

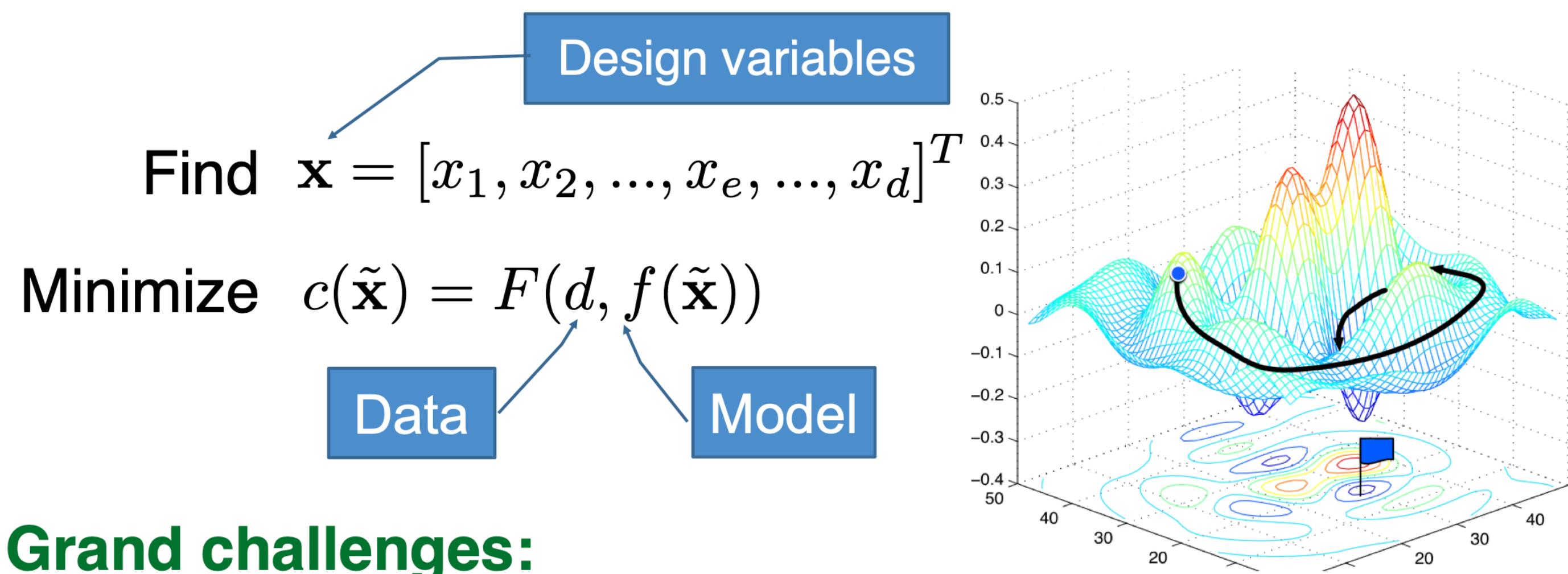
Sirui Bi^{1,2}, Jiaxin Zhang³, Guannan Zhang³

