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APPLICATIONS OF MACHINE LEARNING FOR PROCESS MODELING OF COMPOSITES

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ABSTRACT

Science-based simulation tools such as Finite Element (FE) models are widely used in engineering applications including process modeling of composites. There are inherent limitations associated with these models including trade-off between fidelity and cost, inability to tackle uncertainties such as unknown manufacturing boundary conditions, and difficulties with inverse modeling and optimization of multi-dimensional problems. With the rise of Machine Learning (ML) and data-driven modeling, many branches of science and engineering are exploring the applications of these methods with varying degrees of success. Here we explore current applications of ML in process simulation of composites. With several case studies, it is demonstrated how some of the limitations of traditional science-based models can be addressed using a combined FE-ML approach in the new paradigm of Theory-Guided Machine Learning (TGML). Specifically, case studies are presented for thermo-chemical analysis of composites processing, where surrogate Neural Networks (NN) are developed for near real-time modeling of the manufacturing process.

Keywords: Process Modeling, Machine Learning, Neural Network
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1. INTRODUCTION

Processing of advanced composites is a complex and multi-physics problem during which the material goes through several phase transformations [1–4]. Often, for ease of analysis, this complexity is decoupled for thermo-chemical analysis, flow-compaction analysis, and stress-deformation analysis [5]. In each of these problems, the aim is to express a set of outcomes such as degree of cure, cured ply thickness, and dimensional changes, as a function of process parameters such as temperature and pressure histories. In general, such correlations can be established using the following main approaches:

- Empirical approaches where based on existing theories and experimental observations, closed-form solutions are derived. For example, based on the notion of exponential decay in chemical reactions, cure kinetics in thermoset composites may be represented using Arrhenius type equations for which parameters are obtained via experimental fitting [6]. For the problem of composite processing where the governing laws are complex, high-fidelity and accurate closed-form solutions cannot be obtained. This limits the applicability of such approaches.

- Science-based approaches where the first step is to establish governing physical laws in the form of Partial Differential Equations (PDEs). These are usually obtained based on conservation laws such as mass conservation, momentum conservation and energy conservation [7]. The set of PDEs are then solved using established numerical techniques including Finite Element (FE) methods. FE models are now widely used in every aspect of composite manufacturing and design [5,8–12]. One limitation of such approaches is the trade-off between fidelity and speed [13]. High fidelity FE simulation tools are difficult to characterize and slow to set-up and perform.
- With the rise of Machine Learning (ML) and data-driven modeling approaches, many researchers are exploring the application of such methods to multi-physics problems including processing of composites [13,14]. These are mainly theory-agnostic approaches where no prior knowledge of the underlying physics is needed. The main step in these approaches is to create a dataset of inputs (e.g. process parameters) and desired outputs. The dataset should be large enough to allow for successful training of ML models such as Neural Networks (NN). In these applications, NNs are basically complex and sophisticated data fitting algorithms. The difference with previous approaches is that it does not need an explicit form of the governing laws to establish correlations. One of the main challenges to apply these approaches is creating large physical datasets. The other shortcoming is the so-called brittle AI [15] where outside of the training zone, NN predictions might fail if new data is presented. Compared to FE models, ML models are much faster to the point that they can be used to develop real-time predictive tools.
- Theory-Guided Machine Learning (TGML) or physics-informed machine learning is a new paradigm that combines the best of previous approaches to address their limitations [13,14,16,17]. As oppose to theory-agnostic ML approaches, in these methods, existing theory and domain knowledge is used to guide the training of ML models. For example, established FE tools can be used to create dataset of numerical data instead of physical data. This can be used to train surrogate NN models with comparable accuracy to FE models, but with a fraction of the simulation time.

It is clear that data (experimental or numerical) is the basis of any machine learning model. Given large amount of data such as historical manufacturing data, a variety of ML techniques can be employed for regression (e.g. predicting exotherm during curing) and classification problems (e.g. detecting faulty sensors during manufacturing). ML models have been used in different aspects of composite manufacturing including in-situ defect detection in AFP processing [18], ATL optimization [19], infusion analysis [20,21], cure kinetics characterization [22,23], curing process simulation [13,14,24], machining [25], Nondestructive Inspection (NDI) [26], and assembly [27].

