When Data-efficient Machine Learning Comes to the Rescue: An AI-based Optimization Framework for Advanced Manufacturing

Tutorial Instructors:

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https://github.com/miladramzy/SAMPE2023_Tutorial

Tutorial requirements for participants:

1. Personal laptop
   - Software installation is NOT needed as the codes will be run on the cloud.
2. Internet connection
3. Google (Gmail) account to use Colab notebooks
   - https://accounts.google.com/signup/v2/webcreateaccount?flowName=GlifWebSignIn&flowEntry=SignUp
4. Optional: GitHub account
   - https://github.com/signup?ref_cta=Sign+up&ref_loc=header+logged+out&ref_page=%2F&source=header-home

Content/Agenda

Introductions and motivation (45min)

- AI-based manufacturing era
- Data in advanced manufacturing: challenges with **limited data**
- Coping with limited data: Data-efficient machine learning

Transfer learning (concepts and practical examples) (30min)

- Knowledge transferability of cure cycles in composites manufacturing
- Hybrid with Active Learning

Break (15min)

Physics-informed neural networks (15min)

- PINNs for composites curing process

Multi-fidelity learning (15min)

- MFPINN in Composites heat transfer

Hands-on (coding) practice (45min)

Exit survey and open discussions (15min)

Introduction

PhD candidate at the University of British Columbia

THE UNIVERSITY OF BRITISH COLUMBIA

Master of applied science at the University of British Columbia (2017)
Bachelor of applied science at K. N. Toosi University of Technology (2015)

Data Science and Engineering, Research Cluster Coordinator at Materials and Manufacturing Research Institute (MMRI)

Materials & Manufacturing Research Institute
Experience Innovation with Us

PhD Thesis: Data-Efficient and Uncertainty-Aware Hybrid Machine Learning in Advanced Composites Manufacturing

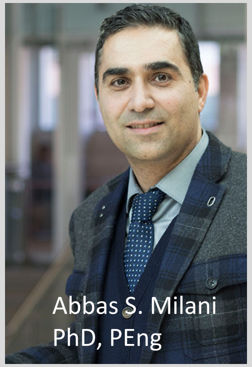
Research interests: Intelligent Manufacturing, Scientific Machine Learning, Transfer Learning, Composites Processing

Web: https://miladramzy.github.io/ | https://www.linkedin.com/in/miladramezankhani/

Introduction

Composites & Optimization Lab (COL)

- *UBC Tier 1 Principal's Research Chair in Sustainable & Smart Manufacturing*
- *Materials and Manufacturing Research Institute (MMRI) Director; CRN Technical Director; Biocomposites Research Cluster Lead; Killam Laureate; Member of Royal Society of Canada*



- Expertise: **Textile Fiber-Reinforced Composites/Biocomposites: Fabrication, Testing, Modeling & Simulation, Industry 5.0 (including Immersive Tech)**
- Related interest: Polymer matrix composites, Forming processes; micro-CT analysis for characterization and mitigation of manufacturing defects
- Web: crno.ok.ubc.ca ; mmri.ubc.ca

Materials and Manufacturing Research Institute

A multi-disciplinary, multi-campus research hub

- Developing a high-impact cluster of research excellence in different sub-areas of materials and manufacturing.
- Expanding collaboration with other UBC Institutes/Centres, and a number of leading national and international research networks and industrial sectors.
- **Ultimate vision**: Be a role model in Canada to link basic and applied research on materials and manufacturing.

Aerospace and Transportation
Materials and Manufacturing

Biomedical and Biological
Materials and Manufacturing

Building and Construction
Materials and Manufacturing

Electromagnetic and Nanoscale
Materials and Manufacturing

Polymer and Natural
Materials and Manufacturing

Data Science and Engineering (Data²)
for Materials and Manufacturing

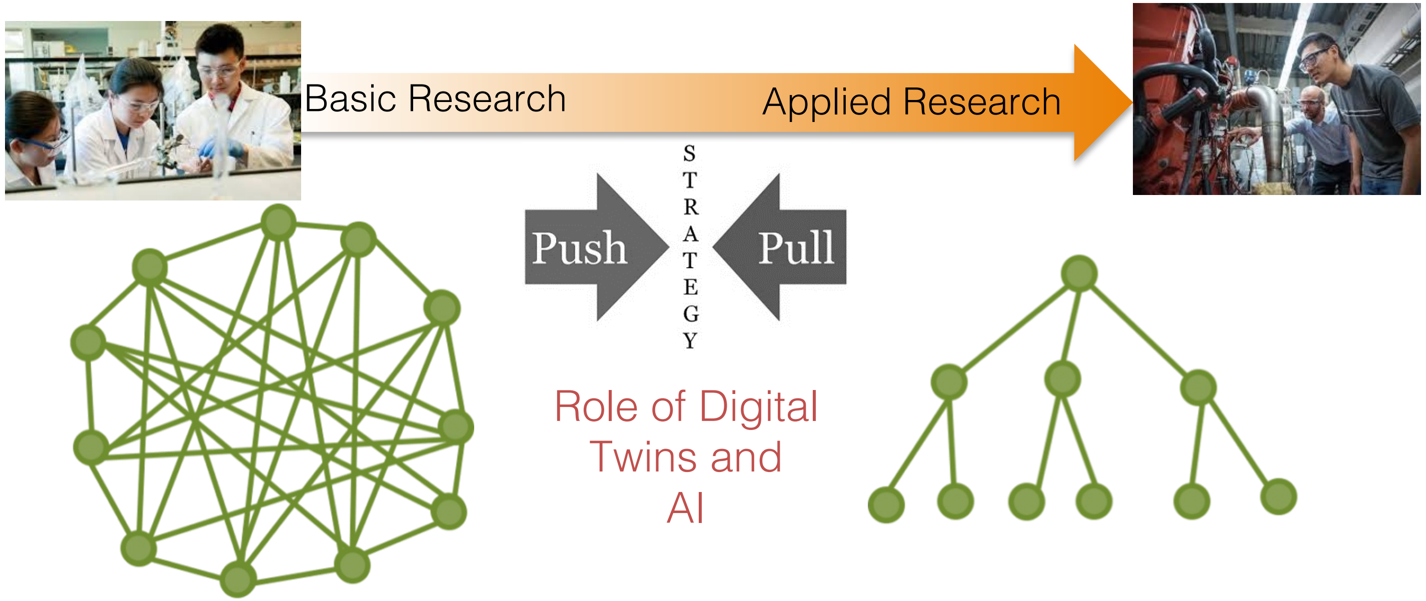
Faculty diversity:

Engineering
Medicine
Health and Exercise Science
Chemistry
Physics
Biology
Statistics & Optimization
Management
Computer Science
Stoical Development
....

https://mmri.ubc.ca/

Emerging Strategic Research Opportunities in the AI era

- **Highly Integrated Basic and Responsive (HIBAR) Research**



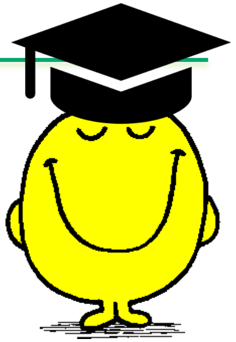
Bottom-up (Capacity Building)

- Generic and autonomous
- Strategic learning and development
- Long-term collaboration
- Team-driven & flexible
- Often lack of short-term application

Top-down (Technology Leadership)

- Well-established short-term vision and application
- Risk-free (industry-driven)
- Often inflexible
- Bureaucracy

Traditional Engineering Education



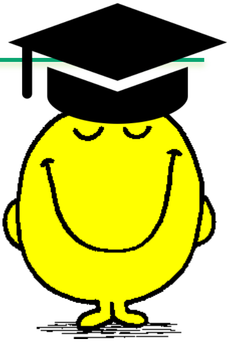
Education

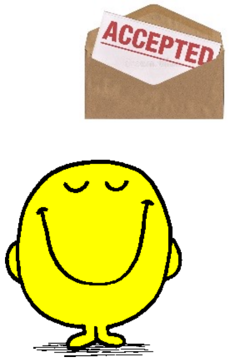
Curriculum-based

- Math
- Science
- Engineering sciences
- Some application of knowledge

Courtesy – Dr. H. Najjaran

Modern Engineering Education





Education

Curriculum-based

- Math
- Science
- Engineering science
- Some application of knowledge

Training

Strategy-based

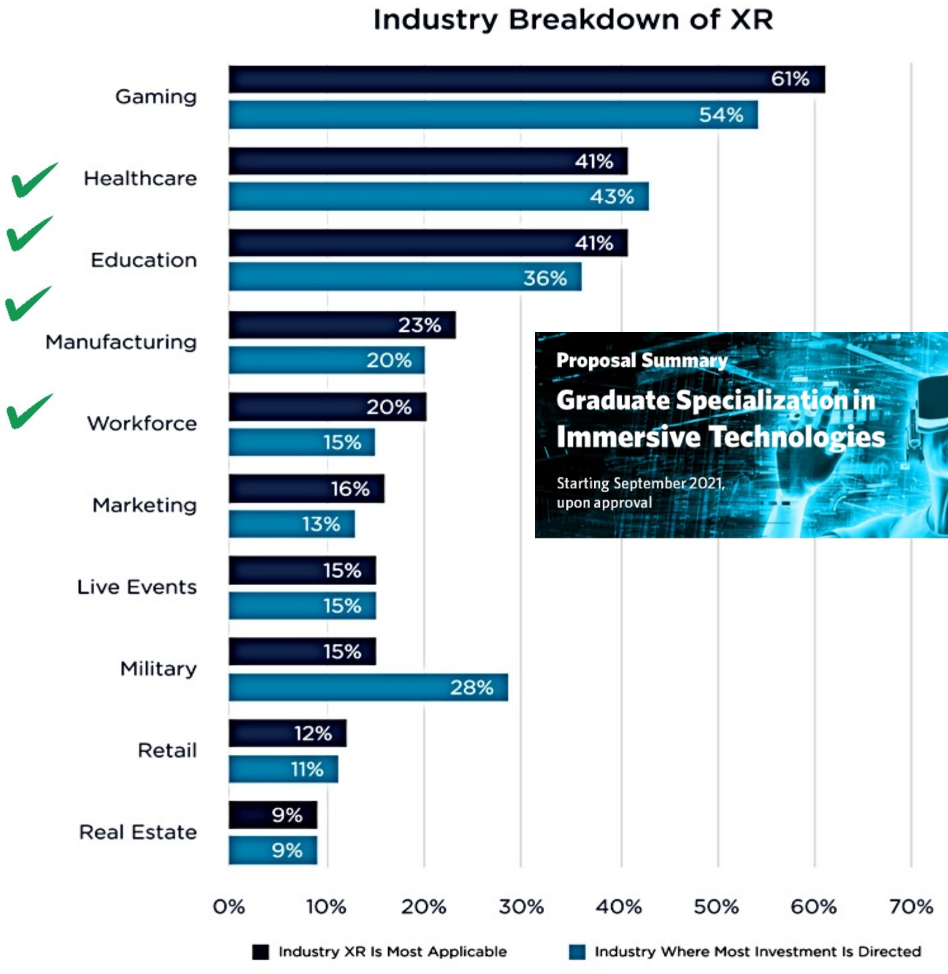
- Design from Day 1
- Soft skills
- Micro-credentials
- Industrial research
- Digital technologies

Courtesy – Dr. H. Najjaran

Collaborative Research and Training Experience (CREATE)

Objectives

- (1) Establish and train a large and diverse cohort of students who will have a strong foundation in fundamental aspects of ITech development through specific course work and multi-faculty research co-supervision;
- (2) Offer a highly interdisciplinary setting, where trainees of varying background practice teamwork and integrate computer science, engineering, health and art perspectives;
- (3) **Support the transition of trainees to highly-skilled careers in immersive technology industries** or academia through professional development opportunities, cutting edge research projects, and real-world experiential learning.
- 10 faculty and 19 industry founding members
- Multiple industry internship opportunities



Data From Perkins Coie

Natural Sciences and Engineering Research Council of Canada

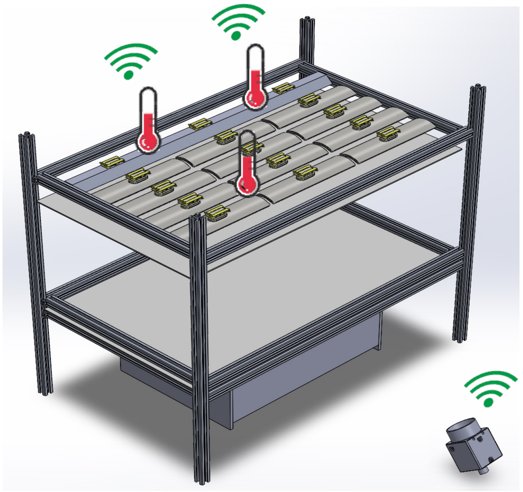
Conseil de Recherches en Sciences Naturelles et en Génie du Canada

NSERC CREATE in Immersive Technologies (CITech)

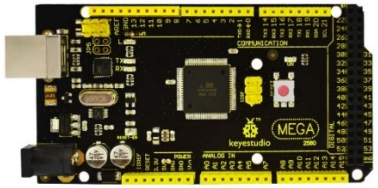
- **Partnership opportunities annually for ~20 industrial projects**

https://citech.ubc.ca/

Sample Project: XR/AI tool development for operators training and process control



Gathering Data to IoT Hub



Meta Learning (Tentative)

Deep Learning

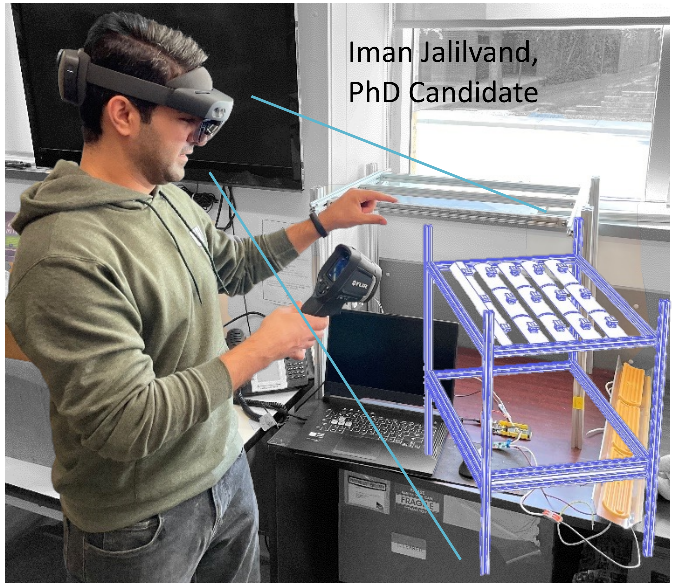
Reinforcement Learning

Input Labelling and categorization

Data Processing

Hyper-parameter tuning

Real-time Monitoring via XR

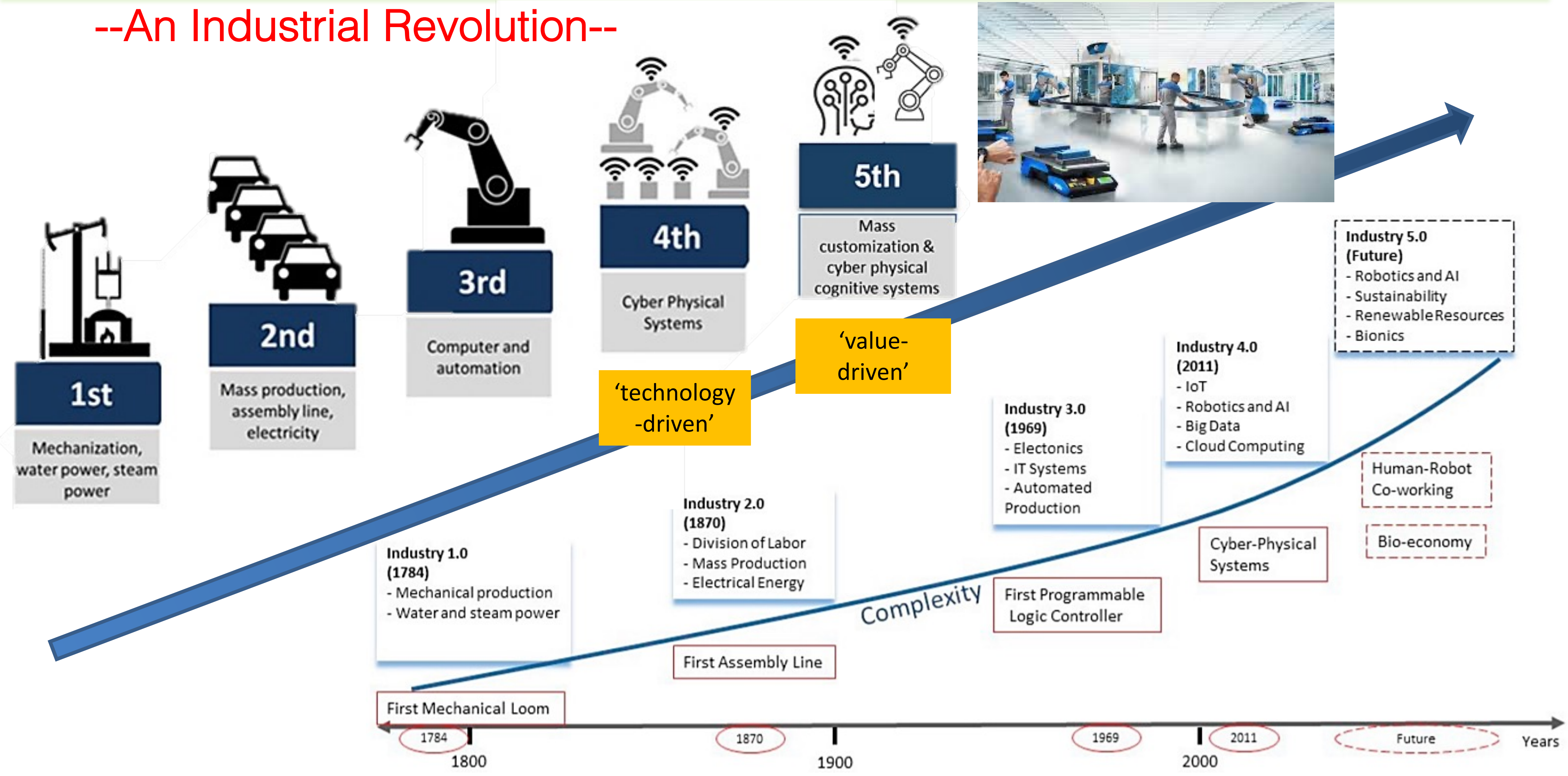


Remote Monitoring

Data Acquisition from IoT Sensors	Data Processing Machine Learning (ML)	Digital Twin Augmented / Mixed Reality (AR / MR)

Smart Factories (of the Future)

--An Industrial Revolution--



Demir et al., Procedia Computer Science 158 (2019) 688–695

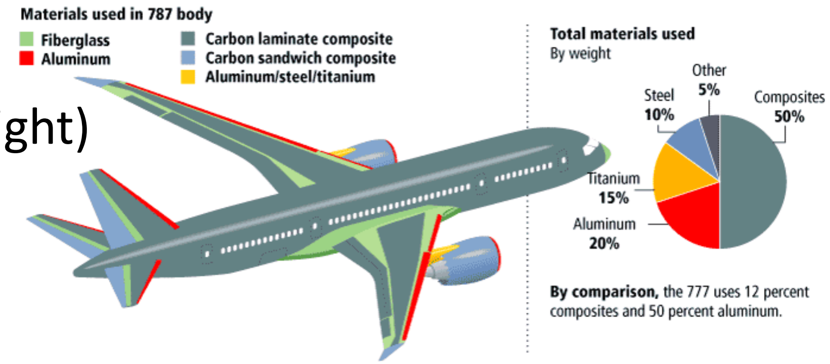
Beyond the Factory 5.0: Digitization of Circular (bio)Economy

