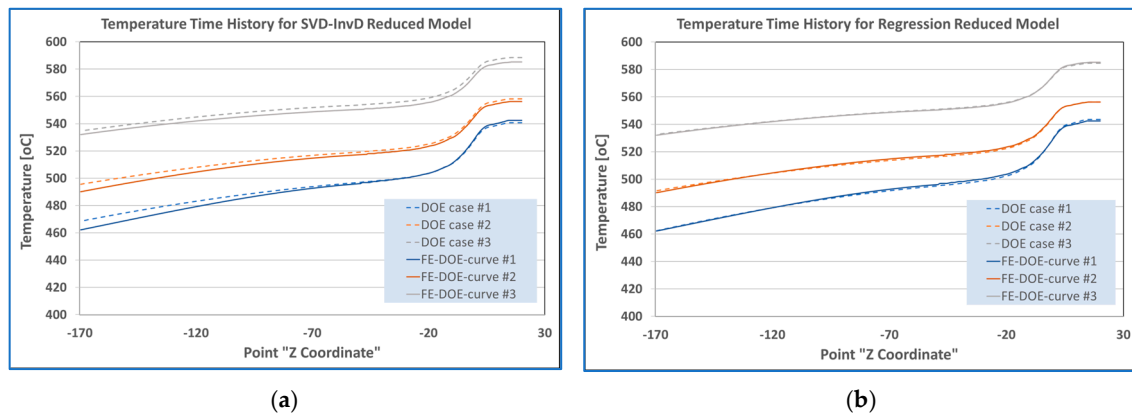


Figure 3. Temperature time histories for reduced models and DOEs for (a) SVD and (b) regression techniques for the extrusion process.

The normalized error graphs for the SVD-InvD and regression techniques are presented in Figure 4 for all three DOEs. The use of symbolic regression or GASR techniques can improve the data model structure, its interoperability, flexibility, and adaptability. The finite element (FE) results for these three validation scenarios are compared with the results from the real-time models. The normalized error percentages are calculated based on the data model predictions for nodes along the extrusion billet, relative to the FE simulation results. The results indicate that the normalized errors are higher at the billet's ends (i.e., at the initial boundary) and near the die, where significant material deformation occurs. The thermo-mechanical phenomena resulting from the material's large deformation as it passes through the die cause temperature fluctuations in this region, which can pose challenges for the accuracy of the data model predictions.

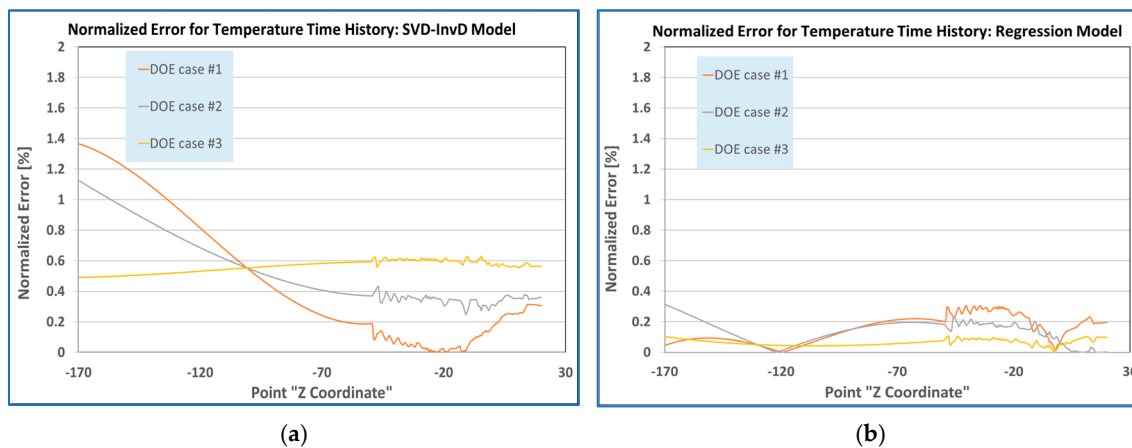


Figure 4. Normalized error graphs for (a) SVD-InvD and (b) regression techniques for the extrusion process.

Similarly, for the real-time models of AM processes, eigen-based and regression solvers were employed to build reduced models to investigate their accuracy and reliability. Although there are no general rules for choosing the best-performing technique for reduced model building, some models perform better in terms of accuracy and reliability for dynamic processes like AM, depending on the nature of the transient data. Figure 5 shows the comparisons of temperature time histories for the DOE results and reduced models, using the SVD-Kriging and SVD-InvD (SVD solver with inverse distance data interpolator)

techniques for a nodal point on the wall during the AM process. Figure 6 shows the normalized transient error graphs for the same SVD-Kriging and SVD-InvD techniques for all three DOEs.

