Multi-Fidelity Surrogate Modeling and Optimization for Multi-Physics Problems

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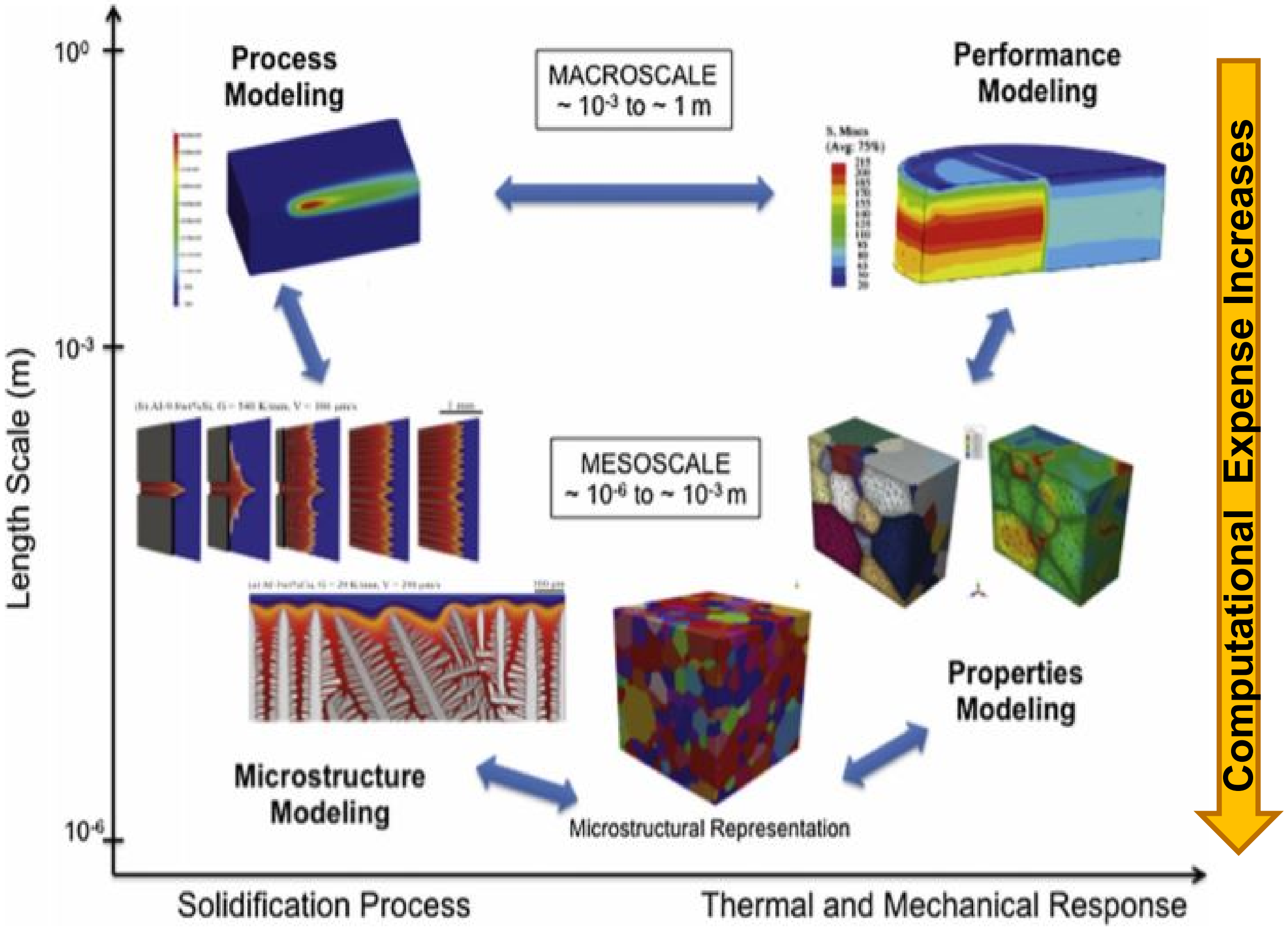
Design Optimization : Budget Restrictions

Expensive Simulations: How to Predict and Optimize?



Existing Gaps in Additive Manufacturing Research

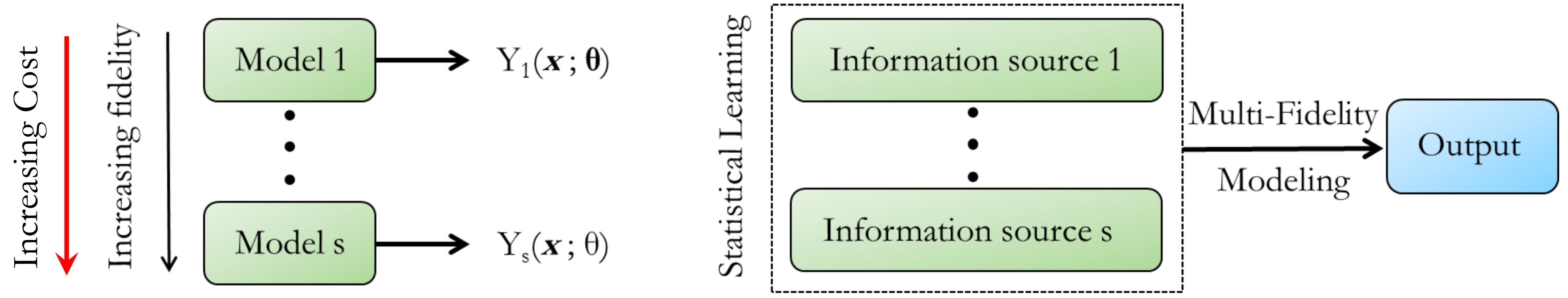
A few unexplored areas till date:

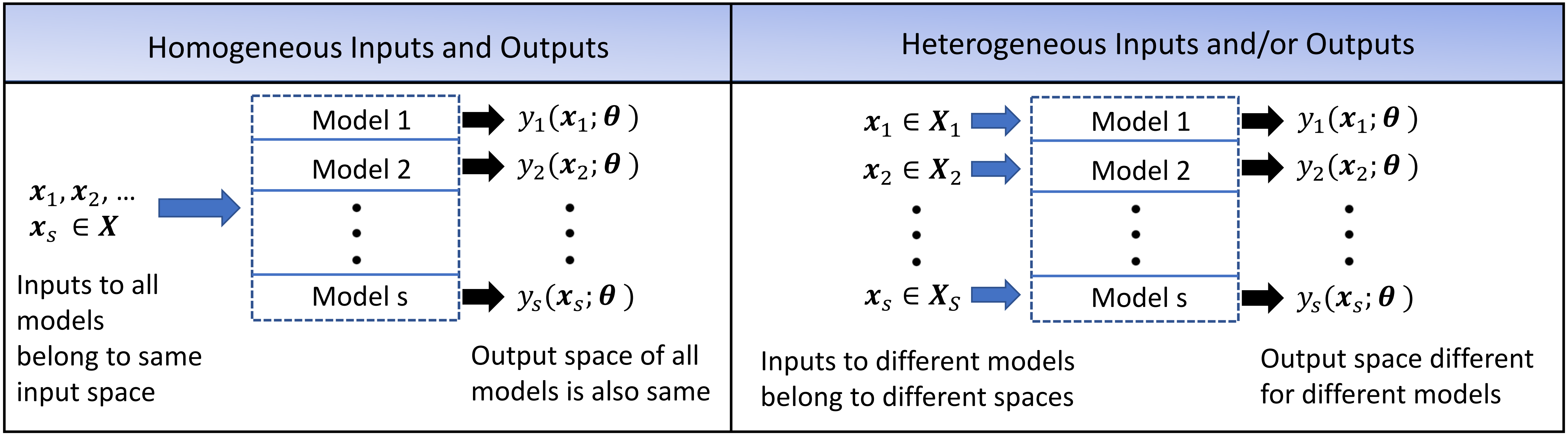
- Process control in AM which involves design optimization with multi-fidelity process models
- Process control strategies that incorporate thermal constraints
- Multi-fidelity modeling when different levels of fidelities have different input spaces, which can happen in multi-scale settings

❑ Address these issues in a generalizable multi-fidelity framework

M.M. Francois et al, Modeling of additive manufacturing processes for metals: Challenges and opportunities, Current Opinion in Solid State and Materials Science, 2017

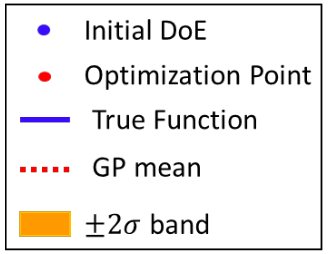
Multi-Fidelity Surrogate Modeling

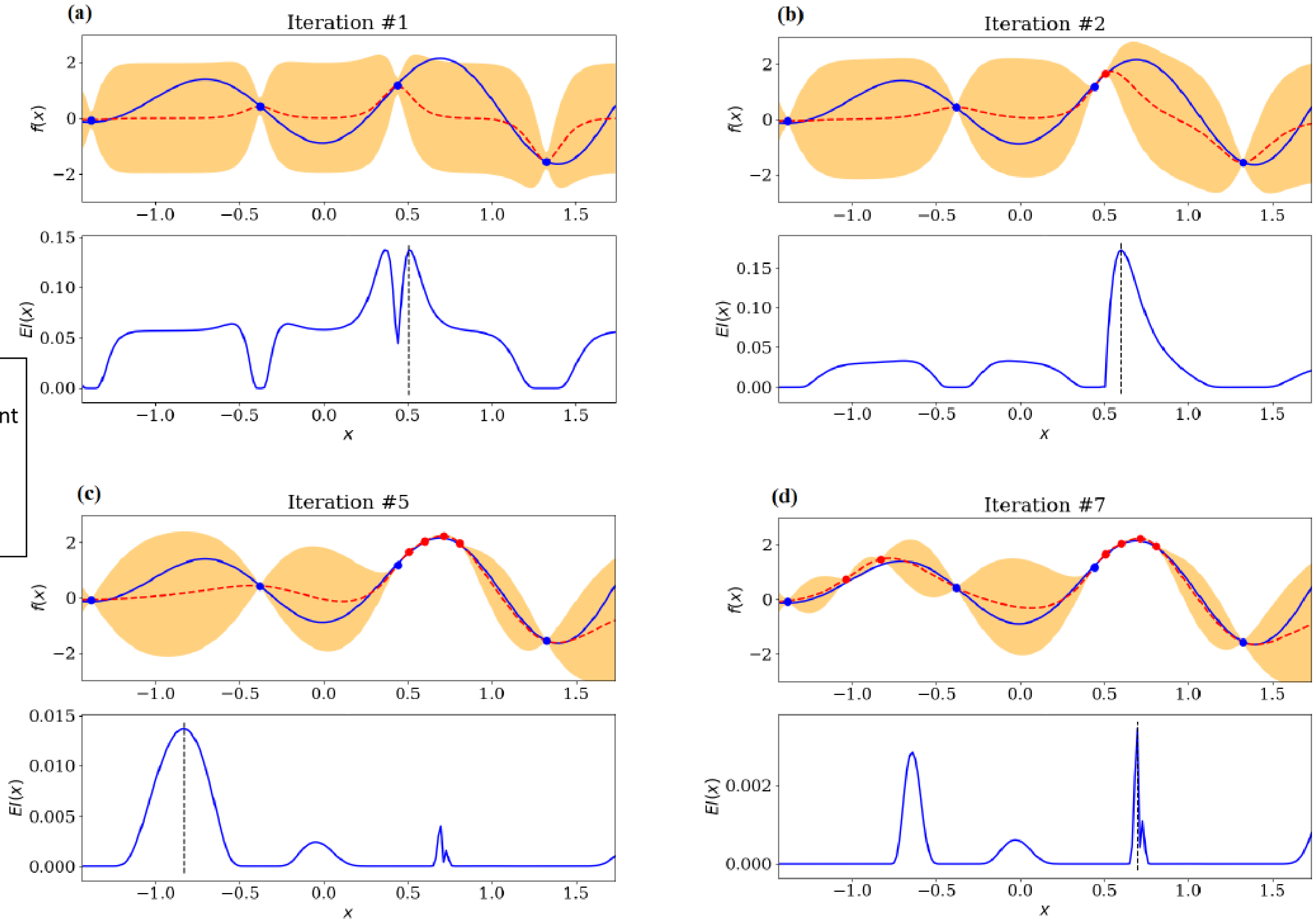




Gaussian Processes & Bayesian Optimization

Exploration ↔ Exploitation

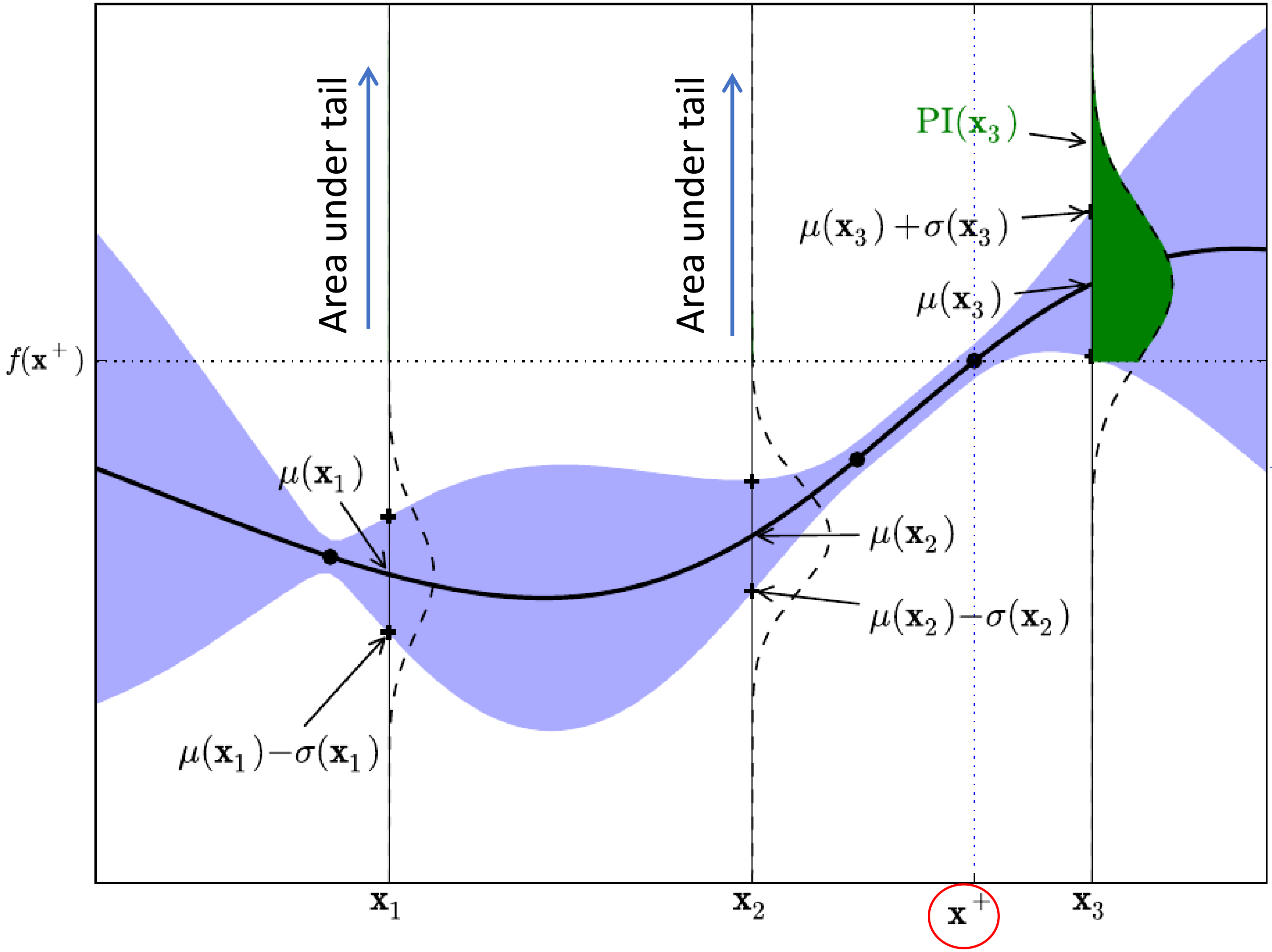




EI (x) :
Acquisition
Function

- GP: Non-parametric probabilistic regression model
- Exploration: Evaluate in locations where variance is large
- Exploitation: Evaluate in locations where mean is high
- Acquisition functions guide the search for optima through active learning

Acquisition Function



- $$\mathrm{PI}(\mathbf{x}) = P(f(\mathbf{x}) \geq f(\mathbf{x}^+)) = \Phi\left(\frac{\mu(\mathbf{x}) - f(\mathbf{x}^+)}{\sigma(\mathbf{x})}\right)$$

$$\mathbf{x}^+ = \mathrm{argmax}_{\mathbf{x}_i \in \mathbf{x}_{1:t}} f(\mathbf{x}_i)$$

