

Versatile Gaussian Process Regression and Bayesian Optimization for Materials Design with Multiscale ICME Models

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Acknowledgment

Joint work with

- SNL: Tim Wildey, Mike Eldred, Bart G van Bloemen Waanders, Kathryn Maupin, John Mitchell, Laura Swiler, Julien Tranchida (now CEA), Aidan Thompson, Theron Rodgers, Hojun Lim, David Montes de Oca Zapiain
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1 Gaussian process / Bayesian optimization

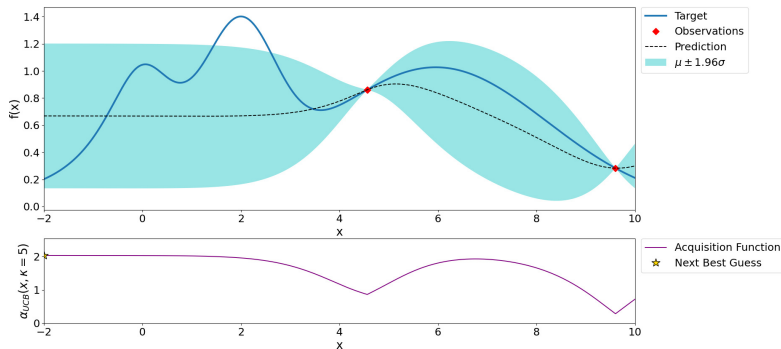
- Demo
- Introduction
- Fundamentals
- Acquisition
- Optimization parallelism

2 ICME applications

3 Conclusion

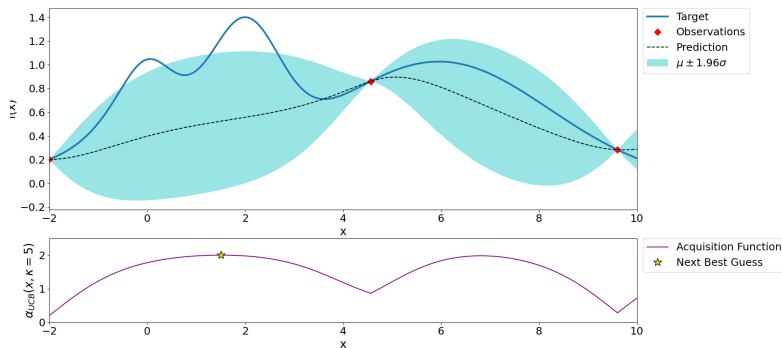
Bayesian optimization - Demo

Bayesian Optimization After 3 Steps



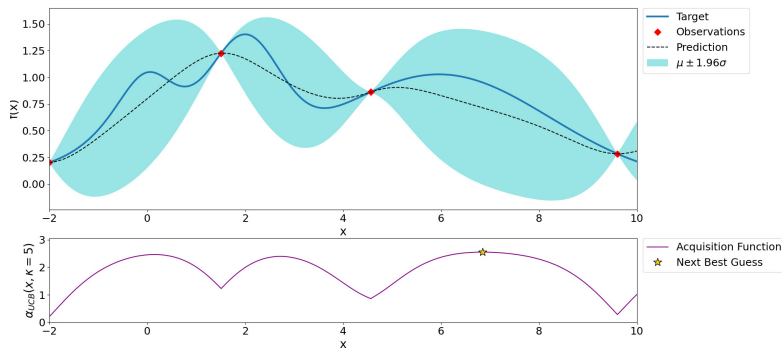
Bayesian optimization - Demo

Bayesian Optimization After 4 Steps



Bayesian optimization - Demo

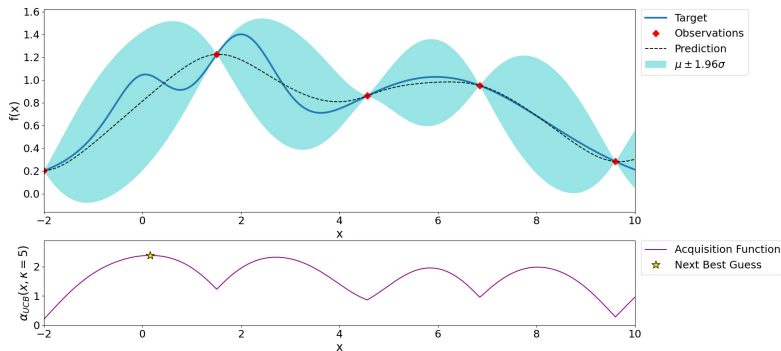
Bayesian Optimization After 5 Steps



Bayesian optimization - Iteration 5

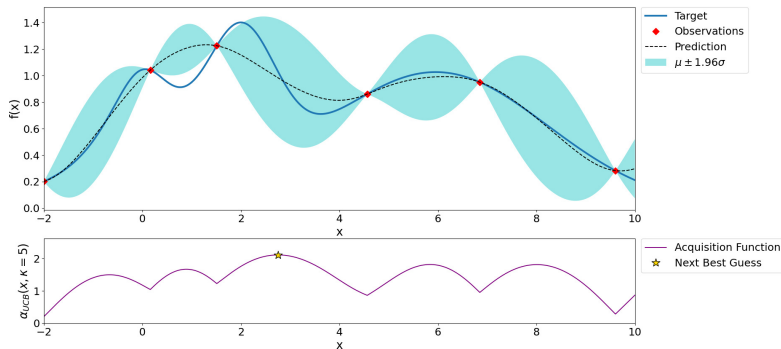
Bayesian optimization - Demo

Bayesian Optimization After 6 Steps



Bayesian optimization - Demo

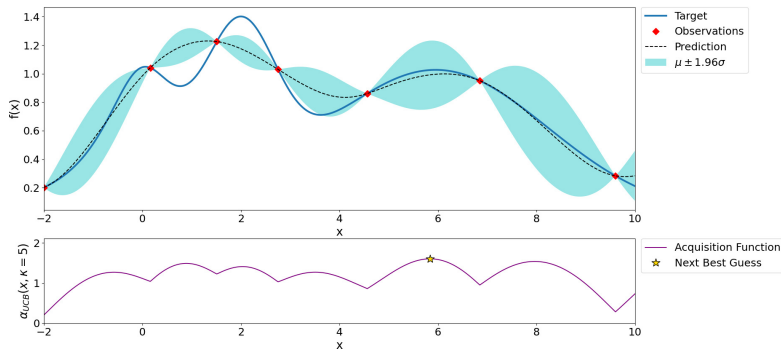
Bayesian Optimization After 7 Steps



Bayesian optimization - Iteration 7

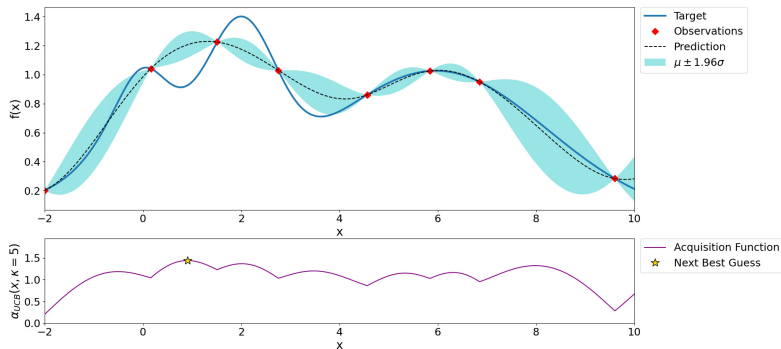
Bayesian optimization - Demo

Bayesian Optimization After 8 Steps



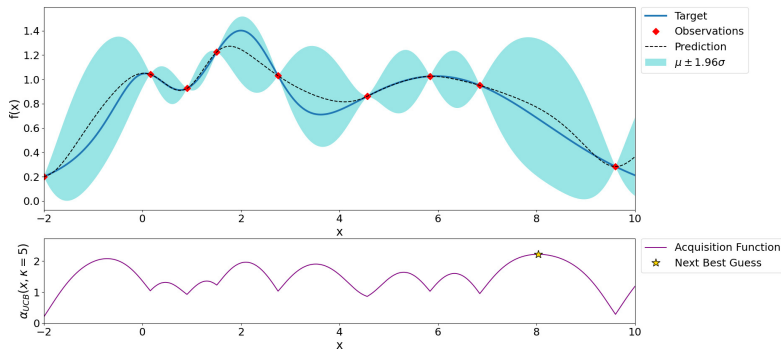
Bayesian optimization - Demo

Bayesian Optimization After 9 Steps



Bayesian optimization - Demo

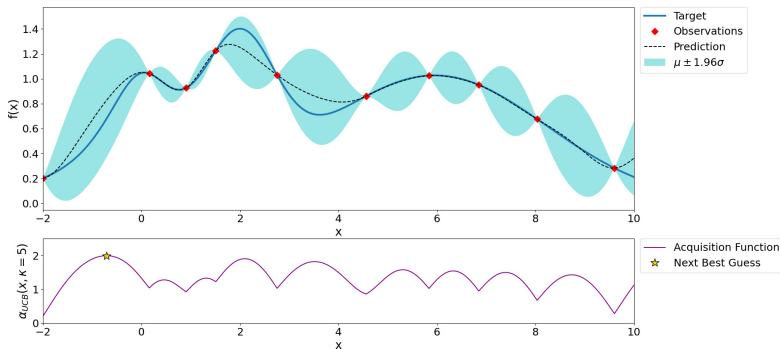
Bayesian Optimization After 10 Steps



Bayesian optimization - Iteration 11

Bayesian optimization - Demo

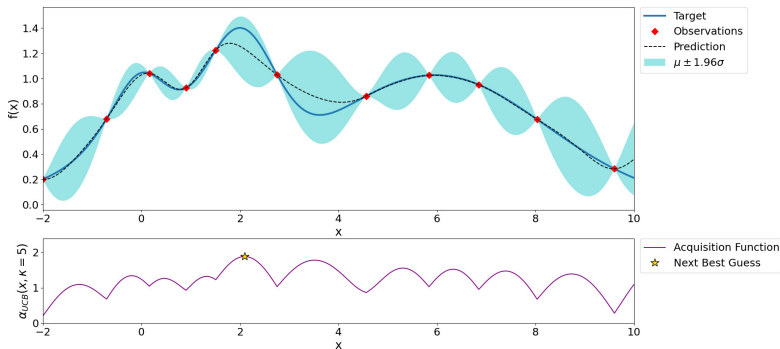
Bayesian Optimization After 11 Steps



Bayesian optimization - Iteration 11

Bayesian optimization - Demo

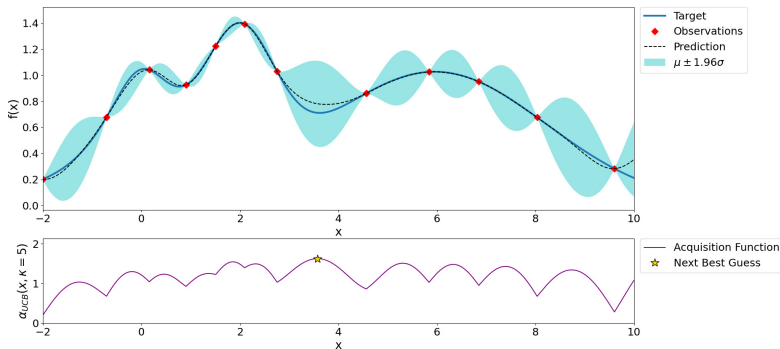
Bayesian Optimization After 12 Steps



Bayesian optimization - Iteration 12

Bayesian optimization - Demo

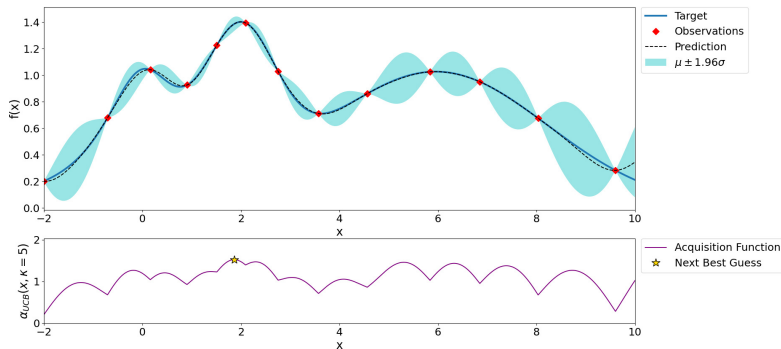
Bayesian Optimization After 13 Steps



Bayesian optimization - Iteration 13

Bayesian optimization - Demo

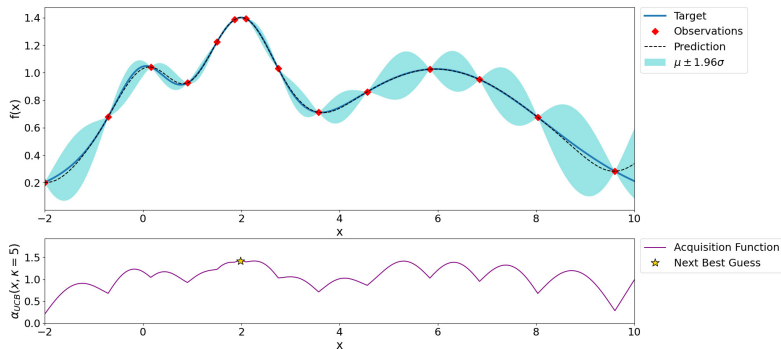
Bayesian Optimization After 14 Steps



Bayesian optimization - Iteration 14

Bayesian optimization - Demo

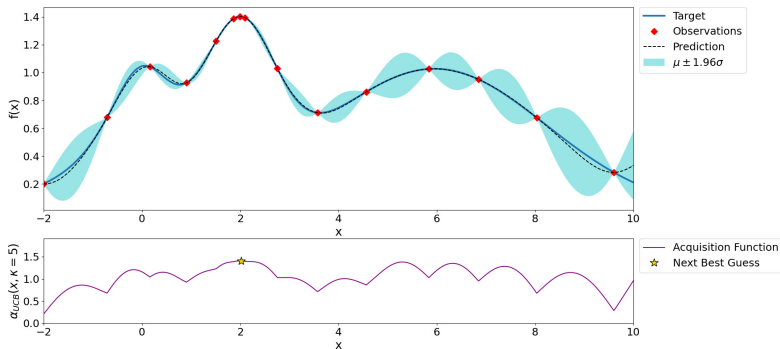
Bayesian Optimization After 15 Steps



Bayesian optimization - Iteration 15

Bayesian optimization - Demo

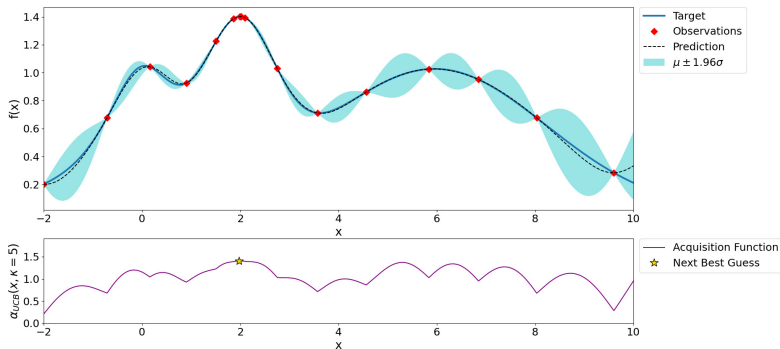
Bayesian Optimization After 16 Steps



Bayesian optimization - Iteration 16

Bayesian optimization - Demo

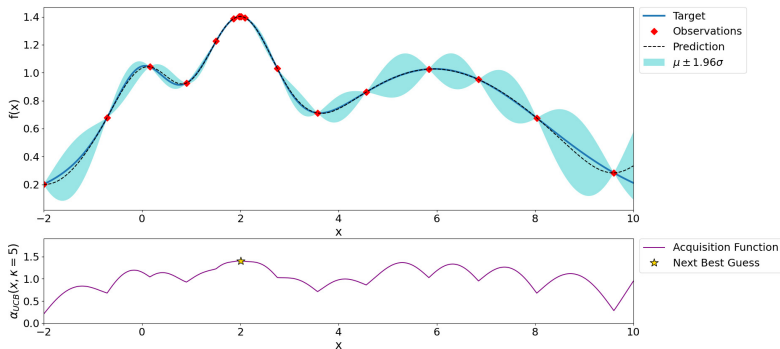
Bayesian Optimization After 17 Steps



Bayesian optimization - Iteration 17

Bayesian optimization - Demo

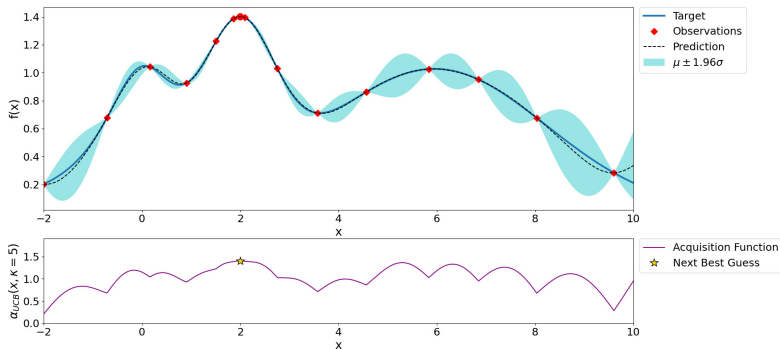
Bayesian Optimization After 18 Steps



Bayesian optimization - Iteration 18

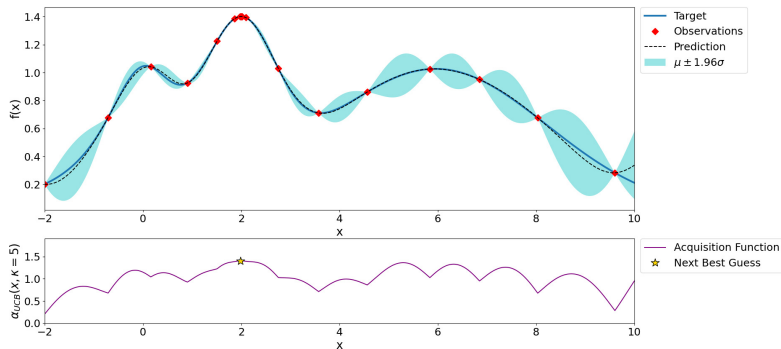
Bayesian optimization - Demo

Bayesian Optimization After 19 Steps



Bayesian optimization - Demo

Bayesian Optimization After 20 Steps



Bayesian optimization - Iteration 20

Advantages/Disadvantages

Bayesian optimization in a nutshell

Bayesian optimization = Gaussian process + sampling strategy

Advantages:

- optimize with uncertainty consideration (e.g. noisy observations)
- active machine learning (balance exploration-exploitation)
- derivative free (avoid computing Jacobian)
- global optimization (convergence in probability to global optimum)
- good convergence rate (provable asymptotic regret)

Disadvantages:

- high-dimensionality
- scalability: computational bottleneck $\mathcal{O}(n^3)$

Bayesian optimization features

very **versatile** (can solve **a lot** of practical problems)

Gaussian process regression:

- multi-task/multi-output
- multi-fidelity
- gradient-enhanced
- physics-constrained (monotonicity, boundedness, convexity, symmetry, etc.)
- stochastic, heteroscedastic: non-Gaussian, student- t
- time-series (forecasting)
- mixed-integer, e.g. discrete/categorical
- scalable to Big Data
- latent variable model
- high-dimensional
- non-stationary kernel

Bayesian optimization:

- constrained on objectives (known + unknown constraints)
- multi-objective optimization (Pareto frontier/optimal, domination)
- batch parallel optimization $\rightarrow$ asynchronous parallel optimization

Classical GP: Fundamentals

Let $\mathcal{D}_n = \{\mathbf{x}_i, y_i\}_{i=1}^n$ denote the set of observations and $\mathbf{x}$ denote an arbitrary test points

$$\mu_n(\mathbf{x}) = \mu_0(\mathbf{x}) + \mathbf{k}(\mathbf{x})^T (\mathbf{K} + \sigma^2 \mathbf{I})^{-1} (\mathbf{y} - \mathbf{m}) \quad (1)$$

$$\sigma_n^2(\mathbf{x}) = k(\mathbf{x}, \mathbf{x}) - \mathbf{k}(\mathbf{x})^T (\mathbf{K} + \sigma^2 \mathbf{I})^{-1} \mathbf{k}(\mathbf{x}) \quad (2)$$

where $\mathbf{k}(\mathbf{x})$ is a vector of covariance terms between $\mathbf{x}$ and $\mathbf{x}_{1:n}$, $\mathbf{K}$ is the *covariance matrix*.

Classical GP: Fundamentals

- assuming **stationary** kernel $\rightarrow k(\mathbf{x}, \mathbf{x}')$ only depends on $r = \|\mathbf{x} - \mathbf{x}'\|$
- the covariance matrix: symmetric positive semidefinite matrix made up of **pairwise** inner products

$$\mathbf{K}_{ij} = k(\mathbf{x}_i, \mathbf{x}_j) = k(\mathbf{x}_j, \mathbf{x}_i) = \mathbf{K}_{ji} \quad (3)$$

- kernel choice: smoothness assumption, e.g. $\mathcal{C}^\infty$
- Matérn kernels:

$$\mathbf{K}_{i,j} = k(\mathbf{x}_i, \mathbf{x}_j) = \theta_0^2 \frac{2^{1-\nu}}{\Gamma(\nu)} (\sqrt{2\nu}r)^\nu K_\nu(\sqrt{2\nu}r), \quad (4)$$

K_ν is a modified Bessel function of the second kind and order ν .

Common kernels:

- $\nu = 1/2$ (very rough): $k_{\text{Matérn}1/2}(\mathbf{x}, \mathbf{x}') = \theta_0^2 \exp(-r)$
- $\nu = 3/2$: $k_{\text{Matérn}3/2}(\mathbf{x}, \mathbf{x}') = \theta_0^2 \exp(-\sqrt{3}r)(1 + \sqrt{3}r)$,
- $\nu = 5/2$: $k_{\text{Matérn}5/2}(\mathbf{x}, \mathbf{x}') = \theta_0^2 \exp(-\sqrt{5}r) \left(1 + \sqrt{5}r + \frac{5}{3}r^2\right)$,
- $\nu \rightarrow \infty$ (very smooth): $k_{\text{sq-exp}}(\mathbf{x}, \mathbf{x}') = \theta_0^2 \exp\left(-\frac{r^2}{2}\right)$

Log (marginal) likelihood function:

$$\log p(\mathbf{y}|\mathbf{x}_{1:n}, \theta) = - \underbrace{\frac{n}{2} \log(2\pi)}_{\text{data likelihood } \downarrow \text{ as } n \uparrow} - \underbrace{\frac{1}{2} \log |\mathbf{K}^\theta + \sigma^2 \mathbf{I}|}_{\text{"complexity" term smoother covariance matrix}} - \underbrace{\frac{1}{2} (\mathbf{y} - \mathbf{m}_\theta)^T (\mathbf{K}^\theta + \sigma^2 \mathbf{I})^{-1} (\mathbf{y} - \mathbf{m}_\theta)}_{\text{"data-fit" term how well model fits data}} \quad (5)$$

Acquisition function: How to pick the next point(s)

- how to pick the next point: **exploitation** (if $\sigma_A^2 = \sigma_B^2$ but $\mu_A > \mu_B$ then choose A) or **exploration** (if $\mu_A = \mu_B$ but $\sigma_A^2 > \sigma_B^2$ then choose A). If
- different flavors:

- 1 **probability of improvement** (PI) (Mockus 1982)

$$\alpha_{\text{PI}}(\mathbf{x}) = \Phi(\gamma(\mathbf{x})), \quad (6)$$

where

$$\gamma(\mathbf{x}) = \frac{\mu(\mathbf{x}) - f(\mathbf{x}_{\text{best}})}{\sigma(\mathbf{x})}, \quad (7)$$

- 2 **expected improvement** (EI) scheme (Huang et al. 2006; Mockus 1975)

$$\alpha_{\text{EI}}(\mathbf{x}) = \sigma(\mathbf{x})[\gamma(\mathbf{x})\Phi(\gamma(\mathbf{x})) + \phi(\gamma(\mathbf{x}))] \quad (8)$$

- 3 **upper confidence bound** (UCB) scheme (Srinivas et al. 2009, 2012)

$$\alpha_{\text{UCB}}(\mathbf{x}) = \mu(\mathbf{x}) + \kappa\sigma(\mathbf{x}), \quad (9)$$

where κ is a hyper-parameter describing the exploitation-exploration balance.

- 4 **pure exploration***:

- maximal MSE $\sigma^2(\mathbf{x}) \Leftrightarrow$ maximal entropy: $\frac{1}{2} \log [2\pi\sigma^2(\mathbf{x})] + \frac{1}{2}$
- maximal IMSE $\int_{\mathbf{x} \in \mathcal{X}} \sigma^2(\mathbf{x})$

- 5 other: KG (generalized EI), MES, PES, etc.

Acquisition function: Reparameterization

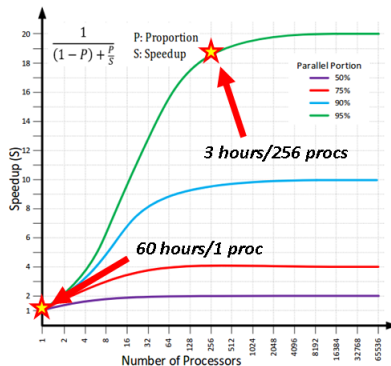
Reparameterization in deep learning by Wilson, Hutter, and Deisenroth 2018.

Table: $1^{+/-}$: right-/left-continuous Heaviside step function; $\text{ReLU} + \text{sigmoid} (\sigma)$
 $+$ softmax: activation function; $\Sigma = \mathbf{L}\mathbf{L}^\top$: Cholesky; $\gamma \sim \mathcal{N}(\mathbf{0}, \Sigma)$ residual

Abbr.	Acquisition function $\mathcal{L}$	Reparameterization
EI	$\mathbb{E}_{\mathbf{y}}[\max(\text{ReLU}(\mathbf{y} - \alpha))]$	$\mathbb{E}_{\mathbf{z}}[\max(\text{ReLU}(\mu + \mathbf{Lz} - \alpha))]$
PI	$\mathbb{E}_{\mathbf{y}}[\max(1^-(\mathbf{y} - \alpha))]$	$\mathbb{E}_{\mathbf{z}}[\max(\sigma(\frac{\mu + \mathbf{Lz} - \alpha}{\tau}))]$
SR	$\mathbb{E}_{\mathbf{y}}[\max(\mathbf{y})]$	$\mathbb{E}_{\mathbf{z}}[\max(\mu + \mathbf{Lz})]$
UCB	$\mathbb{E}_{\mathbf{y}}[\max(\mu + \sqrt{\frac{\beta\pi}{2}} \gamma)]$	$\mathbb{E}_{\mathbf{z}}[\max(\mu + \sqrt{\frac{\beta\pi}{2}} \mathbf{Lz})]$
ES	$-\mathbb{E}_{\mathbf{y}_a}[\mathbf{H}(\mathbb{E}_{\mathbf{y}_b \mathbf{y}_a}[1^+(\mathbf{y}_b - \max(\mathbf{y}_b))])]$	$-\mathbb{E}_{\mathbf{z}_a}[\mathbf{H}(\mathbb{E}_{\mathbf{z}_b}[\text{softmax}(\frac{\mu_{b a} + \mathbf{L}_{b a}\mathbf{z}_b}{\tau})])]$
KG	$\mathbb{E}_{\mathbf{y}_a}[\max(\mu_b + \Sigma_{b,a}\Sigma_{a,a}^{-1}(\mathbf{y}_a - \mu_a))]$	$\mathbb{E}_{\mathbf{z}_a}[\max(\mu_b + \Sigma_{b,a}\Sigma_{a,a}^{-1}\mathbf{L}_a\mathbf{z}_a)]$

Optimization parallelism on HPC for MPI applications

- $P = 0.95 \rightarrow \text{SpeedUp} \approx 20$ times
- **fixed** computational budget: **256** $\times$ 60 CPU hours
- **sequential**: simulation takes 3 hours to finish with 256 procs $\rightarrow$ **20 cases** in 60 hours
- **parallel**: 60 hours (2.5 days) with 1 proc for 1 case $\rightarrow$ **256 cases** in 60 hours

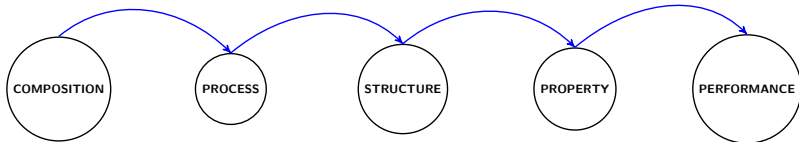


Amdahl's law for parallelization.

- 1 Gaussian process / Bayesian optimization
- 2 ICME applications
 - Overview – MGI with ICME
 - Inverse problems in process-structure (kinetic Monte Carlo)
 - Inverse problems in composition-property (DFT + MD)
 - Inverse problems in structure-property (CPFEM)
- 3 Conclusion

Process-structure-property relationship

- **process**: $\mathbf{x} + \delta, \delta \sim \mathcal{N}[0, \sigma_\delta^2]$ – **deterministic**, controllable within a tolerance δ (in a manufacturing context)
- **(micro)structure** – **random/stochastic**, spatio-temporal, microstructure representations (physics-based vs. data-driven), image (i.e. high-dimensional), limited/scarc data
- **property/performance**: $y = f(\mathbf{x}) + \varepsilon, \varepsilon \sim \mathcal{N}(0, \sigma_\varepsilon^2)$ – **deterministic** with Gaussian noisy observations



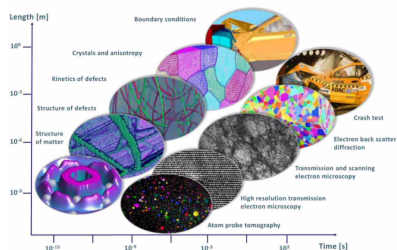
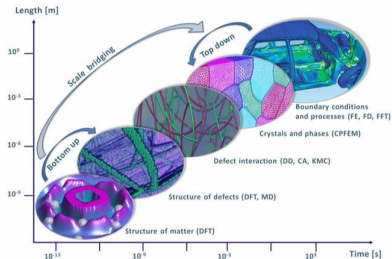
Process-structure-property relationship

Nature of inverse problems

The nature of the input, i.e. deterministic or stochastic, determines the methodology for solving the inverse problem in PSPP.

- for **deterministic variables** in process $\rightarrow$ composition, process $\rightarrow$ structure: Bayesian optimization (or any other optimization methods)
- for **stochastic variables** (typically affiliated with microstructure), such as grain size distribution, orientation distribution, in structure $\rightarrow$ property: Bayesian inference is more appropriate to infer a distribution of features

Multi-scale ICME models as forward models



Courtesy of Prof. Dierk Raabe.

<https://www.dierk-raabe.com/multiscale-modeling/>.

- **Common ICME models:** DFT, MD, PF, CPFEM, kMC, CA, DDD.
- **Multi-physics ICME models:** DFT+MD, PF+CPFEM, kMC+CPFEM, kMC+PF, DDD+CPFEM, MD+CPFEM, PF+kMC, MD+kMC, etc.

Beyond forward ICME models: MGI as inverse problems (2010s)

Materials Genome Initiative for Global Competitiveness

June 2011



US NSTC 2011

MATERIALS GENOME INITIATIVE STRATEGIC PLAN

Materials Genome Initiative
National Science and Technology Council
Committee on Technology
Subcommittee on the Materials Genome Initiative

DECEMBER 2014



Holdren et al. 2014



MATERIALS GENOME INITIATIVE STRATEGIC PLAN

A Report by the
SUBCOMMITTEE ON THE MATERIALS GENOME INITIATIVE
COMMITTEE ON TECHNOLOGY

of the
NATIONAL SCIENCE AND TECHNOLOGY COUNCIL

November 2021

Lander et al. 2021

Beyond forward ICME models: MGI as inverse problems (MGI in 2020s)



The Second Decade of the Materials Genome Initiative

Julie Christodoulou, James A. Frerieders, Linda Sepotich, and Charles A. Warren

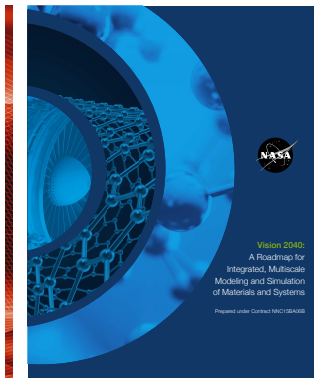
In the past decade, the Materials Genome Initiative (MGI) has been a catalyst for the development of new materials and the acceleration of materials research. The MGI is a national research program that is focused on the development of new materials and the acceleration of materials research. The MGI is a national research program that is focused on the development of new materials and the acceleration of materials research. The MGI is a national research program that is focused on the development of new materials and the acceleration of materials research.