Here first we explore the idea of data and specifically how much data is required to train accurate NN models for composite processing. We then introduce both ML and TGML concepts related to thermo-chemical analysis of composites during processing. Finlay, we present a recent commercial implementation of a TGML model to increase the speed of process simulation tools significantly.

2. 1D THERMO-CHEMICAL ANALYSIS

Consider 1D convective heating of an inert composite part as schematically shown in Figure 1a. As depicted in this figure, assume that a composite tool with a thickness of L is heated with a constant heating rate of T' and a heat transfer coefficient of h. As heating progresses, the temperature at the center of the part lags behind the air temperature. For the steady-state condition, this thermal lag reaches a constant value of ΔT. The part temperature history can be predicted by solving heat transfer equations using FE simulation tools. This can be done using commercially available FE packages such as RAVEN [28] as shown in Figure 1b.

As a first step, we aim to replicate the FE analysis with a surrogate NN model (trained with numerical data) and explore how many data points we need for this purpose. This of course depends on a number of parameters including desired accuracy, complexity of the physical problem, number of input parameters, and architecture and hyper-parameters of the NN model. Recently a comprehensive study was conducted on the effects of NN architecture and hyper-parameters for a similar problem [13]. Following this study, as shown in Figure 2, we will use a optimized NN architecture of 5 hidden layers and 25 nodes per layer to predict the value of thermal lag as a function of 3 input parameters: part thickness, L, heat transfer coefficient, h, and heating rate, T'. Optimized hyper-parameters for the NN model based on the recent study by authors [13] are listed below:

- *Neural Network architecture*: Dense network with 5 hidden layers and 25 nodes per layer as shown in Figure 2.
- *Activation function*: Rectified Linear Unit (ReLU) as defined below:

$$ReLU(z) = max(0, z)$$

- *Loss function*: Mean Squared Error (MSE). Root Mean Squared Error (RMSE) is reported for each training and defined below:

$$RMSE = \sqrt{\frac{\sum (\Delta T_i - \Delta P_i)^2}{N}}$$

  In which ΔT is the thermal lag as precited by FE, ΔP is the thermal lag as predict by NN and N is the total number of data points.

- *Optimization*: Gradient Descent (GD) without regularization and a learning rate of 0.001. Batch size of 50 and training iterations of 200,000.

All training was performed using a high-level API in Python (Version 3.6.8), Tensorflow (Version 1.8.0). In terms of desired accuracy, the NN predictions have to be comparable to FE results. For this, we consider a mean error less than 0.5 ℃ in predictions (i.e. $RMSE < 0.5$ ℃). To train the NN model, first 10,000 FE simulations using RAVEN were conducted. A nominal tooling composite with a through-thickness conductivity of $0.5\ W/mK$ and diffusivity of $0.5 \times 10^{-6}\ m^2/s$ was considered. In each simulation, the tool thickness was randomly varied between 2 and 20 mm, the heat transfer coefficient between 20 and $100\ W/m^2K$, and the heating rate between 1 and 5 °C/min. To study the effect of dataset size, many NN models were trained with different dataset sizes selected from the 10,000 FE simulations. For each training, RMSE was recorded. Results of all training are shown in Figure 3. This shows that as the dataset size increases, the prediction error of NN models decreases as well. Beyond 1,000 datapoints, error becomes almost constant. For the required accuracy of $RMSE < 0.5$ ℃, based on Figure 3, approximately 1,000 datapoints are needed to train NN models.

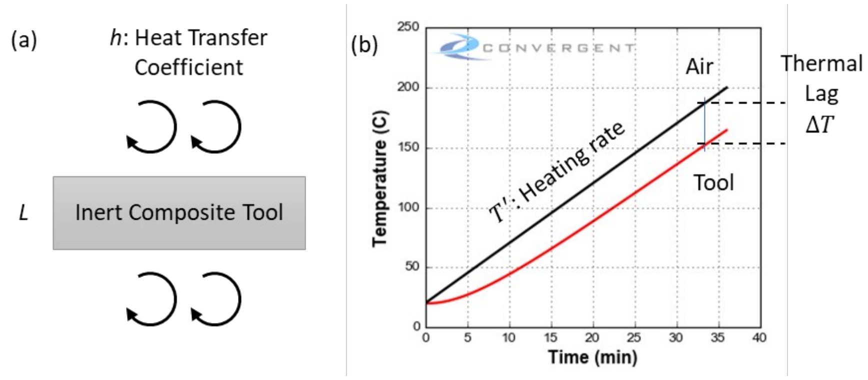

Figure 1: (a) 1D convective heating of an inert composite tool, and (b) temperature history and steady-state thermal lag at the center of the tool subjected to a constant heating rate.