Probability Improvement

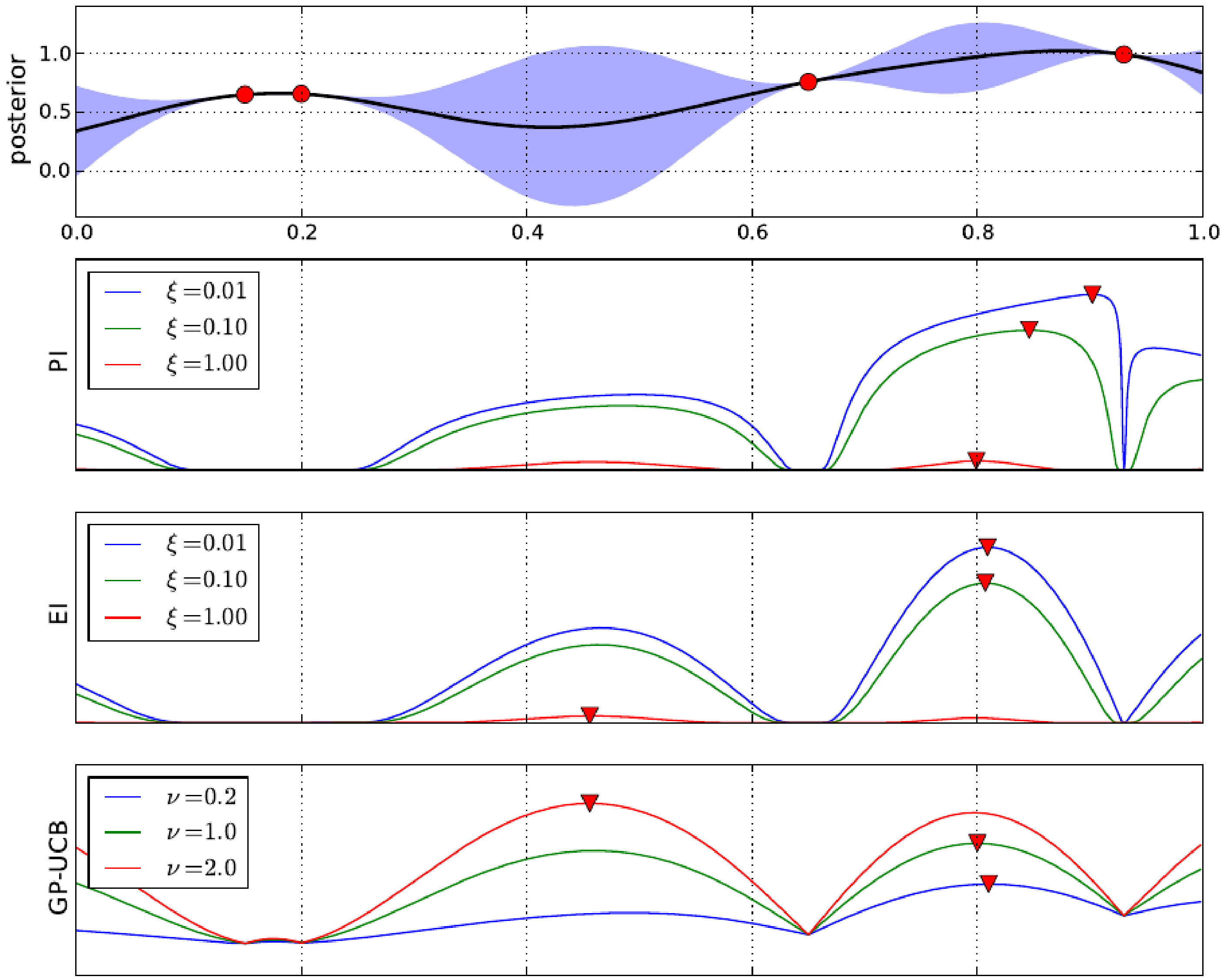
- $$\mathrm{EI}(\mathbf{x}) = \begin{cases} (\mu(\mathbf{x}) - f(\mathbf{x}^+) - \xi)\Phi(Z) + \sigma(\mathbf{x})\phi(Z) & \text{if } \sigma(\mathbf{x}) > 0 \\ 0 & \text{if } \sigma(\mathbf{x}) = 0 \end{cases}$$

$$Z = \begin{cases} \frac{\mu(\mathbf{x}) - f(\mathbf{x}^+) - \xi}{\sigma(\mathbf{x})} & \text{if } \sigma(\mathbf{x}) > 0 \\ 0 & \text{if } \sigma(\mathbf{x}) = 0 \end{cases}$$

Expected Improvement

Bobak Shahriari ; Kevin Swersky ; Ziyu Wang ; Ryan P. Adams ; Nando de Freitas, *Taking the Human Out of the Loop: A Review of Bayesian Optimization,* Progress in Energy and Combustion Science, Volume 49, 2015, Pages 1-39

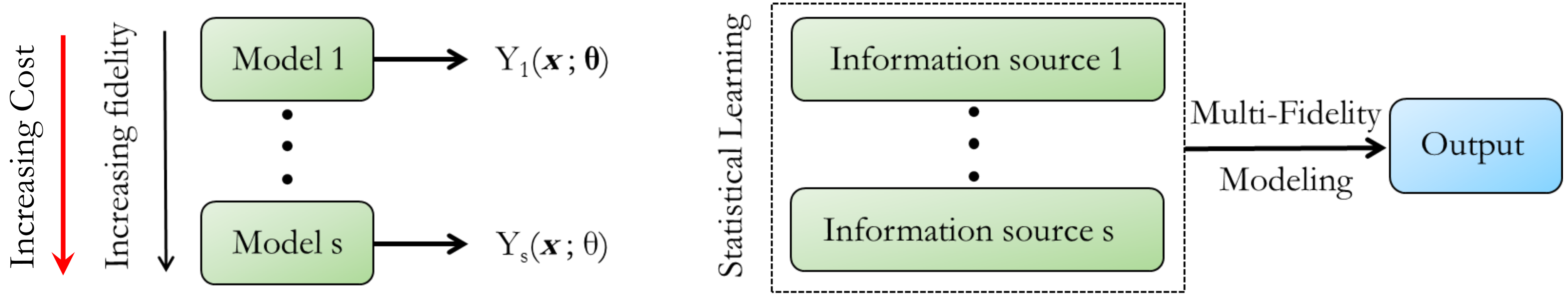
Acquisition Functions



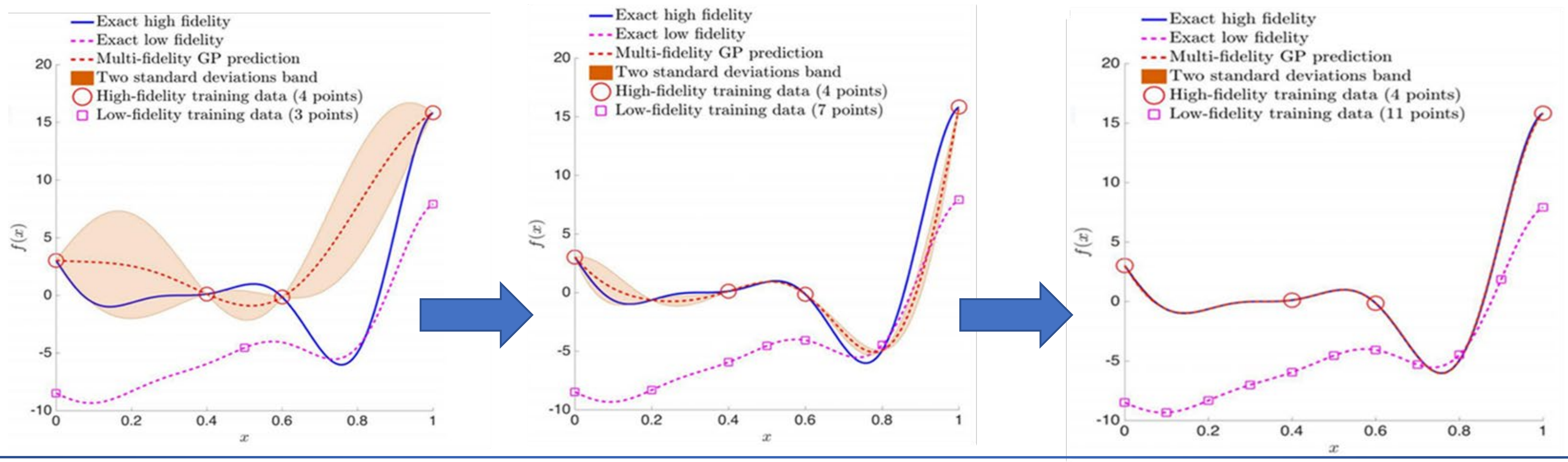
Hyperparameters of the acquisition function can be tuned to suit the exploration vs exploitation trade-off

Bobak Shahriari ; Kevin Swersky ; Ziyu Wang ; Ryan P. Adams ; Nando de Freitas, *Taking the Human Out of the Loop: A Review of Bayesian Optimization,* Progress in Energy and Combustion Science, Volume 49, 2015, Pages 1-39

Multi-Fidelity Surrogate Modeling



Auto-regressive scheme: $f_t(\mathbf{x}) = \rho_{t-1}(\mathbf{x}) f_{t-1}(\mathbf{x}) + \delta_t(\mathbf{x}), \quad t = 2, \ldots, s,$



Courtesy: Paris Perdikaris

Multi-Fidelity Modeling : Mathematical Formulation

Auto-regressive scheme: $f_t(\mathbf{x}) = \rho_{t-1} f_{t-1}(\mathbf{x}) + \delta_t(\mathbf{x}), \quad 2 \leq t \leq Q$ — Q fidelity levels

Multi-fidelity Input

$$\mathbf{X} = \begin{bmatrix} \mathbf{x}_1 \\ \mathbf{x}_2 \end{bmatrix}$$

Multi-fidelity Observations

$$\mathbf{y}_1 = f_1(\mathbf{x}_1) + \epsilon_1$$
$$\mathbf{y}_2 = f_2(\mathbf{x}_2) + \epsilon_2$$

Probabilistic Model

High Fidelity GP → $f_2(\mathbf{x}) = \rho_1 f_1(\mathbf{x}) + \delta(\mathbf{x})$

Low fidelity GP → $f_1(\mathbf{x}) \sim \mathcal{N}(0, k_1(\mathbf{x}, \mathbf{x}'; \boldsymbol{\theta}_1))$

GP → $\delta(\mathbf{x}) \sim \mathcal{N}(0, k_2(\mathbf{x}, \mathbf{x}'; \boldsymbol{\theta}_2))$

$$\epsilon_1 \sim \mathcal{N}(0, \sigma_{\epsilon_1}^2)$$
$$\epsilon_2 \sim \mathcal{N}(0, \sigma_{\epsilon_2}^2)$$

Training:

$$\mathbf{y} = \begin{bmatrix} \mathbf{y}_1 \\ \mathbf{y}_2 \end{bmatrix} \sim \mathcal{N}\left(\mathbf{0}, \begin{bmatrix} k_1(\mathbf{x}_1, \mathbf{x}_1'; \boldsymbol{\theta}_1) + \sigma_{\epsilon_1}^2 I & \rho_1 k_1(\mathbf{x}_1, \mathbf{x}_2'; \boldsymbol{\theta}_1) \\ \rho_1 k_1(\mathbf{x}_2, \mathbf{x}_1'; \boldsymbol{\theta}_1) & \rho_1^2 k_1(\mathbf{x}_2, \mathbf{x}_2'; \boldsymbol{\theta}_1) + k_2(\mathbf{x}_2, \mathbf{x}_2'; \boldsymbol{\theta}_2) + \sigma_{\epsilon_2}^2 I \end{bmatrix}\right)$$

Appropriate choice of kernel function

NLML = $-\log p(\mathbf{y}|\mathbf{X}, \boldsymbol{\theta}_1, \boldsymbol{\theta}_2, \rho_1, \sigma_{\epsilon_1}^2, \sigma_{\epsilon_2}^2) = \frac{1}{2}\log|\mathbf{K}| + \frac{1}{2}\mathbf{y}^T\mathbf{K}^{-1}\mathbf{y} - \frac{N_L + N_H}{2}\log 2\pi$

Prediction:

$$p(f(\boldsymbol{x}^*)|\boldsymbol{y}, \boldsymbol{X}, \boldsymbol{x}^*) \sim \mathcal{N}(f(\boldsymbol{x}^*)|\mu(\boldsymbol{x}^*), \sigma^2(\boldsymbol{x}^*))$$
$$\mu(\boldsymbol{x}^*) = \boldsymbol{k}(\boldsymbol{x}^*, \boldsymbol{X})\boldsymbol{K}^{-1}\boldsymbol{y}$$
$$\sigma(\boldsymbol{x}^*) = \boldsymbol{k}(\boldsymbol{x}^*, \boldsymbol{x}^*) - \boldsymbol{k}(\boldsymbol{x}^*, \boldsymbol{X})\boldsymbol{K}^{-1}\boldsymbol{k}(\boldsymbol{X}, \boldsymbol{x}^*)$$

GP predicting output by incorporating multi-fidelity information

Constrained Bayesian Optimization

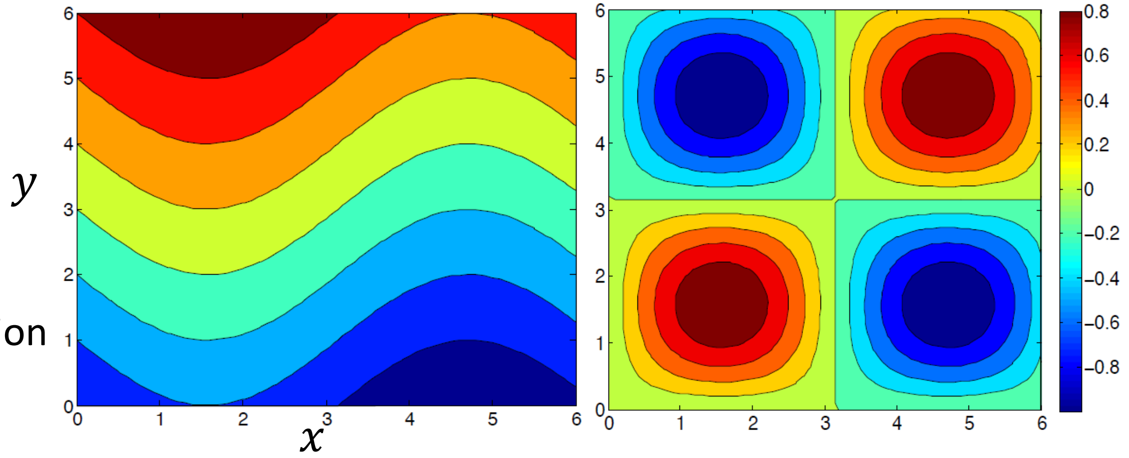
Model the constraint as an additional GP

$$\min_{c(\mathbf{x})\leq\lambda} \ell(\mathbf{x})$$

$$\begin{aligned} EI_C(\hat{\mathbf{x}}) &= \mathbb{E}\left[\tilde{I}_C(\hat{\mathbf{x}})|\hat{\mathbf{x}}\right] \\ &= \mathbb{E}\left[\tilde{\Delta}(\hat{\mathbf{x}})\tilde{I}(\hat{\mathbf{x}})|\hat{\mathbf{x}}\right] \\ &= \mathbb{E}\left[\tilde{\Delta}(\hat{\mathbf{x}})|\hat{\mathbf{x}}\right]\mathbb{E}\left[\tilde{I}(\hat{\mathbf{x}})|\hat{\mathbf{x}}\right] \\ &= PF(\hat{\mathbf{x}})EI(\hat{\mathbf{x}}), \end{aligned}$$

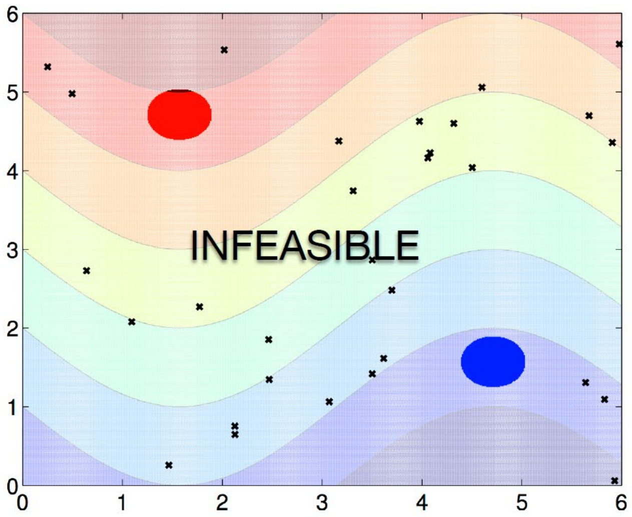
Unconstrained acquisition function

$$PF(\hat{\mathbf{x}}) := Pr\left[\tilde{c}(\mathbf{x}) \leq \lambda\right] = \int_{-\infty}^{\lambda} p(c(\hat{\mathbf{x}})|\hat{\mathbf{x}}, \mathcal{T}_c)dc(\hat{\mathbf{x}})$$

