Uncertainty reduction with multi-model Monte Carlo for crystal plasticity simulations of additively manufactured metals

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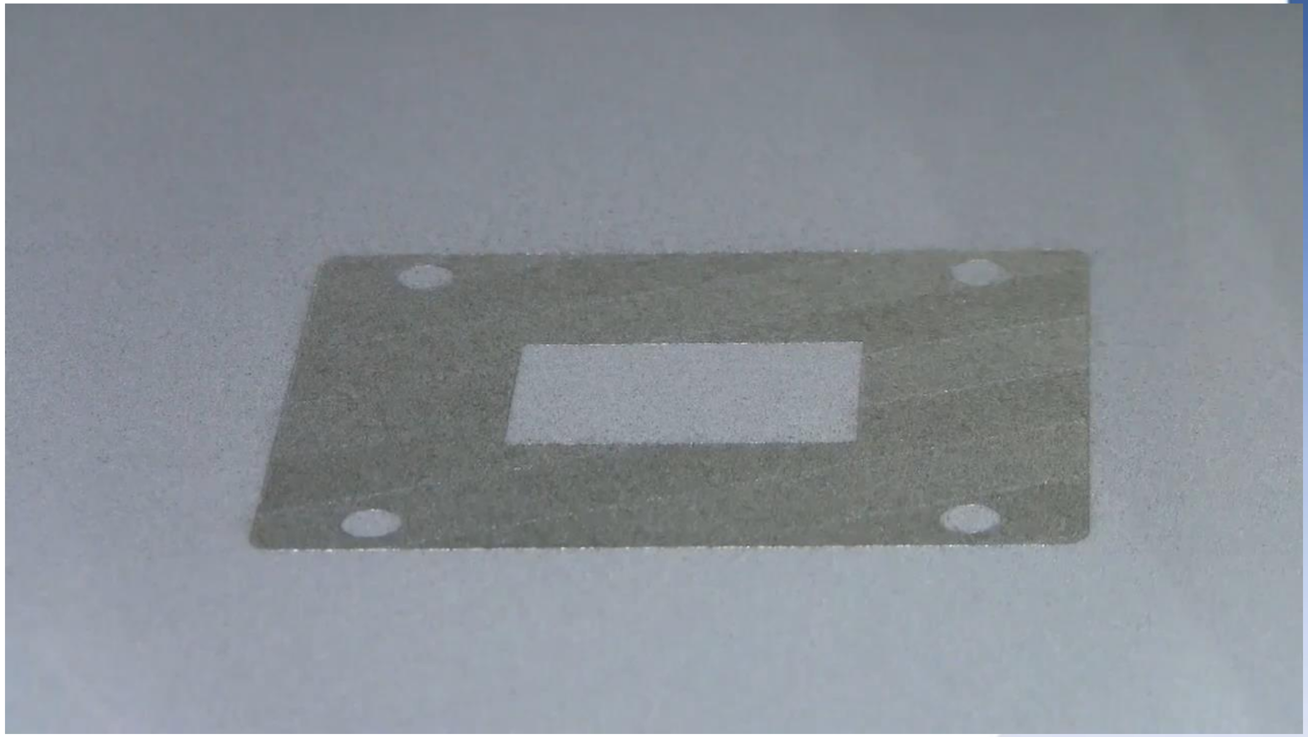
Outline

- Motivation: Additive manufacturing (AM) simulations
- Multi-model Monte Carlo background
  - Monte Carlo (MC) estimation
  - Multi-model MC estimation and variance reduction
- Application to crystal plasticity for AM metals
- Results
- Conclusions

Metal AM background

- Laser powder bed fusion: melt successive layers of powder into a desired shape → efficient production of complex geometries
- Load-bearing aerospace components (airframes, engines) require qualification and certification
- Need to characterize statistical variability in properties/performance → very expensive to rely on experiments alone

Laser powder bed fusion video

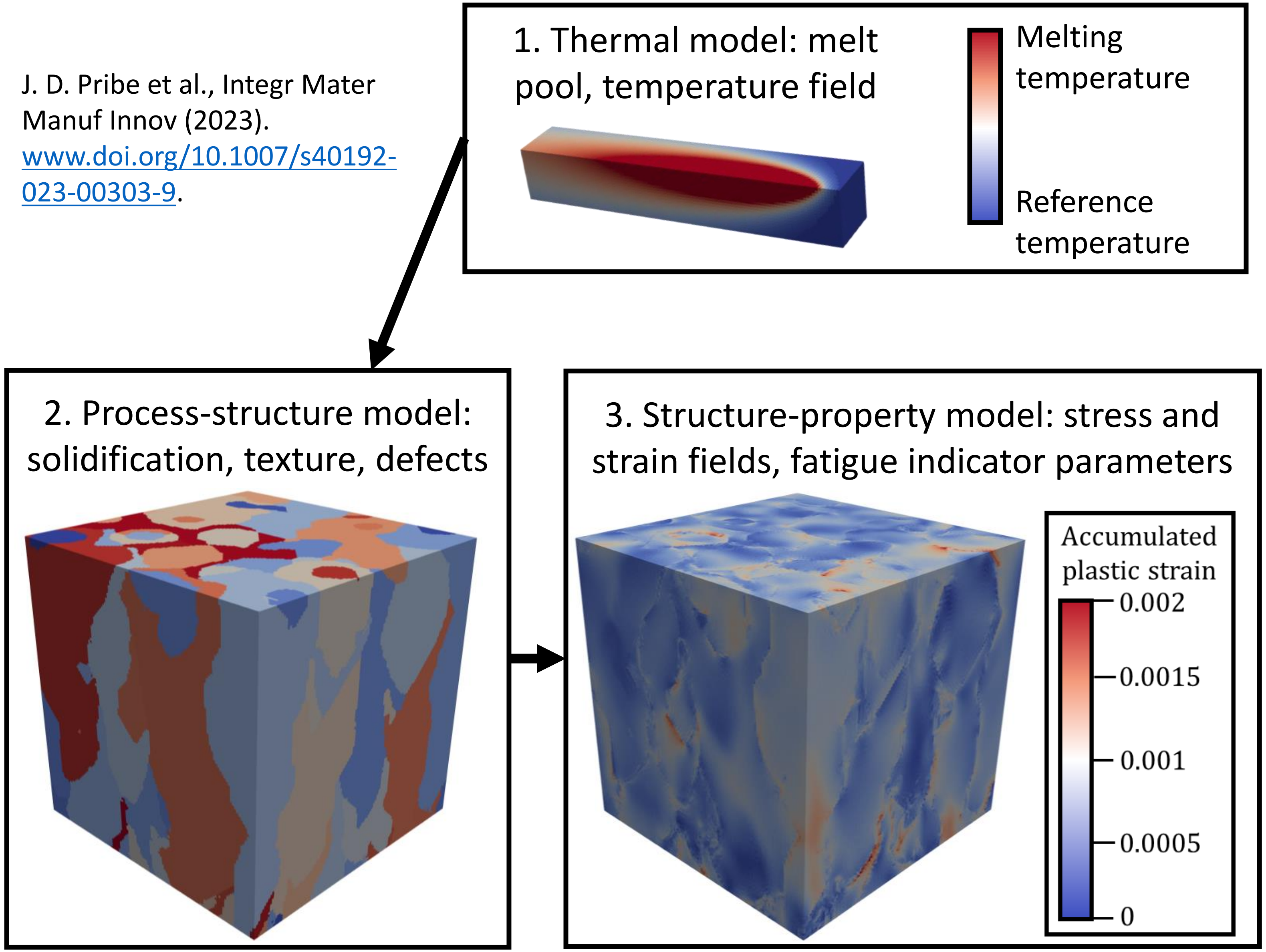


Credit: National Institute of Standards and Technology (NIST)[1]

[1]https://www.nist.gov/video/3d-printing-laser-and-metal-powder; reused as permitted by https://www.nist.gov/oism/copyrights

Motivation: Process-structure-property simulations

J. D. Pribe et al., Integr Mater Manuf Innov (2023). www.doi.org/10.1007/s40192-023-00303-9.

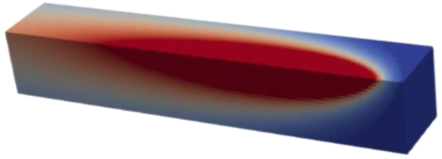


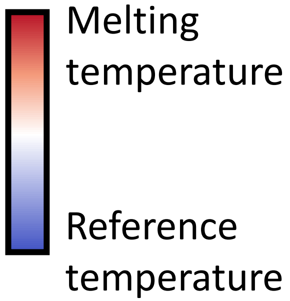
- Process-structure-property (PSP) simulations: understand how process changes/variations influence mechanical quantities of interest (QoIs)
- Need calibration, validation, and uncertainty quantification to build confidence in models

Motivation: PSP simulations with UQ

J. D. Pribe et al., Integr Mater Manuf Innov (2023). www.doi.org/10.1007/s40192-023-00303-9.

1. Thermal model: melt pool, temperature field

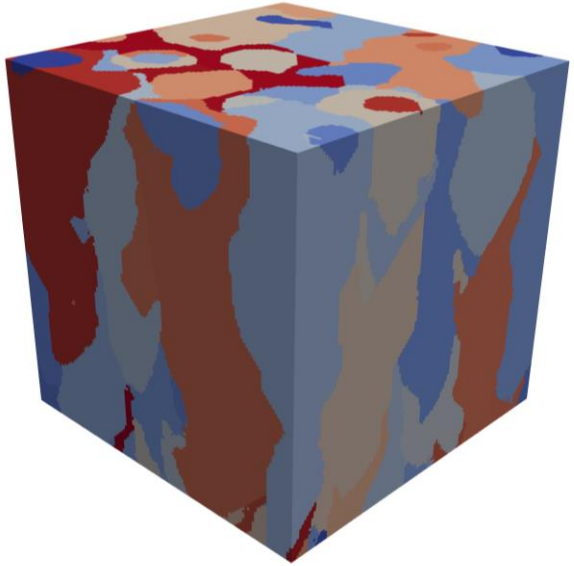




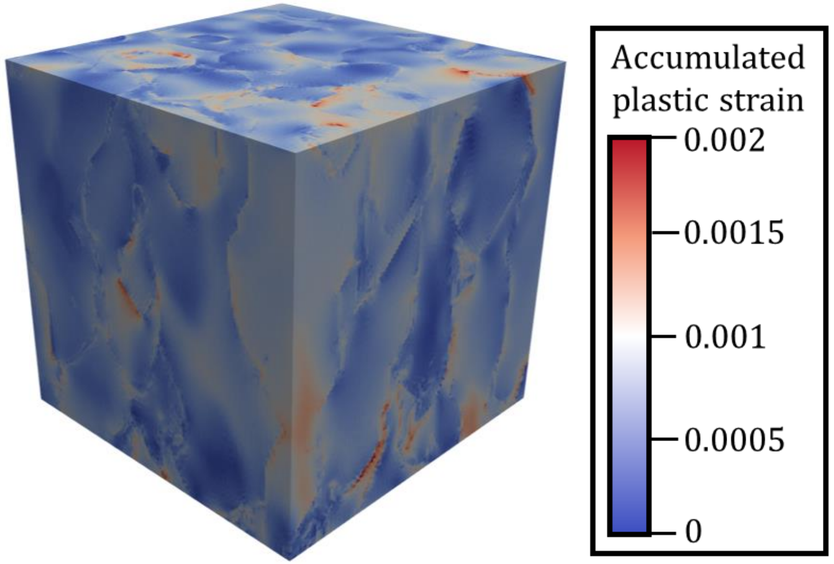
- Repeat simulations to build up statistics on QoIs
- **How to quantify and reduce computational cost?**

