Research Experience

Wei W. Xing（邢炜）

2012
Undergraduate
Automation

Shenzhen University

2012
Ph.D. candidate
Applied Math & Scientific Computing

Center for predictive modeling
University of Warwick
(**QS world university 54th**)

Supervisor: Akeel Shah

2016
Postdoc researcher
Applied Math

School of Engineering
University of Warwick

2017
Postdoc researcher
Scientific Computing & Machine Learning

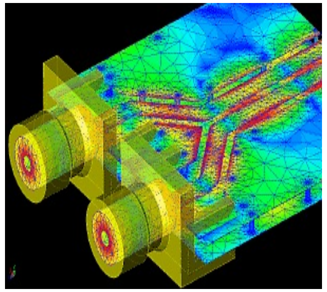
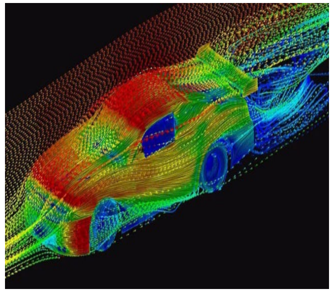
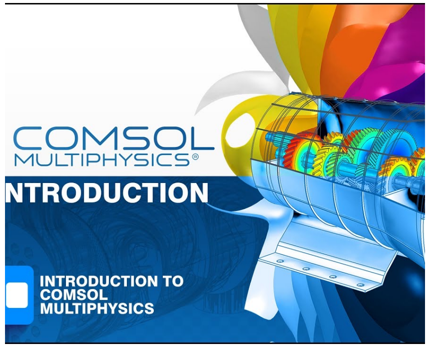
Center for scientific image and scientific computing
University of Utah
(**Top ranked** (CS-RANK) US university in
high-performance computing and visualizat

Supervisor: Mike Kirby / Ross Whitaker(IEEE Fellow)

2020
Assistant Professor
EDA & Machine Learning

School of integrate circuit
Beihang University

Research Interests

Scientific Computing + Machine Learning

A. ML enhanced SC

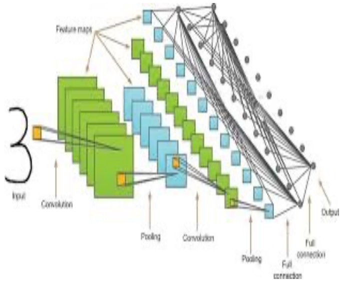
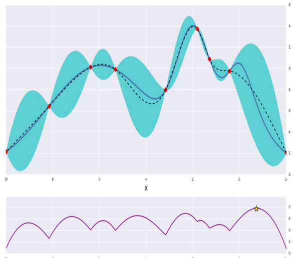
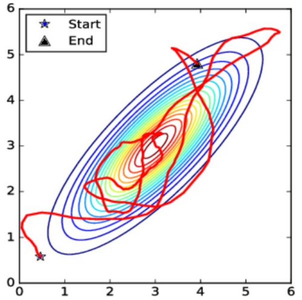
1. Data-driven Spatial-Temporal Field Modeling
2. Multi-fidelity Fusion
3. Machine Learning for Design and Optimization

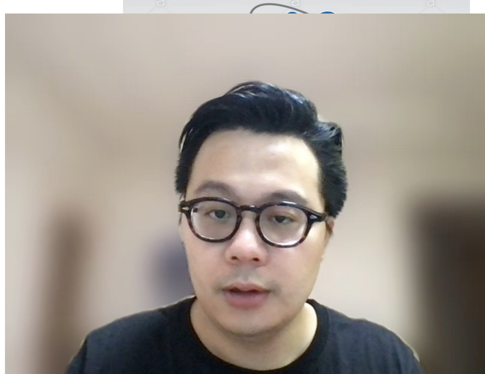
B. SC enhanced ML

1. Physics Informed ML
2. ML Injected Simulation

C. SC+ML for Industry and Application

1. Digital Twins
2. EDA
3. Inverse Problem In Scientific Research



A. ML enhanced SC

Problem definition

Build SC model

#Loop > 1000

Simulations

Analysis

Optimization

Uncertainty quantification

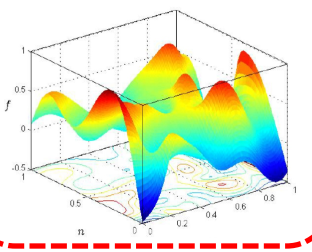
Inverse problem

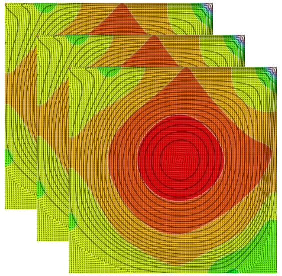
Failure probability

A. The Challenges

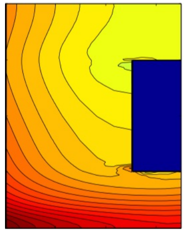
Surrogate model for spatial-temporal problems

Simulations ≈



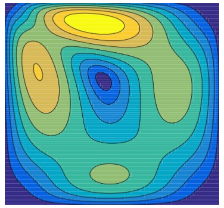


Sequential velocity fields



Steady-state temperature field

Mechanical structure



Chemical Reaction

Challenge:

- Ultra-high dimensionality (100x100x100)
- Coupled fields
- Boundary conditions
- Limited date
- Predictive confidence

A.1. Future Research

1. Generalization of Conservational Kernels:

Utilizing the known conservational law in PDEs to improve a GP surrogate

$$k_r^v(x, x') = \sigma_r^2 \exp\left(\frac{-||x - x'||^2}{2l_r^2}\right) \cdot \left(I - \left(\frac{x - x'}{l_r}\right)\left(\frac{x - x'}{l_r}\right)^T\right)$$

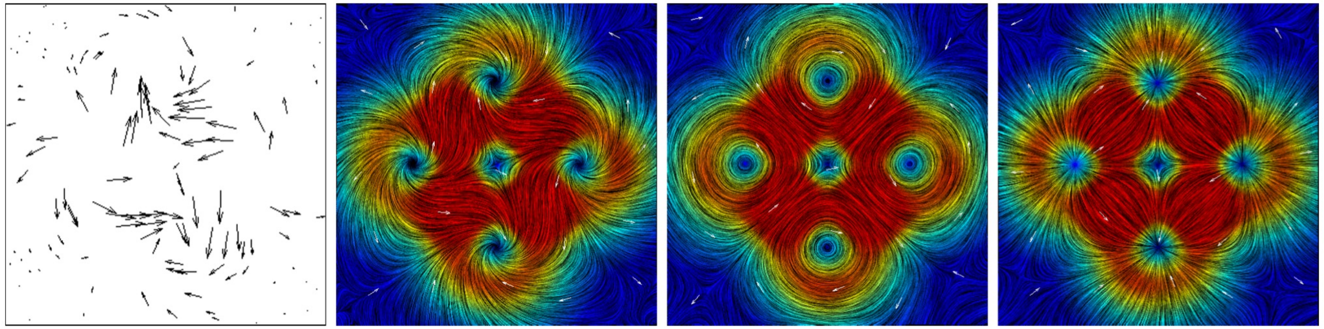


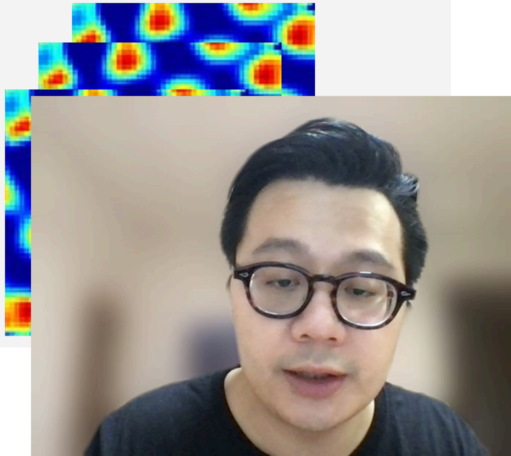
Figure 1. Learning a vector field decomposition: samples, learned field, divergence- and curl-free parts.