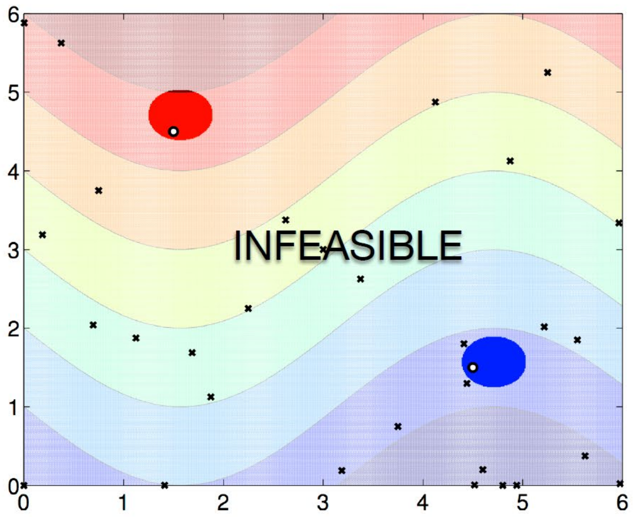


Minimize $l(x, y) = \sin(x) + y$ with $c(x, y) = \sin(x)\sin(y) \leq -0.95$

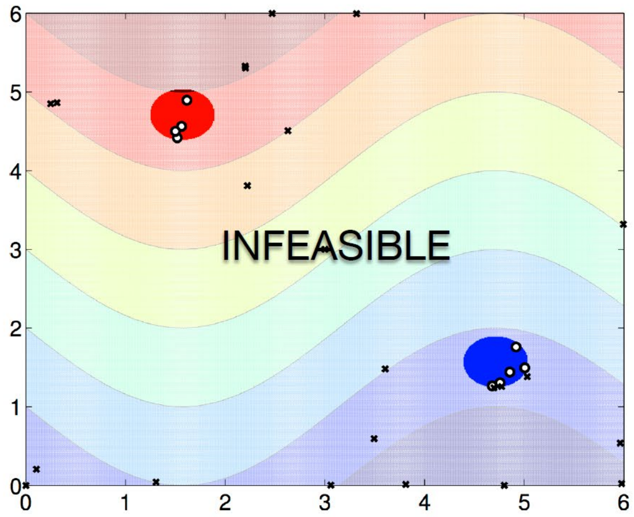
Uniform Sampling



Unconstrained BO



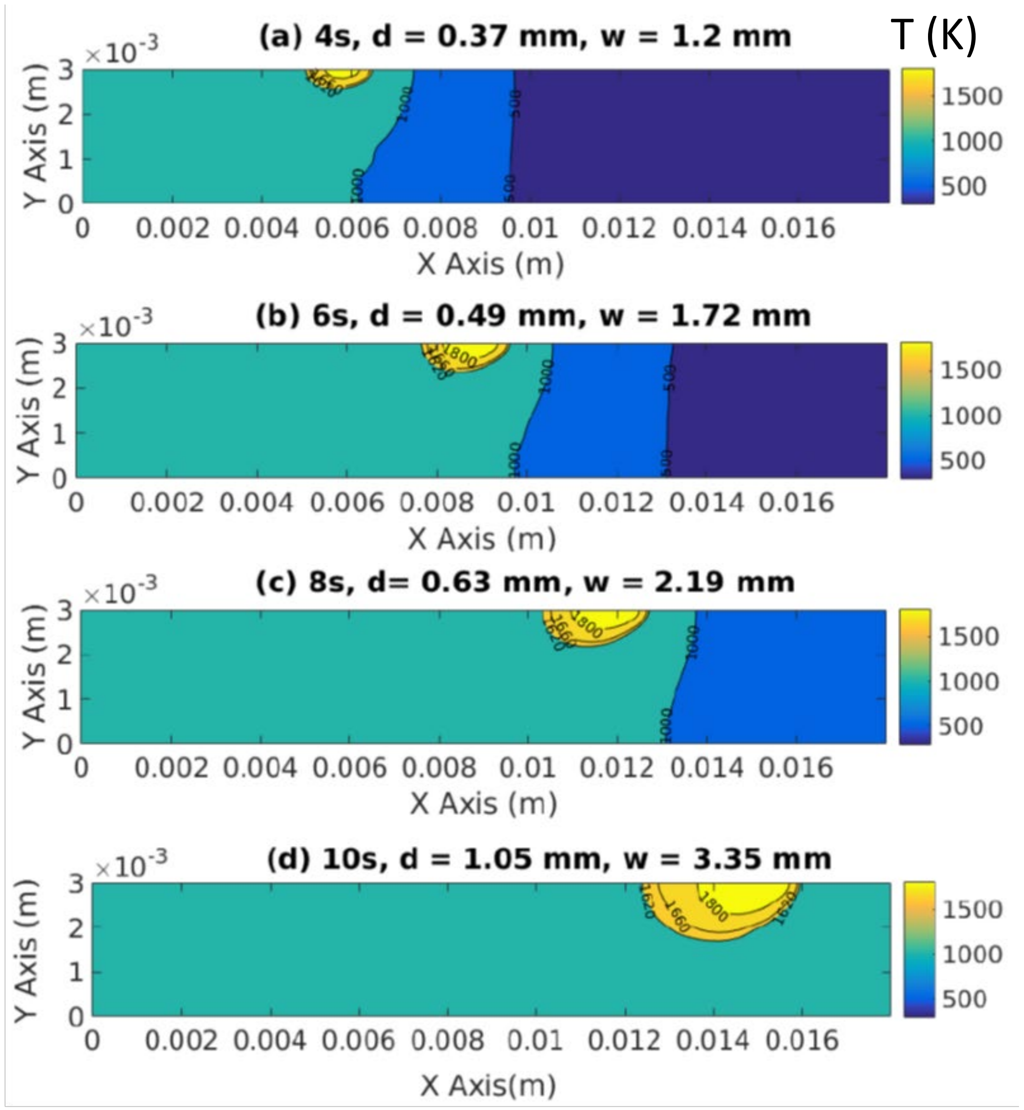
Constrained BO



Data-Driven Process Optimization

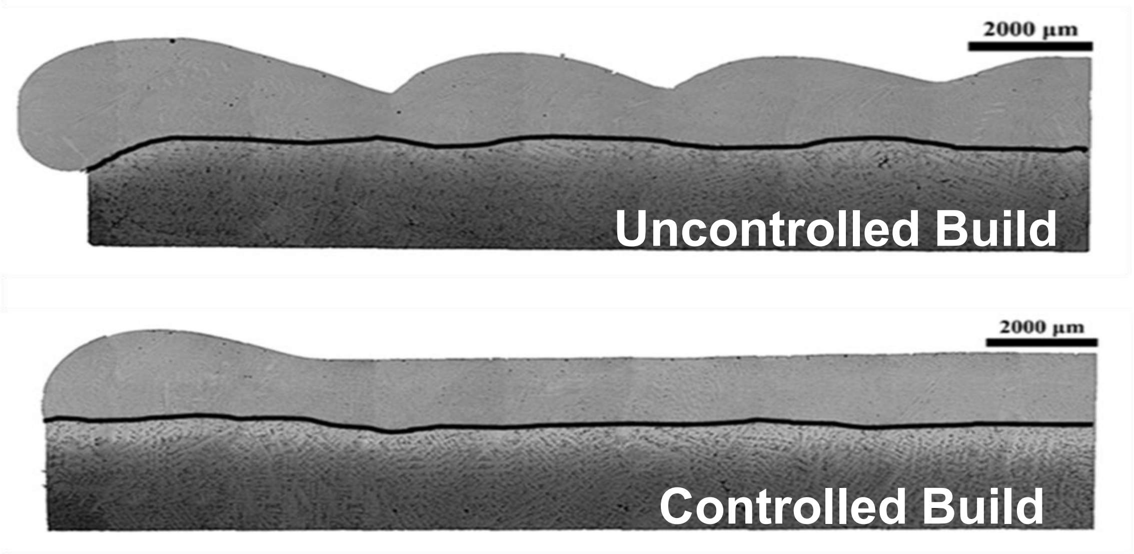
Need for Meltpool Geometry Control

P = 250 W, v = 1.5 mm/s



Uncontrolled Process Parameters

Simulation model: Low-fidelity model, simulates 2-D conductive heat transfer in a finite plate with convective boundary conditions

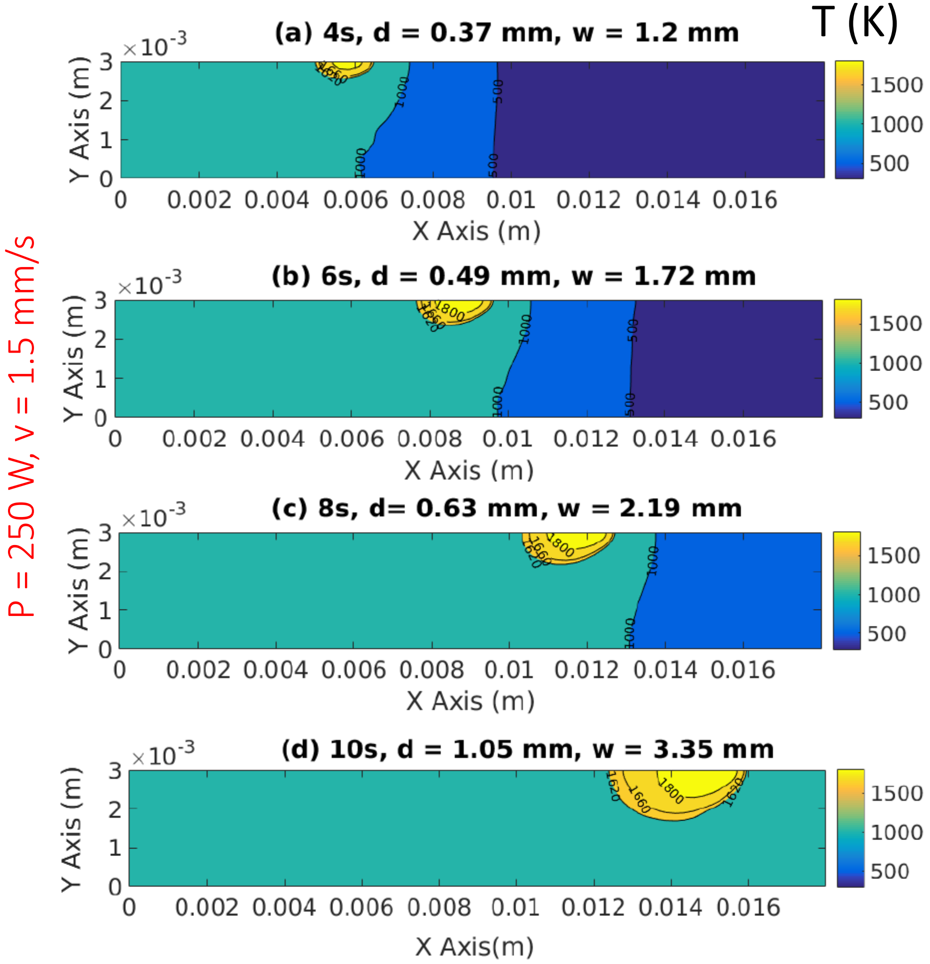


R. Bansal, PhD Thesis, Georgia Institute of Technology, 2013.

Controlling melt pool geometry is essential for maintaining build uniformity

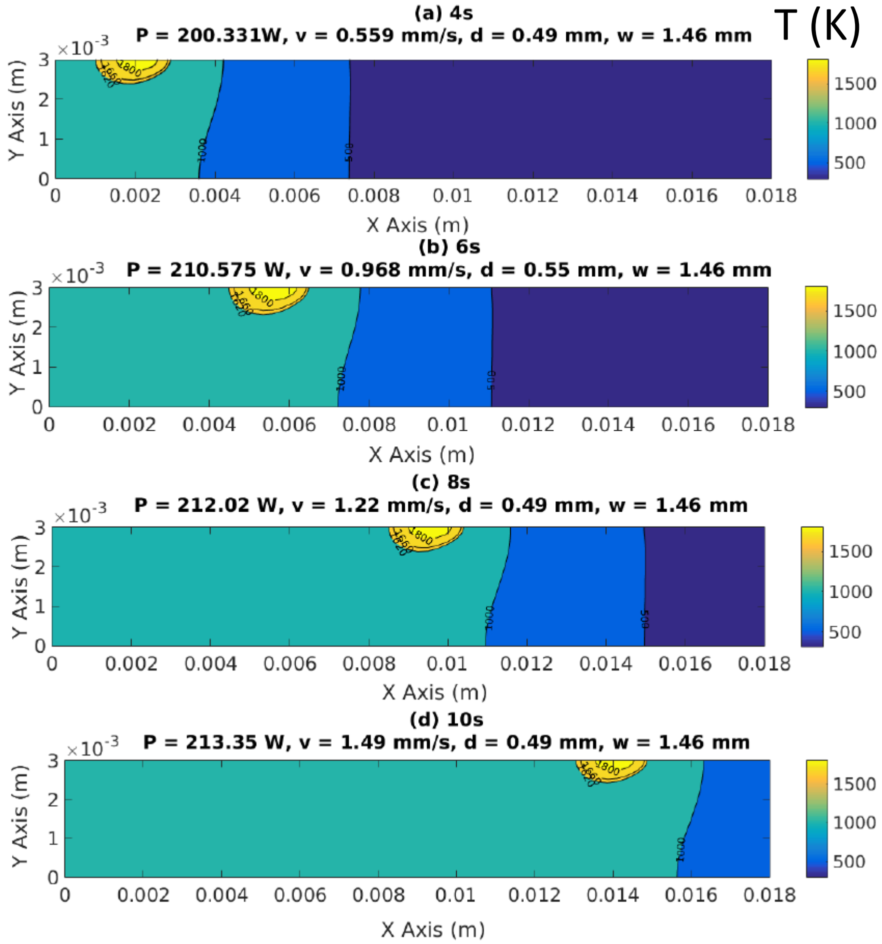
Process Parameter Optimization

Minimize Objective Function: $J \triangleq \left(\alpha \frac{\|d - d^*\|}{\|d^*\|} + (1 - \alpha) \frac{\|w - w^*\|}{\|w^*\|} \right), \quad \alpha \in [0, 1]$



Uncontrolled Process Parameters

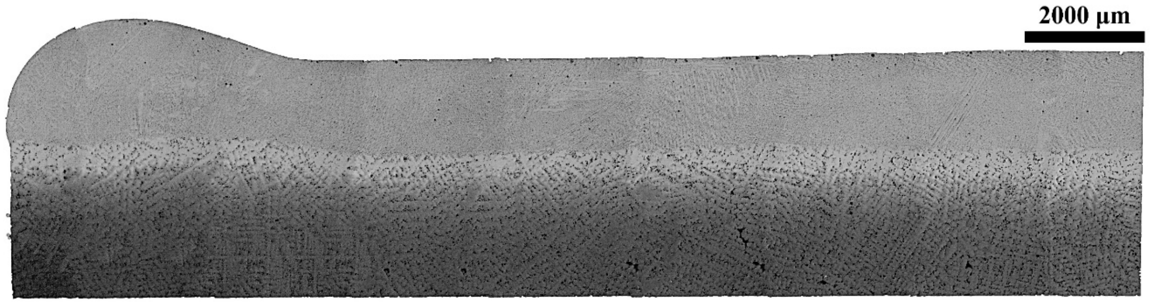
- 20 simulations for GP training
- 10 Optimization iterations

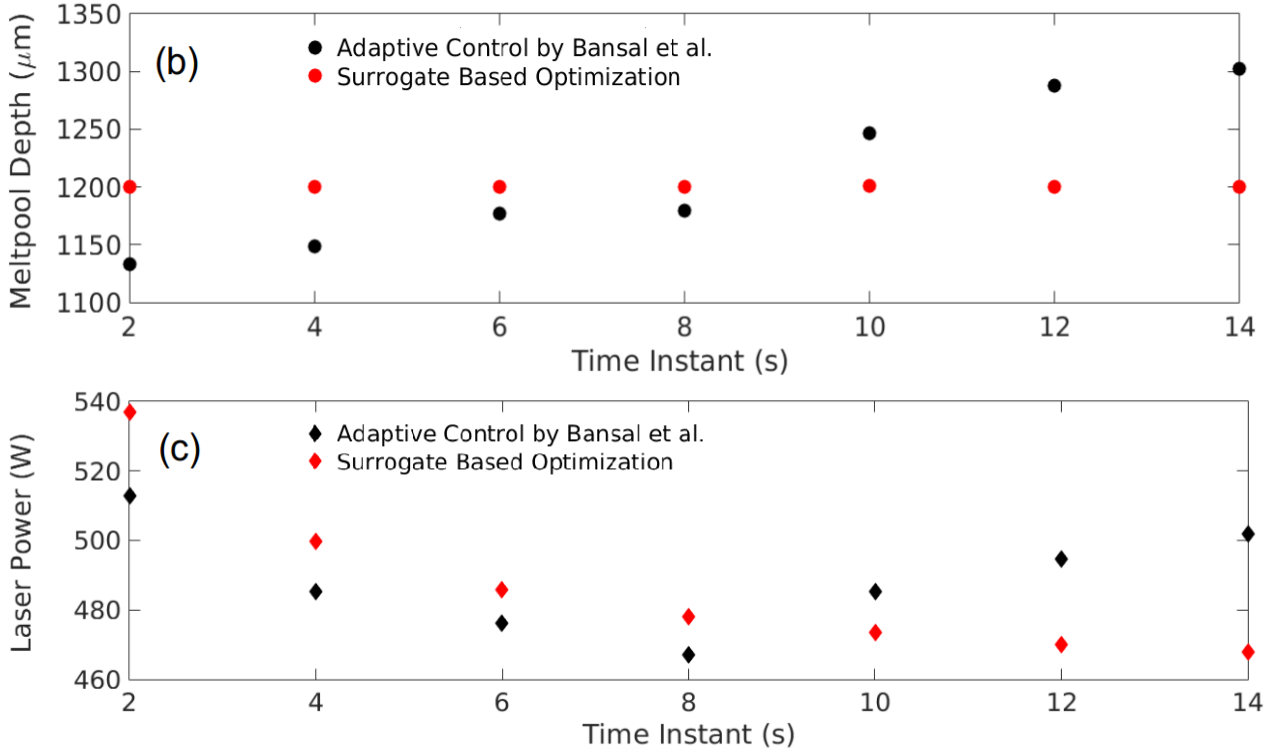


Optimized Process Parameters for d* = 0. 5 mm, w* = 1.5 mm

S. Mondal, D.Gwynn, A. Ray, A. Basak, *Investigation of Melt Pool Geometry Control in Additive Manufacturing using Hybrid Modeling*, Metals 2020, 10(5), 683