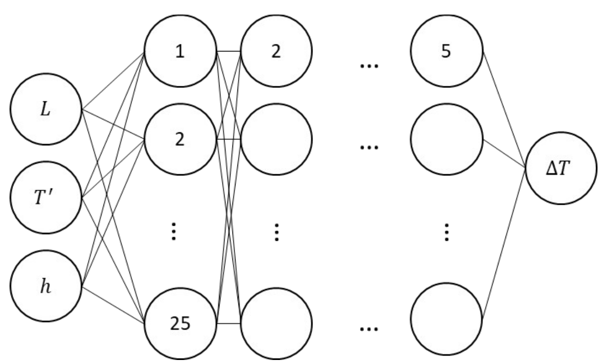

Figure 2: A dense Neural Network (NN) with 5 hidden layers and 25 nodes per hidden layer to predict the steady-state thermal lag during convective heating of a tool as shown in Figure 1.

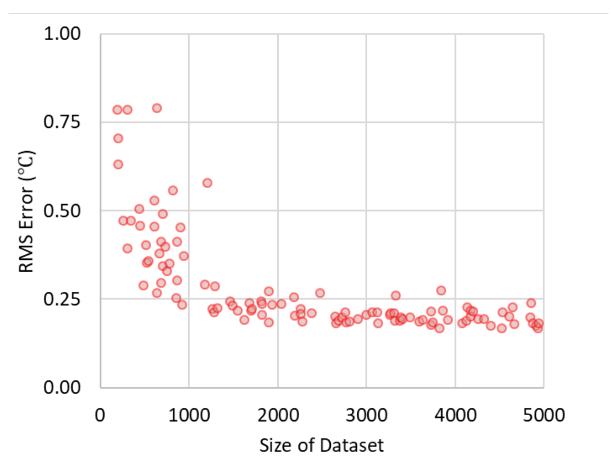

Figure 3: RMSE as a function of dataset size in training of NN models to predict steady-state thermal lag in a tool as shown in Figure 1.

For a more complex case, consider prediction of exotherm and thermal lag in a 1D thermo-chemical analysis of a thermoset composite part on a tool as shown in Figure 4a. For this analysis, a HEXCEL AS4/8552 composite part and an Invar tool are used. Cure kinetics and thermal properties implemented in the RAVEN software were used for FE analysis. Similar to the previous case, we aim to replicate the FE simulation with NN modeling. Here a NN with 4 layers and 10 nodes per layer is considered as shown in Figure 5. The number of input parameters are now increased to 5: part thickness, L_1, tool thickness, L_2, heat transfer coefficient above the part, h_1, heat transfer coefficient below the tool, h_2, and heating rate, T'. Cure cycle is a two-hold cycle with a 1 hour hold at 120 ℃ and 2 hours hold at 180 ℃. Similar to previous case, RAVEN was used to create a dataset for training of NN models to predict exotherm and thermal lag in the part as shown in Figure 4b. Here we compare two types of NN models. In one approach, original FE inputs are used to train NNs (i.e. theory-agnostic ML modeling). In the other approach, first we transform the heating rate as follows and then use it as an input for training (i.e. TGML modeling):