Limitation:

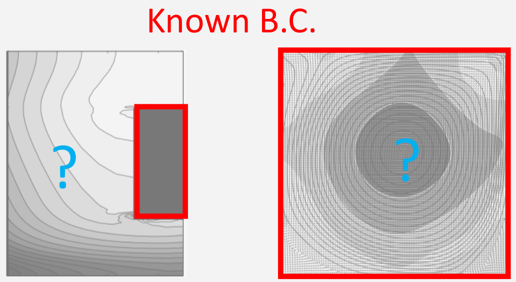
1. Require stationary kernel
2. Scalability
3. Only for one field
4. No knowledge transfer for different system parameters

2. Curse of dimensionality --> blessing of dimensionality:

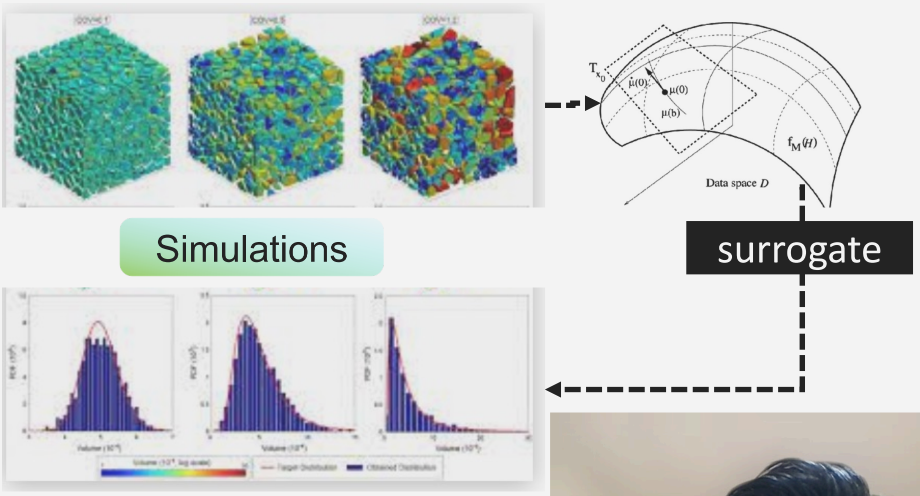
Learning kernels from rich data



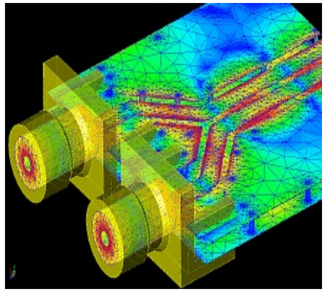
3. Scalable inference with Known B.C.
Scalable inference using tensor product + inducing points

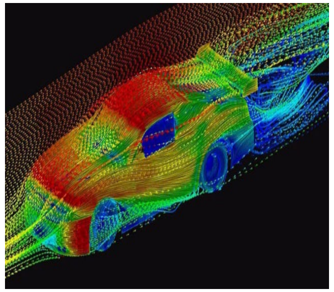


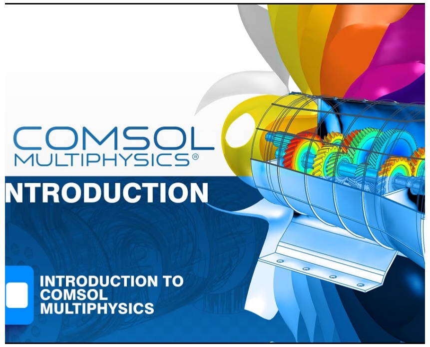
4. Uncertainty quantification for random spatial field inputs
Joint learning with encoder-decoder network and GP



Research Interests







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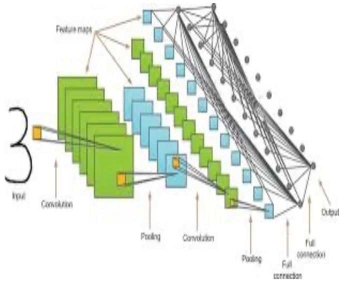

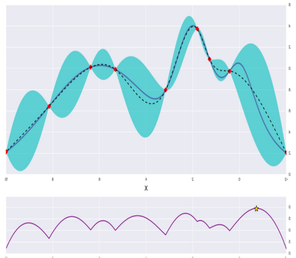

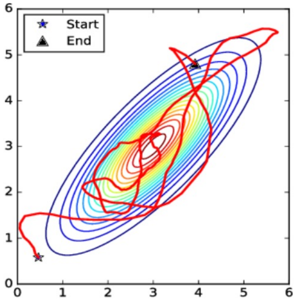

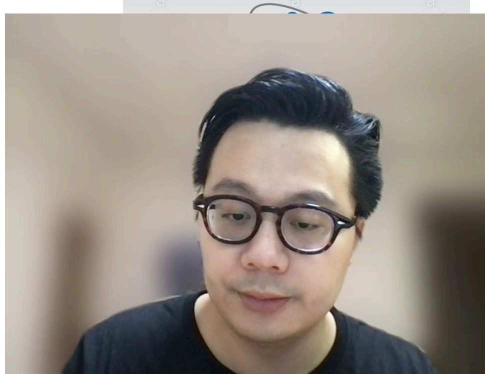

A.2. Multi-Fidelity Motivation

Problem definition

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Loop #1000

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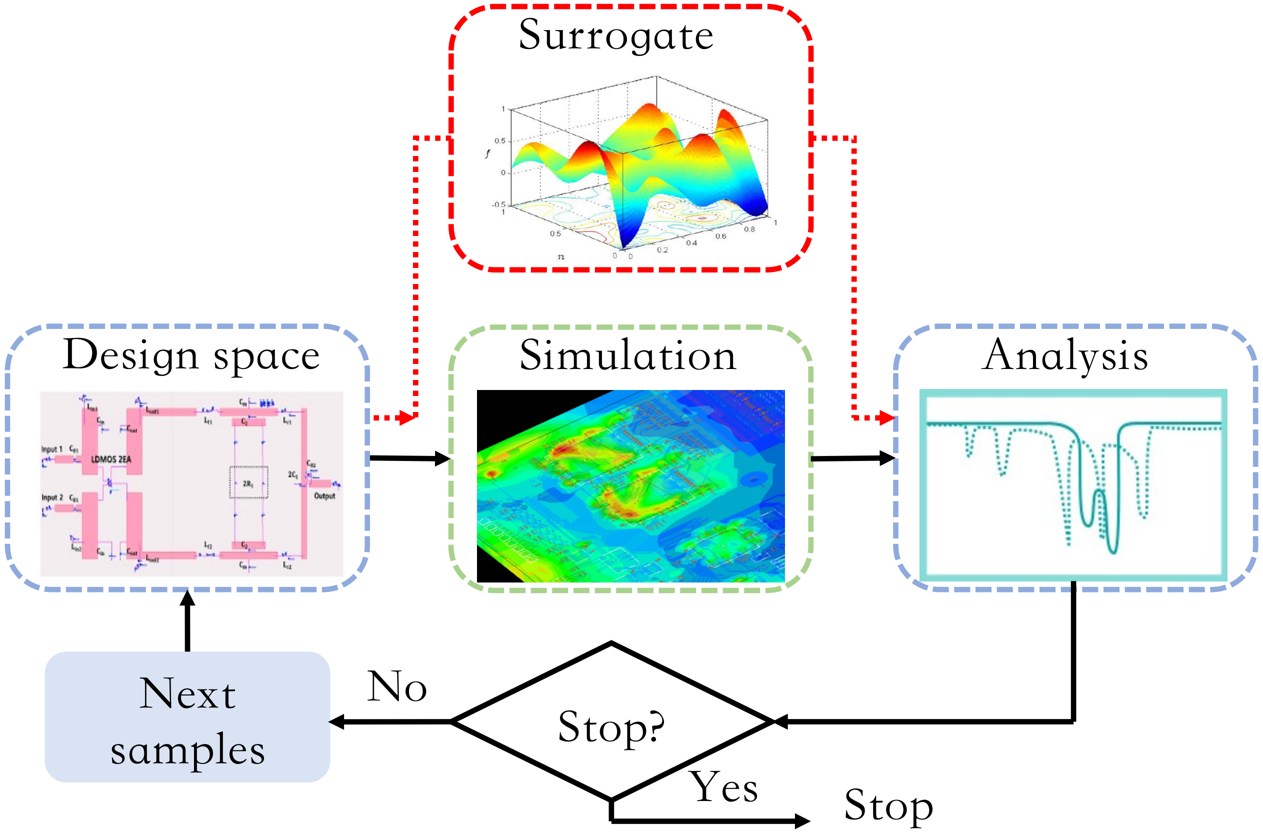
A.2. Multi-Fidelity Motivation

Circuit design optimization as an example:



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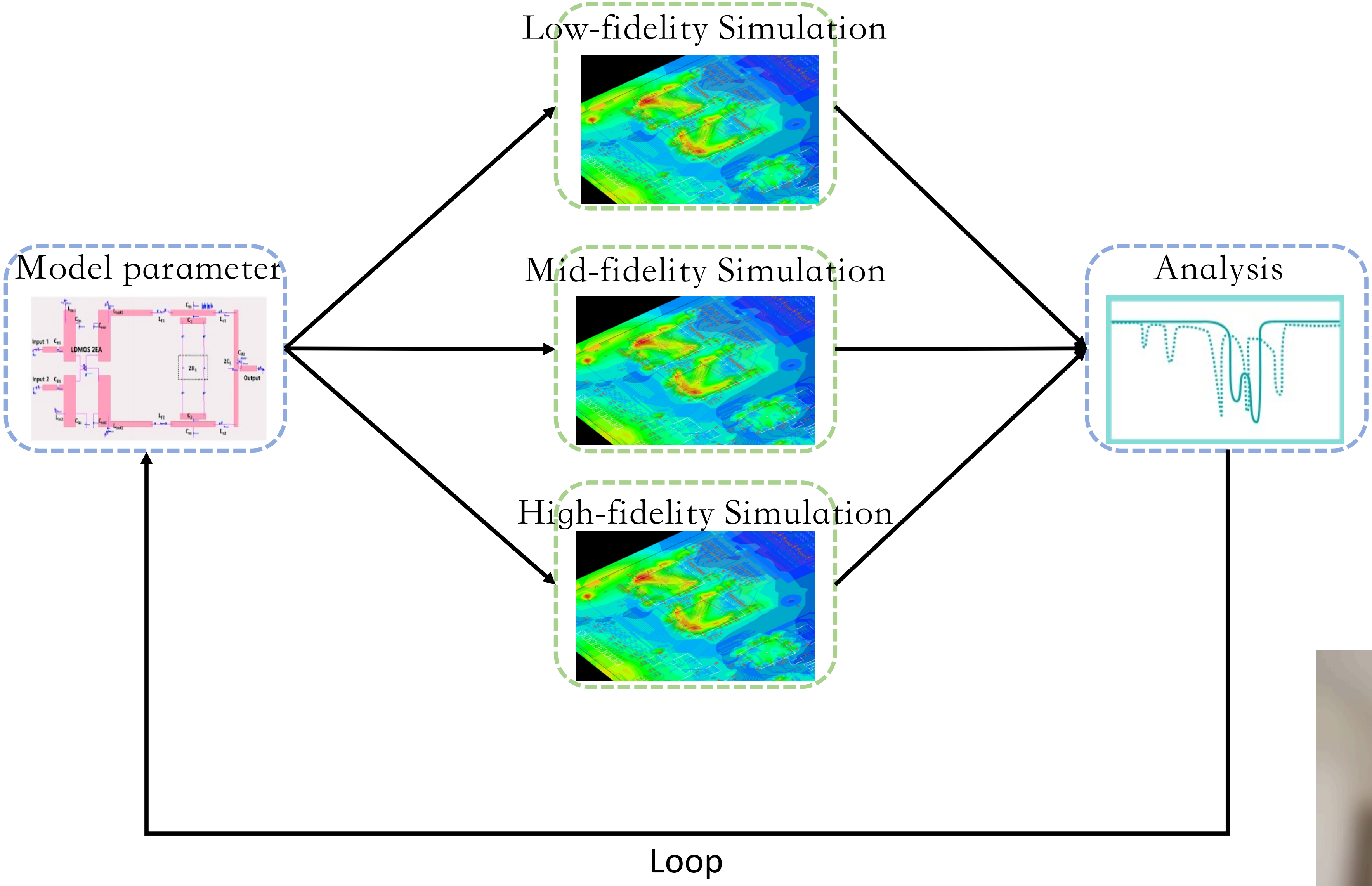

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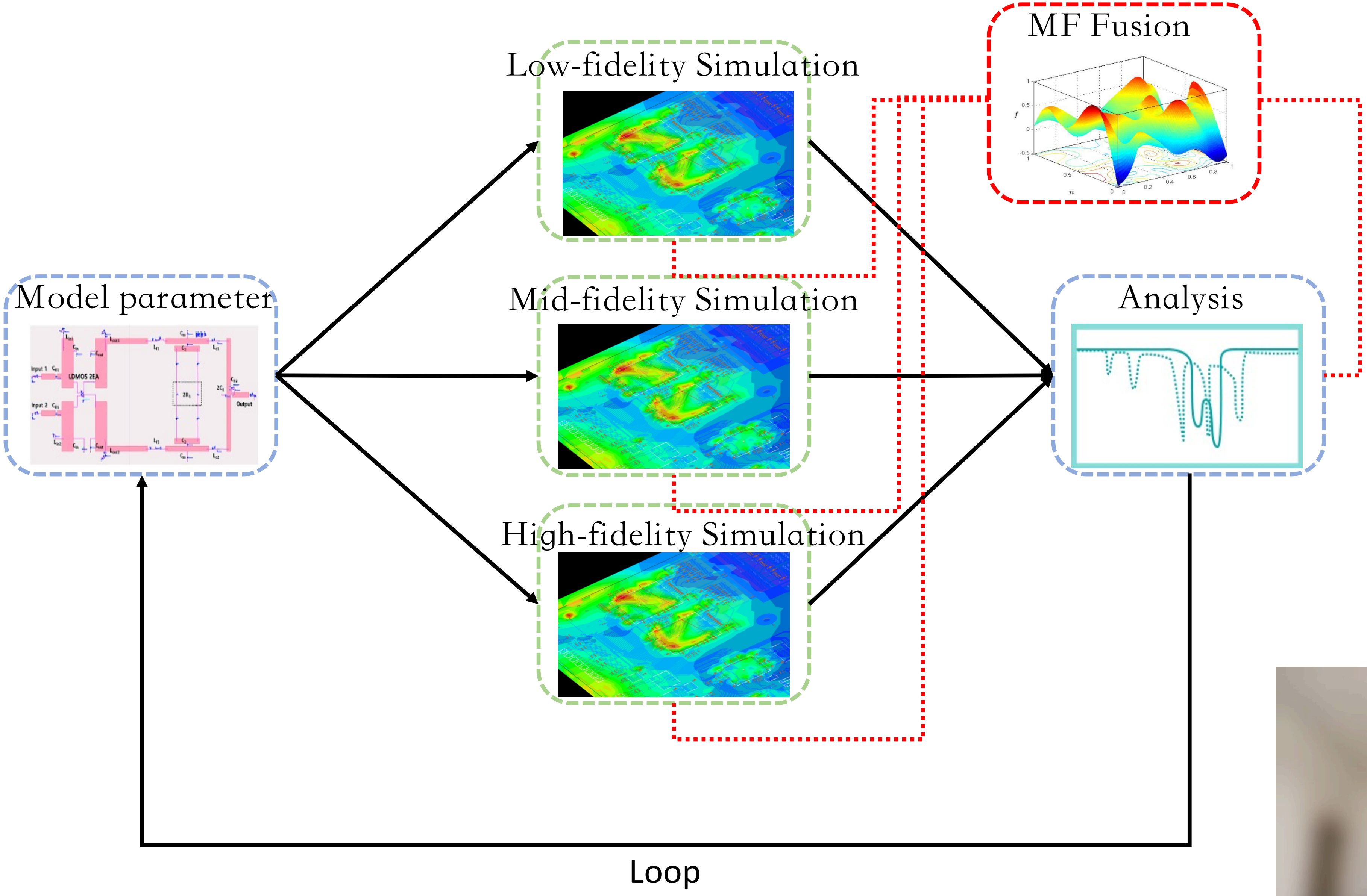
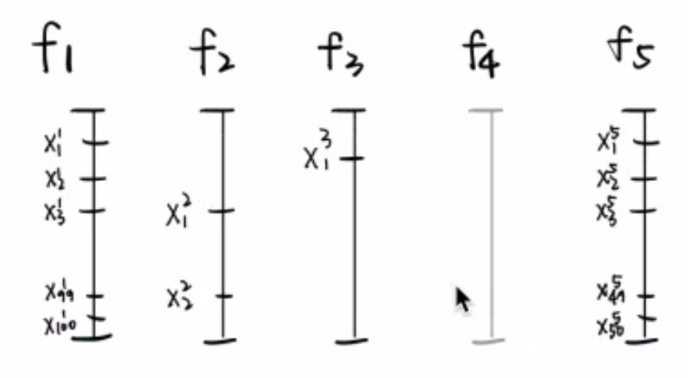


A.2. Multi-Fidelity: Future Work

1. **Multi-Fidelity Fusion with Arbitrary Data**
   1. No more subset requirement.
   2. No more aligned high-dimensional output requirement.
   3. Unlimited number of fidelities