¹Department of Civil and Systems Engineering, Johns Hopkins University

²Computational Sciences and Engineering Division, Oak Ridge National Laboratory

³Computer Science and Mathematics Division, Oak Ridge National Laboratory

Motivation: high-dimensional optimization

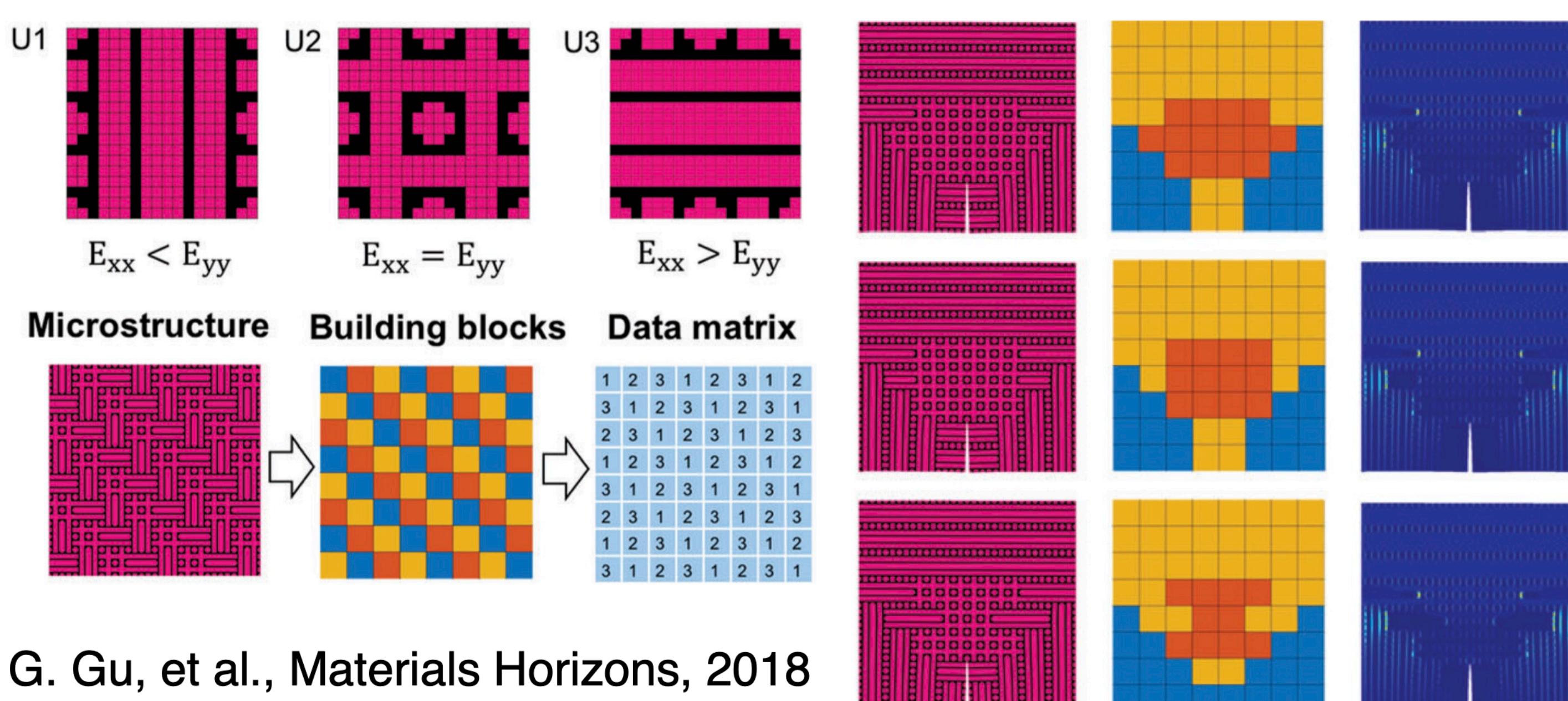


Grand challenges:

- High dimensions: a large number of design variables
- Expensive model simulation: high fidelity
- Sequential optimization: step-by-step search