Meltpool Geometry Control





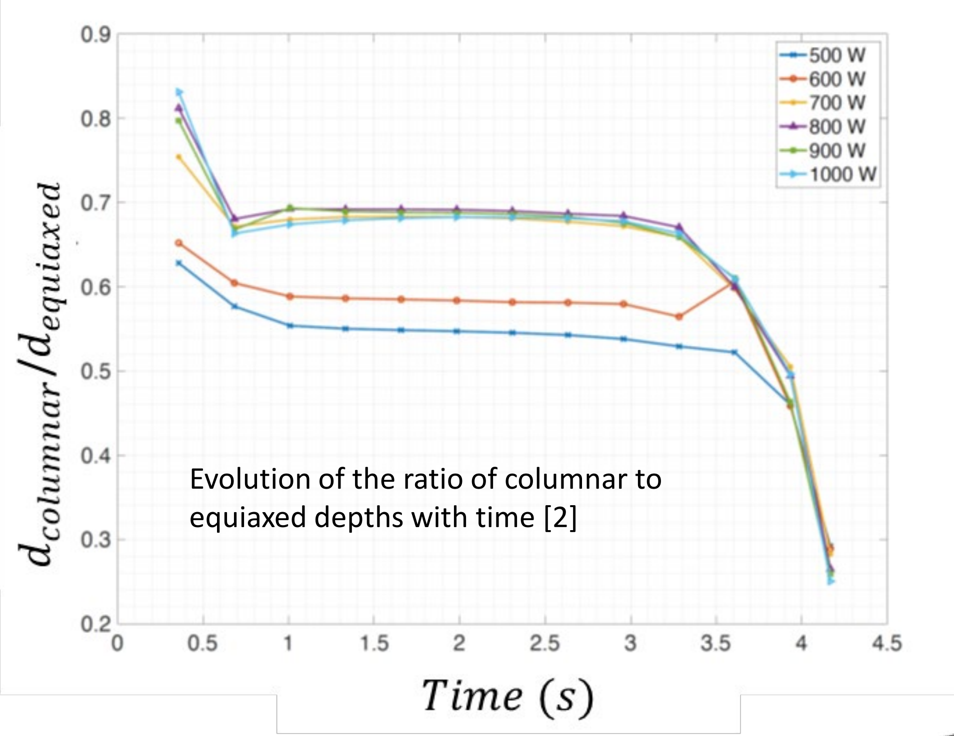
Controlled build process achieved at Georgia Tech using a Model Reference Adaptive Control policy with a constant reference temperature of 1575 ^{o}C

Objective Function

$$J \triangleq -\left(c_1 \frac{|d - d^*|}{|d^*|} + c_2 \frac{|P - P_{min}|}{|P_{max} - P_{min}|}\right)$$

Experimental validation on Rene 80 specimen

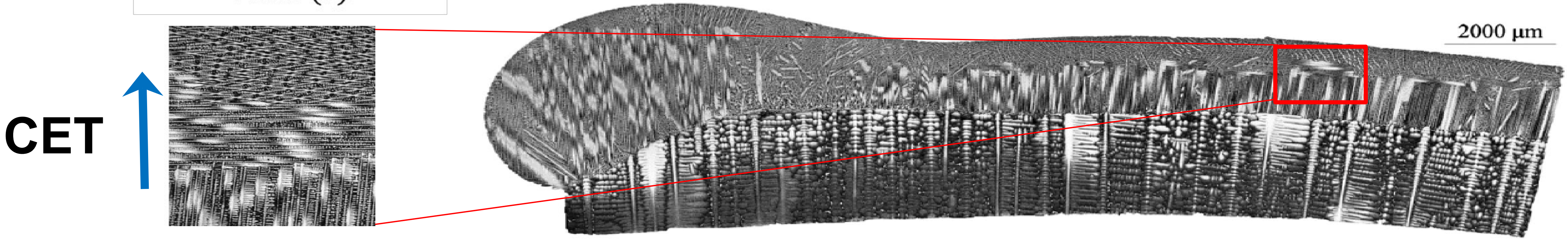
Columnar to Equiaxed Transition (CET)



Evolution of the ratio of columnar to equiaxed depths with time [2]

G: Thermal gradient V: Solidification velocity

- $\frac{G^n}{V}$ reduces with uncontrolled melt pool growth
- CET limits epitaxial single crystal growth
- Need for thermal gradient control



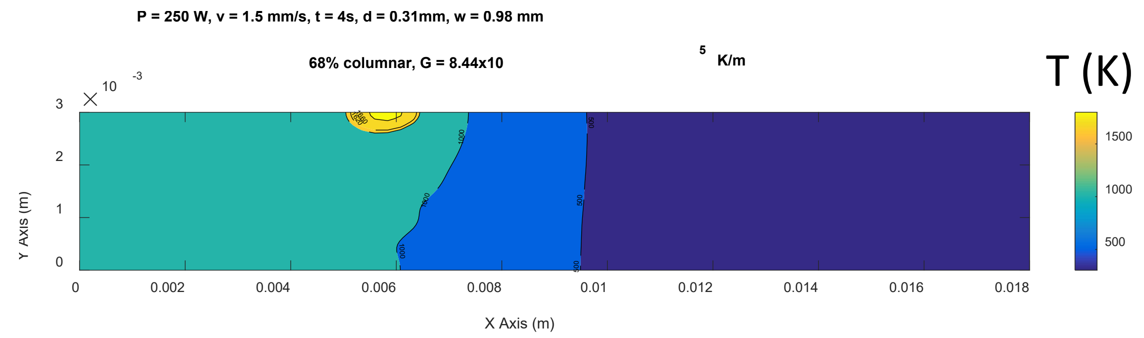
Transverse optical micrograph of Scanning Laser Epitaxy processed CMSX-4 specimen [1]

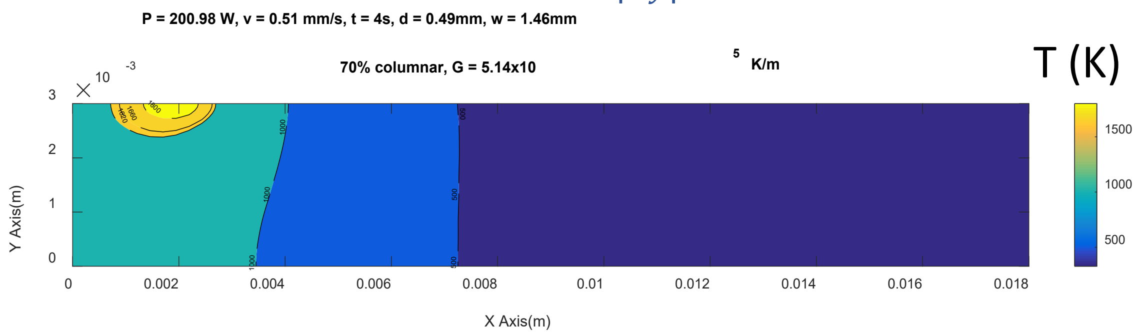
[1] A. Basak, R. Acharya, S. Das, Additive Manufacturing of Single-Crystal Superalloy CMSX-4 Through Scanning Laser Epitaxy: Computational Modeling, Experimental Process Development, and Process Parameter Optimization , Metallurgical and Material Transactions A, 2016 Metallurgical and Materials Transactions A.
[2] Image Courtesy: Nandana Menon

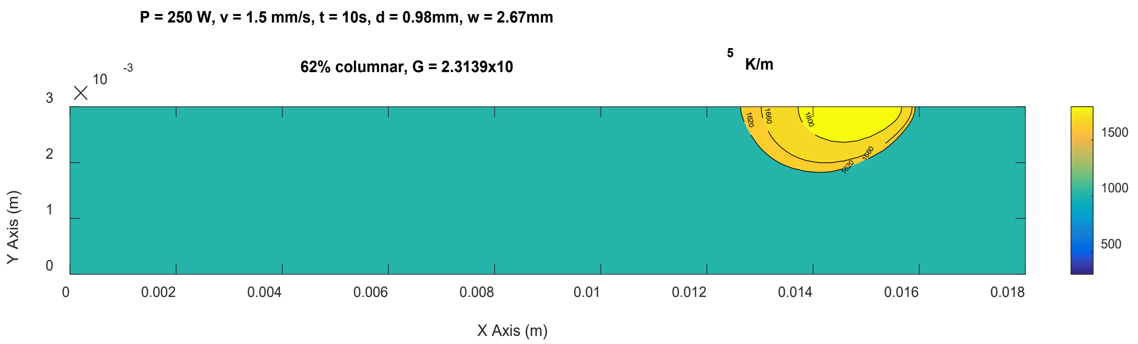
Constrained Melt pool Geometry Control

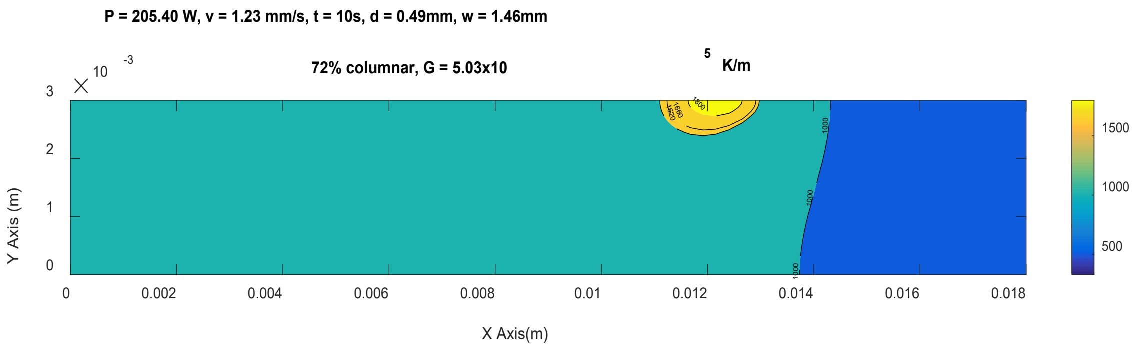
Minimize Objective Function : $J \triangleq \left(\frac{\|d - d^*\|}{\|d^*\|} + \frac{\|w - w^*\|}{\|w^*\|} \right)$ Subject to: **Columnar growth > 70%**

Columnar growth percentage ≜ percentage of nodes inside the melt pool that has $|G_y| > |G_x|$







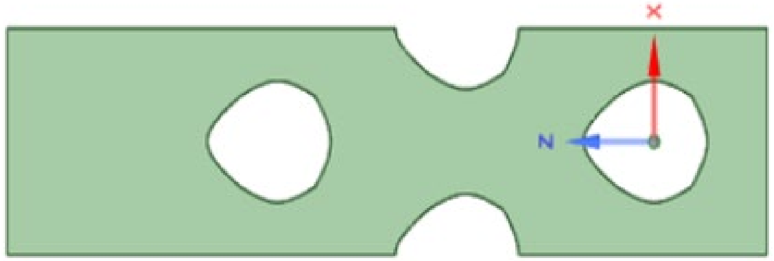


Uncontrolled Geometry : Columnar growth percentage drops

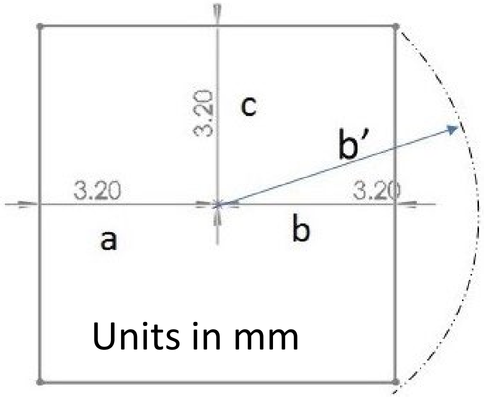
Controlled Geometry maintains columnar growth percentage

[1] S. Mondal, D. Gwynn, N. Menon, A. Ray, A. Basak, Selection of Process Parameters for Controlling Microstructural Properties in Additive Manufacturing: A Machine Learning Based Approach, TMS 2020, San Diego, California, USA

Comparison with Genetic Algorithm: Shape Optimization of Pin Fin Arrays

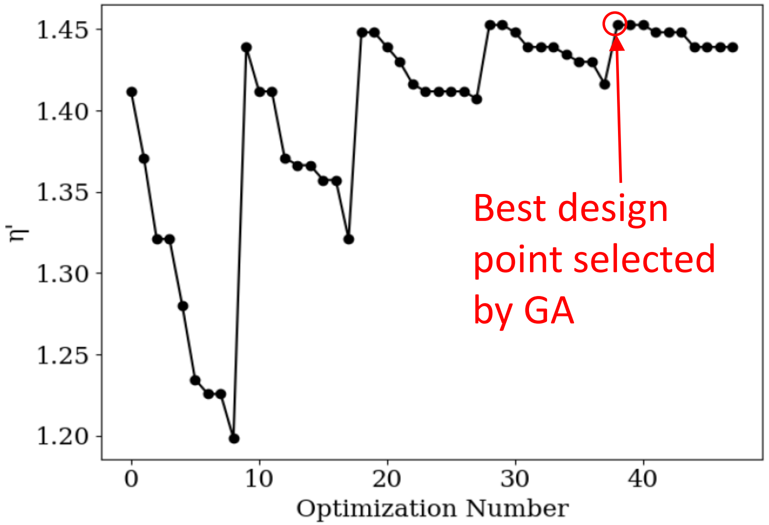


Problem: Optimize the shape of pin fin arrays for internal blade cooling in gas turbines. Collaborative work with University of Central Florida. Simulator: RANS CFD



- 3 parameter shape optimization
- Objective: Maximize thermal performance efficiency

Genetic Algorithm (GA)



Number of Function evaluations during Optimization

GA	BO
40	5

50 initial DoE for both

BO optima 1.2% greater than GA optima

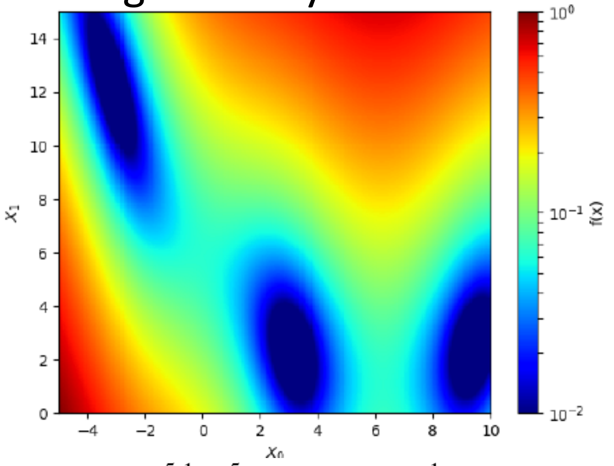
Accelerated search for optimum using BO

[1] S. Ghosh, S. Mondal, JS Kapat, A. Ray, *Parametric Shape Optimization of Pin Fin Arrays Using Surrogate Model Based Bayesian Methods*, Journal of Thermophysics and Heat Transfer, in press

[2] S. Ghosh, S. Mondal, JS Kapat, A. Ray, *Shape Optimization of Pin Fin Arrays Using Gaussian Process Surrogate Models Under Design Constraints*, GT2020-15277, accepted in ASME 2020 Turbo Expo, 2020

