Development of Uncertainty-Guided Deep Learning with Application to Thermal Fluid Closures

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NEKVAC/NUC Workshop
“Multiphysics Model Validation”
June 27-29, 2017

Outline

- Introduction
- Technical background overview
- Formulation of the framework
- Case study
- Type-II machine learning (work in progress)

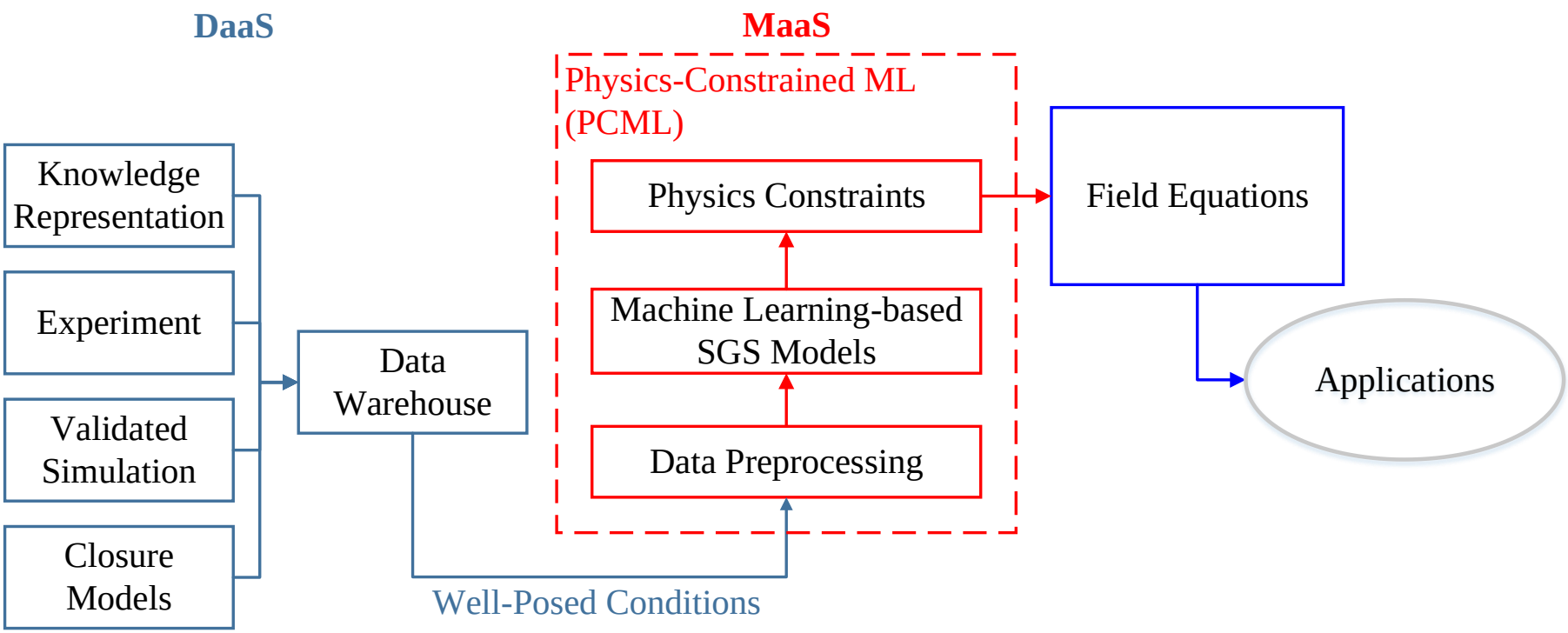
Motivation

- Sub-grid-scale (SGS) physics models (or so-called closure relations) determines the accuracy of thermal-fluid modeling, and it is essential for simulation codes.

- "Big" data in thermal-hydraulics are available with the invention of measurement equipment such as inferred and PIV (Particle image velocimetry) camera.

- Deep learning (DL) is a universal approximator [Hinton, 1989], and can discover the underlying correlations behind the data to achieve the cost-effective closure development for
  - new geometries, new coolants or system conditions, particularly in newly designed systems.

Physics-Constrained ML for Thermal Fluids



aaS: as a Service

(D, M): (Data, Method)

SGS: Sub-Grid-Scale

Objectives

- We will develop the uncertainty guided deep learning framework for developing fluid dynamics closures.
  - Allow thermo-fluid codes to have the features of
    - Robustness
    - Reliability
    - Adaptability
    - Extensibility

+ Predictability

  - Benefit not only system-level codes but also computational multi-fluid dynamics simulations (not DNS).

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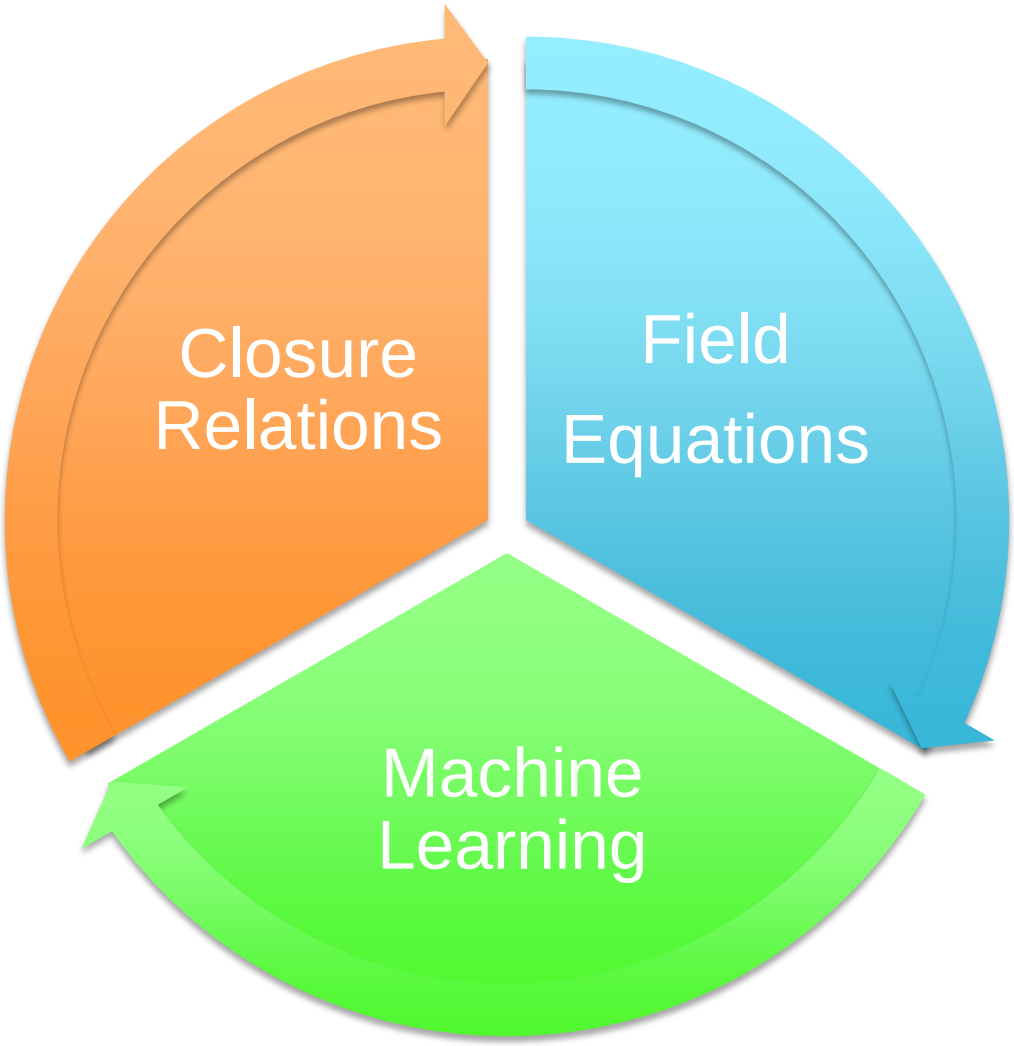
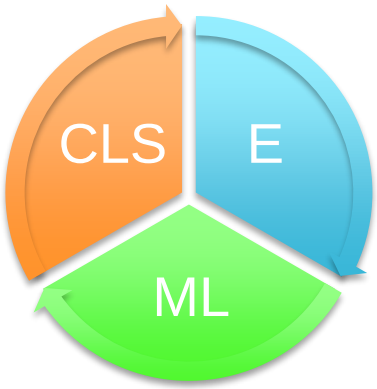
Introduction



Conservation Equations



- Two-phase mixture model (TMM) [Doster, 2015]
  - Mass

$$A_x \frac{\partial \rho}{\partial t} + \frac{\partial \rho v A_x}{\partial z} = 0$$

  - Momentum

$$A_x \frac{\partial \rho v}{\partial t} + \frac{\partial \rho v v A_x}{\partial z} = -A_x \frac{\partial P}{\partial z} - \tau_w P_w + \rho g_z A_x - \frac{\partial}{\partial z}\left[\frac{\alpha_g \rho_g \alpha_l \rho_l}{\rho}(v_g - v_l)^2\right] A_x$$

  - Energy

$$A_x \frac{\partial \rho u}{\partial t} + \frac{\partial \rho u v A_x}{\partial z} = -P \frac{\partial v A_x}{\partial z} + q_w'' P_w - \frac{\partial}{\partial z}\left[\frac{\alpha_g \rho_g \alpha_l \rho_l}{\rho}(u_g - u_l)(v_g - v_l)\right] A_x + P \frac{\partial}{\partial z}\left[\frac{\alpha_g \rho_g \alpha_l \rho_l}{\rho}(\upsilon_g - \upsilon_l)(v_g - v_l)\right] A_x$$

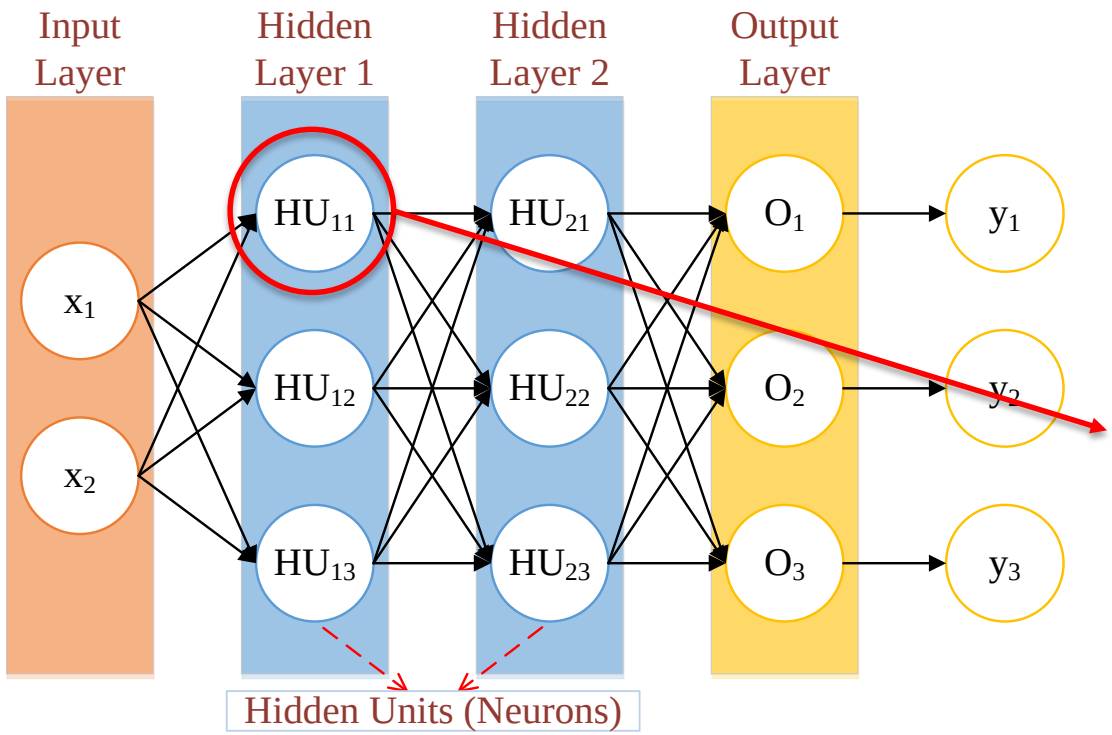
Data assimilation by Machine Learning

- The data assimilation in this work is different from the definition by meteorologists.
- Our goal is to have a relax function form that can assimilate the data to enable cost-effective closure model development.

