A study on using image-based machine learning methods to develop surrogate models of stamp forming simulations

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ABSTRACT
In design for forming, it is becoming increasingly significant to develop surrogate models of high-fidelity finite element analysis (FEA) simulations of forming processes, to achieve effective component feasibility assessment as well as process and component optimizations. However, surrogate models using traditional scalar-based machine learning methods (SBMLMs) fall short on accuracy and generalizability. This is because SBMLMs fail to harness the location information available from the simulations. To overcome this shortcoming, the theoretical feasibility and practical advantages of innovatively applying image-based machine learning methods (IBMLMs) in developing surrogate models of sheet stamp forming simulations are explored in this study. To demonstrate the advantages of IBMLMs, the effect of the location information on both design variables and simulated physical fields is firstly proposed and analyzed. Based
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on a sheet steel stamping case study, a Res-SE-U-Net IBMLM surrogate model of stamping simulations is then developed and compared with a baseline multi-layer perceptron (MLP) SBMLM surrogate model. The results show that the IBMLM model is advantageous over the MLP SBMLM model in accuracy, generalizability, robustness, and informativeness. This paper presents a promising methodology in leveraging IBMLMs as surrogate models to make maximum use of information from stamp forming FEA results. Future prospective studies that are inspired by this paper are also discussed.

Key words: stamp forming, machine learning, FEA, IBMLM, SBMLM, MLP, Res-SE-U-Net

1. Introduction

In the design of metal forming processes, design candidates that are defined by design variables are evaluated by numerical simulations, such as finite element analysis (FEA) [1,2]. The simulation results are then used to optimize the design candidates in design optimization. However, these simulations are computationally intensive and time consuming, which makes trial-and-error design optimization impractical. To facilitate the optimization process, an effectual method is to construct surrogate models that are trained on a limited number of simulation results [3]. In surrogate modelling, the design variables of the design candidates are regarded as inputs, while the corresponding simulation results are regarded as outputs. The surrogate models learn the mapping relationship from the inputs to the outputs, which can be used to rapidly predict metal forming simulation results in design optimization.

To construct surrogate models, machine learning methods have been widely used. Traditionally, the scalar-based machine learning method (SBMLM) is commonly used, which downscales both the design variables and the simulation results to scalar-

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based metrics. In recent years, SBMLMs have been widely applied to design optimization tasks [4-7]. Despite this impact, SBMLMs usually suffer from several shortcomings. Firstly, SBMLM surrogate models generally fail to extract a bijective mapping relationship from inputs to outputs. This makes the models not just inaccurate, but also non-generalizable. Secondly, it is difficult to apply SBMLMs to scenarios where the location information of the simulation results is of vast importance. This information cannot be represented by hard-coded scalar metrics. Typical examples of these scenarios include thinning distributions analysis, punch impact line analysis, microstructure evolution, and damage [8]. These two shortcomings are mostly due to the information losses caused by the downscaling process.

To overcome these shortcomings, a representation that is superior to scalars is required to mitigate the information loss when down-sampling into single scalar values. This leads to image-based machine learning methods (IBMLMs), where both the design variables and simulation results are represented as images, which retain their full spatial information. Based on these images, a bijective mapping relationship can be extracted using IBMLMs, which is more accurate and more generalizable compared with those extracted using SBMLMs. Though the use of IBMLMs as surrogate models is still at an early stage of development, they have been investigated in several studies. Early studies of IBMLMs mainly focused on fluid dynamics, since the image-like nature of Eulerian meshing in most fluid-dynamics simulations are suitable for using IBMLMs [9-11]. Recently, IBMLMs have been extended to special scenarios of solid mechanics, such as sheet forming [12-15] and additive manufacturing [16-18]. This is because the inputs

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and outputs in these special scenarios can be represented by 2D images. To extend
IBMLMs to more general scenarios of solid mechanics, further studies are under
investigation [19-22].

In this article, the theoretical feasibility and practical advantages of IBMLMs
are studied. The objective of this article is to analyze the theoretical feasibility of
IBMLMs and validate their practical advantages compared with SBMLMs for developing
surrogate models of stamp forming simulations. In section 2, the pipelines of SBMLMs
and IBMLMs are discussed in detail. To demonstrate the advantage of location
information in IBMLMs, a simplistic, half-symmetric stamp forming FEA model is
analyzed. Details of the specific SBMLM and IBMLM representative models used in this
study are also discussed. In section 3, the details of the dataset and the machine
learning models used in this study are discussed. The dataset of a cold metal forming
case was established, which was then divided into a training set and a test set. A MLP
SBMLM model and a Res-SE-U-Net IBMLM model were developed. In section 4, the
results of the SBMLM model and the IBMLM model are compared and discussed from
three aspects, including interpolation performance, extrapolation performance, and
informativeness. In section 5, conclusions about IBMLMs are stated, and the bright
outlook of IBMLMs is demonstrated.

2. Theory & Methodology

IBMLMs have been separately discussed and investigated in multiple domains. In
the domain of fluid dynamics, a convolutional neural network (CNN) model was

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developed to predict steady flows in a representative, early-stage study [23]. In the domain of topology optimization, deep neural networks (DNNs) have been applied to learn the structural features of optimization results [24,25]. In the domain of solid mechanics, a multi-channel residual CNN, namely StressNet, was firstly developed to predict the image-based stress fields of multiple 2D cantilever structures under varying boundary conditions [14]. Based on StressNet, normalization modules were leveraged to further improve the accuracy of DNNs in predicting the stress concentrations in heterogeneous media, such as composite materials [26].

It is noteworthy that in the studies discussed above, the geometries and simulation results are compatible with IBMLMs since they are naturally represented by pixels or voxels. To extend IBMLMs to the realm of nonlinear solid mechanics, complex 3D geometries and strong nonlinearities are the major obstacles. Several studies have attempted to apply CNNs to crash simulations [27,28]. However, these studies were limited to reconstruction tasks, which could not be used for fast predictions.