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James A. Frerieders is a senior advisor at the National Science Foundation (NSF), where he leads the Materials Genome Initiative (MGI) program. He is also a senior advisor at the National Science Foundation (NSF), where he leads the Materials Genome Initiative (MGI) program. He is also a senior advisor at the National Science Foundation (NSF), where he leads the Materials Genome Initiative (MGI) program.

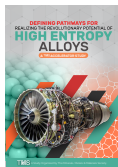
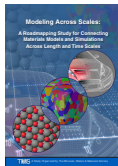
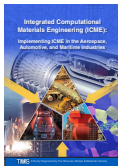
Linda Sepotich is a senior advisor at the National Science Foundation (NSF), where she leads the Materials Genome Initiative (MGI) program. She is also a senior advisor at the National Science Foundation (NSF), where she leads the Materials Genome Initiative (MGI) program. She is also a senior advisor at the National Science Foundation (NSF), where she leads the Materials Genome Initiative (MGI) program.

Charles A. Warren is a senior advisor at the National Science Foundation (NSF), where he leads the Materials Genome Initiative (MGI) program. He is also a senior advisor at the National Science Foundation (NSF), where he leads the Materials Genome Initiative (MGI) program. He is also a senior advisor at the National Science Foundation (NSF), where he leads the Materials Genome Initiative (MGI) program.



Liu et al. 2018

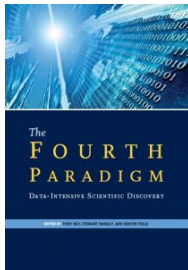
TMS Studies



DOE Office of Science / ASCR-BES-FES



Beyond forward ICME models: MGI as inverse problems



The Fourth Paradigm:
Data-Intensive Scientific
Discovery Hey, Tansley,
Tolle, et al. 2009.

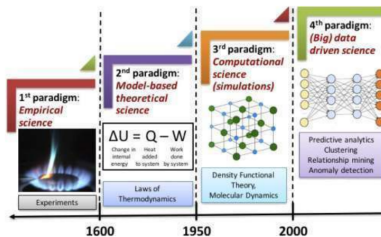


FIG. 1. The four paradigms of science: empirical, theoretical, computational, and data-driven.

The four paradigms of science: **empirical**, **theoretical**, **computational**, and **AI**. Agrawal and Choudhary 2016.

- ICME is the 3rd paradigm,
- AI is the 4th paradigm,
- Is SciML the 5th?

Beyond forward ICME models: MGI as inverse problems

Challenges:

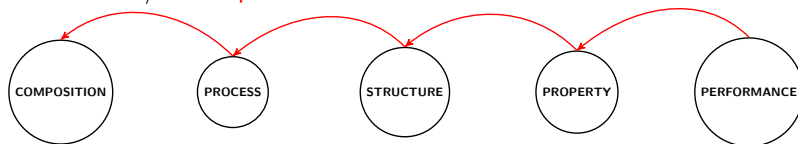
- optimization under (microstructure-induced) uncertainty
- small (sparse) + noisy datasets, high-dimensional
- high computational cost for ICME models → sample-efficient

Goals:

- traditional approach: 20+ years
- accelerate materials design by “2× at a fraction of the cost” (original)

Accelerators:

- ICME: experimental² → computational³
- ML/AI: computational³ → ML⁴



GP advantages

What are Gaussian process regression and Bayesian optimization useful for?

- (multiscale) **design optimization** under **microstructure-induced uncertainty**, e.g. manufacturing, chemical processing, AM, materials discovery,
- ICME **model calibration** (e.g. CPFE, DDD, kMC, MD, DFT, PF)
- **surrogate model** (ML) for forward and inverse UQ,
- **AutoML** for materials applications, e.g. tuning other ML hyper-parameters, such as AdaBoost and RandomForest,
- **automation, taking human out of the loop**, in both experimental and computational context.

Why are they useful?

- flexible – easy to modify to suit your needs,
- versatile – solve many problems in theory and practice,
- not too many hyper-parameters,
- optimization under (microstructure-induced) uncertainty,
- rigorous on mathematical ground: analytical convergence rate (both GP and BO),
- work well on small datasets with low- to intermediate-dimensional problems.

When is GP not useful?

- emulates field responses,
- spatial-temporal problems.

Inverse problems in process-structure

(joint work w/ Laura Swiler, John Mitchell, Tim Wildey, Theron Rodgers)

Reference

Anh Tran et al. (2020a). “An active-learning high-throughput microstructure calibration framework for process-structure linkage in materials informatics”. In: *Acta Materialia* 194, pp. 80–92

Problem statement:

- There exists a forward tool $f(\cdot)$ to **predict** microstructure, $u = f(x)$ (represented as images)
- Given a **target** u^* (represented as images)
- Task: **find** x^* such that $f(x^*) = u^* \approx u$

$\approx$ is defined in the sense of statistical equivalence for microstructures, $p_{\mathcal{D}}$ is the p.d.f. of statistical microstructure descriptors $\mathcal{D}$, i.e.

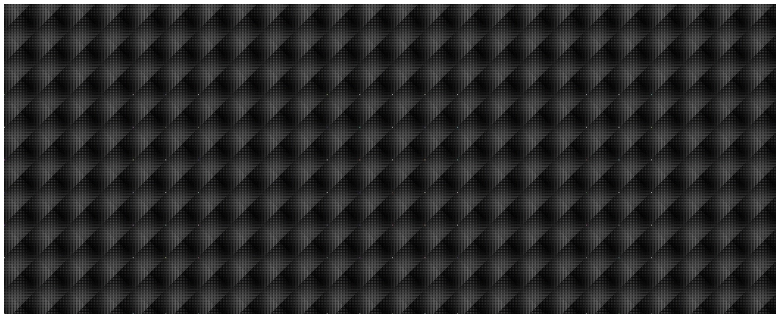
$$p_{\mathcal{D}} : \Omega \rightarrow L^1 : p_{\mathcal{D}}(u^*) \approx p_{\mathcal{D}}(u) \quad (10)$$

$$d(p_{\mathcal{D}}(u^*), p_{\mathcal{D}}(u)) \leq \text{TOL} \quad (11)$$

Hint: quantitatively differentiate microstructures using statistical microstructure descriptors

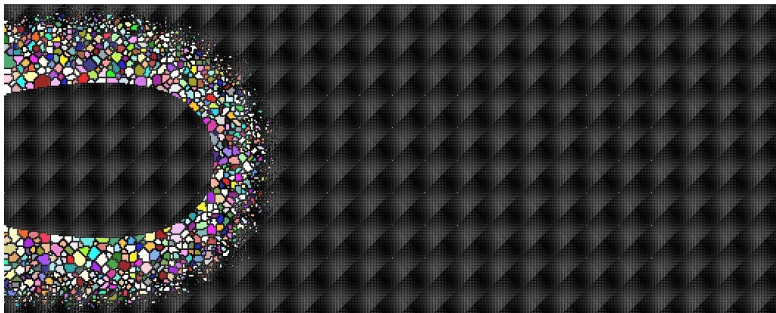
Inverse problems in process-structure

(joint work w/ Laura Swiler, John Mitchell, Tim Wildey, Theron Rodgers)



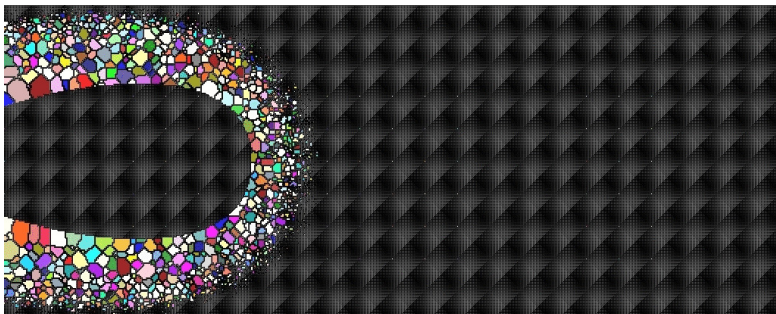
Inverse problems in process-structure

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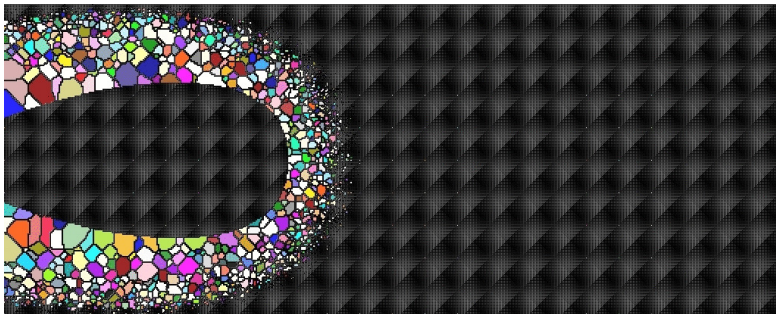
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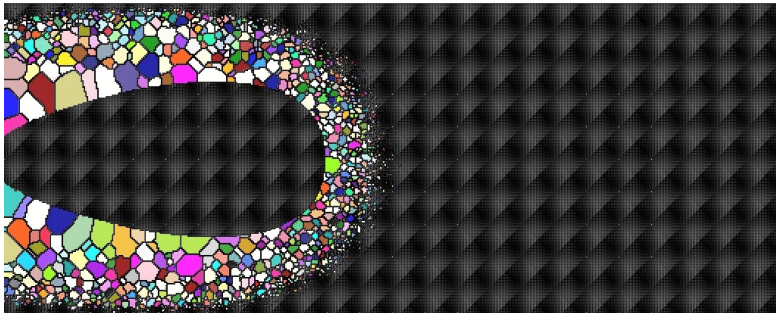
Inverse problems in process-structure

(joint work w/ Laura Swiler, John Mitchell, Tim Wildey, Theron Rodgers)



