SYSTEMS ENGINEERING RESEARCH CENTER

Physics-informed Machine Learning for System Intelligence

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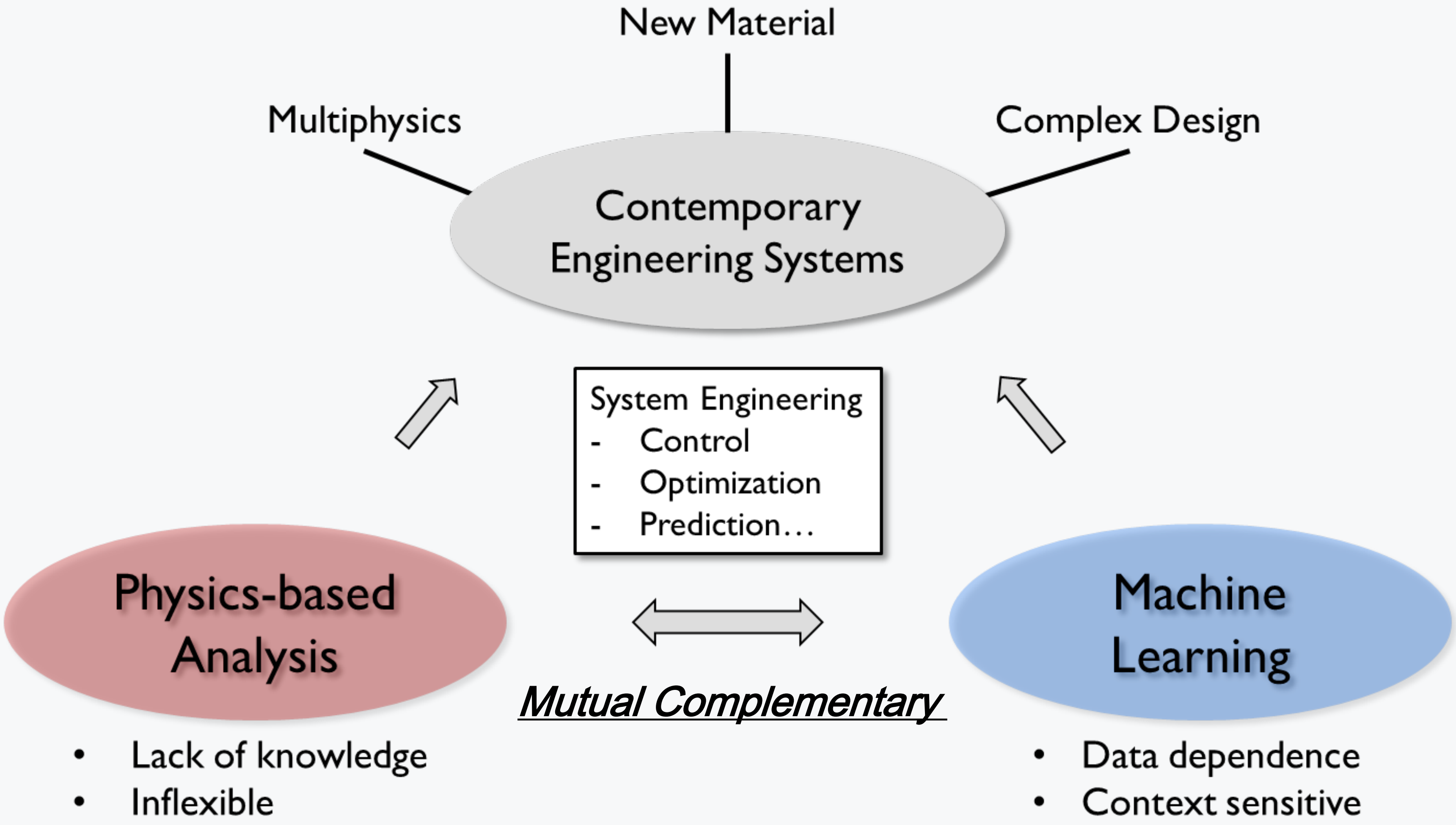
SERC DOCTORAL STUDENT FORUM 2022

Introduction



New Material

Multiphysics

Complex Design

Contemporary Engineering Systems

System Engineering
- Control
- Optimization
- Prediction…

Physics-based Analysis

- Lack of knowledge
- Inflexible

Mutual Complementary

Machine Learning

- Data dependence
- Context sensitive

Motivation

- Example 1: Composite fuselage assembly (aircraft manufacturing)
  - ➢ The shape control process is subject to:
    (i) intrinsic uncertainty; (ii) material complexity; and (iii) failure risks
  - ➢ Conventional control theory is suboptimal and time-consuming (trial-and-error)

