Data-informed Multiscale Modeling of Additive Materials

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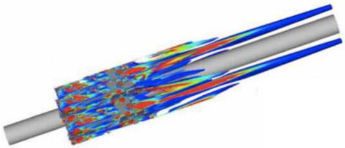
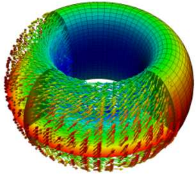
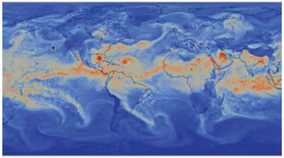
Motivation

Flow in Nuclear Reactor (Turbulent CFD)

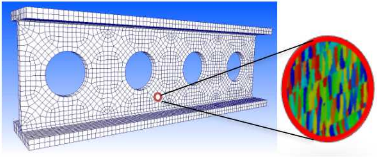


Tokamak Equilibrium (MHD)





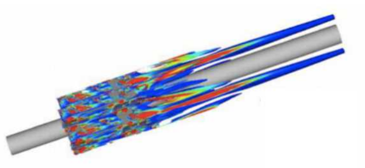
Climate Modeling



Multi-scale Materials Modeling

Motivation

Flow in Nuclear Reactor (Turbulent CFD)



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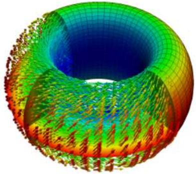
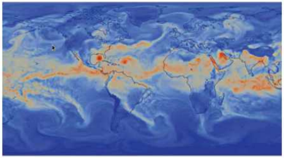
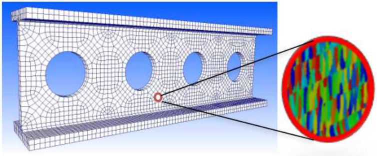


We are working to develop **data-informed** models ...