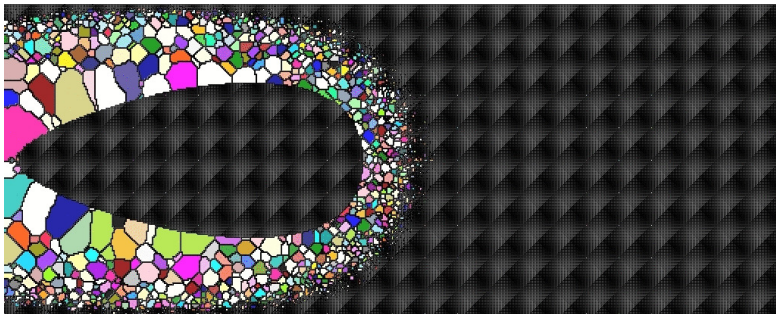
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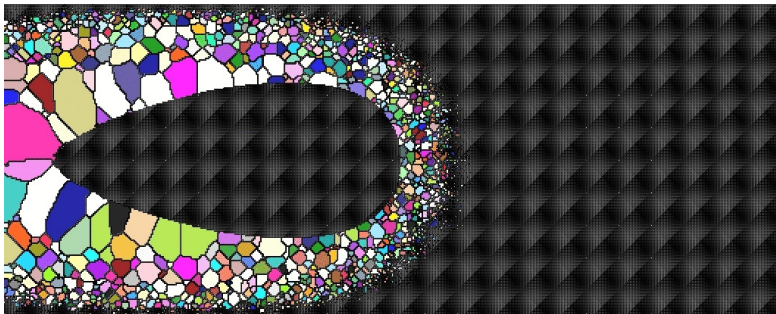
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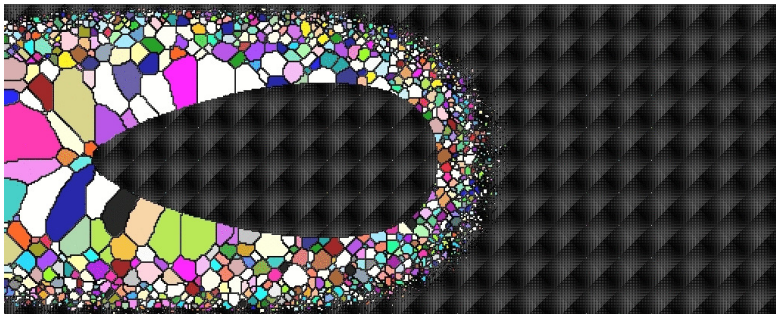
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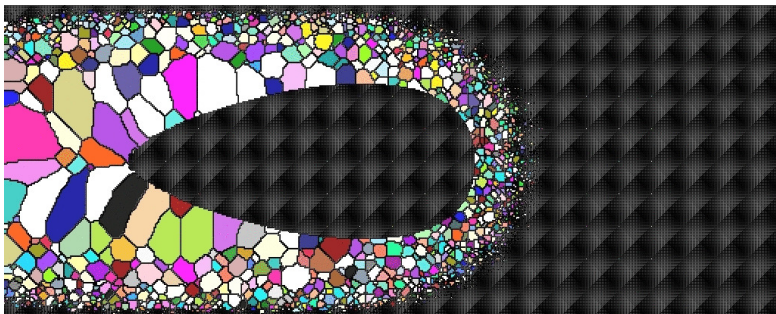
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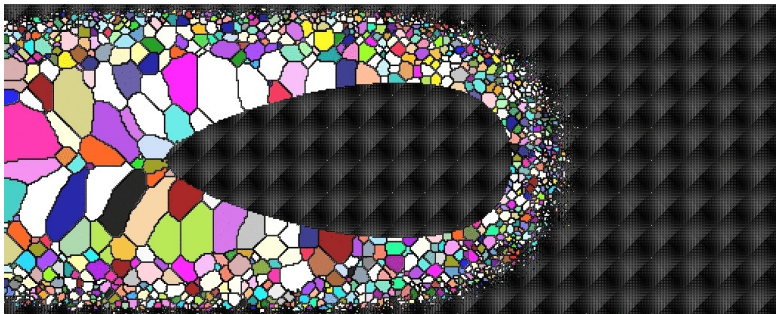
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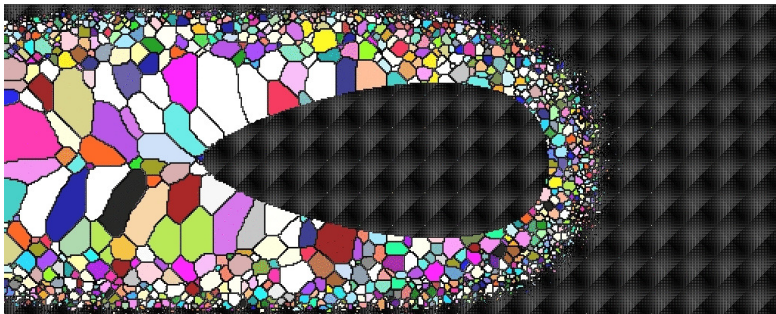
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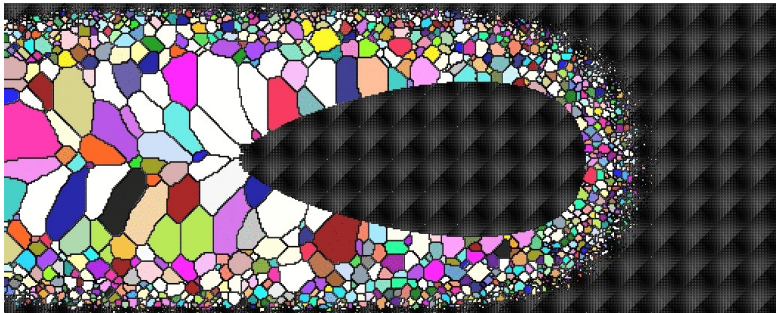
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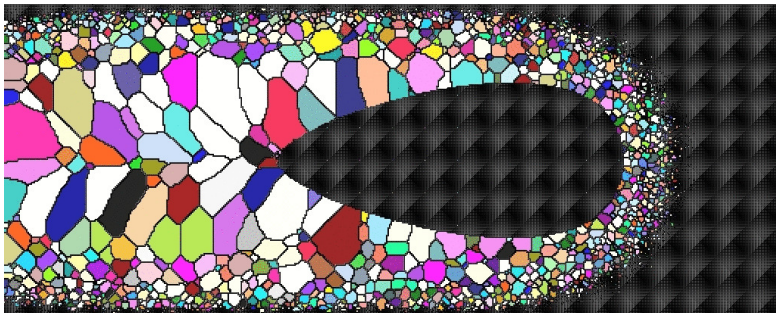
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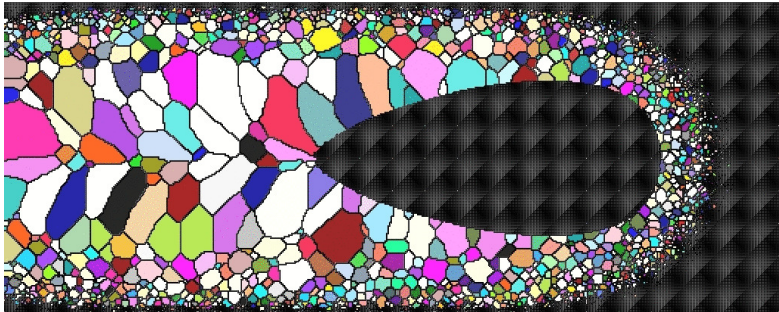
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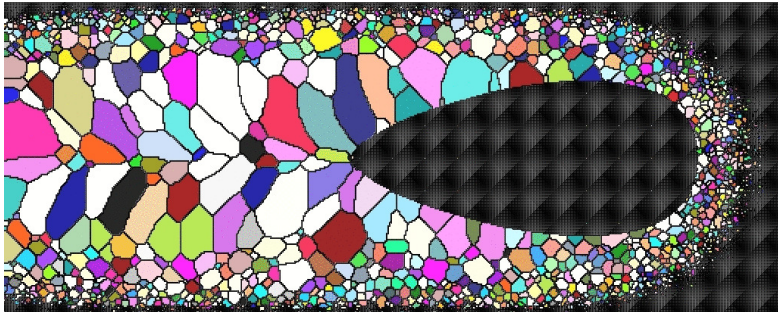
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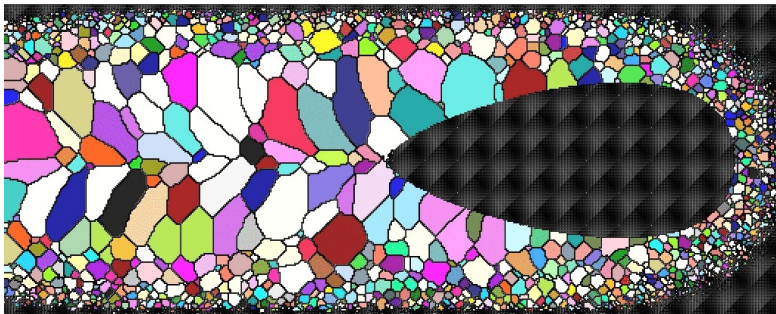
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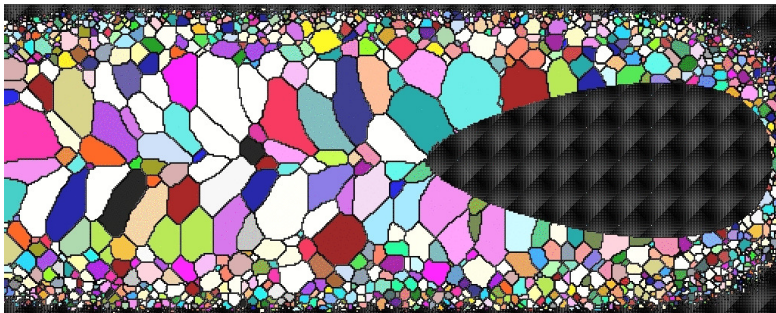
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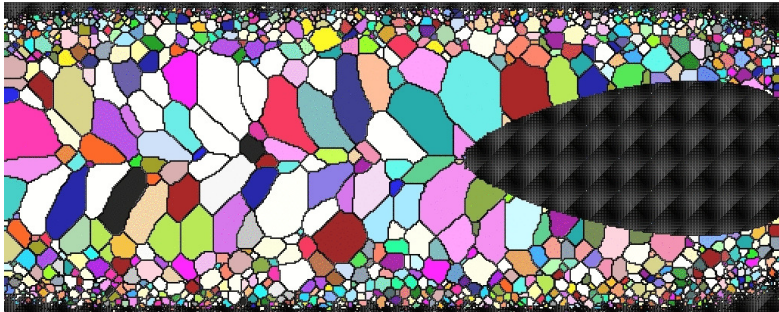
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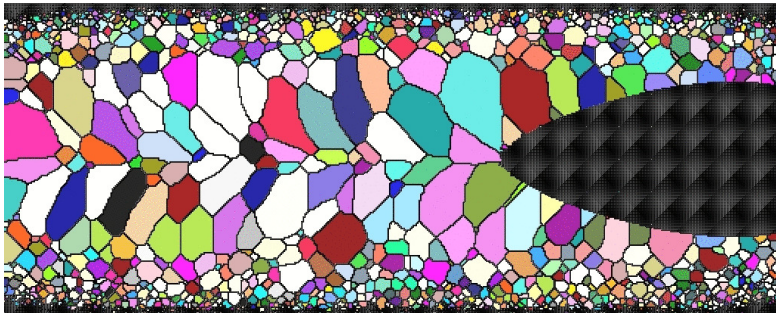
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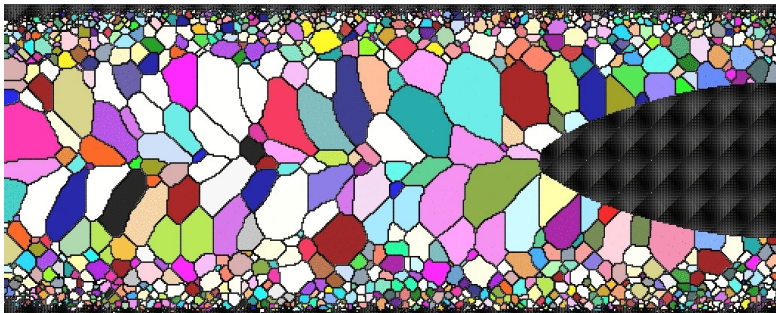
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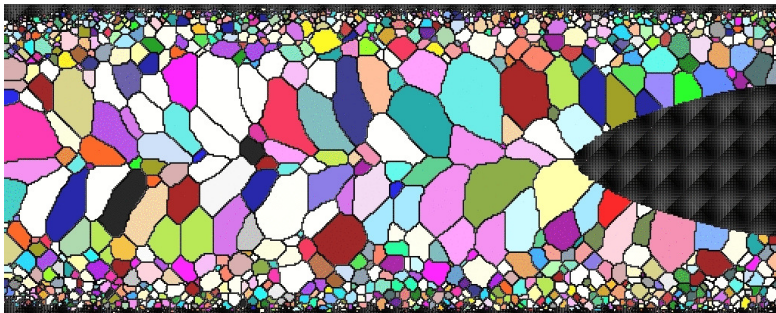
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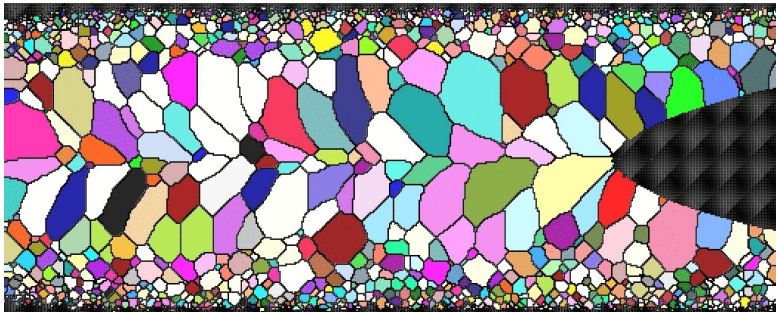
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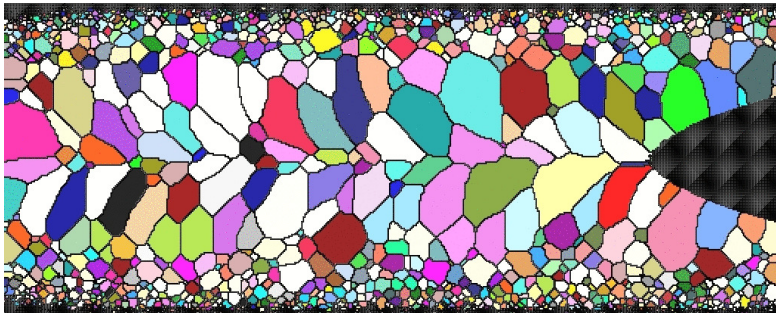
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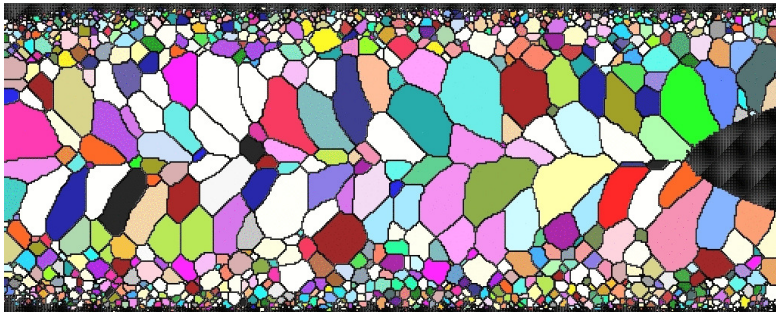
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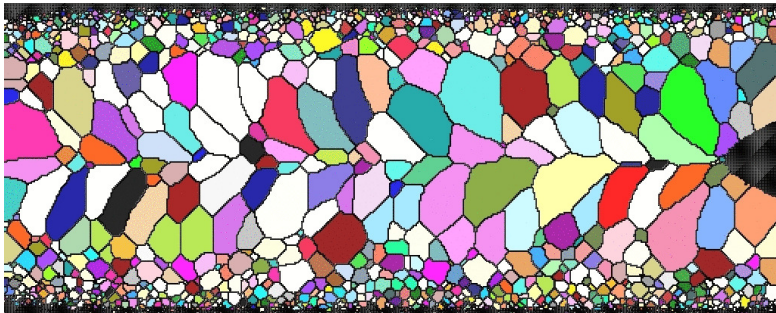
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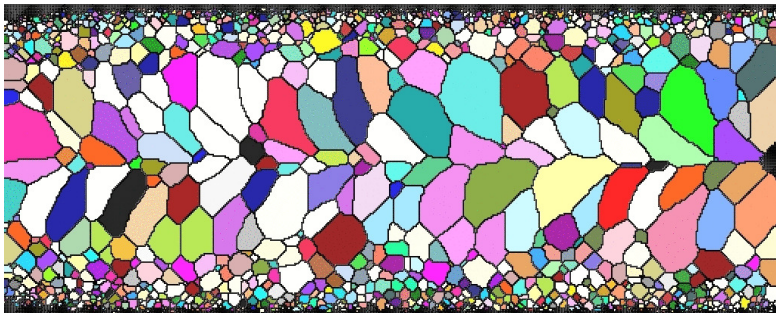
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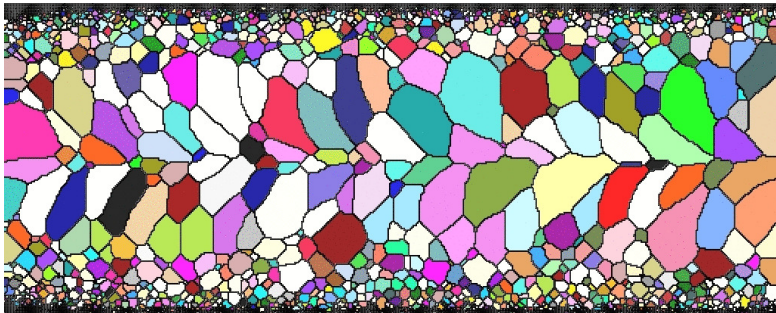
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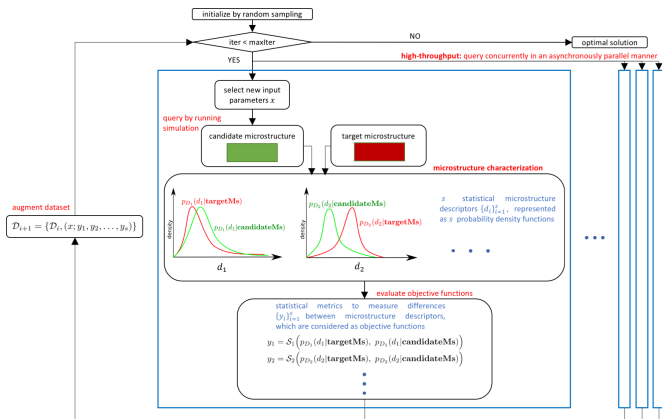
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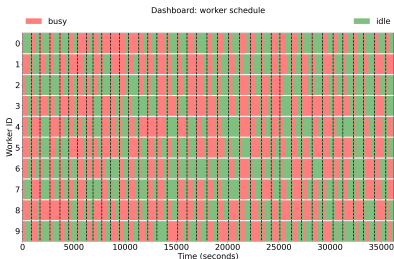
An asynchronous parallel Bayesian optimization workflow for inverse problems in process-structure linkage.

Inverse problems in process-structure

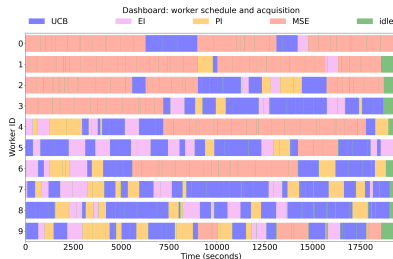
(joint work w/ Laura Swiler, John Mitchell, Tim Wildey, Theron Rodgers)

Reference

An asynchronous parallel constrained Bayesian optimization [Anh Tran et al. \(2022\)](#). “aphBO-2GP-3B: a budgeted asynchronous parallel multi-acquisition functions for constrained Bayesian optimization on high-performing computing architecture”. In: *Structural and Multidisciplinary Optimization* 65.4, pp. 1–45.



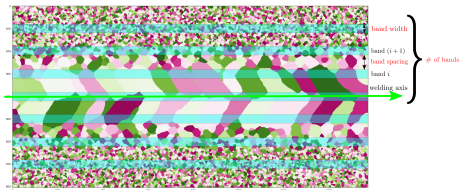
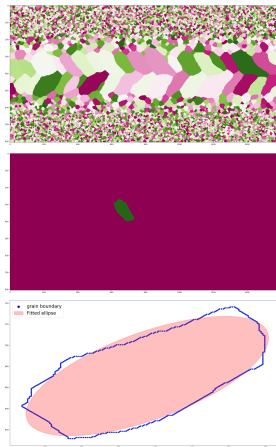
Batch-sequential parallel



Multi- α asynchronous parallel

Inverse problems in process-structure

(joint work w/ Laura Swiler, John Mitchell, Tim Wildey, Theron Rodgers)

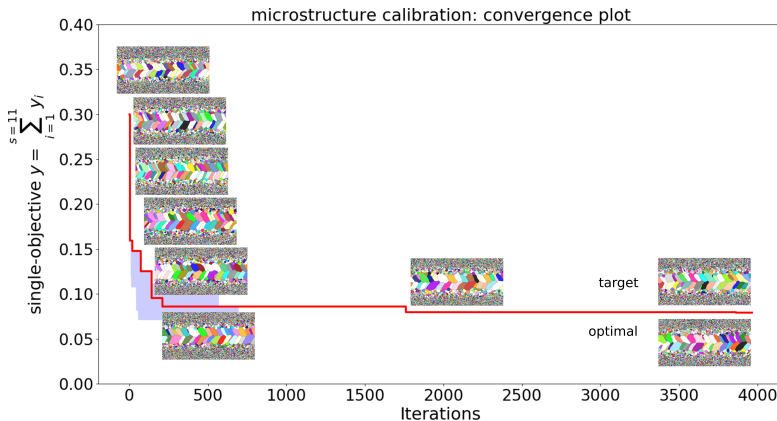


Collecting **local** and **global** statistical microstructure descriptors given a microstructure.

Convert multi-objective optimization to single-objective optimization by scalarization.

Inverse problems in process-structure

(joint work w/ Laura Swiler, John Mitchell, Tim Wildey, Theron Rodgers)



Reverse engineering an AM specimen through kinetic Monte Carlo (SPPARKS).

Inverse problems in composition-property

(joint work w/ Julien Tranchida, Aidan Thompson, Tim Wildey)

Reference

Active learning from chemical composition space to material property
Anh Tran et al. (2020b). “Multi-fidelity machine-learning with uncertainty quantification and Bayesian optimization for materials design: Application to ternary random alloys”. In: *The Journal of Chemical Physics* 153 (7), p. 074705.