Despite these obstacles, IBMLMs have shown promise when applied to several special scenarios of nonlinear solid mechanics. One of these scenarios is forming. This is because the geometries in forming processes can be projected to 2D images from the top view, while forming simulation results can also be plotted onto undeformed blank configurations as 2D images. Several pioneering studies have been published on this topic. J. Pfrommer and C. Zimmerling originally applied IBMLMs to predict the simulation images of a composite forming process [29]. By counting in more elements of simulation results, IBMLMs outperformed SBMLMs. This original method was further

extended to handle varying geometries using pattern recognition or CNNs [30,31]. In a subsequent article, the progress in the development of IBMLMs in forming was summarized [32]. Recently, these developed IBMLM models were combined with reinforcement learning to optimize manufacturing process parameters [33].

Based on these studies, it seems promising to further develop IBMLMs for rapid prediction and optimization of forming processes. However, most of the studies regarded IBMLMs as black boxes. The underlying theory on the advantages of IBMLMs has barely been discussed. To fill this gap, the present paper will discuss and verify the effect of location information, which potentially makes IBMLMs advantageous. This verification will be made by using a half-symmetric metal forming model.

To elaborate, the pipeline of metal forming simulations and surrogate models is presented in Fig 1. At the beginning, scalar-based design variables are defined by engineers and then modelled by computer-aided design (CAD) programs. This leads to image-based design variables, including projected geometry images, distribution images of binder pressures and thickness. These CAD models are processed through FEA solvers to acquire image-based simulation results, which include multiple physical fields. To extract the mapping relationship from the design variables to the simulation results, surrogate models are required. Traditionally, due to the lack of advanced representations and modelling tools, the simulation images are downscaled to several critical scalar metrics, such as maximum strain. As shown by Fig 1 (a), this downscaling leads to SBMLMs, which bridge scalar-based design variables and simulation results. It is obvious that the topological relationships of the geometric design variables and the

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distributions of the simulated physical fields are discarded when using a scalar-based representation. This leads to the loss of location information of both the design variables and the simulation results. This information loss is considered to be responsible for the inaccuracy and non-generalizability of SBMLMs. To include location information in training processes, IBMLMs have thus been developed as shown in Fig 1 (b), which directly bridges the images of both design variables and simulation results. IBMLMs are promising in terms of better accuracy and generalizability, because they are trained with integrated location information. It should be noted that 3D geometries are projected to geometry contours representing drawing depth from the top view; 3D FEA results are mapped back to the undeformed configuration, which can be dealt with as 2D images.

In section 2, the effect of location information will be further elaborated, and the methodologies of both SBMLMs and IBMLMs will be discussed. In subsection 2.1, a half-symmetric metal forming case will be discussed to further illustrate the effect of location information. In subsection 2.2, the multi-layer perceptron (MLP) will be introduced as a typical method of SBMLMs. In subsection 2.3, the CNN will be introduced as a typical method of IBMLMs. In particular, CNNs enhanced by multiple blocks, namely Res-SE-U-Nets, will be discussed and then utilized to develop the IBMLM model in this study.

2.1 The effect of location information of FEA results

To explain the effect of location information, a case study was tested based on a symmetric half-model. In this case study, both the SBMLM and IBMLM models were

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used to predict the maximum equivalent plastic strain (denoted Max. PEEQ) of a metal sheet stamping simulation. The settings of this case study are shown in Fig 2 (a). As can be seen in both the Isometric view and the top view, a symmetric boundary condition was added to the edge of the half model. Note that the binder is partitioned into two sections along another symmetric line, named Binder I and Binder II in this case study. The die was constrained in all degrees of freedom, while the punch and binders were allowed to move along the z axis. The stamping direction was along the negative direction of z axis, and the punch velocity was set to 100 mm/s. Two binder pressures, denoted $BP1$ and $BP2$, are applied to the two separated binders. Cold rolled, drawing quality (CRDQ) steel was used as the blank material, and its flow stress-strain curve is presented in Fig 2 (b). Punch, die and binders were all set to be rigid. Based on these settings, PEEQ fields can be calculated and the maximum value of which is denoted as Max. PEEQ.

In this case study, the two binder pressure values, vectorized as $(BP1, BP2)$, are regarded as design variables. As shown in Fig 2 (c), there are only two samples defined in training set. The BP vector of the first sample is (1, 5), while that of the second is (5, 1). Their ground truth (denoted GT) Max. PEEQ results are both 0.7302, since the two binders are symmetric to their partition line. There is only one sample in the test set. The BP vector is (3, 3), which adopted the averaged value of the two training samples. The GT Max. PEEQ of the test sample is 0.6348, which is lower than the averaged output of the training samples. The ground truth equivalent plastic strain (GT PEEQ) fields of all three samples are presented in Fig 2 (d), where $BP1$ and $BP2$ refers to the binder

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pressure of binder I and binder II; Max. PEEQ refers to the maximum value of equivalent plastic strain.

Based on the two-sample training set, both the SBMLM and IBMLM models were trained to predict the Max. PEEQ of the test sample. Since no prior knowledge about the mapping relationship was known beforehand, a linear prior was given to the SBMLM and IBMLM models. Subsequently, the three *GT* Max. PEEQ and two *PD* Max. PEEQ can be plotted as a 3D graph, where the two independent variables were (*BP1*, *BP2*), while the dependent variable was Max. PEEQ. For the sake of visualization, in Fig 3 (a), this 3D graph is projected onto a 2D graph by equivalently replacing (*BP1*, *BP2*) with (*BP1-BP2*), which presents a plot of Max. PEEQ versus (*BP1-BP2*). In this figure, the two square symbols refer to the *GT* of the training samples; the diamond symbol refers to the *GT* of the test sample; and the dot symbol refers to the prediction of SBMLM, which was determined by calculating the averaged Max. PEEQ of the two training samples. The triangle refers to the prediction of the IBMLM model, which was given by calculating the averaged PEEQ of the two training samples at each pixel. To illustrate, the *GT* PEEQ fields of *S1*, *S2*, *S3* c the *PD* PEEQ fields of *S3* are placed beside each symbol. It is observed that the IBMLM model remarkably outperforms the SBMLM model in accuracy and clarity. When comparing the *GT* PEEQ fields and *PD* PEEQ fields in Fig 3 (b), common patterns were observed at most locations apart from the discrepancy, which was due to strong, local nonlinearities, at the regions circled in red.