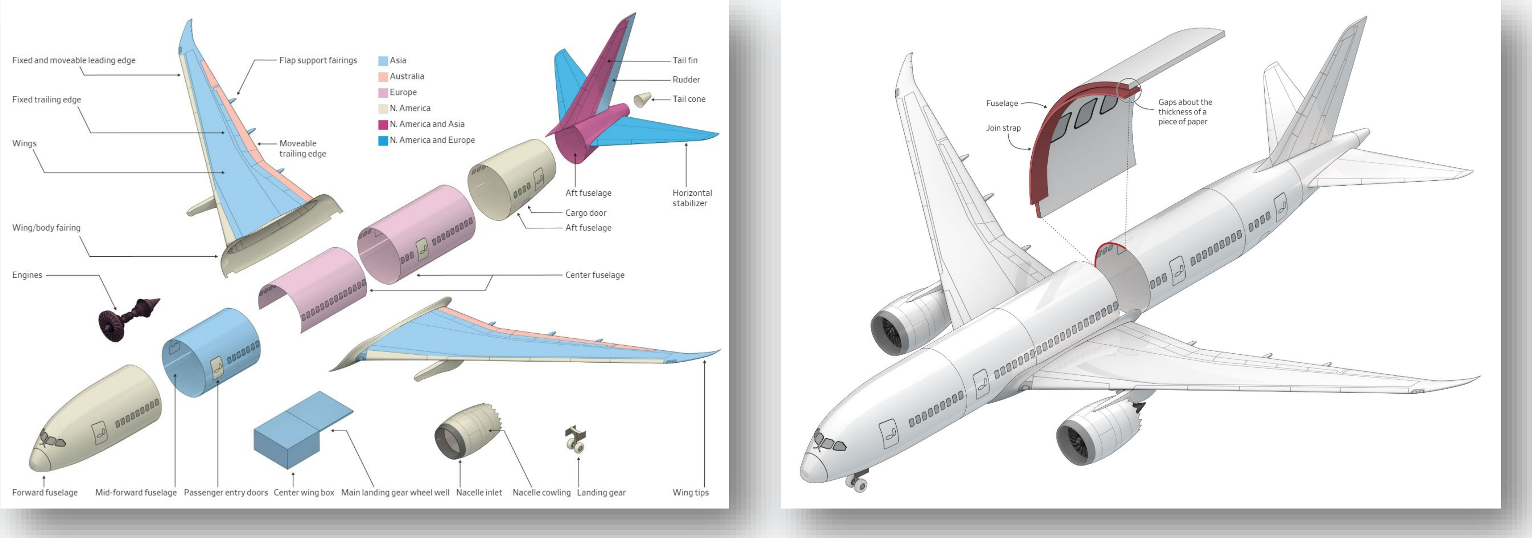


Fig 1. Subsections of Boeing 787. (from Tangel and J. R. Brinson, "What's holding back Boeing's 787 Dreamliner?" WSJ, June 26 2022)

Fig 2. Shape control process

Motivation

- Example 2: Multiphysics material analysis
  - ➢ Response is extremely complex to interpret existing physics
  - ➢ Uncertainty quantification is intractable with physics
  - ➢ Conventional design of experiment (DoE) is inefficient

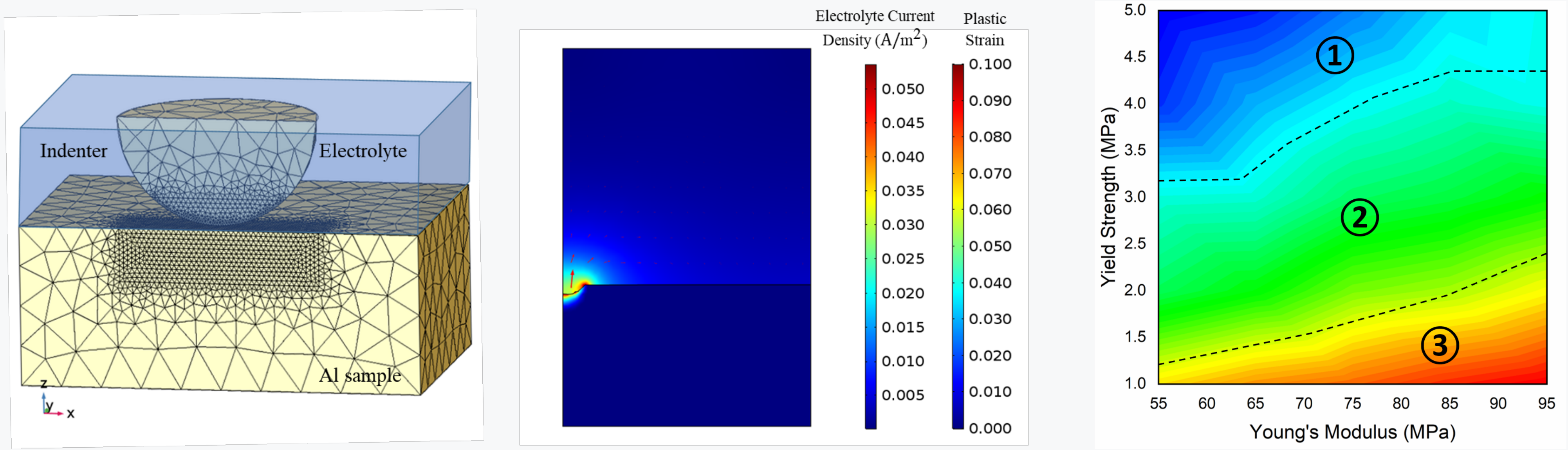


Fig 3. Tribocorrosion analysis for Al alloys (from Wang et al. "Multiphysics modeling and uncertainty quantification of tribocorrosion in aluminum alloys." *Corrosion Science* 178 (2021): 109095.)

Research Overview

Physics-informed Machine Learning for System Informatics

Physical Characteristics	Uncertainty	Heterogeneity	Implicit Constraint
Solution	Uncertainty Quantification	Divide-and-Conquer	Constraint Model
Method	NNGP considering Input Uncertainty (NNGPIU)	Partitioned Active Learning (PAL)	Physics-constrained Active Learning (PhysCAL)
Usage	Modeling	Data Acquisition	
Applications	Simulation, Control, Design Optimization, etc.		

Neural Network GP considering Input Uncertainty

- Motivation: Surrogate modeling of complex system under input uncertainty

Problem Property

Material Property

- *Nonlinear*
- *Anisotropic*

Process Property

- *Heterogeneous Parts*
- *Input Uncertainty*

Desired Model

Neural Network Gaussian Process (NNGP)

- *High Model Capacity: Deep Structure*
- *Uncertainty Quantification (UQ)*
- *Limitation:*
  How to consider Input Uncertainty?