- Establishing new, smart supply chains

Application in Composites Manufacturing

Composite materials offer many advantages

- Excellent properties (e.g. strength-to-weight, stiffness-to-weight)
- Boeing 777 -> 787; 10% lower fuel burn per seat



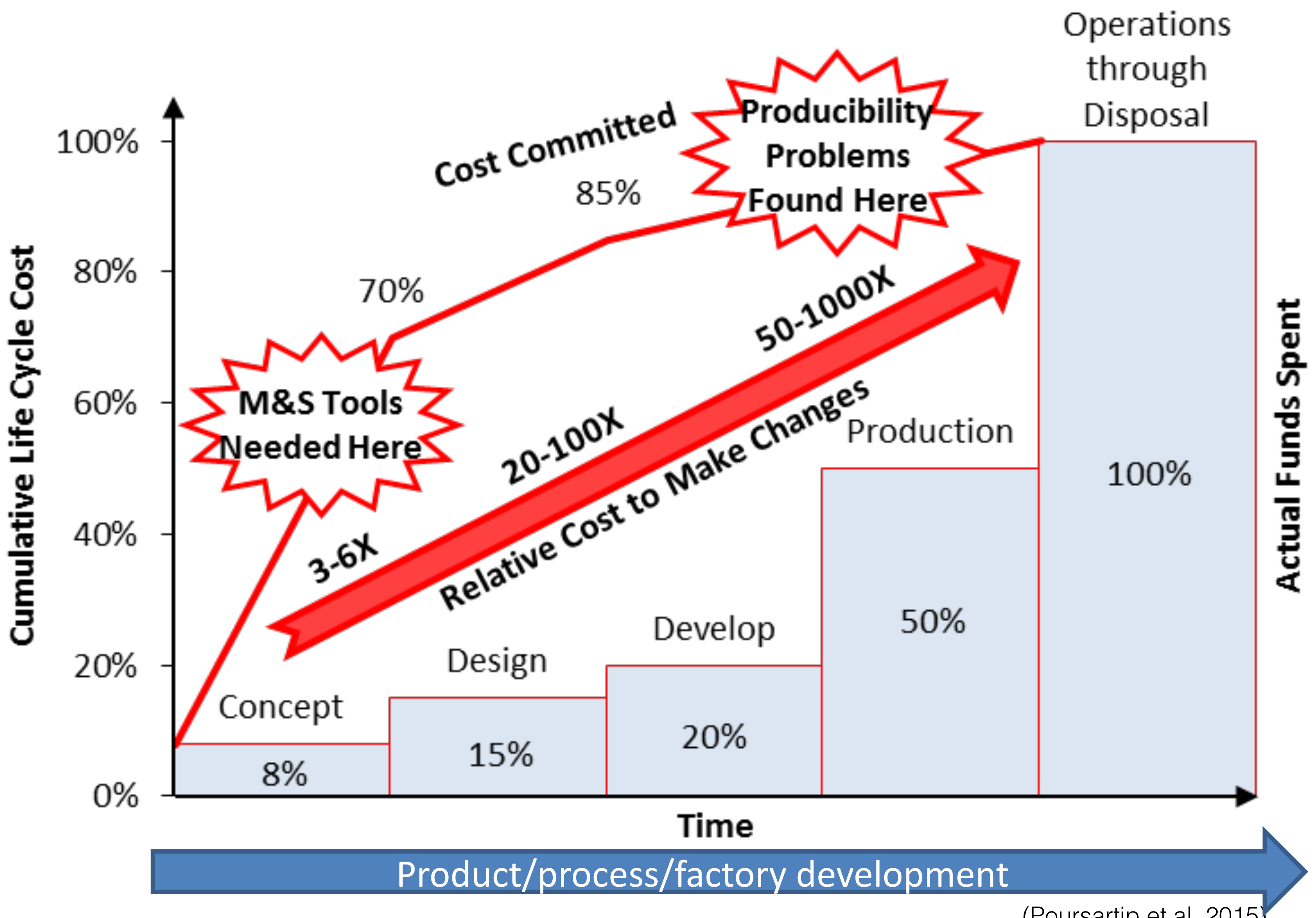
Challenges

- Material properties and processing conditions highly coupled
- Many discreet parts, often cured in **batches** to reduce cost
- **In-situ decision-making**; long lead-time for white-box tools
- Incremental changes; some already close to process tolerance



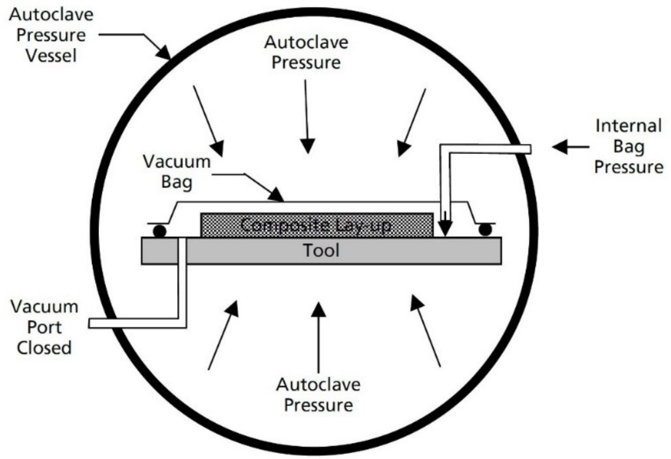



Role of Digital Twins to Reduce Cost for Composites Businesses



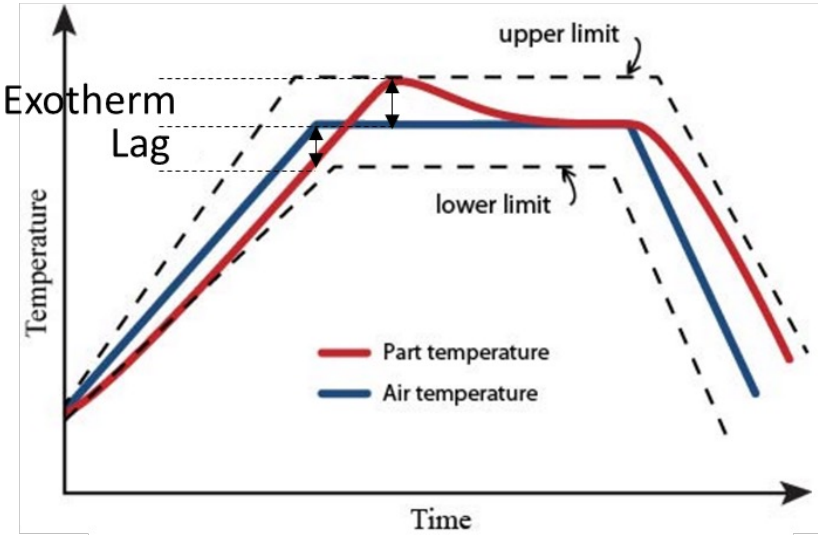
(Poursartip et al, 2015)

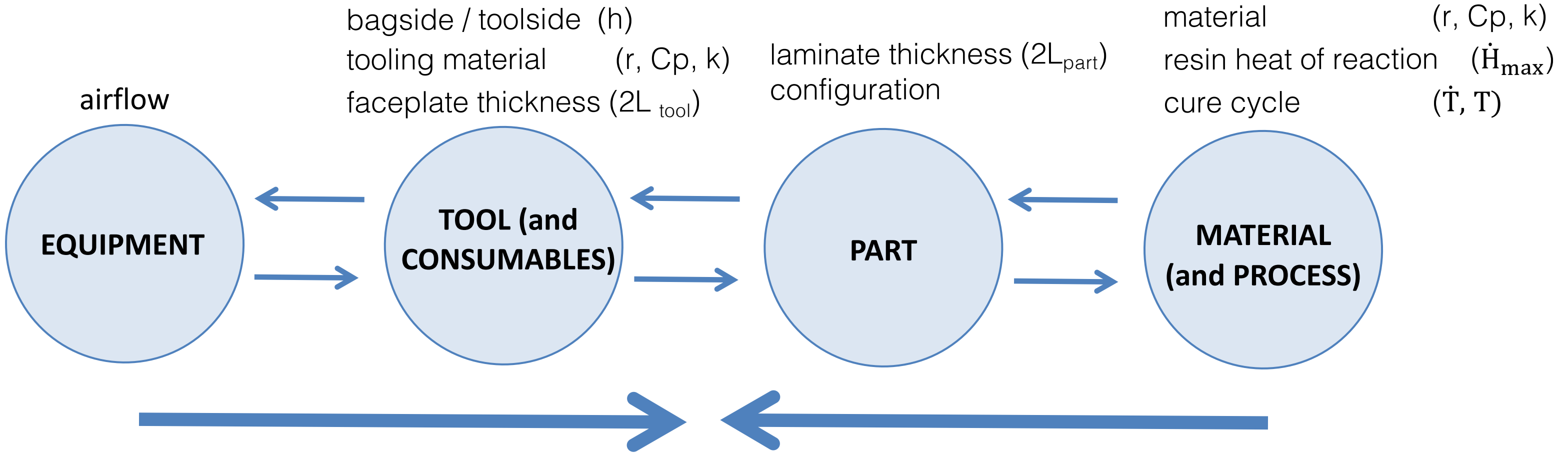
Autoclave Processing Example



Loading a “bus-stop” style autoclave run cycle [Polek, 2014]

Typical Quality Metric:





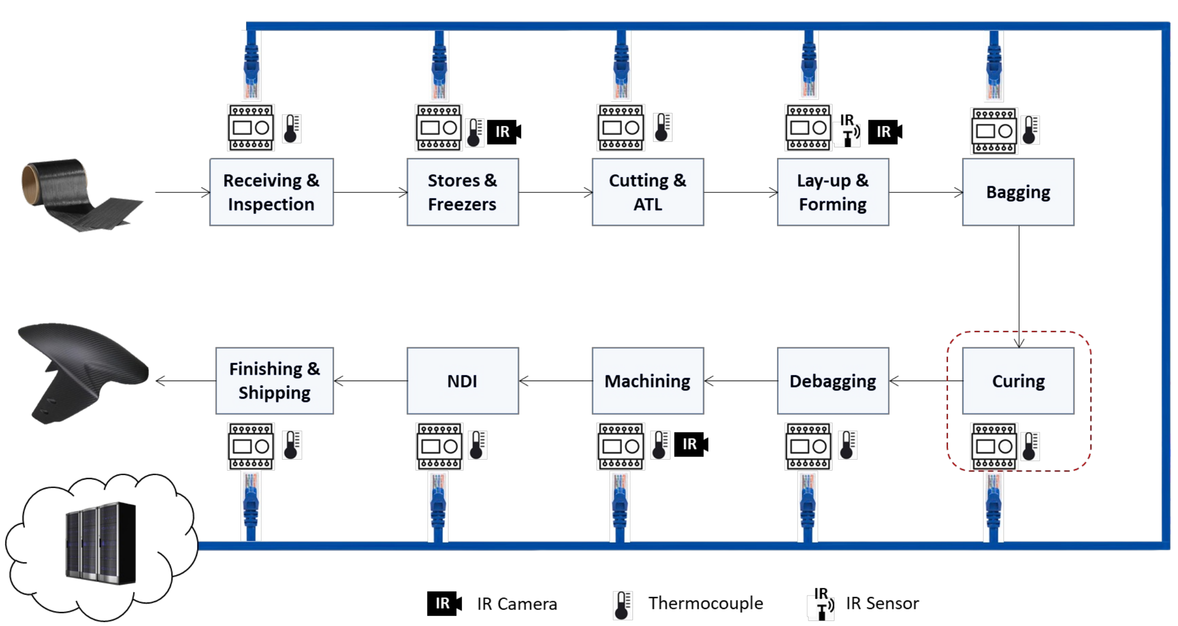
BOUNDARY CONDITIONS

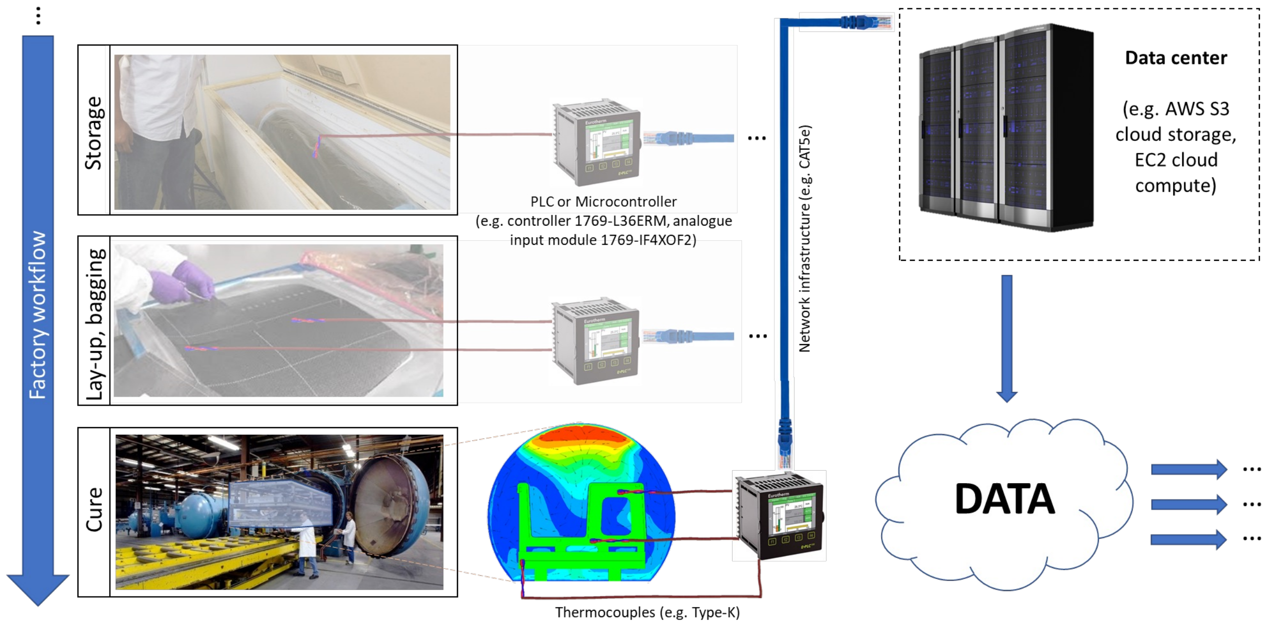
(convective heat transfer in autoclaves and ovens)

SENSTITIVITY TO THERMAL HISTORY OUTCOMES

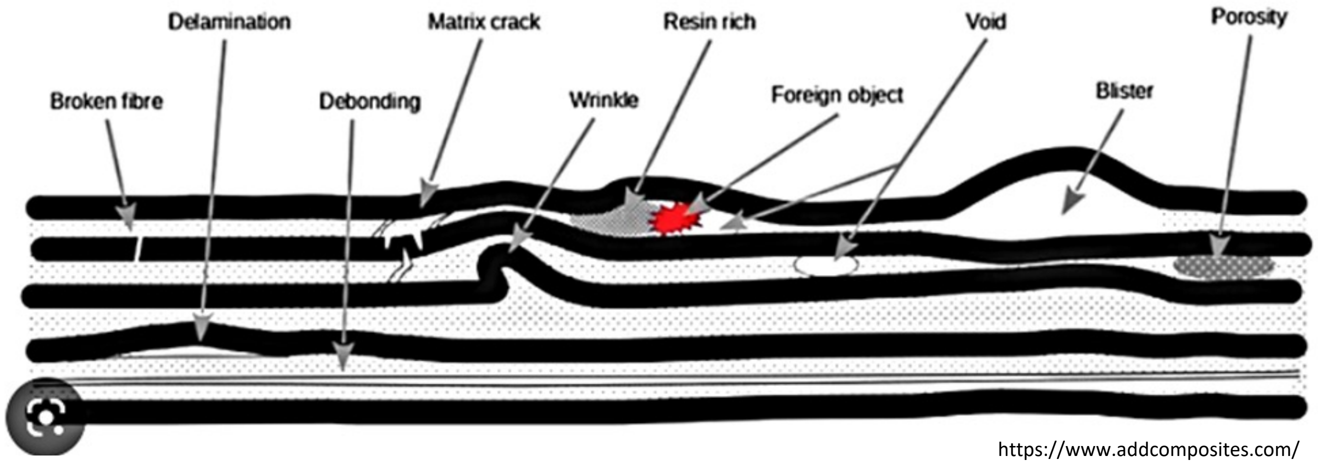
max. exotherm (T_{max})
max. thermal lag (ΔT_{SS})
final degree of cure (DOC)

Smart Composites Manufacturing





Typical defects induced at different stages of the processing:



https://www.addcomposites.com/

Data conundrum in smart manufacturing

Integration of data-driven technologies into intelligent manufacturing processes:

- Sensing technologies
- Cloud computing
- AI and machine learning

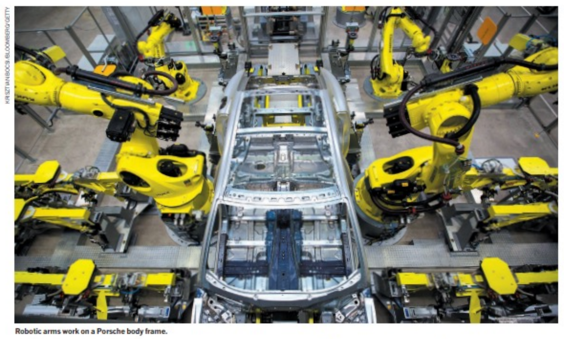
5 Vs of big data

Volume	Variety	Velocity	Veracity	Value

Big data in advanced manufacturing (**Product quality and design data**):

Volume ⟹ Limited and insufficient for machine learning tasks.

Value ⟹ Available data does not fully describe the input and output space.



nature

Robotic arms work on a Porsche body frame.

Smart manufacturing must embrace big data

Study and model industrial processes to save money, energy and materials, urges **Andrew Kusiak**.

Manufacturing is getting smart. Companies are increasingly using sensors and wireless technologies to capture data at all stages of a product's life. These range from material properties and the temperatures and vibrations of equipment to the logistics of supply chains and customer details. Truck engines beam back data on speed, fuel consumption and oil temperature to manufacturers and fleet operators. Optical scanners are used to spot defects in printed electronics circuits[1].

But big data is a long way from transforming manufacturing. Leading industries — computing, energy and aircraft and semiconductor manufacturing — face data gaps. Most companies do not know what to do with the data they have, let alone how to interpret them to improve their processes and products. Businesses compete and usually operate in isolation. They lack software and modelling systems to analyse data.