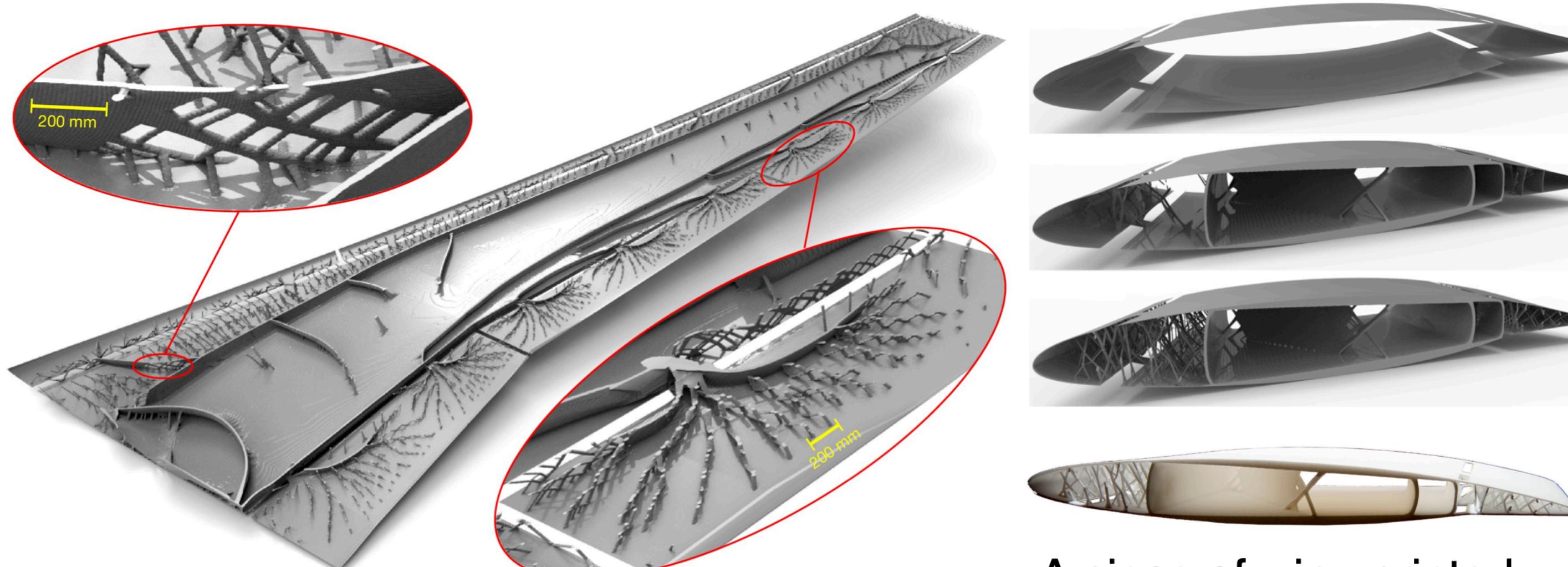
Driving application: AM material design

Design optimization for advanced composite materials with *Additive Manufacturing*



G. Gu, et al., Materials Horizons, 2018

Computational morphogenesis for optimized wing design



N. Aage, et al., Nature, 2017

High dimensional optimization with expensive simulation

Method: scalable ML-based optimization

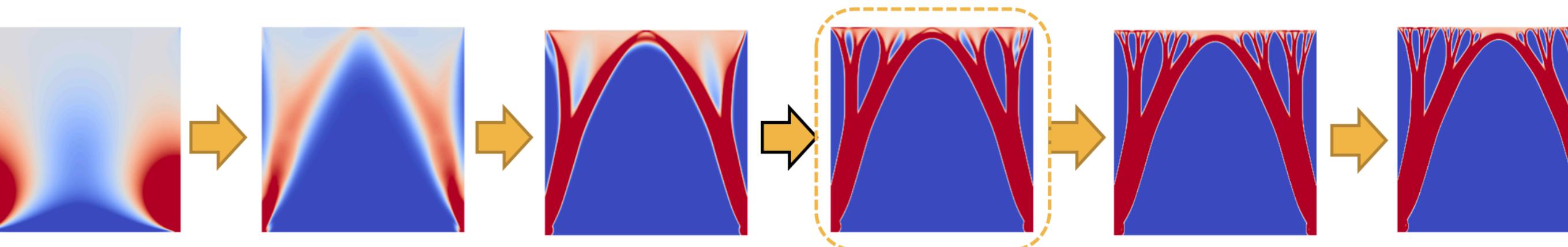
Optimal path guided learning with local sampling

- Optimal path is low dimensional (ideally, 1d)
- Local sampling - closely follow optimal path