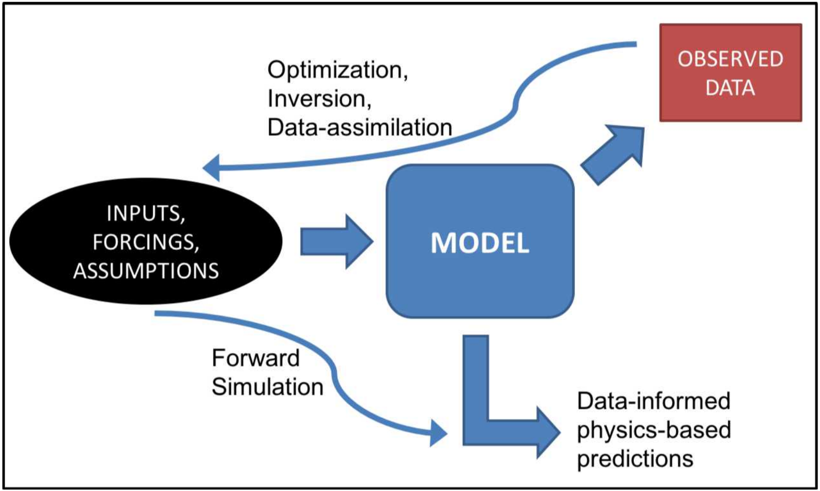


Climate Modeling

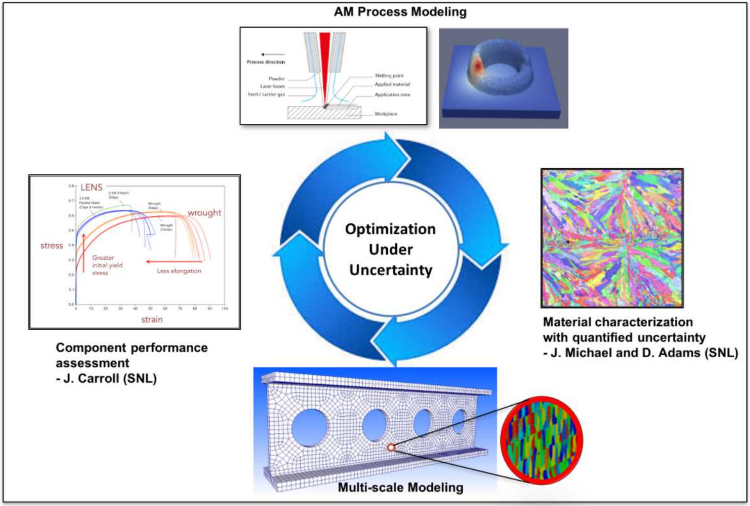


Multi-scale Materials Modeling

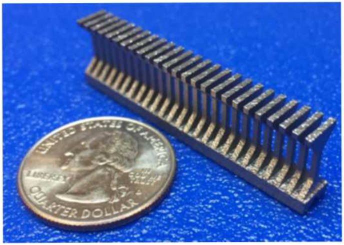
Data-informed Physics-Based Predictions

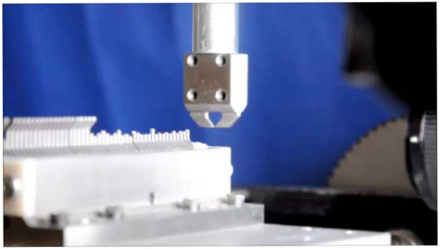


Predict/Control Performance of Additive Manufacturing of Materials and Components with Quantified Uncertainty

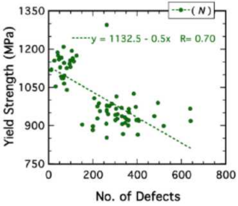


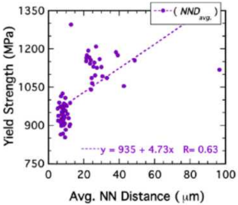
High-throughput Testing of Dog-bone Exemplar

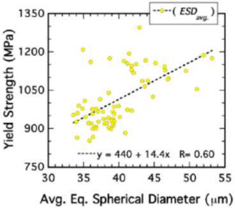


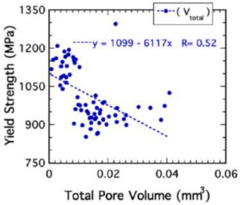


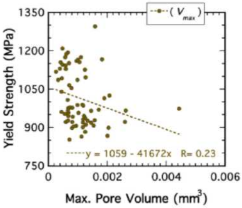
Assessing Statistical Correlations











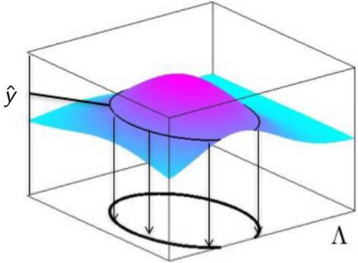
In relation to Y.S.

Measure	R value	R^2
No. of Defects	-0.705	0.50
Avg. NN Distance (mm)	0.631	0.40
Avg. ESD (mm)	0.601	0.36
Max CSA Redux (mm^2)	-0.581	0.38
Total Pore Volume (mm^3)	-0.518	0.27
Avg. Defect Vol. (mm^3)	0.500	0.25
Max CSA Redux (%)	-0.486	0.24
Maximum Pore Size	-0.257	0.07

Key Question:

Can we use this data to inform a physics-based computational model?

A Deterministic Inverse Problem



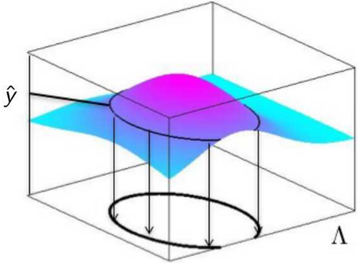
QoI response surface

2D parameter space

Problem

Given a deterministic observation, $\hat{y}$, find $\lambda \in \Lambda$ such that $D(\lambda) = \hat{y}$.