Yet smart manufacturing can make industry more efficient, profitable and sustainable. Minimizing the distances over which products and components are transported reduces costs — financial and environmental. Computer modelling can identify risks and pinch points. It can, for example, anticipate impacts from deliveries delayed by extreme weather, a situation that affect the electronics industry after Thailand's major floods in 2011. Similarly,

6 APRIL 2017 | VOL 544 | NATURE | 23

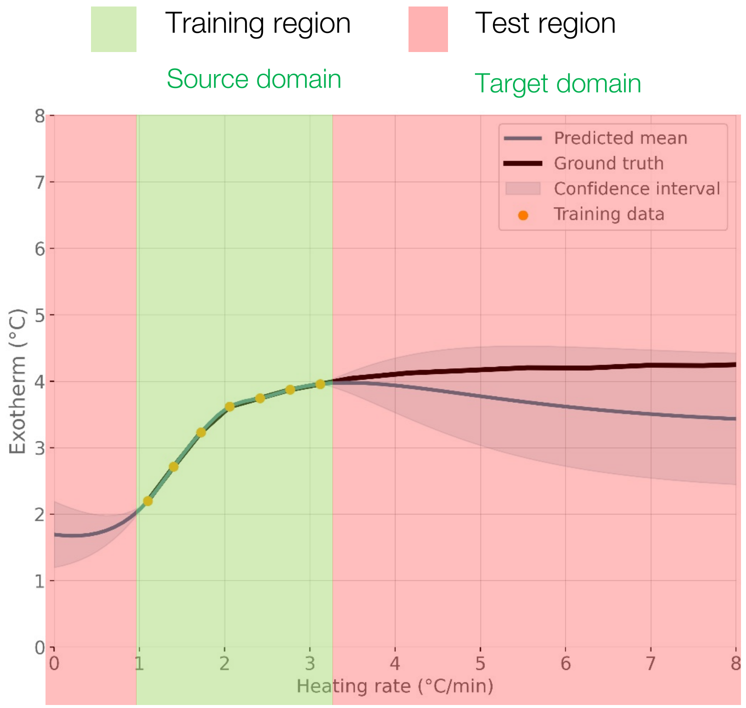
Kusiak A., 2017

Data-efficient machine learning

Conventional ML models assumption about data:

- Training set size is sufficient for developing the model.
- The training and test data are drawn from the same probability distribution:

$$p_{training}(x) = p_{test}(x)$$



Overcome the shortfalls of data-driven ML for smart manufacturing applications by developing a learning framework that can concurrently:

1. Establish reliable prediction models for complex manufacturing processes in the presence of limited labelled data.
2. Be immune (robust) against domain (e.g., new material) shifts during the production/design.

Data-Efficient Machine Learning

01
Transfer learning

02
Physics-informed ML

03
Multi-fidelity learning

Transfer learning - Example

Large dataset of cat images

Classification task
(is this an image of a cat?)

→ Black box model →

Data is sufficient → Good prediction performance

Limited number of dog images

Classification task
(is this an image of a dog?)

→ Black box model →

Data is limited → Poor prediction performance

Transfer learning - Example

Large dataset of cat images

Classification task
(is this an image of a cat?)

Black box model

Data is sufficient → Good prediction performance

Knowledge transfer

Limited number of dog images

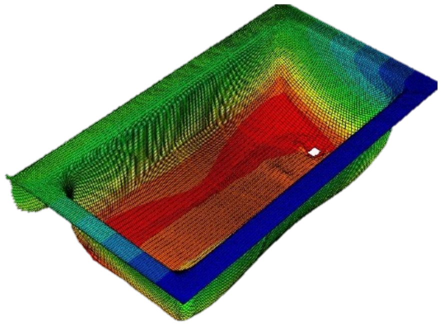
Classification task
(is this an image of a dog?)

Black box model

Data is limited, but relevant knowledge is transferred → Good prediction performance

Transfer learning – Advanced thermoforming

Inexpensive FE simulations (abundant)



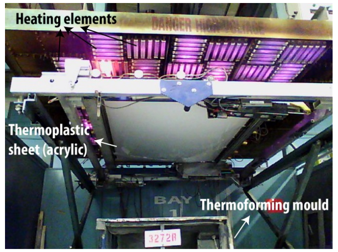
Regression task
(Predicting manufactured part's quality)

Black box model

Data is sufficient → Good prediction performance

Knowledge transfer

Costly and time-consuming in-situ data collection (limited)

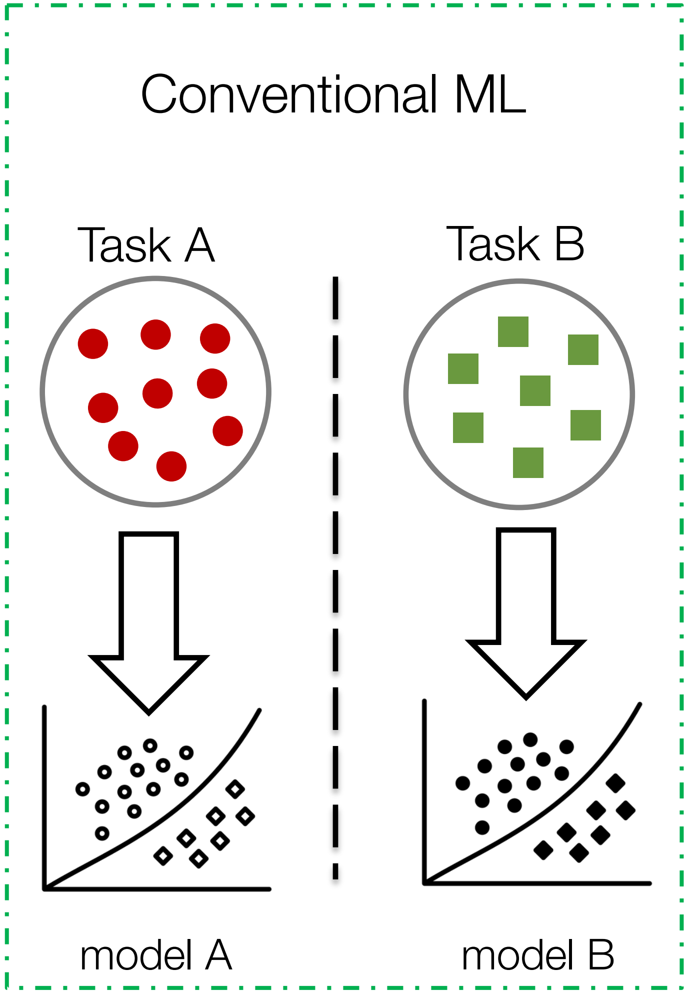


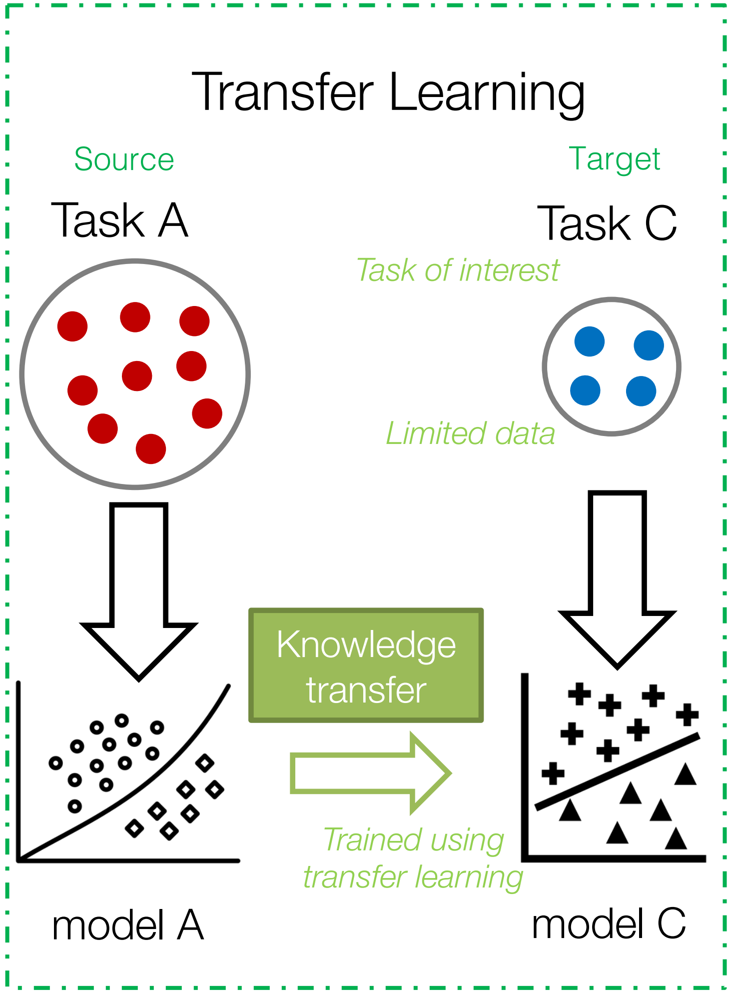
Regression task
(Predicting manufactured part's quality)

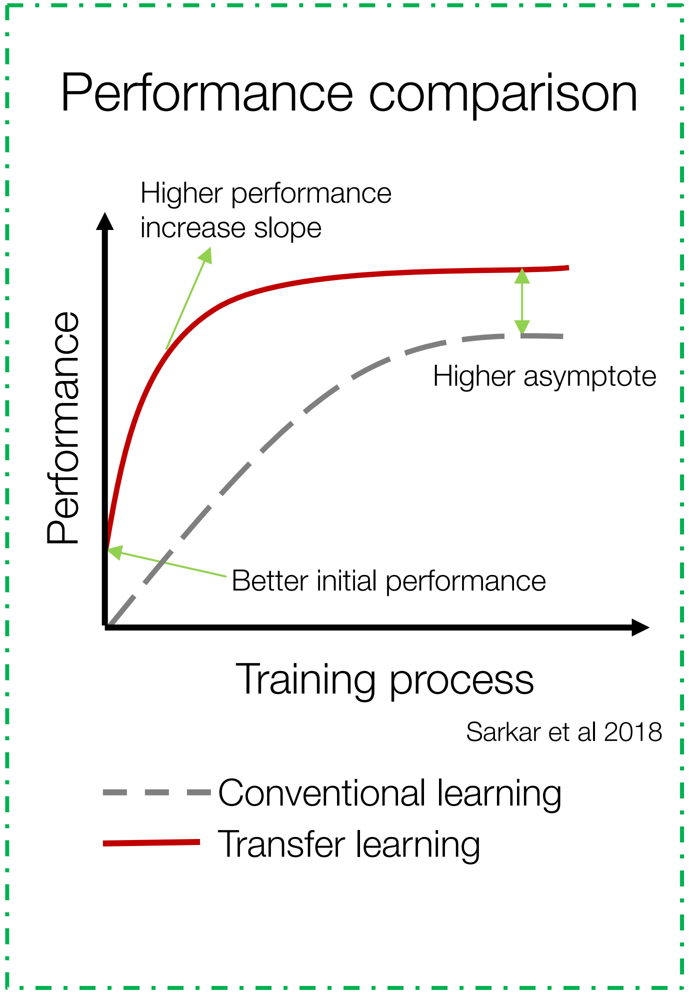
Black box model

Data is limited, but relevant knowledge is transferred → Good prediction performance

Transfer Learning – Architecture







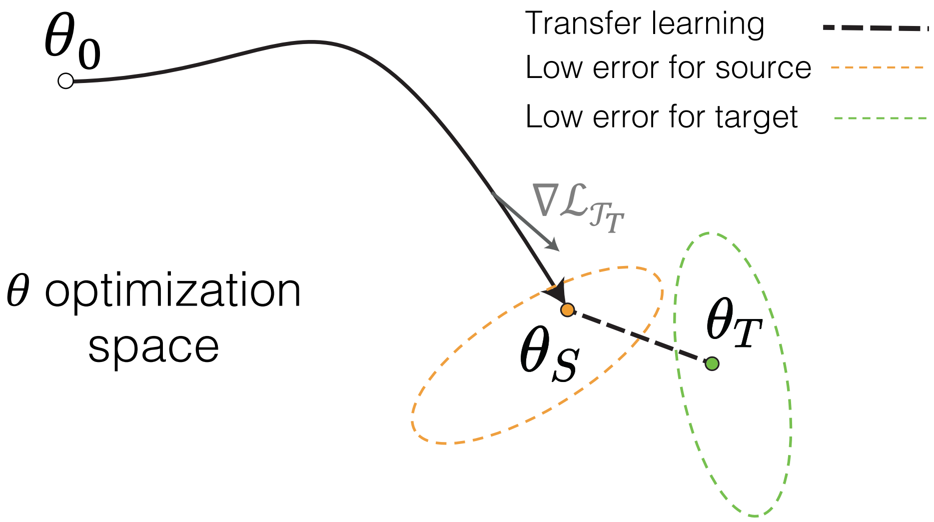
Transfer learning – Neural networks

A neural network model NN is expressed by a parametrized function $f(\theta)$.

Learned (optimized) parameters of the source task $\mathcal{T}_s \rightarrow \theta_s$

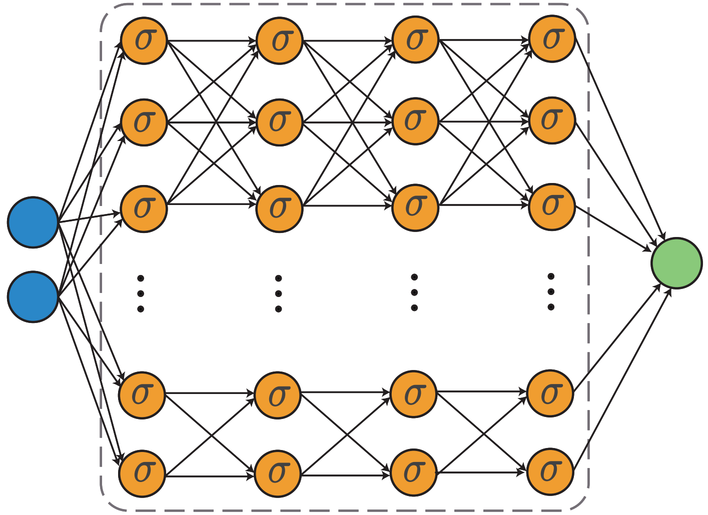
$$\theta_T \leftarrow \theta_S - \alpha \nabla_{\theta_S} \mathcal{L}_{\mathcal{T}_T}(f_\theta)$$

Small changes in the parameters will provide necessary improvements toward learning the target task.



Source task: $\mathcal{T}_s$

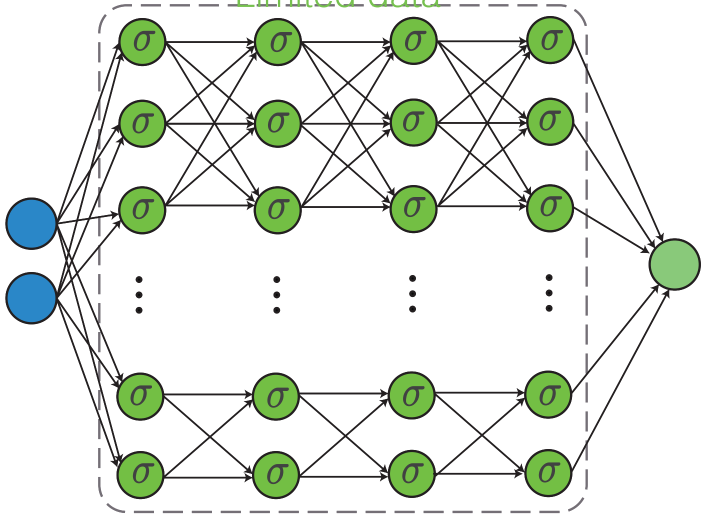
Abundant data



Initialize the target network with the optimized parameters of the source network