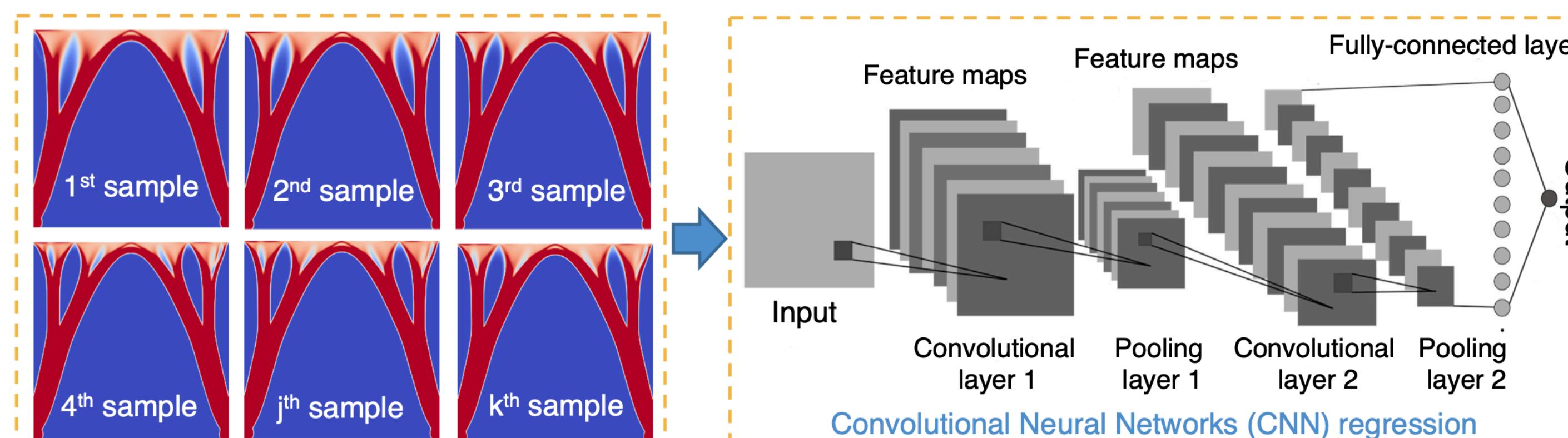
$$\tilde{x}_{\max}^j = \max \{ \tilde{x}^{(j-1)}, \tilde{x}^{(j-2)}, \dots, \tilde{x}^{(j-w)} \}$$

$$\tilde{x}_{\min}^j = \min \{ \tilde{x}^{(j-1)}, \tilde{x}^{(j-2)}, \dots, \tilde{x}^{(j-w)} \}$$

$$\tilde{x}_{rs}^j = U(\tilde{x}_{\max}^j + \delta, \tilde{x}_{\min}^j - \delta) \text{ Dimension reduction}$$