Problem statement:

- Multiple forward ICME models that share the same inputs and outputs:
 - MD-MLIAP: low-fidelity (low accuracy, low cost)
 - DFT: high-fidelity (high accuracy, high cost)
- Exploit correlation between low- and high-fidelity models
- Input: chemical composition
- Output/QoI: bulk modulus B_0
- What chemical composition would optimize the QoI?

Inverse problems in composition-property

(joint work w/ Julien Tranchida, Aidan Thompson, Tim Wildey)

Ab-initio:

- DFT implemented in Quantum ESPRESSO
- **high** cost + **high** accuracy
→ **high**-fidelity

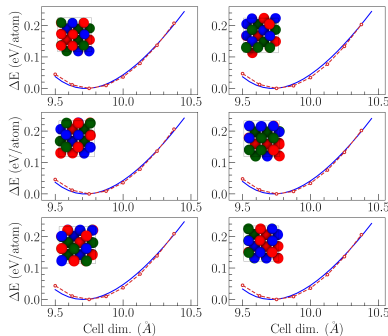
MD:

- MD with ML interatomic potential (SNAP)
- orders of magnitude faster
- **low** cost + **low** accuracy
→ **low**-fidelity

Birch-Murnaghan polynomials for B_0 :

$$E(V) = E_0 + \frac{9V_0 B_0}{16} \left\{ B_0' \left[\left(\frac{V_0}{V} \right)^{\frac{2}{3}} - 1 \right]^3 + \left[\left(\frac{V_0}{V} \right)^{\frac{2}{3}} - 1 \right]^2 \left[6 - 4 \left(\frac{V_0}{V} \right)^{\frac{2}{3}} \right] \right\}$$

(12)



EOS calculations for 6 configs. —: DFT; —: MD+SNAP

Inverse problems in composition-property

(joint work w/ Julien Tranchida, Aidan Thompson, Tim Wildey)

Kennedy and O'Hagan 2000: a chain of **auto-regressive model** connecting across fidelity hierarchy, bottom-up approach.

- Consider s levels of fidelity model $\{y_t(\mathbf{x})\}_{t=1}^s$ with $y_1(\mathbf{x})$ as the lowest fidelity-level, $y_s(\mathbf{x})$ as the highest fidelity-level, the auto-regressive model assumes:

$$y_t(\mathbf{x}) = \rho_{t-1}y_{t-1}(\mathbf{x}) + \delta_t(\mathbf{x}), \quad 1 \leq t \leq s \quad (13)$$

- Bi-fidelity covariance matrix

$$\tilde{\mathbf{K}} = \begin{pmatrix} \sigma_L^2 \mathbf{K}_L(\mathbf{x}_L, \mathbf{x}_L) & \rho \sigma_L^2 \mathbf{K}_L(\mathbf{x}_L, \mathbf{x}_H) \\ \rho \sigma_L^2 \mathbf{K}_L(\mathbf{x}_H, \mathbf{x}_L) & \rho^2 \sigma_L^2 \mathbf{K}_L(\mathbf{x}_H, \mathbf{x}_H) + \sigma_D^2 \mathbf{K}_D(\mathbf{x}_H, \mathbf{x}_H) \end{pmatrix} \quad (14)$$

- Log marginal likelihood

$$\log p(\tilde{\mathbf{y}}|\mathbf{x}_{1:n_L+n_H}, \tilde{\theta}) = -\frac{1}{2}(\tilde{\mathbf{y}} - \tilde{\mathbf{m}})^T (\tilde{\mathbf{K}}^{\tilde{\theta}} + \sigma^2 \mathbf{I})^{-1} (\tilde{\mathbf{y}} - \tilde{\mathbf{m}}) - \frac{1}{2} \log |\tilde{\mathbf{K}}^{\tilde{\theta}} + \sigma^2 \mathbf{I}| - \frac{n_H + n_L}{2} \log(2\pi) \quad (15)$$

- Selection of fidelity-level to query

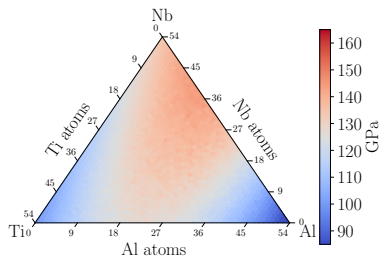
$$t^* = \underset{t}{\operatorname{argmin}} \left(\mathbf{C}_t \int_{\mathcal{X}} \sigma^2(\mathbf{x}) d\mathbf{x} \right), \quad (16)$$

$\mathbf{C}_t$: computational cost at level t .

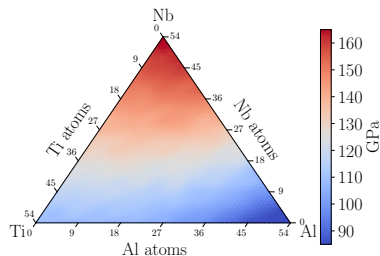
Inverse problems in composition-property

(joint work w/ Julien Tranchida, Aidan Thompson, Tim Wildey)

$R^2 = 0.7122$: not exactly the same



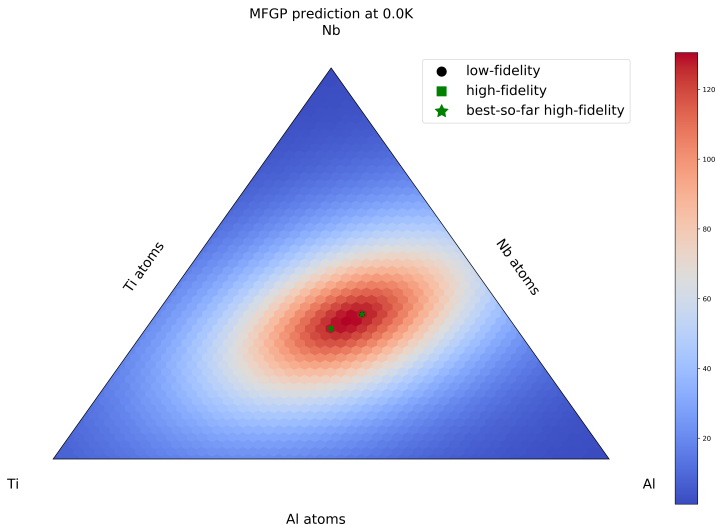
Low-fidelity: MD with SNAP potential.



Multi-fidelity GP $\approx$ high-fidelity: DFT.