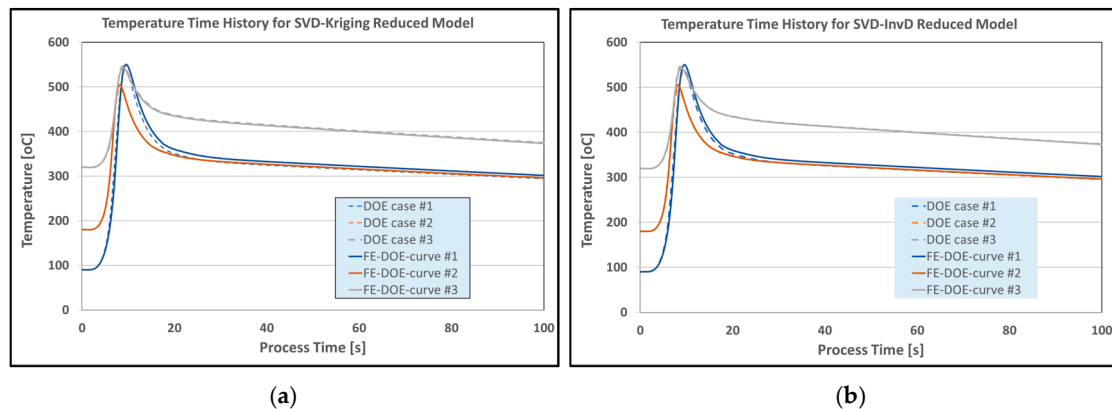


Figure 5. Temperature time histories for reduced models and DOEs for (a) SVD-Kriging and (b) SVD-InvD techniques for the AM process.

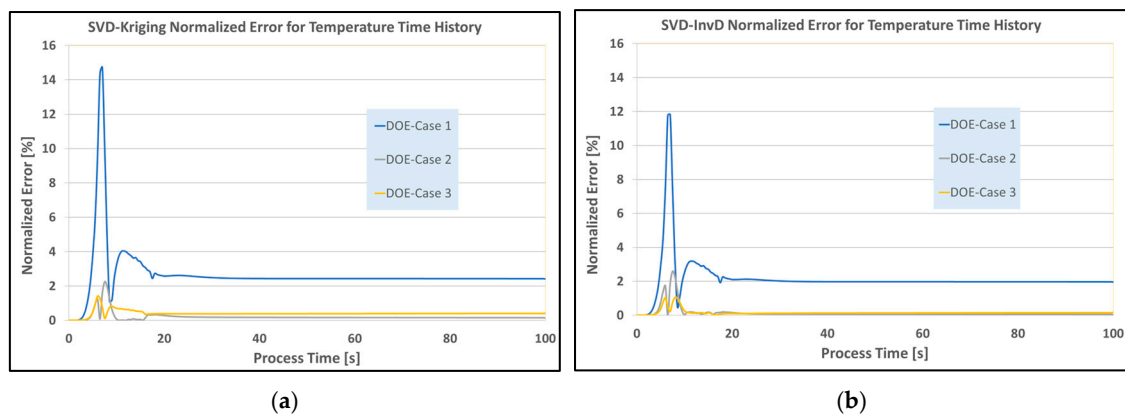


Figure 6. Normalized error graphs for (a) SVD-Kriging and (b) SVD-InvD techniques for the AM process.

Clustering and SVM techniques have not been employed for these processes due to the sensitivity of predictions to initial conditions, the limited number of process data clusters, difficulties in choosing the appropriate kernel, and sensitivity to regularization parameters.

5. Discussion

Numerical simulations, analytical approaches, and extensive experimental activities have long been used to model manufacturing processes. These methods have been widely employed for initial design and offline optimization, considering multi-physical and multi-scale aspects. However, computational complexities and CPU time often limit the application of these methods for real-time control and optimization. Conversely, real-time data models can enhance prediction–correction schemes for material processes, though challenges related to their accuracy, efficiency, and reliability remain. Material processes are inherently multi-physical, often involving high rates of heating and cooling during production, as well as changes in material state from fluid to solid or vice versa. Therefore, the performance of these real-time models depends on data quality, the quantity of available data, the rate of changes within the data, and the complexity of the system being modeled.

The results presented here show that these models can reasonably predict the transient responses of the AM and extrusion processes. Although the process databases for both

AM and extrusion cases are limited in size, the available data have balanced distributions within the multi-dimensional search spaces (e.g., limits of the processing parameters for manufacturing machines). However, as observed from the real-time responses, coping with high heating/cooling rates (e.g., the passage of the torch over a measuring point in the AM process) and fitting into the initial process conditions (e.g., initial temperature) remain challenging tasks for these models. The rapid changes in data patterns (e.g., temperature, strain rate, etc.) often pose challenges to data models, as new predictions can become erroneous due to high data gradients. Therefore, additional data training and learning may be necessary to train the data models for these highly dynamic processes.

To investigate the performance of real-time models in predicting high heating/cooling rates and their ability to fit initial process conditions, a further study was conducted to compare the accuracy of different model-building techniques. Figure 7a shows the average maximum errors (over three DOEs) and the deviation of initial conditions (in percentages) for four popular model-building techniques: SVD-RBF (SVD solver with radial basis function interpolator), SVD-Kriging, SVD-InvD, and regression techniques. Figure 7b shows the time history of the average normalized errors (over three DOEs) with the calculated rate of temperature changes. Figure 8 also shows the computational time for the FE simulations and real-time models for both the extrusion and AM case studies.