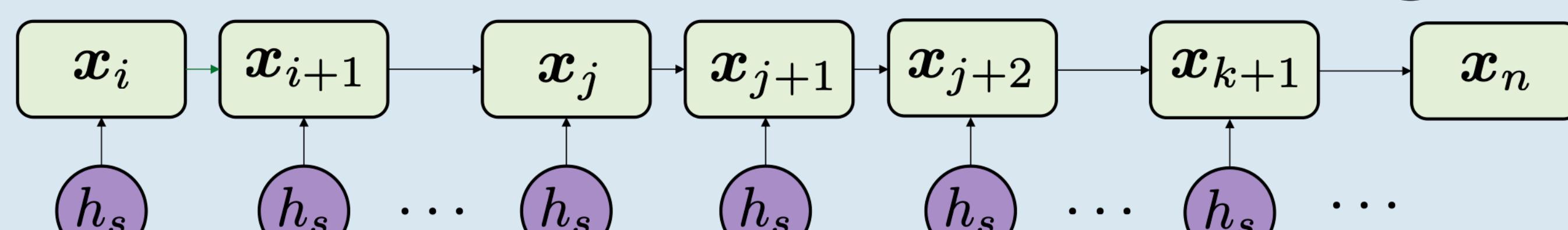


- Low-dimensional ML model (e.g., CNN) trained by local data

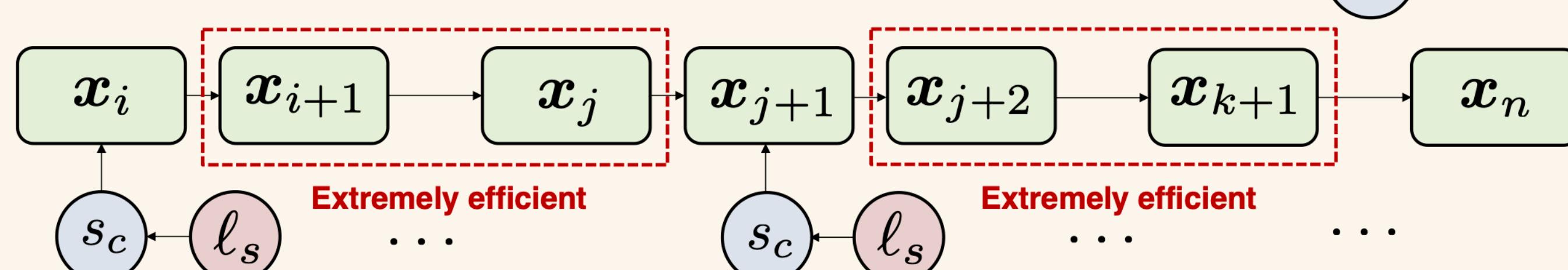


Scalable implementation (CPU+GPU) on Summit

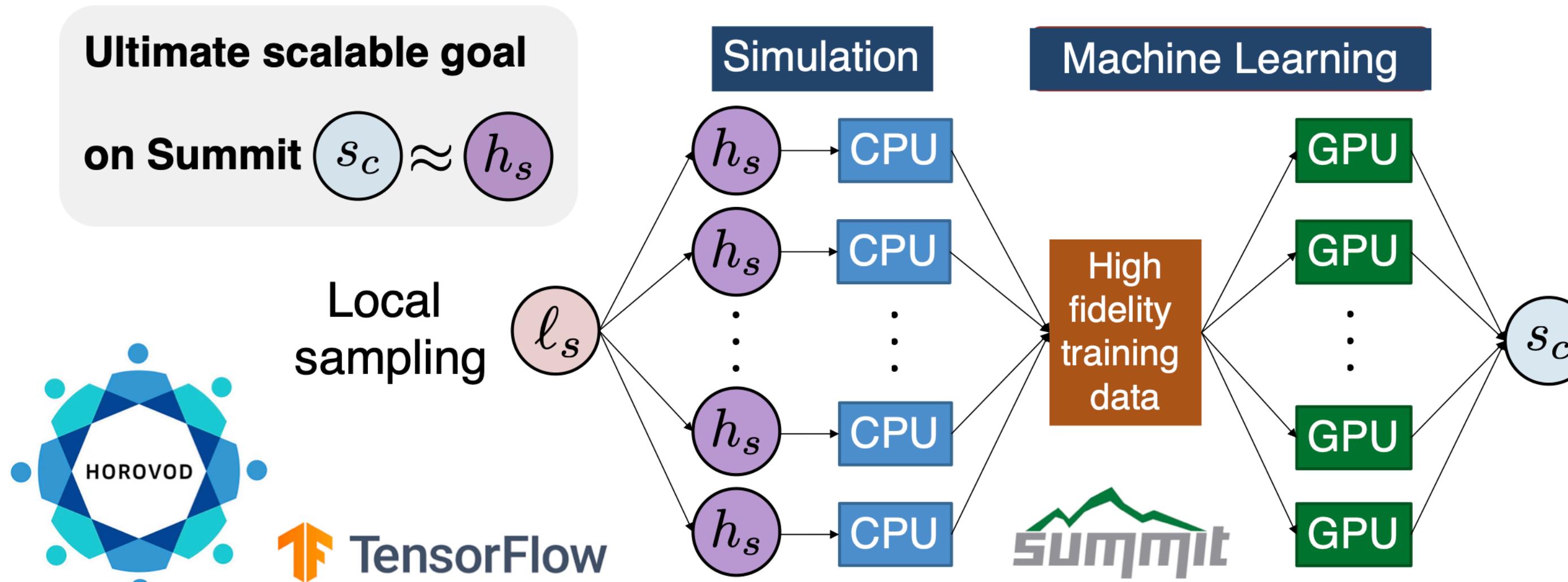
Sequential optimization with iterative high fidelity simulations (h_s)