Conventional Approach

Gaussian Processes

- *Pros: Capability of UQ*
- *Cons: Shallow Structure*

Deep Neural Networks

- *Pros: High Expressivity*
- *Cons: Intractable UQ*

- Neural network Gaussian process (NNGP)
  - Gaussian process (GP) induced from infinite-width random deep neural networks
  - Nonstationary GP with deep architecture using composite kernels

Neural Network GP considering Input Uncertainty

- Method details

Problem Formulation

$$\underbrace{\boxed{y(x)}}_{\substack{\text{Actual}\\ \text{Observation}}} = \underbrace{\boxed{f}}_{\substack{\text{Target Function}\\ \sim NNGP(\mu^L, k^L)}}(x + \underbrace{\boxed{u}}_{\substack{\text{Input Noise}\\ \sim \mathcal{U}(0, \sigma_u^2)}}) + \underbrace{\boxed{\epsilon},}_{\substack{\text{Observation Noise}\\ \sim \mathcal{N}(0, \sigma_\epsilon^2)}} \qquad x \in \Omega$$

NNGP

$$\begin{aligned} k_{NNGP}(x, x') &= \mathrm{Cov}[y(x), y(x')] \\ &\neq \underline{\mathrm{Cov}[f(x), f(x')]} \end{aligned}$$

Ignore Input Noise
$(u, u' = 0)$

NNGPIU (Our Proposal)

$$\begin{aligned} k_{NNGPIU}(x, x') &= \mathrm{Cov}[y(x), y(x')] \\ &= \mathrm{Cov}[f(x+u), f(x'+u') | u, u'] \\ &\rightarrow \underline{\mathbb{E}_{u,u'}[f(x+u) f(x'+u')]} \end{aligned}$$

Expectation over Input Noises

- *MC Approximation for Kernel (m: # Input Noise (u) Samples; $u \sim \mathcal{U}$)*

$$\tilde{k}^L_{NNGPIU}(x, x') \approx \begin{cases} \frac{1}{m^2} \sum_{i,j} k^L(x + u_i, x' + u_j), & x \neq x' \\ \frac{1}{m} \sum_i k^L(x + u_i, x + u_i), & x = x' \\ \frac{1}{m} \sum_i k^L(x + u_i, x_*), & x_*: \textit{New Input} \end{cases}$$

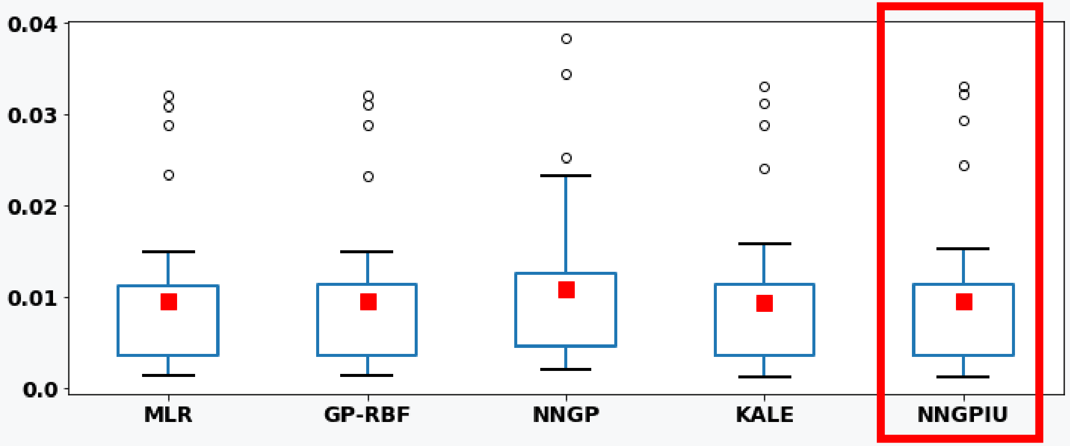
__Proposition 1.__ NNGPIU is a Best Linear Unbiased Predictor (BLUP) of $f(x_*)$, which is subject to input noise, where x_* is an unobserved input.

$$\arg\min_{\beta} \| f(x_{new}) - \beta^\top y \|^2 = k^L_{NNGPIU}(x, X) \left[K^L_{NNGPIU}(X, X) + \sigma_\epsilon^2 I \right]^{-1}.$$

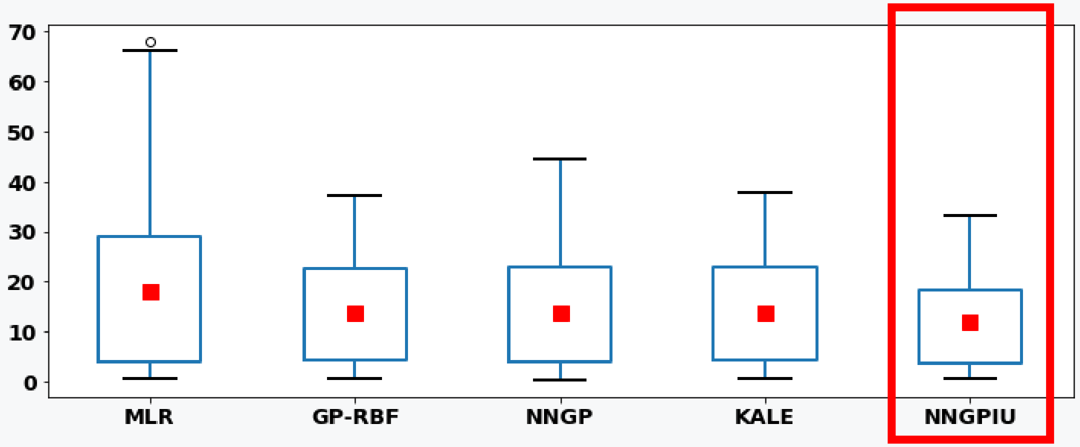
Neural Network GP considering Input Uncertainty