To explain the better performance of the IBMLM model, it is noted that the Max. PEEQ values of the two training samples are equal in quantity but differ in

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locations. Based on the linear prior, the SBMLM model can give only the average of the Max. PEEQ values; the IBMLM model, on the other hand, performs a pixel-wise operation to generate the predicted (*PD*) strain field (*SF*), and the Max. PEEQ of predicted *PD* strain field (*SF*) is then taken as the *PD* Max. PEEQ. The pixel-wise operation takes into consideration the location differences of both the binder pressures and the Max. PEEQ. Generally speaking, SBMLM models establish a many-to-one mapping from scalar-based design parameters to scalar-based simulation results, which is not an invertible mapping; However, IBMLM models establish a one-to-one mapping by incorporating location information. It is obvious that the one-to-one mapping is bijective and easier to learn. The potential advantage of IBMLM can be inferred from the results, as the IBMLM model in this case study reduces the absolute error from 0.0954 to 0.0490, and the relative error from 15.02% to 7.719%.

The advantages of IBMLMs, which demonstrates the positive effect of including location information, will be even more prominent with more complex datasets and nonlinear priors. It should be noted that the effect of location information usually has an implicit influence on the performance of surrogate models, which is case-dependent.

The case study in this section is intended to provide an intuitive example. In the remainder of this Section 2, specific techniques of SBMLMs and IBMLMs will be discussed.

2.2 MLP SBMLM model

As a comparison to the IBMLM model, in this paper, a SBMLM model was established. To establish this end-to-end scalar model, a MLP is the most suitable

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method. A MLP, in a narrow sense, is a typical structure of feedforward artificial neural networks (ANNs), which is comprised of an input layer, an output layer, and multiple hidden layers. The neurons of two adjacent layers are fully connected, where each connection is assigned with a weight. Fig 4 presents a MLP consisting of L hidden layers. In the i^{th} layer ($i = 1, 2, \dots, L$), there are n_i neurons. In feedforward, the value of each neuron is calculated as:

$$a_j^i = A \left(\sum_{k=1}^{n^{i-1}} (w_{kj}^i a_k^{i-1} + b_j^i) \right), i = 1, 2, \dots, L + 1; j = 1, 2, \dots, n^i \quad (1)$$

where the superscript refers to the layer number and the subscript refers to the neuron number in a certain layer. To clarify, a superscript of 0 refers to the input layer, while a superscript of $L+1$ refers to the output layer. a_j^i refers to the value of the j^{th} neuron in the i^{th} layer. Specially, a_1^{L+1} equals to the output $\hat{Y}$. w_{kj}^i refers to the weight of the connection from the k^{th} neuron in the $(i - 1)^{th}$ layer to the j^{th} neuron in the i^{th} layer. b_j^i refers to the bias term in the i^{th} layer. $A(\cdot)$ refers to an activation function.

2.3 Res-SE-U-Net IBMLM model

To establish an IBMLM model, CNNs were utilized in this paper. A major strength of CNNs is that they can hierarchically extract location information, which makes CNNs suitable for IBMLMs [34]. Since 2014, multiple architectures of modern deep CNNs have been proposed [35-38]. Among these architectures, the Res-SE-U-Net was selected, which has been proven to be effective in image-to-image generating tasks [14]. In this subsection, the two components, U-Net and Res-SE blocks, will be illustrated.

U-Nets were originally applied in the domain of biomedical image segmentation, which was an image-to-image generating tasks [39]. As shown in Fig 5, a

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typical U-Net features a skip connection, which can reinforce information flow in the neural network. U-Nets have been successfully applied in a number of IBMLM models. N. Thuerey et. al. developed a U-Net model to quickly predict the results of Reynolds-averaged Navier-Stokes simulations [40]. This model was further enhanced by physics-driven methods and applied to predicting steady heat conduction simulations [41]. Other IBMLM models using U-Nets [42-44] are not be described at length in this paper.

A U-Net serves as the backbone of a Res-SE-U-Net. To further enhance its predicting capability, Res-SE blocks can be integrated into U-Nets, where 'Res' refers to the residual connection mechanism and 'SE' refers to the squeeze-excitation channel-wise attention mechanism. The whole Res-SE block is shown in Fig 6 (a) and the nested SE block is further illustrated in Fig 6 (b). To elaborate, the input x of a Res-SE block is firstly processed into $u \in R^{H \times W \times C}$ by two integrated conv layers, where H, W, and C denote the height, width, and channel number, respectively. An integrated conv layer refers to a conv layer that is followed by a batch normalization layer (BN) and an activation layer. An SE block is then attached after the two integrated conv layers. The specific architecture of an SE block is shown in Fig 6 (b). In an SE block, the input tensor u is reduced to $w \in R^C$ by a global pooling layer. w is downscaled to $p \in R^{C/r}$ by a fully connected layer (FC+Activation), where r refers to the reduction ratio of a SE block. p is then upscaled to $q \in R^C$ by another fully connected layer (FC+Sigmoid). q is reshaped to $e \in R^{H \times W \times C}$ that has the same dimensions as u . The SE block output v is then

calculated by the Hadamard product of u and e . v is then processed by the activation function $F(\cdot)$ in Fig 6 (a). The Res-SE block output y is calculated by adding x to $F(v)$.