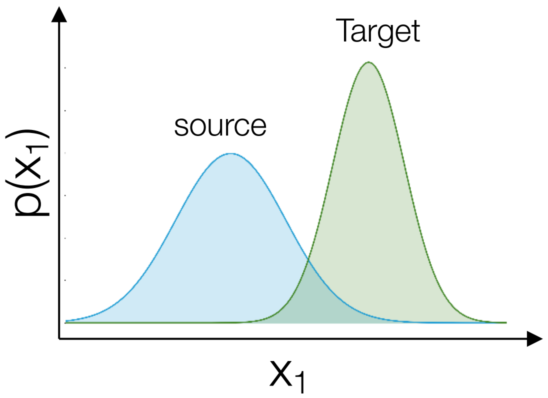
Target task: $\mathcal{T}_T$

Limited data

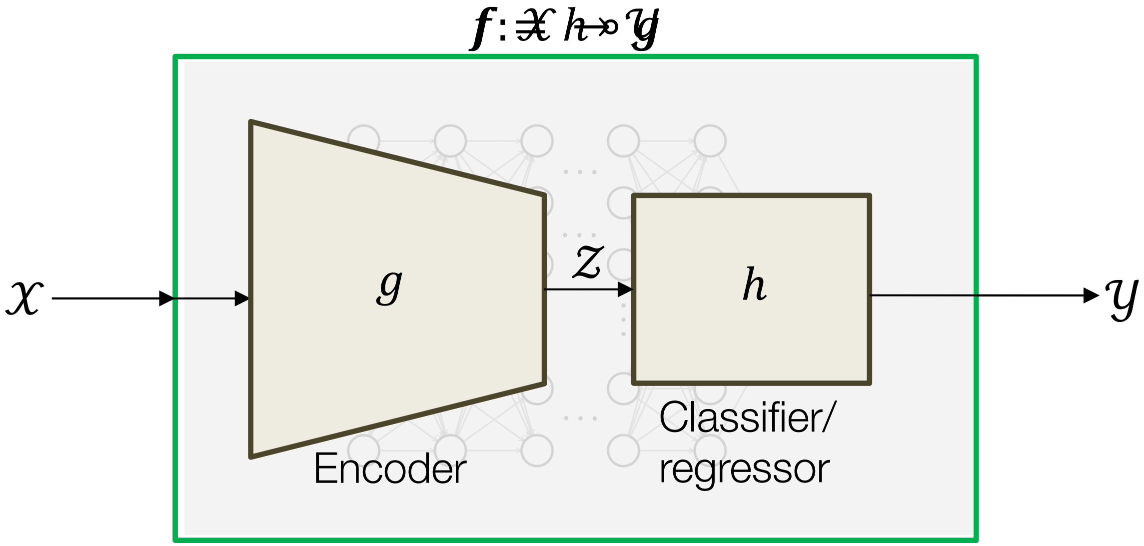


Transfer learning – Categories

Covariate shift



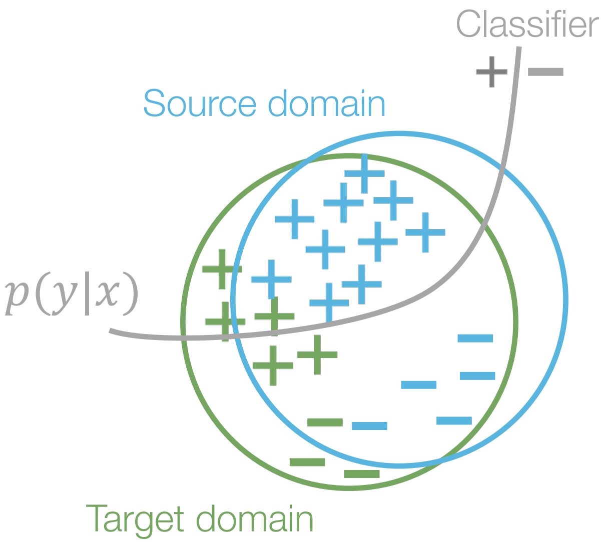
$p(x^s) \neq p(x^t)$



$g: \mathcal{X} \to \mathcal{Z}$ $\quad$ $h: \mathcal{Z} \to \mathcal{Y}$

Domain		Task	
$\mathcal{X}$	$p(x)$	$\mathcal{Y}$	$p(y\|x)$

Inductive transfer learning

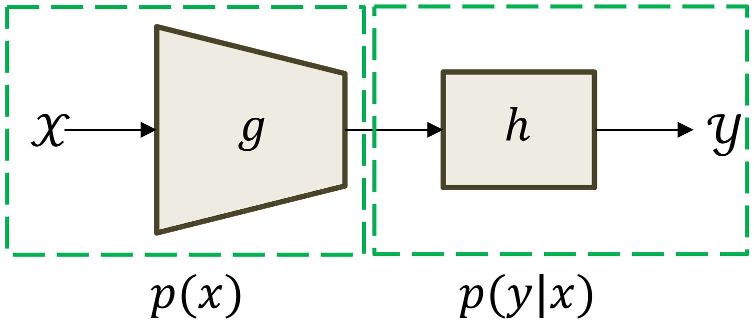


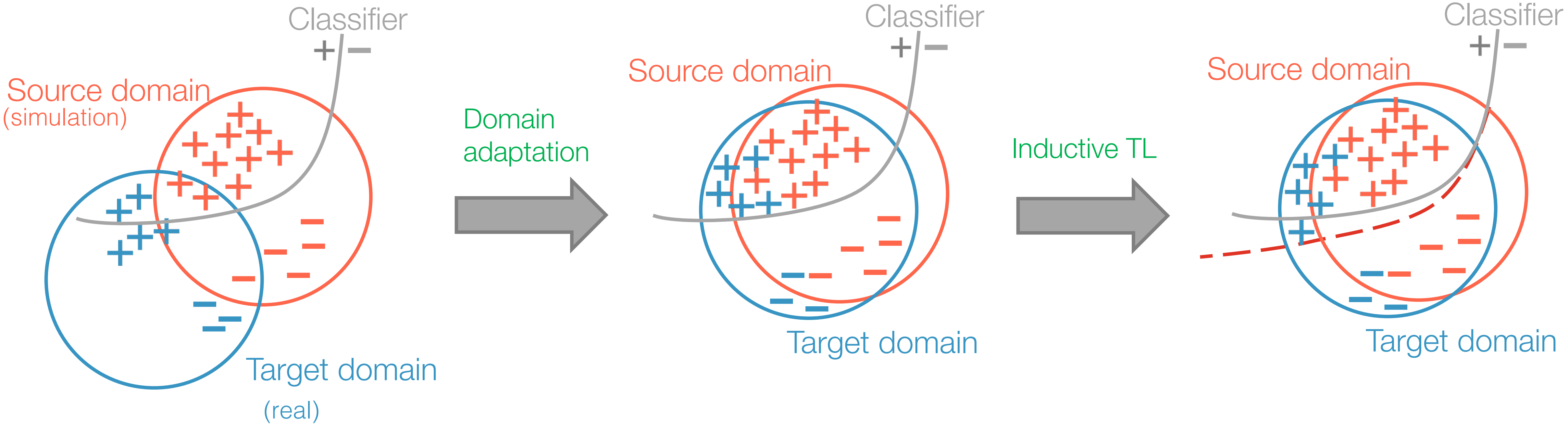
$p(y^s|x) \neq p(y^t|x)$

Transfer learning - Functionality

How does transfer learning help?

- Domain shift and dataset bias: Domain Adaptation
- Discrepancy in mapping functions: Inductive TL





Transfer learning in manufacturing applications

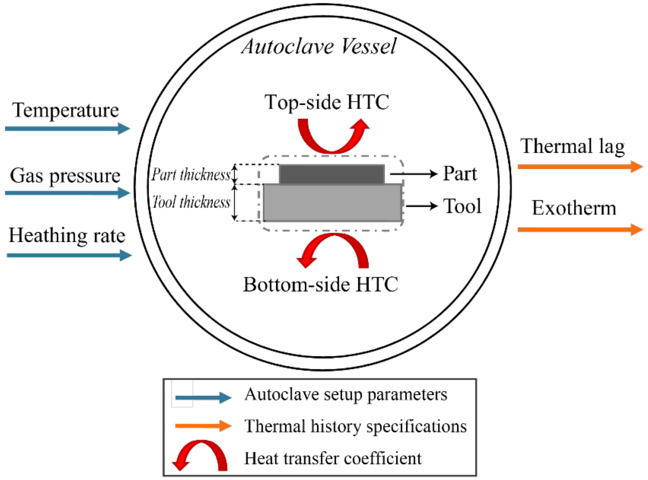
Limited data | Imbalanced classes | Complex domain

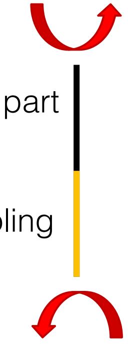
Potential solutions:

1. Collecting in-situ big and balanced data
   - Not practical in many industrial applications
   - Time consuming and expensive
2. Develop high fidelity simulations:
   - Time consuming
   - Not *fully* resembles the real world due to the process complexity and uncertainties
3. Transfer learning:
   - Low to medium-fidelity numerical models
   - Limited and imbalanced data

Case study 1: Knowledge transferability of cure cycles - Methodology

Courtesy of Boeing Company





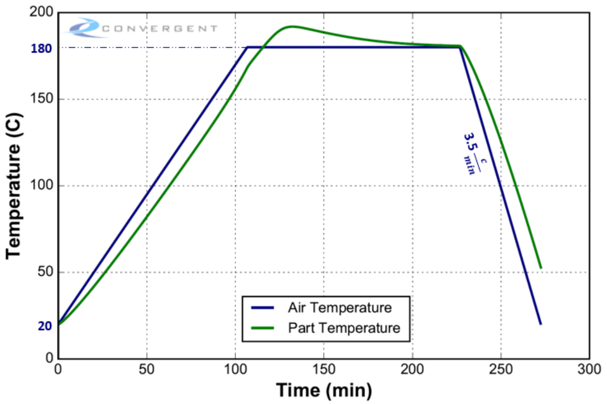
Source model

- Cure cycle 1: **1-hold** cure cycle: (20-180C), then hold for 2hrs, then (180-20C cool down at 3.5C/min)
- **44000** training/validation data

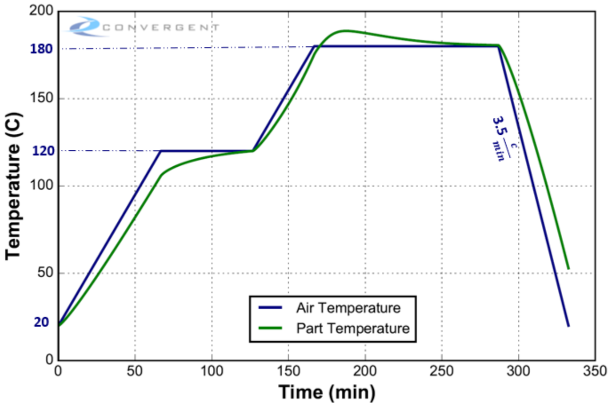
Target model

- Cure cycle 2**: 2-hold** cure cycle: (20-120C), then hold for 1hr, then (120-180C), hold for 2hrs, then (180-20C cool down at 3.5C/min)
- 500 (<1%) training/validation data

Source model



Target model



Case study 1: Knowledge transferability of cure cycles - Methodology

Source model
- Cure cycle 1: **1-hold** cure cycle: (20-180C), then hold for 2hrs, then (180-20C cool down at 3.5C/min)
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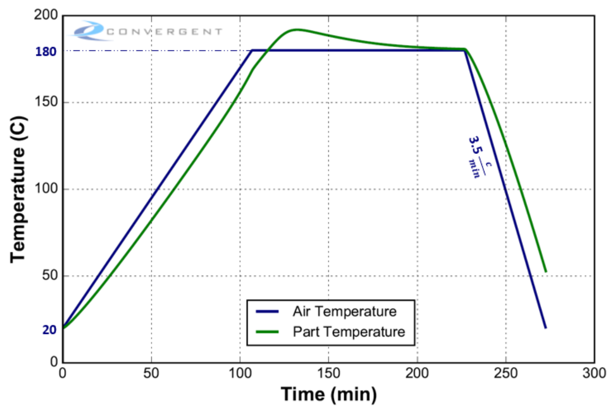
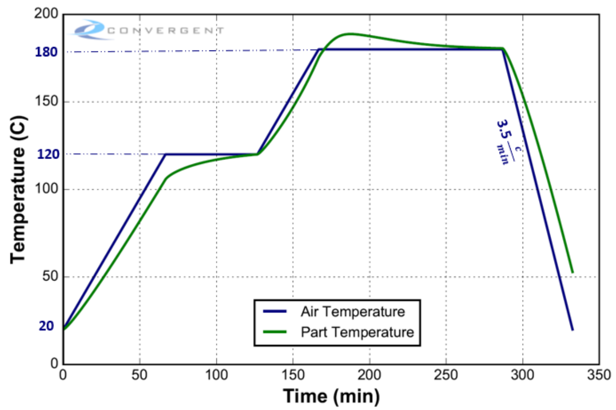
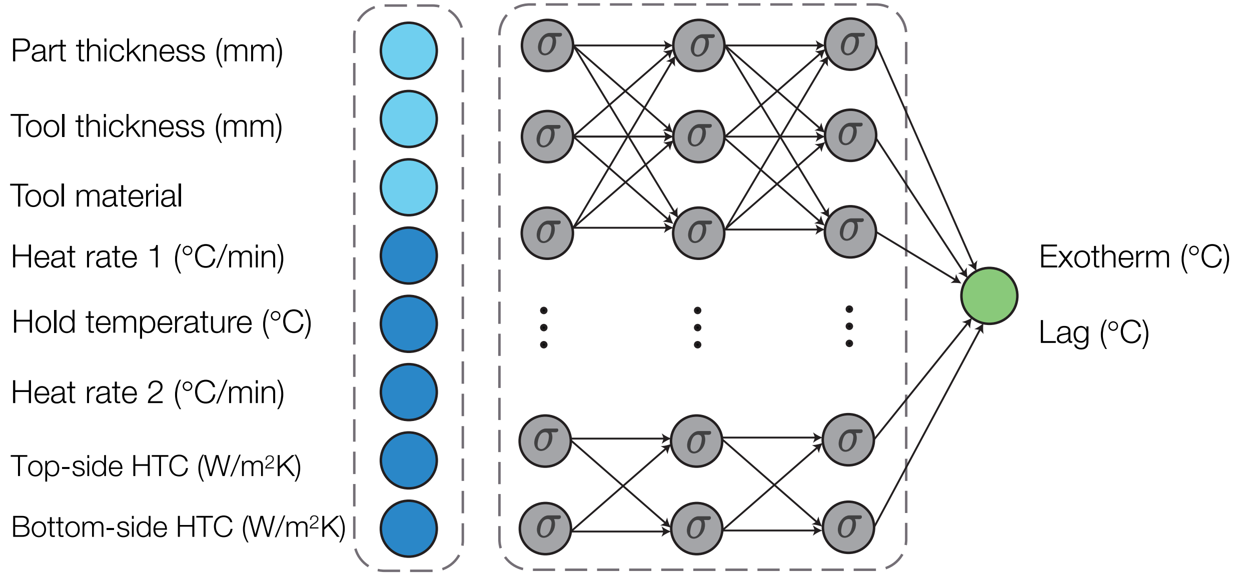
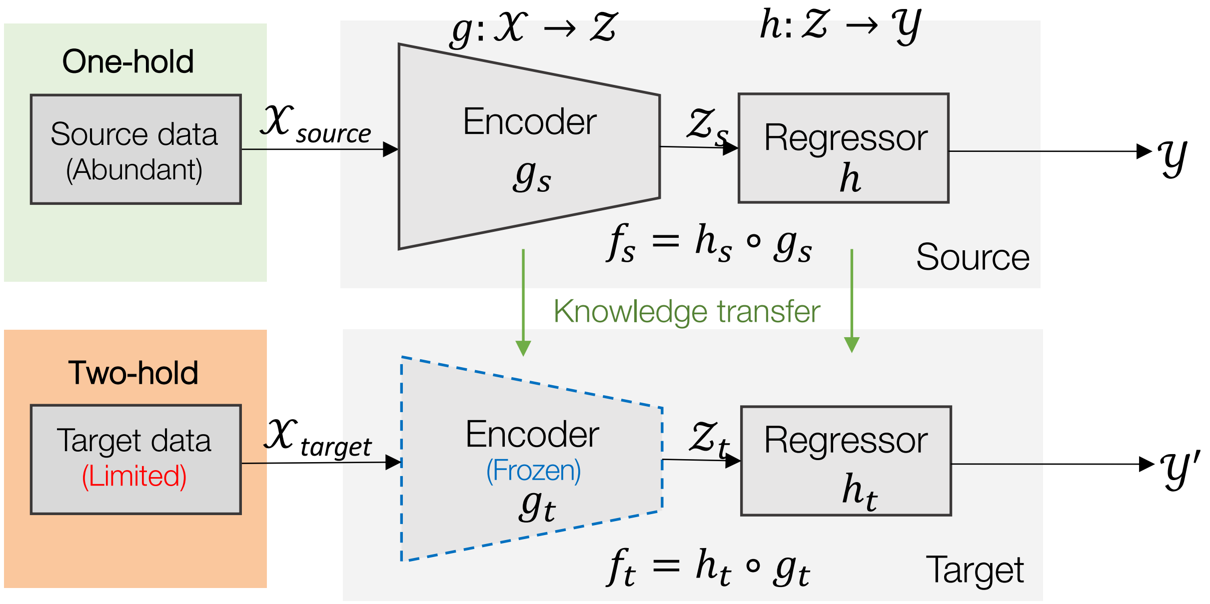
Source model



Target model



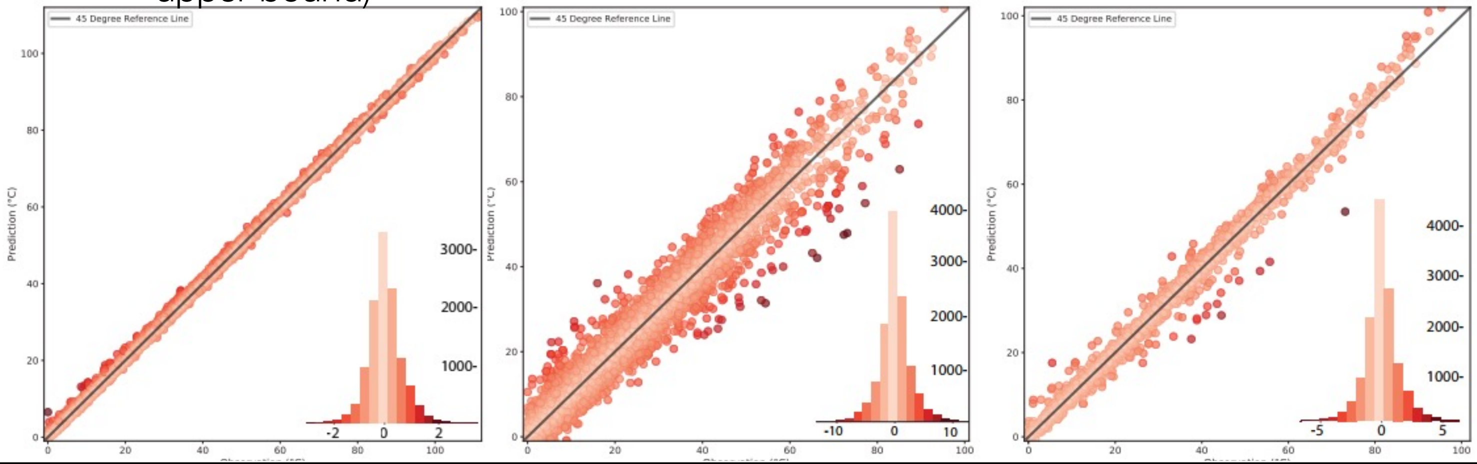




Case study 1: Knowledge transferability of cure cycles - Results

Exotherm

Conventional ML on full (44000) target dataset (Ideal upper bound)	Conventional ML on limited (500) target dataset	Transfer learning on limited (500) target dataset



Metric	Traditional ML on full target dataset	Traditional ML on limited target dataset	Transfer learning
Training time(s)	863	143	38
RMSE (°C)	0.162	17.273	0.84
R-squared	0.999	0.88	0.96

$$RMSE = \sqrt{\frac{1}{k}\sum_{i=1}^{k}(y_i - \hat{y}_i)^2}$$

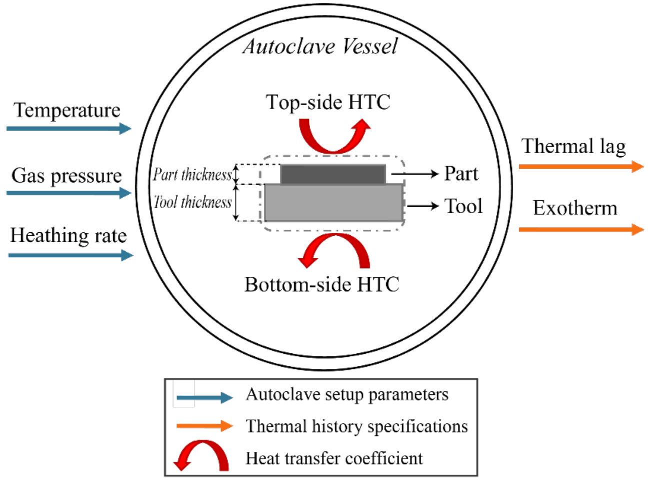
$$R^2 = 1 - \frac{\sum_{i=1}^{k}(y_i - \hat{y}_i)^2}{\sum_{i=1}^{k}(y_i - \bar{y})^2}$$

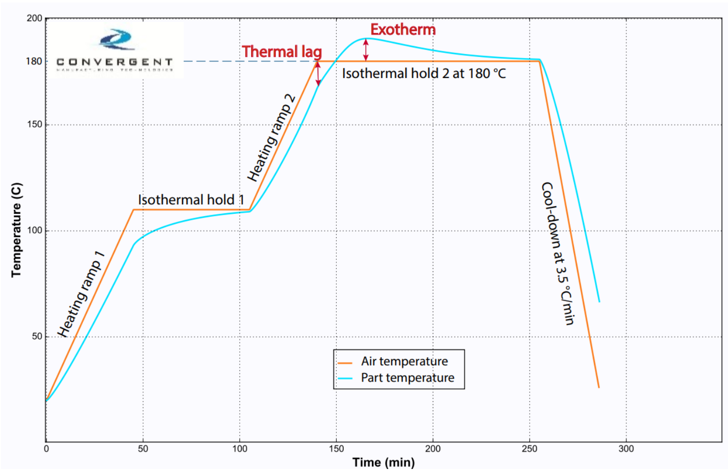
Ramezankhani, M., et al. "**Making costly manufacturing smart with transfer learning under limited data: A case study on composites autoclave processing**" 2021. Journal of Manufacturing Systems.