- Application to composite fuselage shape control

Deformation



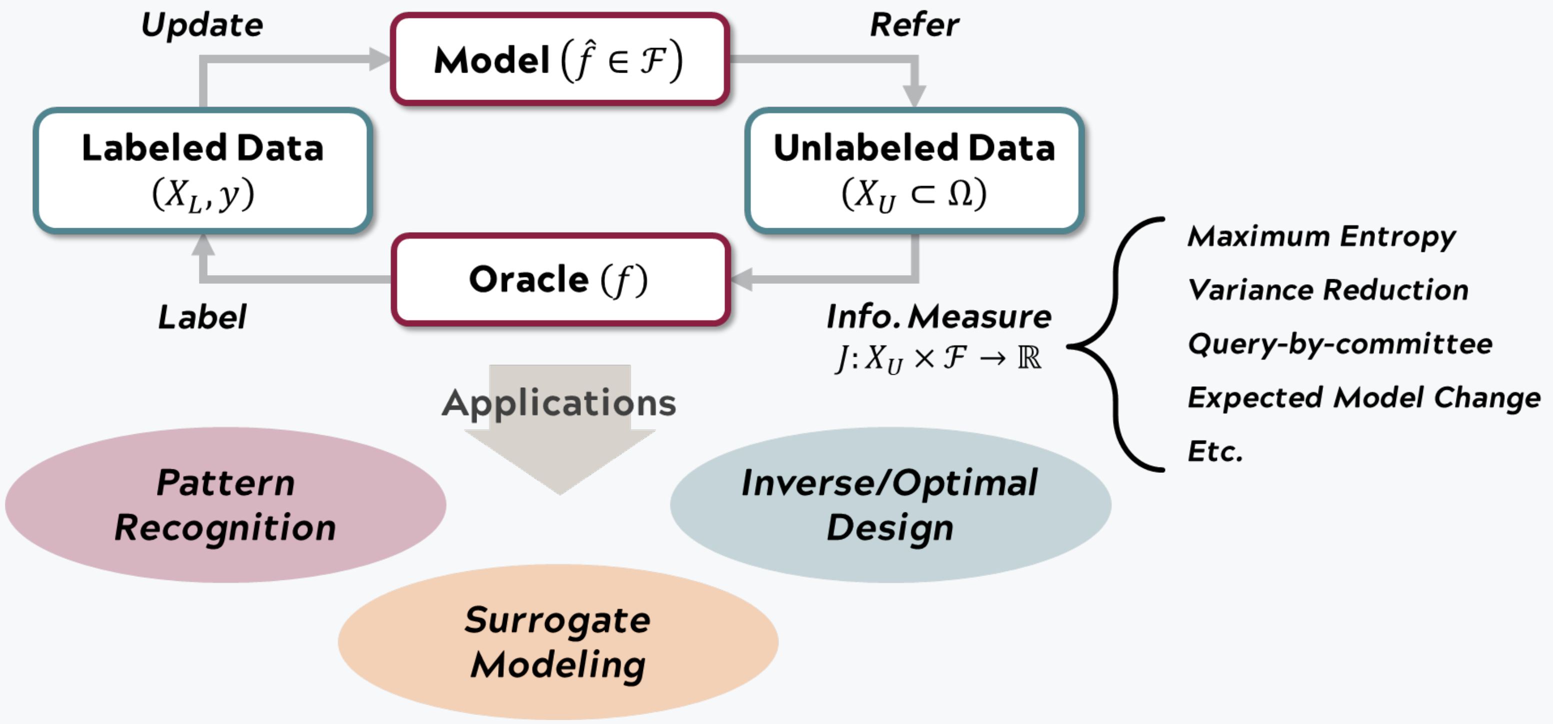
Residual Stress



Model	*Linear*	*Shallow GP*	*NNGP*	*KALE*	*NNGPIU*
MAE (× 10^{-3} in)	9.37	9.42	10.84	9.29	9.35
MAE (psi)	18.143	13.668	13.619	13.742	11.884

Partitioned Active Learning

- Motivation: Optimal design for heterogeneous systems



Update

Model ($\hat{f} \in \mathcal{F}$)

Refer

Labeled Data (X_L, y)

Unlabeled Data $(X_U \subset \Omega)$

Oracle (f)

Label

Info. Measure $J: X_U \times \mathcal{F} \rightarrow \mathbb{R}$

Maximum Entropy
Variance Reduction
Query-by-committee
Expected Model Change
Etc.