The Res-SE blocks discussed above have been combined with U-Nets in several studies [14,45,46]. A remarkable increase in accuracy was observed using these Res-SE-U-Nets. In this present paper, a Res-SE-U-Net will be developed based on these two components, i.e. U-Net and Res-SE blocks, to establish IBMLM models.

3. Dataset & Specific surrogate models

To verify the superiority of IBMLMs which benefit from location information, specific SBMLM and IBMLM models were developed and compared based on a dataset of metal forming FEA simulations. This dataset was composed of N pairs of design variables and simulation results, where N refers to the number of samples. Subsequently, the dataset was divided into a training set and a test set. A MLP model was developed as an SBMLM surrogate model, which predicted the scalar simulation results, namely the Max. PEEQ, on the basis of the scalar design variables; and a Res-SE-U-Net model was developed as an IBMLM model, which predicted the image simulation results, namely the entire PEEQ fields, based on images of the design variables.

For comparability, activation functions, optimizers, loss functions are identical for both the MLP and Res-SE-U-Net. The rectified linear unit (ReLU) was selected as the activation function [47]. The Adam algorithm was used to train both models [48]. To

evaluate the performance of the trained networks, two metrics were selected, namely the mean squared error (MSE) and the maximum PEEQ error (MPE):

$$\text{MSE} = \frac{1}{n} \sum_{i=1}^n (p_i^{PD} - p_i^{GT})^2 \quad (2)$$

$$\text{MPE} = |\max(p^{PD}) - \max(p^{GT})| \quad (3)$$

where n refers to the total number of outputs; p refers to the output vector while p_i refers to the i^{th} component of p . In particular, in the Res-SE-U-Net, p refers to the equivalent plastic strain (denoted as PEEQ) in the output image of the PEEQ field and n refers to the total number of pixels of the image, while p_i refers to the value of PEEQ at the i^{th} pixel of the image. A superscript of PD refers to the predicted value, while GT refers to the ground truth value. MSE was used as the loss function in the training processes of both models. MPE was used to evaluate the capability of both models to predict the Max. PEEQ. To illustrate the ability of IBMLMs in alleviating overfitting, numerical techniques, such as regularization terms, were not included in either model.

In subsection 3.1, the dataset will be further elaborated upon, based on which an interpolation task and an extrapolation task will be defined. In subsection 3.2, the architectures and parameters of the MLP will be demonstrated. In subsection 3.3, the architectures and parameters of the Res-SE-U-Net will be demonstrated.

3.1 A simplistic dataset of cold steel stamping simulations

In this study, a simplistic dataset of cold steel stamping simulations, which comprised 1,080 samples, was established to demonstrate the performance of IBMLMs. Once the performance of IBMLMs are demonstrated and validated on this dataset, they can be readily extended to more practical and complex scenarios of metal stamp

forming. The setup of this dataset is shown in Fig 7, where the left figure shows the CAD model of a designed geometry and the right figure shows the FEA model in Abaqus. Each sample in the dataset is determined by five scalar variables that highlighted in green, namely $R1$, $R2$, $R3$, BP , and T . To clarify, the first three variables refer to the three radii values that determine the designed geometries; BP refers to binder pressure; and T refers to blank thickness. Other geometric parameters, including $C1$, $C2$ and $C3$, are fixed in this dataset. The values of $C1$, $C2$, $C3$ are 25 mm, 40 mm, 40 mm, respectively. The quarter blank is a square sized 70 mm $\times$ 70 mm. In the FEA model, the blank is meshed to 2,500 square pixels sized 14 mm $\times$ 14 mm.

Each radius value, namely $R1$, $R2$, or $R3$, takes one value from [6 mm, 8 mm, 10 mm]. This leads to 27 designs using full factorial sampling. For brevity, these 27 designed geometries are numbered from Geo1 to Geo27. In the FEA model of each Geo, the BP could take on any of 20 values evenly spaced from 0.25 MPa to 5 MPa; the T could take on a value of 1 mm or 1.5 mm. In total, this dataset contains $27 \times 20 \times 2 = 1,080$ samples. The initially ordered, unshuffled sequence of these samples is presented in Table 1.

The samples in this dataset are uniformly shuffled and then divided into a training set and a test set by a test ratio of 10%, which is regarded as an interpolation task. In this interpolation task, the test set is uniformly sampled from the whole dataset. Besides the interpolation task, an extrapolation task is defined in this study by directly dividing the samples in the unshuffled order. This unshuffled order leads to the fact that the design space (i.e. the dimensional range of the box radii $R1$, $R2$, and $R3$ in this case MANU-21-1029, Li.

study) of the test set, corresponding to all samples of Geo27 and parts of the samples of Geo26 (illustrated in Table 1), are never covered by the training set. Therefore, this extrapolation task could demonstrate the generalizability and information extraction capability of the SBMLM and IBMLM models.

The dataset size is intentionally set to a small number (1,080) instead of a large number as used in other studies [14, 31]. The purpose of this small dataset is to verify the claim that IBMLMs can deal with given design problems without relying on big data. The scale of the dataset is flexible as long as it contains sufficient information on the corresponding design problem. To further illustrate the location information, four simulation results with different BP values, for Geo1 and $T=1.0$ mm, are presented in Fig 8. It can be observed that wrinkles occur under the lowest binder pressure (0.25 MPa). These simulation results, from left to right, show an evolution of spatial features containing the location information - for example, the location where Max. PEEQ lies. This evolution cannot be captured by SBMLMs. This observation qualitatively demonstrates the necessity of using IBMLMs.

It should be noted that the Max. PEEQ value of samples in the dataset ranges from 0.6366 to 0.9639. It is fully acknowledged that most metal alloys cannot achieve such high level of plastic strain without fracture under cold stamping in practice. However, since the focus of this study is the validation of IBMLMs, the constitutive material model adopted here did not take failure criteria into account. Once the method of IBMLMs is validated, new stamping simulation datasets incorporating more

comprehensive material and process modelling can be employed for practical application.