Case study 2: **Hybrid** Material transfer in composites processing

Source material: AS4/8552 (Abundant historical data) --> Target material: AS4/8551 (No data; to be sampled/limited)

Classification problem:
Pass/Fail per part's **thermal history**



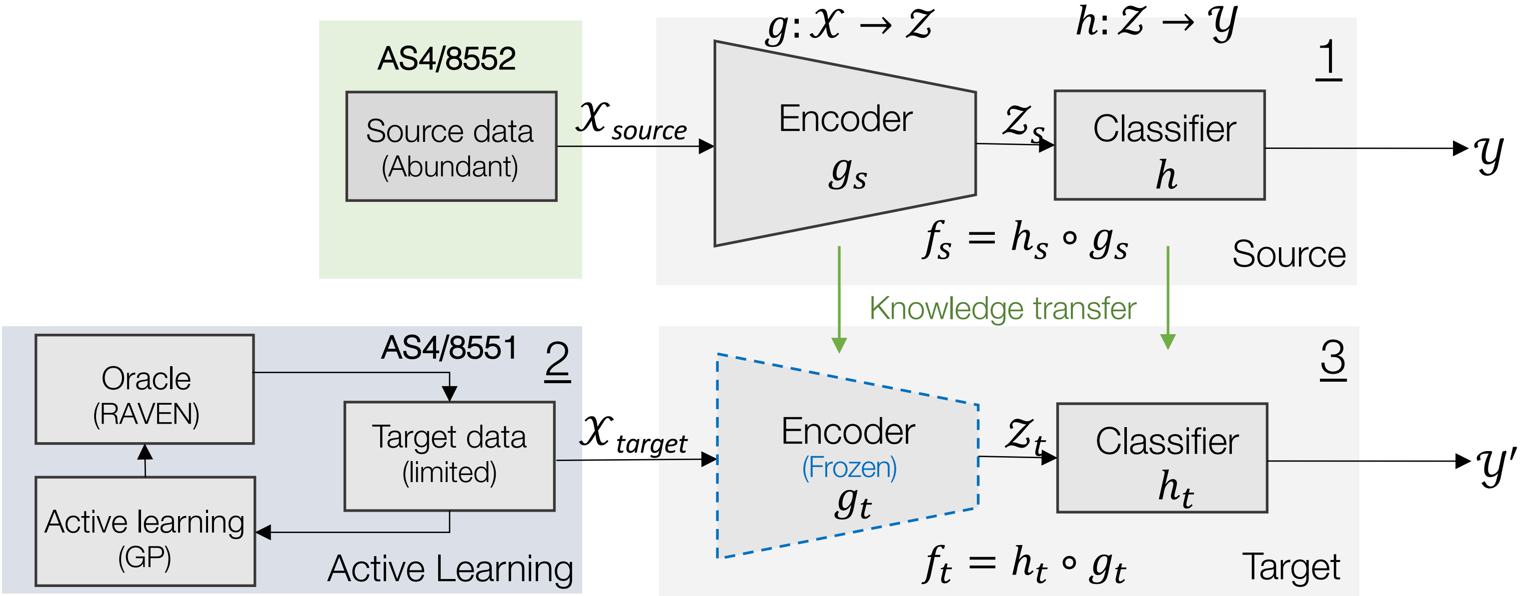


Active Learning: The unknown function of interest (i.e., mapping between inputs and outputs) is learned by minimizing the **uncertainty** about the posterior distribution.

Differential entropy (STD): $x^* = \mathrm{argmax}_{x \in \mathcal{D}_{\mathrm{Pool}}} v$

Decision boundary: $x^* = \mathrm{argmin}_{x \in \mathcal{D}_{\mathrm{Pool}}} |\bar{y}|$

Uncertainty: $x^* = \mathrm{argmin}_{x \in \mathcal{D}_{\mathrm{Pool}}} \frac{|\bar{y}|}{\sqrt{v + \sigma_n{}^2}}$



Ramezankhani, M., et al. "**An Active Transfer Learning (ATL) Framework for Smart Manufacturing with Limited Data: Case Study on Material Transfer in Composites Processing**" 2021 IEEE International Conference on Industrial Cyber Physical Systems (ICPS)

Case study 2: **Hybrid** Material transfer in composites processing – results

Gaussian Processes (GP) classification:

$$p(y^*|x^*, X, f) \sim \mathcal{N}(\bar{y}^*, v^*)$$

$$\bar{y}^* = K(x^*, X)[K(X,X) + \sigma_n^2 I]^{-1} y$$

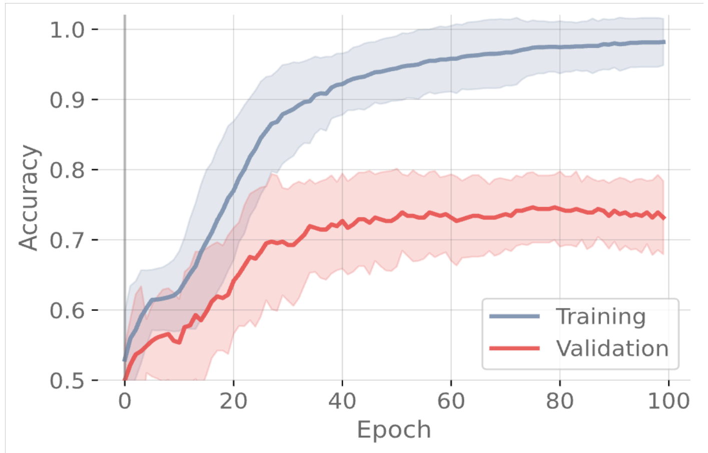
$$v^* = K(x^*, X^*) - K(x^*, X)[K(X,X) + \sigma_n^2 I]^{-1} K(X, x^*)$$

In GP:
Maximize *differential entropy score*:

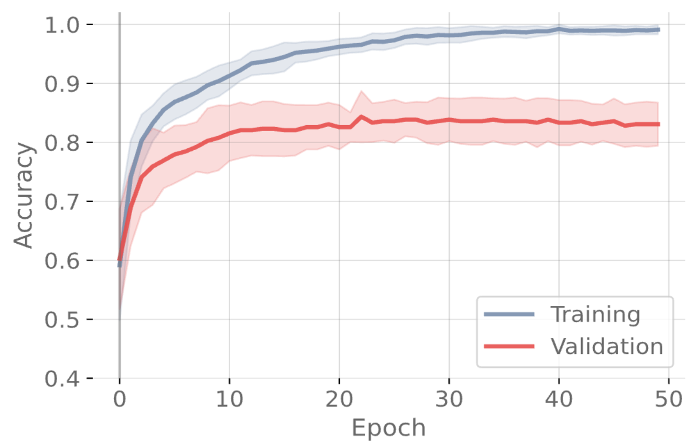
$$\Delta_j \triangleq H[p(y_j)] - H[p^{new}(y_j)]$$

Equivalent to finding the point with the **highest variance**

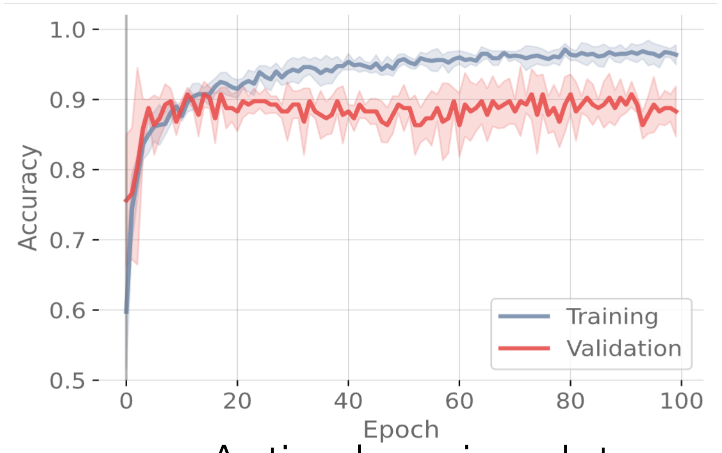
Model	Target Test Accuracy
Upper-bound	94.64 %
ATL	**91.9 %**
TL	87.88 %
AL	86.2 %
Random	80.08 %



Randomly generated data



Active learning data



Active learning data
+ Transfer learning

Case study 2: **Hybrid** Material transfer in composites processing – results

Gaussian Processes (GP) classification:

$$p(y^*|x^*,X,f) \sim \mathcal{N}(\bar{y}^*, v^*)$$

$$\bar{y}^* = K(x^*,X)[K(X,X)+\sigma_n^2 I]^{-1}y$$

$$v^* = K(x^*,X^*) - K(x^*,X)[K(X,X)+\sigma_n^2 I]^{-1}K(X,x^*)$$

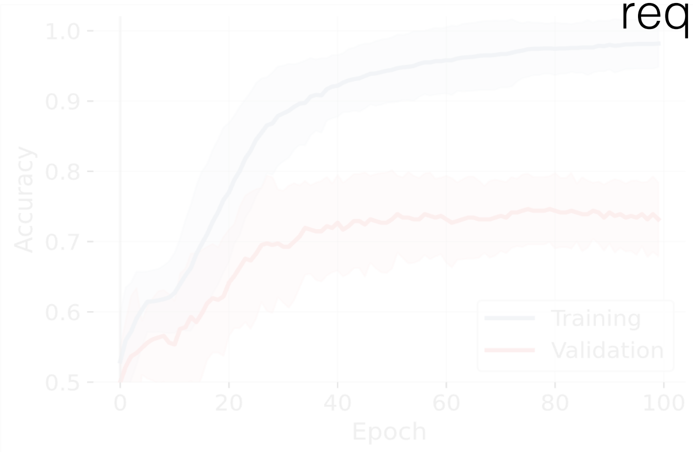
In GP:
Maximize *differential entropy score*:

$$\Delta_j \triangleq H[p(y_j)] - H[p^{new}(y_j)]$$

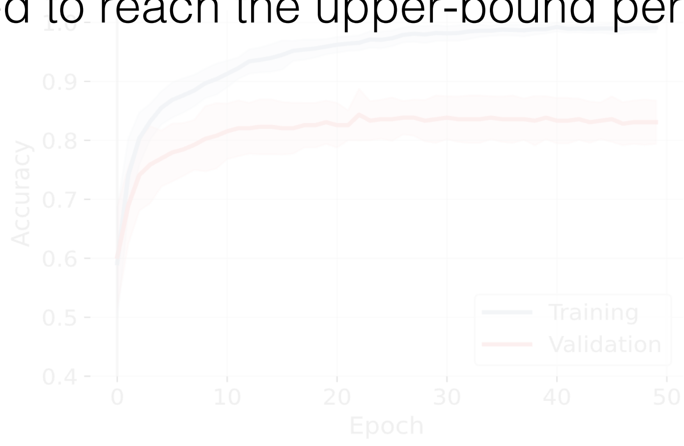
Equivalent to finding the point w

Model	Target Test Accuracy
Upper-bound	94.64 %
ATL	**91.9 %**
TL	87.88 %
AL	86.2 %
Random	80.08 %

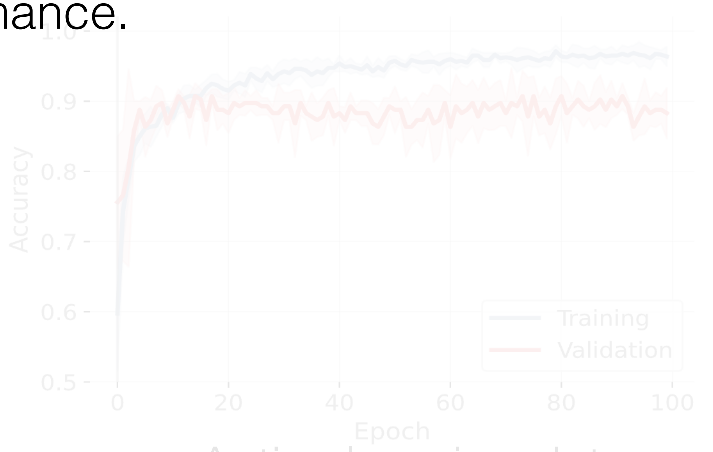
The new Active Transfer Learning (ATL) method achieved comparable results with only **5%** of data required to reach the upper-bound performance.



Randomly generated data



Active learning data



Active learning data + Transfer learning

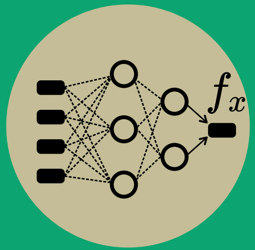
Break

(15 minutes)

Data-Efficient Machine Learning

01
Transfer learning

02
Physics-informed ML



03
Multi-fidelity learning

Physics-informed neural networks

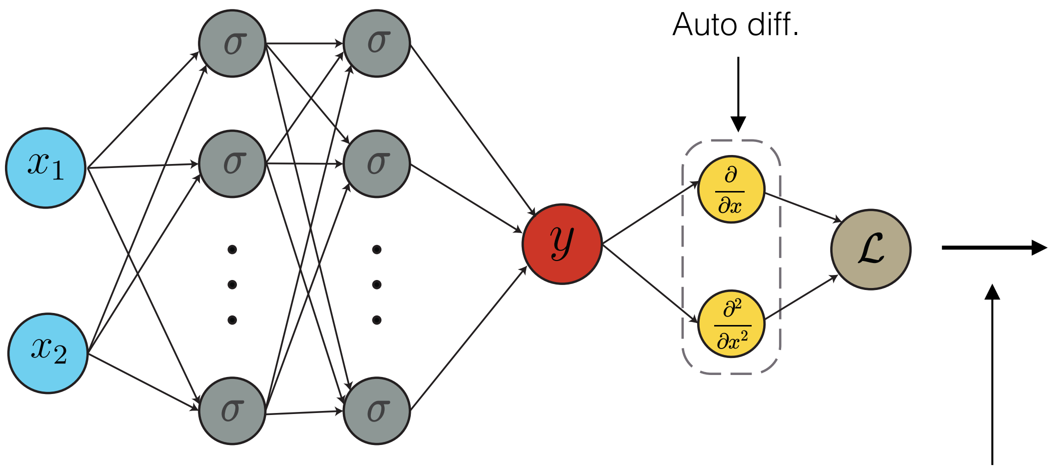
- Physics-informed neural networks (**PINNs**) infer a continuous latent function u(x, t), the solution to a system of nonlinear partial differential equations (PDE)[1].
- The solution of PDE, $u(x,t)$, is approximated by a deep neural network $f_\theta(x,t)$:

$$\boldsymbol{u}_t + \mathcal{N}_{\boldsymbol{x}}[\boldsymbol{u}] = 0, \qquad \boldsymbol{x} \in \Omega, t \in [0,T]$$ PDE

$$\boldsymbol{u}(\boldsymbol{x},0) = h(\boldsymbol{x}), \qquad x \in \Omega$$
$$\boldsymbol{u}(\boldsymbol{x},t) = g(\boldsymbol{x},t), \qquad t \in [0,T], \boldsymbol{x} \in \partial\Omega$$ BC & IC

$$\boldsymbol{r}_\theta(\boldsymbol{x},t) := \frac{\partial}{\partial t} f_\theta(\boldsymbol{x},t) + \mathcal{N}_{\boldsymbol{x}}[f_\theta(\boldsymbol{x},t)]$$ Residual

$f_\theta(x,t)$

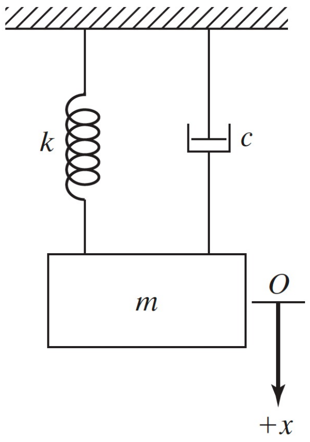


$$\left\{ \begin{aligned} \mathcal{L}_r &= \frac{1}{N_r}\sum_{i=1}^{N_r}\left[\boldsymbol{r}(\boldsymbol{x}_r^i, t_r^i)\right]^2 \\ \mathcal{L}_{u_b} &= \frac{1}{N_b}\sum_{i=1}^{N_b}\left[\boldsymbol{u}(\boldsymbol{x}_b^i, t_b^i) - g_b^i\right]^2 \\ \mathcal{L}_{u_0} &= \frac{1}{N_0}\sum_{i=1}^{N_0}\left[\boldsymbol{u}(\boldsymbol{x}_0^i, 0) - h_0^i\right]^2 \end{aligned} \right.$$

Minimize L to satisfy PDE, BC and IC

PINNs – Illustrative example

Free vibration with viscous damping:



Governing equation:

$$m\ddot{x} + c\dot{x} + kx = 0$$

Solution:

$$x(t) = X_0 e^{-\zeta\omega_n t} \sin\left(\sqrt{1-\zeta^2}\omega_n t + \phi_0\right)$$

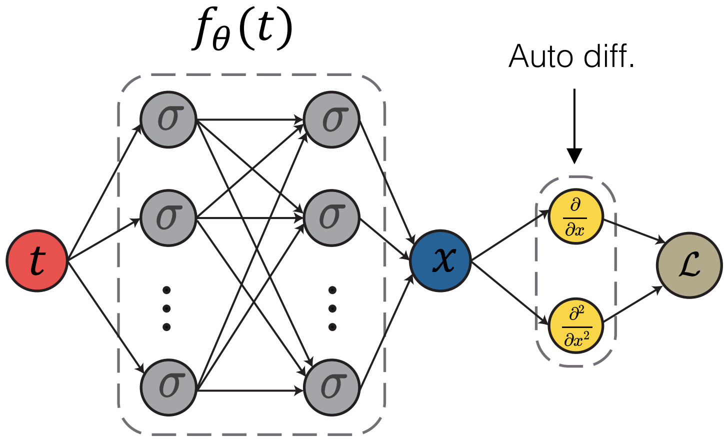
where:

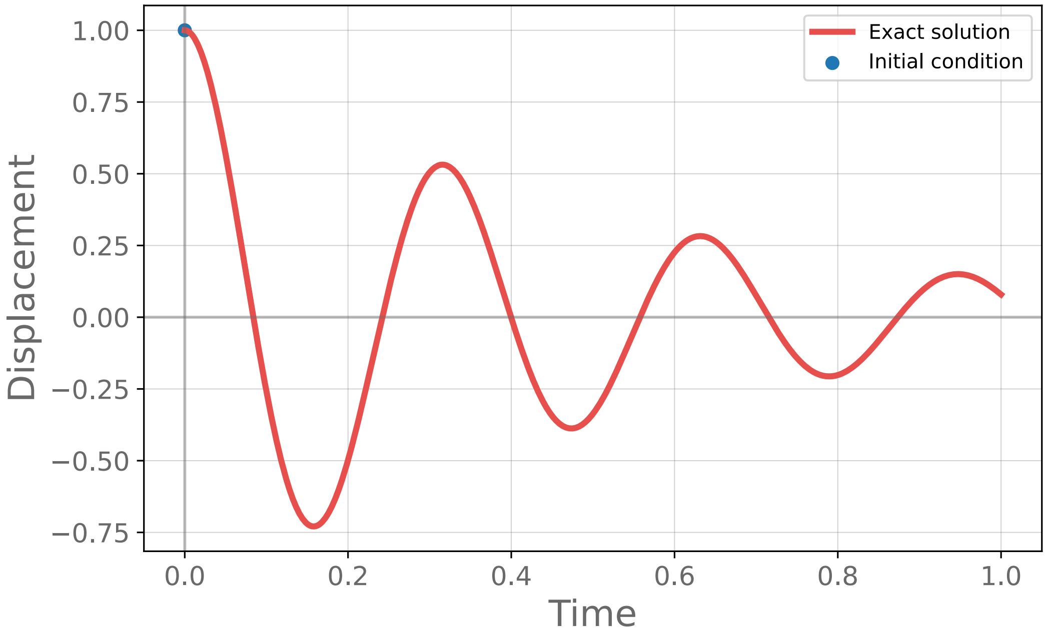
$$X_0 = \frac{\sqrt{x_0^2\omega_n^2 + \dot{x}^2 + 2x_0\dot{x}_0\zeta\omega_n}}{\omega_n\sqrt{1-\zeta^2}} \qquad \phi_0 = \tan^{-1}\left(\frac{x_0\omega_n}{\dot{x}_0 + \zeta\omega_n x_0}\right)$$