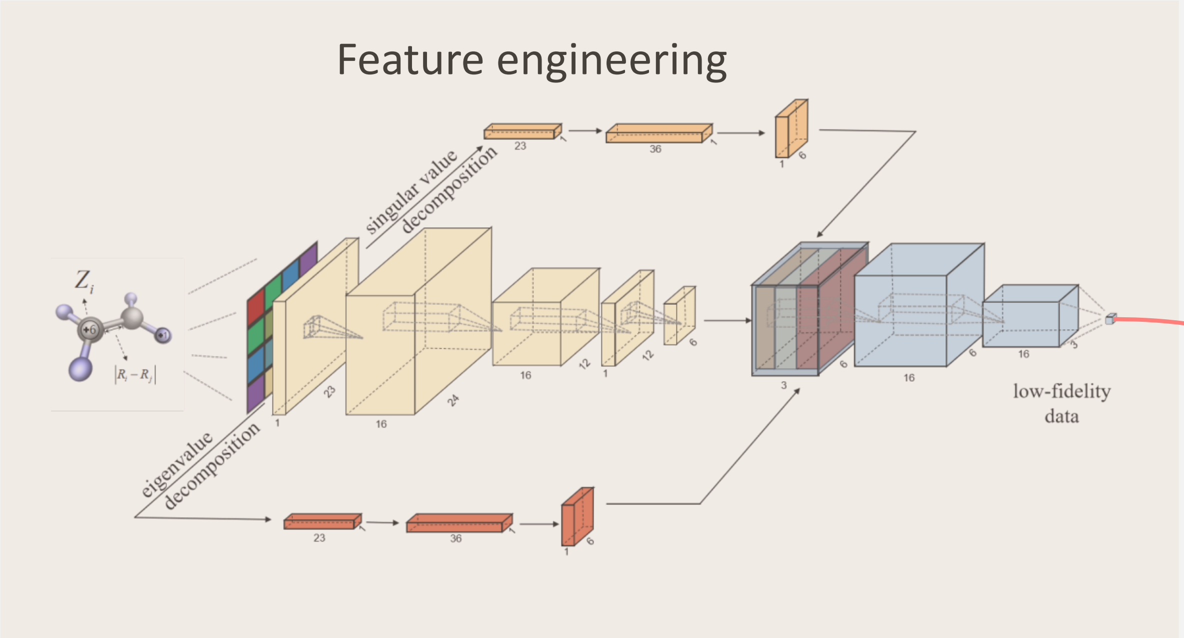


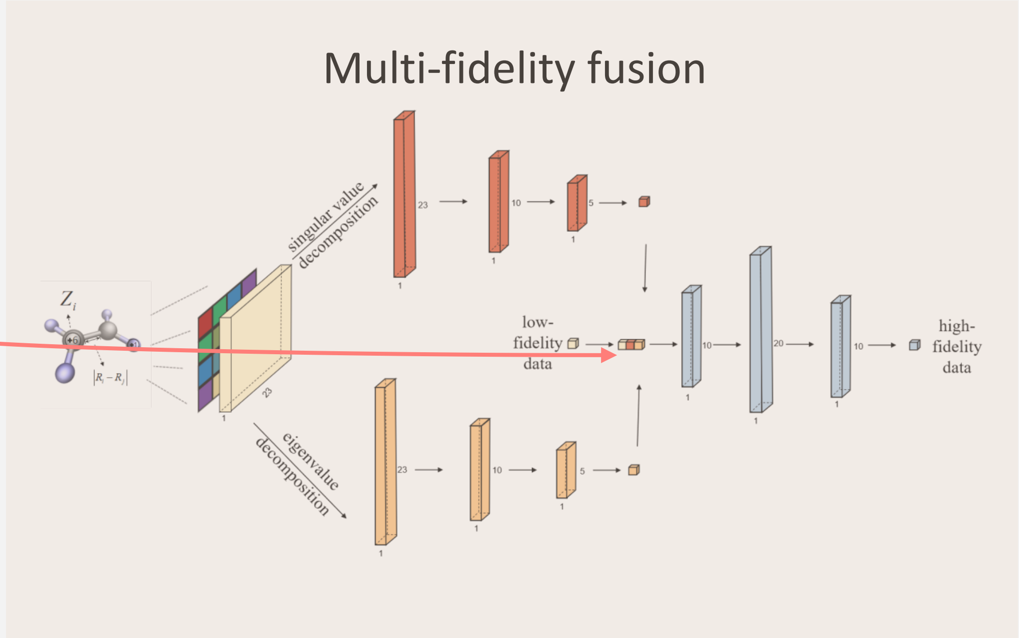
2. **Automatic efficient surrogate**

   Active learning based on entropy reduction + parallelization

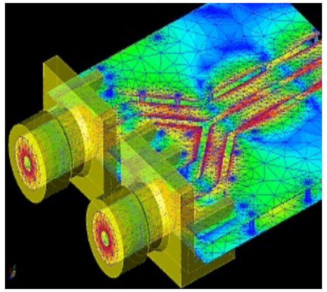
3. **Meta-learning in multi-fidelity**
   1. Learning the kernel function throughout multi-fidelity data
   2. Bayesian neural network (with scalable tensor variational posterior) with weight sharing
   3. Learning the manifold of correlation using CNF or NeuralODE

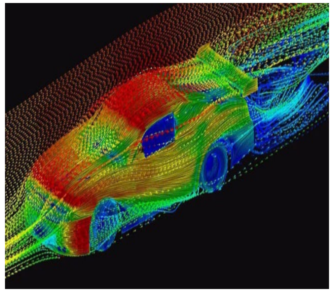
6. Multi-Fidelity fusion for electronic structure calculation

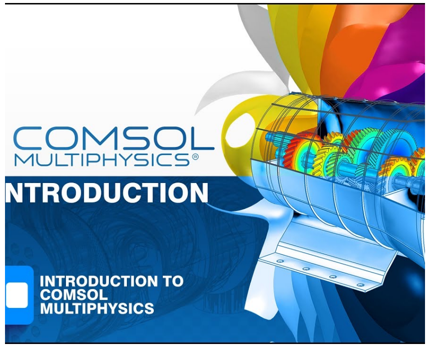




Research Interests







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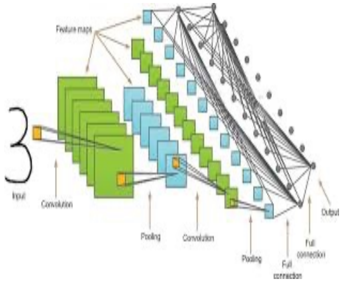
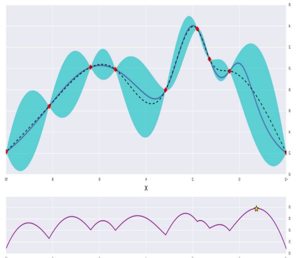
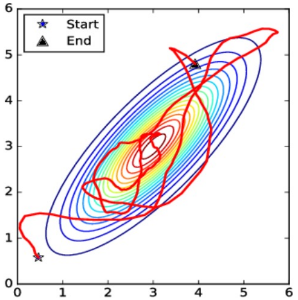
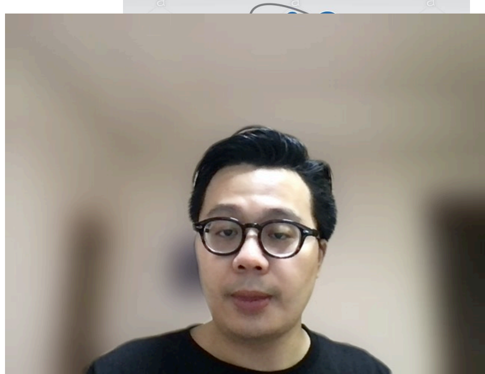
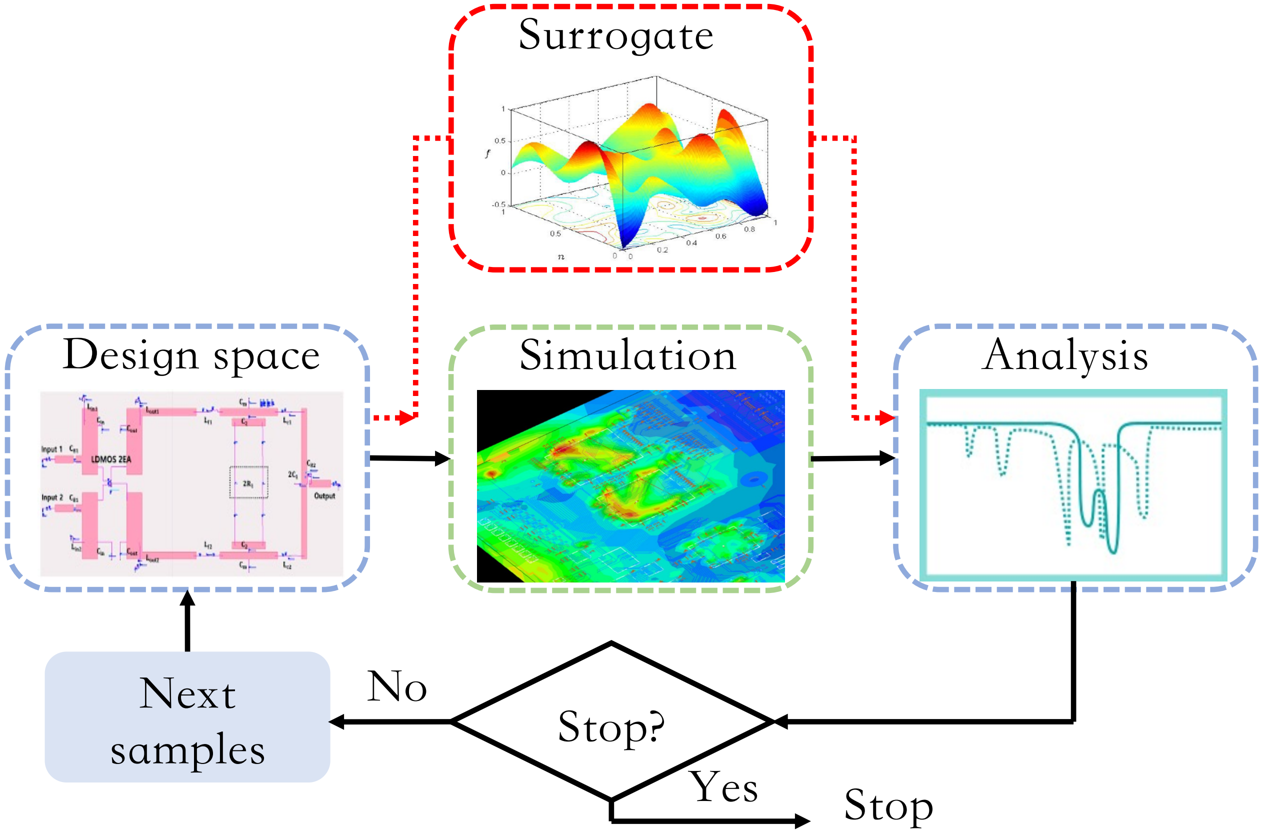