Repeat simulations

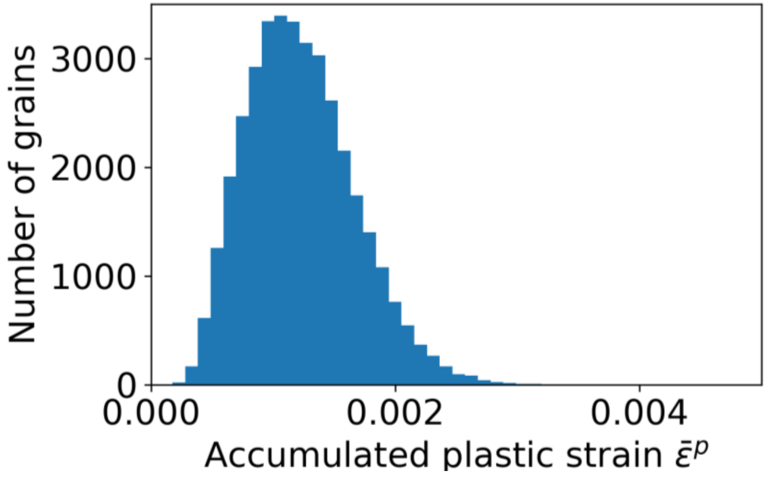
2. Process-structure model: solidification, texture, defects



3. Structure-property model: stress and strain fields, fatigue indicator parameters

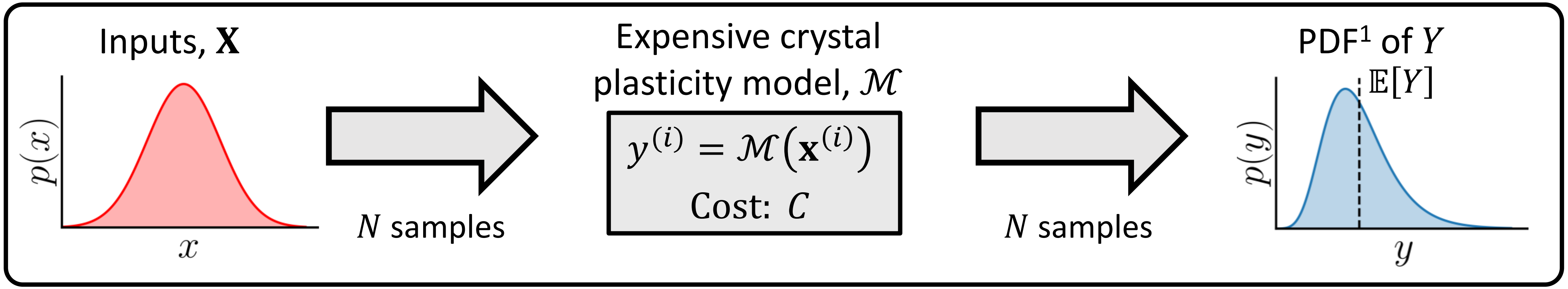


Fatigue indicator parameter statistics



MC estimation

Problem: estimate the expected value, $\mathbb{E}[Y]$, for a QoI, Y



[1]PDF: probability density function

MC estimator: $\mathbb{E}[Y] \approx \hat{Y}(\mathbf{x}) = \frac{1}{N}\sum_{i=1}^{N} \mathcal{M}(\mathbf{x}^{(i)})$ $\quad \mathbf{x} = \{\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(N)}\}$ (input samples)

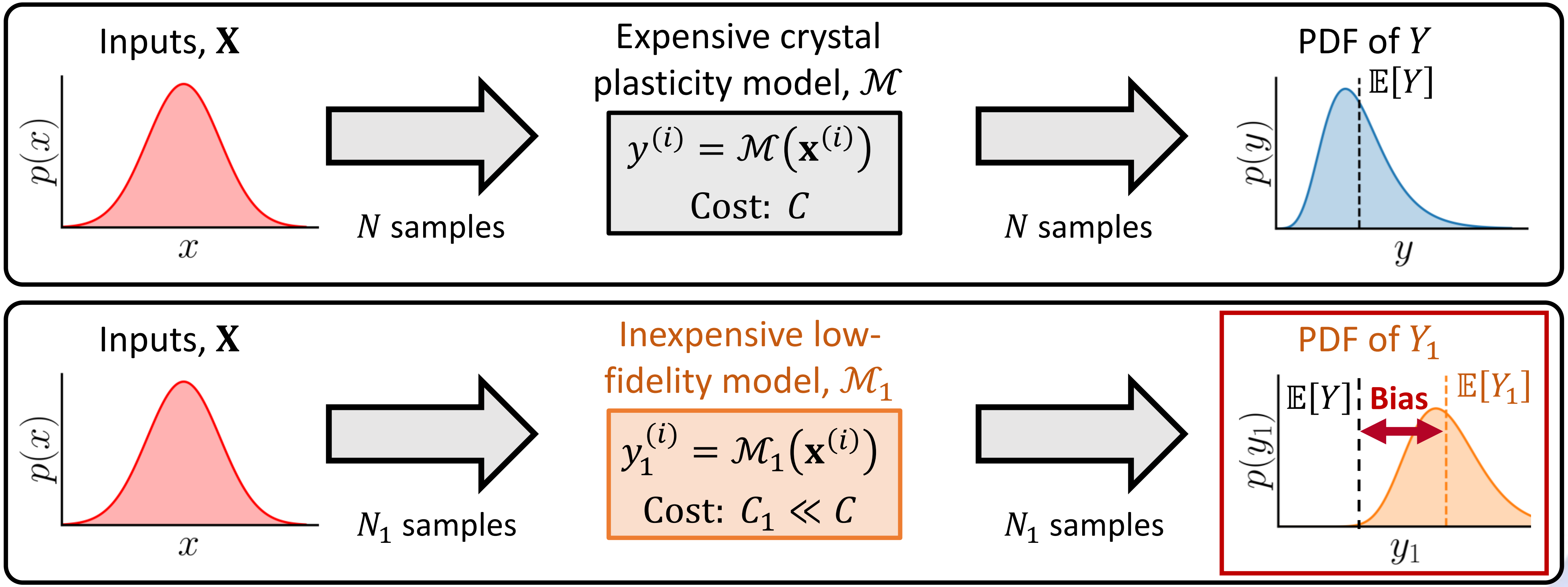
Total cost: $\hat{C} = NC$

Mean-squared error: (MSE) $\mathrm{MSE}(\hat{Y}) = \mathrm{Bias}[\hat{Y}]^2 + \mathbb{V}\mathrm{ar}[\hat{Y}] = \mathbb{V}\mathrm{ar}[Y]/N$ (Bias → 0)

- Unbiased estimator → **guaranteed convergence** $(\mathbb{E}[\hat{Y}] = \mathbb{E}[Y])$
- MSE convergence rate is $1/N$ → **prohibitive cost** for expensive, high-fidelity models

MC estimation

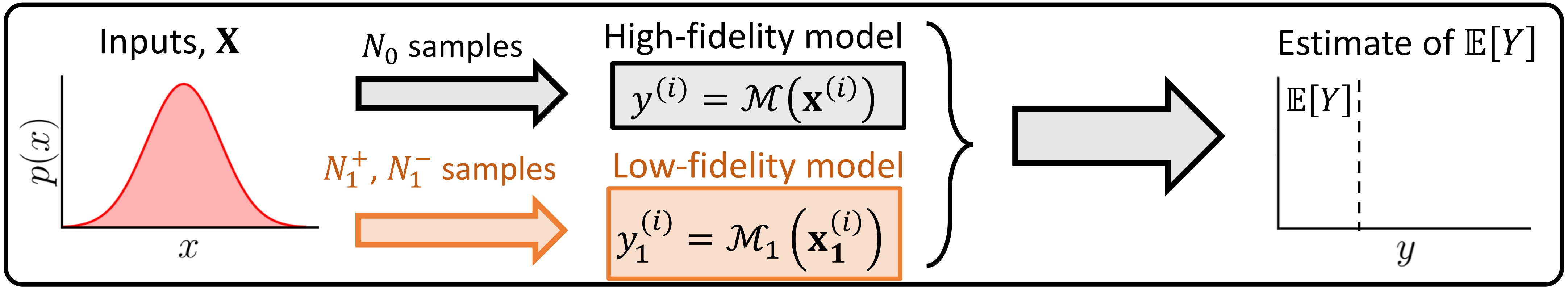
Problem: estimate the expected value, $\mathbb{E}[Y]$, for a QoI, Y



- Biased estimator → **irreducible error** ($\mathbb{E}[Y_1] \neq \mathbb{E}[Y]$)
- $C_1 \ll C$ → efficient **variance reduction** (cheap samples relative to high-fidelity model)

Multi-model MC estimation

Problem: estimate the expected value, $\mathbb{E}[Y]$, for a QoI, Y



Multi-model MC estimator[1]: $\mathbb{E}[Y] \approx \tilde{Y}_{MM} = \hat{Y}(\mathbf{x_0}) + \alpha_1 \left(\hat{Y}_1(\mathbf{x}_1^+) - \hat{Y}_1(\mathbf{x}_1^-)\right)$

High-fidelity: N_0 samples

Low-fidelity: N_1 samples

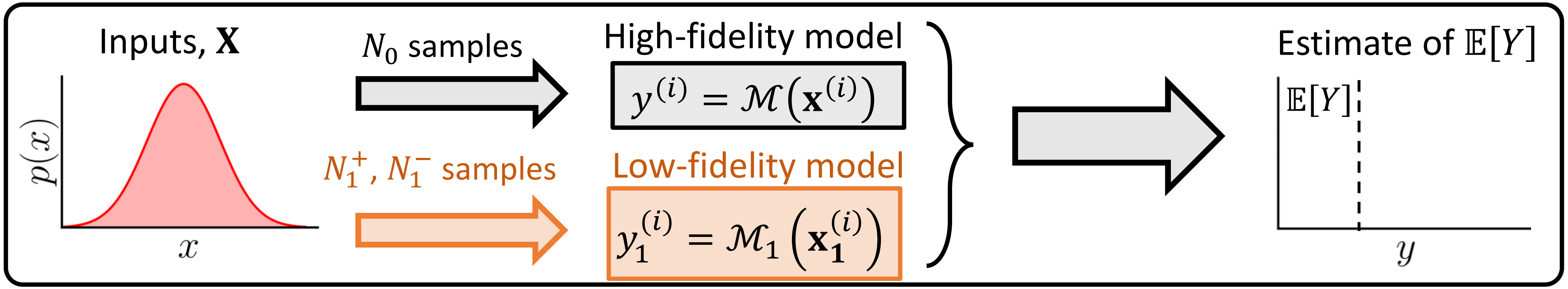
High-fidelity with sample set $\mathbf{x_0}$

Low-fidelity with two different sample sets ($\mathbf{x}_1^+$ and $\mathbf{x}_1^-$)

[1]Based on approximate control variates approaches: A.A. Gorodetsky et al., J Comput Phys. 408 (2020) 109257. https://doi.org/10.1016/j.jcp.2020.109257.