System specification:

$$m = 1\,kg, k = 100\,\frac{N}{m}, c = 2\,\frac{N\text{–}s}{m}$$

$$x_0 = 1\,m, \dot{x}_0 = 0\,\frac{m}{s}$$





PINNs – Illustrative example

Governing equation:

$$m\ddot{x} + c\dot{x} + kx = 0$$

System specification:

$$m = 1\,kg, k = 100\frac{N}{m}, c = 2\frac{kg}{2}$$

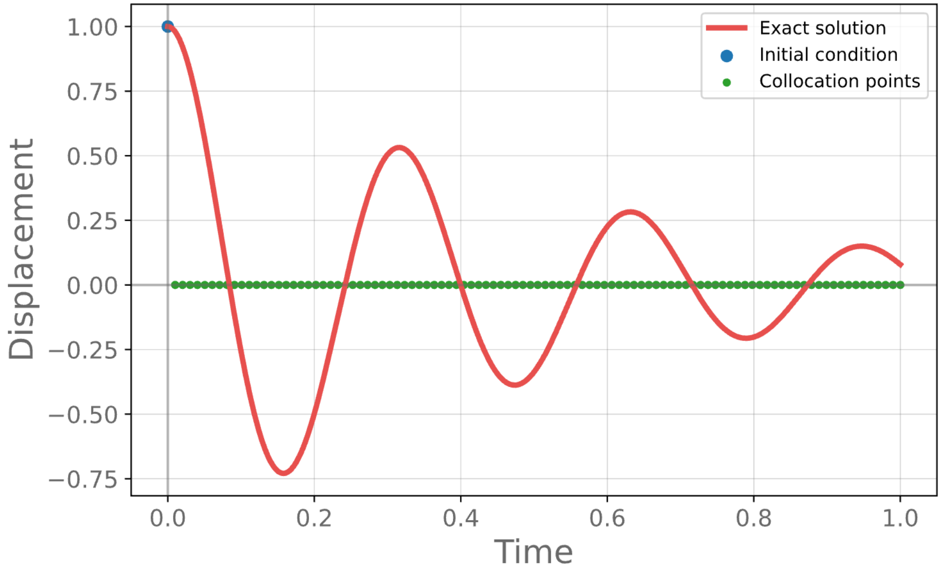
$$x_0 = 1\,m, \dot{x}_0 = 0\frac{m}{s}$$

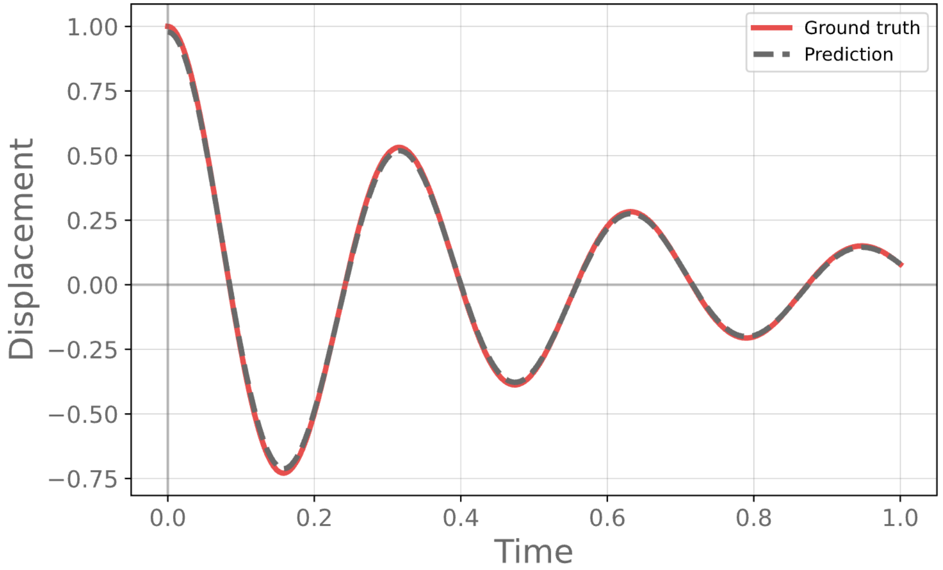
Loss terms:

$$\mathcal{L}_r = \frac{1}{N_r}\sum_{i=1}^{N_r}\left[\boldsymbol{r}(\boldsymbol{x}_r^i, t_r^i)\right]^2 = \frac{1}{N_r}\sum_{i=1}^{N_r}\left[m\frac{\partial^2 f_\theta(t)}{\partial t^2} + c\frac{\partial f_\theta(t)}{\partial t} + kf_\theta(t)\right]^2$$

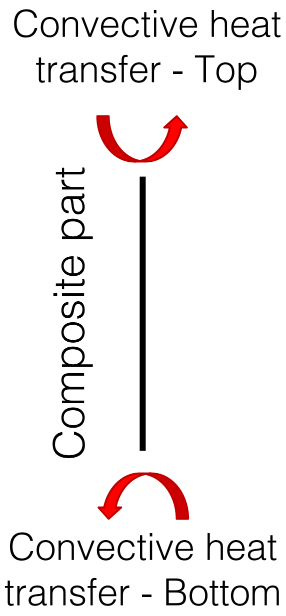
$$\mathcal{L}_{u_0} = \frac{1}{N_0}\sum_{i=1}^{N_0}\left[\boldsymbol{u}(\boldsymbol{x}_0^i, 0) - h_0^i\right]^2 = \frac{1}{N_0}\sum_{i=1}^{N_0}\left[f_\theta(t_0) - 1\right]^2$$

$$\mathcal{L}_{\dot{u}_0} = \frac{1}{N_0}\sum_{i=1}^{N_0}\left[\dot{u}(\boldsymbol{x}_0^i, 0) - h_0^i\right]^2 = \frac{1}{N_0}\sum_{i=1}^{N_0}\left[\frac{\partial f_\theta(t_0)}{\partial t} - 0\right]^2$$





Case study 2: PINNs for composites curing process



Governing equations (1D composite part):

$$\rho C_P \frac{\partial T}{\partial t} = k \frac{\partial^2 T}{\partial x^2} + \nu_r \rho_r H_r \frac{\partial \alpha}{\partial t} \quad \text{and}$$

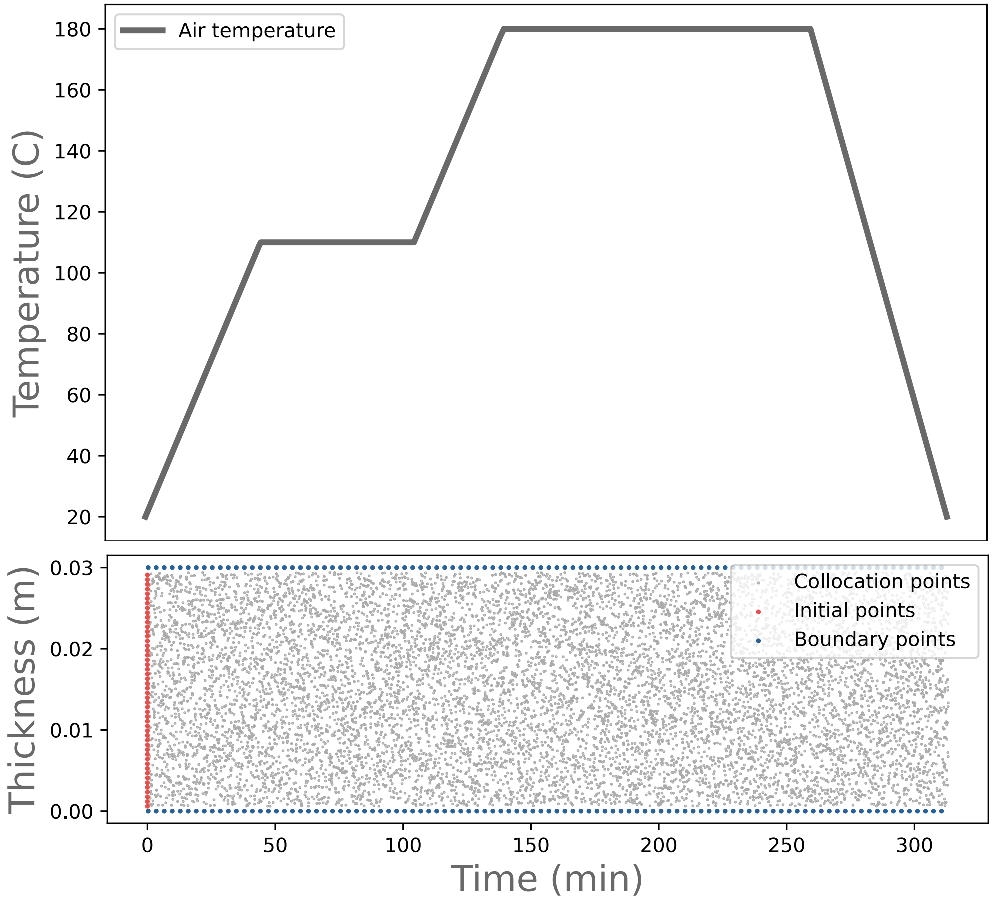
$$\frac{\partial \alpha}{\partial t} = g(T, \alpha)$$

Initial and boundary conditions:

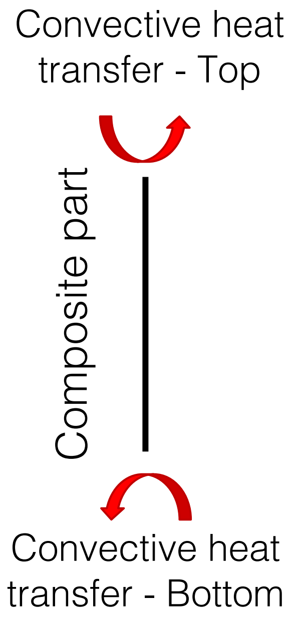
$$h_b(T|_{x=0} - T_a) = k \frac{\partial T}{\partial x}|_{x=0}$$

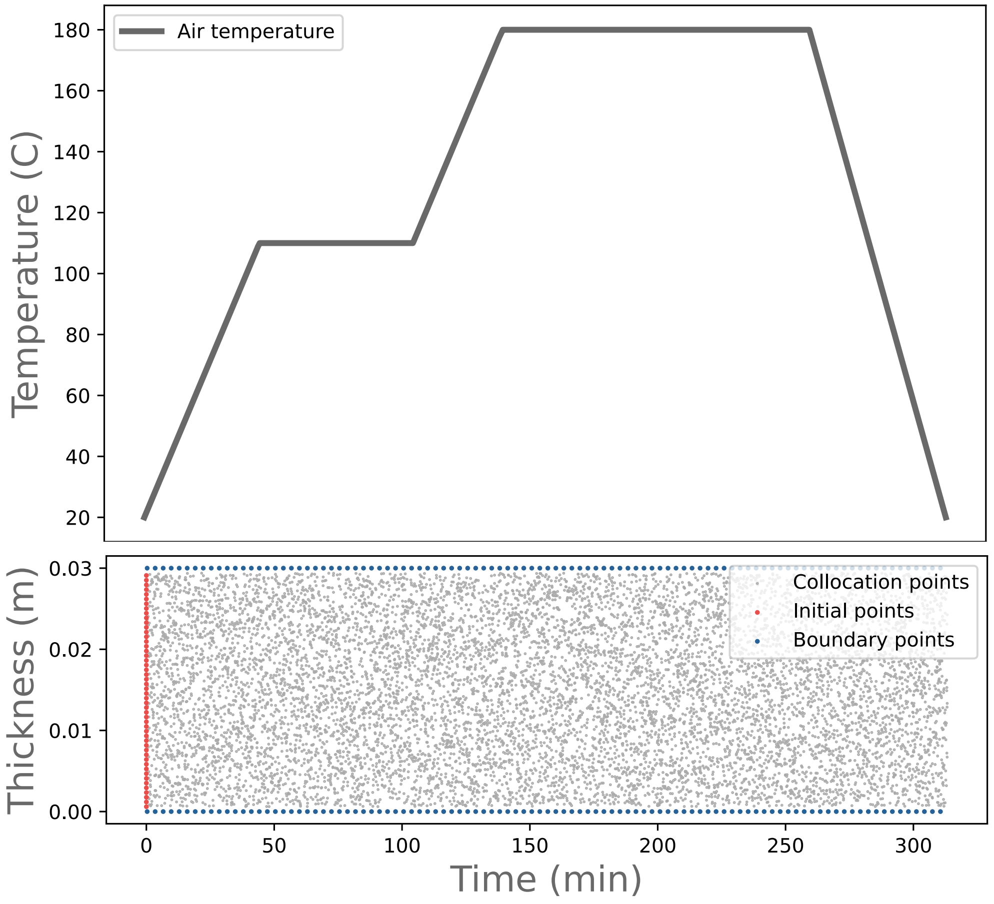
$$h_t(T_a - T|_{x=L}) = k \frac{\partial T}{\partial x}|_{x=L}$$

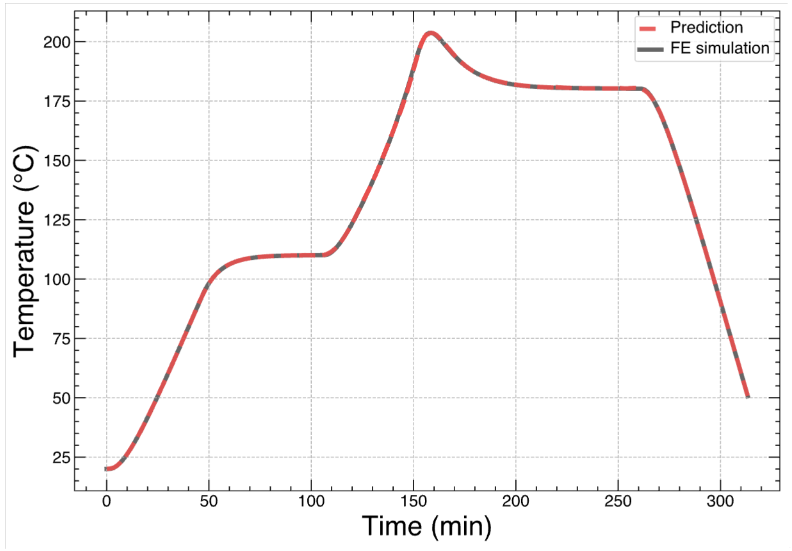
$$T|_{t=0} = T_0$$

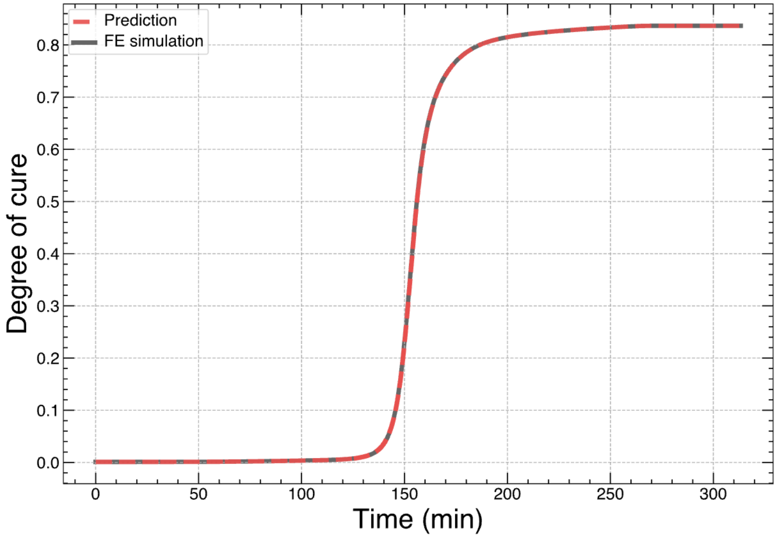


Case study 2: PINNs for composites curing process





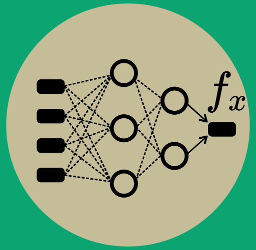




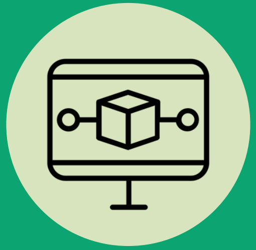
Data-Efficient Machine Learning

01
Transfer learning

02
Physics-informed ML



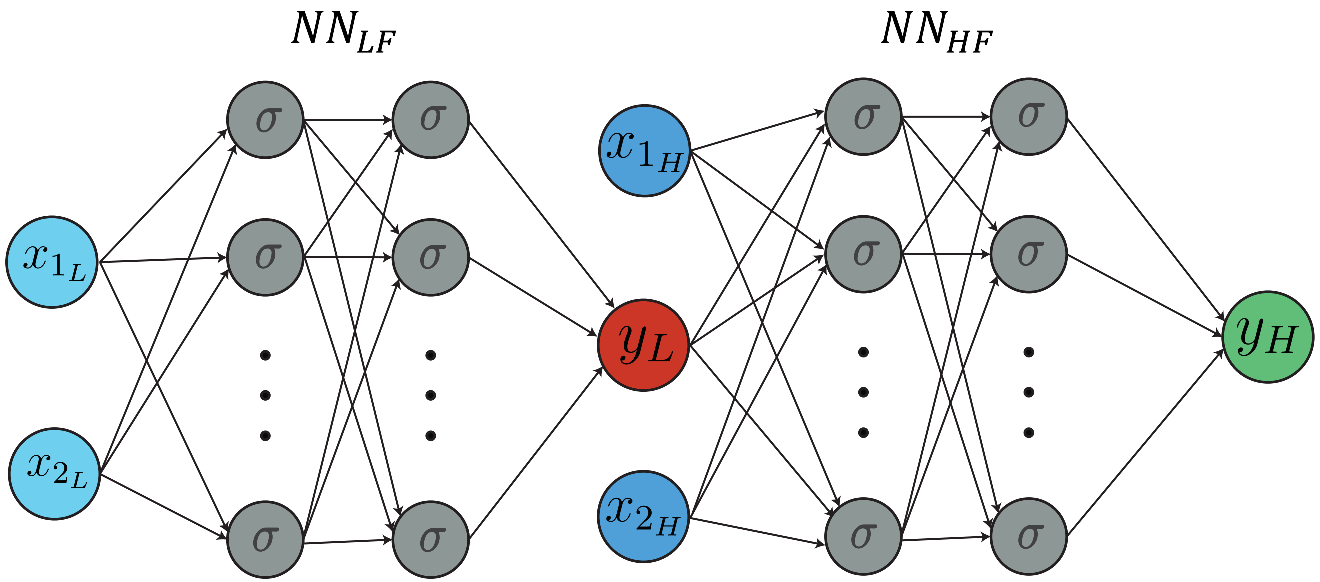
03
Multi-fidelity learning



Multi-fidelity learning

- A sub-category of transfer learning aiming at discovering the linear and nonlinear relationships between the low-fidelity (LF) and high-fidelity (HF) data (*Source and target*).
  - Accurate but costly HF data are limited → experimental measurements
  - Less accurate but cheap LF data are abundant → synthetic data from FE simulation

- **Idea**: LF data provides useful info about the behavior of HF data → reduces the necessity to obtain many HF data
- **Goal**: Identify the cross-correlation (**linear** and **nonlinear**) between the LF and HF data.