Tribe	Problem	Master Algorithm
Symbolists	Knowledge Composition	Inverse Deduction
Evolutionaries	Structure Discovery	Genetic Programming
Analogizers	Similarity	Support Vector Machine
Connectionists	Credit Assignment	Backpropagation
Bayesians	Uncertainty	Probabilistic Inference

Deep learning - model structure

- Neural networks (NNs) with more than two layers are deep learning (DL) [Heaton, 2015].
- More layers are expected to capture data behaviors well, but it may suffer from overfitting issues.
  - No theorem to guide the selection of NN hyperparameters
- Multilayer NNs are universal approximators [Hornik, 1989].



Deep means multilayer

Activation Functions

Sigmoid

$$f(x) = \frac{1}{1+e^{-x}}$$

ReLU (Rectified Linear Unit)

$$f(x) = \max(0, x)$$

$$HU_{11}(\mathbf{x}) = \sigma\left(\sum_{i=1}^{2} w_{1i}x_i + b_{11}\right)$$

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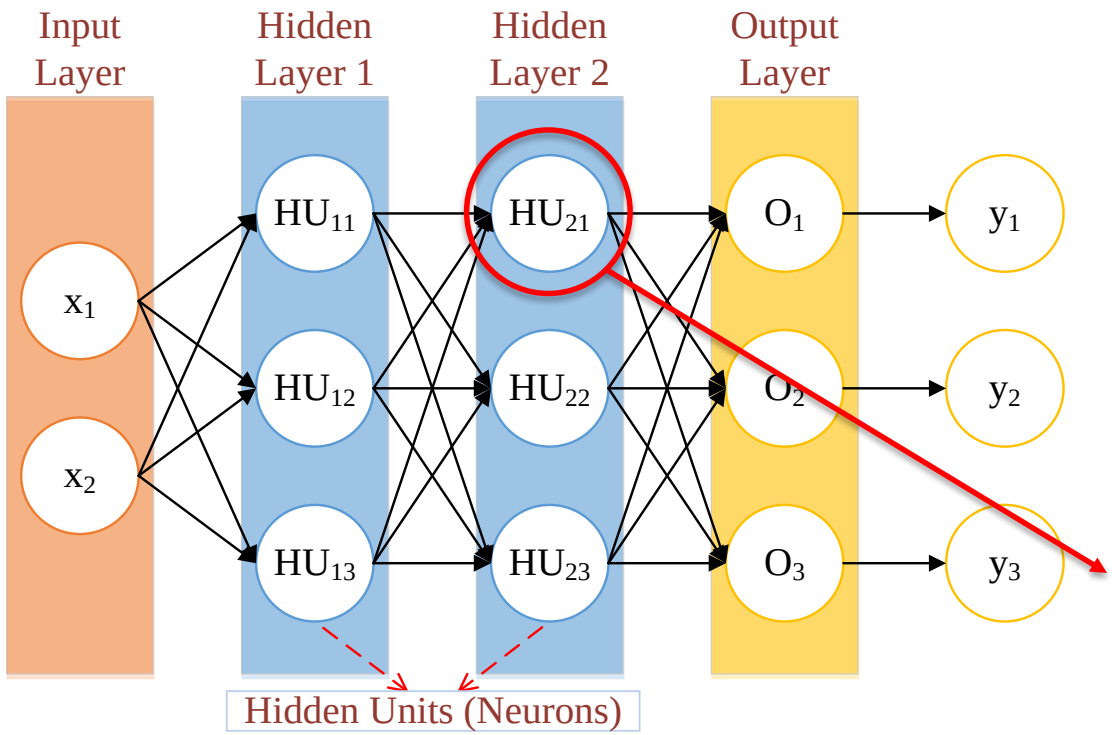

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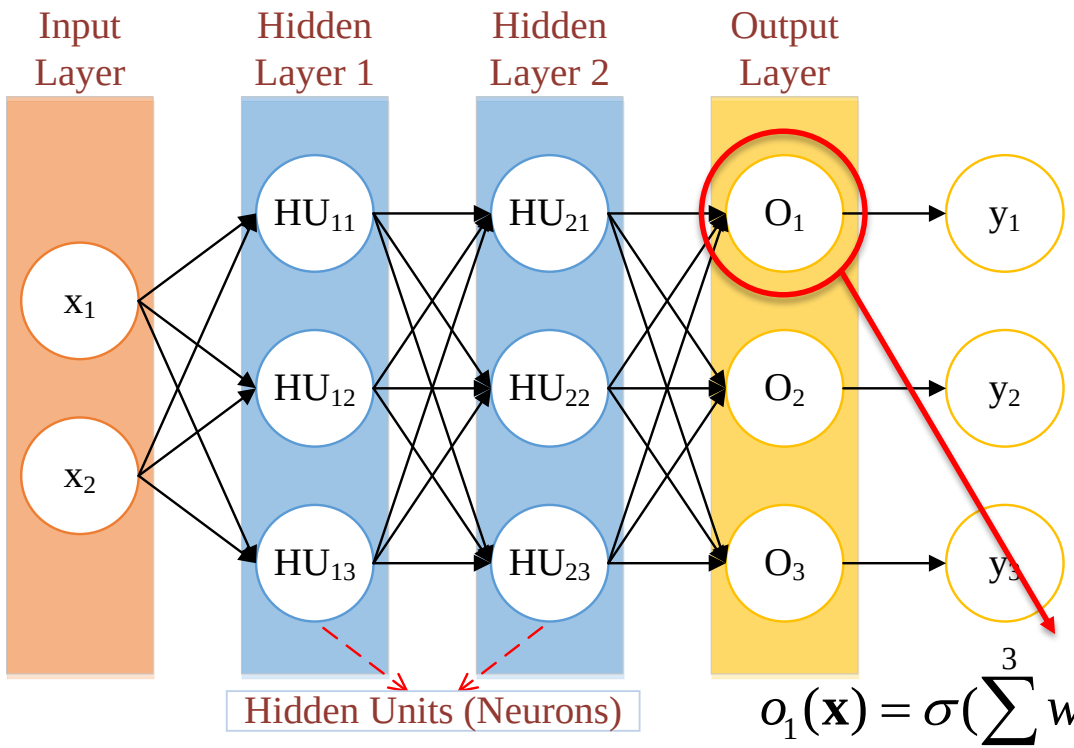

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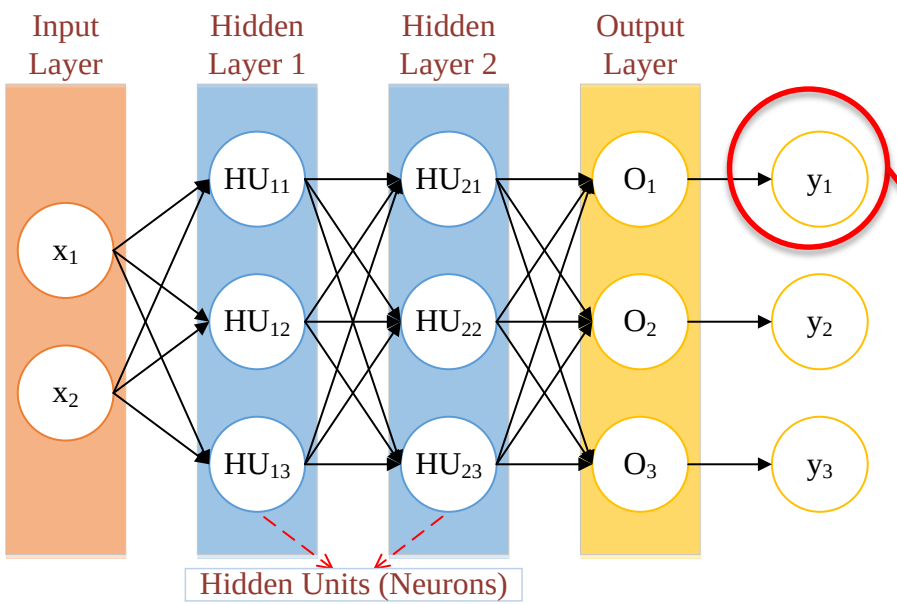
$$o_1(\mathbf{x}) = \sigma\left(\sum_{i=1}^{3} w_{oi} HU_{2i} + b_{o1}\right)$$