Multi-model MC estimation

Problem: estimate the expected value, $\mathbb{E}[Y]$, for a QoI, Y



Multi-model MC estimator: $\mathbb{E}[Y] \approx \tilde{Y}_{MM} = \hat{Y}(\mathbf{x_0}) + \alpha_1\left(\hat{Y}_1(\mathbf{x}_1^+) - \hat{Y}_1(\mathbf{x}_1^-)\right)$

High-fidelity: N_0 samples
Low-fidelity: N_1 samples

- Unbiased estimator → **guaranteed convergence** $\left(\mathbb{E}[\tilde{Y}_{MM}] = \mathbb{E}[\hat{Y}] = \mathbb{E}[Y]\right)$
- Error depends only on variance → how to efficiently reduce $\mathbb{V}\mathrm{ar}[\tilde{Y}_{MM}]$?[1]
  - Decreases with **increasing correlation** between models
  - Optimal **sample allocation,** $\{\mathbf{x}_0, \mathbf{x}_1^+, \mathbf{x}_1^-\}$**, and weight,** α_1, minimize cost given a **target variance (accuracy)**
  - Equivalently: minimize variance given a **target cost**, $\hat{C}$

[1]A.A. Gorodetsky et al., J Comput Phys. 408 (2020) 109257. https://doi.org/10.1016/j.jcp.2020.109257.

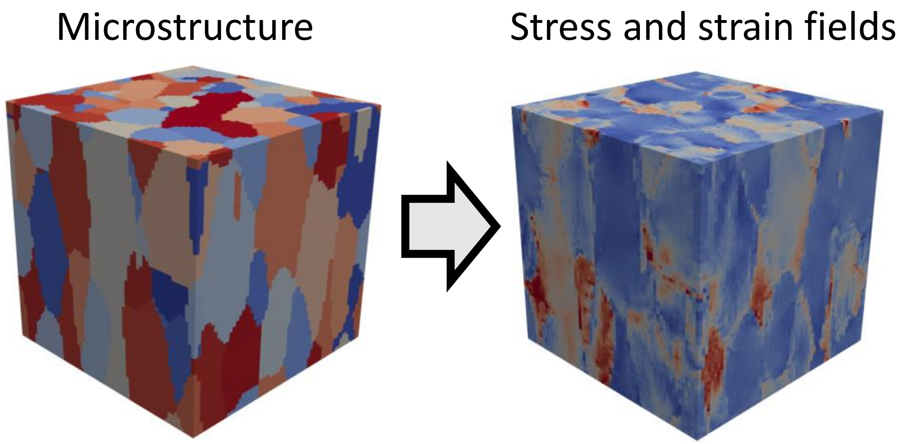
Multi-model MC summary

- **Low cost** and **high correlation with high-fidelity model** are desirable
- Can extend to **any number of low-fidelity models and QoIs**

$$\tilde{Y}_{MM} = \hat{Y}(\mathbf{x_0}) + \sum_{j=1}^{M} \alpha_j \left(\hat{Y}_j(\mathbf{x_j^+}) - \hat{Y}_j(\mathbf{x_j^-}) \right)$$

M: number of low-fidelity models

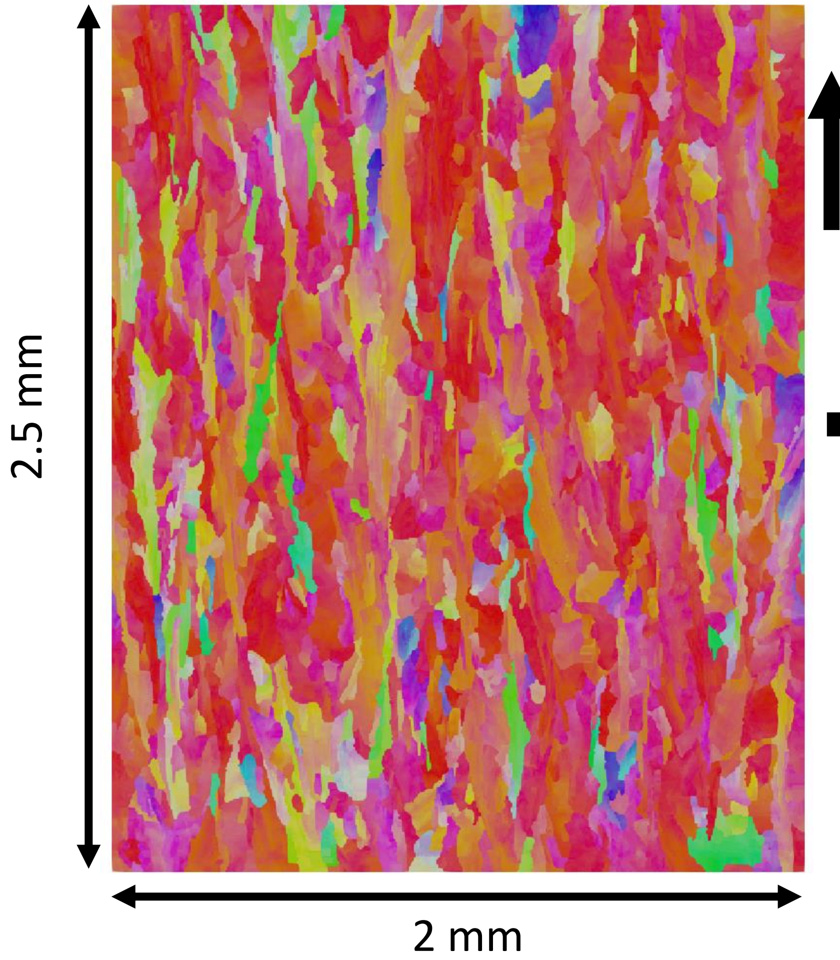
- Application (here: crystal plasticity simulations of AM microstructures)
  - Sample input space
  - Choose QoIs
  - Choose high- and low-fidelity model(s)
  - Estimate model covariances for each QoI
  - Solve optimization to minimize variance for target cost

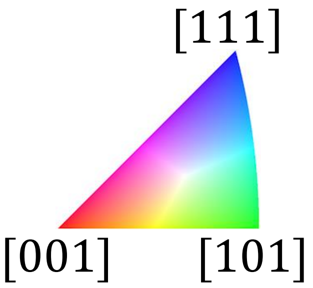


Details on optimization and sample allocation in G.F. Bomarito et al., J Comput Phys. 451 (2022) 110882. https://doi.org/10.1016/j.jcp.2021.110882.

Application to crystal plasticity

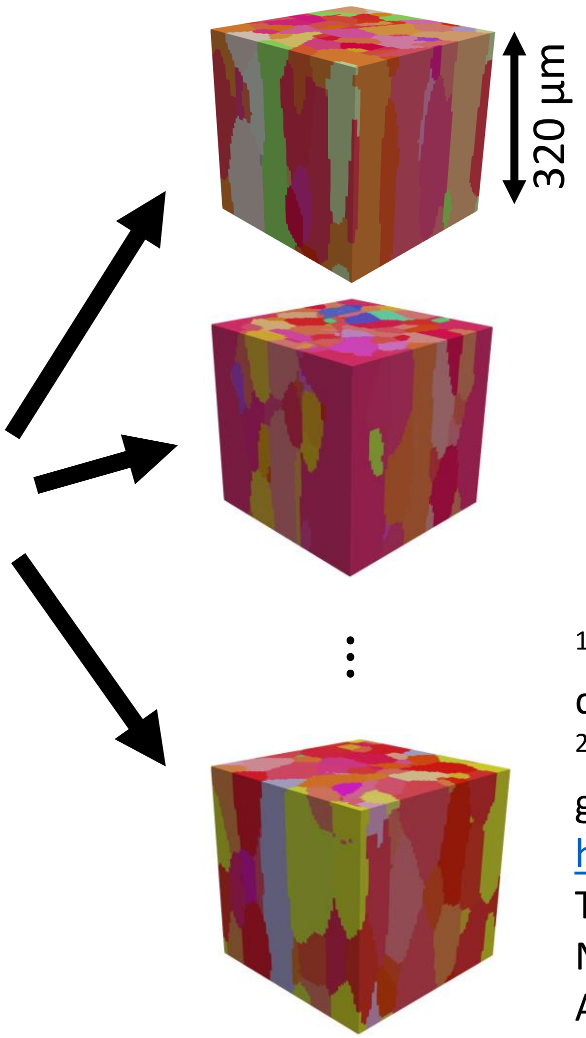
- Create AM-relevant microstructures based on Inconel 718 EBSD[1] data





Generate statistically equivalent samples[2]

Microstructure samples



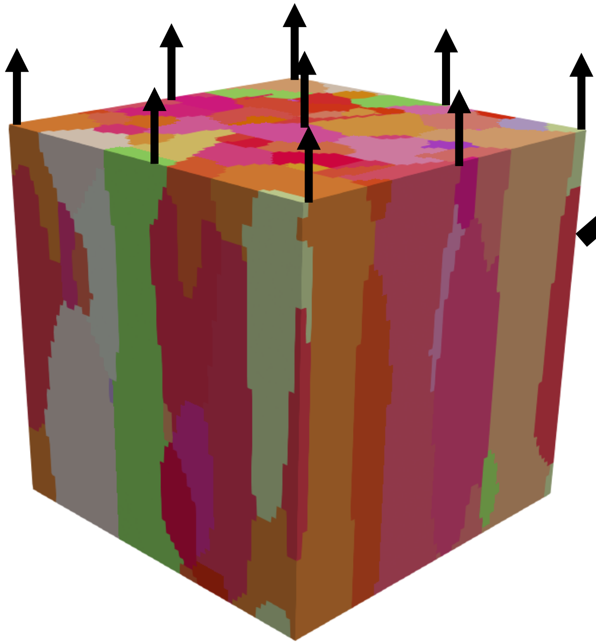
[1]EBSD: electron backscatter diffraction

[2]Statistics extracted and samples generated using DREAM.3D: http://dream3d.bluequartz.net/. This is not an endorsement by the National Aeronautics and Space Administration (NASA)