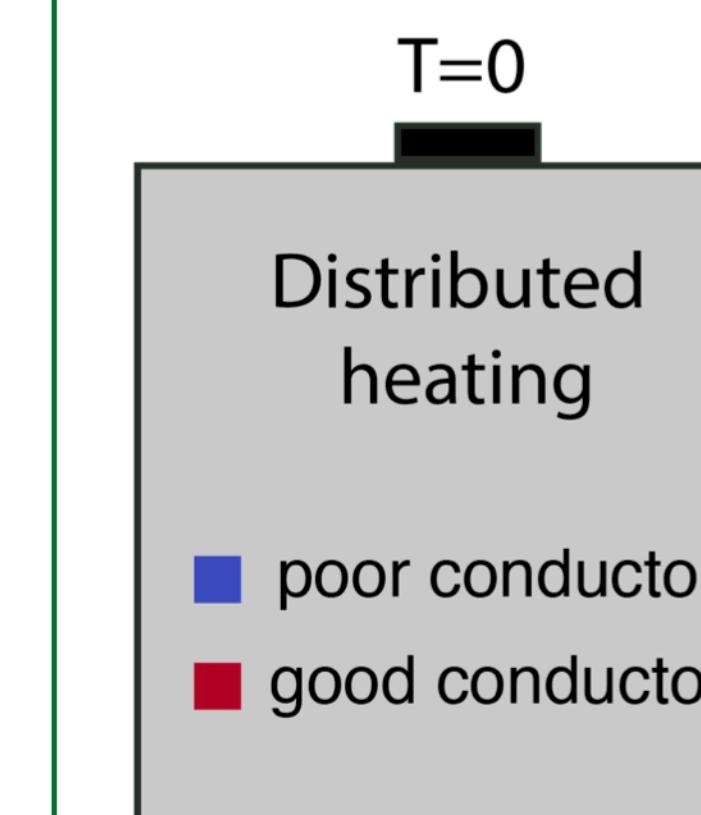
Scalable ML-based optimization with interval CNN learned (s_c)



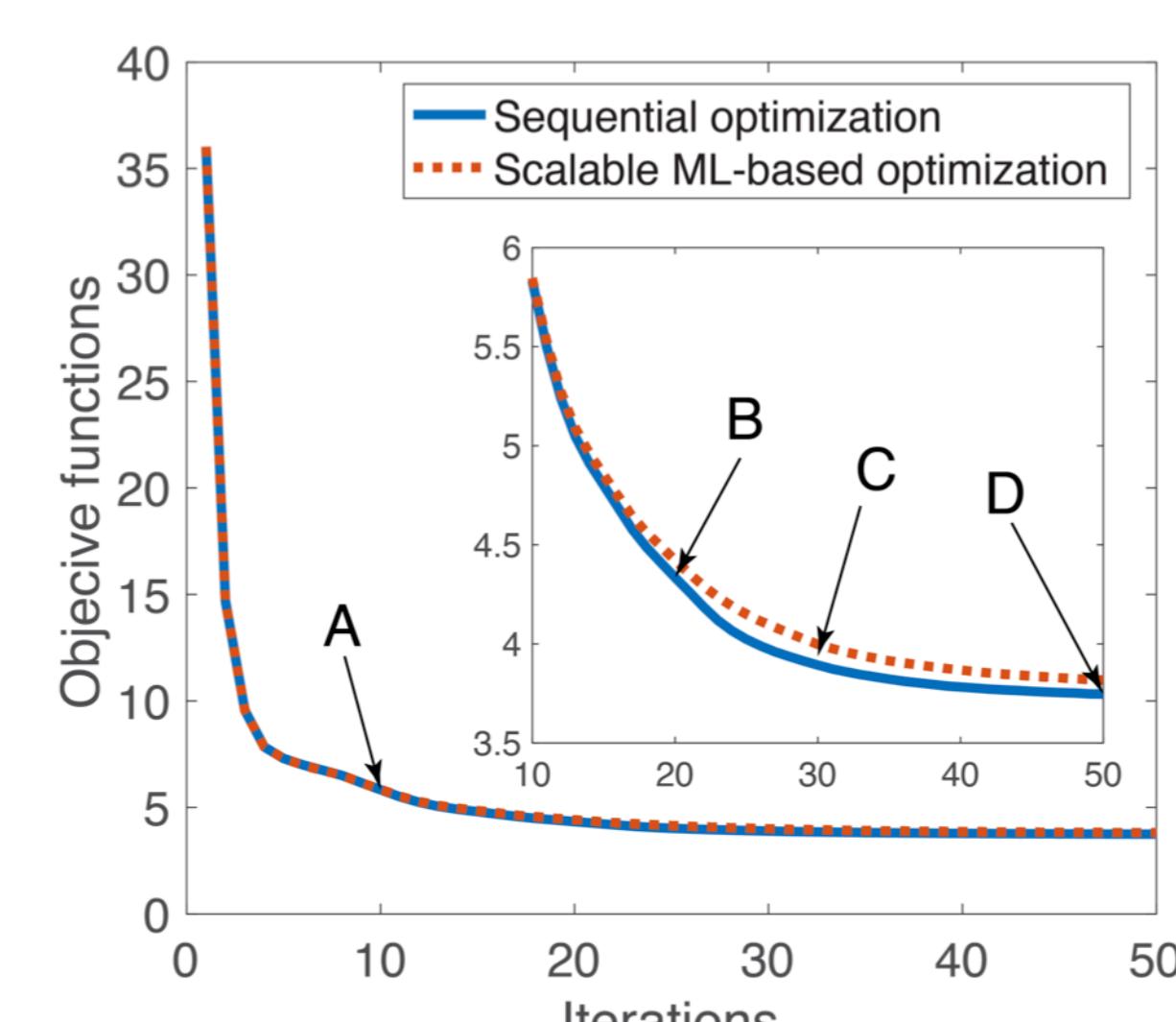
Time cost: parallel simulation + scalable ML ≈ high fidelity simulation