Deep learning - model structure



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$$o_1(\mathbf{x}) = \sigma(\sum_{i=1}^{3} w_{oi} HU_{2i} + b_{o1})$$

$$\hat{y}(\mathbf{x}) = o_1(\mathbf{x})$$

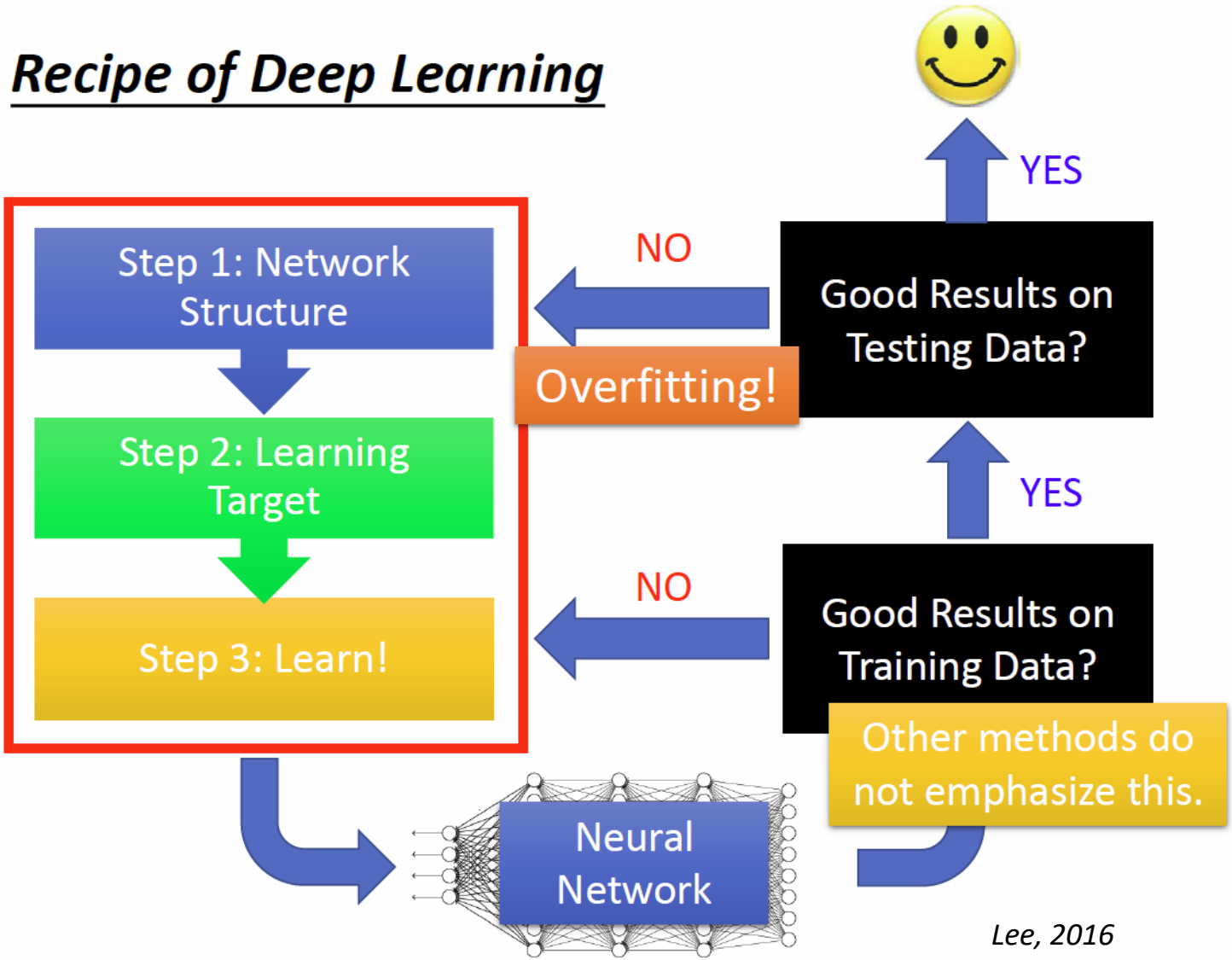
L2 norm (loss function)

$$L = \frac{1}{2N} \sum_{i=1}^{N} \left(y_i - \hat{y}_i \right)^2$$

Stochastic Gradient Descent

$$w^{n+1} = w^n - \eta \frac{\partial L}{\partial w^n}$$

Deep learning - workflow



Lee, 2016

Deep learning – frameworks

Configuration File	Programmatic Generation
Caffe	Theano
Microsoft Cognitive Toolkit	Tensorflow
	Torch

		Languages	Tutorials and training materials	CNN modeling capability	RNN modeling capability	Architecture: easy-to-use and modular front end	Speed	Multiple GPU support	Keras compatible
Academic	Theano	Python, C++	++	++	++	+	++	+	+
Google	Tensor-Flow	Python	+++	+++	++	+++	++	++	+
Facebook	Torch	Lua, Python (new)	+	+++	++	++	+++	++	
Berkeley AI Research	Caffe	C++	+	++		+	+	+	
Amazon	MXNet	R, Python, Julia, Scala	++	++	+	++	++	+++	
Intel Nervana	Neon	Python	+	++	+	+	++	+	
Microsoft	CNTK	C++	+	+	+++	+	++	+	

http://www.svds.com/getting-started-deep-learning/

Related work

	Problem	Method	Data
Tryggvason	Isothermal bubbly flow (VF < 0.1)	2-layer feedforward NN	DNS → TFM
Duraisamy	Turbulent flow	Field-inversion (Bayesian)	DNS → RANS
Xiao	Turbulent flow	Random forest regression	DNS → RANS

- There is no ML application for thermal-hydraulics yet.
- There is no PDE-constrained DL application yet.
- Although 2-layer NN has been applied to the isothermal bubbly flow case, the previous work does not indicate the method to select
  - NN hyperparameters
  - and the requirements of datasets.

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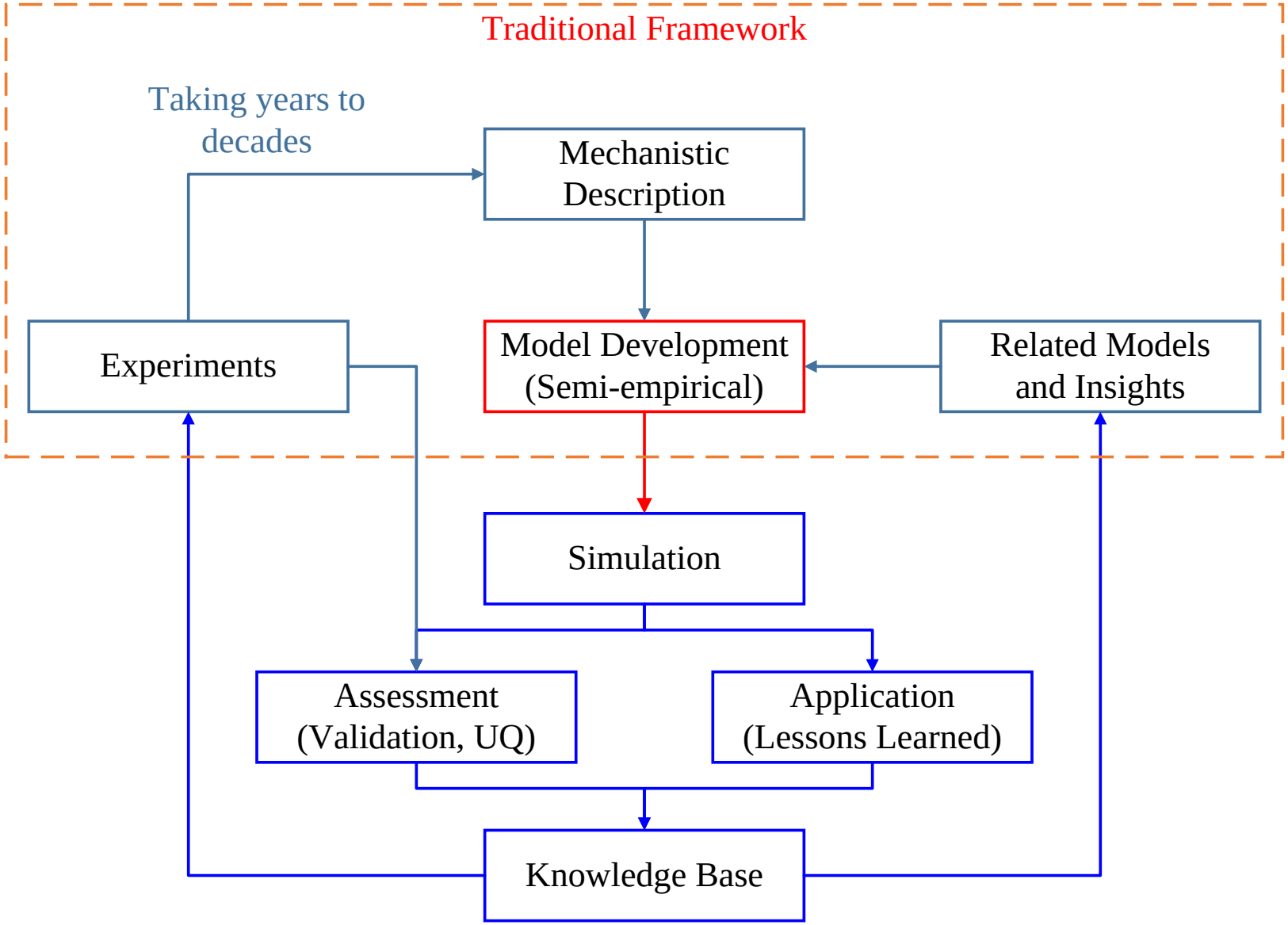
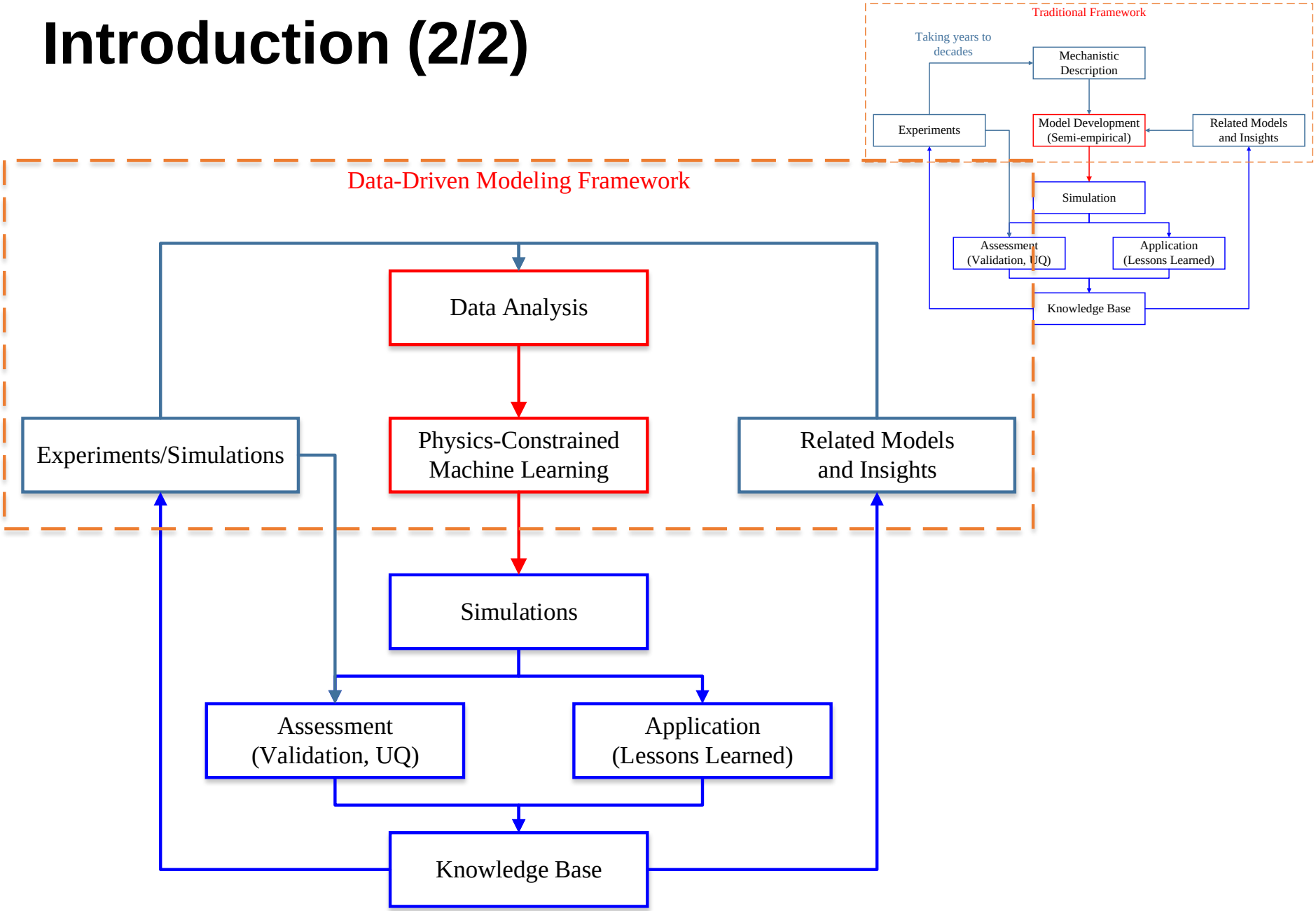
Introduction (1/2)