Application to crystal plasticity

- Create AM-relevant microstructures based on Inconel 718 EBSD data
- Choose QoIs to extract from crystal plasticity simulations

Microstructure sample with loading (1% strain) in build direction



Crystal plasticity model

Aggregate QoI
- Yield strength (YS)

Grain-scale QoIs (one value per grain)
- Equivalent stress, $\bar{\boldsymbol{\sigma}}_{\boldsymbol{g}}$
- Shear strain, $\boldsymbol{\gamma}_{\boldsymbol{g}}$
- Fatemi-Socie parameter (related to crack initiation), $\boldsymbol{FS}_{\boldsymbol{g}}$

Mean across all grains

$\text{mean}(\bar{\sigma}_g)$
$\text{mean}(\gamma_g)$
$\text{mean}(FS_g)$

Max across all grains

$\max(\bar{\sigma}_g)$
$\max(\gamma_g)$
$\max(FS_g)$

Application to crystal plasticity

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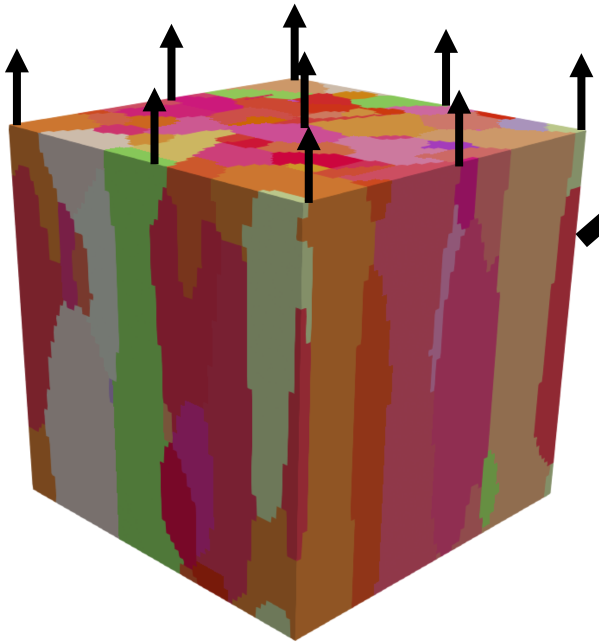

Crystal plasticity model

<u>Aggregate QoI</u>
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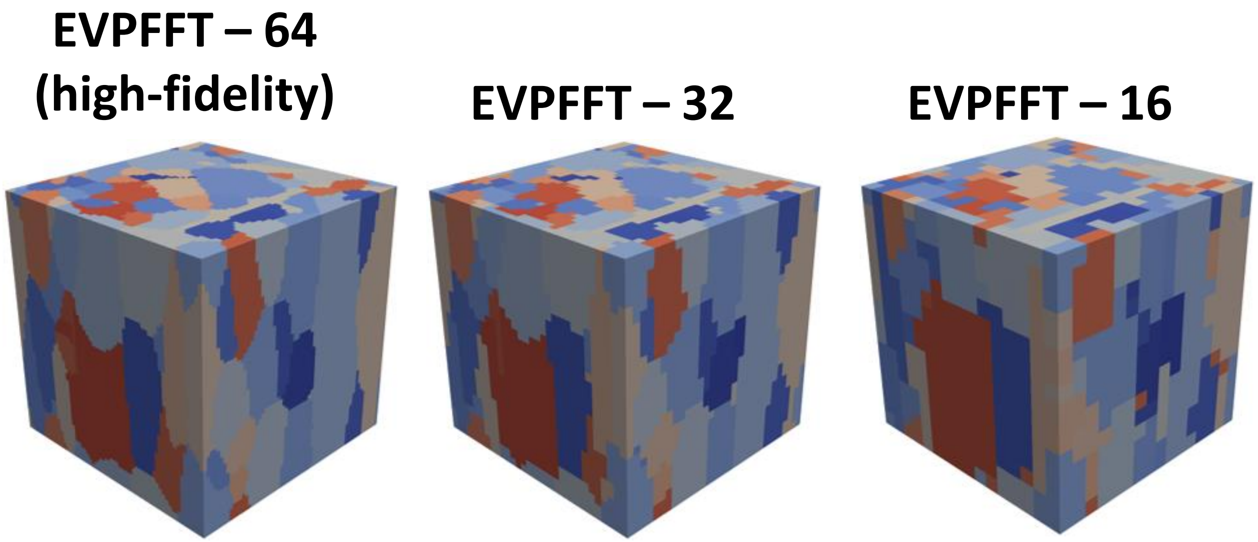
$\text{mean}(\gamma_g)$
$\text{mean}(FS_g)$

Max across all grains

$\max(\bar{\sigma}_g)$
$\max(\gamma_g)$
$\max(FS_g)$

High- and low-fidelity models

Three-dimensional full-field simulations



Model names refer to resolution (EVPFFT – 64 has $64 \times 64 \times 64$ voxel resolution with 5-µm voxel size)

EVPFFT: elasto-viscoplastic fast Fourier transform model[1]

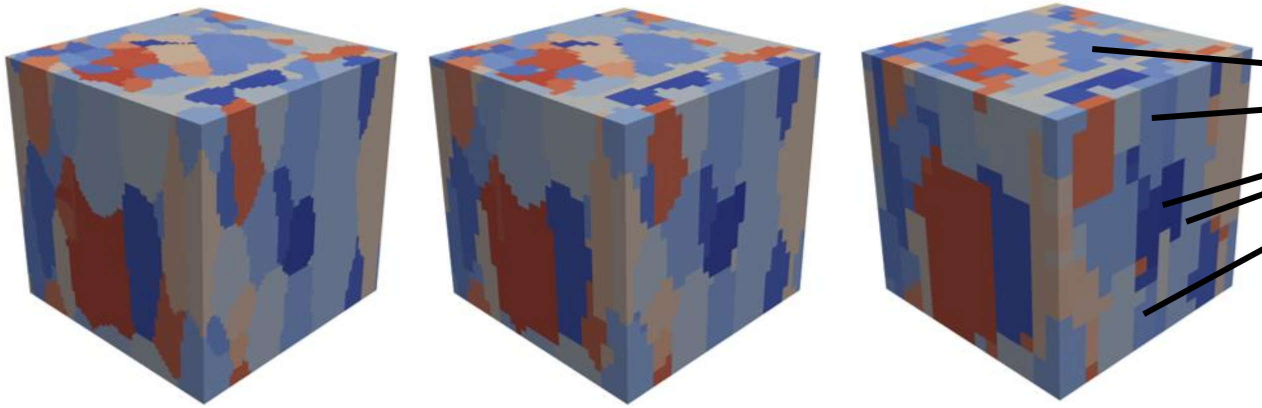
- Calculate stress and strain for **all voxels**
- Generate low-fidelity models by coarsening the discretization

[1] R.A. Lebensohn et al., Int J Plast. 32–33 (2012) 59–69. https://doi.org/10.1016/j.ijplas.2011.12.005.

High- and low-fidelity models

Three-dimensional full-field simulations

EVPFFT – 64 (high-fidelity) **EVPFFT – 32** **EVPFFT – 16**



Extract geometry and orientation information for each grain

- Volume
- Aspect ratios
- Crystallographic orientation

VPSC[1]: self-consistent homogenization-based formulation

- Solve for **grain-average** stresses and strains
- Different linearization schemes → three different models

Model	Cost
EVPFFT – 64	**~33 min.**
EVPFFT – 32	~3.5 min.
EVPFFT – 16	~0.4 min.

Model	Cost
VPSC – affine	~1 sec.
VPSC – FC	~1 sec.
VPSC – tangent	~1 sec.

[1]Viscoplastic self-consistent formulation

R.A. Lebensohn, C.N. Tomé, Acta Metall et Mater. 41 (1993) 2611–2624. https://doi.org/10.1016/0956-7151(93)90130-K.

Results to be shown

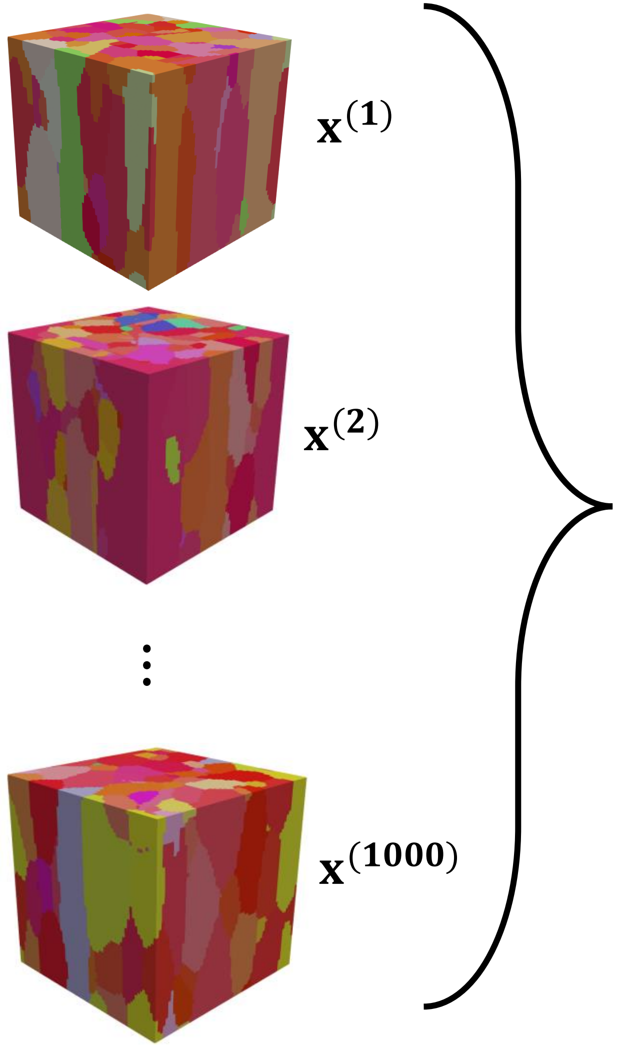
- Pilot samples → correlations between high- and low-fidelity models
- Multi-model MC variance reduction, optimal sample allocation, and verification
- Consider two sets of QoIs
  - Yield strength and mean grain-scale QoIs only ("mean QoIs")
  - All seven QoIs ("mean QoIs" and "max QoIs" together)