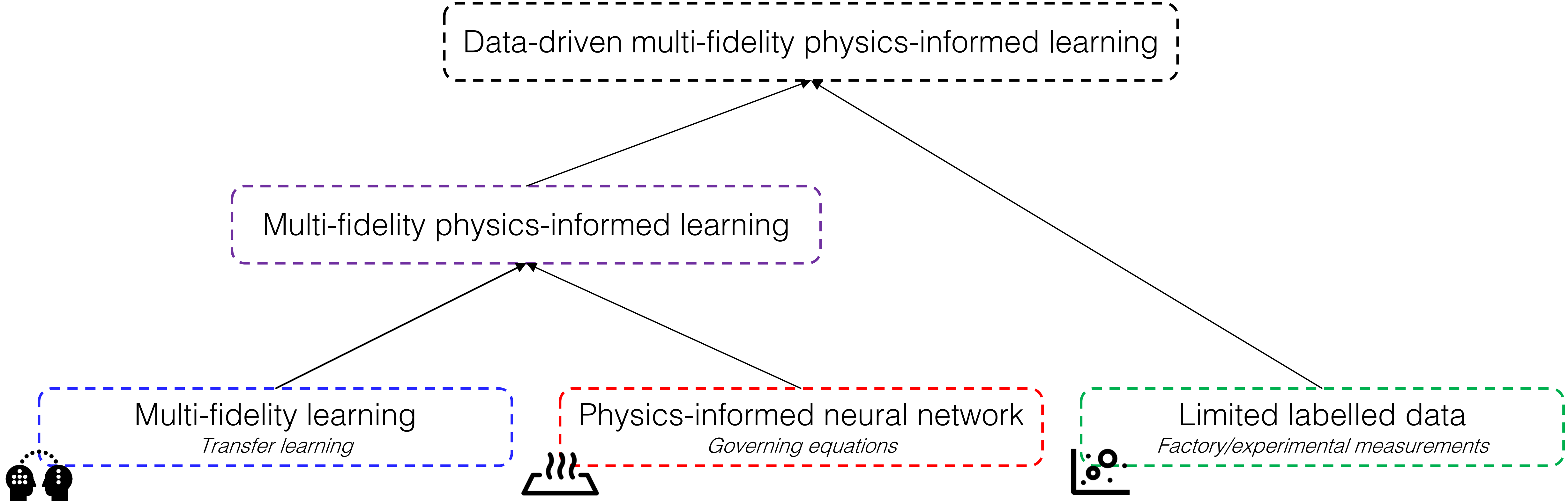
$$y_{HF} = \mathcal{F}(y_{LF}, x)$$

$$MSE = MSE_{y_{LF}} + MSE_{y_{HF}}$$

$$MSE_{y_{LF}} = \frac{1}{N_{y_{LF}}} \sum_{i=1}^{N_{y_{LF}}} (|y_{LF}^{*} - y_{LF}|^2)$$

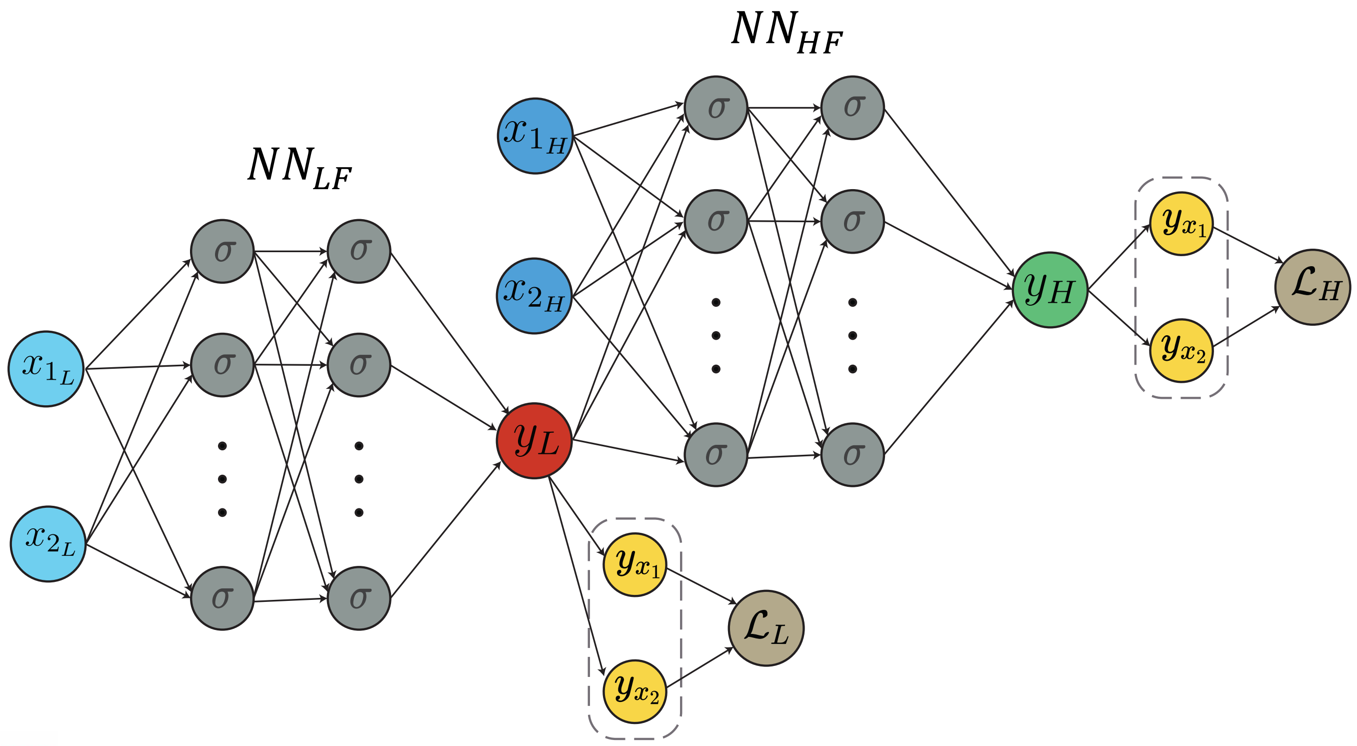
$$MSE_{y_{HF}} = \frac{1}{N_{y_{HF}}} \sum_{i=1}^{N_{y_{HF}}} (|y_{HF}^{*} - y_{HF}|^2)$$

Knowledge integration: data, physics and relevant prior tasks



Multi-fidelity physics-informed learning

- Incorporating the governing physics as inductive biases to the training of **MFPINN**.
- Using partial differential equations (PDEs) that describe the behavior of the system by adding them to the loss functions as regularizes.
- Outperforms both **data-driven** and **data-agnostic** approaches.



$$MSE = MSE_{y_{LF}} + MSE_{y_{HF}} + MSE_{f_e}$$

$$MSE_{f_e} = \mathcal{L}_L + \mathcal{L}_H$$

$$MSE_{y_{LF}} = \frac{1}{N_{y_{LF}}} \sum_{i=1}^{N_{y_{LF}}} (|y_{LF}^* - y_{LF}|^2)$$

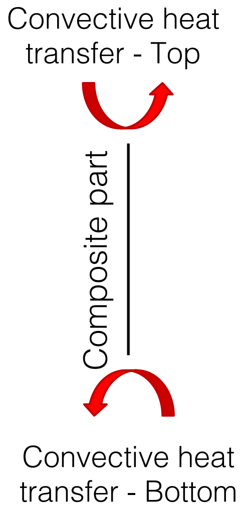
$$MSE_{y_{HF}} = \frac{1}{N_{y_{HF}}} \sum_{i=1}^{N_{y_{HF}}} (|y_{HF}^* - y_{HF}|^2)$$

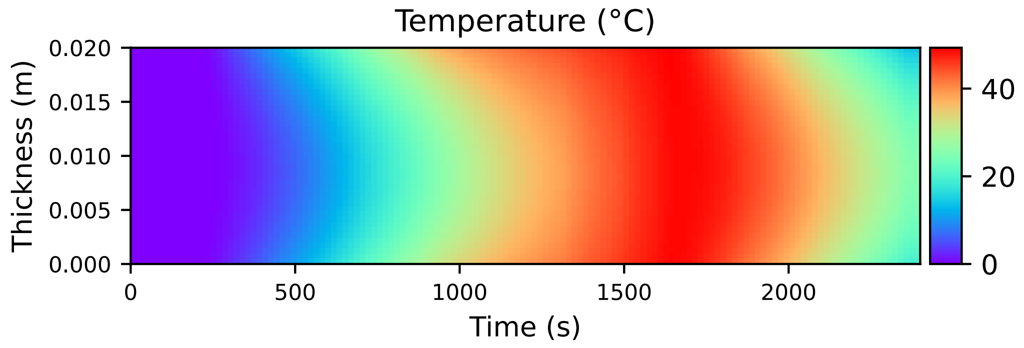
$$MSE_{f_e} = \frac{1}{N_{f_e}} \sum_{i=1}^{N_f} (|f_e^* - f_e|^2)$$

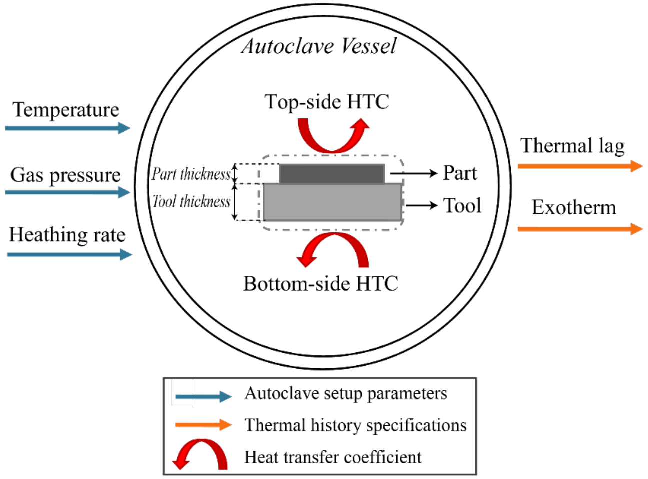
f_e: Inductive biases

- Initial conditions
- Boundary conditions
- Governing PDEs

Case study 3: MFPINN in Composites heat transfer







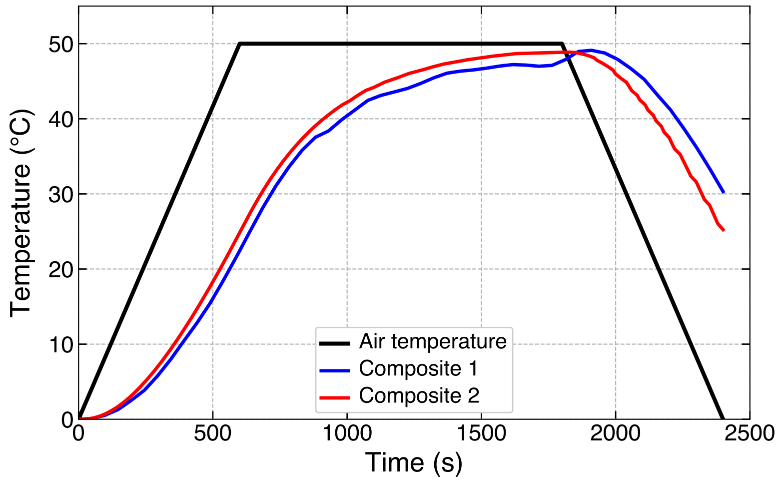
Governing equations:

$$\frac{\partial T}{\partial t} - \alpha \frac{\partial^2 T}{\partial x^2} = 0$$

$$h_b(T|_{x=0} - T_a) = k \frac{\partial T}{\partial x}|_{x=0}$$

$$h_t(T_a - T|_{x=L}) = k \frac{\partial T}{\partial x}|_{x=L}$$

$$T|_{t=0} = T_0$$

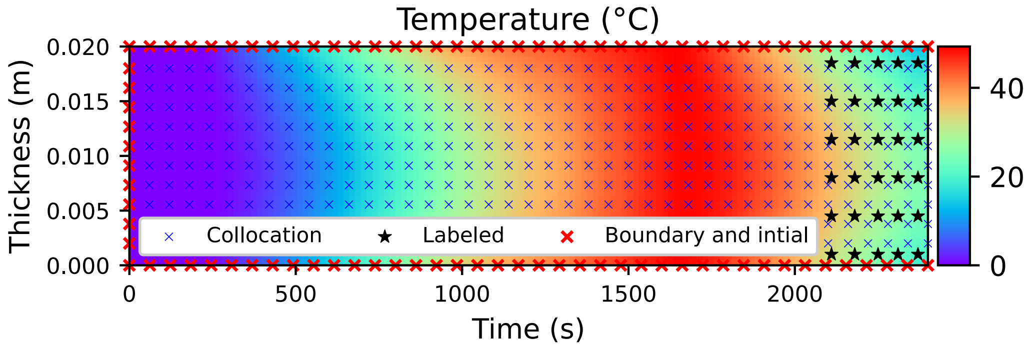


Parameters	Composite 1 (Low-fidelity)	Composite 2 (High-fidelity)
Part length(mm)	20	20
Density (kg/m³)	1573	1581.26
Conductivity (w/mK)	0.47	0.702
Specific heat capacity (J/kgK)	967	1080.22
HTC - top (W/m²K)	100	100
HTC - bottom (W/m²K)	50	50
Initial temperature (°C)	0	0

CRN Composites Research Network

Case study 3: MFPINN in Composites heat transfer

	Scenarios	Description
1	PINN	Train PINN on HF (Composite 2) system (LF data excluded)
2	PINN with labeled data	Train PINN on HF (Composite 2) system including limited labeled HF data
3	MFPINN	Train PINN on HF (Composite 2) system using LF system (Composite 1) prediction from LF network
4	MFPINN with labeled data	Train PINN on HF (Composite 2) system using LF system (Composite 1) prediction from LF network and limited labeled HF data



Case study 3: MFPINN in Composites heat transfer

Source material
(Abundant)

$k = 0.47$ W/m K

$\rho = 1573$ kg/m^3

$C_p = 967$ J/kg K

Target material
(Limited)

$k = 0.638$ W/m K

$\rho = 1581.2$ kg/m^3

$C_p = 1080.2$J/kg K

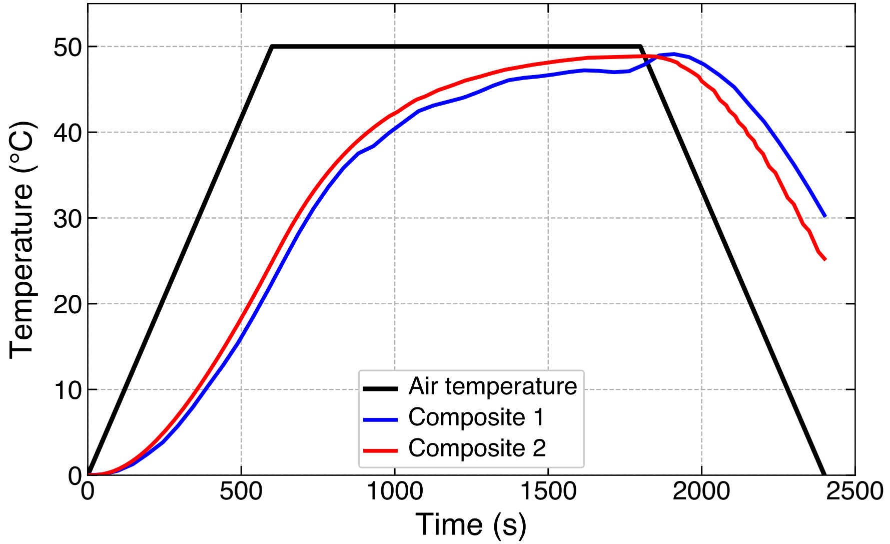
Governing equations:

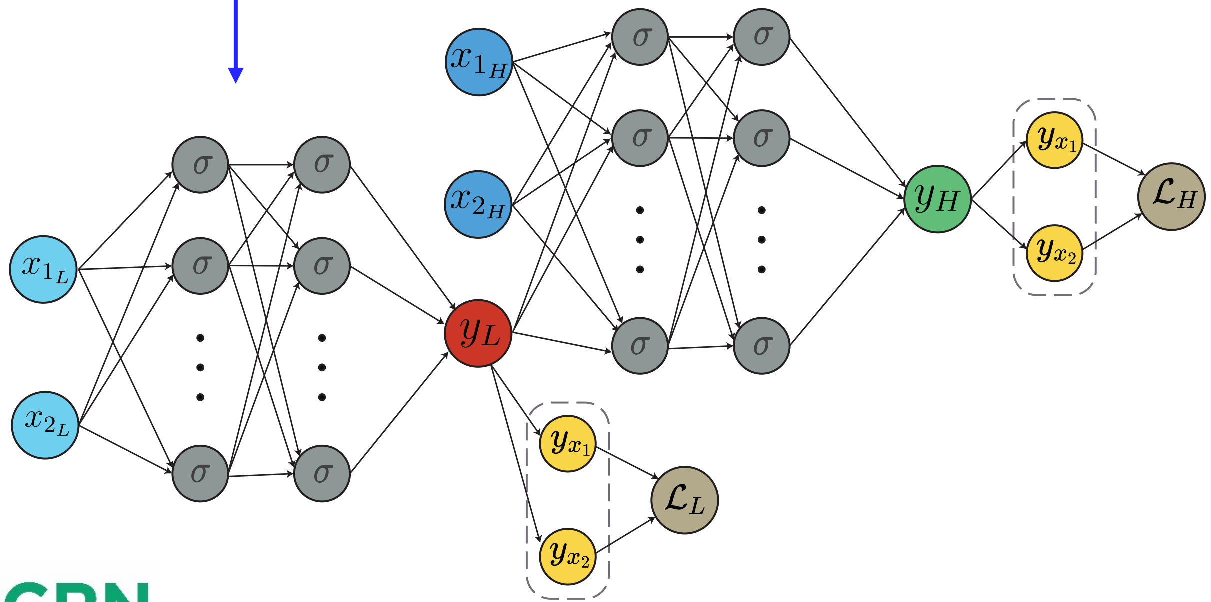
$$\frac{\partial T}{\partial t} - \alpha \frac{\partial^2 T}{\partial x^2} = 0$$