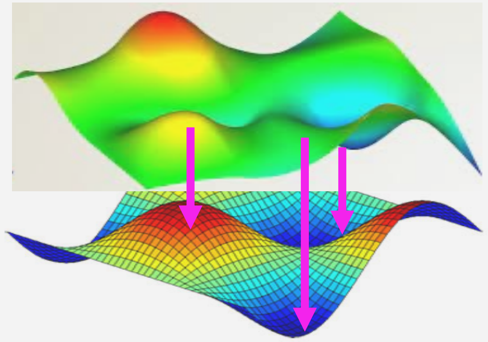
A.3. Bayesian Optimization: Motivation



A.3. Future Research

1. Multi-Fidelity Bayesian optimization

- Infinite fidelity
- Cost-aware
- Parallel



2. BO with uncertainty, e.g., yield optimization

- Bayesian quadrature
- Feature selection
- Transfer learning
- Better acquisition function and parallelization

Yield analysis: $g(x) \equiv \int_{v} I(f_k(x, v))p(v)dv$

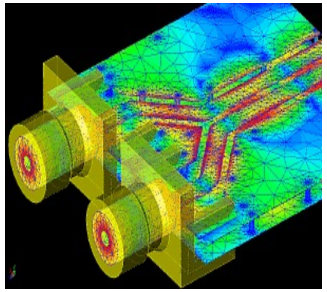
Yield Optimization: $x^* = argmax_{\{x \in X\}} g(x)$

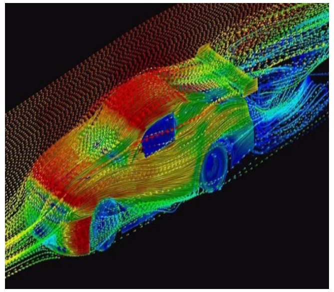
Where SPICE simulation $z_k = f_k(x, v)$

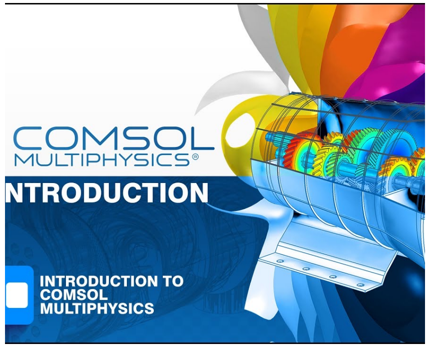
Indication function $I(x, v) = \begin{cases} 1 & z_k \leq z_0 \\ 0 & z_k > z_0 \end{cases}$

3. Mix-variable (Ordinal + categorical + continuous variables) Bayesian optimization

Research Interests







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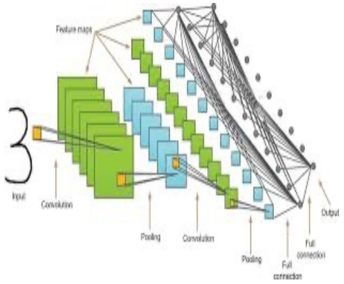
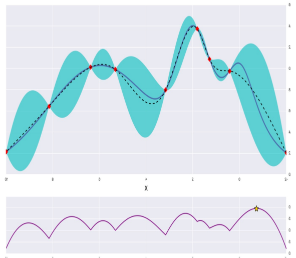
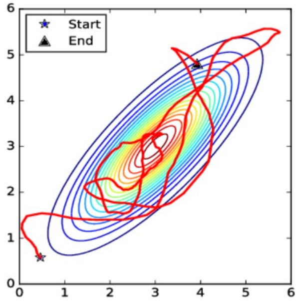
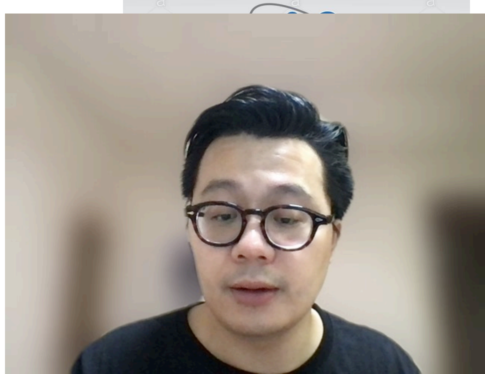








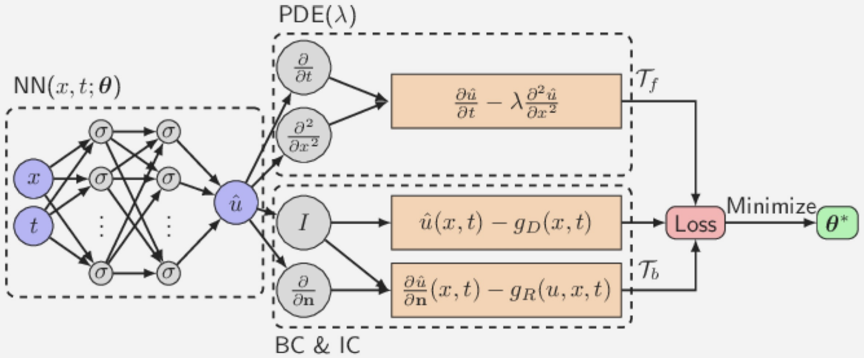
PINN: Physics-informed neural networks

Classic NN:

$$\mathcal{L}(\theta) := \underbrace{\mathcal{L}_u(\theta)}_{\text{Data fit}}$$

PINN:

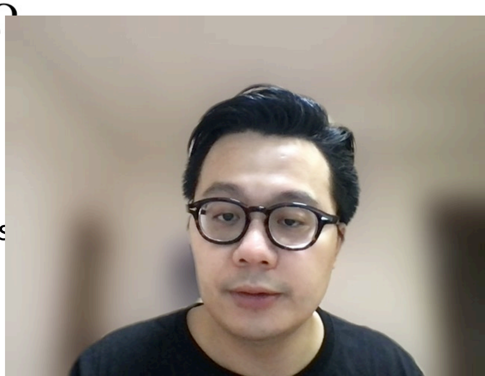
$$\mathcal{L}(\theta) := \underbrace{\mathcal{L}_u(\theta)}_{\text{Data fit}} + \underbrace{\mathcal{L}_r(\theta)}_{\text{PDE residual}} + \underbrace{\mathcal{L}_{u_0}(\theta)}_{\text{ICs fit}} + \underbrace{\mathcal{L}_{u_b}(\theta)}_{\text{BCs fit}}$$



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

$$\boldsymbol{u}(\boldsymbol{x}, 0) = h(\boldsymbol{x}), \quad x \in \Omega$$

$$\boldsymbol{u}(\boldsymbol{x}, t) = g(\boldsymbol{x}, t), \quad t \in$$

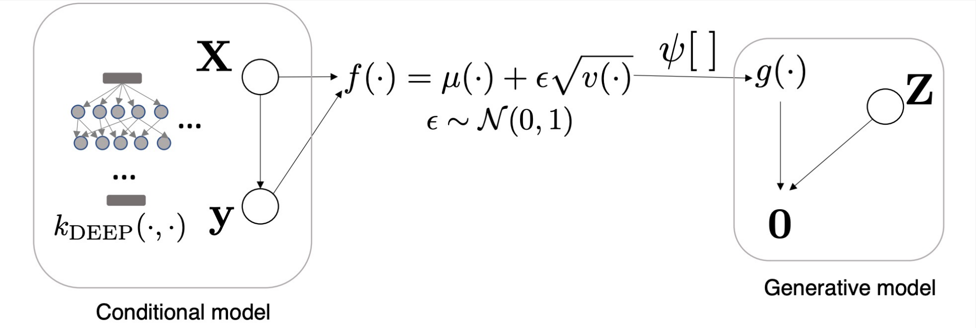


[1] Raissi, M., Perdikaris, P., & Karniadakis, G. E. (2019). Physics-informed neural networks: A deep learning framework for solving forward and inverse problems differential equations. Journal of Computational Physics, 378, 686-707.
[2] Lagaris, I. E., Likas, A., & Fotiadis, D. I. (1998). Artificial neural networks for solving ordinary and partial differential equations.
[3] Psichogios, D. C., & Ungar, L. H. (1992). A hybrid neural network-first principles approach to process modeling.