3.2 Development of the MLP

In the present study, to provide a baseline for the IBMLM model, a MLP was developed to establish an SBMLM model. This MLP contained 6 hidden layers, the architecture and parameters of which are illustrated in Fig 9. The inputs of the MLP were scalar-based design variables, vectors of $R1, R2, \text{ and } R3, BP, T$. The output of the MLP was the Max. PEEQ. Other settings of the MLP, including activation functions, optimizers, loss functions and regularization terms, are fixed according to the discussion at the beginning of section 3.

Compared with CNNs, MLP models are notably more vulnerable to gradient problems, which may lead to an unfair comparison between the MLP SBMLM and the Res-SE-U-Net IBMLM models. To rectify this, the neuron number parameters of this MLP model were appropriately tweaked to reflect the average learning capability of MLPs, which prevents under-fitting and over-fitting. For brevity, only the final architecture and parameters are presented in Fig 9.

3.3 Development of the Res-SE-U-Net

To predict PEEQ fields on the deformed architecture, the Res-SE-U-Net contained two branches, namely Res-SE-U-Net-PEEQ and Res-SE-U-Net-Disp, and both branches shared the same architecture. Based on design variables represented by images, Res-SE-U-Net-PEEQ predicted the image-based PEEQ field, while Res-SE-U-Net-Disp predicted the x, y, z components of the image-based displacement fields. The PD PEEQ and PD MANU-21-1029, Li.

displacement fields were plotted on the undeformed configuration, i.e. the flat blank, for purposes of comparison with the *GT* PEEQ fields and *GT* displacement fields, respectively. *PD* as-deformed components can be created based on the *PD* displacement fields. Subsequently, the *PD* PEEQ fields can be mapped onto the *PD* as-deformed components.

To represent the design variables in 2D-images, the geometric design of each sample was firstly projected to the blank plane sized $70\text{ mm} \times 70\text{ mm}$ from the top view and then discretized into a grid sized 199^2 . The contour map represents the drawing depth, varying with the design configuration of radii $R1$, $R2$ and $R3$. This image based geometric information constituted the first channel of the inputs. To uniformly represent the other parameters in images, the distributions of *BP* and *T* were also projected to the blank plane and discretized into grids of the same size. Image-based *BP* and *T* constituted the second and the third channel of the inputs, respectively. Eventually, the processing/projection of all design variables into imaged based information led to inputs sized $199^2 \times 3$, containing 3 channels. After the processing of the design variables, simulation results of each sample were similarly projected. To further elaborate, the PEEQ fields and X, Y, and Z displacement fields were plotted on the undeformed blank that was discretized into 50^2 pixels. This processing/operation led to outputs sized $50^2 \times 1$ for Res-SE-U-Net-PEEQ, and outputs sized $50^2 \times 3$ for Res-SE-U-Net-Disp. Based on these image-based inputs and outputs, an unified architecture was developed for both Res-SE-U-Net-PEEQ and Res-SE-U-Net-Disp. This architecture was

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composed of three modules, namely downsample, upsample, and Res-SE blocks. In the downsample module, the GT image-based design variables were gradually reduced to feature images sized $12^2 \times 512$ by a series of conv layers. Meanwhile, the channel number was gradually increased from 3 to 512, which aimed to extract the location information of the design variables. These feature images were then processed by 6 serial Res-SE blocks after the downsample module and then imported to the upsample module. In the upscale module, the feature images sized 12^2 were gradually expanded by 8 transposed conv layers, each of which was followed by a BN layer and a ReLU activation function, to the output sized 50^2 for Res-SE-U-Net-PEEQ, representing the processed/projected/flattened PD simulation result of plastic strain fields. In particular, skip connections were applied between the downsample module and the upsample module to enhance the capability of information extraction.

The workflows of Res-SE-U-Net-PEEQ and Res-SE-U-Net-Disp are illustrated in Fig 10, while the parameters of CNN and transposed conv layers in the unified architecture are listed in Table 2. Other settings of the Res-SE-U-Net, including activation functions, optimizers, loss functions and regularization terms, complied with the settings of the MLP according to the discussion in section 3.

4. Results & Discussion

The MLP SBMLM model (SBMLM for short in section 4) and Res-SE-U-Net IBMLM model (IBMLM for short in section 4) were evaluated respectively on both the interpolation task and the extrapolation task. To evaluate their accuracy and

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generalizability, four scalar metrics were applied: MPE (maximum PEEQ error) on the training set, MPE on the test set, LMSE (logarithmic mean square error) on the training set, and LMSE on the test set. These scalar metrics were calculated for each model and then compared. To evaluate the capability of IBMLM in predicting PEEQ distributions, an image metric, namely pixel-wise error (PWE), is applied. PWE can visualize the difference between the an IBMLM *PD* PEEQ field and a *GT* PEEQ field on the undeformed configuration.

All codes were written in Pytorch. Both models were run on an NVIDIA Quadro RTX 5000 GPU. To demonstrate the results of the four models after convergence, the epoch number on the interpolation task was set to 8,000, while that on the extrapolation task was set to 4,000. For both models, the thread number was set to 4, and the batch size was set to 54. Evaluation results on the interpolation task are discussed in subsection 4.1, while those on the extrapolation task are discussed in subsection 4.2. The advantages of the IBMLM in informativeness are demonstrated in subsection 4.3.

4.1 Evaluation results on the interpolation task

An interpolation task was designed to evaluate the capability of IBMLM in accurately predicting the Max. PEEQ, which was evaluated by MPE. It should be noted that the loss function of SBMLM was exactly equal to the square of MPE, while the loss function of IBMLM did not explicitly contain MPE. It was thus anticipated that SBMLM should perform well in MPE, while the performance of IBMLM was not guaranteed.