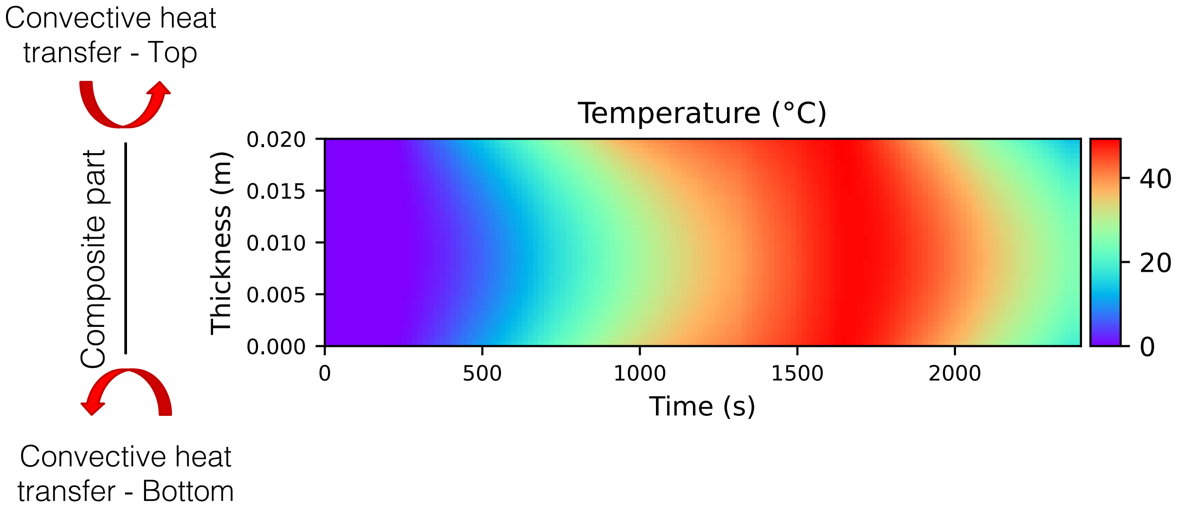
$$h_b(T|_{x=0} - T_a) = k\frac{\partial T}{\partial x}|_{x=0}$$

$$h_t(T_a - T|_{x=L}) = k\frac{\partial T}{\partial x}|_{x=L}$$

$$T|_{t=0} = T_0$$

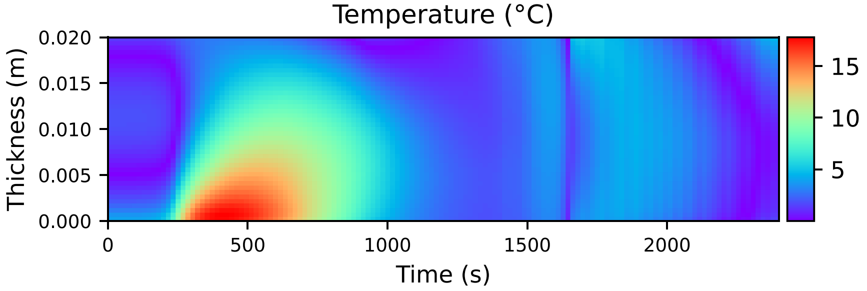




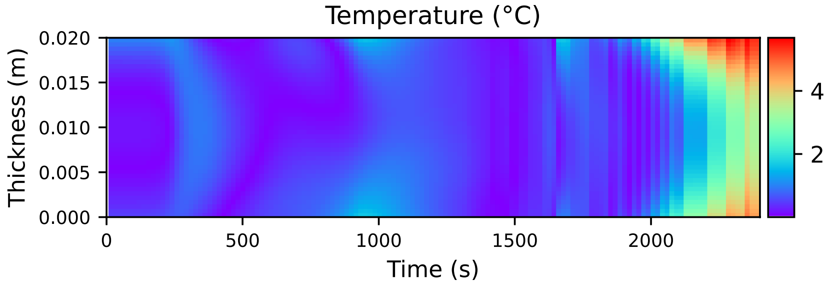


Case study 3: MFPINN in Composites heat transfer

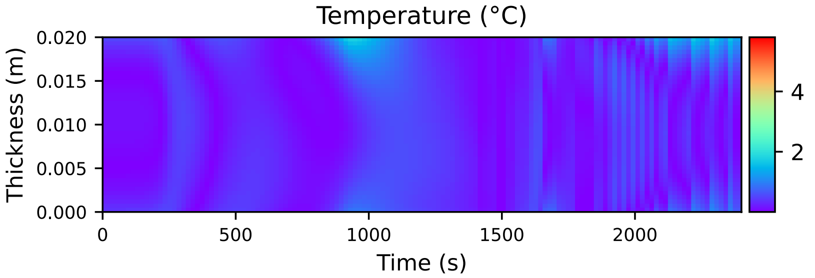
PINN
Trained on PDE only

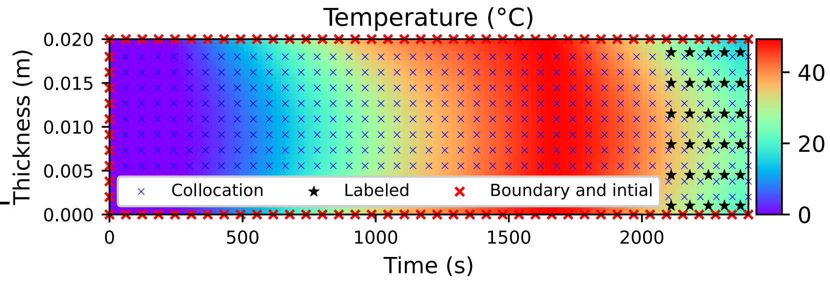


MFPINN
Trained on PDE only (no HF data)



MFPINN
Trained on PDE + HF data





Generalization performance (Relative L2 error) of developed models [3]

	Scenarios	Training time (s)		Labeled Training points		Relative L_2 ($\times 10^{-2}$) error*
		Source (LF)	Target (HF)	Source (LF)	Target (HF)	
1	PINN	--	32	--	90	12.9
2	PINN with labeled data	--	32	--	90 + 30	5.1
3	MFPINN	697	38	4,500	90 (2%)	2.8
4	MFPINN with labeled data	697	39	4,500	90 + 30 (3%)	1.7

40,000 Collocation points (for calculating PDE residuals) are used for all scenarios

* Relative L_2 error: $E = \sqrt{\dfrac{\sum_j \left(y_j^* - y_j\right)^2}{\sum y_j^2}}$

Ramezankhani, M., et al. "**A Data-driven Multi-fidelity Physics-informed Learning Framework for Smart Manufacturing: A Composites Processing Case Study**" 2022 IEEE International Conference on Industrial Cyber Physical Systems (ICPS)

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Hands-on coding in Python

https://github.com/miladramzy/SAMPE2023_Tutorial

Thank you

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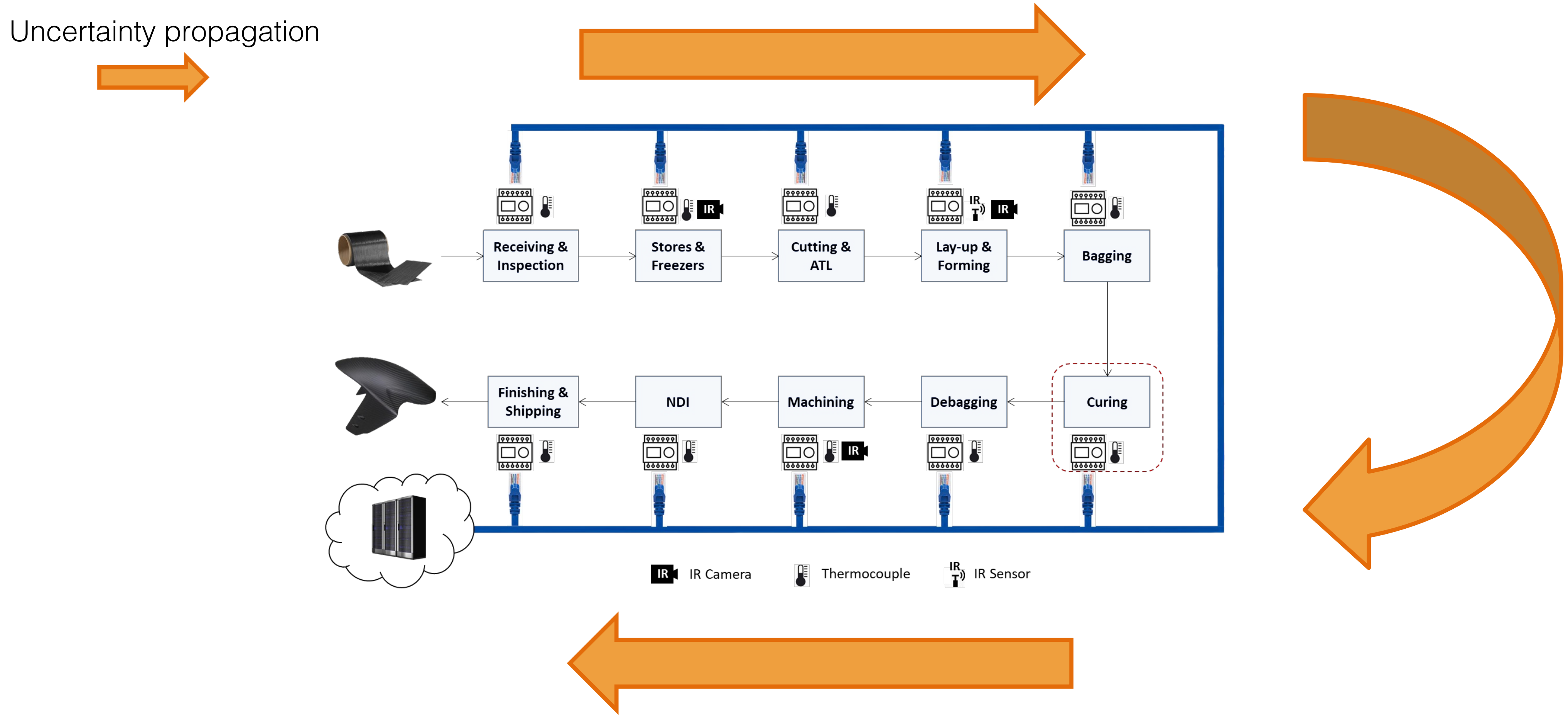
Supporting slides

- Incorporating Uncertainty Factors in AI-based Advanced Manufacturing



Bayesian inference for neural networks

- Unlike conventional deep learning approaches, in Bayesian deep learning (BDL), a posterior distribution $p(w \mid \mathcal{D})$ over model parameters w is inferred after observing data $\mathcal{D}$[4].

- Bayes' rule: $$p(w \mid \mathcal{D}) \propto p(\mathcal{D} \mid w)p(w)$$

- Once the posterior is derived, the model prediction for a new test point is given by:
$$p(y \mid x, \mathcal{D}) = \int_w p(y \mid x, w)p(w \mid \mathcal{D})dw$$

- BDL provides:
  - Accurate predictions
  - Uncertainties estimate → **Active learning** and **decision-making under uncertainty**

- Inference with BDL is challenging: requires calculating a posterior that is very **high-dimensional** and **non-convex** → approximating the posterior:
  - Variational inference
  - Drop-out methods
  - Monte Carlo family

Hamiltonian Monte Carlo

- Classical MCMC algorithms perform poorly in high dimensional spaces→ they rely on a form of *random search* based on local perturbations.
- HMC leverages *gradient information* to guide the local moves. HMC builds on *Hamiltonian mechanics* with (θ, v) representing the *position* and *momentum* of the particle in the energy landspace:

$$\mathcal{H}(\theta, v) \triangleq \mathcal{E}(\theta) + \mathcal{K}(v)$$

- In a statistical setting, we often take the potential energy to be:

$$\mathcal{E}(\boldsymbol{\theta}) = -\log \tilde{p}(\boldsymbol{\theta})$$

$$\mathcal{K}(\boldsymbol{v}) = \frac{1}{2}\boldsymbol{v}^{\top}\boldsymbol{\Sigma}^{-1}\boldsymbol{v}$$

- An auxiliary momentum term is introduced to further guide the search to the typical set, the neighbourhood that most contributes to expectations (approximating the parameter space).

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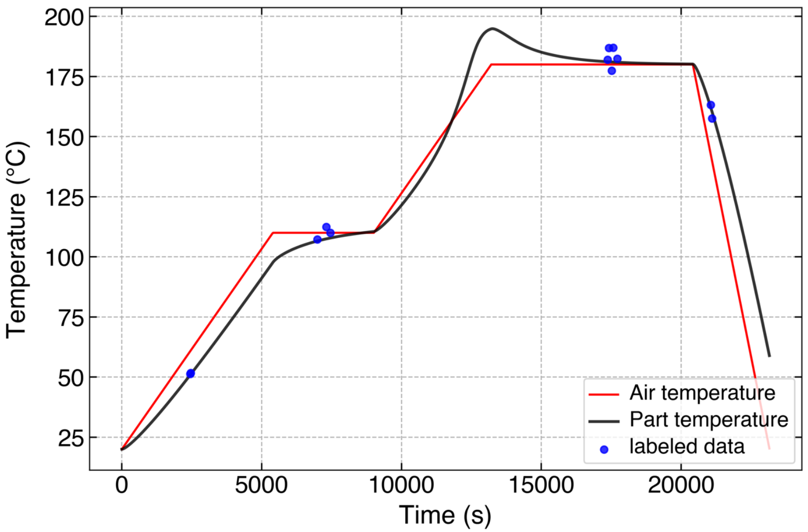
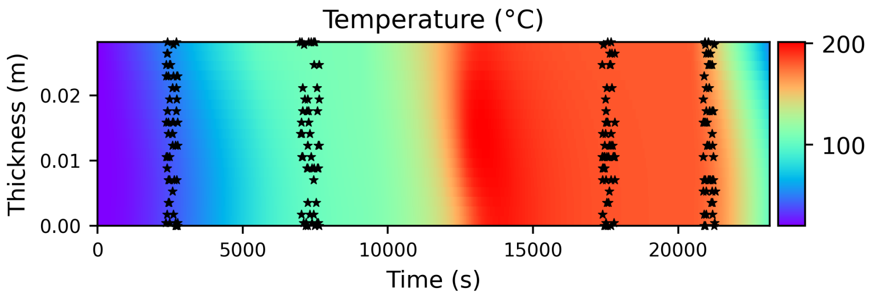
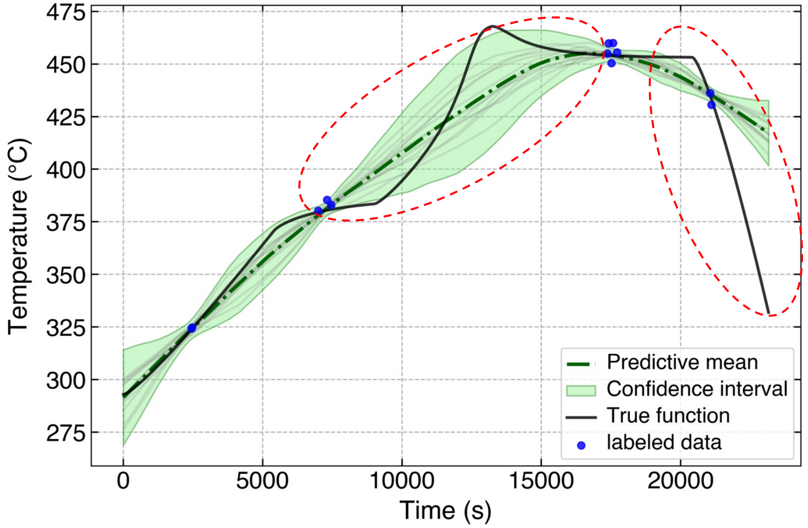
Bayesian multi-fidelity physics-informed learning: Curing process

- **Case study**: curing process of a composite part (AS4-8552) with a 2-hold cure cycle. AS4-8551 simulation is used as LF data.
- Posterior approximation: Hamiltonian Monte Carlo.
- A neural network with three hidden layers (100-100-100-100) is implemented.
- *Noisy* data ($\sigma = 0.02$) at multiple locations (through thickness) are used in the training.



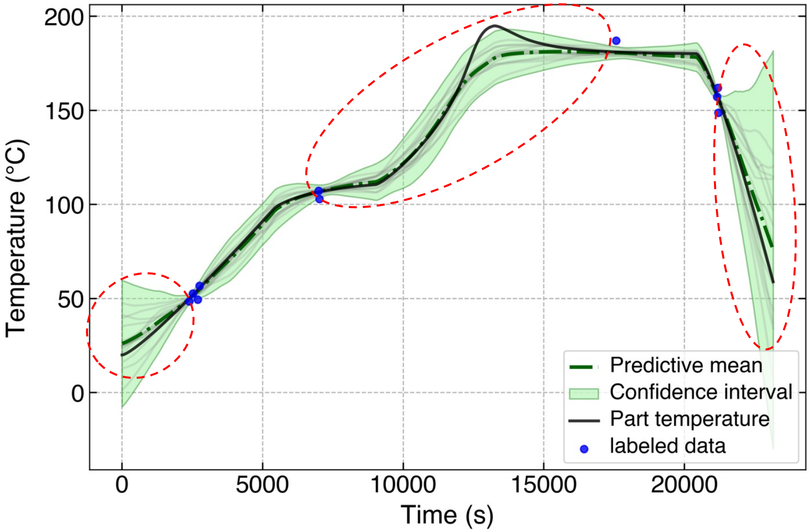


HMC-NN



✓ Uncertainties estimate
✗ Generalization
✗ Accuracy
✗ Extrapolation

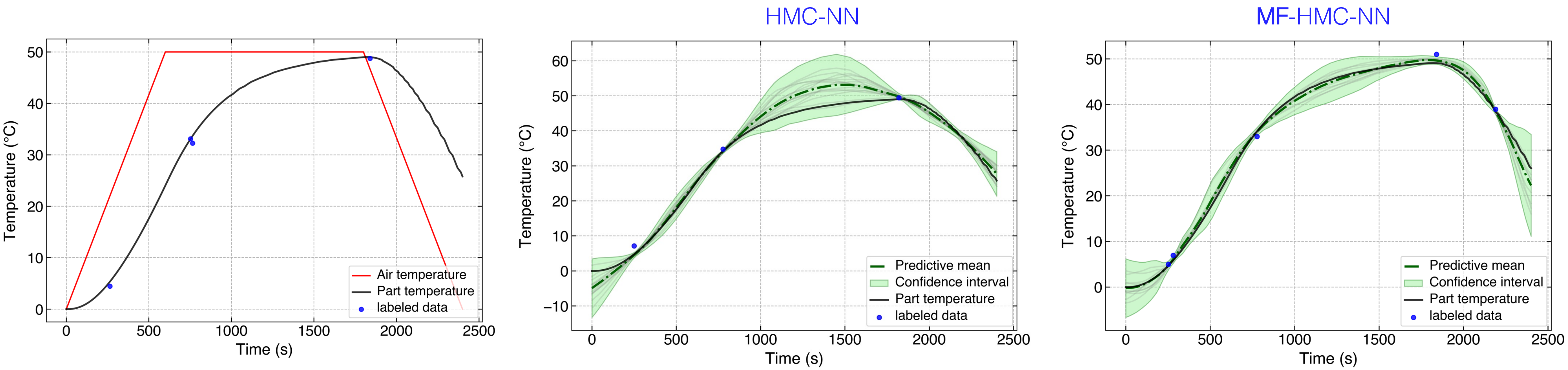
MF-HMC-NN



✓ Uncertainties estimate
✓ Generalization
– Accuracy
✗ Extrapolation

Bayesian multi-fidelity physics-informed learning: Heat transfer

- **Case study**: Heat transfer of a **cured** composite part with a 1-hold cure cycle.
- Posterior approximation: Hamiltonian Monte Carlo.
- A neural network with three hidden layers (100-100-100-100) is implemented.
- *Noisy* data ($\sigma = 0.02$) at multiple locations (through thickness) are used in the training.



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