$$f(T') = \frac{1}{1+e^{-T'}} - 0.6$$

This is to consider the exponential effect of heating rate on exotherm. For the considered range of input parameters, and with low heating rates below 0.6 ℃/min, exotherm is negligible in the part. As the heating rate is increased, exotherm also increases. However, eventually the exotherm reaches a constant value and becomes independent of heating rate. This is because for fast heating rates, curing occurs at the final hold and not during the second heat-up step. As such, the effect of heating rate on exotherm becomes exponential [13]. This understanding of the physical problem is used here to help training of ML models. The effect of this transformation is shown in Figure 6. This shows that the NN models that are trained with this transformation are more accurate than the models that are not trained with this transformation. This observation is generally true independent of the dataset size. The NN models with transformed heating rates, reach a stable RMSE value below 0.5 ℃/min beyond 500 datapoints. On the other hand, the NN models that are trained with original heating rates reach this value beyond 750 data points. This shows that TGML modeling reduces the required number of datapoints for training. In addition, this can better capture the behavior of the physical problem even outside of the training zone [13]. This is shown in Figure 8 where predictions of exotherm using three methods are compared: NN model trained with the original heating rate, NN model trained with the transformed heating rate and FE analysis. This is to predict exotherm as a function of heating rate for a 10 mm part on a 12 mm tool, and heat transfer coefficients of 60 and 40 W/m^2K. The training zone for heating rate was between 1 and 5 ℃/min as highlighted in Figure 8. This shows that while predictions within the training zone are quite similar, outside of the training zone, predations using the NN model trained with original heating rates are incorrect. In comparison, FE analysis and TGML model have very similar results even outside of the training zone. This is because training with a transformed heating rate, captures the underlying physics and ensures consistency even outside of the training zone.

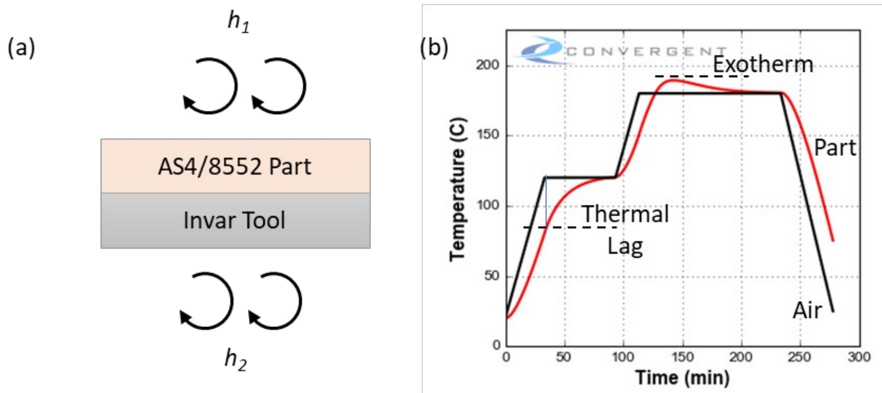

Figure 4: (a) 1D representation of convective heating and curing of a composite part on a tool, and (b) prediction of the thermal history at the center of the part using RAVEN software.

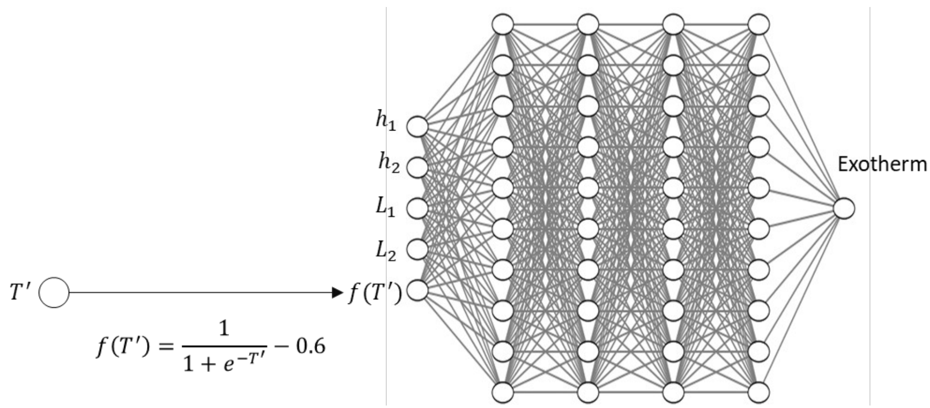

Figure 5: A TGML NN model to predict exotherm in 1D thermo-chemical analysis of a composite part using a transformed heating rate.