Therefore, this task can be used to certify whether IBMLM really can extract inherent features of design variables and PEEQ fields that guarantee the MPE accuracy.

The results of the four scalar metrics on the interpolation task are illustrated in Fig 11 (a) (b) (c) (d). In each figure, one of the four metrics are compared between SBMLM and IBMLM. To clarify the amplitude fluctuation of MSE, logarithmic MSE (LMSE) is used in Fig 11 (c) (d) instead of the original MSE. For comparability, the MPEs of samples in both models are sorted in ascending order, respectively on the training set and test set.

As can be seen in Fig 11 (a) (b), both models performed well in the accuracy of Max. PEEQ, while IBMLM slightly outperformed SBMLM in generalizability according to Fig 11 (b). In Fig 11 (c), the curves of LMSE on the training set are plotted for both models. Both curves decrease to the same order of magnitude of -6 after 5000 epochs. However, the fluctuation amplitude of the SBMLM curve is significantly larger than that of the IBMLM curve. In Fig 11 (d), the curves of LMSE on the test set are plotted for both models. The IBMLM test error converges after 1500 epochs, whereas the SBMLM curve still fluctuates acutely after 8000 epochs. Fig 11 (c) (d) show the better convergency and robustness of IBMLM over SBMLM, which are of vast importance in practical applications. This advantage of convergency and robustness is because IBMLM converts the surrogate model to an easy-to-train bijective mapping relationship. To elaborate further, in SBMLM, a certain set of scalar-based design variables can be uniquely mapped to a certain Max. PEEQ, but not the opposite. In IBMLM, a certain set of image-

based design variables can be reversibly mapped to certain PEEQ fields. This bijective mapping relationship can significantly improve the capability of IBMLM.

To conclude, on the interpolation task, both models performed well in accuracy, whilst IBMLM performed better in generalizability, convergency, and robustness. As mentioned above, even though MPE was not explicitly contained in the loss function of IBMLM, IBMLM still slightly outperformed SBMLM. This indicates that the IBMLM indeed extracted the inherent features of simulation results, which led to accurate predictions.

4.2 Evaluation results on the extrapolation task

An extrapolation task, in which the test geometries were unseen (see section 3.1), was designed to test the generalizability of both models. The results of the four scalar metrics on the extrapolation task are presented in Fig 12 (a) (b) (c) (d). In Fig 12 (a), the training set performance of both models on the extrapolation task was as good as that on the interpolation task. In Fig 12 (b), IBMLM significantly outperformed SBMLM on the test set of the extrapolation task, while SBMLM was severely overfitted. This can be explained by the fact that Geo parameters in the test set were completely unseen in the training set. When facing unseen geometries, SBMLM failed to generalize because the parameterized radii values were literally isolated scalars without interrelationships, and the location information of the PEEQ fields was lost. IBMLM, on the other hand, was still able to generalize, since both the geometries and the simulation results were treated as images that preserved complete interrelationships and location information. In Fig 12 (c), both curves of IBMLM and SBMLM converge to MANU-21-1029, Li.

the same order of magnitude. In Fig 12 (d), IBMLM stabilized around -3.7 after 1,000 epochs, whereas SBMLM still oscillates around -3.2 after 4,000 epochs.

To further stress the importance of the extrapolation evaluation, a comparison of test set performances on both tasks are presented in Fig 13 (a) (b). It is observed that both SBMLM and IBMLM performed better on the interpolation task. This is because the training set in the interpolation task gave better coverage of the ranges of design variables than the training set in the extrapolation task. To better cover the ranges of design variables, advanced sampling strategies can be adopted, which are not detailed in this paper (A van Beek, et. al., 2020). Despite these strategies, it is impossible to guarantee a perfect sampling and eradicate the effects of extrapolation in practical industries when confronting complicated and non-isometric geometries [50].

4.3 Capability of IBMLM to analyze location information

A critical advantage of IBMLM is that they can deal with scenarios where the performance metrics are distributions of simulation results instead of scalars, such as plastic strain fields and displacement fields (as shown in this study), or thinning fields, punch impact lines, and microstructure distributions, which are also important performance indicators in sheet metal forming. To evaluate the capability of IBMLM to extract features and predict the distribution of PEEQ, pixel-wise errors (PWEs) are used. PWEs are calculated as the pixel-wise difference between a *GT* PEEQ field and its IBMLM PDE PEEQ field, both on the undeformed configuration:

$$PWE_i = (PEEQ_i^{GT} - PEEQ_i^{PD}), i = 1, 2, \dots, n \quad (4)$$

where n refers to the total number of pixels, $PEEQ_i^{GT}$ refers to the GT PEEQ at the i^{th} pixel, $PEEQ_i^{PD}$ refers to the PD PEEQ at the i^{th} pixel. The GT , PD PEEQ fields and corresponding PWEs of several typical cases are visualized in Fig 13. In Fig 13 (a), 6 cases from the training set are presented. The PD PEEQ fields are practically identical with the GT PEEQ fields, while the PWEs are low and evenly distributed. In Fig 13 (b), 6 cases from the test set are presented. It is observed that the PWEs of these test cases are higher than those of the training cases. However, the extreme values of the PWEs are mostly centralized in zones of sensitive features, such as the tail on the lower left of test Case2. Mostly, these extreme PWEs slightly tampered with the locations of the sensitive features instead of radically transforming the whole distribution. Therefore, these extreme PWEs are acceptable. Moreover, it can be seen that the overall PEEQ distribution is well maintained.

Based on the discussions above, it is affirmed that IBMLM are capable of extracting location information and predicting the distributions of PEEQ. A striking advantage of IBMLM is informativeness. To elaborate, suspicious outliers of predictions in IBMLM are embodied as uncommon distributions of PEEQ fields. Uncommon distributions of physical fields can provide more information for researchers to judge the existence and possible cause of errors. On the other hand, suspicious outliers in SBMLM are only embodied as extreme scalar values. Extreme values are only indicative of the possibility of errors, which cannot help researchers to make a judgement or locate the possible errors.