Introduction (2/2)

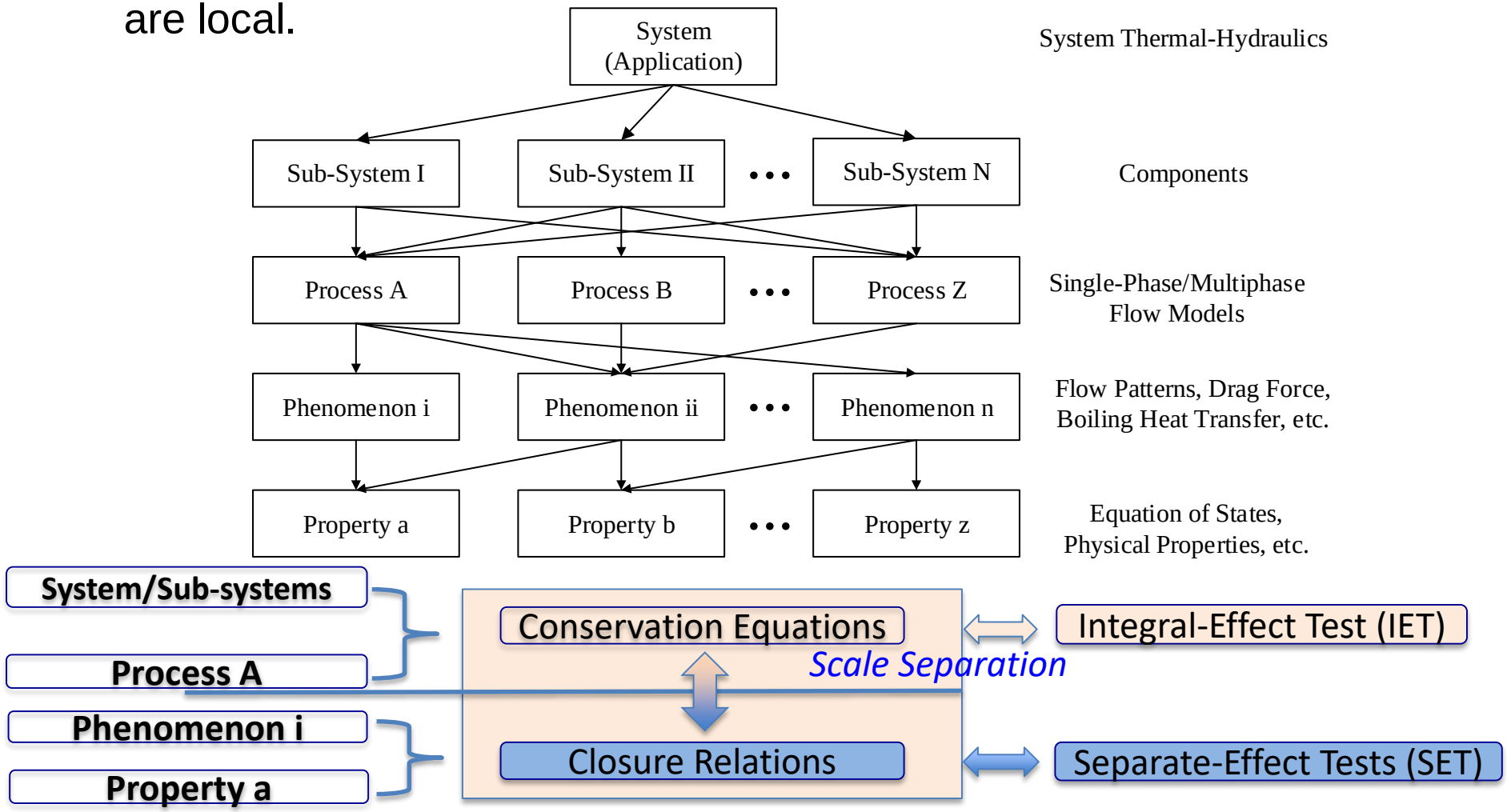


Method of manufactured data (MMD)

- To evaluate the framework, the present work proposes a method of manufactured data (MMD) as surrogates for actual datasets in real-life applications.
- The MMD applies a computer code with high-fidelity models to generate numerical solutions
  - for training and benchmark purposes.
- The “high fidelity” here refers to models which have been more **extensively adjusted** and **assessed** to be trustworthy for conditions under consideration.
- Both training and benchmark datasets can be generated with
  - different degree of detail (homogenization, amount).
  - controlled uncertainty (“manufactured errors and biases”).

Physics-constrained machine learning

- PCML problems involve PDE models with sub-grid-scale (SGS) physics models that are scale separable, for which closure relations are local.

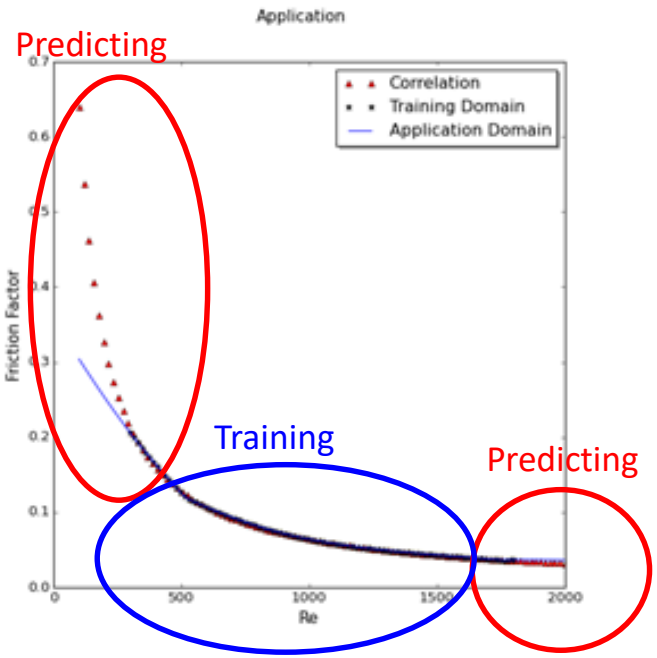


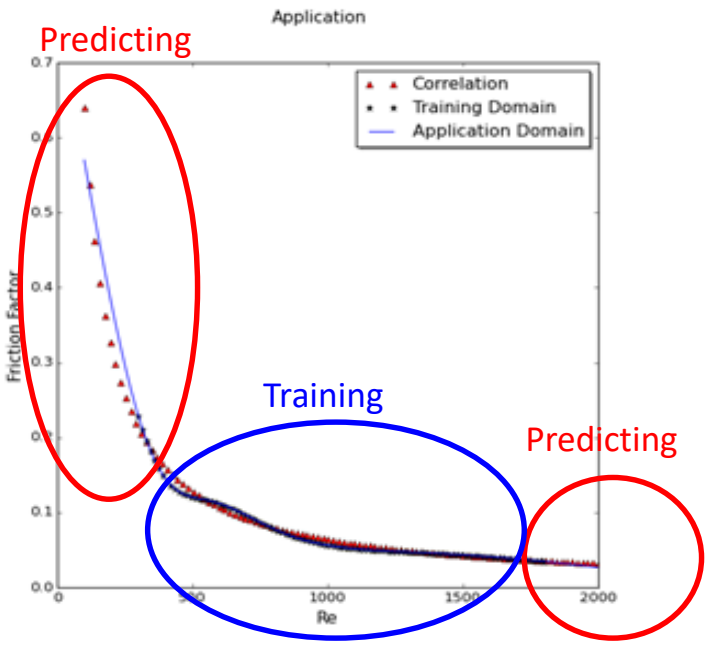
Issues of using DL in thermal fluid (1/6)

- Questions
  - What is the uncertainty in DL due to different weight initialization?
  - How to select Tikhonov regularization parameters to increase the predictability?
  - What is the uncertainty due to different DNN structures?
  - How to increase the training accuracy for DNN while using multiple datasets?
  - What are the criteria to search the optimal DL-based fluid closures for field equations?

Issues of using DL in thermal fluid (2/6)

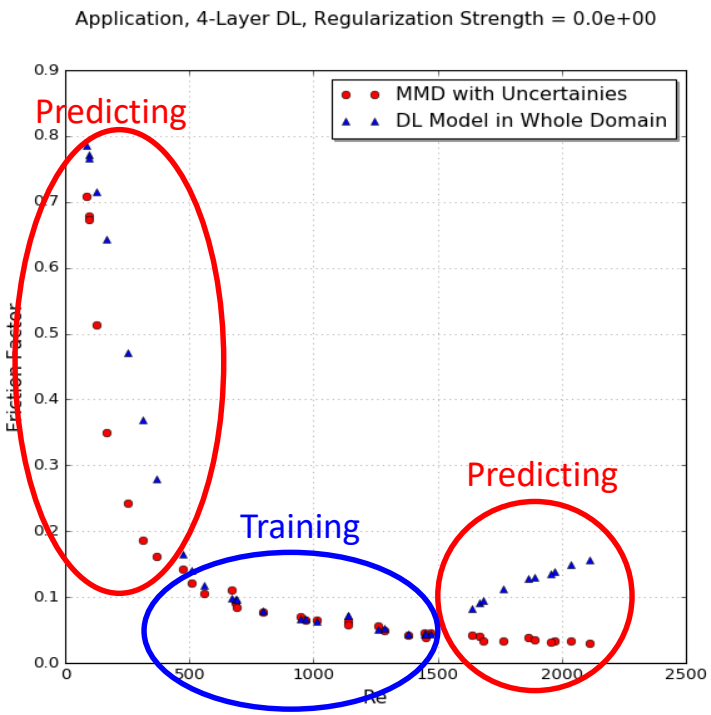
- Understand the uncertainties in DL by different weight initialization.
  - "*Remember that all models are wrong; the practical question is how wrong do they have to be to not be useful*," George E.P. Box.
  - The goal of uncertainty quantification is to evaluate and minimize uncertainties associated with experiments and models.
  - DL with the same structure can result in different predictabilities due to parameter uncertainties. The following figures identify this fact by using DL-based friction closures with different parameters.