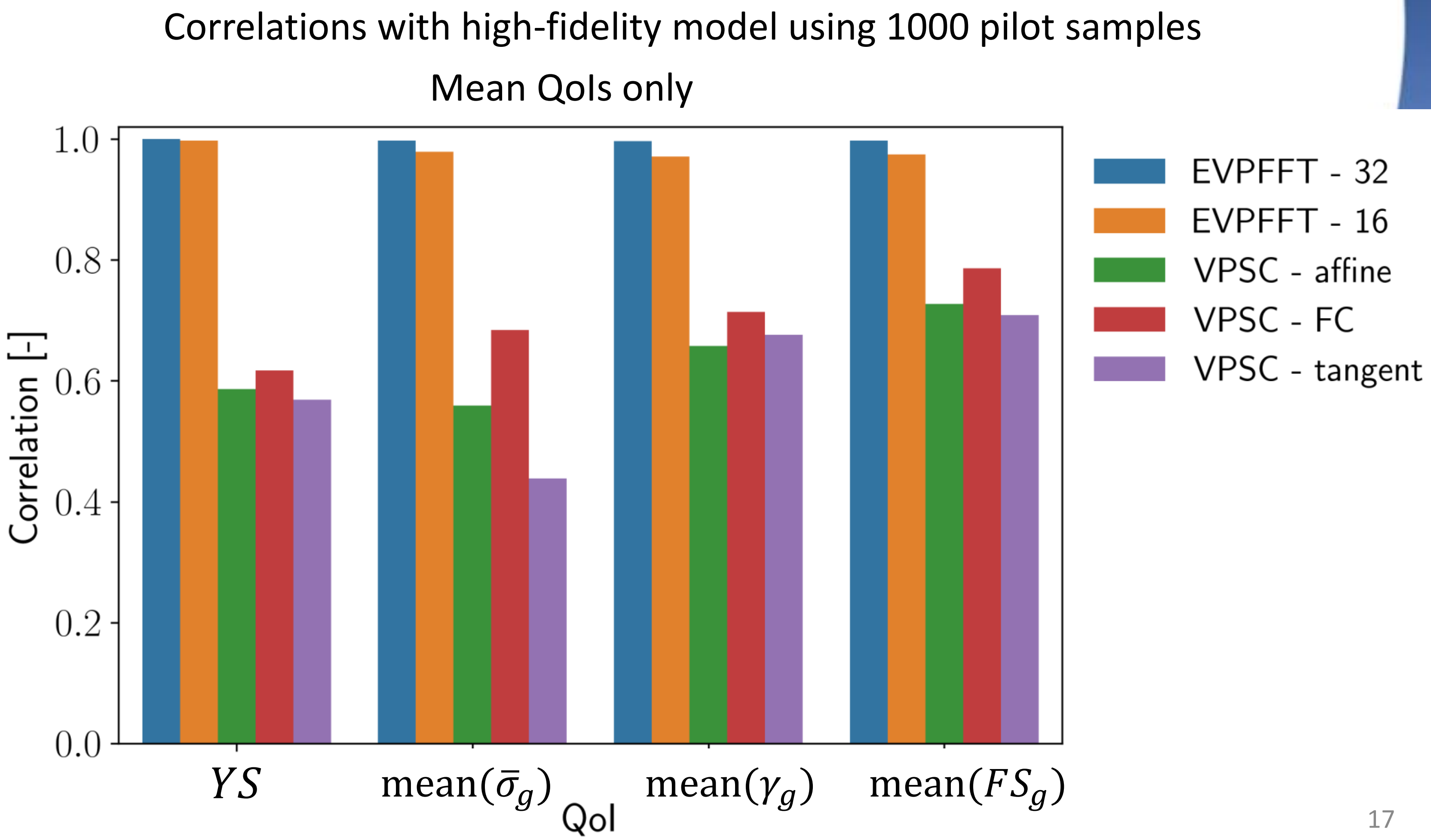
<u>Aggregate QoI</u>
- Yield strength (YS)

<u>Grain-scale QoIs</u>
- mean($\bar{\sigma}_g$), max($\bar{\sigma}_g$)
- mean(γ_g), max(γ_g)
- mean(FS_g), max(FS_g)

Model correlations, mean QoIs

- Estimate covariances between models using pilot samples

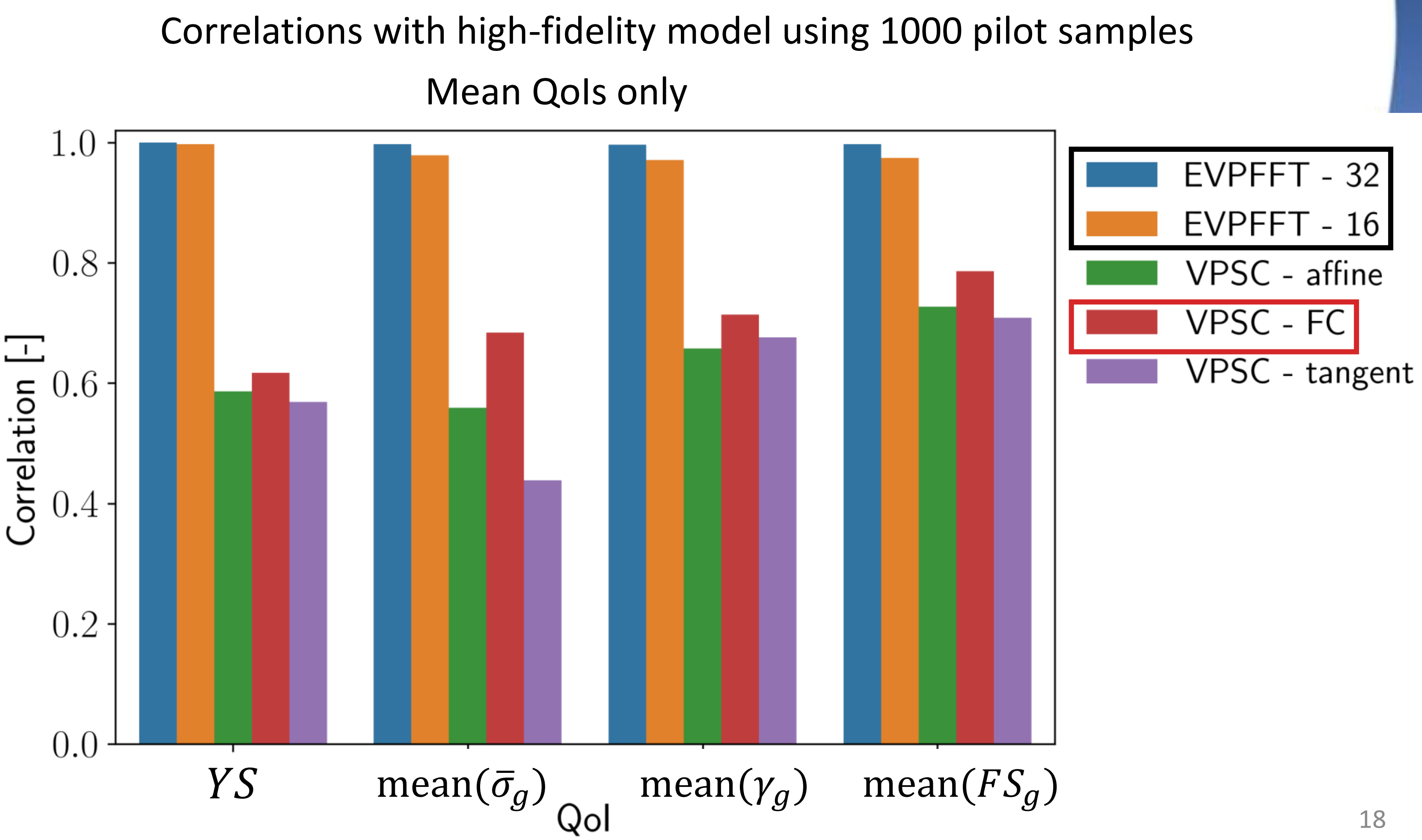




Model correlations, mean QoIs

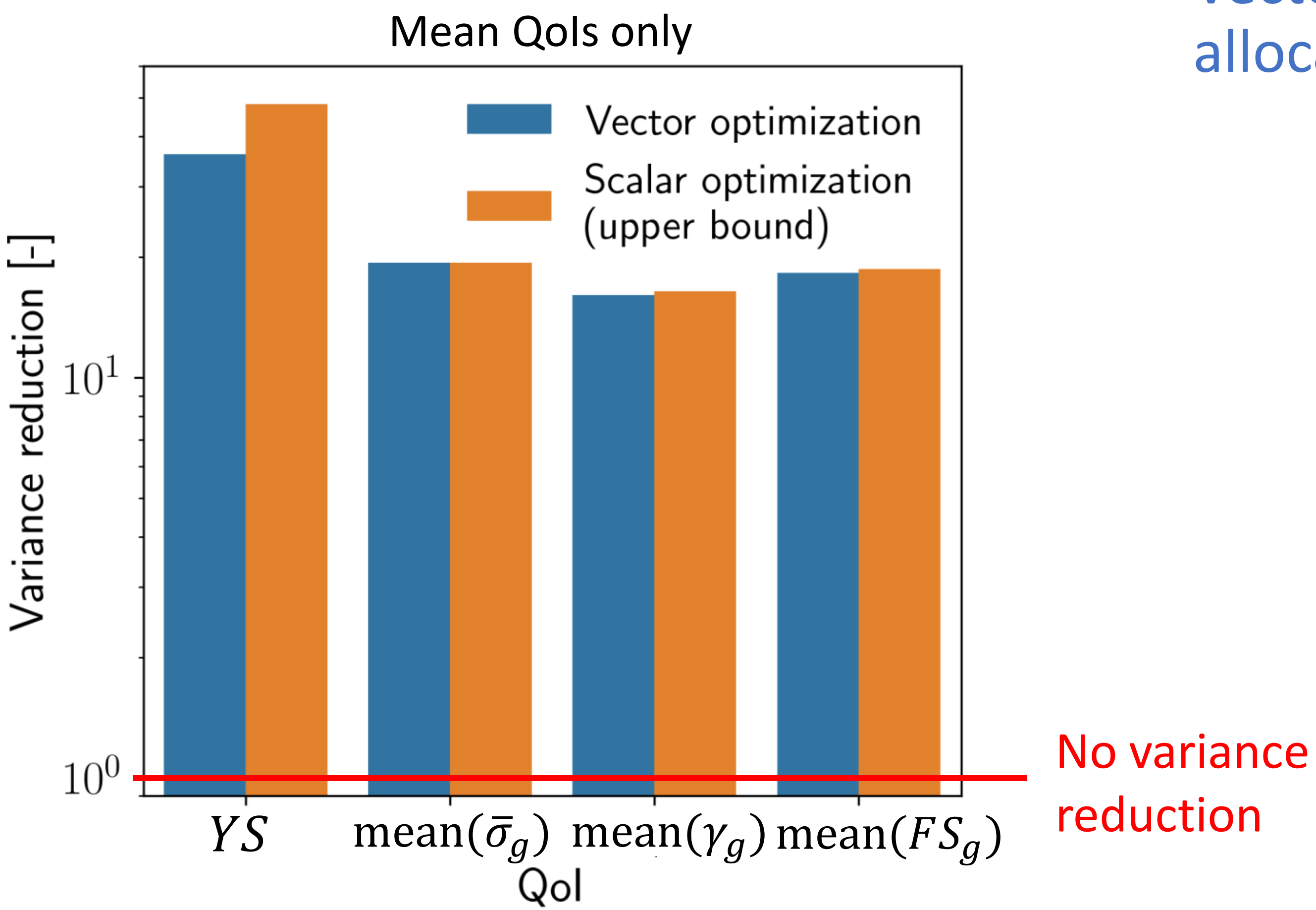
- Estimate covariances between models using pilot samples