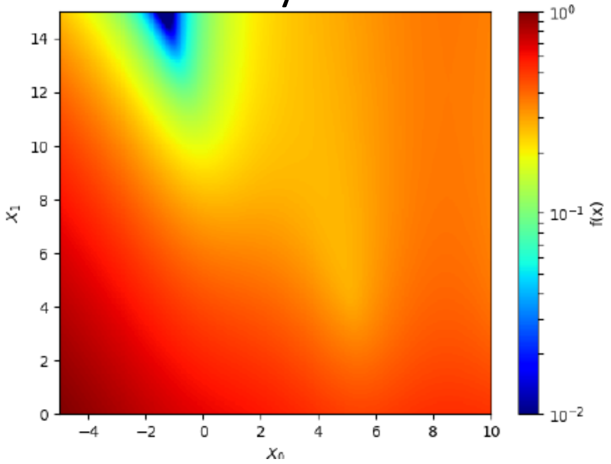
2-D Problem : Complex Discrepancies

High Fidelity Function

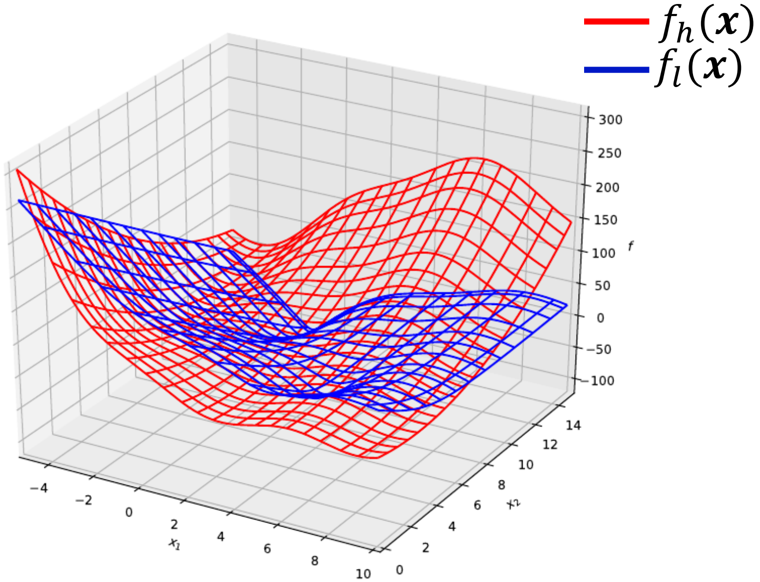


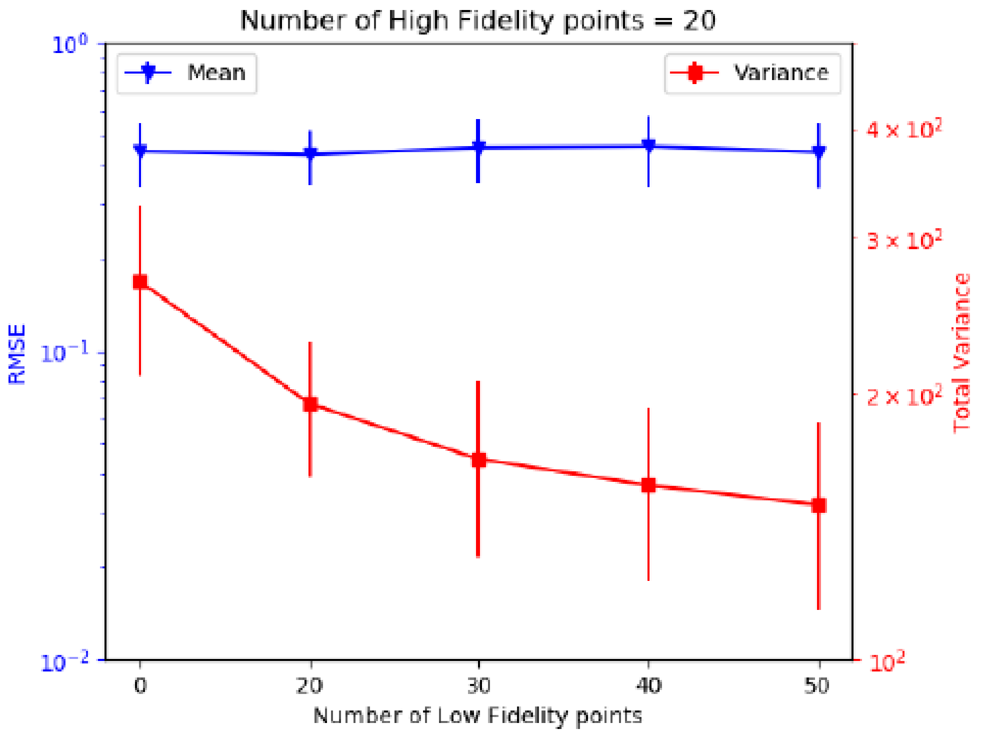
$$f_h(\mathbf{x}) = (x_2 - \frac{5.1}{4\pi^2} + \frac{5}{\pi}x_1 - 6)^2 + 10(1 - \frac{1}{8\pi})cos(x_1) + 10$$

Low Fidelity Function



$$f_l(\mathbf{x}) = (10\sqrt{f_h(\mathbf{x}-2)} + 2(x_1 - 2.5) - 3(3x_2 - 7) - 1$$





- Global Variance Reduction with LF points

RMSE: Root Mean Squared Error

SFGP and MFGP Algorithms

Single Fidelity Gaussian Process (SFGP) based Optimization

1. Start with surrogate models of objective and constraints from initial HF data
2. Sample HF point as $\text{argmax}_{\mathbf{x}} EI_c(\mathbf{x})$
3. Add the HF point with its objective and constraints for retraining the surrogates
4. Repeat 2-3 for $N_{iteration}$ times, which is the number of HF optimization iterations

$$\text{EI}(\mathbf{x}) = \begin{cases} (\mu(\mathbf{x}) - f(\mathbf{x}^+) - \xi)\Phi(Z) + \sigma(\mathbf{x})\phi(Z) & \text{if } \sigma(\mathbf{x}) > 0 \\ 0 & \text{if } \sigma(\mathbf{x}) = 0 \end{cases}$$

$$Z = \begin{cases} \frac{\mu(\mathbf{x}) - f(\mathbf{x}^+) - \xi}{\sigma(\mathbf{x})} & \text{if } \sigma(\mathbf{x}) > 0 \\ 0 & \text{if } \sigma(\mathbf{x}) = 0 \end{cases}$$

$$EI_c(\mathbf{x}) = PF(\mathbf{x})EI(\mathbf{x})$$

Multi-Fidelity Gaussian Process (MFGP) based Optimization

Algorithm 1 Multifidelity Optimization Routine

Require: Start with surrogate models of objective and constraints from initial HF/LF data

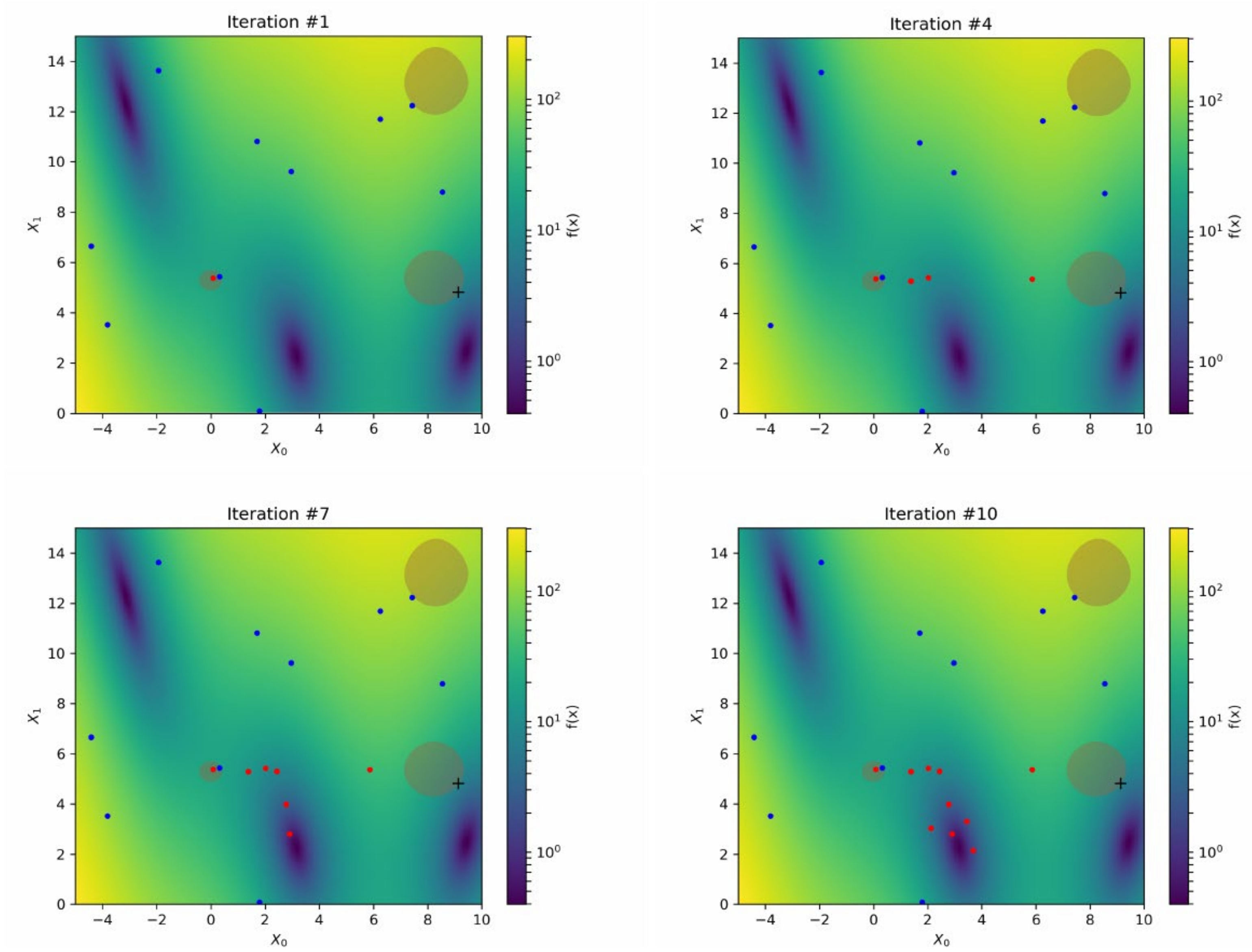
```
for N_iteration optimizations steps do
    Sample HF point as argmax_x EI_c(x)
    Add the HF point with its objective and constraints to the surrogate model
    Retrain the surrogate model
    for N_ratio times do
        Sample LF point as argmax_x GP − MI(x) with constraint penalization
        Add the LF point back to the surrogate model with its objective and constraints
        Retrain the surrogate model
    end for
end for
```

Mean ↑ Variance ↑

$$GP - MI_c(\mathbf{x}) = PF(\mathbf{x})(\mu_t(\mathbf{x}) + \phi_t(\mathbf{x}))$$

S. Sarkar, S. Mondal, M. Joly, M. Lynch, S. Bopardikar, R. Acharya, P. Perdikaris, *Multi-Fidelity and Multi-Scale Bayesian Framework for High-Dimensional Engineering Design and Calibration*, ASME Journal of Mechanical Design

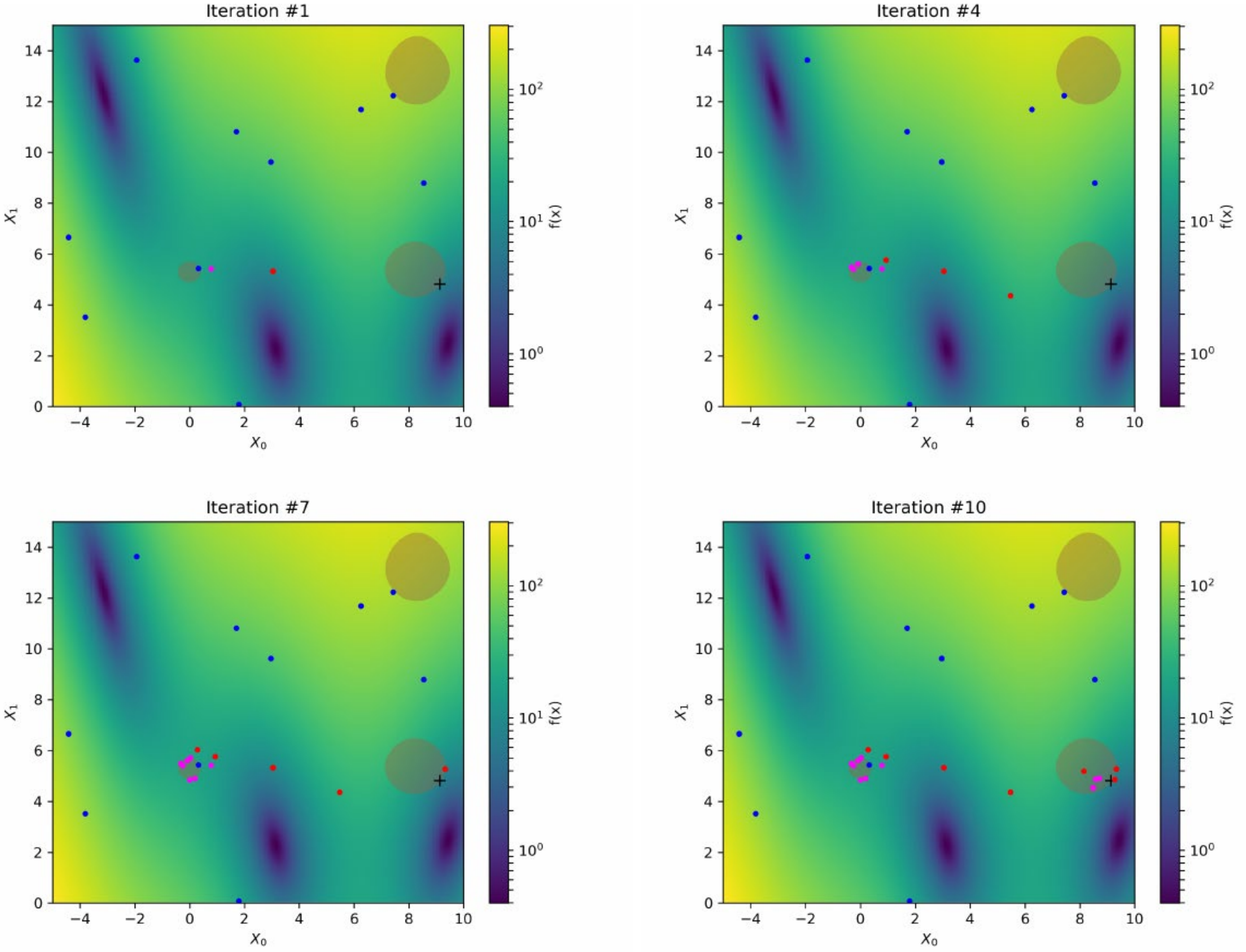
Case A: Constraint violation with SFGP



$N_H = 10$ LHS

(Latin Hypercube Samples for DoE)