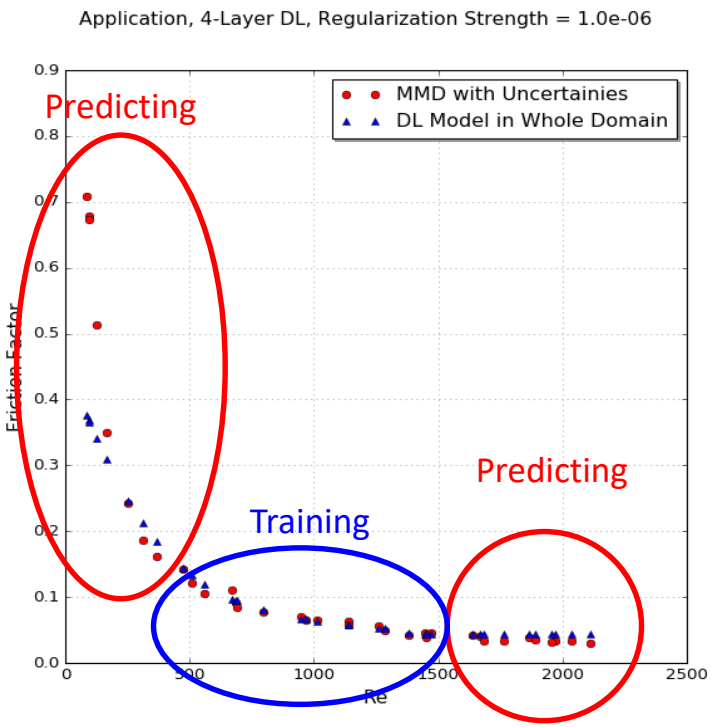




Issues of using DL in thermal fluid (3/6)

- Understand how to use Tikhonov regularization to increase the predictability.
  - DL model tends to over fit the noisy dataset.
  - The following figures shows the regularization can increase the prediction for DL-based friction closures. The question is how to systematically determine the regularization parameters to obtain DL-based fluid closures with robustness.





Issues of using DL in thermal fluid (4/6)

- Understand the uncertainty due to different DNN structures and datasets.
  - The Euclidean loss of DNN with the layer number more than 3 will converge to a larger value then DNN with less layers. Fig. 1 depicts the results by 1-training dataset, and the wiggle in the figure is due to lack of training datasets.

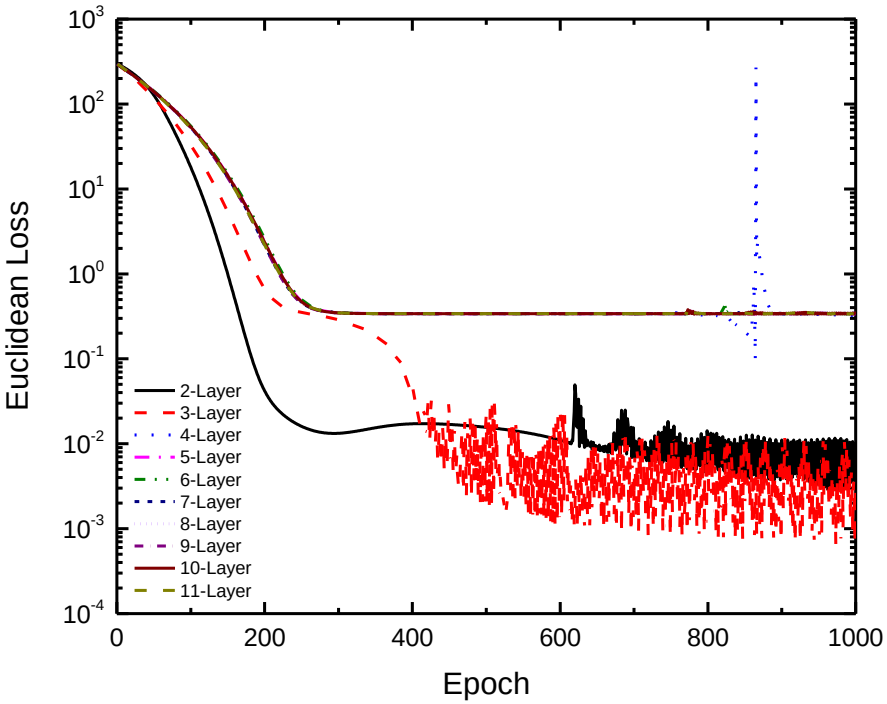


Fig. 1 DNN with 1-training dataset

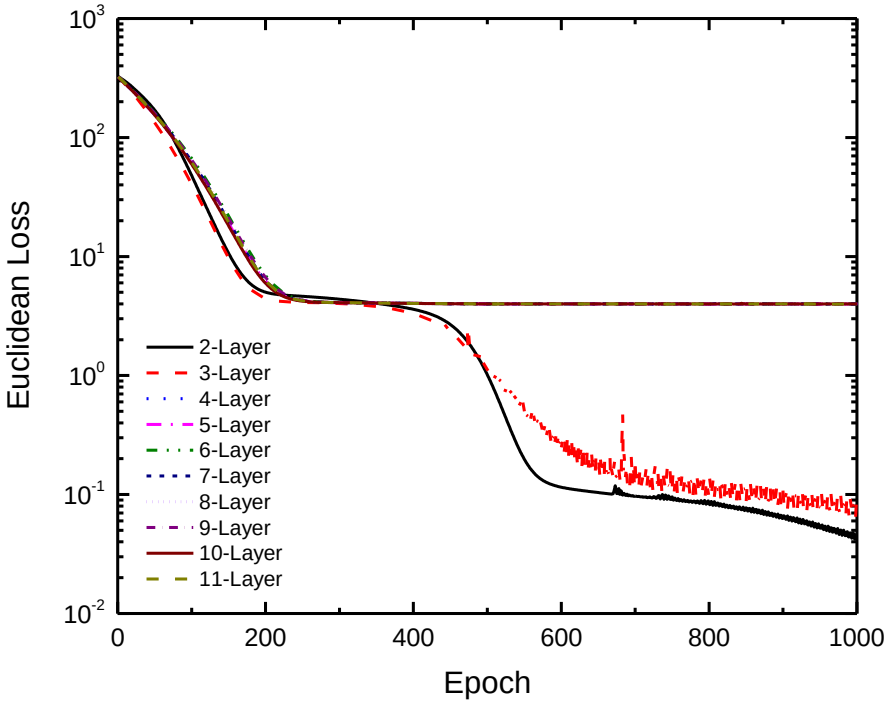


Fig. 2 DNN with 9-training dataset

Issues of using DL in thermal fluid (5/6)

- Understand the difficulty of training DNN while using multiple datasets.
  - The Euclidean loss of DNN with more layers and training datasets tend to saturate at a higher value than DNN with less layers and training data.
  - Fig. 1 depicts the comparison of Euclidean losses by using different datasets and different DNN structures. The black and red dash lines show the results by fully connected feedforward NN with 6 layers.
  - In order to obtain accurate results for DNN with training dataset more than 1, we implement batch normalization (BN) [Ioffe, 2015] into DNN model. The blue line shows that BN can help DNN to achieve lower Euclidean loss.

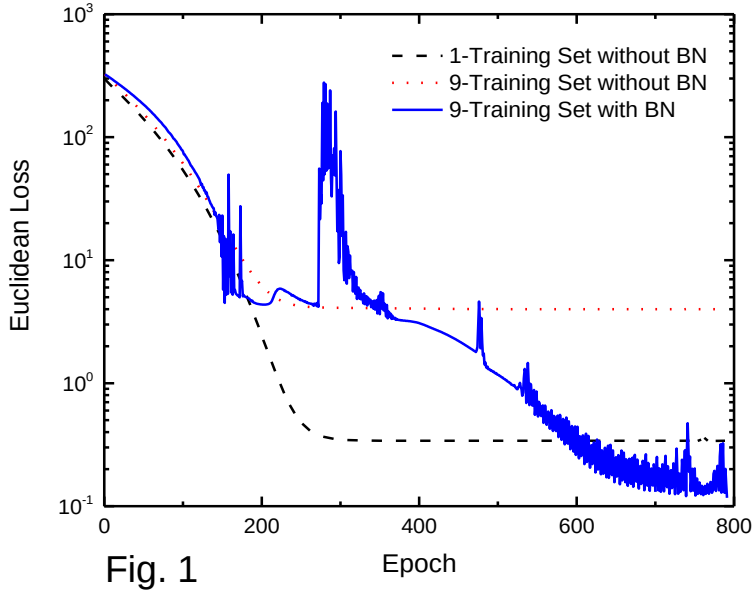
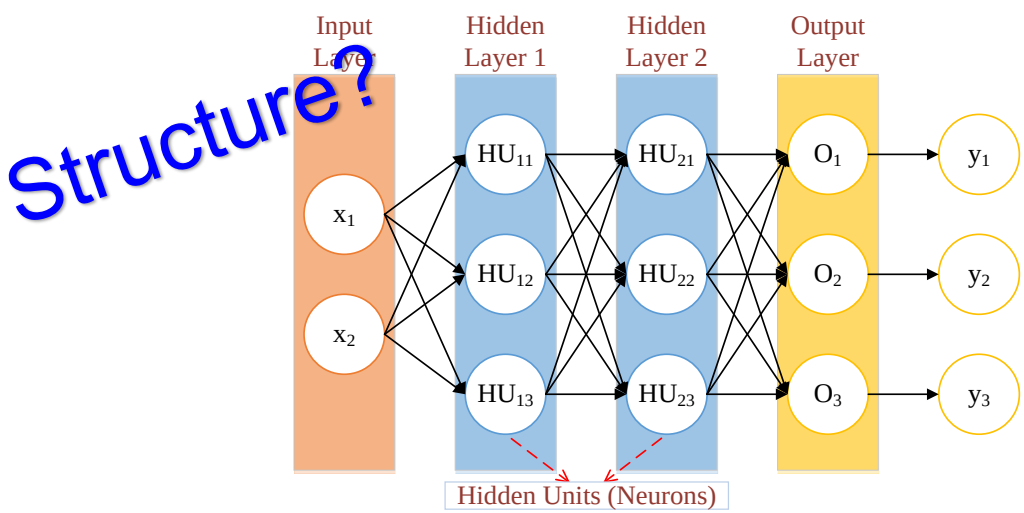


Fig. 1

Issues of using DL in thermal fluid (6/6)

- Understand how to define the criteria to search the optimal DL-based fluid closures for field equations.
  - Inferring a model from data belongs to ill-posed problem that the solution may not exist.
  - Hadamard's principles on well-posedness
    - A solution should exist.
    - The solution should be unique.
    - The solution should continuously depend on the data.
  - Requirements of well-posedness
  - Requirements of minimum training datasets



Requirements of well-posedness

- The output behavior of DL-based model should change continuously with the insight for the given problems.
  - "Insight" is the current best knowledge toward the problems

- We define model complexity (MC) and model-insight consistence (MIC) factors as:

$$\text{Model Complexity } (MC) = \frac{\left|\frac{\partial M}{\partial Par}\right| - \left|\frac{\partial I}{\partial Par}\right|}{\left|\frac{\partial I}{\partial Par}\right|}$$

$$\text{Model Insight Consistence } (MIC) = 1 - MC$$

Ex. Friction Factor

$$I \propto \mathrm{Re}^{-1}$$

$$M = sigmoid\left(\sum_{i=1}^{5} HU_{k-1,i} w_{kji} + b_{kj}\right)$$

- Model insight consistence factor dose not represent the model accuracy; instead, it is an indicator to check if the DL-based model achieves the given requirement.