A Deterministic Inverse Problem



QoI response surface

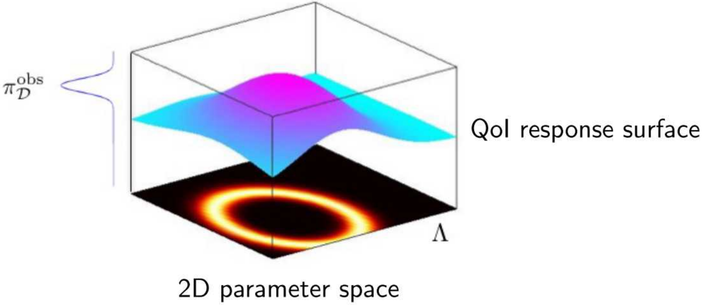
2D parameter space

Problem

Given a deterministic observation, $\hat{y}$, find $\lambda \in \Lambda$ such that $D(\lambda) = \hat{y}$.

- Solutions may not be unique without additional assumptions.
- Requires solving several deterministic forward problems.

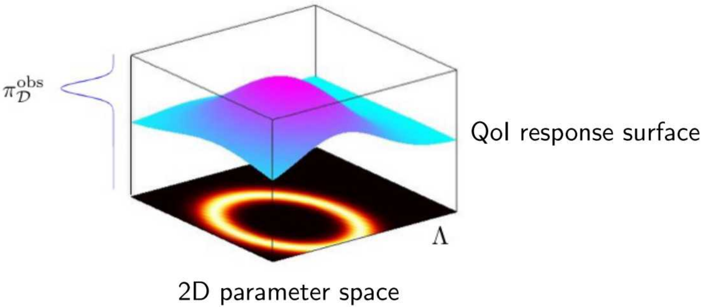
A Stochastic Inverse Problem



Problem

Given a probability density on observations, find a probability density on Λ such that the push-forward matches the given density on the observed data.

A Stochastic Inverse Problem

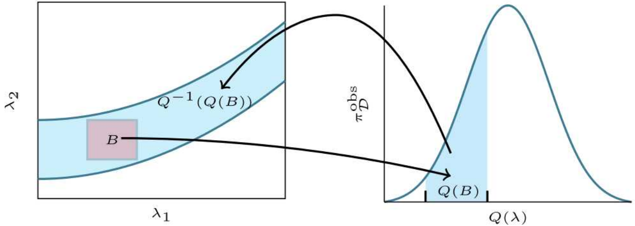


Problem

Given a probability density on observations, find a probability density on Λ such that the push-forward matches the given density on the observed data.

- Solutions may not be unique without additional assumptions.
- We only need to solve a **single stochastic forward problem.**

A Solution to the Stochastic Inverse Problem

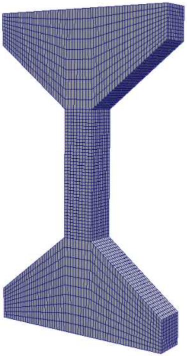


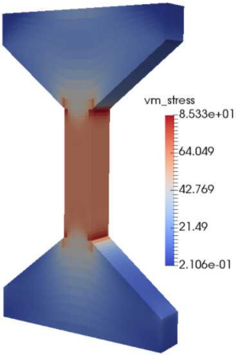
We use measure theory and Bayes' rule to construct a posterior density:

$$\pi_\Lambda^{\text{post}}(\lambda) = \pi_\Lambda^{\text{prior}}(\lambda)\frac{\pi_{\mathcal{D}}^{\text{obs}}(D(\lambda))}{\pi_{\mathcal{D}}^{D(\text{prior})}(D(\lambda))}.$$

- $\pi_\Lambda^{\text{prior}}$ is the **given** prior
- $\pi_{\mathcal{D}}^{\text{obs}}$ is the **given** distribution of the data
- **Computing** $\pi_{\mathcal{D}}^{D(\text{prior})}$ requires a forward propagation of the prior.
- For more details, see: "Combining Push-forward Measures and Bayes Rule to Construct Consistent Solutions to Stochastic Inverse Problems", BJW. SISC 40 (2), 2018.