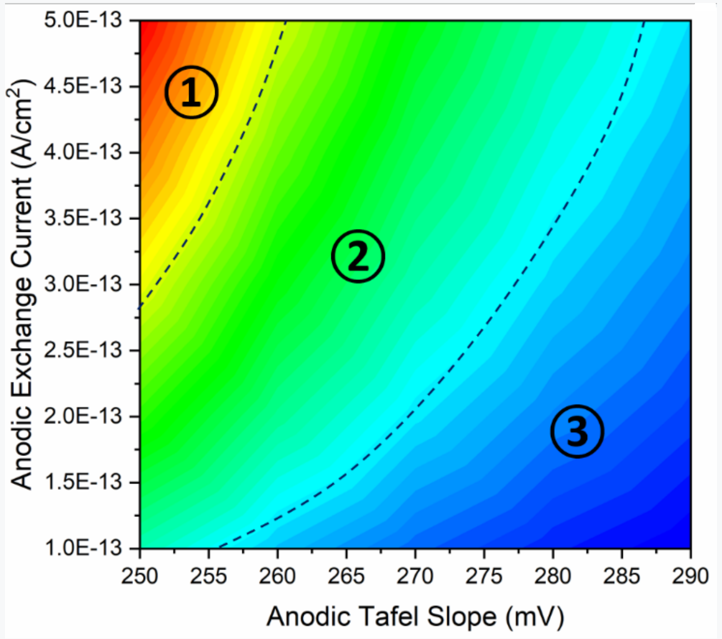
Applications

Pattern Recognition

Inverse/Optimal Design

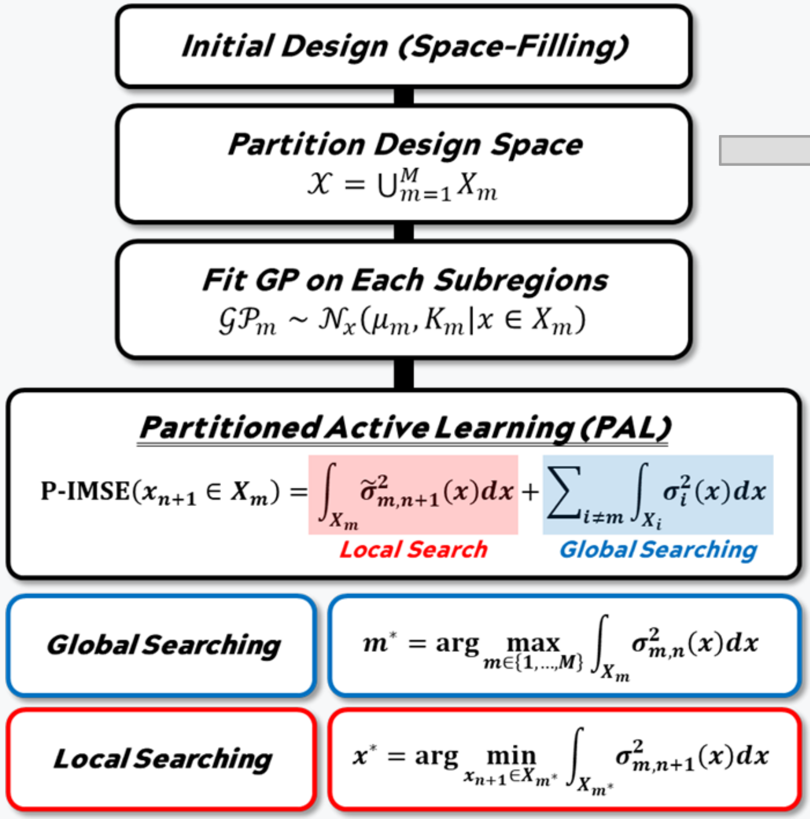
Surrogate Modeling

Fig 4. Corrosive Rates of Al Alloys



Partitioned Active Learning

- Method details



Initial Design (Space-Filling)

Partition Design Space
$\mathcal{X} = \cup_{m=1}^{M} X_m$

Fit GP on Each Subregions
$\mathcal{GP}_m \sim \mathcal{N}_x(\mu_m, K_m | x \in X_m)$

Partitioned Active Learning (PAL)

$$\text{P-IMSE}(x_{n+1} \in X_m) = \underbrace{\int_{X_m} \tilde{\sigma}^2_{m,n+1}(x)dx}_{\text{Local Search}} + \underbrace{\sum_{i \neq m} \int_{X_i} \sigma_i^2(x)dx}_{\text{Global Searching}}$$

Global Searching

$$m^* = \arg \max_{m \in \{1,\ldots,M\}} \int_{X_m} \sigma^2_{m,n}(x)dx$$

Local Searching

$$x^* = \arg \min_{x_{n+1} \in X_{m^*}} \int_{X_{m^*}} \sigma^2_{m,n+1}(x)dx$$

** Iterate until the "Budget" is consumed or "Desired-Accuracy" is achieved*

Heterogeneity-based Partitioning

- Compute heterogeneous feature for (X, y):

$$h(x) = \underbrace{\text{avg}\left(\frac{d(y_i, y)}{d(x_i, x)}; x_i \in N_r(x)\right)}_{\boxed{\text{Finite difference}}}, \text{ or } \underbrace{\text{Var}\left(y_i; x_i \in N_r(x)\right)}_{\boxed{\text{Variance}}}$$

- Implement mean-shift for $(X, h) \rightarrow (X, h, m)$
- Train SVC on (X, m)

Consequently, Partitioned Active Learning (PAL) achieves:

i) ***Reduction of Numerical Cost*** **in Optimal Location Search**

- Matrix Inversion: $\mathcal{O}(N^3) \rightarrow \Sigma_{\mathrm{m}} \mathcal{O}(n_m^3),\ \Sigma_{\mathrm{m}} n_m = N$

- # Candidates: $\text{Card}(X_{cand}) \rightarrow \Pr(x \in X_{m^*})\text{Card}(X_{cand})$

*** Assuming X_{cand} uniformly spread out in $\mathcal{X}$**

ii) ***More Accurate Search*** **via Localized GPs**

For each region ($m \in \{1, \ldots, M\}$), $x \in X_m$,

$$\sigma^2_{m,\,n_m}(x) = k_m(x) - k_m^\top(x, X_{n_m})K^{-1}_{m,n_m} k_m(x, X_{n_m}).$$