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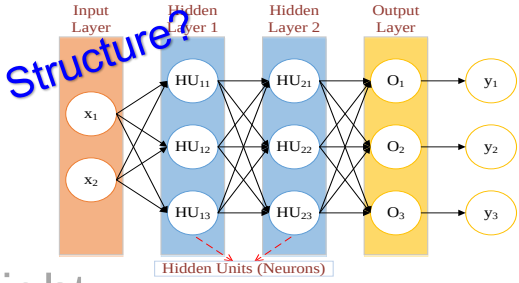
  - Requirements of formulating well-posed DL-based closures for fluid simulations
- Type-II machine learning (work in progress)

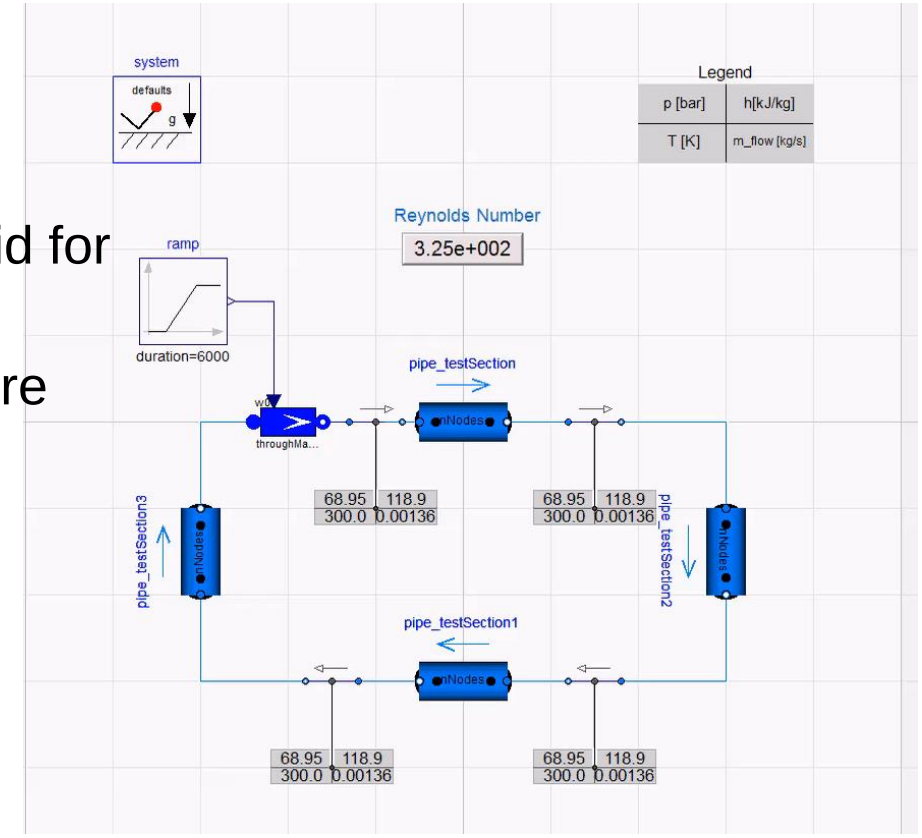
The purpose of the testing task



- Questions
  - What is the uncertainty in DL due to different weight initialization?
  - How to select Tikhonov regularization parameters to increase the predictability?
  - What is the uncertainty due to different DNN structures?
    - What the DNN structure can produce optimal results?
  - How to increase the training accuracy for DNN while using multiple datasets?
  - What are the criteria to search the optimal DL-based fluid closures for field equations?
    - Can model-insight consistence (MIC) factor be the screening criterion to recognize whether DL-based closures are well-posed?

Problem formulation

- Applying manufactured data
  - Assuming the global model is valid for local application
- Developing a DL-based friction closure



$$\frac{\partial(\rho A)}{\partial t}+\frac{\partial(\rho A v)}{\partial x}=0$$

$$\frac{\partial(\rho v A)}{\partial t}+\frac{\partial(\rho v^2 A)}{\partial x}=-A\frac{\partial p}{\partial x}-F_F-A\rho g\frac{\partial z}{\partial x}$$

$$F_F=\frac{1}{2}\rho v|v|fS$$

$$f=aRe^b$$

$$f=DL(Re)$$

S: circumference
f: Fanning friction factor
DL: deep learning

Parameters	Values
Pipe length (m)	2
Pipe diameter (m)	6.25×10^{-3}
Flow rate (kg/s)	4.06×10^{-4} – 8.6×10^{-3}
Re (experiment)	100 – 2000
Re (training)	300 – 1800

Data processing and results (1/2)

- Regularize DL-based closures by insights
- Prevent model outputs from a sudden gradient change

$$\text{Model Complexity } (MC) = \frac{\left|\frac{\partial M}{\partial Par}\right| - \left|\frac{\partial I}{\partial Par}\right|}{\left|\frac{\partial I}{\partial Par}\right|}$$

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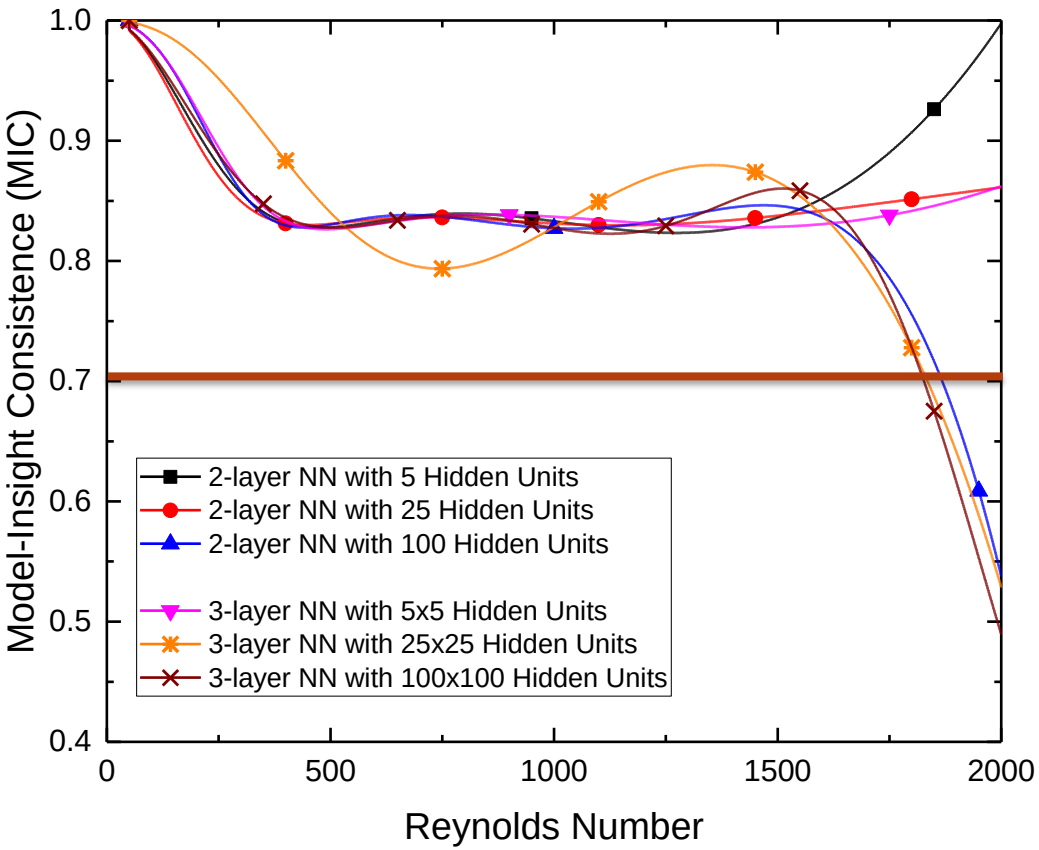
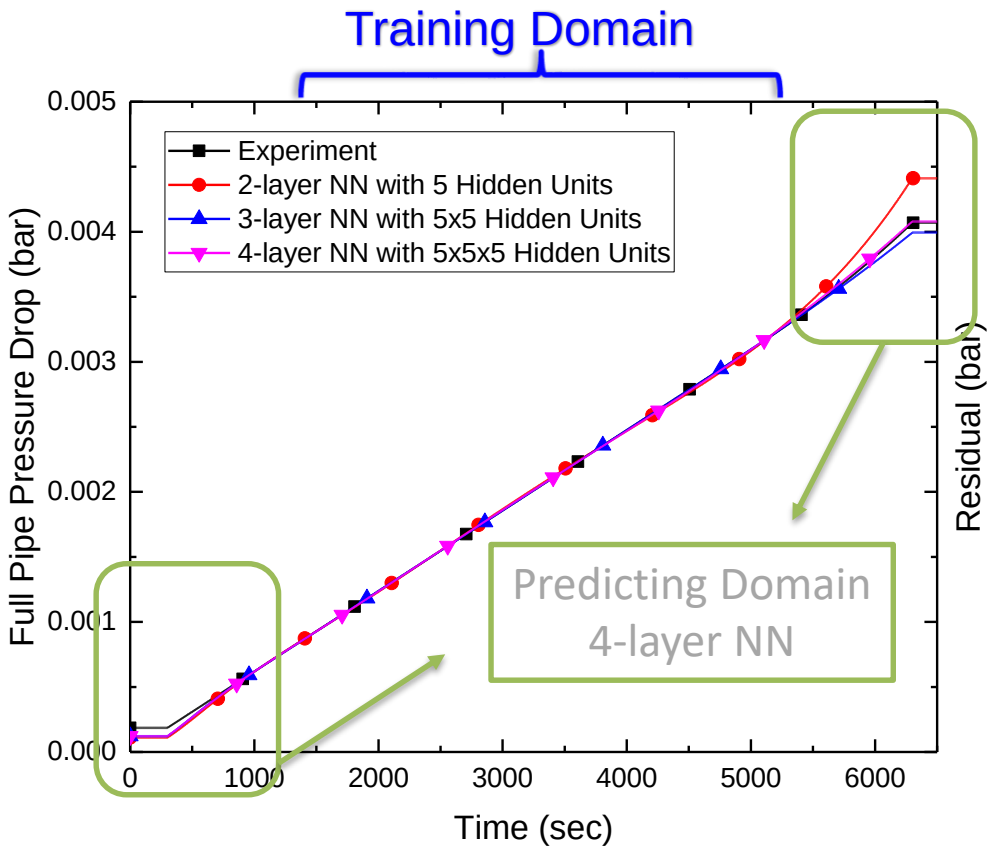
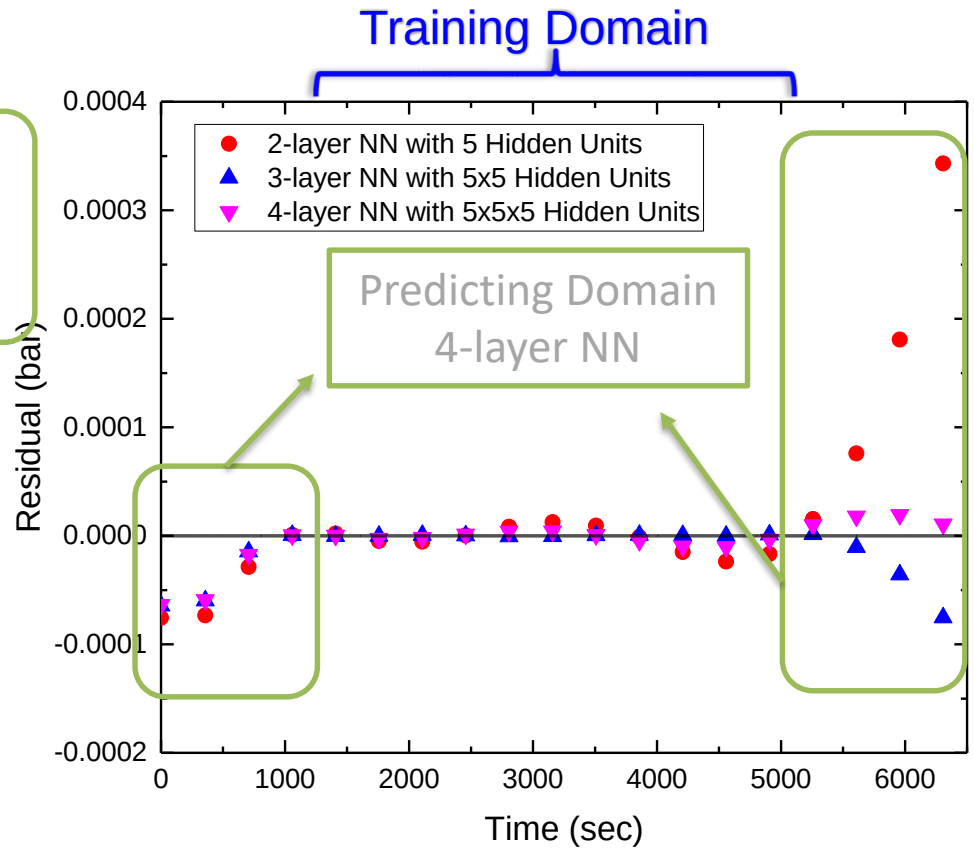