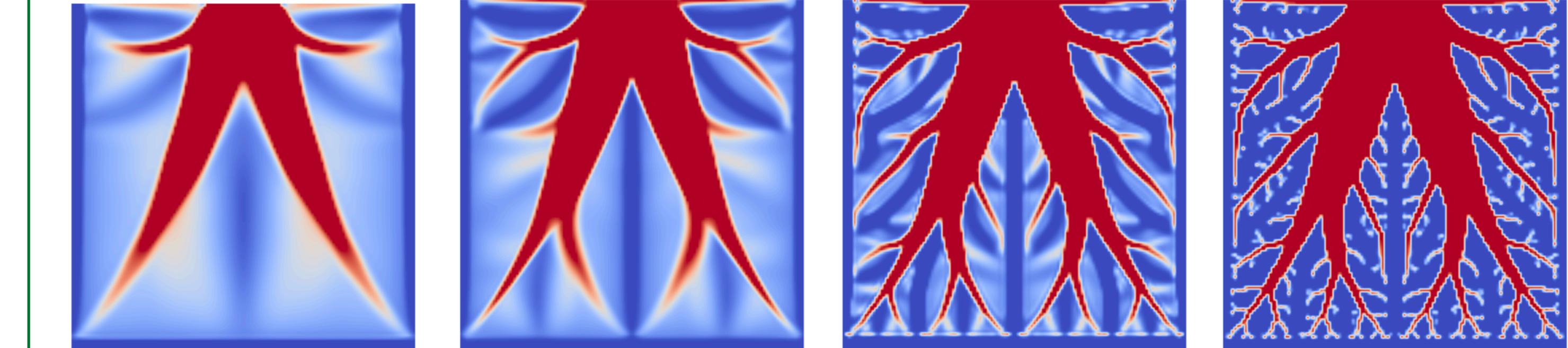
Results: two materials heat conduction



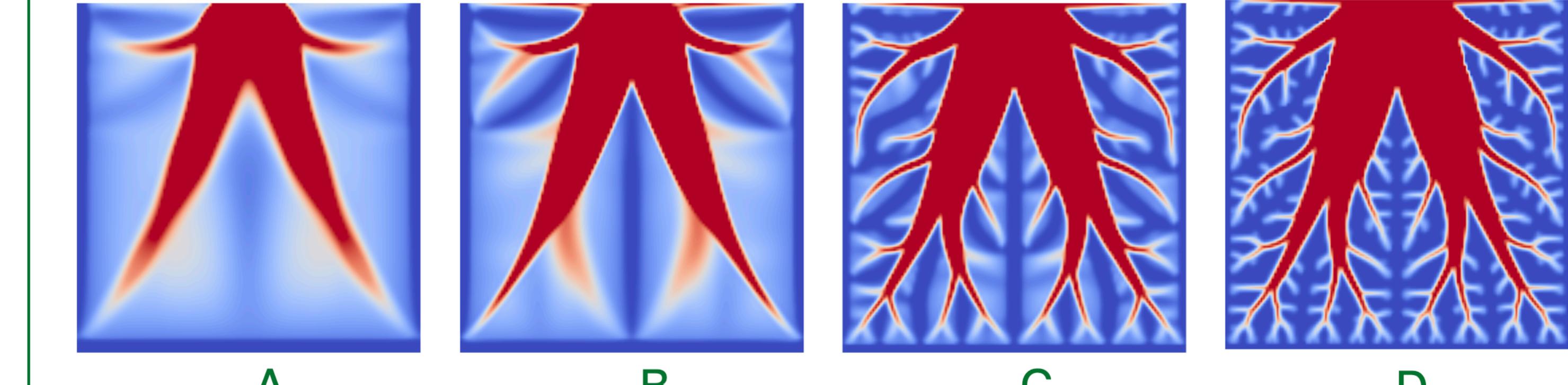
60% "good" thermal materials, $k_1 = 1.0$
40% "poor" thermal materials, $k_2 = 0.001$