Partitioned Active Learning

- 2-D simulation result

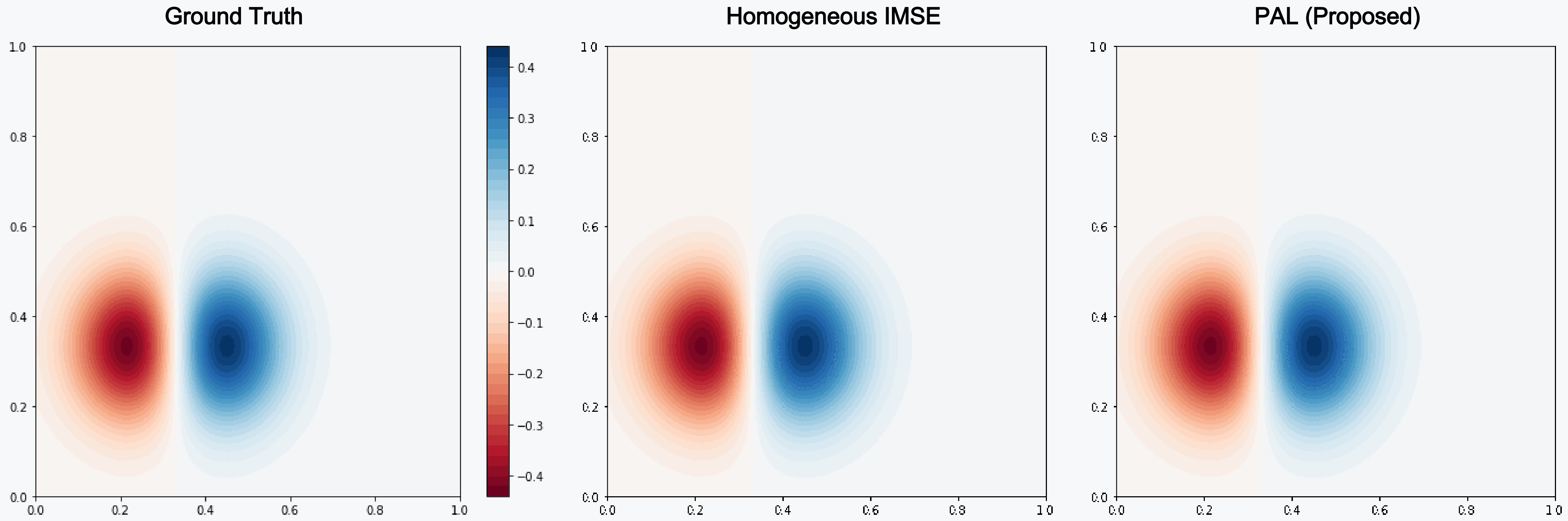
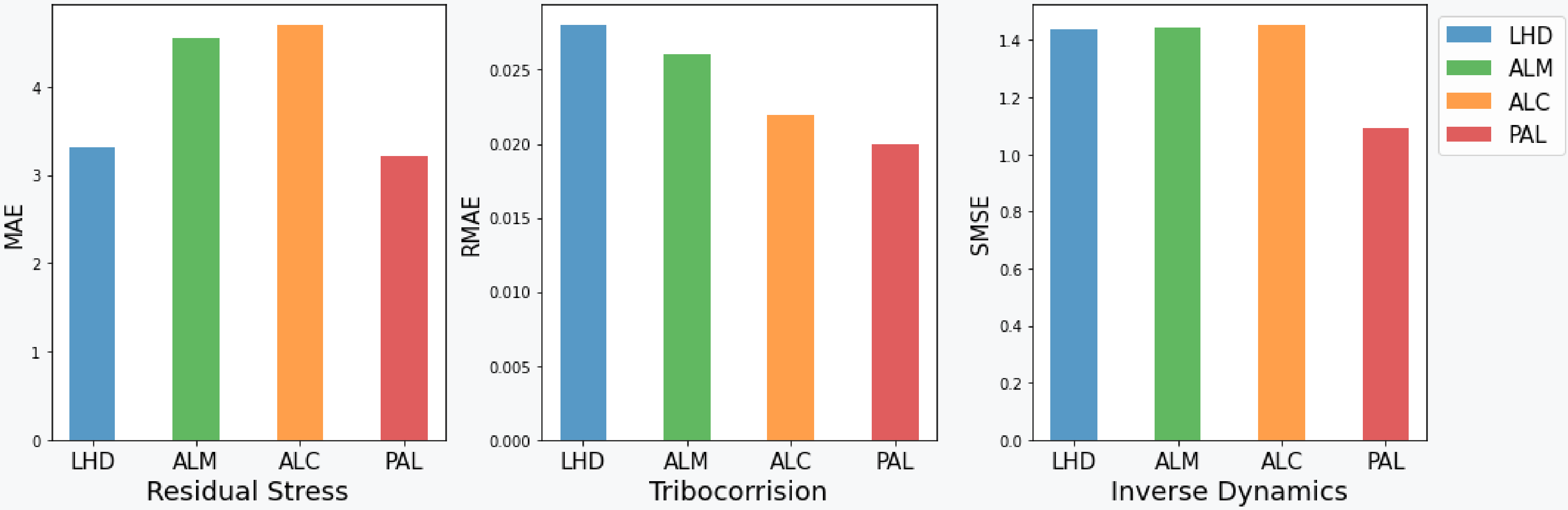


Fig 5. Comparison between ALC and PAL in 2-D simulation

Partitioned Active Learning

- Case study results

Case	Input Dims	Output Dims
Residual stress in shape control	10	1
Tribocorrosion rates of Al alloys	6	1
Inverse dynamics of robotic arm	21	7



Physics-constrained Active Learning

- Motivation: avoid system failures in physics-constrained systems
- Underestimating implicit constraints in active learning may induce:
  - ➢ Fatal system failures
  - ➢ Incompliant models