An Illustrative Example





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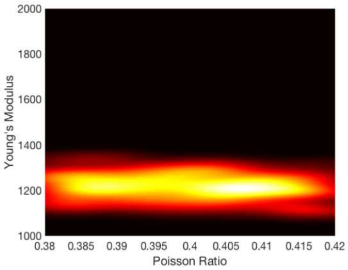
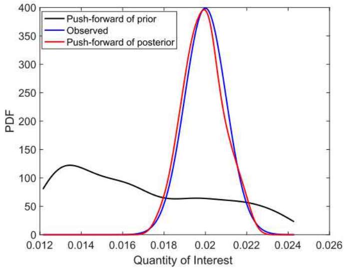
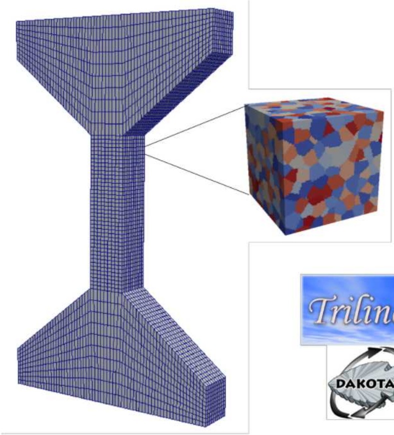




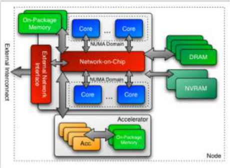
Perspective on Multiscale Modeling and Simulation



Dynamic/adaptive subgrid model selection,
Goal-oriented error estimates,
Machine learning (classification),
Homogenized elastic, crystal elasticity, crystal plasticity, etc.,
FEM, HDG, Multiscale hybridized, FE^2, etc.,
Multiphysics (thermo-chemo-mechanical),
Stochastic subgrid models,
Leverage emerging computational architectures

Trilinos

DAKOTA



Generalized Multiscale Mortar/Hybridized Formulation

Local/Fine Scale Problems

On each element $K_i \in \mathcal{T}_H$, we solve the local fine-scale problem:

$$\begin{cases} \frac{\partial \mathbf{u}_i}{\partial t} + \nabla \cdot \mathbf{F}_i(\mathbf{u}_i) = \mathbf{G}(\mathbf{u}_i), & \text{in } K_i \times (0, T], \\ \mathbf{u}_i = \mathbf{g}, & \text{on } \partial K_i \cap \partial\Omega \times (0, T], \\ \mathbf{u}_i = \boldsymbol{\lambda}, & \text{on } \Gamma_i \times (0, T], \\ \mathbf{u}_i = \mathbf{u}_0, & \text{on } K_i, \quad t = 0. \end{cases}$$

where $\boldsymbol{\lambda} = \mathbf{u}|_{\Gamma_i}$.

Generalized Multiscale Mortar/Hybridized Formulation

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where $\boldsymbol{\lambda} = \mathbf{u}|_{\Gamma_i}$.

Global/Coarse Scale Problem

Continuity and conservation of the appropriate fields across interfaces:

$$\begin{cases} \mathbf{u}_i = \mathbf{u}_j, \\ -\mathbf{F}_i(\mathbf{u}_i) \cdot \mathbf{n}_i = \mathbf{F}_j(\mathbf{u}_j) \cdot \mathbf{n}_j \end{cases} \quad \text{on } \Gamma_{i,j} \times (0, T]$$

where $\mathbf{n}_i$ is the outwards facing normal to $\partial\Omega_i$.

Conclusions and Future Work

- Our goal is to develop **data-informed physics-based** models
- Many approaches exist for incorporating data into a simulation
- The **consistent Bayesian** approach provides a robust approach for inverting a distribution
- **Multiscale mortar/hybridized methods** provide a mathematically elegant concurrent multiscale framework
- Consistent variational formulation (enables adjoints for optimization)
- Easily extends to multiphysics applications
- Modeling philosophy can be implemented at the element level which recovers many modern discretization techniques with specific choices for discretization, fluxes, etc.

Thanks! Questions?

Acknowledgments

T. Wildey's work was supported by the U.S. Department of Energy, Office of Science, Early Career Research Program.

Thank you for your attention!

Questions?