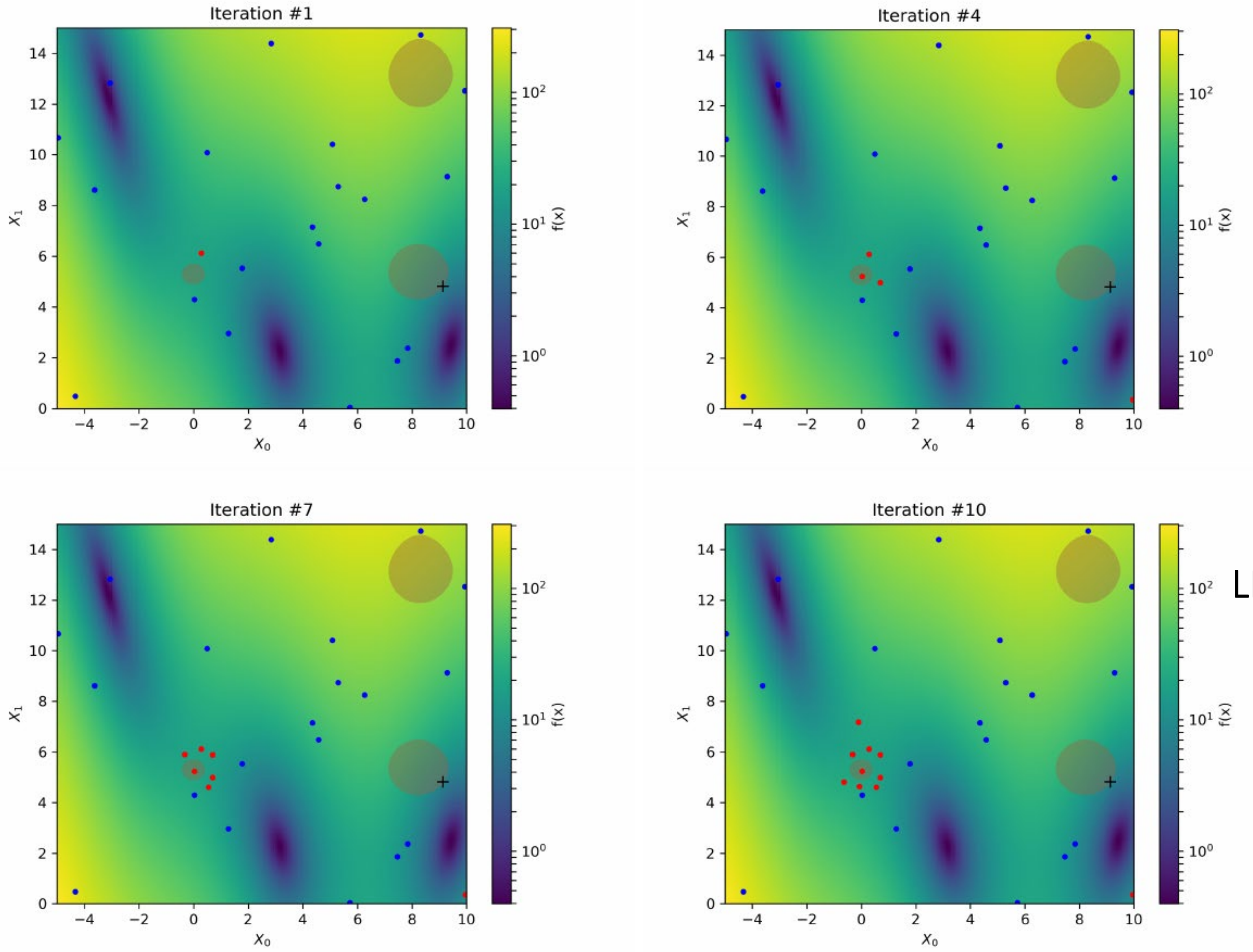
Case A: Constraint satisfied with MFGP



$N_H = 10$ LHS

$N_L = 20$ LHS

Case B : Non-optimal convergence with SFGP



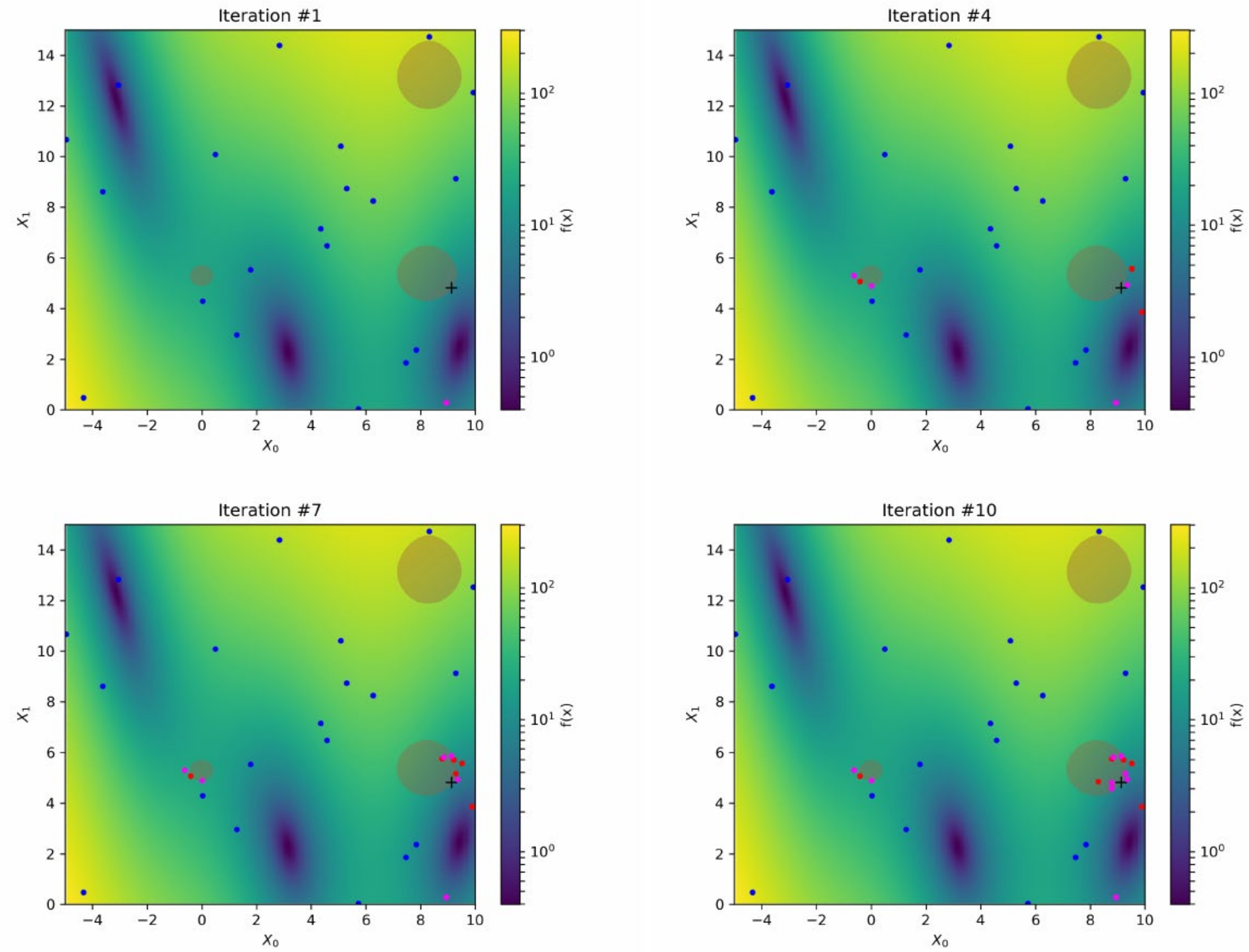
- Initial DoE
- Optimization iterations

$N_H = 20$ LHS

LHS : Latin Hypercube Sampling for initial Design of Experiments (DoE)

S. Sarkar, S. Mondal, M. Joly, M. Lynch, S. Bopardikar, R. Acharya, P. Perdikaris, *Multi-Fidelity and Multi-Scale Bayesian Framework for High-Dimensional Engineering Design and Calibration*, ASME Journal of Mechanical Design

Case B : Convergence with MFGP



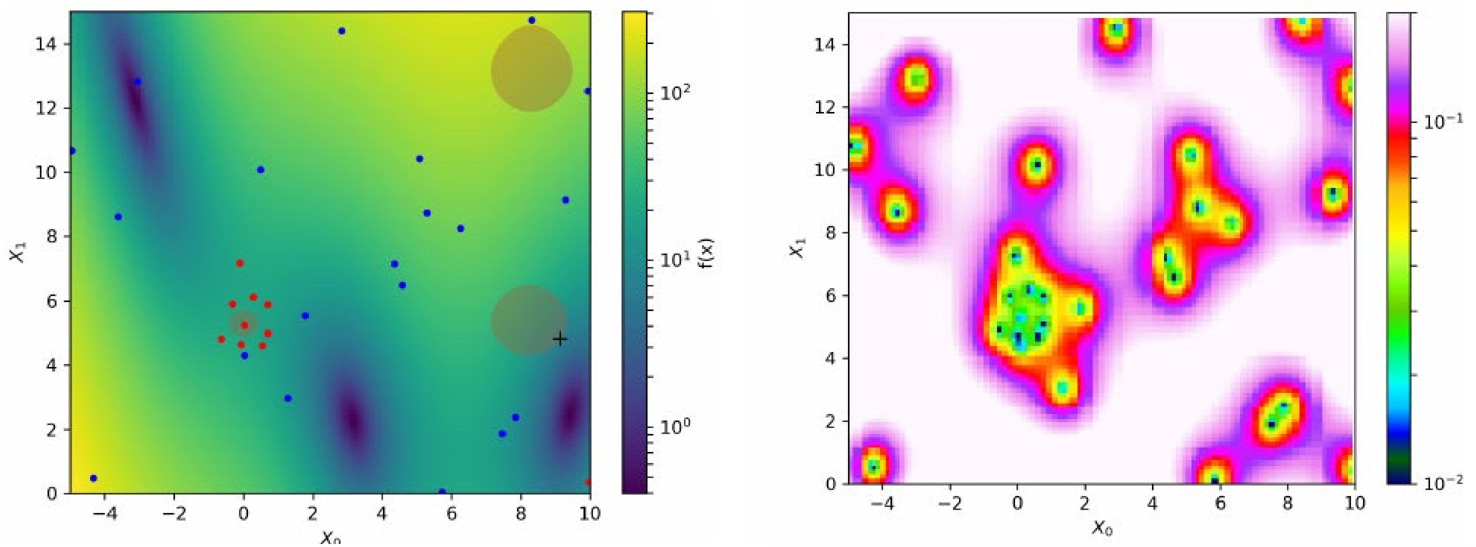
- Initial DoE
- HF Optimization iterations
- LF Optimization iterations

N_H = 20 LHS

N_L = 40 LHS

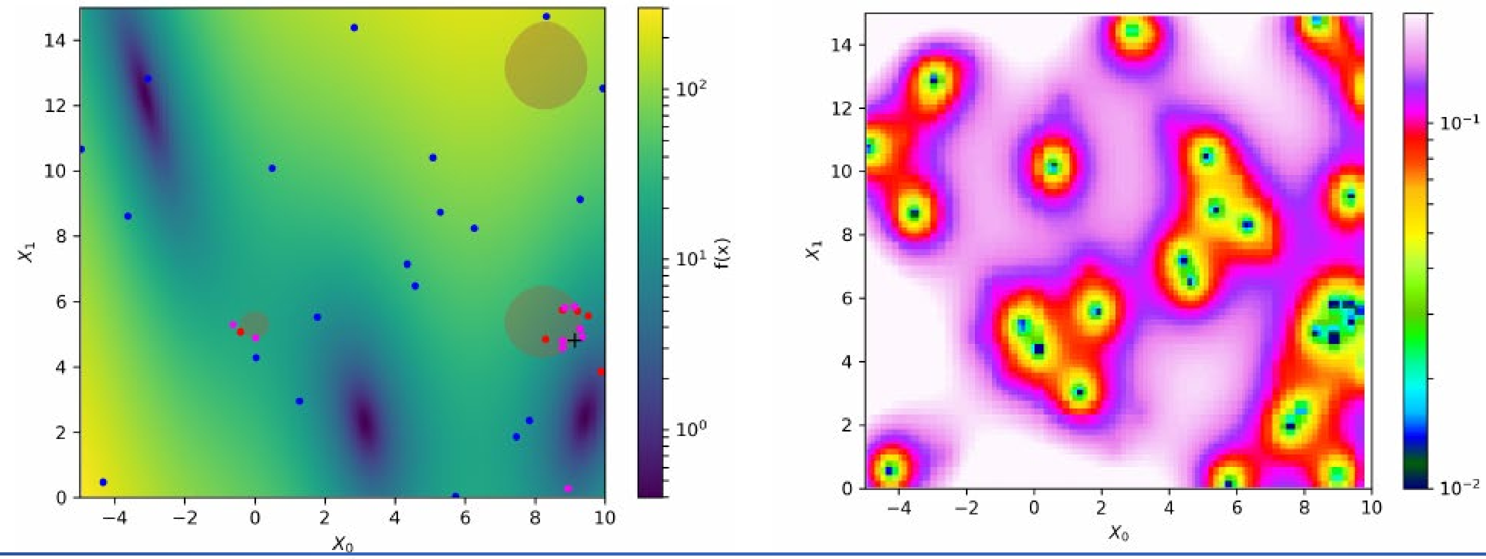
S. Sarkar, S. Mondal, M. Joly, M. Lynch, S. Bopardikar, R. Acharya, P. Perdikaris, *Multi-Fidelity and Multi-Scale Bayesian Framework for High-Dimensional Engineering Design and Calibration*, ASME Journal of Mechanical Design

Uncertainty Reduction in MFGP



SFGP

$N_H = 20$ LHS



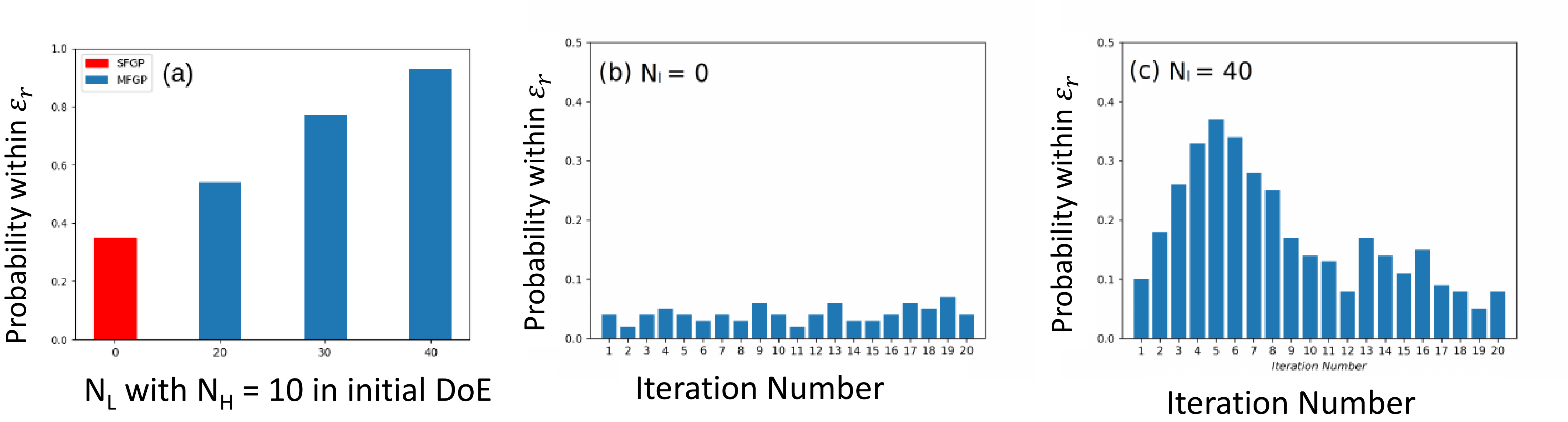
MFGP

$N_H = 20$ LHS

$N_L = 40$ LHS

S. Sarkar, S. Mondal, M. Joly, M. Lynch, S. Bopardikar, R. Acharya, P. Perdikaris, *Multi-Fidelity and Multi-Scale Bayesian Framework for High-Dimensional Engineering Design and Calibration*, ASME Journal of Mechanical Design

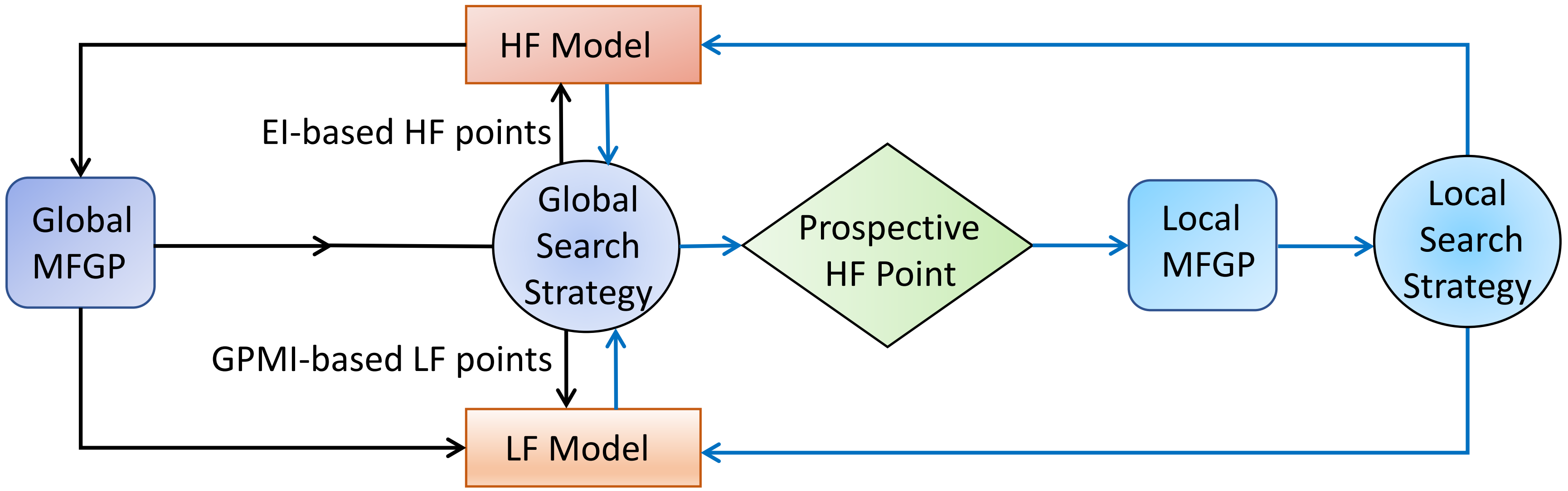
Probabilistic Performance in Branin function Optimization



(a) Probability of $e_r < 0.06$ at subsequent Bayesian Optimization iterations with initial $N_h = 10$ and variable N_l for Island constraint. Convergence rates with (b) SFGP and (c) MFGP having $N_l = 40$.