1. Physics informed Bayesian model

Finished work:

Physics-informed deep kernel learning (AISTAT2021)



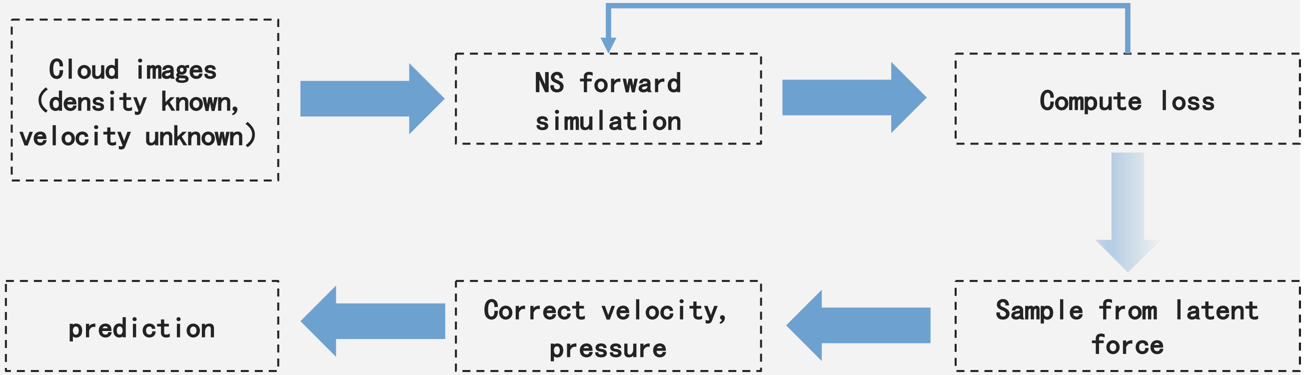
$$
\begin{aligned}
&p(\mathbf{y}, \mathbf{0}, \mathbf{Z}, \epsilon, \mathbf{g} | \mathbf{X}) \\
&= p(\mathbf{y}|\mathbf{X}) p(\mathbf{Z}) p(\epsilon) p(\mathbf{g}|\epsilon, \mathbf{X}, \mathbf{y}) p(\mathbf{0}|\mathbf{g}, \mathbf{Z}) \\
&= \mathcal{N}(\mathbf{y}|\mathbf{0}, \mathbf{K} + \tau^{-1}\mathbf{I}) p(\mathbf{Z}) \mathcal{N}(\epsilon|0,1) \\
&\cdot \prod_{j=1}^{m} \delta\left(\widetilde{g}_j - h(\mathbf{z}_j, \epsilon)\right) \mathcal{N}(\mathbf{0}|\mathbf{g}, \mathbf{\Sigma}).
\end{aligned}
$$

2. ML-Injected Simulations

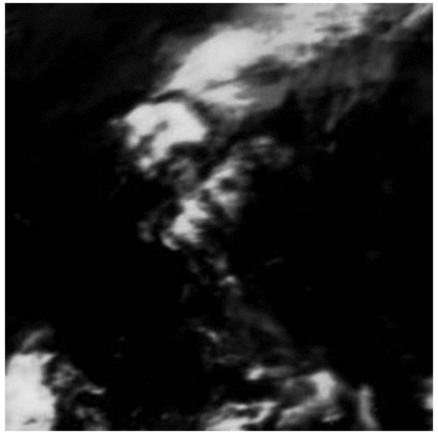
NS equation

$$
\begin{cases}
\dfrac{\partial \mathbf{u}}{\partial t} = -(\mathbf{u}\cdot\nabla)\mathbf{u} + \nu\nabla^2\mathbf{u} + \mathbf{f} - \nabla \boldsymbol{p} \\[2ex]
\dfrac{\partial \boldsymbol{\rho}}{\partial t} = -(\mathbf{u}\cdot\nabla)\boldsymbol{\rho} + \kappa\nabla^2\boldsymbol{\rho} + \boldsymbol{S} \\[2ex]
\nabla\cdot\mathbf{u} = \mathbf{0}
\end{cases}
$$

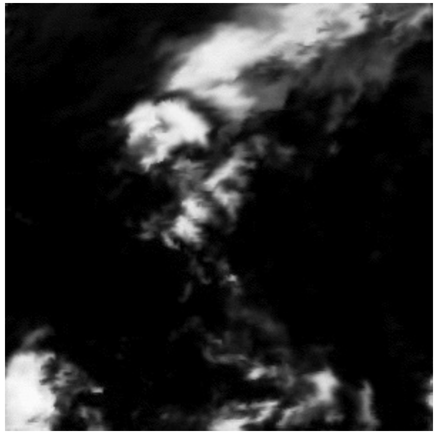
Velocity field is altered the PDE system + external forced



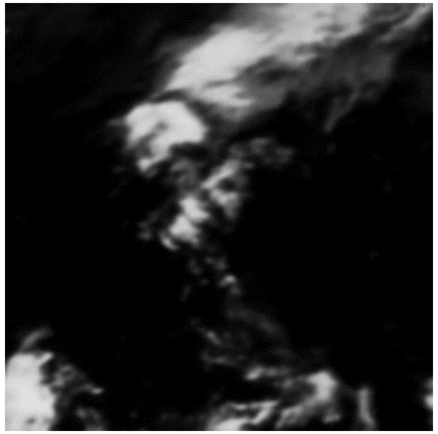
Cloud forecasting



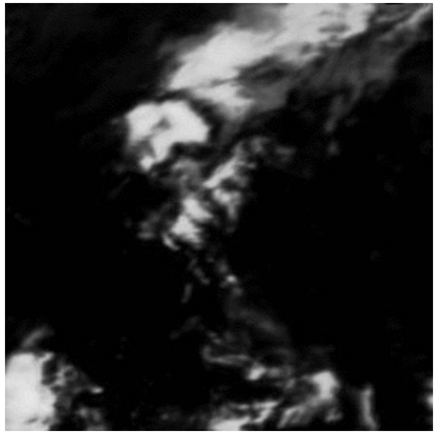
Truth



ML + Physics

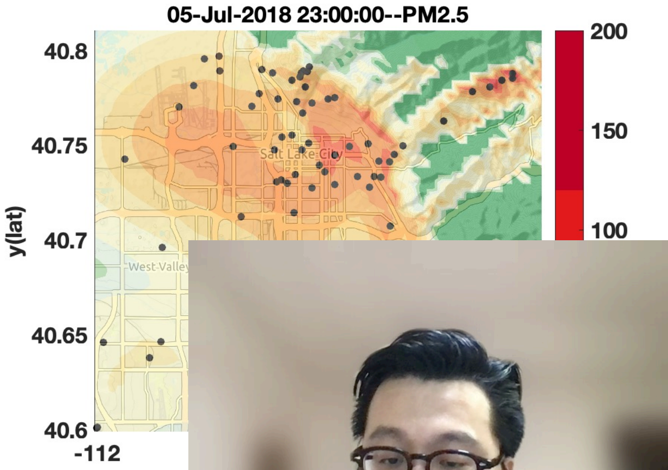


Pred-RNN



Flow

PM2.5 forcasting

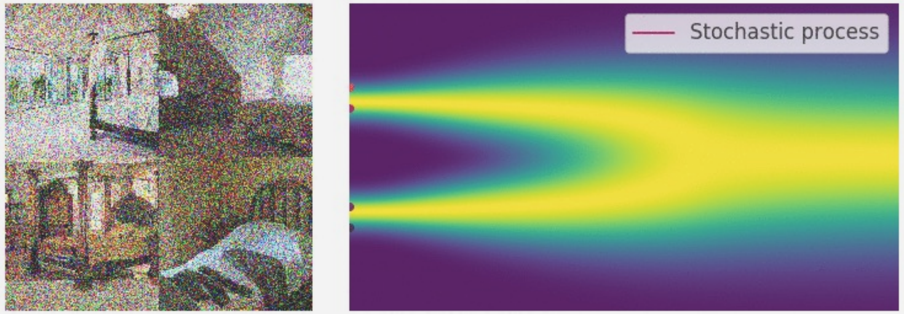


*B.3. Denoising Diffusion Probabilistic Models

OPEN AI's DALL·E 2

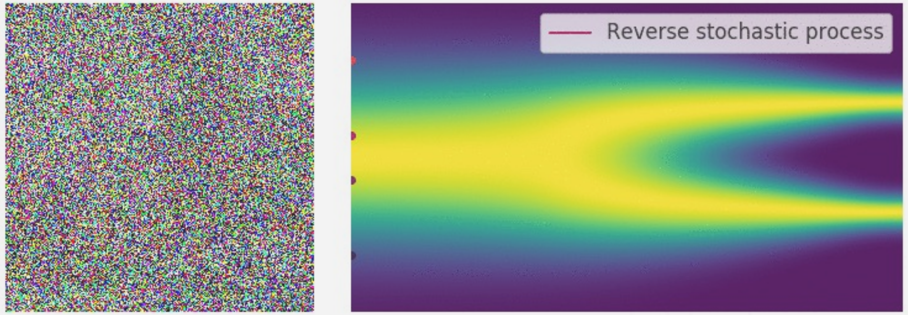
Inputs:
An astronaut
riding a horse
as a pencil drawing