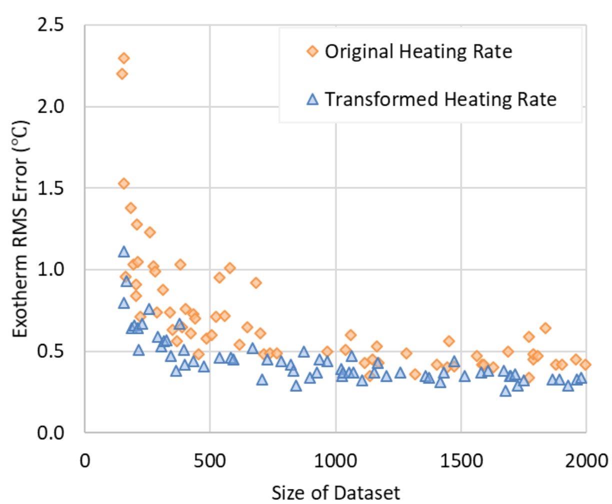

Figure 6: RMSE in predicting exotherm as a function of dataset size for theory-agnostic NN models and theory-guided NN models.

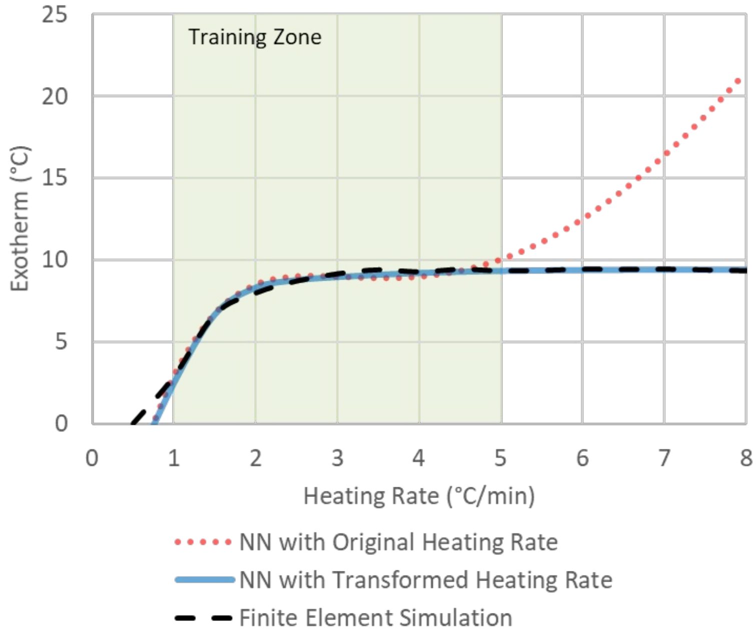

Figure 7: Comparison of predictions of exotherm using three methods: NN model with original heating rate, NN model with transformed heating rate and FE analysis.

3. IMPLEMENTATION AND APPLICATION

In this section, we consider the application of developed surrogate NN models in increasing the speed of process simulation in composites. During the conceptual design phase of aerospace composite parts, it becomes necessary to quickly assess the manufacturability of the part. This is usually done by conducting full 3D thermo-chemical analysis of the part and tool. Since details of the design including part and tool thicknesses, and cure cycle parameters are not set in the conceptual design phase, it becomes important to quickly assess many design iterations at this step. Two established approaches may be taken for this analysis:

- Full 3D thermo-chemical analysis using software packages such as COMPRO in ABAQUS [29]. For a complex part such as a composite wing skin, analysis might take at best several hours. Analysis of design iterations might take several days on a typical engineering workstation.
- Since during heating of thin parts on thin tools, the through-thickness heat transfer is the dominant heat transfer mechanism, the 3D problem may be divided into several 1D zones to conduct 1D FE simulations. Convergent Manufacturing Technologies has developed a commercial design aid, the Composites Producibility Assessment – Thermal Analysis (CPA-TA), as a plugin for CATIA V5 which can be used for this purpose. For a given wing skin as shown in Figure 8, this decreases the analysis time significantly to less than an hour on a typical engineering workstation. Although this is an approximate approach, in the conceptual design phase, the accuracy is good enough for making quick decisions.