One thing to note is that the magnitudes of PWEs seem high compared with those of MSEs and MPEs mentioned above. However, this comparison is pointless, because MSEs and MPEs are used to contrast the accuracy and generalizability between SBMLM and IBMLM, while PWEs are used to evaluate the capability of IBMLM of extracting location information. Furthermore, although the distributions are well maintained, small local discrepancies in adjacent pixels between the *PD* and *GT* images may result in local patches of large PWE. Since the overall distribution is of interest, these local discrepancies can be interpreted as numerical noise. To mitigate this, more advanced metrics will be investigated in future studies to evaluate the information extraction capability of IBMLM.

where n refers to the total number of pixels, md_i refers to the magnitude of displacements at the i^{th} pixel. As can be seen in Fig 15, the highest maximum errors of the magnitude of displacements (MEMD) across the dataset is below 1.5 *mm* and the highest average errors of the magnitude of displacements (AEMD) across the dataset is below 0.25 *mm*. Given that the *GT* displacements are one order of magnitude larger than MEMD and two larger than AEMD, the accuracy of the *PD* displacement fields is acceptable. In Fig 16, based on the acceptable *PD* displacement fields, *PD* PEEQ fields are projected and compared with *GT* PEEQ fields on the deformed configuration. This capability of IBMLM in predicting the deformed configuration can further enhance the informativeness of IBMLM and extend IBMLM to more scenarios, such as springback prediction.

As discussed, this paper is a pioneering work to apply image-based machine learning methods (IBMLM) to metal forming problems for the first time. Thus, it focuses more on theory than practical applications and sampling strategies. Therefore, the numerical experiment is based on a simple and virtual cold stamping case and the dataset may have been overly sampled. Although this dataset is much smaller than those in the literature [14, 31], there is good potential to further reduce the dataset in practice. In reports on commercial applications in other fields with similar problems [51,52], the datasets contained less than 100 samples and IBMLM significantly outperformed SBMLM. In next step studies, advanced sampling strategies, such as active learning, will be further investigated to improve computation efficiency.

5. Conclusion & Outlook

In this study, a Res-SE-U-Net IBMLM surrogate model was innovatively applied to predicting the physical fields (plastic strain and displacement fields) of stamp forming simulations. Compared with SBMLM, the IBMLM proved to be more accurate, generalizable, robust, and informative. It was seen that the loss curve of the IBMLM converged faster and with greater stability when compared with that of the SBMLM. When tackling an extrapolation task, IBMLM succeeded in extracting common features and giving plausible predictions to a certain degree, while SBMLM failed to generalize.

In terms of theories and interpretability, the assumption of location information was intuitively and quantitatively validated through a two-sample case in section 2.1, which has not been discussed in most existing studies about IBMLM. Based on this assumption, the advantage of IBMLM can be summarized as extracting more

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information from given datasets, which was proven to be valid even with small datasets.

Meanwhile, the predictions obtained from IBMLM provide more location information

for engineers to evaluate and accurately calibrate the IBMLM surrogate models.

Despite these efforts and achievements, IBMLM suffers from the problem of training time. For example, in the interpolation task, a 1,500-epoch training process of the IBMLM model, which was sufficient for convergence, took 3.75 hours, while that of the SBMLM model took 0.8 hours. This was because IBMLMs take full images as inputs and outputs, which increases the computational complexity when compared to the scalars used in SBMLM. However, thanks to the image-based and non-parameterized representation, IBMLM is empowered to be scalable and generalizable. IBMLM can benefit from transferring learning and integrating data from multiple sources, while SBMLM is severely restricted by a specific parameterization [51,52]. This considerably reduces the time spent on sampling and simulations, which make up most of the computation time. Therefore, IBMLM models are time-saving in the long run. Moreover, it has been observed that IBMLM models are easier to optimize due to their robustness. Lightweight IBMLM architectures can thus be designed to further mitigate the computational burden.

In future studies, IBMLM will be extensively investigated in more complex metal forming scenarios. Firstly, the design principles of the architecture will be studied to boost performance. Secondly, multiple machine learning methods and techniques, such as generative models and physics-based priors, will be leveraged. Thirdly, IBMLM models show promise to be transferred to multiple scenarios, particularly where it is

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necessary to represent the simulation results by images. Furthermore, IBMLM models will be embedded in inverse problems, such as optimizing the metal forming manufacturing parameters based on cost performance considerations. Datasets of specific materials and manufacturing methods will also be established for training virtual manufacturing experts using IBMLM.

ACKNOWLEDGMENT

The funding support from Shougang Group Co., Ltd. Research Institute of Technology for this research is much appreciated. The research was performed at the Shougang-Imperial Lab for lightweight steel-based systems for impact resistant automotive applications at Imperial College London. Haosu Zhou acknowledges the Chinese Scholarship Council and Imperial College London for his scholarship. The authors would like to thank Hamid Reza Attar for his assistance in the final revision of this paper.