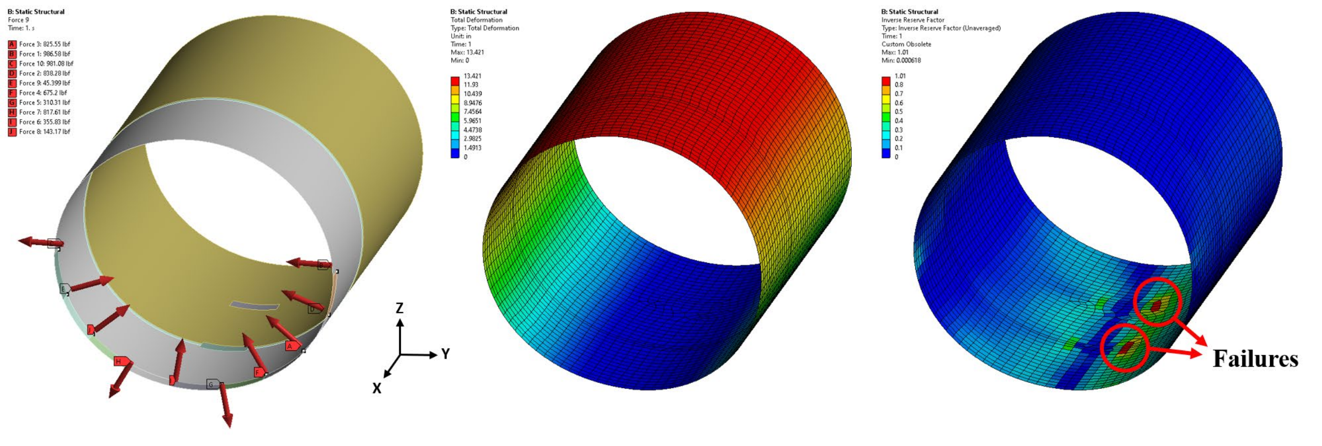


Fig 6. Composite fuselage shape control inducing material failures

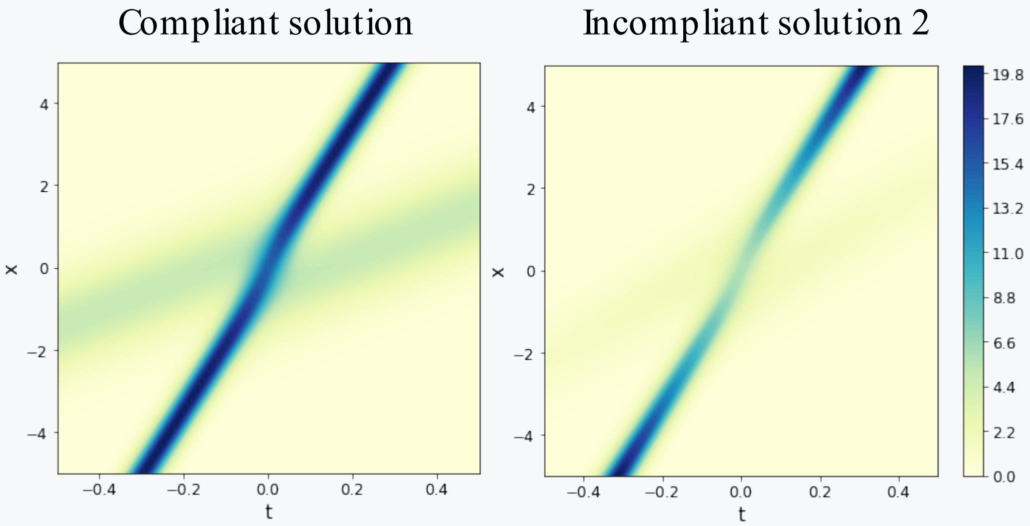
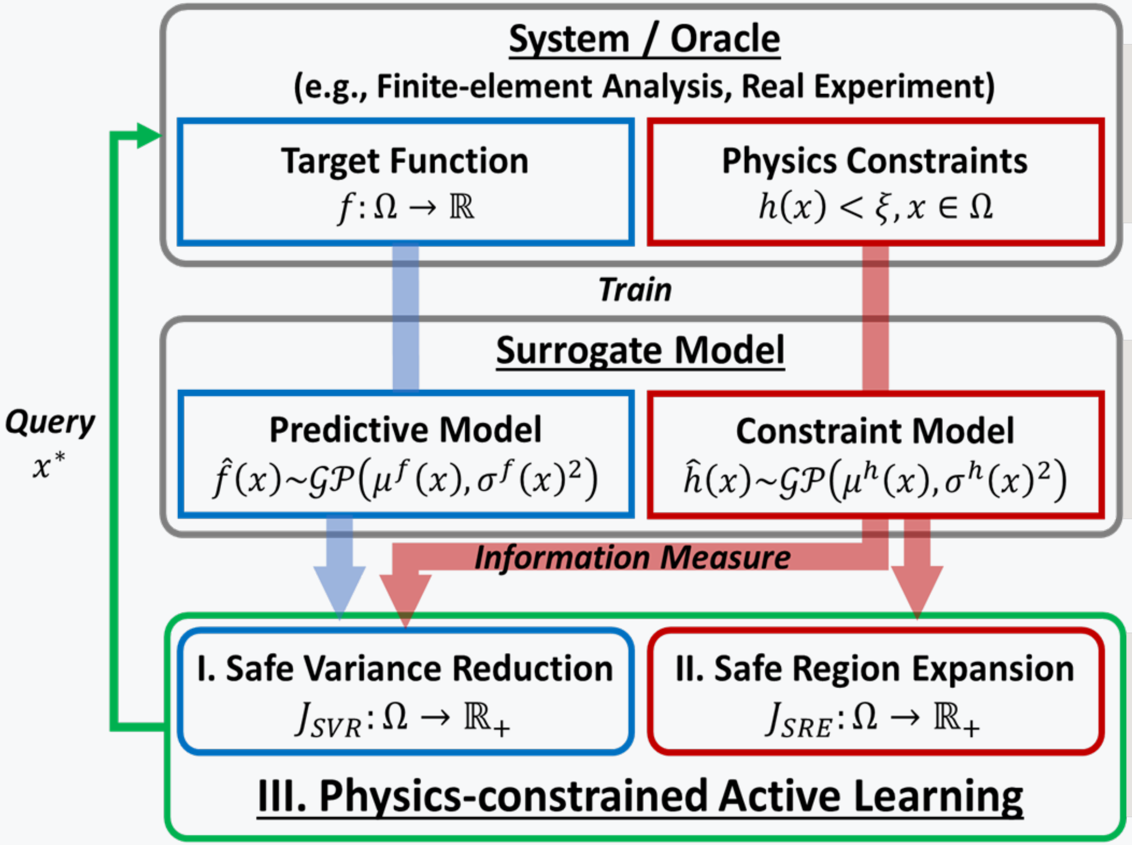