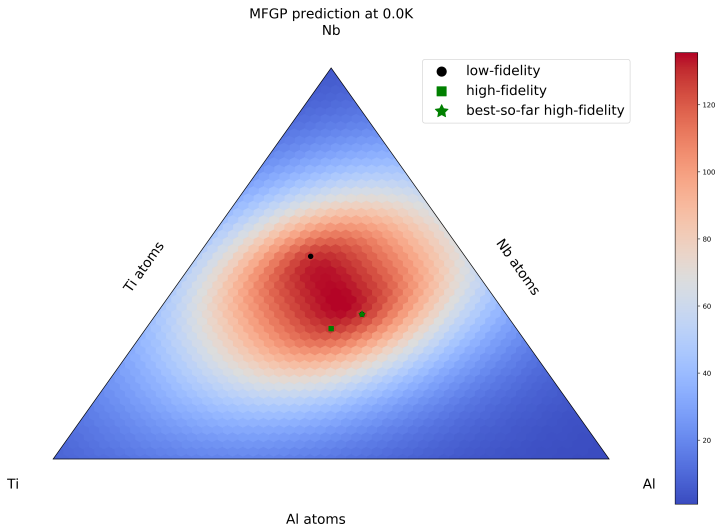
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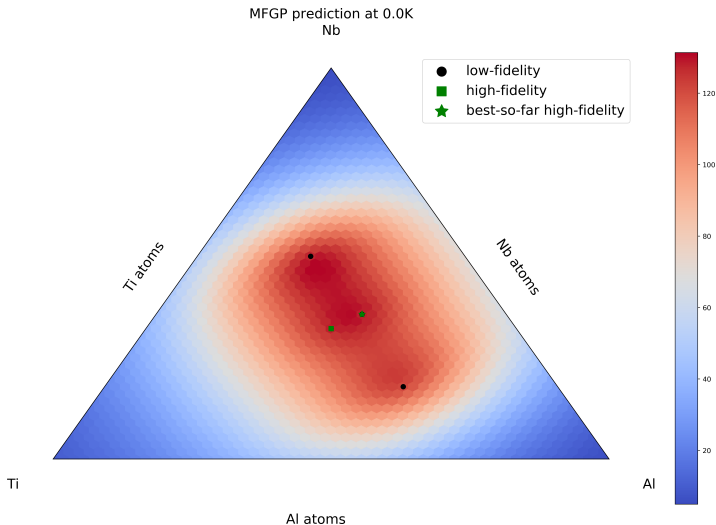
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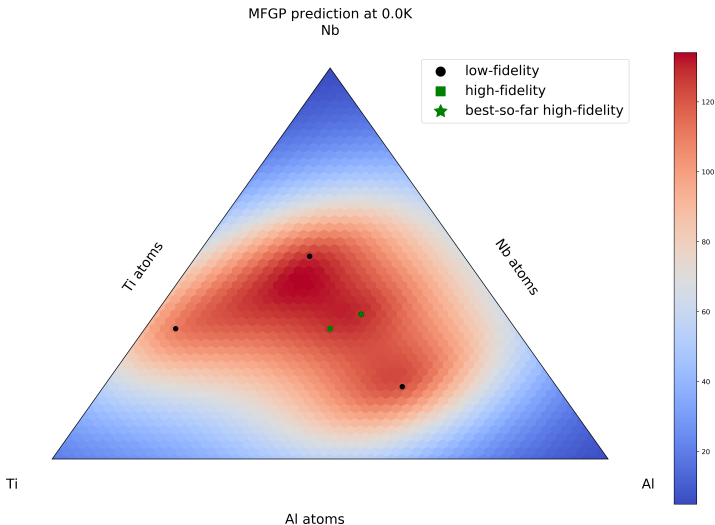
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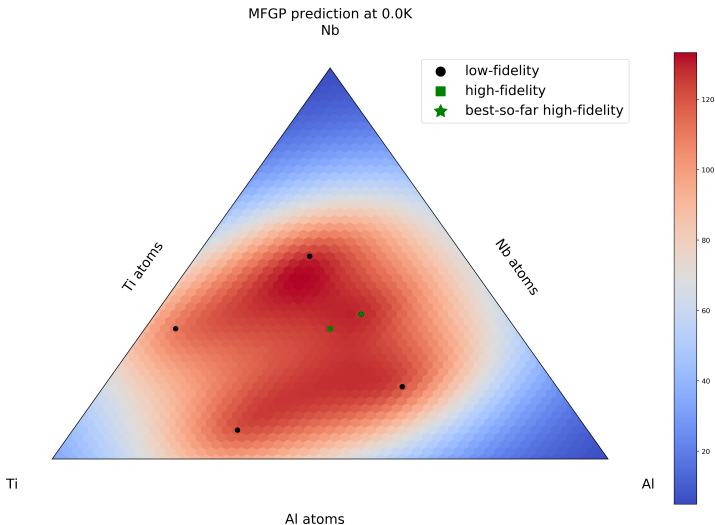
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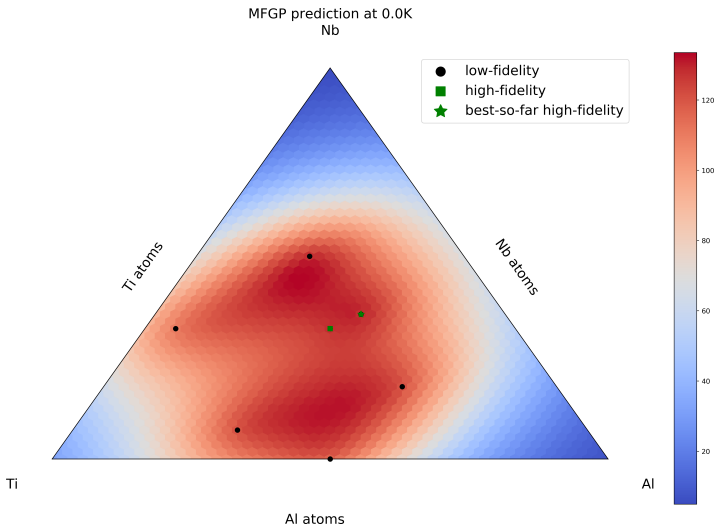
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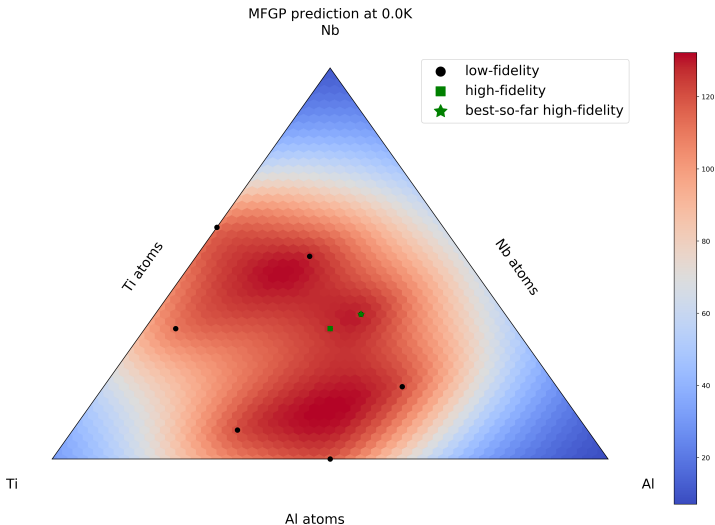
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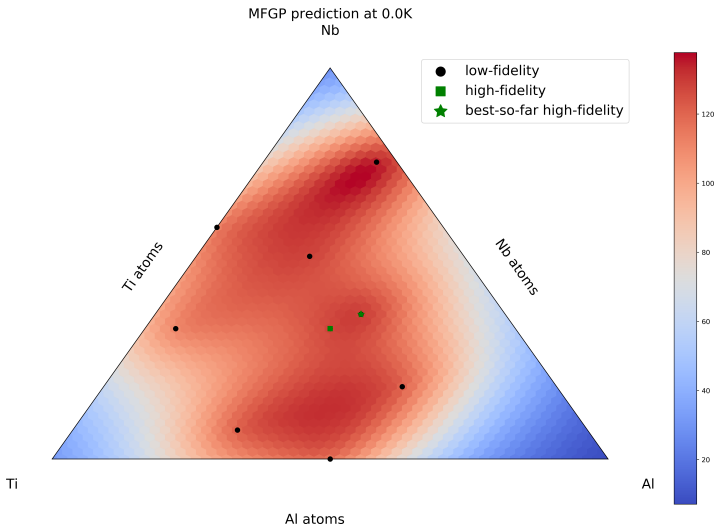
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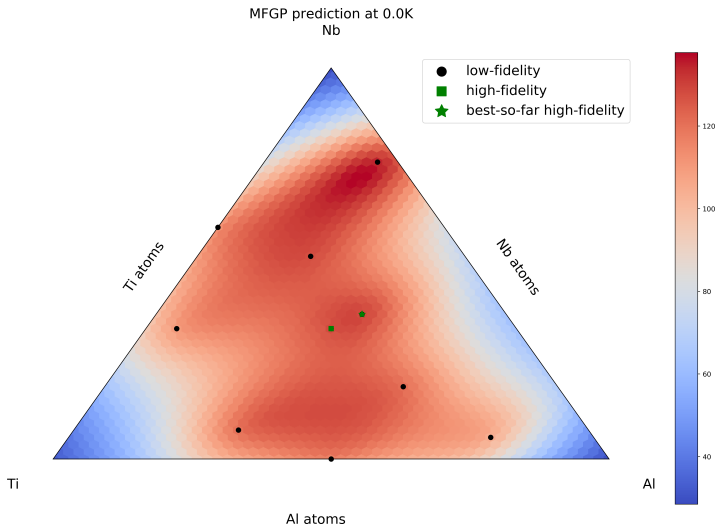
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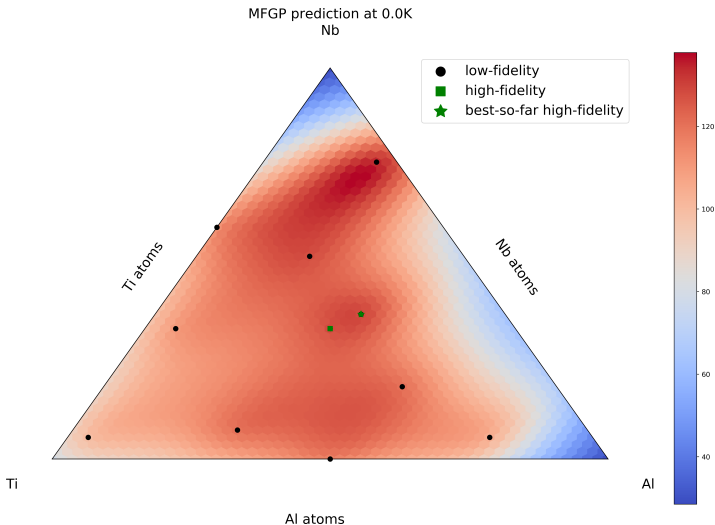
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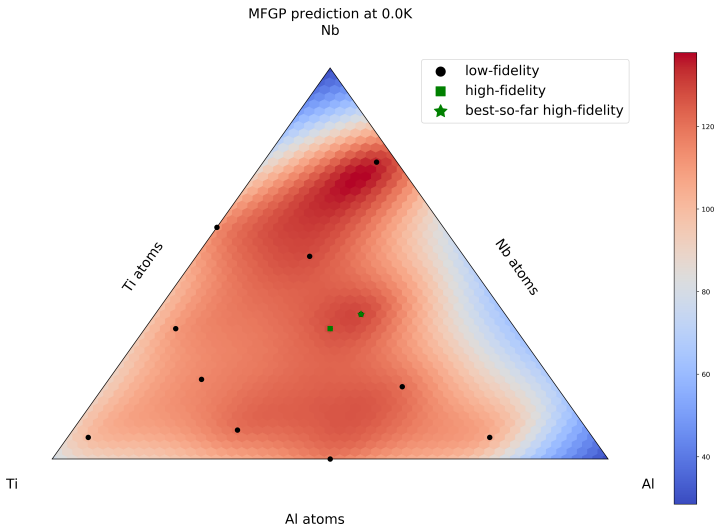
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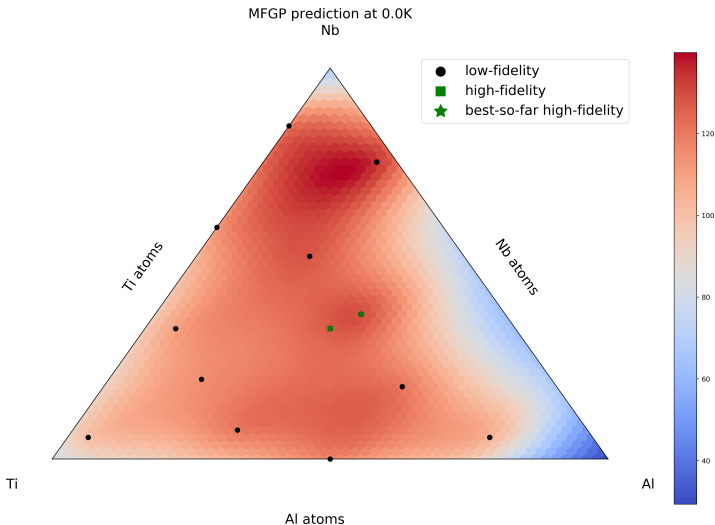
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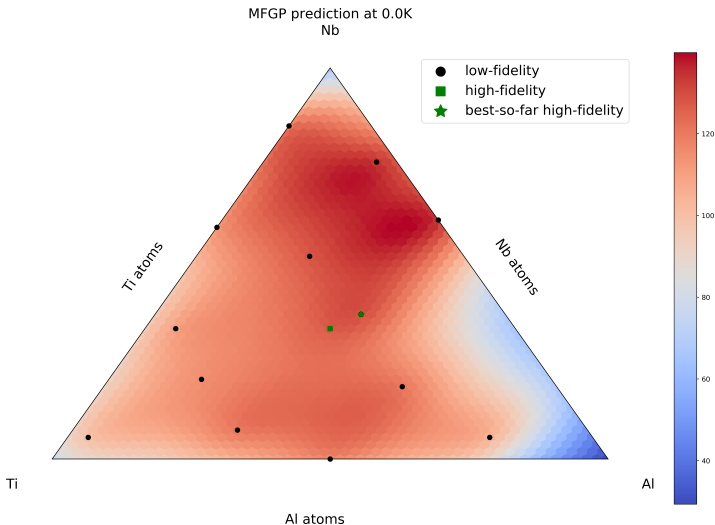
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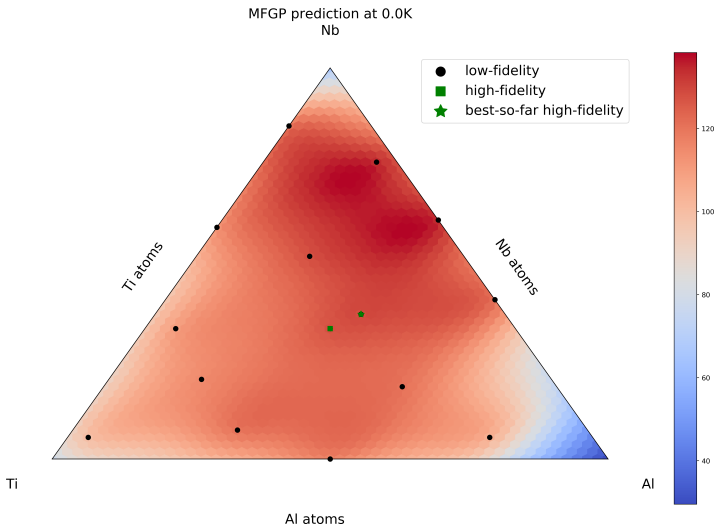
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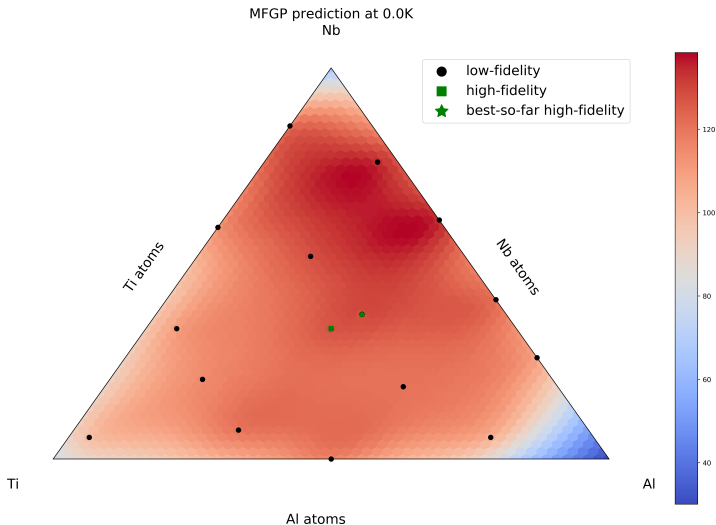
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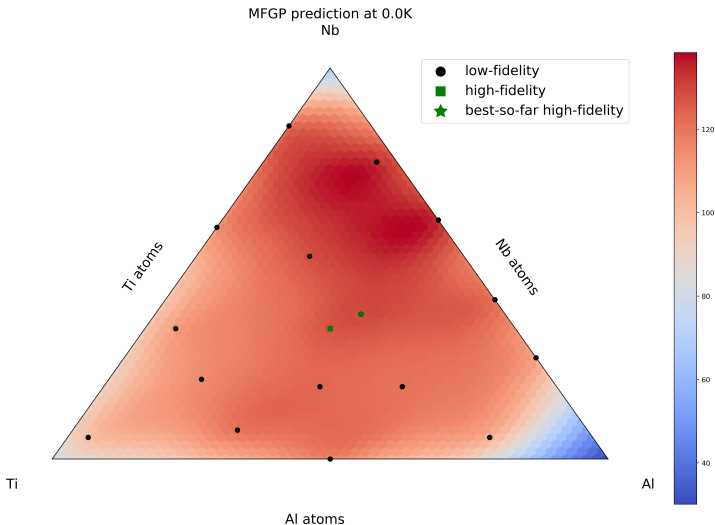
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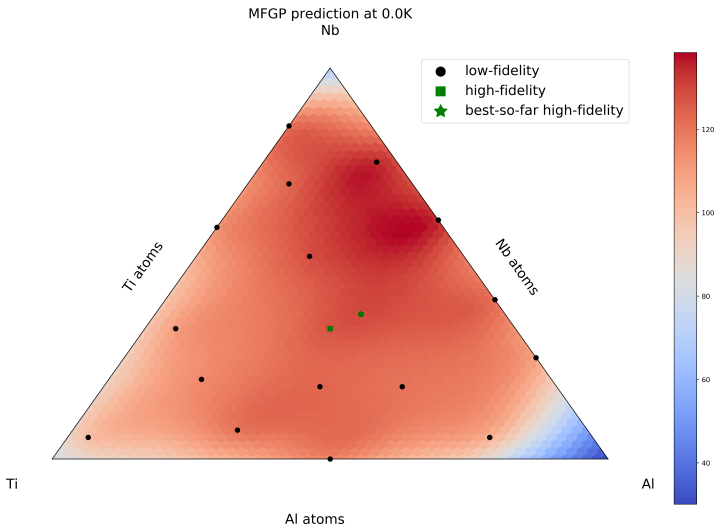
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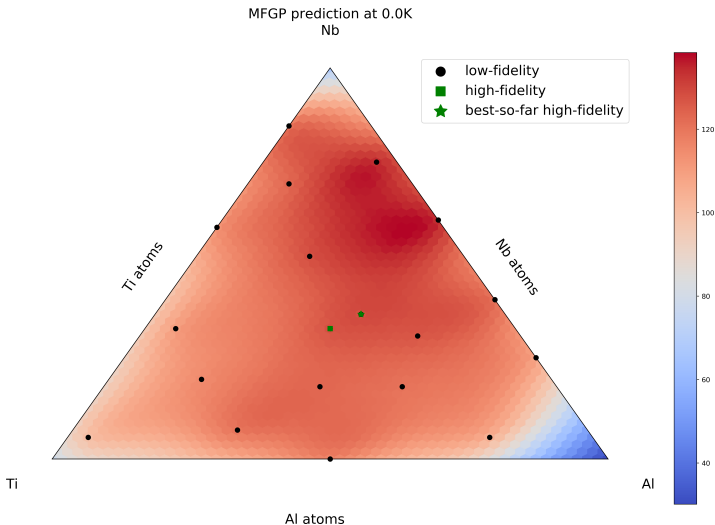
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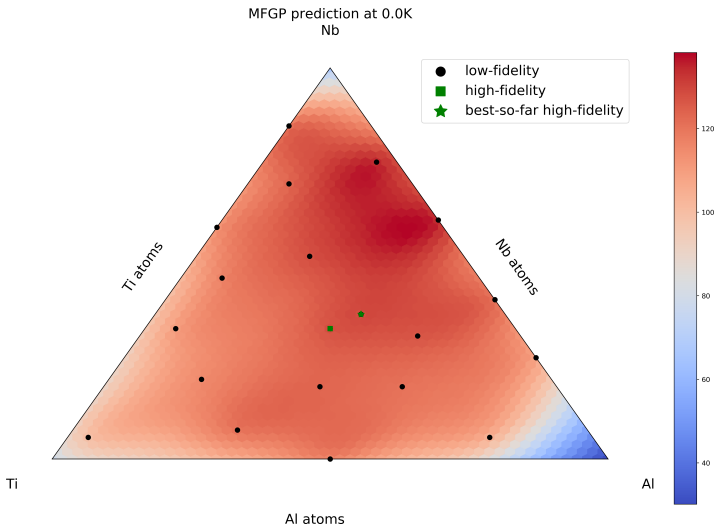
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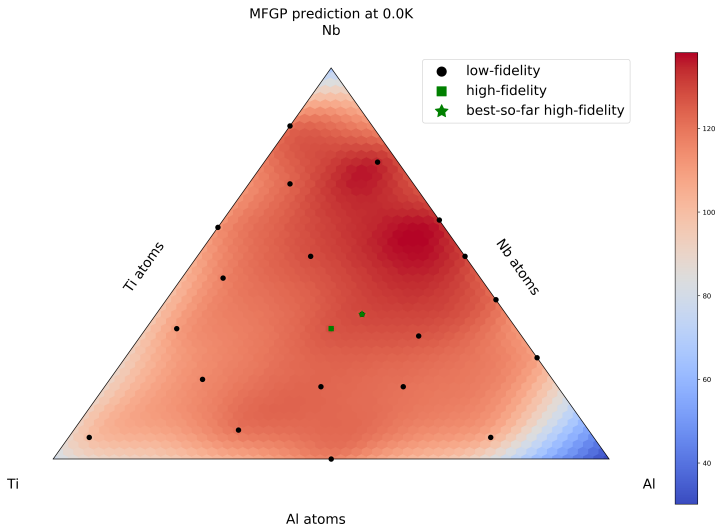
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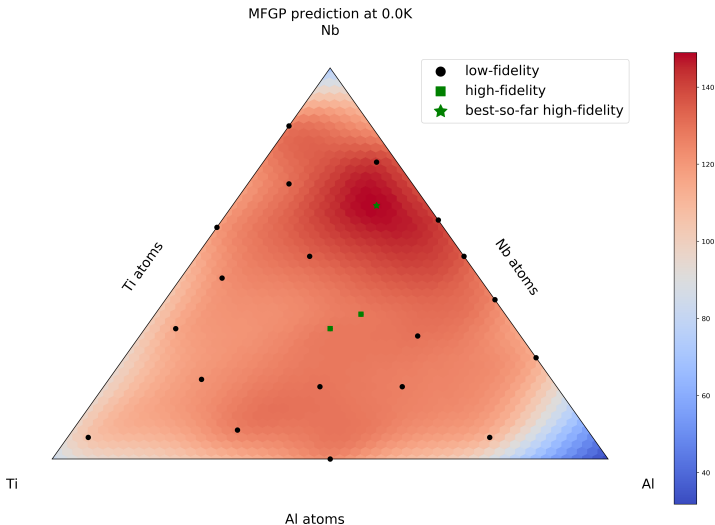
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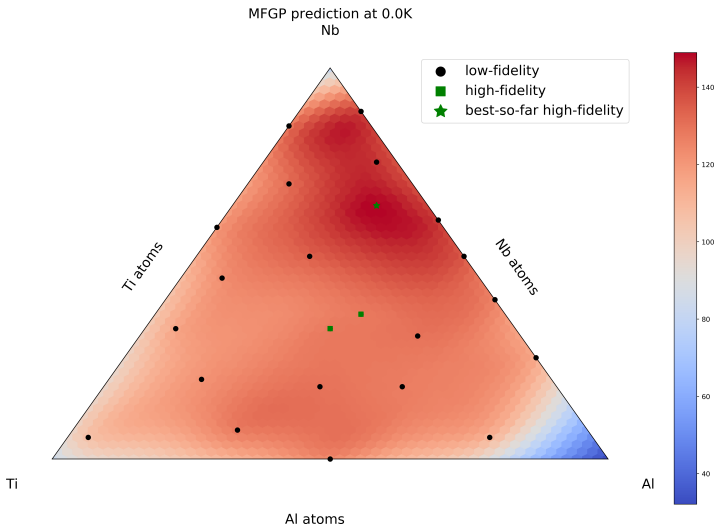
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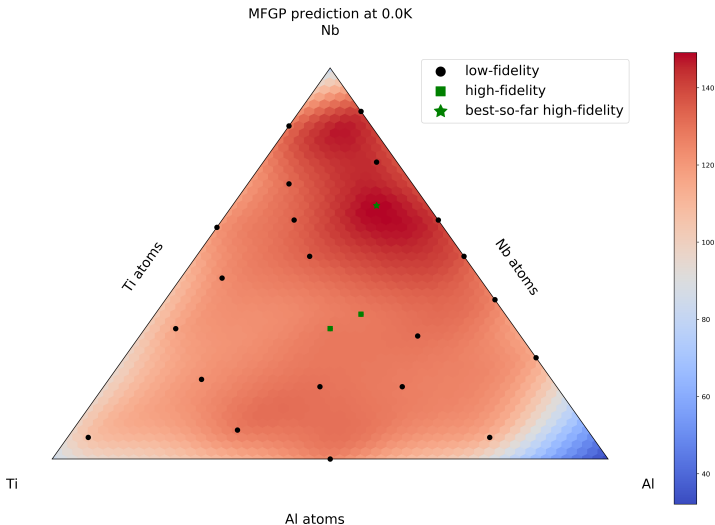
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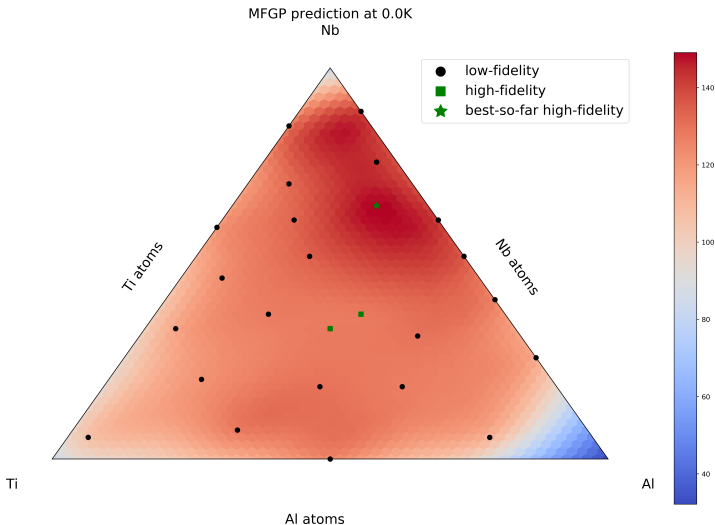
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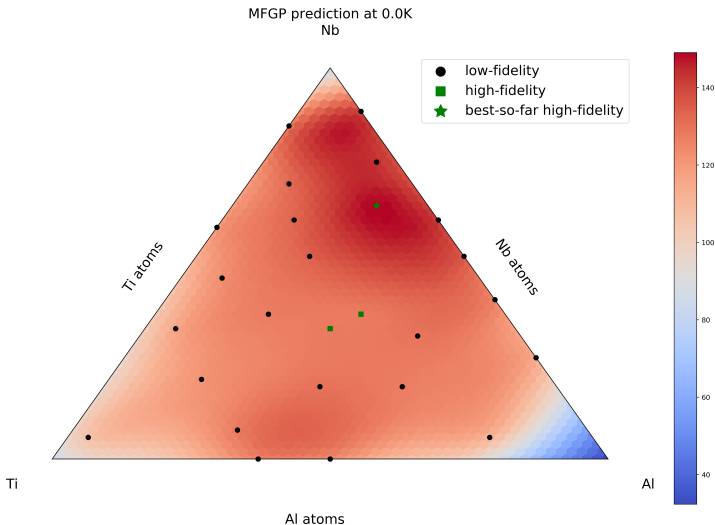
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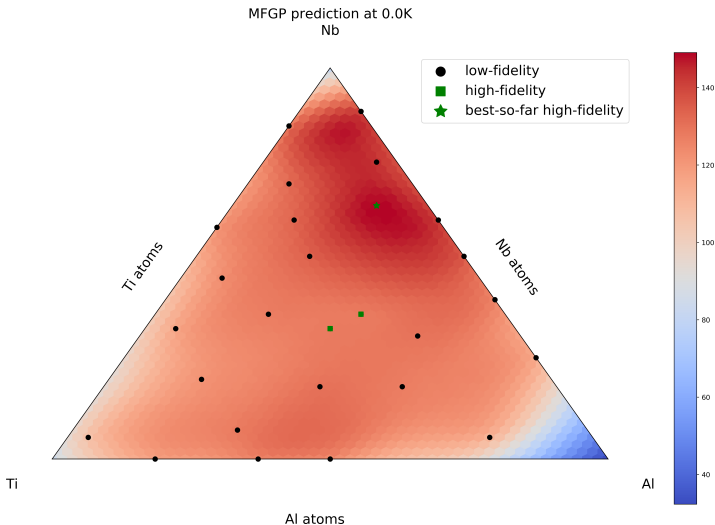
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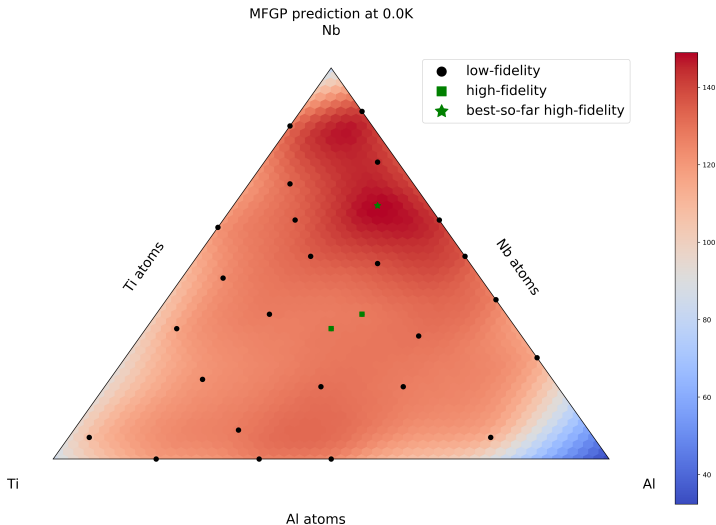
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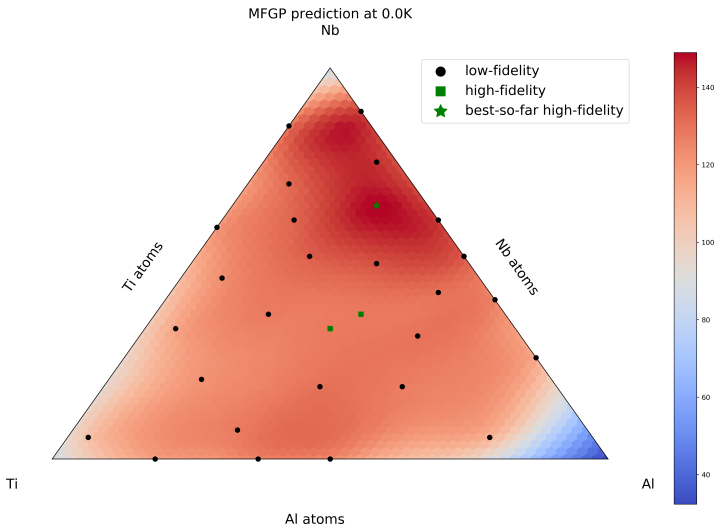
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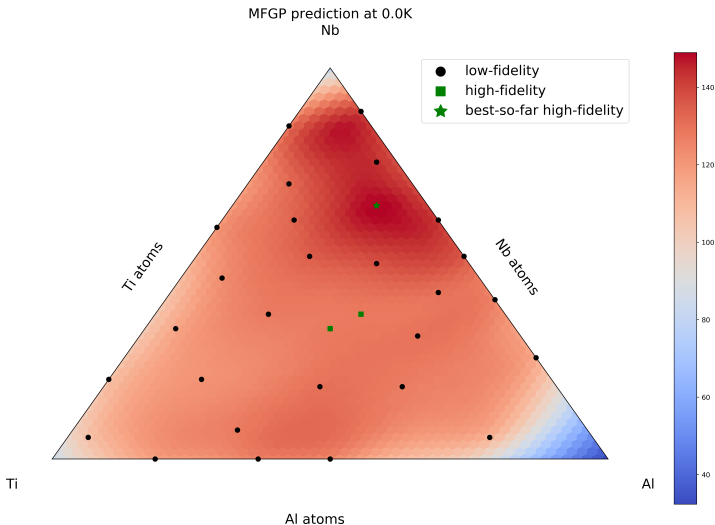
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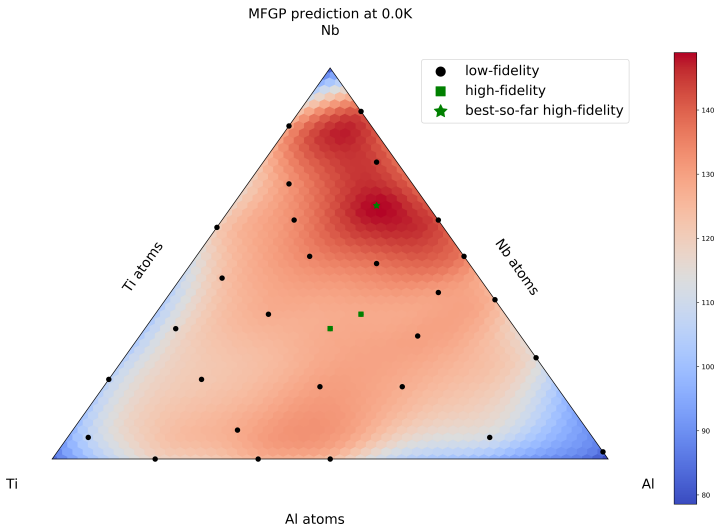
Inverse problems in composition-property