Perturbing data with an SDE



Langevin dynamics

Reversing the SDE for sample generation

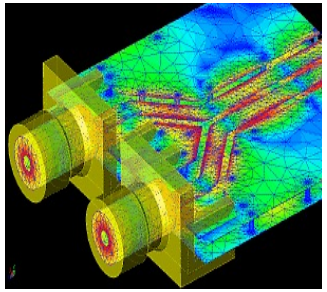


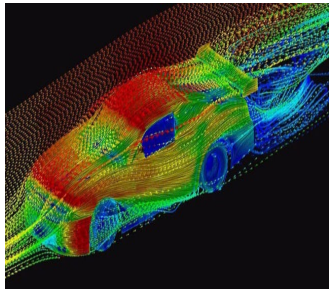
Reverse Langevin dynamics

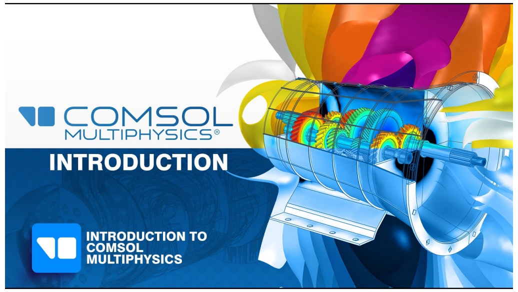
A better SDE and faster solver?

https://yang-song.github.io/blog/2021/score/

Research Interests







Scientific Computing + Machine Learning

A. ML enhanced SC

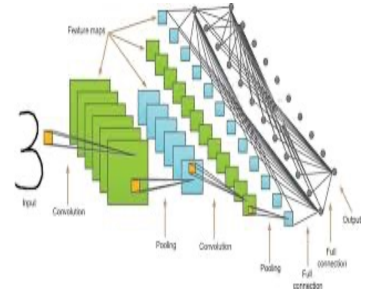
1. Data-driven Spatial-Temporal Field Modeling
2. Multi-fidelity Fusion
3. Machine Learning for Design and Optimization

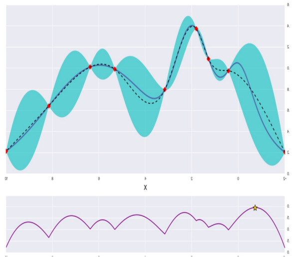
B. SC enhanced ML

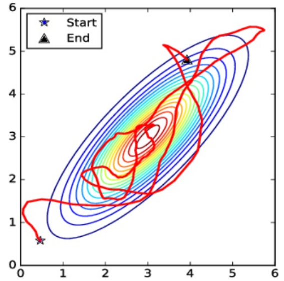
1. Physics Informed ML
2. ML Injected Simulation

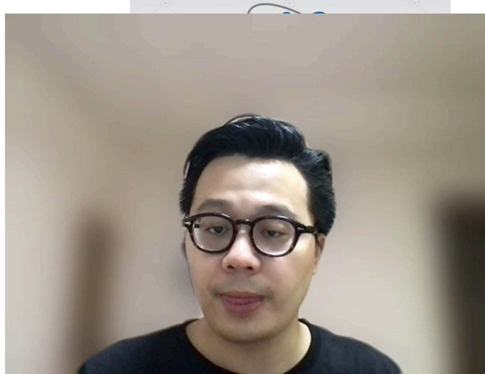
C. SC+ML for Industry and Application

1. Digital Twins
2. EDA
3. Inverse Problem In Scientific Research

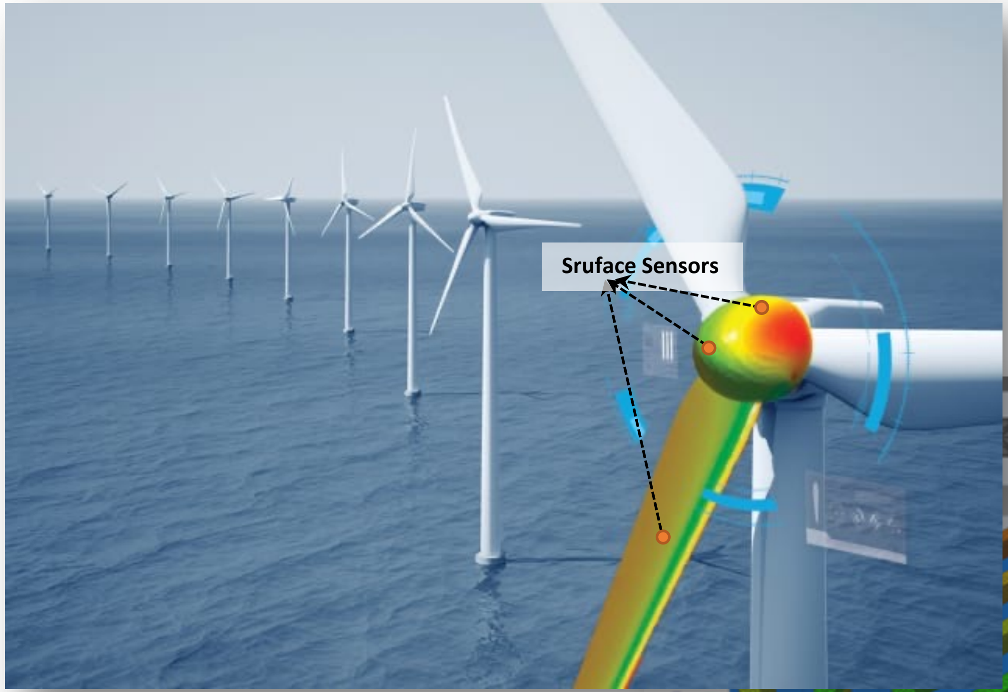


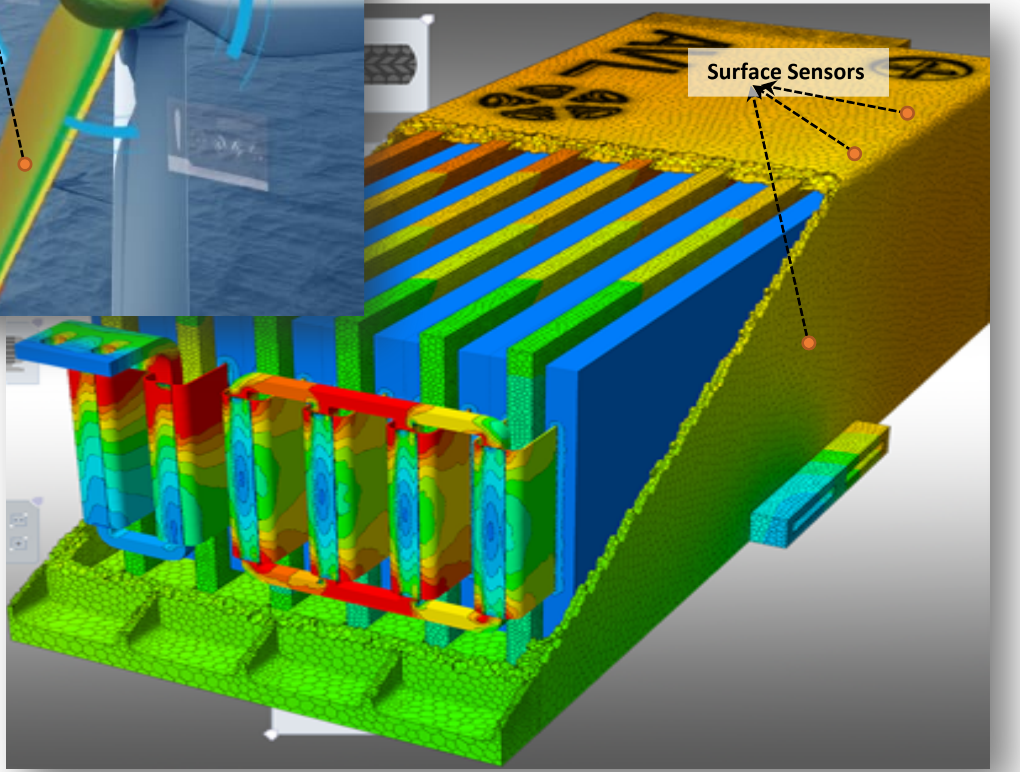


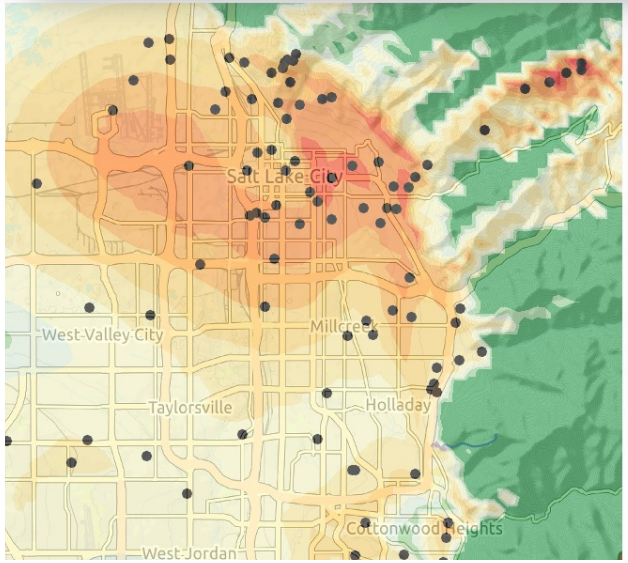




C.1. Bayesian Digital Twins Automata





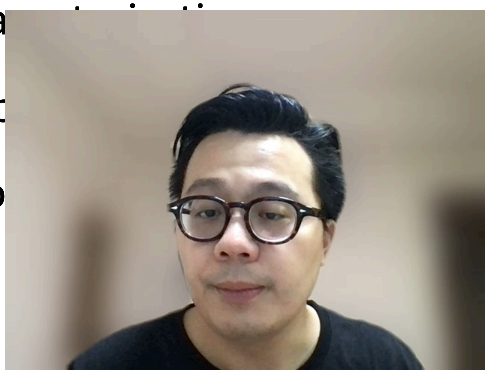


A Bayesian model for:

- Real-time filed report and forecast
- Real-time UQ
- Abnormal detection
- Optimal sensor deployment
- Automatic deployment through active learning

Core Techniques:

- Gaussian process
- Tensor para
- Bayesian op
- Physics info
- Inpainting



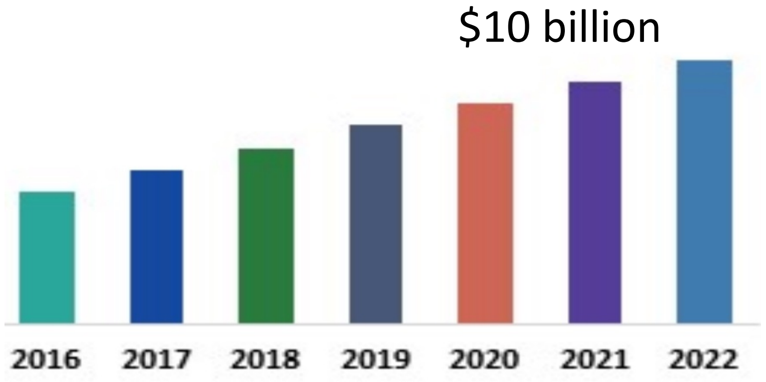
C.2. Electronic Design Automation

- Market size was valued at about 10 billion dollars in 2021
- CAGR of 9.1% from 2022 to 2030.
- ML becomes the next theme

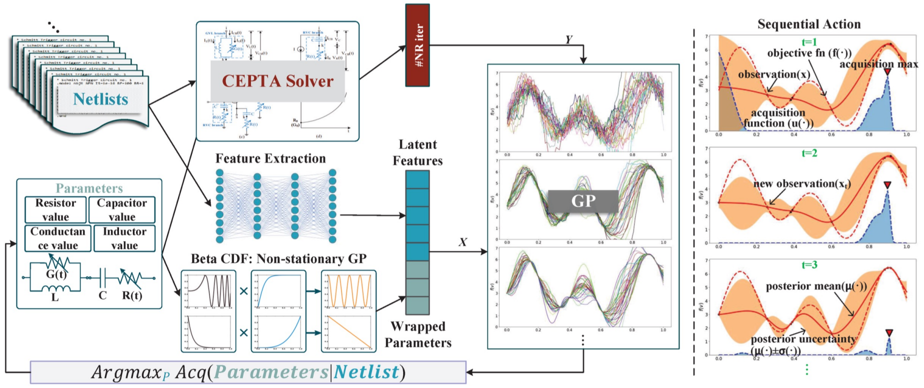
My works

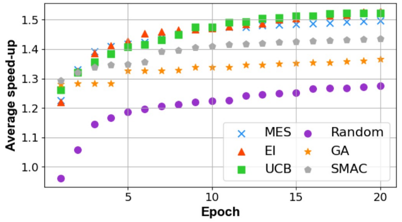
- Reinforcement learning adaptive stepping for SPICE speed up (DAC2022)
- Novel Bayesian yield optimization framework (DAC2022)
- First AI-accelerated SPICE solver of 2.3x-3.5x speed up (TODAES under revision)
- High-dimensional yield estimation (ICCAD2022 under view)

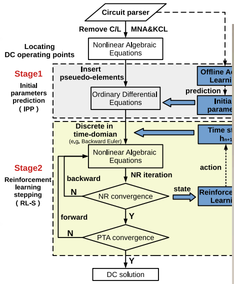
Grant: 800k

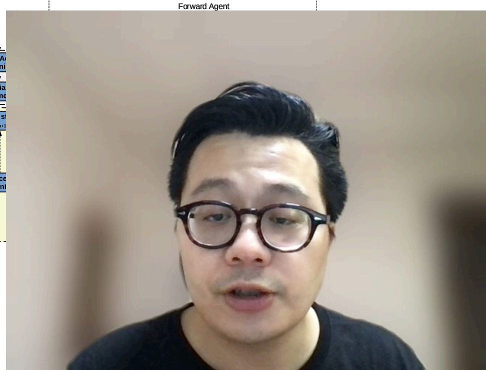


Source : IndustryARC Analysis, Expert Insights



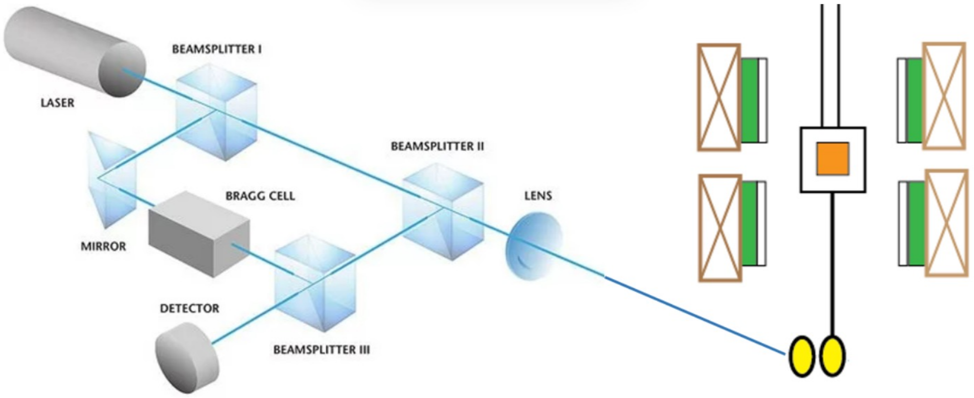


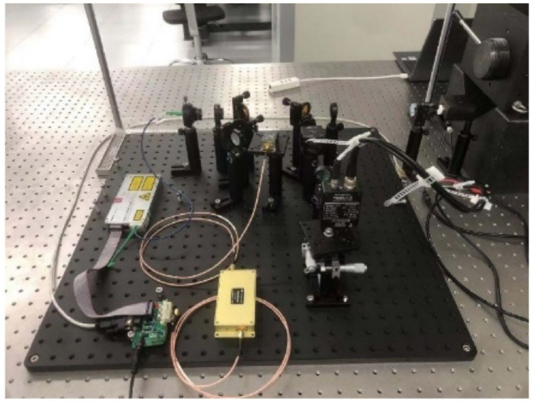


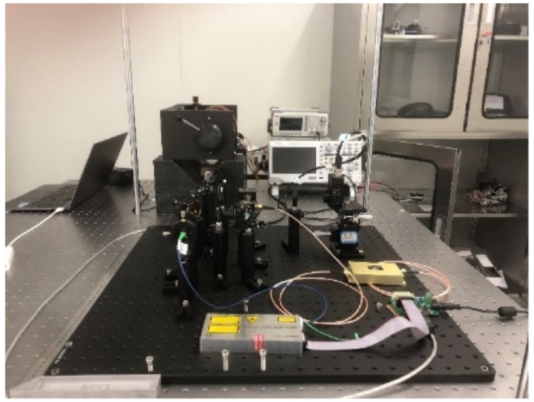


C.3. ML Enhanced Industry Instrument

Laser Doppler Vibrometer: A classic inverse problem







$$u(t) = A cos[2\pi f_a t - \frac{4\pi}{\lambda} R(t)]$$

R(t) is the target harmonical vibration

Grant: 1 million

Recap: research map

Multi-fidelity fusion

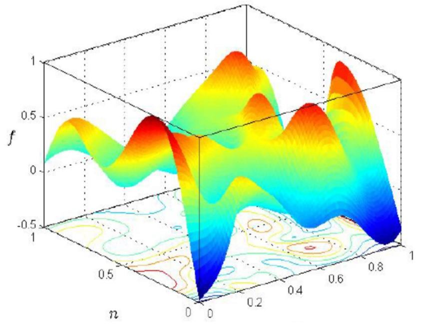
Meta learning

Neural ODE

Physics knowledge

Active learning & BO

Spatial-temporal surrogate



Better engineering process

Optimization

Uncertainty quantification

Inverse problem

Failure probability

Accelerate solvers

…

Digital twins & Hybrid models