- Coarse EVPFFT models are strongly correlated with high-fidelity model
- VPSC – FC has best correlation across all four QoIs



Variance reduction, mean QoIs

Variance reduction for multi-model MC relative to standard MC for $\hat{C} = 100$ high-fidelity simulations

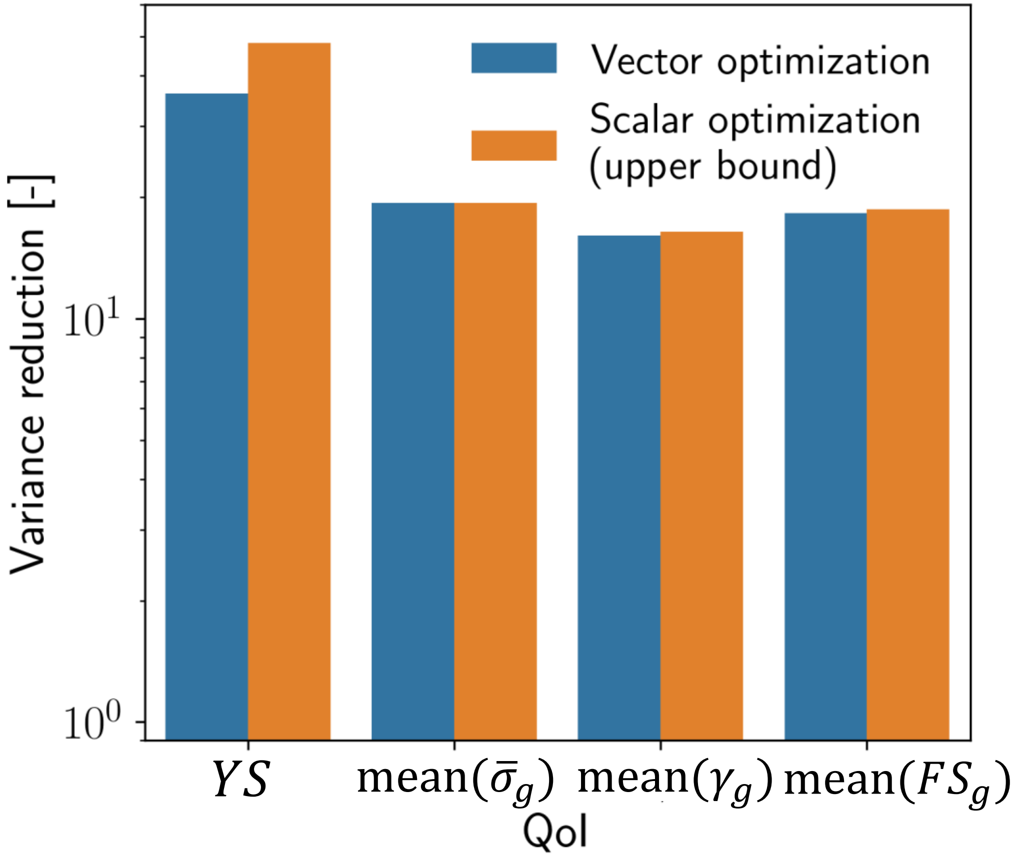


- Scalar optimization: upper bound; optimize sample allocation for each individual QoI
- Vector optimization: optimize sample allocation for all QoIs shown in the chart

Sample allocation, mean QoIs

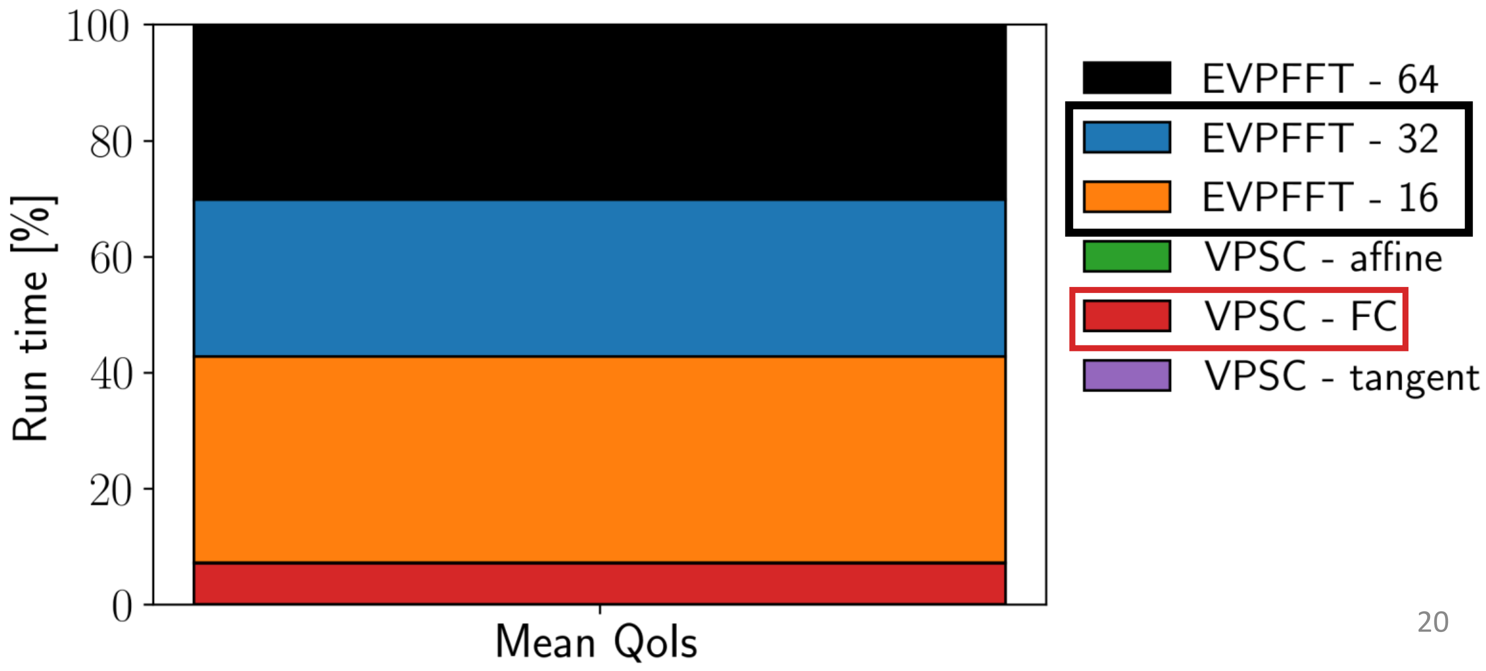
Variance reduction for multi-model MC relative to standard MC for $\hat{C} = 100$ high-fidelity simulations

Mean QoIs only



- Significant allocation to coarse full-field models
- VPSC – FC is the only homogenized model with a significant number of samples

Sample allocations for vector optimization



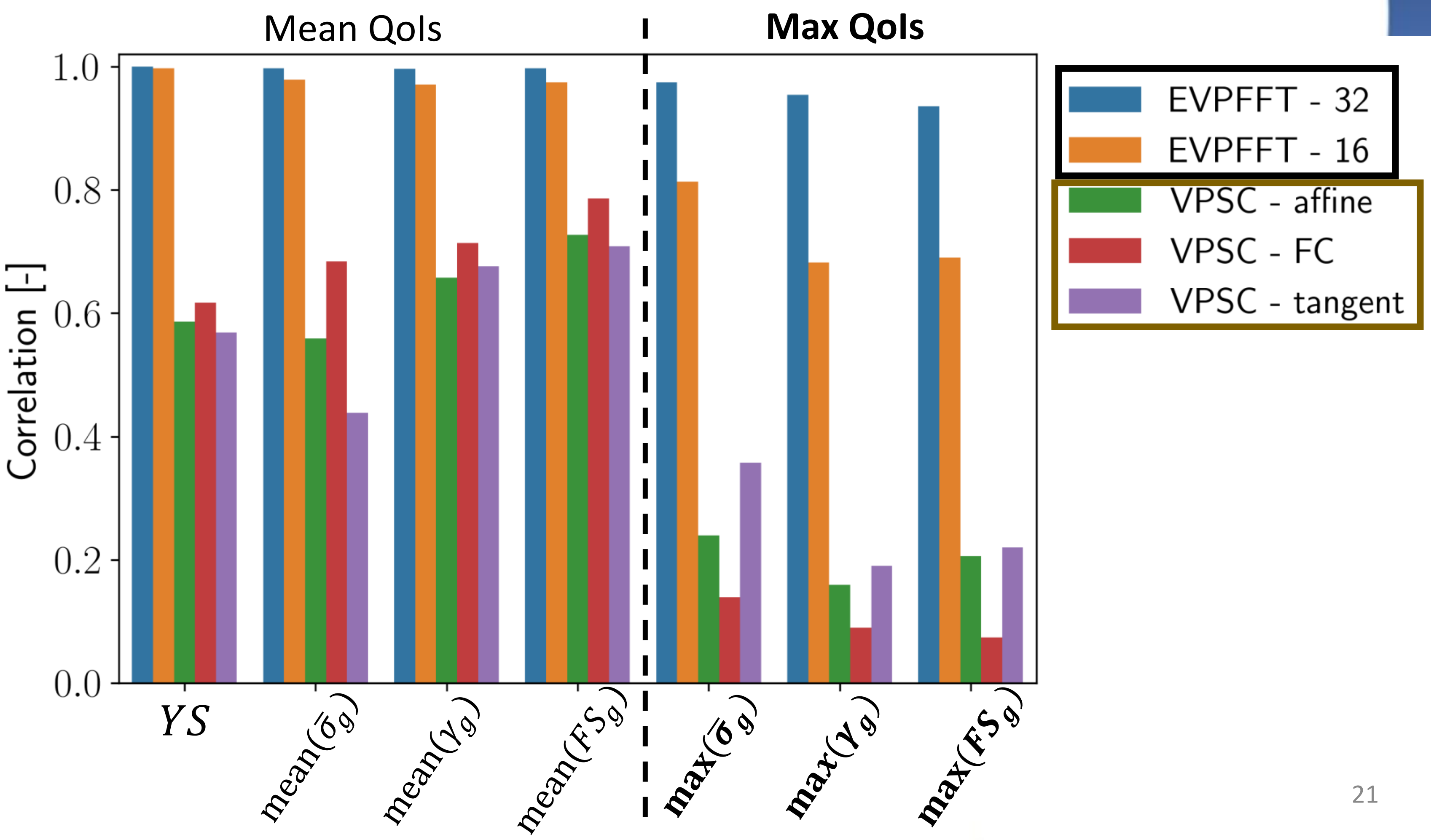
Model correlations, all QoIs

- Estimate covariances between models using pilot samples

- Max. grain-scale QoIs:
  All correlations are lower
  - Consistent with refinement studies: coarse mesh is worse near hotspots