(joint work w/ Julien Tranchida, Aidan Thompson, Tim Wildey)



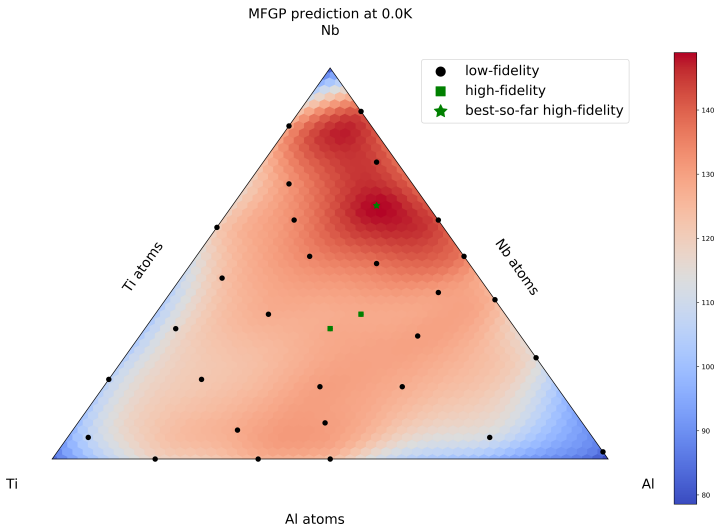
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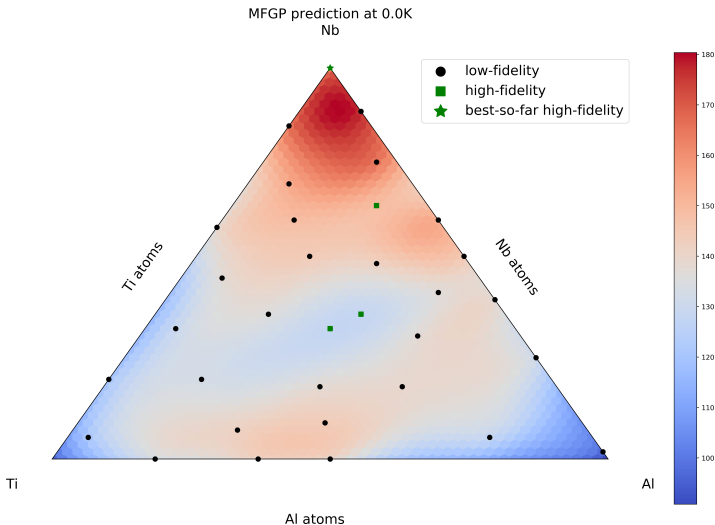
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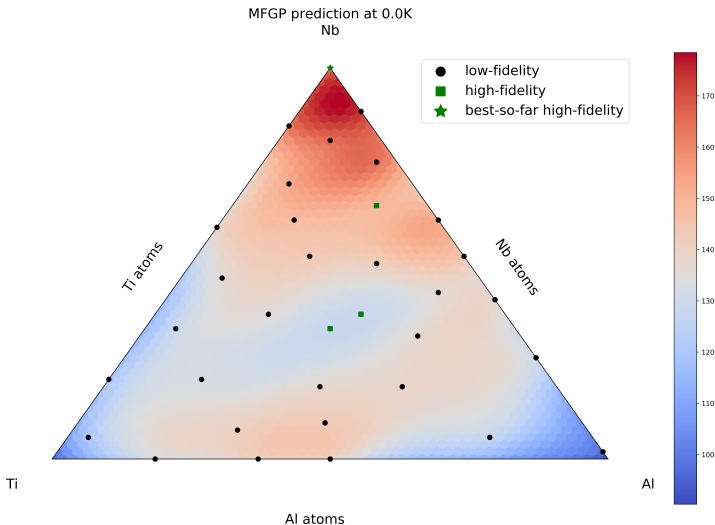
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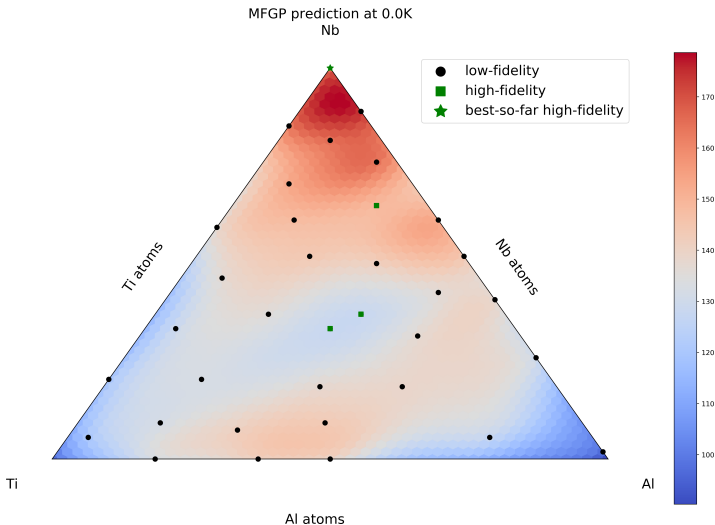
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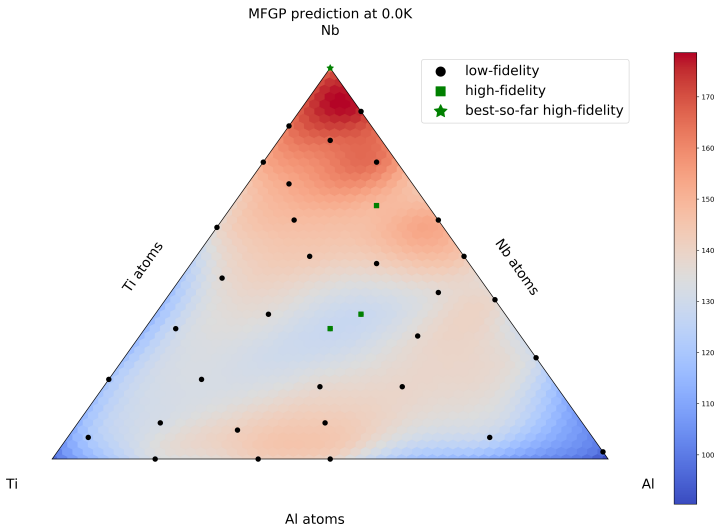
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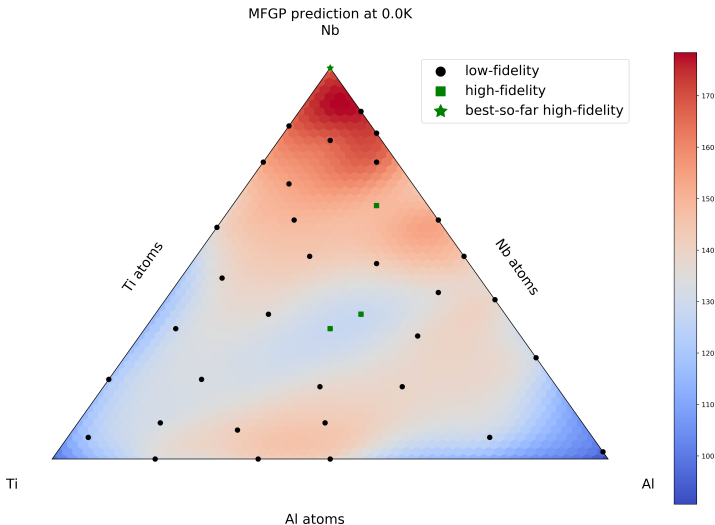
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Inverse problems in composition-property

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Inverse problems in structure-property

(joint work w/ Tim Wildey, Hojun Lim)

Reference

Anh Tran and Tim Wildey (2020). "Solving stochastic inverse problems for property-structure linkages using data-consistent inversion and machine learning". In: *JOM* 73, pp. 72–89

Ingredients:

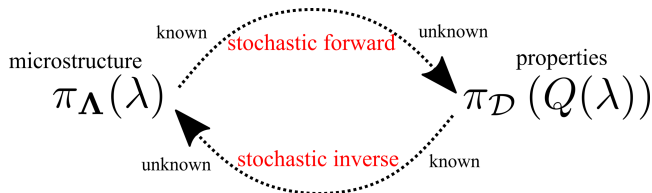
- 1 Crystal plasticity finite element as forward ICME model
- 2 **Heteroscedastic** Gaussian process as ML model for microstructure - homogenized materials property relationship
- 3 A data-consistent UQ technique (Butler, Jakeman, and Wildey 2018a,b) to solve a stochastic inverse problem (on ML model)

Inverse problems in structure-property

(joint work w/ Tim Wildey, Hojun Lim)

Problem statement:

- Given a deterministic or stochastic map (either analytical as Hall-Petch or numerical ML) **from microstructure features to homogenized materials**,
- Given a (target) distribution of homogenized materials properties,
- Task: **infer** a data-consistent distribution of microstructure features, in the sense that **forward propagation of this microstructure feature distribution matches the target distribution on homogenized materials properties**

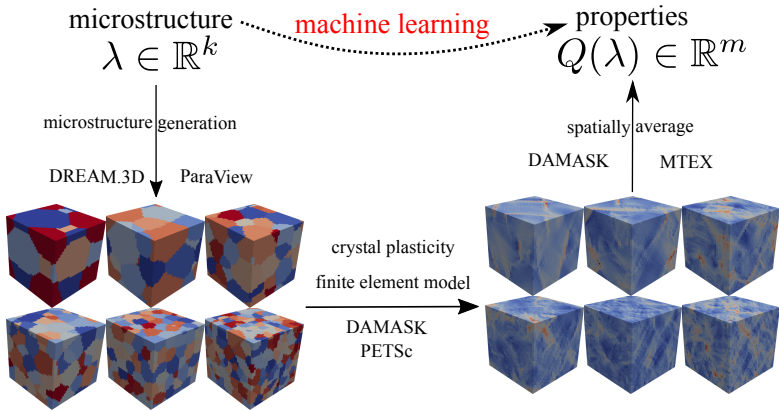


Stochastic Forward: given uncertain input $\lambda \rightarrow$ uncertain output $Q(\lambda)$;

Stochastic Inverse: given uncertain output $Q(\lambda) \rightarrow$ uncertain input λ .