Average results over 100 different initializations

Proposed MFGP Optimization Framework

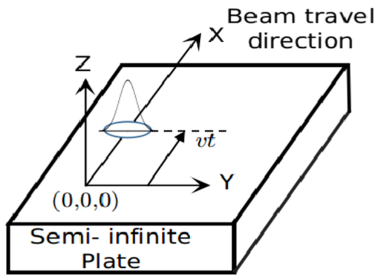


Parallel Global-Local Optimization Strategy

- Prospective HF Point: Improved objective with constraint satisfaction
- Multi-instance HF point selection through hierarchical clustering of EI Acquisition function
- Multi-instance LF point selection through hierarchical clustering of GP-MI Acquisition function

Melt pool Geometry Control: MFGP

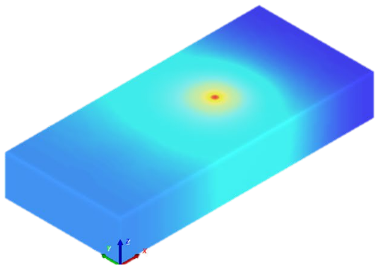
❑ **Low Fidelity (LF) Model : Eagar-Tsai's Analytical Model**



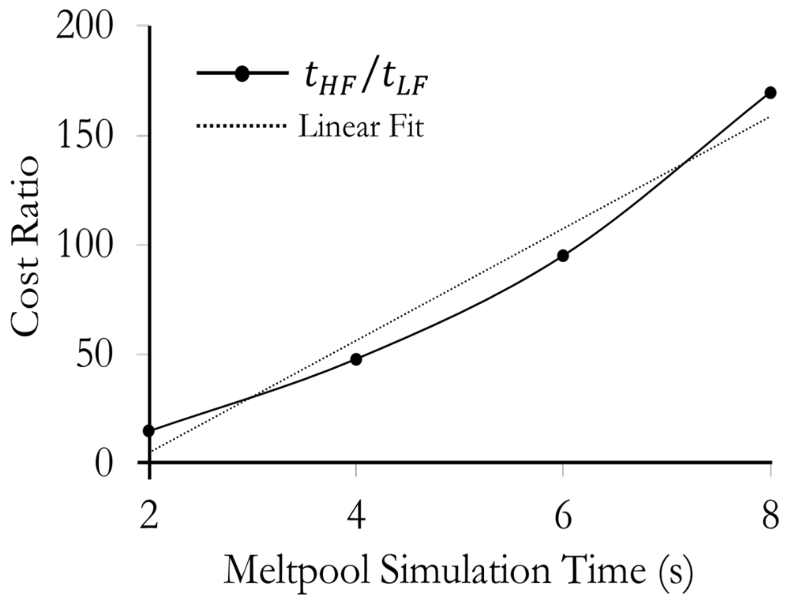
- **Analytical heat transfer model in 3D**
- **Convective/radiative heat transfer ignored**
- **Temperature independent thermophysical properties**
- **Semi-infinite substrate, implying negligible rise of surface temperature with time**
- **Phase change of substrate material ignored**

$$T(x,y,z,t) = \frac{\alpha q}{\pi\rho c\sqrt{4\pi a}}\int_0^t \frac{(t-t')^{-\frac{1}{2}}}{2a(t-t')+\sigma^2}\, e^{-\frac{(x-vt')^2+y^2}{4a(t-t')+2\sigma^2}-\frac{z^2}{4a(t-t')}}dt'$$

❑ **High Fidelity (HF) Model: Autodesk Netfabb DED Simulation**



- **Non-linear decoupled 3D transient FEM**
- **Radiative and Convective losses**
- **Temperature dependent thermophysical properties**
- **Includes Marangoni convection effect**



❑ **Cost Ratio**

- **Cost of HF model significantly higher than LF model**
- **Cost increases with simulation time**
- **Need to optimize within budget constraints**

GOAL: Optimize process parameters in a multi-fidelity setting for a controlled build height under budget limitations

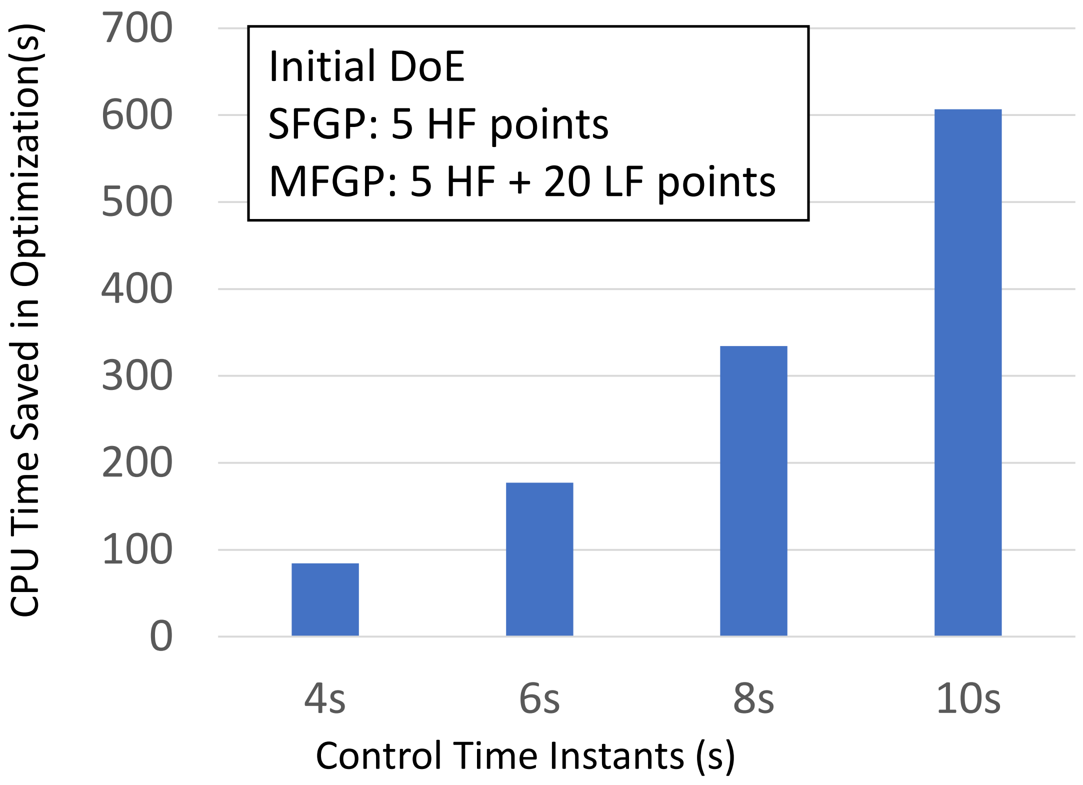
[1] S. Mondal, N. Menon, D. Gwynn, A. Ray, A. Basak, *Multi-Fidelity Surrogate Assisted Framework for Prediction and Control of Meltpool Geometry in Additive Manufacturing Processes*, **Invited Poster**, ICME Gap Analysis in Materials Informatics: Databases, Machine Learning, and Data-Driven Design, TMS 2020, San Diego, California, USA

Melt pool Geometry Control: MFGP

- CPU Time Saved = $(t_{HF} - t_{LF})(\bar{N}_{SFGP} - \bar{N}_{MFGP}) - \bar{N}_{MFGP}\, t_{LF}$

$\bar{N}_{SFGP}$: Average # of optimization steps using SFGP

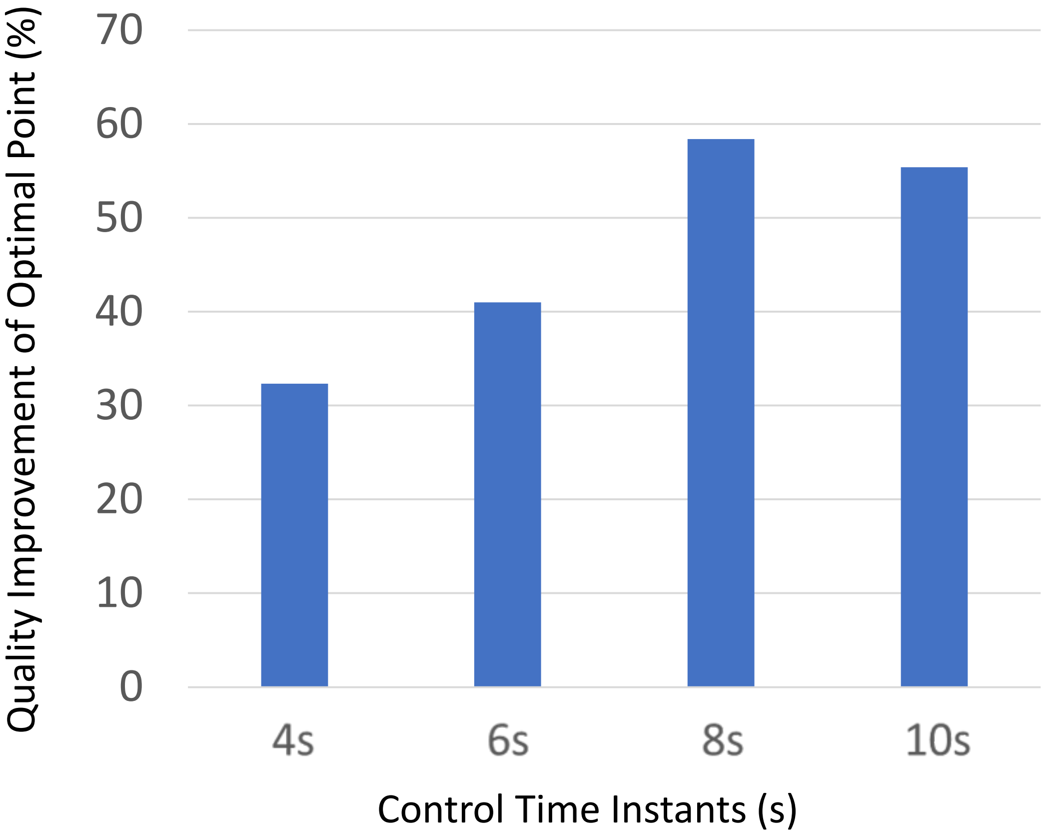
$\bar{N}_{MFGP}$: Average # of optimization steps using MFGP



Significant Cost Savings

- Quality Improvement = $\frac{RMSE_{SFGP} - RMSE_{MFGP}}{RMSE_{SFGP}} \times 100\%$

$$RMSE = \|d^* - d_{opt}\|_2$$



Improved Optimal Points

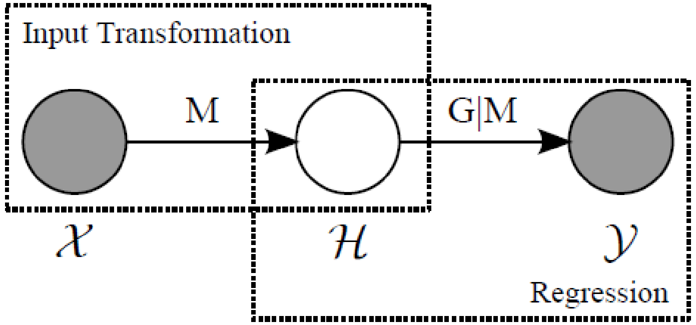
Ongoing Extensions and Future Work

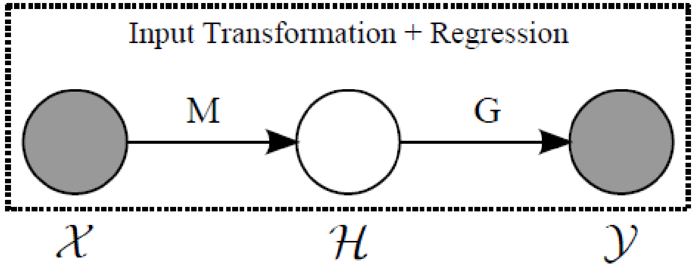
- Developing Multi-Fidelity strategies for internal flow simulations in fuel injectors, with an aim to speed up emulator design

- Developing Multi-Fidelity framework for melt pool geometry control with microstructural constraints ⟶ Multi-scale Multi-fidelity modeling optimization

- Manifold Learning: Handling heterogeneity of the possibly high dimensional input space through a supervised dimension reduction ⟶ Required when high and low fidelities have different input spaces, need to learn from common subspace

- Deep MFGPs: Handling discontinuities across fidelity levels ⟶ Required for handling more general correlations/discrepancies across fidelity levels





$$\tilde{k}(\boldsymbol{x}_p, \boldsymbol{x}_q) = k\left(M(\boldsymbol{x}_p), M(\boldsymbol{x}_q)\right)$$

R. Calandra, J. Peters, C.E. Rasmussen, M Deisenroth. *Manifold Gaussian Processes for Regression,* ArXiv Preprints, 2014

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(United Technologies Research Center, now Raytheon Technologies)

Dr. Shaunak Bopardikar (Michigan State)

Dr. Jayanta Kapat, Shinjan Ghosh (University of Central Florida)

Current extensions in Multiphase flow simulations at Argonne:

Dr. Gina Magnotti, Dr. Roberto Torelli (ES)
Dr. Bethany Lusch (ALCF)

Bottomline : A less accurate model is not always bad !

THANK YOU!

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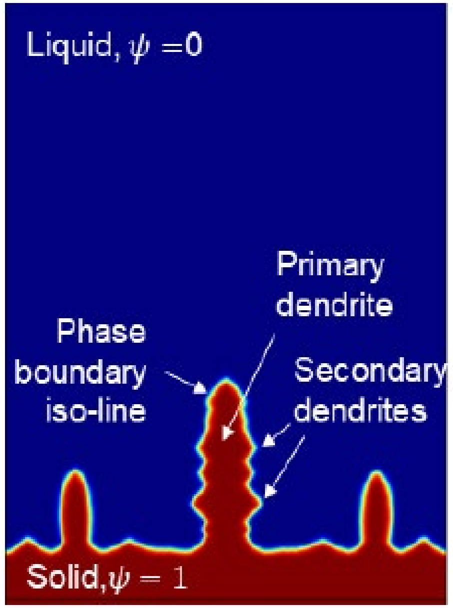
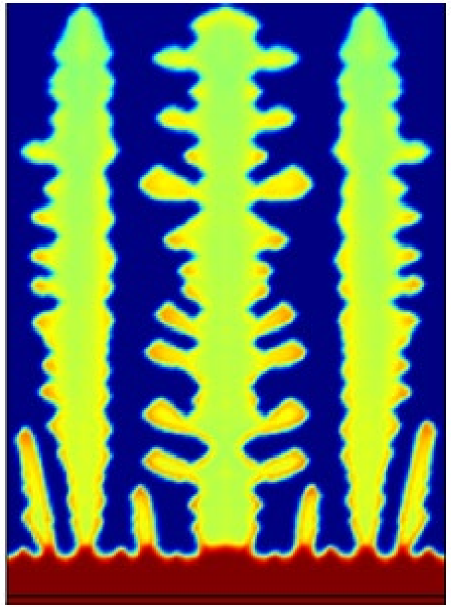
Backup Slides

Calibration of Phase-Field Model



Well Calibrated Model



Poorly Calibrated Model

Phase Field Equation [1]:

$$\tau_C \frac{\partial \psi}{\partial t} = \tilde{\varepsilon}^2 \nabla . \left(\begin{pmatrix} \eta^2 & -\eta\eta' \\ \eta\eta' & \eta^2 \end{pmatrix} \nabla \psi \right) + \psi(1-\psi)\left(\psi - \frac{1}{2} + m\right)$$

$$m = (\alpha/\pi)\left[\gamma[T_m - T + m_L(c_l - c_0)]\right]$$

Objective: Obtain a sharp (crisp) interface between solid and liquid phases
Constraint: Avoid phase distributions that are too planar

System contains several numerical constants that need to be tuned to match experiments

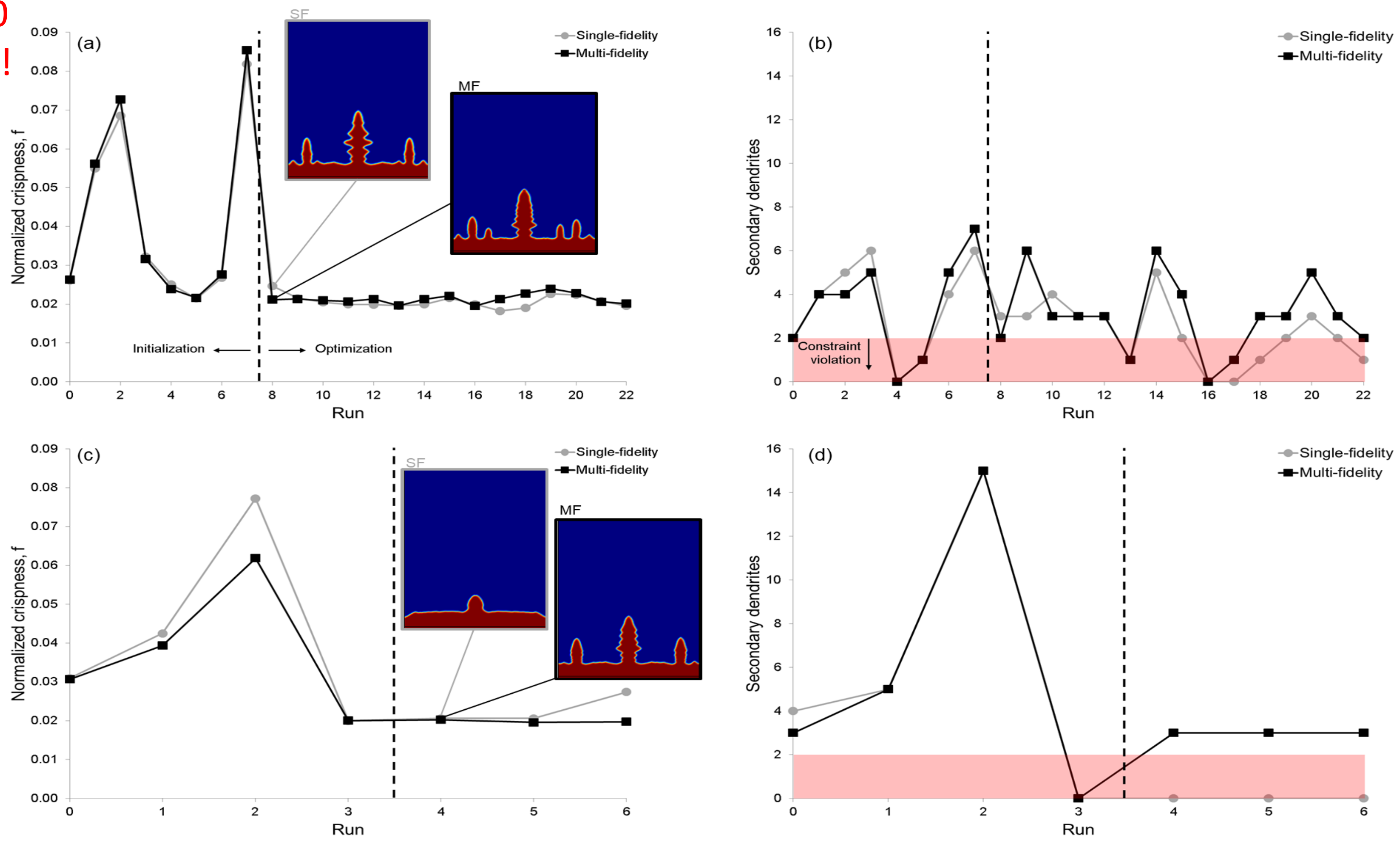
α : slope parameter
$\tilde{\varepsilon}$: constant representing penalty for interface thickness
τ_C : Fitting parameter

Ranadip Acharya, John A. Sharon, Alexander Staroselsky. *Prediction of microstructure in laser powder bed fusion process*. Acta Materialia 124 (2017) 360 - 371

Multi-Fidelity and Multi-Scale Bayesian Framework for High-Dimensional Engineering Design and Calibration, S. Sarkar, S. Mondal, M. Joly, M. Lynch, S. Bopardikar, R. Acharya, P. Perdikaris, ASME Journal of Mechanical Design

Minimize a normalized crispness metric subject to number of secondary dendrites ≥2

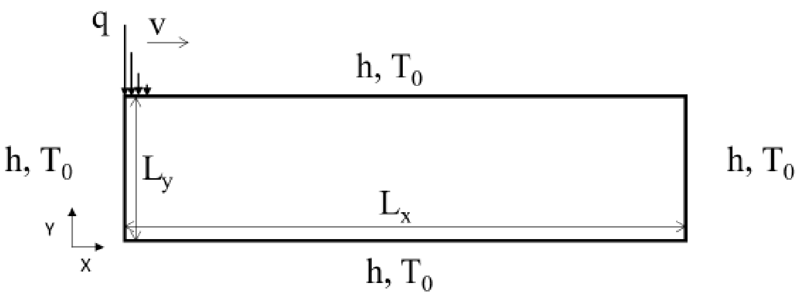
Manual tuning took ~100 iterations!