Data processing and results (2/2)



Full pipe pressure drop in both training and predicting domains by DL-based friction closures



Residual of full pipe pressure drop in both training and predicting domains by DL-based friction closures

Main findings

- Model-insight consistence (MIC) factor can be a screening criterion that guides the search for the optimal DL model.
- Optimal DL models are defined as:
  - They have the maximal predictive capability.
  - By Occam's razor principle, they are deep neural networks with the simplest structure that captures the insights and the data within the uncertainty range.
- This case study is limited to model fully developed laminar flow using the simple closure model with a single scaling parameter, Re.
  - A broader case study is a must to characterize usefulness of the MIC factor in more complex processes
  - "Insight" is subject to multiple scaling parameters and various sources of uncertainty such as pressure loss due to spacer grids.

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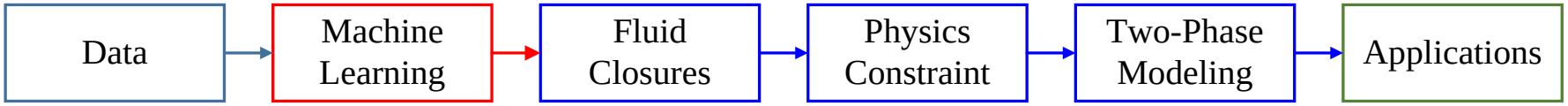
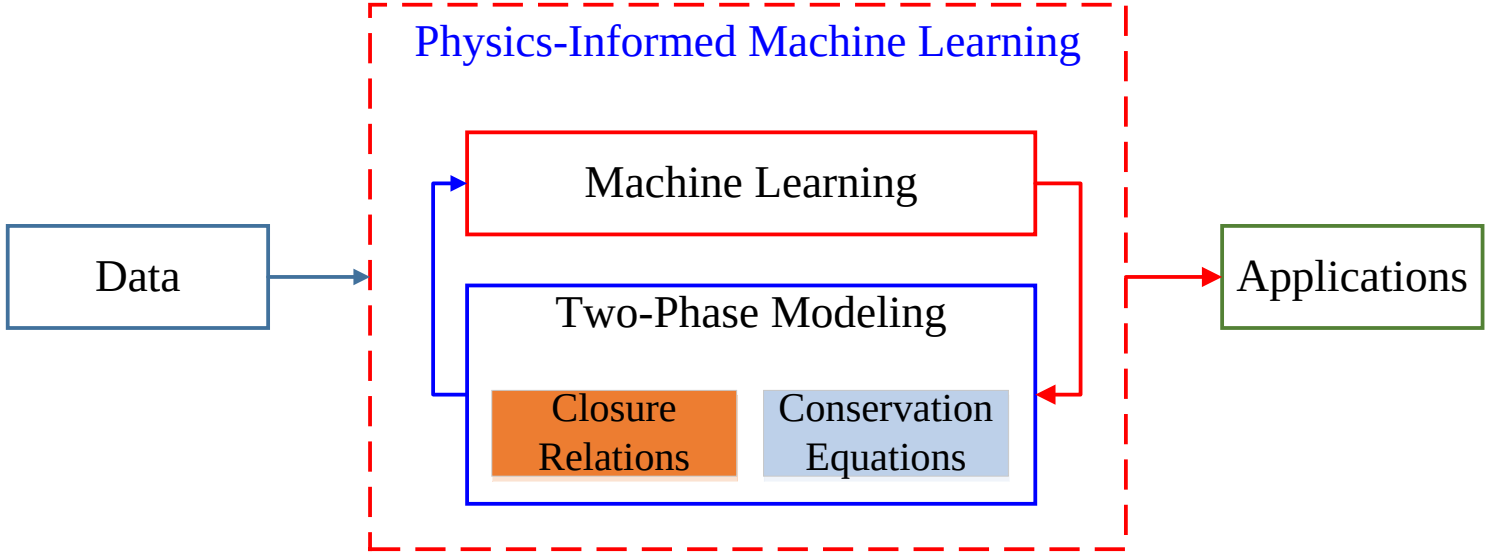
- Classification of machine learning (ML)

Type-I ML, Physics-Constrained ML



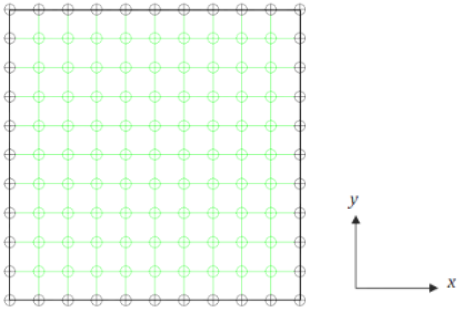
Type-II ML, Physics-Informed ML



Technical approach (1/2)

- 2D steady-state heat conduction equation with *k*(T)

$$\frac{\partial}{\partial x}\left(k\frac{\partial T}{\partial x}\right)+\frac{\partial}{\partial y}\left(k\frac{\partial T}{\partial y}\right)=0$$



https://www.codeproject.com/articles/1087025/using-python-to-solve-computational-physics-proble

- Geometry
  - square geometry with length equal to 1 cm
- Model assumptions
  - Temperature dependent thermal conductivity [W/(cm-K)]

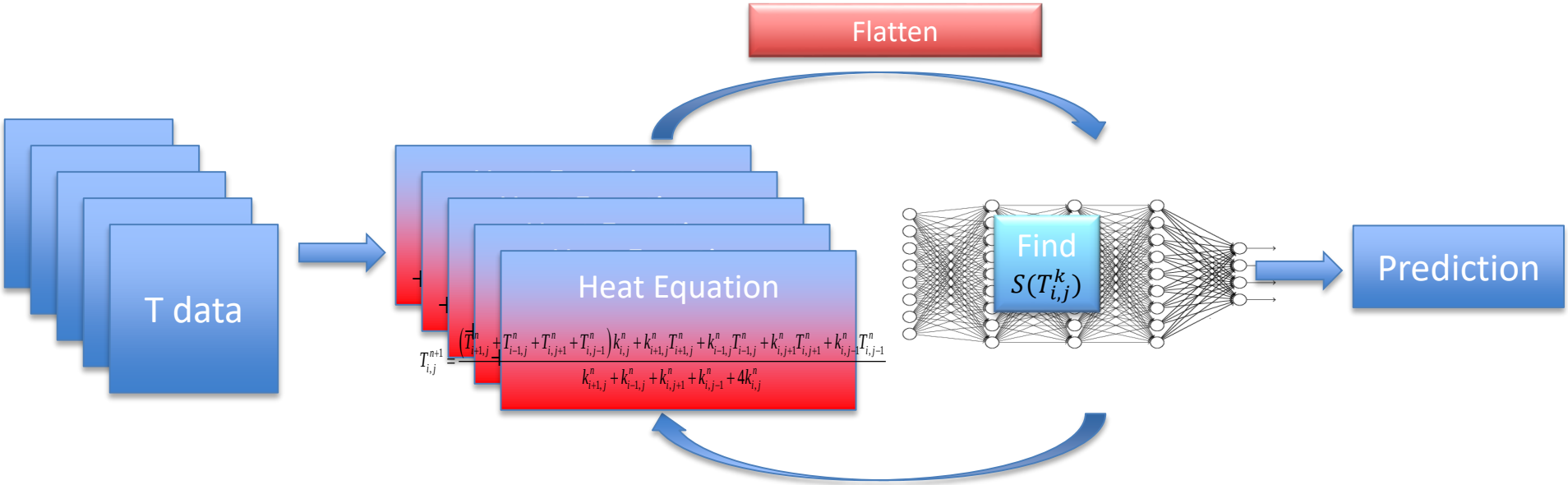
$$k=\frac{1}{11.75+0.0235T}$$

  - Dirichlet boundary conditions
- Numerical discretization (Patankar, 1980)
  - 21 grids on each side ($\Delta x=\Delta y=\Delta h=0.05cm$)
  - piecewise-linear temperature and *k* profile between the grids
  - centered formula of order $O(h^2)$

$$T_{i,j}^{n+1}=\frac{\left(T_{i+1,j}^{n}+T_{i-1,j}^{n}+T_{i,j+1}^{n}+T_{i,j-1}^{n}\right)k_{i,j}^{n}+k_{i+1,j}^{n}T_{i+1,j}^{n}+k_{i-1,j}^{n}T_{i-1,j}^{n}+k_{i,j+1}^{n}T_{i,j+1}^{n}+k_{i,j-1}^{n}T_{i,j-1}^{n}}{k_{i+1,j}^{n}+k_{i-1,j}^{n}+k_{i,j+1}^{n}+k_{i,j-1}^{n}+4k_{i,j}^{n}}$$