Inverse problems in structure-property

(joint work w/ Tim Wildey, Hojun Lim)



Microstructure-homogenized properties map over an ensemble of microstructures with a **heteroscedastic GP**.

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Steps:

- 1 Parameterize *deterministic* λ as microstructure features, e.g. average grain size, location/scale/shape parameters for Weibull, exponential, extreme value distribution, etc.
- 2 Sample N microstructure RVE (DREAM.3D)
- 3 Run crystal plasticity over an ensemble of RVEs (DAMASK)
- 4 Estimate quantities of interest $Q(\lambda)$ by Monte Carlo average
- 5 Approximate $Q(\cdot)$ by a heteroscedastic Gaussian process regression
- 6 Infer the distribution of microstructure features (Butler, Jakeman, and Wildey 2018a,b)

$$\pi_{\Lambda}^{\text{updated}}(\lambda) = \pi_{\Lambda}^{\text{init}}(\lambda) \frac{\pi_{\mathcal{D}}^{\text{obs}}(\lambda)}{\pi_{\mathcal{D}}^{Q(\text{init})}(\lambda)}, \quad \lambda \in \Lambda \quad (17)$$

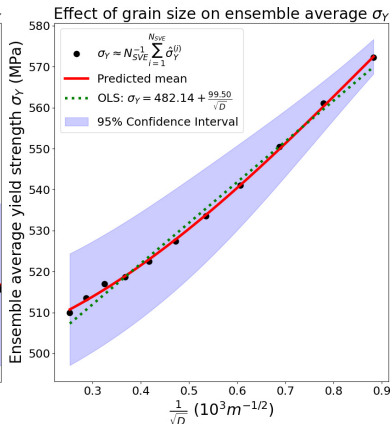
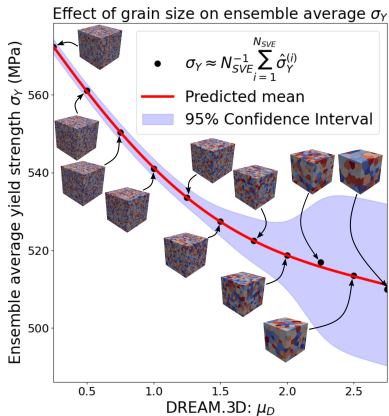
- 7 Sample $\pi_{\Lambda}^{\text{updated}}(\lambda)$ by rejection sampling

Inverse problems in structure-property

(joint work w/ Tim Wildey, Hojun Lim)

Ensemble average yield stress via Monte Carlo with different grain sizes

Comparison: GP (ML/UQ) and the Hall-Petch (ordinary least square)

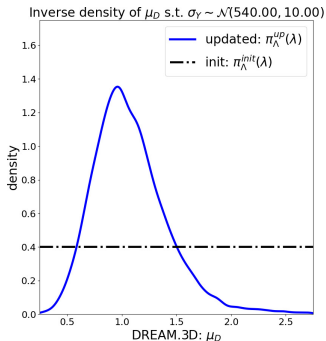


Noise depends on grain size!

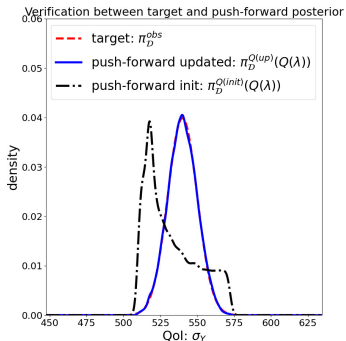
Inverse problems in structure-property

(joint work w/ Tim Wildey, Hojun Lim)

Initial density and updated density:
normal case



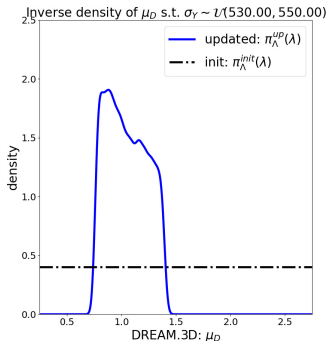
Comparison: Distributions of materials properties



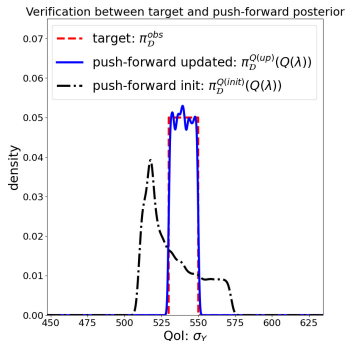
Inverse problems in structure-property

(joint work w/ Tim Wildey, Hojun Lim)

Initial density and updated density:
uniform case



Comparison: Distributions of materials properties



Conclusion

Takeaway message

Gaussian process is a versatile machine learning, uncertainty quantification, and (global) optimization toolbox for multiscale ICME applications.

In this talk, we:

- introduce a gentle tutorial to Gaussian process and Bayesian optimization
- demonstrate with multiscale ICME applications (all are open-source)
 - density functional theory: Quantum ESPRESSO
 - molecular dynamics: LAMMPS
 - kinetic Monte Carlo: SPPARKS
 - crystal plasticity finite element: DREAM.3D + DAMASK

Thank you for your time and listening.

References

Methodology:

- Anh Tran et al. (2022). "aphBO-2GP-3B: a budgeted asynchronous parallel multi-acquisition functions for constrained Bayesian optimization on high-performing computing architecture". In: *Structural and Multidisciplinary Optimization* 65.4, pp. 1–45
- Anh Tran (Aug. 2021). "Scalable³-BO: Big Data meets HPC - A scalable asynchronous parallel high-dimensional Bayesian optimization framework on supercomputers". In: *Proceedings of the ASME 2021 IDETC/CIE*, vol. Volume 1: 41th Computers and Information in Engineering Conference. International Design Engineering Technical Conferences and Computers and Information in Engineering Conference. American Society of Mechanical Engineers
- Anh Tran et al. (Aug. 2020c). "srMO-BO-3GP: A sequential regularized multi-objective constrained Bayesian optimization for design applications". In: *Proceedings of the ASME 2020 IDETC/CIE*, vol. Volume 1: 40th Computers and Information in Engineering Conference. International Design Engineering Technical Conferences and Computers and Information in Engineering Conference. American Society of Mechanical Engineers
- Anh Tran, Tim Wildey, and Scott McCann (2020). "sMF-BO-2CoGP: A sequential multi-fidelity constrained Bayesian optimization for design applications". In: *Journal of Computing and Information Science in Engineering* 20.3, pp. 1–15
- Anh Tran, Tim Wildey, and Scott McCann (Aug. 2019). "sBF-BO-2CoGP: A sequential bi-fidelity constrained Bayesian optimization for design applications". In: *Proceedings of the ASME 2019 IDETC/CIE*, vol. Volume 1: 39th Computers and Information in Engineering Conference. International Design Engineering Technical Conferences and Computers and Information in Engineering Conference. V001T02A073. American Society of Mechanical Engineers
- Anh Tran, Minh Tran, and Yan Wang (2019). "Constrained mixed-integer Gaussian mixture Bayesian optimization and its applications in designing fractal and auxetic metamaterials". In: *Structural and Multidisciplinary Optimization* 59 (6), pp. 2131–2154
- Anh Tran et al. (2019a). "pBO-2GP-3B: A batch parallel known/unknown constrained Bayesian optimization with feasibility classification and its applications in computational fluid dynamics". In: *Computer Methods in Applied Mechanics and Engineering* 347, pp. 827–852

Applications:

- Anh Tran and Tim Wildey (2020). "Solving stochastic inverse problems for property-structure linkages using data-consistent inversion and machine learning". In: *JOM* 73, pp. 72–89
- Anh Tran et al. (2020b). "Multi-fidelity machine-learning with uncertainty quantification and Bayesian optimization for materials design: Application to ternary random alloys". In: *The Journal of Chemical Physics* 153 (7), p. 074705
- Anh Tran et al. (2020a). "An active-learning high-throughput microstructure calibration framework for process-structure linkage in materials informatics". In: *Acta Materialia* 194, pp. 80–92
- Stefano Travaglini et al. (2020). "Computational optimization study of transcatheter aortic valve leaflet design using porcine and bovine leaflets". In: *Journal of Biomechanical Engineering* 142 (1)
- Anh Tran et al. (2019b). "WearGP: A computationally efficient machine learning framework for local erosive wear predictions via nodal Gaussian processes". In: *Wear* 422, pp. 9–26
- Anh Tran, Lijuan He, and Yan Wang (2018). "An efficient first-principles saddle point searching method based on distributed kriging metamodels". In: *ASCE-ASME Journal of Risk and Uncertainty in Engineering Systems, Part B: Mechanical Engineering* 4.1, p. 011006

References I

-  Agrawal, Ankit and Alok Choudhary (2016). “Perspective: Materials informatics and big data: Realization of the “fourth paradigm” of science in materials science”. In: *APL Materials* 4.5, p. 053208.
-  Butler, T, J Jakeman, and T Wildey (2018a). “Combining push-forward measures and Bayes’ rule to construct consistent solutions to stochastic inverse problems”. In: *SIAM Journal on Scientific Computing* 40.2, A984–A1011.
-  — (2018b). “Convergence of Probability Densities Using Approximate Models for Forward and Inverse Problems in Uncertainty Quantification”. In: *SIAM Journal on Scientific Computing* 40.5, A3523–A3548.
-  Christodoulou, Julie et al. (2021). *The second decade of the Materials Genome Initiative*.
-  Hey, Tony, Stewart Tansley, Kristin M Tolle, et al. (2009). *The fourth paradigm: data-intensive scientific discovery*. Vol. 1. Microsoft research Redmond, WA.

References II

-  Holdren, John P et al. (2014). “Materials genome initiative strategic plan (2014)”. In: *National Science And Technology Council*.
-  Huang, Deng et al. (2006). “Global optimization of stochastic black-box systems via sequential kriging meta-models”. In: *Journal of Global Optimization* 34.3, pp. 441–466.
-  Kennedy, Marc C and Anthony O’Hagan (2000). “Predicting the output from a complex computer code when fast approximations are available”. In: *Biometrika* 87.1, pp. 1–13.
-  Lander, Eric et al. (2021). “Materials genome initiative strategic plan (2021)”. In: *National Science And Technology Council*.
-  Liu, Xuan et al. (2018). *Vision 2040: a roadmap for integrated, multiscale modeling and simulation of materials and systems*. Tech. rep.
-  Mockus, Jonas (1975). “On Bayesian methods for seeking the extremum”. In: *Optimization Techniques IFIP Technical Conference*. Springer, pp. 400–404.
-  — (1982). “The Bayesian approach to global optimization”. In: *System Modeling and Optimization*, pp. 473–481.

References III

-  Pablo, Juan J de et al. (2019). “New frontiers for the materials genome initiative”. In: *npj Computational Materials* 5.1, pp. 1–23.
-  Srinivas, Niranjana et al. (2009). “Gaussian process optimization in the bandit setting: No regret and experimental design”. In: *arXiv preprint arXiv:0912.3995*.
-  Srinivas, Niranjana et al. (2012). “Information-theoretic regret bounds for Gaussian process optimization in the bandit setting”. In: *IEEE Transactions on Information Theory* 58.5, pp. 3250–3265.
-  Tran, Anh (Aug. 2021). “Scalable³-BO: Big Data meets HPC - A scalable asynchronous parallel high-dimensional Bayesian optimization framework on supercomputers”. In: *Proceedings of the ASME 2021 IDETC/CIE*. Vol. Volume 1: 41th Computers and Information in Engineering Conference. International Design Engineering Technical Conferences and Computers and Information in Engineering Conference. American Society of Mechanical Engineers.

References IV



Tran, Anh, Lijuan He, and Yan Wang (2018). “An efficient first-principles saddle point searching method based on distributed kriging metamodels”. In: *ASCE-ASME Journal of Risk and Uncertainty in Engineering Systems, Part B: Mechanical Engineering* 4.1, p. 011006.



Tran, Anh, Minh Tran, and Yan Wang (2019). “Constrained mixed-integer Gaussian mixture Bayesian optimization and its applications in designing fractal and auxetic metamaterials”. In: *Structural and Multidisciplinary Optimization* 59 (6), pp. 2131–2154.



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References V



Tran, Anh, Tim Wildey, and Scott McCann (Aug. 2019).
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— (2020). “sMF-BO-2CoGP: A sequential multi-fidelity constrained Bayesian optimization for design applications”. In: *Journal of Computing and Information Science in Engineering* 20.3, pp. 1–15.



Tran, Anh et al. (2019a). “pBO-2GP-3B: A batch parallel known/unknown constrained Bayesian optimization with feasibility classification and its applications in computational fluid dynamics”. In: *Computer Methods in Applied Mechanics and Engineering* 347, pp. 827–852.



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References VI



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Tran, Anh et al. (2020b). “Multi-fidelity machine-learning with uncertainty quantification and Bayesian optimization for materials design: Application to ternary random alloys”. In: *The Journal of Chemical Physics* 153 (7), p. 074705.



Tran, Anh et al. (Aug. 2020c). “srMO-BO-3GP: A sequential regularized multi-objective constrained Bayesian optimization for design applications”. In: *Proceedings of the ASME 2020 IDETC/CIE*. Vol. Volume 1: 40th Computers and Information in Engineering Conference. International Design Engineering Technical Conferences and Computers and Information in Engineering Conference. American Society of Mechanical Engineers.

References VII

-  Tran, Anh et al. (2022). “aphBO-2GP-3B: a budgeted asynchronous parallel multi-acquisition functions for constrained Bayesian optimization on high-performing computing architecture”. In: *Structural and Multidisciplinary Optimization* 65.4, pp. 1–45.
-  Travaglini, Stefano et al. (2020). “Computational optimization study of transcatheter aortic valve leaflet design using porcine and bovine leaflets”. In: *Journal of Biomechanical Engineering* 142 (1).
-  US NSTC (2011). *Materials Genome Initiative for global competitiveness*. Executive Office of the President, National Science and Technology Council.
-  Wilson, James, Frank Hutter, and Marc Deisenroth (2018). “Maximizing acquisition functions for Bayesian optimization”. In: *Advances in Neural Information Processing Systems* 31, pp. 9884–9895.