Although 1D analysis increases the speed of simulation significantly, it is still not fast enough to fully explore the design spectrum. The speed of simulation can be further increased using the trained TGML models described in previous section. These models were recently implemented in

CPA-TA in CATIA to predict a series of outcomes including exotherm, thermal lag and minimum viscosity during processing [14]. For design iterations, the entire wing skin was analyzed using three different temperature cycles by varying heating rates and three different tool thicknesses. This was equivalent of conducting 270 1D analyses. For comparison, the same simulation was conducted using FE and then using TGML models. Comparison of simulation time is shown in Table 1. This shows a significant speed gain where simulation time is decreased from about half an hour to only 2 seconds on a typical engineering workstation. Out of 2 seconds, about 1.5 seconds was used to initialize libraries in the CPA-TA code while analysis time was only about 0.5 seconds. This is a significant gain in simulation speed to the point of virtually developing real-time predictive tools for composite processing.

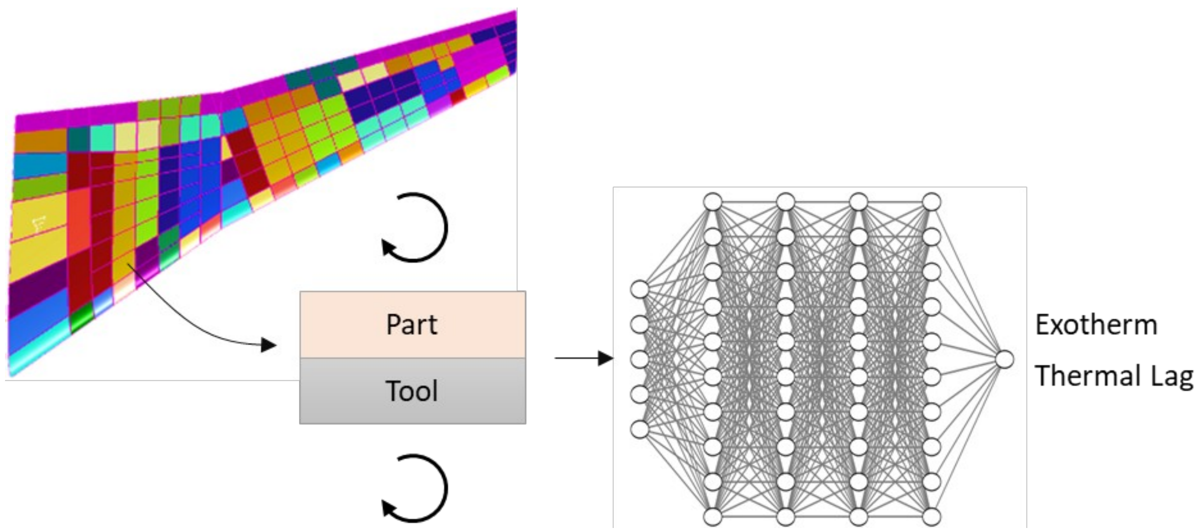

Figure 8: Thermo-chemical analysis of a composite wing skin by dividing it into 1D zones to use surrogate NN models.

Table 1: Comparison of different methods for thermo-chemical analysis of a composite wing skin.

Analysis Method	1 x 3D FE simulation	270 x 1D FE Simulations	270 x NN Simulations
Commercial Software	COMPRO in ABAQUS	CPA-TA in CATIA V5	CPA-TA in CATIA V5
Simulation Time on a Workstation	Several hours	27 minutes	2 seconds

4. SUMMARY

In this paper, application of ML and TGML for process modeling of composites is presented. It is shown that for simple 1D problems, about 1000 datapoints is needed to successfully train surrogate NN models. By including theory in training of NN models (i.e. TGML), the required datapoints may be decreased while physical consistency in solutions is ensured. With trained surrogate NN models, simulation speed can be increased significantly to the point of developing near real-time simulation capability. A recent commercial application of the TGML models to assess producibility of composite parts using 1D thermo-chemical analysis is presented. It is shown that analysis with design iterations for an entire composite wing skin can be conducted in about 2 seconds on a typical engineering workstation. This is a significant gain compared to half an hour simulation time using 1D FE simulation, and several hours/days using 3D FE simulation.

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