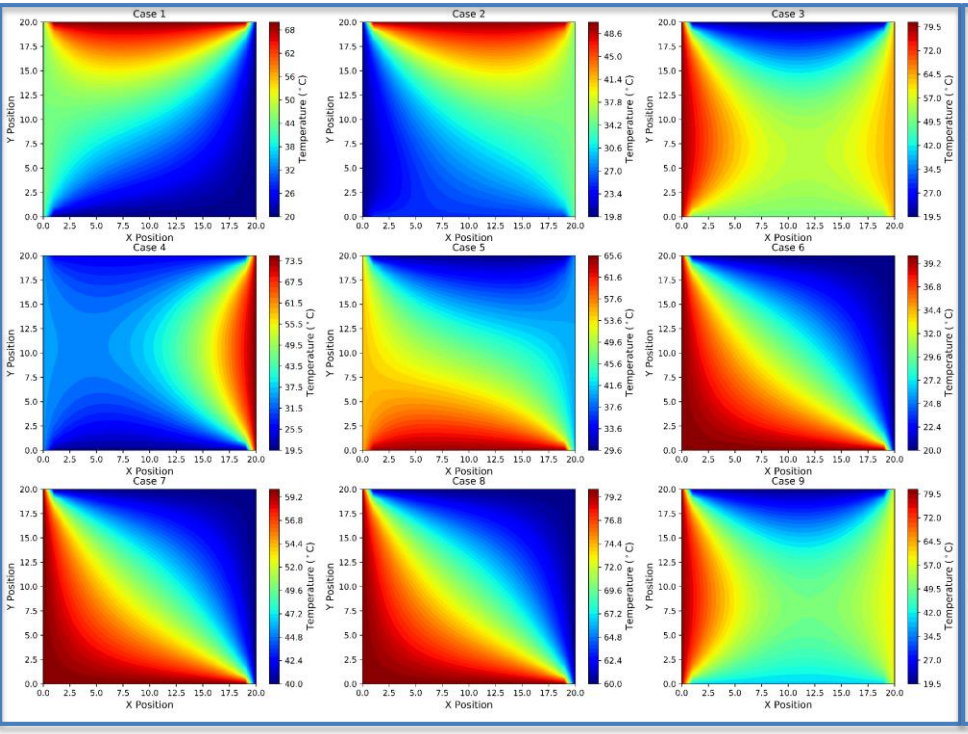
Technical approach (2/2)

- Deep learning library - Tensorflow (v 1.0.0)
  - Train DNN to construct *k* from data
  - Accelerate PDE solutions by GPU
    - 2D steady-state heat diffusion

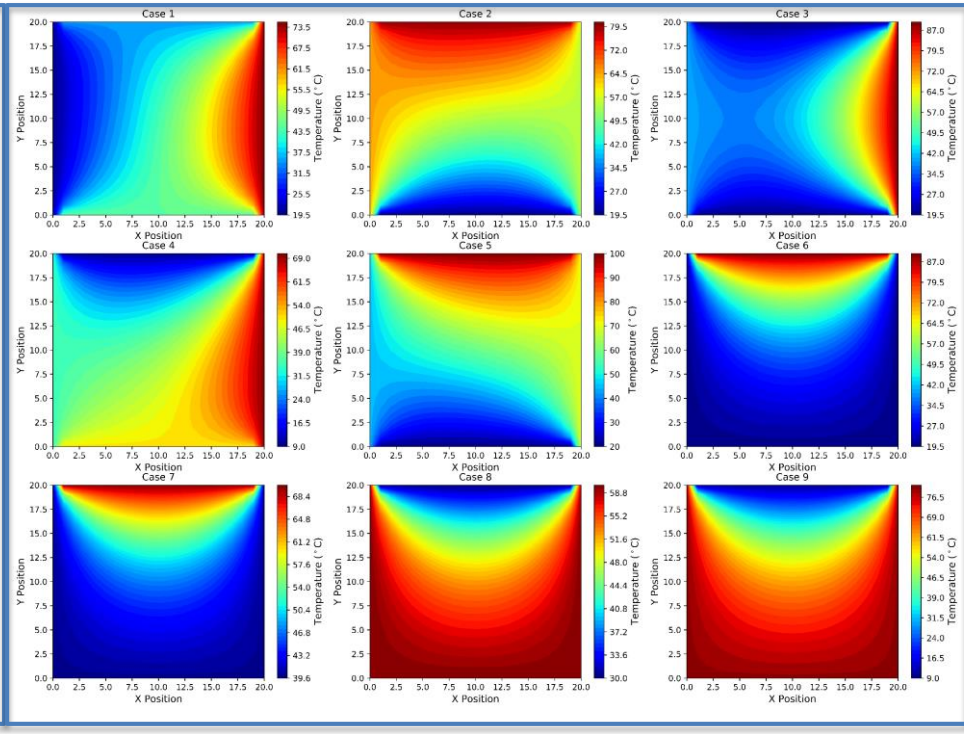


Method of manufactured data (MMD)

- Compare training and predicting datasets.
  - different temperature profiles



Training datasets



Predicting datasets

Results of type-I and type-II ML with k(T)

- Compare predicting results between type-I and type-II training

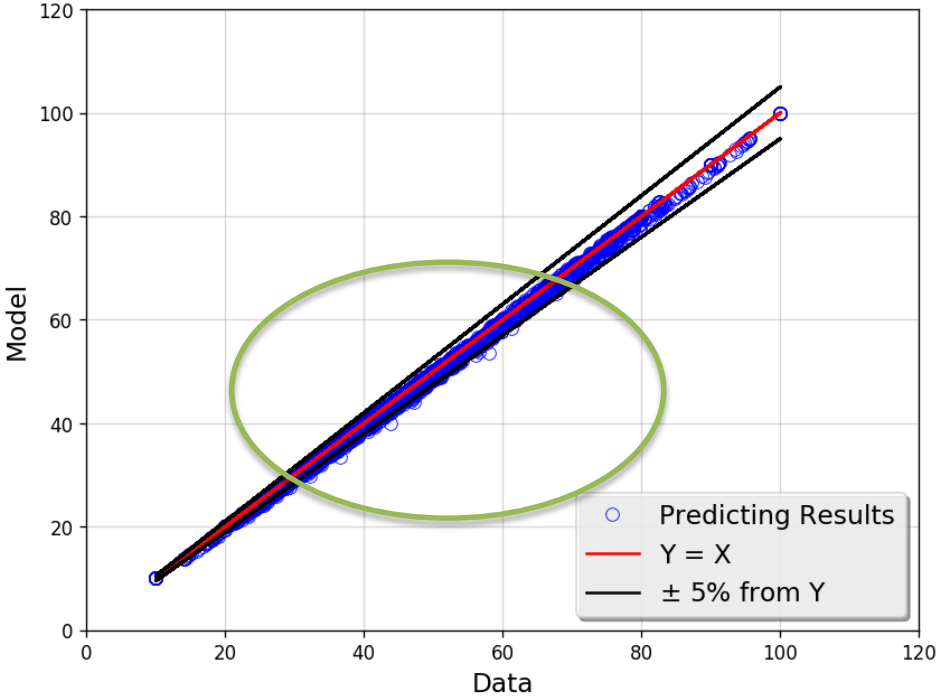


Fig. 1 Predicting the temperature profiles by type-I training

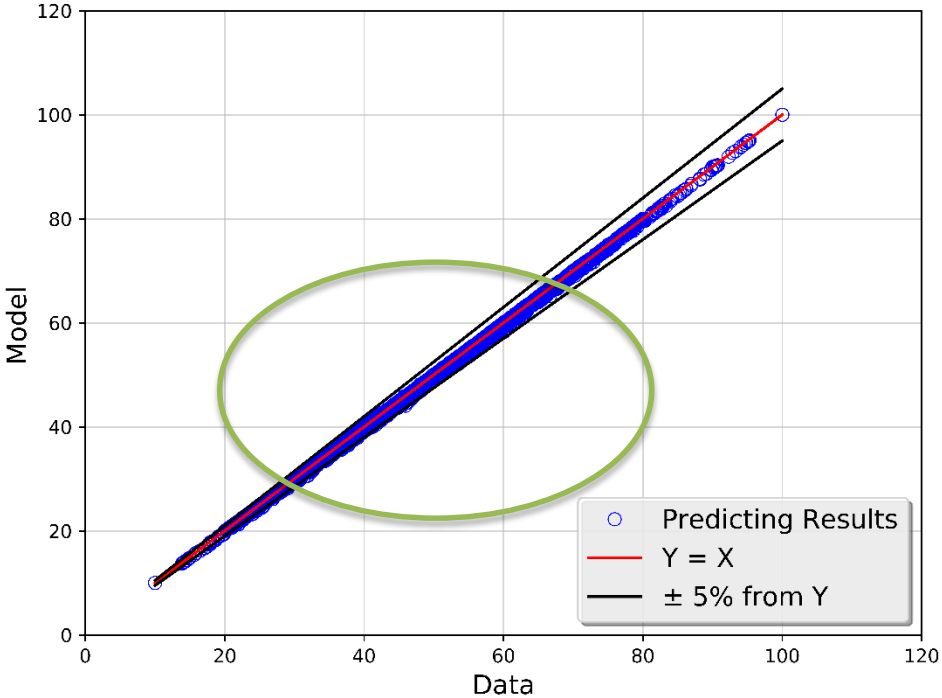


Fig. 2 Predicting the temperature profiles by type-II training

Main findings (work in progress)

- Tensorflow can accelerate the solution of PDE by GPU that make the type-II training becomes possible.

- Type-II training makes the temperature dependent conductivity model tightly couple with PDE. The results is more consistent with the data than type-I training.

- This nonlinear task confirms that the stochastic gradient descent (SGD) algorithm can search the optimal solution for type-II ML problems.

Thank you very much!

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