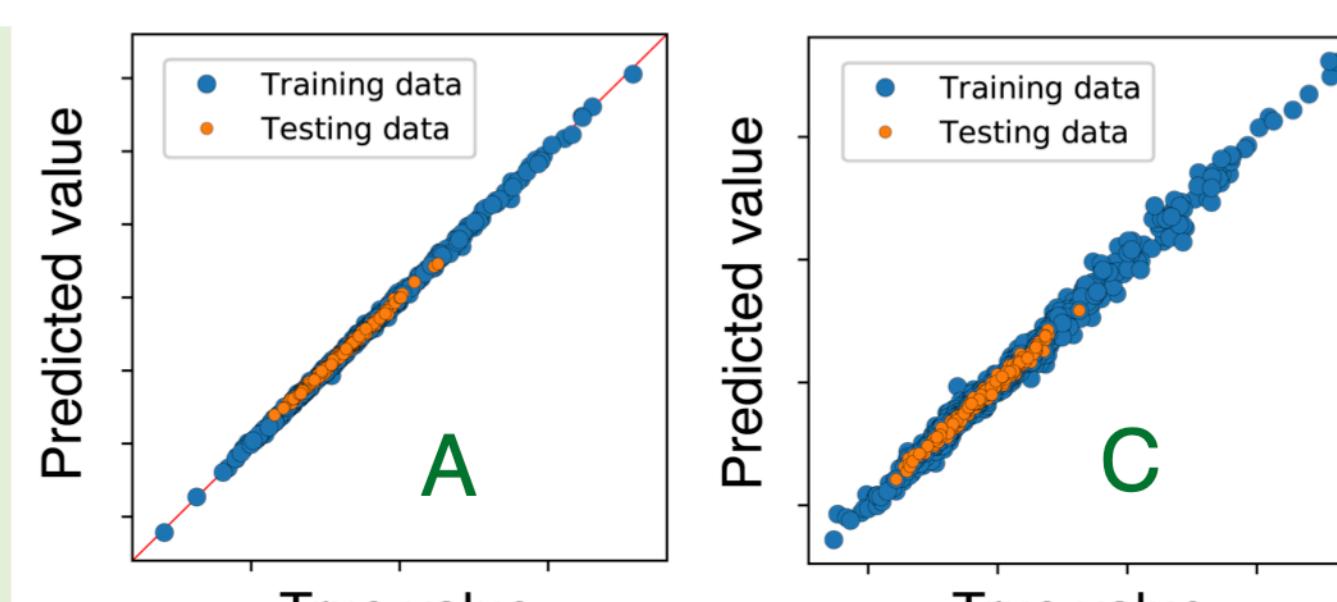
Sequential optimization: 50 expensive simulations



Scalable ML- optimization: 5 CNN-based learning



- Finite element for simulation: 128x128 mesh (up to 1024x1024) - expensive
- Local sampling: 10,000 total data
- Training: 32 nodes (192 GPUs) on Summit
- Time cost: 15% of classical method



Significant reduction of 85% time cost with acceleration 6.7x

Summary and future work

- Improve scalability and optimality for complex design requirement
 - high resolution, b) irregular design domain, c) multi-material, d) 3D
- Adaptive local sampling strategy: dimension reduction