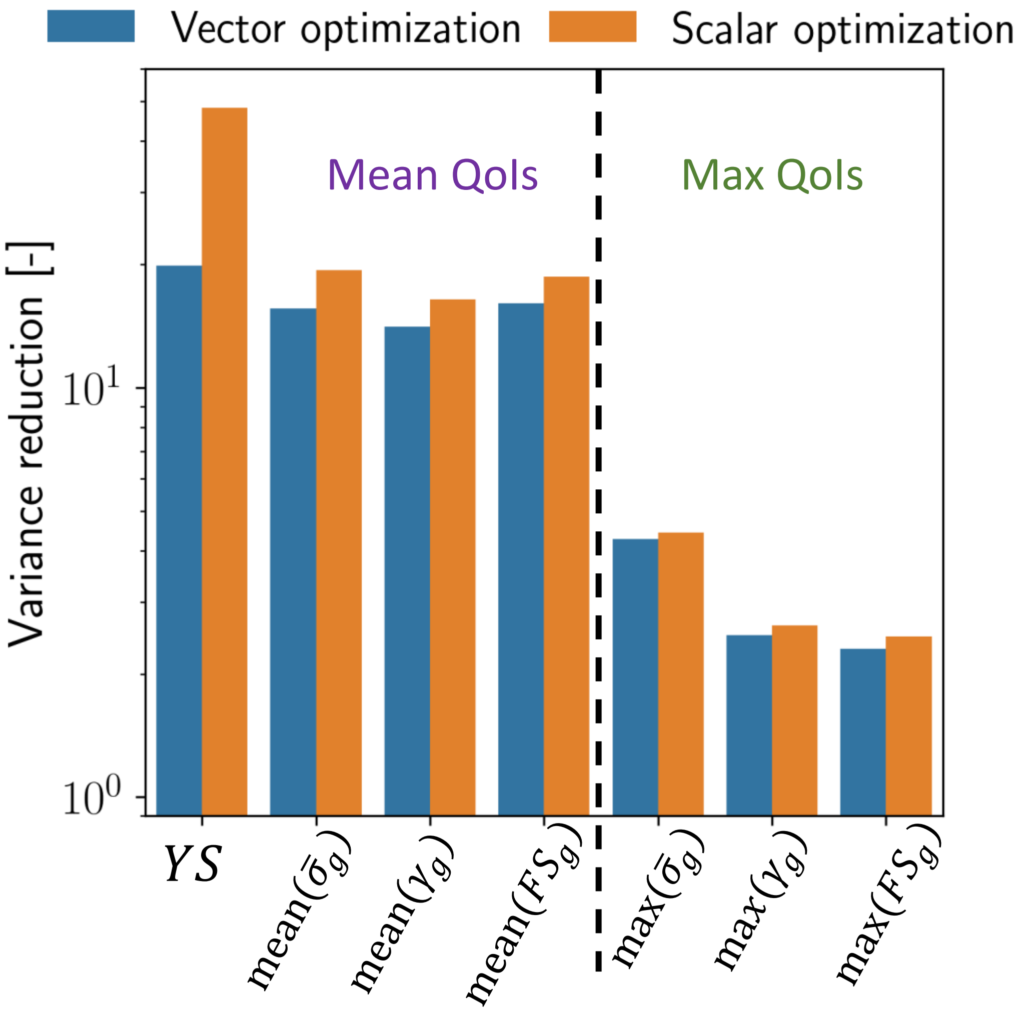
- Not obvious which VPSC models are the most useful across all QoIs

Correlations with high-fidelity model using 1000 pilot samples



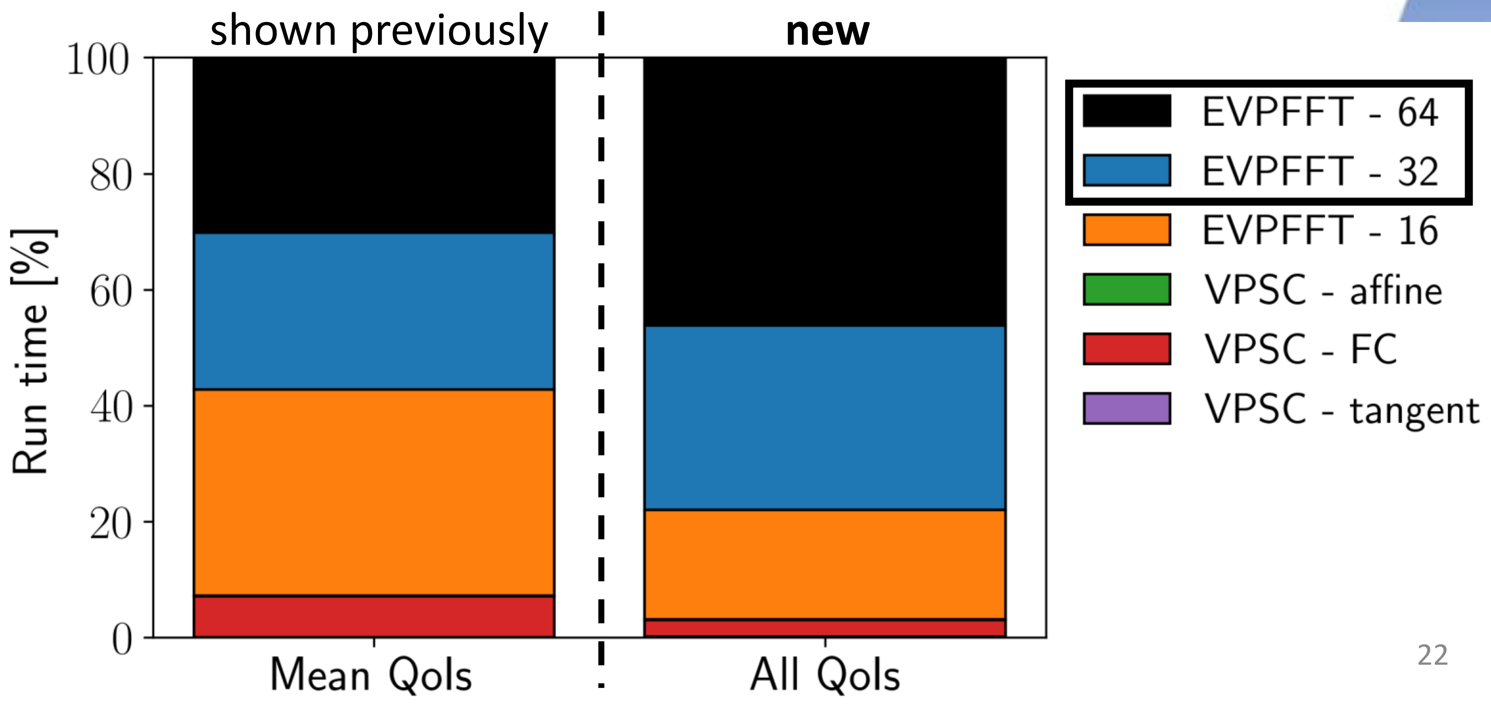
Variance reduction and sample allocation, all QoIs

Variance reduction for $\hat{C} = 100$ high-fidelity simulations; optimization with all QoIs



- Less variance reduction for max QoIs
- Mean QoIs are less optimized than before
- More time allocated to high-fidelity model and first low-fidelity model

Sample allocations – comparison between QoI sets



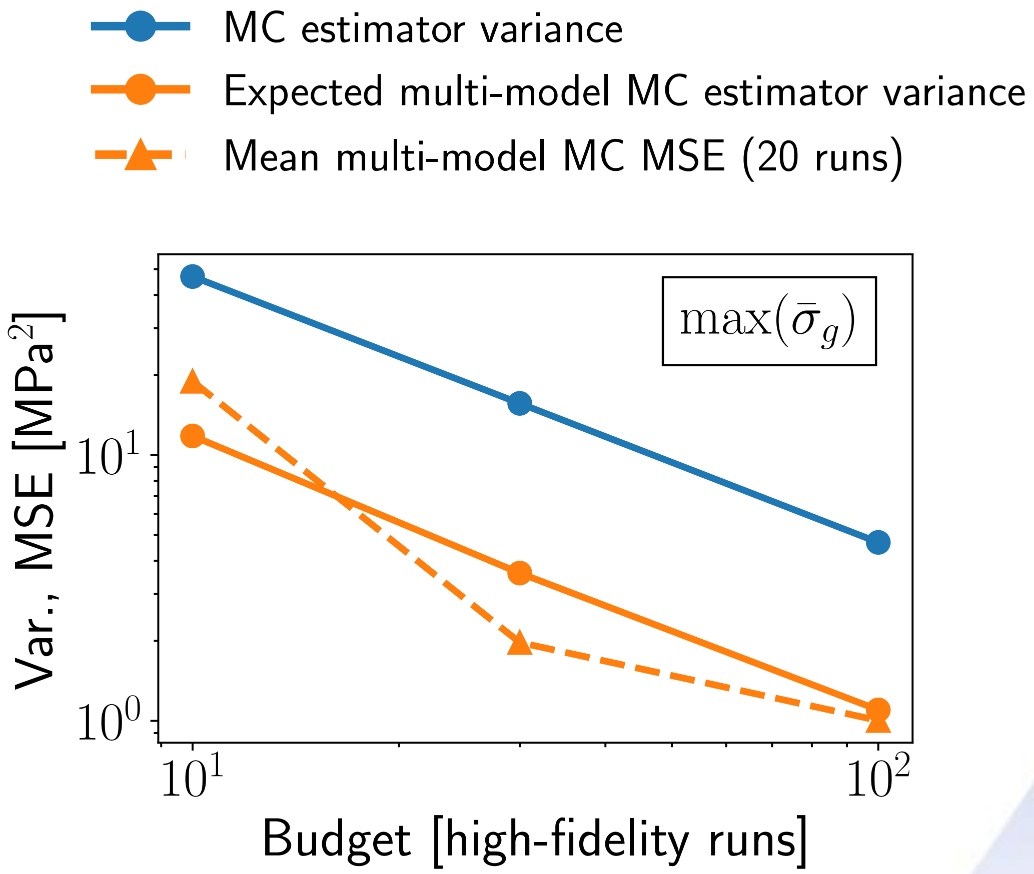
Multi-model MC estimator verification

Estimate of the actual multi-model MC mean-squared error:

$$\mathrm{MSE}[\tilde{Y}_{MM}] \approx \frac{1}{20}\sum_{i=1}^{20}\left(\tilde{Y}_{MM}^{(i)} - \hat{Y}_{\mathrm{ref}}\right)^2$$