- Good agreement within ~10 ML optimizations
- MFGP yields more compliant solutions
- Better learning of the narrow feasibility region

Multi-Fidelity and Multi-Scale Bayesian Framework for High-Dimensional Engineering Design and Calibration, S. Sarkar, S. Mondal, M. Joly, M. Lynch, S. Bopardikar, R. Acharya, P. Perdikaris, ASME Journal of Mechanical Design

Directed Energy Deposition: 2D Model for Thermal Field



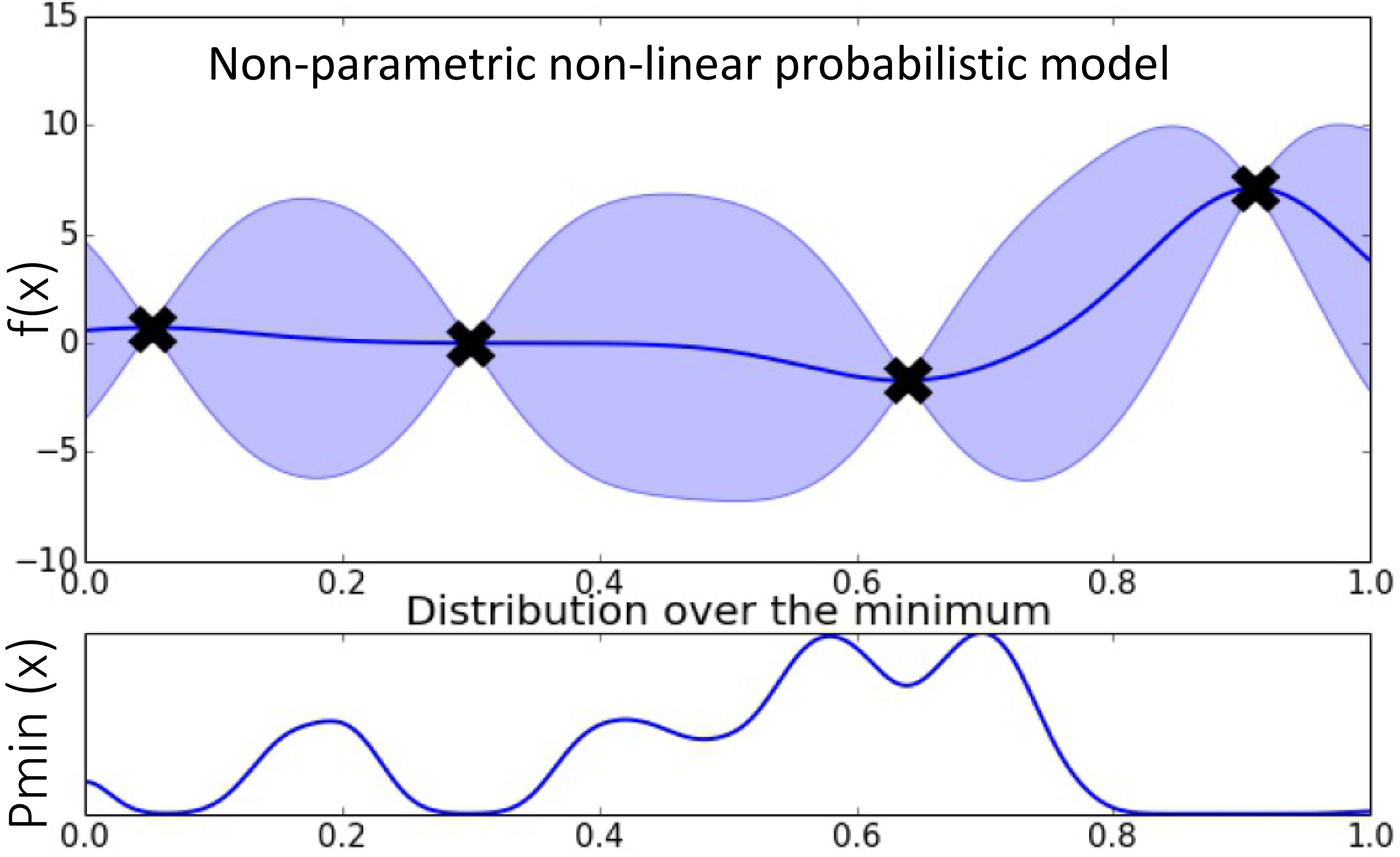
$$T(x,y,\theta) = T_0 + \frac{\alpha}{k}\int_{\tau=0}^{\theta}\int_{x'=0}^{L_x} G(x,y,\theta|x',y',\tau)|_{y'=0}\, q''(x',\tau)dx'd\tau$$

Traversing Gaussian Laser Beam : $q''(x',\tau) = \frac{\tilde{P}(\tau)}{\sigma\sqrt{2\pi}} e^{-\frac{1}{2}(\frac{x'-v\tau}{\sigma})^2}$

Assumptions:

- Simplistic 2D heat conduction model with convective boundary conditions
- Single Phase Model
- Temperature independence assumption of CMSX4 thermophyscial proterties
- Radiative heat loss ignored

Motivation: Gaussian Process Modeling



Gaussian Process Regression

- Stochastic process : Collection of random variables {β(x):x∈ X}; X :index set (operating conditions in our case)
- GP : stochastic process, s.t. any finite set of random variables is jointly Gaussian.

➢ For any finite set $x_1, x_2, .., x_n$∈ X :

$$\begin{bmatrix} \boldsymbol{\beta(x_1)} \\ \cdot \\ \cdot \\ \boldsymbol{\beta(x_n)} \end{bmatrix} \sim \boldsymbol{N} \left(\begin{bmatrix} \boldsymbol{m(x_1)} \\ \cdot \\ \cdot \\ \boldsymbol{m(x_n)} \end{bmatrix}, \begin{bmatrix} \boldsymbol{k(x_1, x_1)} \dots \boldsymbol{k(x_1, x_n)} \\ \cdot\cdot \\ \cdot\cdot \\ \boldsymbol{k(x_n, x_1)} \dots \boldsymbol{k(x_n, x_n)} \end{bmatrix} \right) \quad .....(1)$$

where mean function m($x_1) = E[\beta(x_1)]$; covariance function $k(x_1, x_n) = E[(\beta(x_1) - m(x_1))(\beta(x_n) - m(x_n))]$

- Non-parametric: No assumptions have been made about the function form of β(x).

Covariance functions

- Covariance function:
- Has to be a non-negative definite covariance matrix for any set of points.
- Some examples:
  - SEARD : $k(x,z) = \alpha^2 \exp(-\frac{(x-z)^T P^{-1}(x-z)}{2})$
  - Linear : $k\ (\mathrm{x},\mathrm{z}) = \alpha x^T z + \gamma$

- Mean functions:

  Constant : m(x)=c

  Linear : m(x)=$\sum_{i=1}^{D} a_i x_i$
- Hyperparameters : α, γ, P, c, a

SEARD: Squared Exponential Automatic Relevance Determination- The matrix P represents relevance determination (feature selection)—which feature is most important in predicting response.

- Given $\{(x^i, y^i)\}$, where $\boldsymbol{x^i}$: **operating condition**; $\boldsymbol{y^i}$: **system response**-

  Assume : $\boldsymbol{y^i = \beta(x^i) + \varepsilon^i \,;\, \varepsilon \sim N(0, \sigma^2);\, \beta \sim GP(0, k(.,.))}$

Let $D_{train} = \{(x^i_{train}, y^i_{train})\}$, *i*=1 to n; $D_{test} = \{(x^i_{test}, unknown\ y^i_{test})\}$, *i*=1 to m.

Operating conditions: [combustor length; inlet velocity; equivalence ratio]- 3 dimensional vector

System Response: Rms of the pressure fluctuations

- Considering the concatenated set of training ($X_{train} = \{x^i_{train}\}$) and testing data ($X_{test} = \{x^i_{test}\}$) together i.e. $[X_{train}\ X_{test}]$, by (1) :

$$\begin{bmatrix} \boldsymbol{\beta(X_{train})} \\ \boldsymbol{\beta(X_{test})} \end{bmatrix} \mid \boldsymbol{X_{train}, X_{test} \sim N\left(0, \begin{bmatrix} k(X_{train}, X_{train}) & k(X_{train}, X_{test}) \\ k(X_{test}, X_{train}) & k(X_{test}, X_{test}) \end{bmatrix}\right)}$$

where $k(X_{train}, X_{test}) \in R^{nxm}$ *and* $k(X_{train}, X_{test})_{ij}$ =k(x^i_{train}, x^j_{test}); similarly for others.

- Being i.i.d, $\begin{bmatrix}\varepsilon_{train} \\ \varepsilon_{test}\end{bmatrix} \sim N\left(0, \begin{pmatrix}\sigma^2 I & 0 \\ 0 & \sigma^2 I\end{pmatrix}\right)$
- Sum of independent Gaussians is Gaussian:

$$\begin{bmatrix}\boldsymbol{Y_{train}} \\ \boldsymbol{Y_{test}}\end{bmatrix} | \boldsymbol{X_{train}}, \boldsymbol{X_{test}} \sim \mathrm{N}\left(\mathbf{0}, \begin{bmatrix}\boldsymbol{k(X_{train}, X_{train}) + \sigma^2 I} & \boldsymbol{k(X_{train}, X_{test})} \\ \boldsymbol{k(X_{test}, X_{train})} & \boldsymbol{k(X_{test}, X_{test}) + \sigma^2 I}\end{bmatrix}\right)$$

- Using the rules for conditioning of Gaussians on Gaussians,

$$\boldsymbol{Y_{test}} | \boldsymbol{Y_{train}}, \boldsymbol{X_{train}}, \boldsymbol{X_{test}} \sim \boldsymbol{N(\mu_{test}, \Sigma_{test})}$$

$$\boldsymbol{\mu_{test}} = \boldsymbol{k(X_{test}, X_{train})(k(X_{train}, X_{train}) + \sigma^2 I)^{-1} Y_{train}}$$

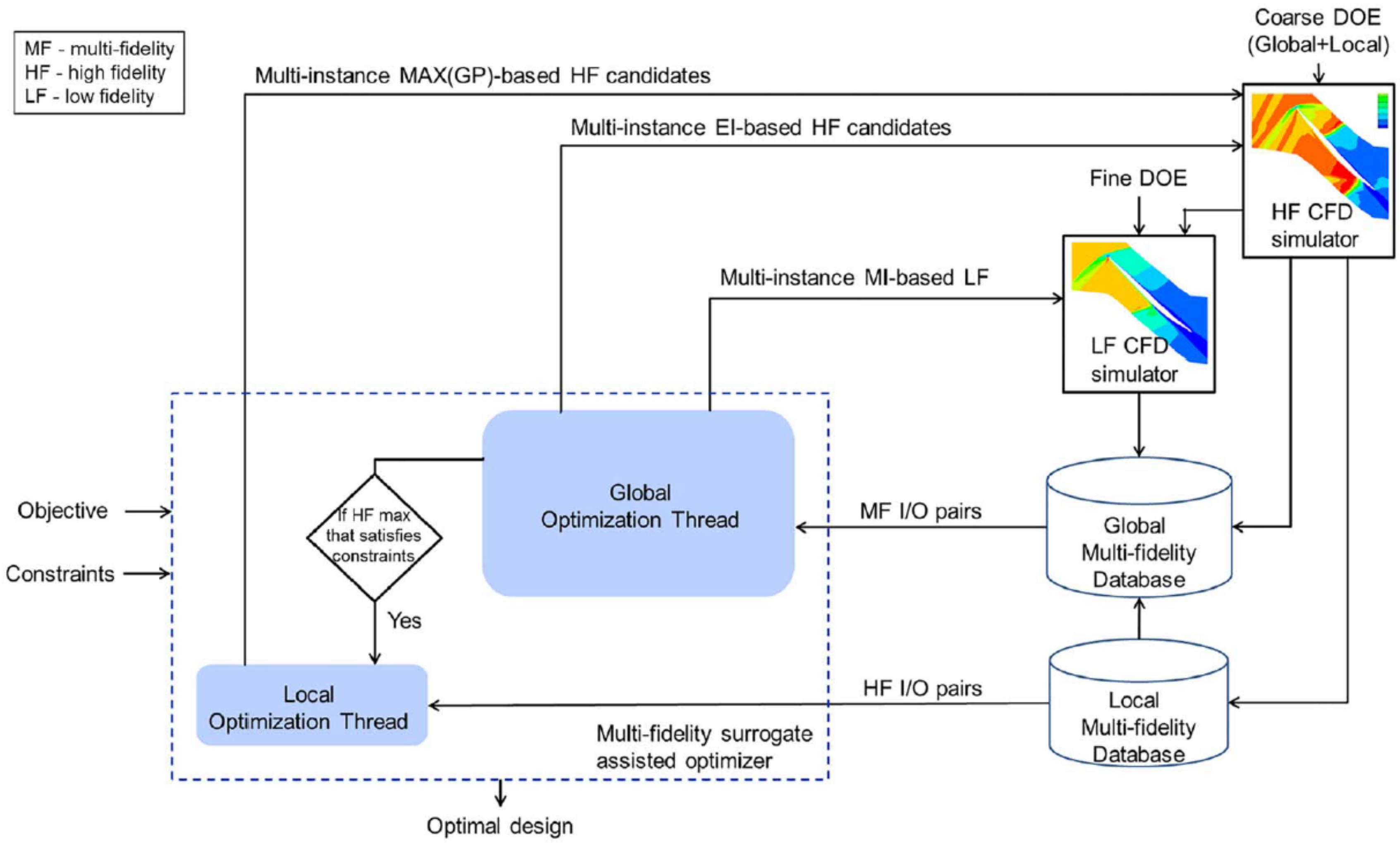
$$\boldsymbol{\Sigma_{test}} = \boldsymbol{k(X_{test}, X_{test}) + \sigma^2 I - k(X_{test}, X_{train})\left(k(X_{train}, X_{train}) + \sigma^2 I\right)^{-1} k(X_{train}, X_{test})} \dots \dots (\mathbf{2})$$

If instead of zero mean, a certain mean function is assumed,

- $\boldsymbol{\mu_{test}} = \boldsymbol{m(X_{test}) + k(X_{test}, X_{train})\left(k(X_{train}, X_{train}) + \sigma^2 I\right)^{-1}(Y_{train} - m(X_{train}))}$**……(3)**

Features of GP

- Y determined by covariance function and mean function forms chosen by user.
- Hyperparameters of the mean and covariance functions are optimized. (ML estimation)
- Avoids overfitting
  - Tries to use simple models
  - User‘s domain knowledge can be used to choose forms of mean and covariance functions together with setting informative priors for hyperparameters
- Disadvantage: Can be computationally expensive for large batch of training data



Multifidelity multiscale optimization architecture for turbomachinery design