NOMENCLATURE

FEA	Finite element analysis
SBMLM	Scalar-based machine learning method
IBMLM	Image-based machine learning method
MLP	Multi-layer perceptron
CNN	Convolutional neural network
DNN	Deep neural network

CAD	Computer-aided design
PEEQ	Equivalent plastic strain
CRDQ	Cold rolled, drawing quality
<i>GT</i>	Ground truth
<i>PD</i>	Predicted
<i>SF</i>	Strain fields
<i>S1</i>	Strain fields 1
<i>S2</i>	Strain fields 2
<i>S3</i>	Strain fields 3
ANN	Artificial neural network
<i>BN</i>	Batch normalization
<i>FC</i>	Fully connected layer
<i>SE</i>	Squeeze-Excitation
Res	Residual-connection mechanism
ReLU	Rectified linear unit
MSE	Mean squared error
MPE	Maximum PEEQ error
<i>R1</i>	Radius 1

<i>R2</i>	Radius 2
<i>R3</i>	Radius 3
<i>BP</i>	Blank pressure
<i>BP1</i>	Blank pressure 1
<i>BP2</i>	Blank pressure 2
<i>C1</i>	Constant 1
<i>C2</i>	Constant 2
<i>C3</i>	Constant 3
MPa	Mega pascal
Geo	Geometry
LMSE	Logarithmic mean square error
PWE	Pixel-wise error
MEMD	Maximum errors of the magnitude of displacements
AEMD	Average errors of the magnitude of displacements

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Figure Captions List

- Fig. 1 Pipelines of surrogate models: (a) scalar-based machine learning methods (SBMLM) based surrogate models; (b) image-based machine learning methods (IBMLM) based surrogate models.
- Fig. 2 A surrogate model with two training samples to illustrate the location information of FEA results:
 (a) setup of a half-symmetric model with varying binder pressures;
 (b) stress-strain curve of the material used in the simulation;
 (c) two training samples and one test sample: the ground truth (GT) PEEQ of Sample 1, Sample 2 and Sample 3.
- Fig. 3 Max. PEEQ predictions of SBMLM and IBMLM models both under linear assumption:
 (a) plot of Max. PEEQ versus (BP1-BP2), where BP refers to the binder pressure; (b) comparison between the ground truth (GT) PEEQ and the predicted (PD) PEEQ by using IBMLM of the test sample.
- Fig. 4 The schematic of a Multi-Layer Perceptron (MLP) for SBMLM.
- Fig. 5 The schematic of a U-Net and skip connection mechanisms.
- Fig. 6 Composition of Res-SE block.
- Fig. 7 Setup of a model metal forming simulation: a quarter CAD model of the designed geometry and a FEA model in Abaqus.

- Fig. 8 PEEQ fields under increasing binder pressure.
- Fig. 9 The architectures and parameters of the Multi-Layer Perceptron used in this study.
- Fig. 10 (a) The workflow of Res-SE-U-Net-PEEQ (b) The workflow of Res-SE-U-Net-Disp. Note: The two networks share a similar architecture, but differ in the channel number of the output layer. They are trained as two separate networks with different parameters.
- Fig. 11 Interpolation performance of SBMLM and IBMLM:
 (a) maximum PEEQ error (MPE) on the training set and (b) MPE on the test set; (c) logarithm mean square error (LMSE) loss on the training set and (d) LMSE loss on the test set.
- Fig. 12 Extrapolation performance of SBMLM and IBMLM:
 (a) MPE (maximum PEEQ error) on the training set and (b) MPE on the test set; (c) LMSE (logarithm mean square error) loss on the training set and (d) LMSE loss on the test set.
- Fig. 13 Comparison between the ground truth (GT) PEEQ fields and the predicted (PD) PEEQ fields: cases in (a) training set and (b) test set.
- Fig. 14 Certification of the accuracy of predicted displacement fields: (a) maximum errors of the magnitude of displacements (MEMD) and (b) average errors of the magnitude of displacements (AEMD).

Fig. 15 Fig. 15 Example PEEQ fields on the deformed configuration: (a) predicted;
(b) ground truth.

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Table Caption List

Table 1	Dataset of the quarter-model metal forming simulation samples in an unshuffled order, splitting the training set (90%) and test set (10%) for the extrapolation task.
Table 2	Architecture parameters of the Res-SE-U-Net

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(c) logarithm mean square error (LMSE) loss on the training set and (d) LMSE loss on the test set.

Fig. 12 Extrapolation performance of SBMLM and IBMLM

(a) MPE (maximum PEEQ error) on the training set and (b) MPE on the test set;
(c) LMSE (logarithm mean square error) loss on the training set and (d) LMSE loss on the test set.

(a)

Fig. 13 Comparison between the ground truth (GT) PEEQ fields and the predicted (PD) PEEQ fields: cases in (a) training set and (b) test set.

Fig. 14 Certification of the accuracy of predicted displacement fields: (a) maximum errors of the magnitude of displacements (MEMD) and (b) average errors of the magnitude of displacements (AEMD).

(a)

(b)

Fig. 15 Example PEEQ fields on the deformed configuration: (a) predicted; (b) ground truth.

Table. 1 Dataset of the quarter-model metal forming simulation samples in an unshuffled order, splitting the training set (90%) and test set (10%) for the extrapolation task.

Geo	Geo1					...	Geo25						...	Geo27					
BF	BP1		...	BP20		...	...	BP6		BP7		...	...	BP1		...	BP20		
T	T1	T2	...	T1	T2	...	...	T1	T2	T1	T2	...	...	T1	T2	...	T1	T2	
90% samples										10% samples									

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Table. 2 Architecture parameters of the Res-SE-U-Net

Layer	Downscale			Upscale			Res-blocks
Number	Kernel	Stride	Padding	Kernel	Stride	Padding	<ul style="list-style-type: none">• Number of blocks: 6• CNN layers in each block: Kernel (3,3) Stride (1,1) Padding (1,1)• Reduction ratio in SE blocks: R=16
1	(1,1)	(1,1)	(0,0)	(3,3)	(1,1)	(1,1)	
2	(11,11)	(2,2)	(5,5)	(3,3)	(1,1)	(1,1)	
3	(8,8)	(2,2)	(3,3)	(3,3)	(1,1)	(1,1)	
4	(6,6)	(2,2)	(2,2)	(3,3)	(2,2)	(0,0)	
5	(3,3)	(1,1)	(1,1)	(3,3)	(1,1)	(1,1)	
6	(3,3)	(2,2)	(0,0)	(3,3)	(1,1)	(1,1)	
7	(3,3)	(1,1)	(1,1)	(6,6)	(2,2)	(2,2)	
8				(3,3)	(1,1)	(1,1)	

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