Should converge to multi-model MC estimator variance

Reference solution using 10^4 high-fidelity runs



Conclusions

- Multi-model MC: reduce variance by optimizing sample allocation across high- and low-fidelity models
  - Best low-fidelity models and inexpensive and highly-correlated with the high-fidelity model
- Multi-model MC estimator is about $2\times$ to $20\times$ more efficient than standard MC for crystal plasticity QoIs
- More reliance on high-fidelity model for maximum grain-scale QoIs (characteristic of crack initiation hotspots)
- Remaining challenges:
  - Effective low-fidelity models for extreme-value QoIs (machine learning?)
  - Efficiently using pilot samples

Acknowledgements

- This work was supported by the NASA Aeronautics Research Mission Directorate (ARMD) Transformational Tools and Technologies (TTT) project

- The authors also thank:
  - Ricardo Lebensohn from Los Alamos National Laboratory for sharing the serial/distribution version of the EVPFFT code
  - Wes Tayon and Bryan Koscielny for completing the EBSD scans

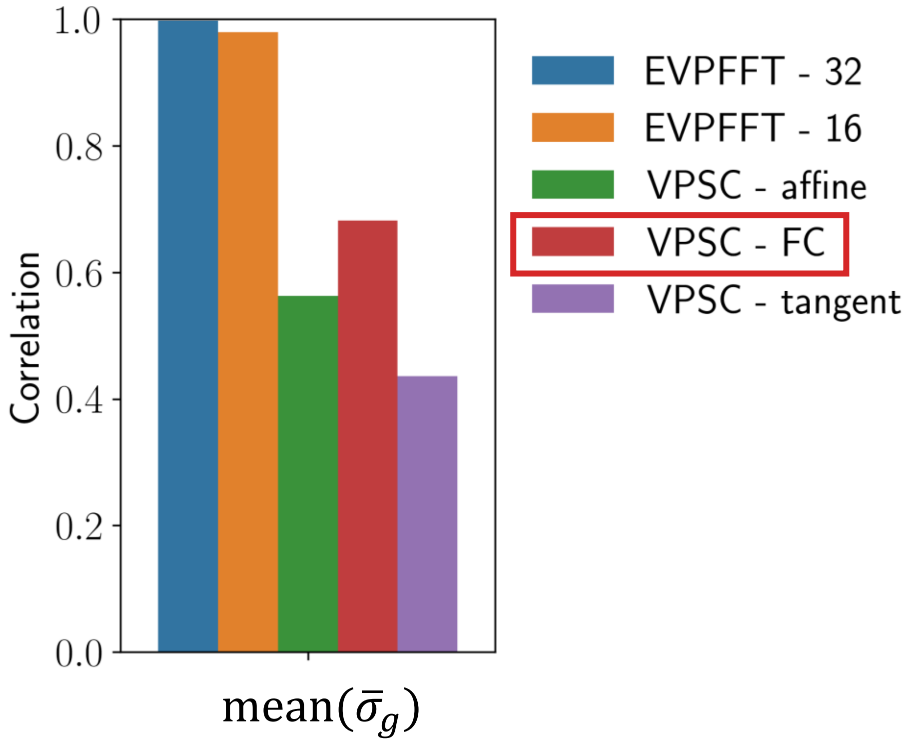
- MXMCPy – Multi-model Monte Carlo in Python: https://github.com/nasa/MXMCPy →

- Contact information: joshua.pribe@nasa.gov

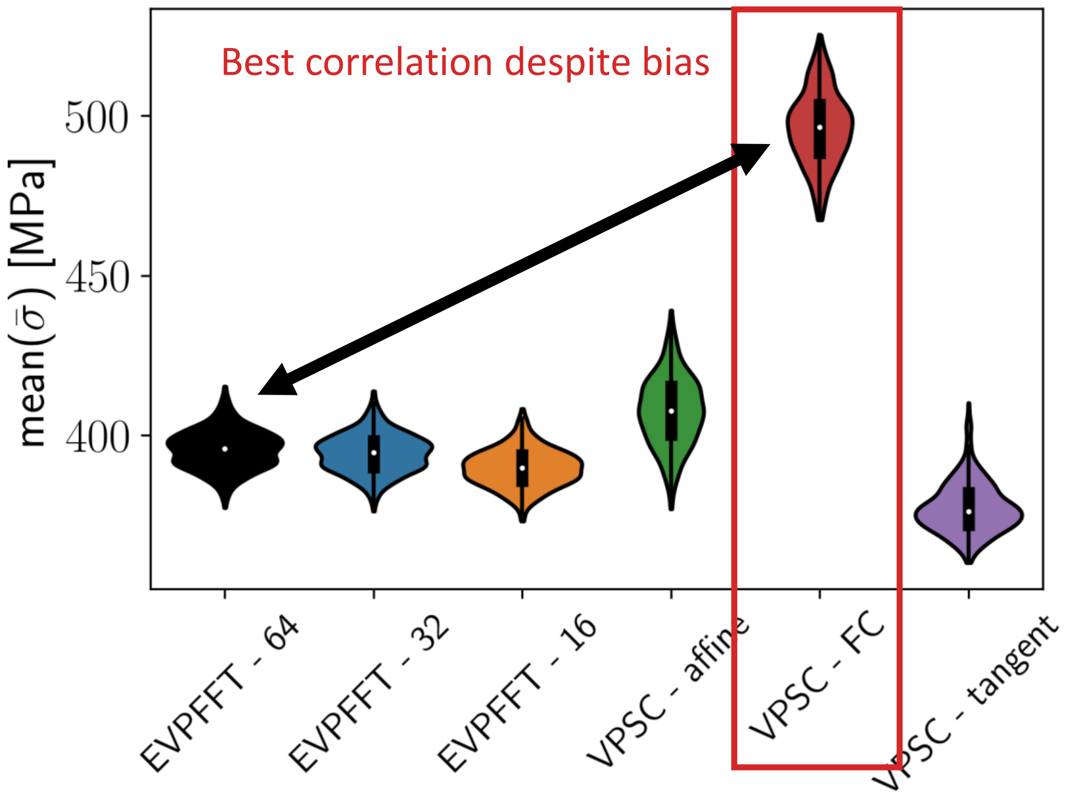
Biased low-fidelity models

- Biased low-fidelity models are fine, if trends are correlated with the high-fidelity model

Correlations with high-fidelity mean grain-scale equivalent stress



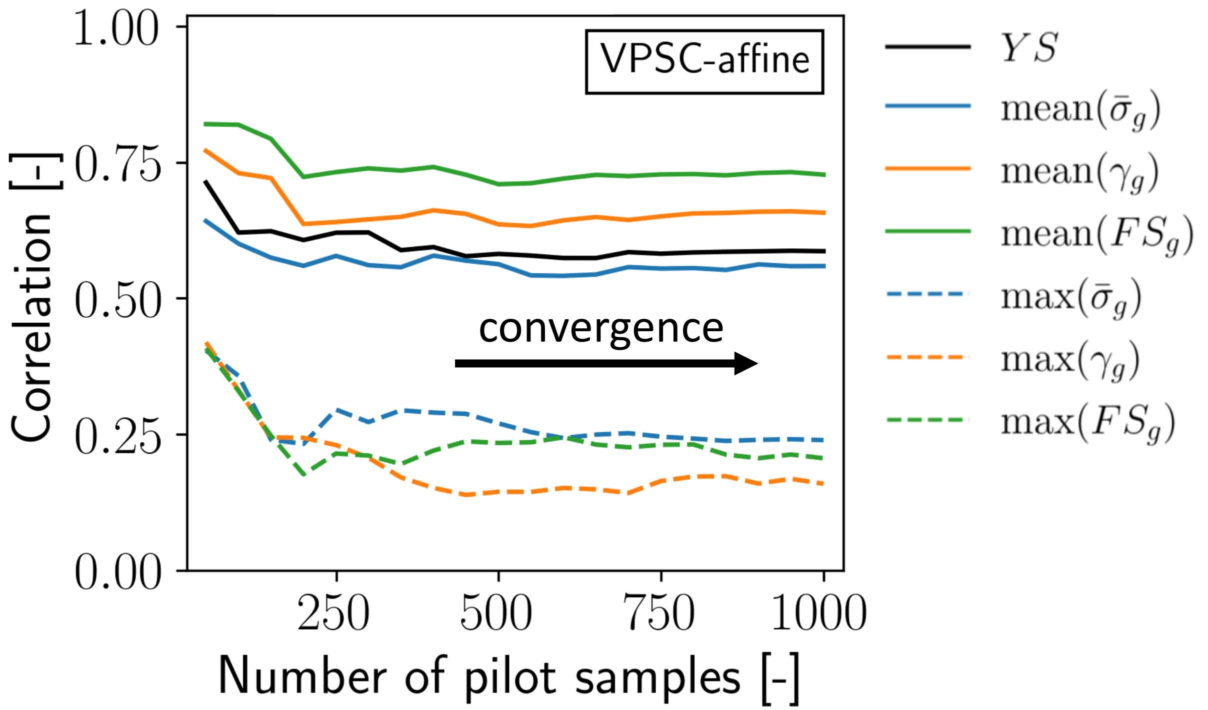
Violin plots of mean grain-scale equivalent stress from 500 pilot samples



Correlation convergence

- Biased low-fidelity models are fine, if trends are correlated with the high-fidelity model
- Cost of pilot samples is non-trivial[1]

Correlation of VPSC – affine with high-fidelity model with increasing pilot samples



[1]T. Pham, A.A. Gorodetsky, SIAM/ASA J. Uncertainty Quantification. 10 (2022) 1250–1292. https://doi.org/10.1137/21M1390426.

Multi-model MC optimization

Estimator: $\tilde{Y}_{MM} = \hat{Y}(\mathbf{x_0}) + \sum_{j=1}^{M} \alpha_j \left(\hat{Y}_j(\mathbf{x_j^+}) - \hat{Y}_j(\mathbf{x_j^-})\right)$

Cost: $\tilde{C} = N_0 C + N_1 C_1 + \cdots + N_M C_M \qquad N_j = N_j^+ + N_j^-$

Goal: select weights, $\boldsymbol{\alpha}$, and sample allocation, $\{\mathbf{x}\} = \{\mathbf{x_0}, \mathbf{x_1^+}, \mathbf{x_1^-}, \dots, \mathbf{x_M^+}, \mathbf{x_M^-}\}$, to yield the most accurate estimator given cost constraint, $\hat{C}$

$$\boldsymbol{\alpha}, \{\mathbf{x}\}^{opt} = \underset{\boldsymbol{\alpha}, \{\mathbf{x}\}}{\arg\min}\ \mathbb{V}\mathrm{ar}[\tilde{Y}(\boldsymbol{\alpha}, \{\mathbf{x}\})]$$
$$\text{s.t. } \tilde{C} \leq \hat{C}$$

Details in G.F. Bomarito et al., J Comput Phys. 451 (2022) 110882. https://doi.org/10.1016/j.jcp.2021.110882.