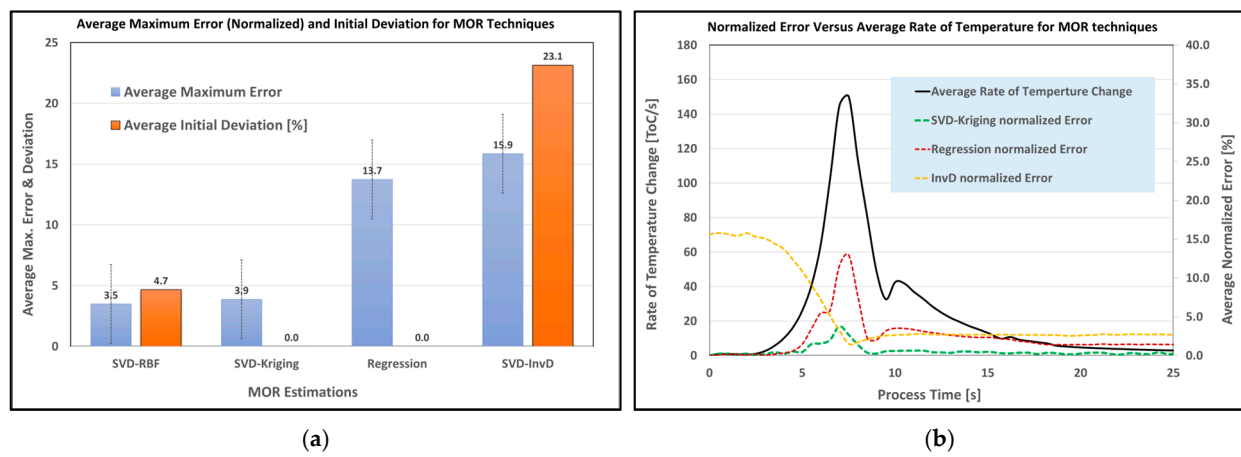


Figure 7. (a) Average maximum errors (over three DOEs) and deviation of initial conditions (in percentages); (b) correlation for rate of temperature changes with normalized errors for real-time models.

Extrusion Scenario	Model Description	Computational time [sec]	AM Scenario	Model Description	Computational time [sec]
FE	Init. scenarios	480	FE	Init. scenarios	2880
FE_DOE	DOE scenarios	480	FE_DOE	DOE scenarios	2880
MOR SVD_RBF	Eigen-based MOR	1.1	MOR SVD_RBF	Eigen-based MOR	0.8
MOR SVD_Kriging	Eigen-based MOR	1.2	MOR SVD_Kriging	Eigen-based MOR	0.9
MOR SVD_InvD	Eigen-based MOR	1.1	MOR SVD_InvD	Eigen-based MOR	0.8
MOR Regression	Regression MOR	1.3	MOR Regression	Regression MOR	0.9

Figure 8. Numerical simulations and MOR computational CPU times for (a) extrusion and (b) AM processes.

As observed from these figures, the real-time models exhibit some degree of temperature rate dependency and deviations from the initial process conditions. However, for both the extrusion and AM processes in this study, the SVD-Kriging and regression techniques demonstrate superior performance in predicting the thermal transient responses.

The size and distribution of process data within the data space can significantly impact prediction accuracy. A balanced data search space with even data density can lead to better results. Additionally, the right combination of data solvers and interpolators, along with appropriate data training, can create more efficient data models for material processes.

6. Conclusions

The use of dimensional-reduction techniques and their associated real-time models for material processes like casting, extrusion, and additive manufacturing is becoming increasingly popular and valuable for industrial production. These tools can optimize manufacturing processes, improve product quality, enhance the predictive–corrective power of real-time adjustments, and reduce costs and time by avoiding lengthy trial-and-error loops. Nevertheless, challenges related to the employment of these techniques remain (e.g., rate dependency and fitting to initial conditions), and these have been elaborated upon within the manuscript.

In the first part of the paper, descriptions of some MOR techniques (e.g., POD, regression, etc.) and their applications for dynamic material processes like extrusion and AM were presented, along with some elaborations on data science aspects of these new techniques. In the second part of the paper, real-time model-building exercises for practical case studies were explained, and their challenges related to accuracy, heat rate dependency, and thermal initial boundary conditions were examined. The results presented here show that for extrusion process modeling, the developed SVD-InvD and regression methods can produce reasonable results in real time. For AM process modeling, SVD-Kriging and SVD-InvD, with some extra data training, can be employed to produce reasonable results even when the heating/cooling rate is high. With further machine learning training for the process database, even better results can be achieved for high-gradient heating/cooling processes. This would help develop efficient process control schemes, allowing for real-time optimization using both live and offline process data.

Although there are many combinations of popular data “solver–interpolator”, not all of them are suitable for material process modeling. In this research, after investigating different combinations, the best-performing ones (i.e., SVD, regression) have been employed for the extrusion and AM process applications. These data models can produce reasonably accurate real-time results with a small-sized process database. Future publications will explore real-time model-building exercises for other multi-physical processes, such as casting.

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