Fig 7. Data-driven solutions of the Korteweg-de Vries (KdV)-Burgers equation

Physics-constrained Active Learning

- Method overview



System / Oracle

(e.g., Finite-element Analysis, Real Experiment)

Target Function

$f : \Omega \rightarrow \mathbb{R}$

Physics Constraints

$h(x) < \xi, x \in \Omega$

Train

Surrogate Model

Predictive Model

$\hat{f}(x) \sim \mathcal{GP}\left(\mu^f(x), \sigma^f(x)^2\right)$

Constraint Model

$\hat{h}(x) \sim \mathcal{GP}\left(\mu^h(x), \sigma^h(x)^2\right)$

Information Measure

Query

x^*

I. Safe Variance Reduction

$J_{SVR} : \Omega \rightarrow \mathbb{R}_+$

II. Safe Region Expansion

$J_{SRE} : \Omega \rightarrow \mathbb{R}_+$

III. Physics-constrained Active Learning

- The system consists of two functions
- Assume functions are bounded in RKHS

- Maintain two surrogate GPs
- Surrogate models are utilized for info. measure

- Reduce model variance over the safe region
- Expand the explorable safe region
- Integrate two tasks

Physics-constrained Active Learning

- Method details

I. Safe Variance Reduction (SVR)

- Consider *two-level safe regions* with the constraint model as

$$S\ (S^+) = \left\{x \,\middle|\, \Pr\left(\hat{h}(x) < \xi\right) < 1 - \gamma\ (\gamma^+)\right\} \text{ with } S \subseteq S^+$$

- Choose $x \in S$ that *reduces the model variance* over S^+ the most

$$J_{SVR}(x \in S) = \int_{S^+} \mathrm{Var}\left(\hat{f}(s)\right) d\lambda(s) - \int_{S^+} \mathrm{Var}\left(\hat{f}(s|x)\right) d\lambda(s)$$

* Note: S: safe region, S^+: progressive safe region, λ: measure on Ω

II. Safe Region Expansion (SRE)

- Choose the most informative data to *expand the explorable region*
- Incorporate *uncertainty* and *closeness* to the safe boundary

$$J_{SRE}(x \in S) = \eta^2\left(\Phi^h(\xi) - \Phi^h(\xi - \eta)\right) - \int_{\xi-\eta}^{\xi} (h - \xi)^2 \phi^h(x)\, dh$$

Uncertainty *Closeness*

* Note: $\eta = \alpha\sigma^h(x)\ (\alpha > 0)$, $\Phi^{\mathrm{h}}(\cdot)$, ϕ^h: CDF, PDF of $\hat{h}(\cdot)$

III. Harmonizing Acquisition Functions

- Preference parameter (w): adjust balance between two criteria
- Multi-objective optimization formulation with Pareto optimality

$$x^* = \arg\max_{x \in S}\ (1 - w)\, J_{SVR}(x) + w\, J_{SRE}(x)\,, w \in [0, 1]$$

IV. Theoretical Properties

- Proposition 1. *(Failure Probability)* For N-sampling, the failure-averse active learning has the probability of failure $\zeta = N\gamma$.
- Proposition 2. *(Asymptotic Convergence)* As $n \to \infty$, the acquisition function and S converge to zero and a subset of the true safe region.

Physics-constrained Active Learning

- Application to composite fuselage shape control
  - Target function: fuselage deformation (10 actuators)
  - Constraint: composite material failure criterion (Tsai-Wu criterion)

Tsai-Wu criterion

$$\sum_{i=1}^{2}\left(\frac{1}{\sigma_i^T}-\frac{1}{\sigma_i^C}\right)\sigma_1+\frac{\sigma_i^2}{\sigma_i^T\sigma_i^C}+\left(\frac{\tau_{12}}{\tau_{12}^F}\right)^2-\frac{\sigma_1\sigma_2}{\sigma_1^T\sigma_1^C\sigma_2^T\sigma_2^C}\geq\frac{1}{MS}$$

MS (Margin of safety)=1.25

  - 20 initial samples + 20 samples with AL (10 replications)
  - Result

Methods	**Random**		**Max Entropy**		**IMSE**		**SEGP**		**Proposed Method**	
	MAE	**# Fail**	**MAE**	**# Fail**	**MAE**	**# Fail**	**MAE**	**# Fail**	**MAE**	**# Fail**
Mean (Std/μm)	**5.383 (2.345)**	**0.4 (0.5)**	**2.244 (0.470)**	**4.1 (0.3)**	**2.046 (0.441)**	**3.8 (0.6)**	**2.297 (0.305)**	**1.0 (0.8)**	**2.832 (0.518)**	**0.1 (0.3)**

Summary and Conclusion

Topic	Challenges	Contributions	Further Applications
NNGP Considering Input Uncertainty	- *Low expressivity (GP)* - *Data-inefficient (DNN)* - Cannot address *input uncertainty (NNGP)*	- Developed data-efficient and highly expressive model that considers input uncertainty	- Modeling of complex systems with limited data - Systems subject to intrinsic input uncertainty
Partitioned Active Learning	- Hindered learning by system *heterogeneity*	- Incorporate the region classifier to *improve the validity of data importance* - Hierarchical acquisition function with improved *computational cost*	- Multiphysics systems - Geostatistics, human health subject to ecologic heterogeneity
Physics-constrained Active Learning	- *Implicit constraints* associated with system failure	- *Development of acquisition functions* with implicit constraints - Utilizing multi-objective optimization for *the flexibility of AL*	- Solving PDE problems - Optimizing control policy with implicit constraints

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