ARL-HTMDEC Kickoff Meeting, July 2022

Development and deployment of a Bayesian framework for the accelerated machine learning of multiscale physics controlling material responses in extreme environments

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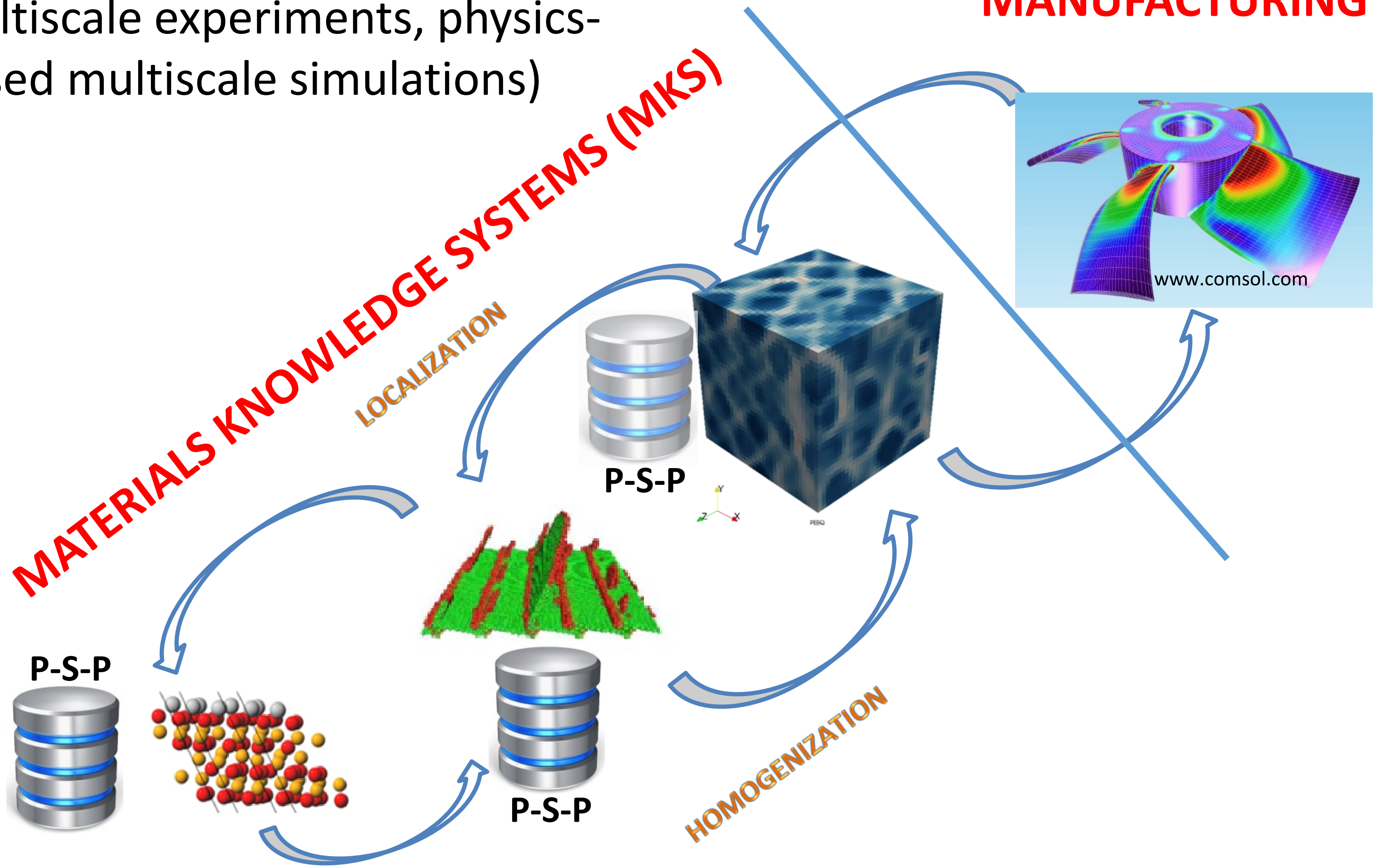
Uncertain Materials Knowledge Systems

Objective fusion of disparate data from heterogeneous sources (e.g., multiscale experiments, physics-based multiscale simulations)



Bayesian Learning Framework for PSP Linkages

<u>Notation</u>

$\mathcal{P}$ Set of Process Variable
$\boldsymbol{\mu}$ Material Structure
P Properties
$\boldsymbol{\varphi}$ Governing Physics
$\boldsymbol{\Sigma}$ Co-variance
$\boldsymbol{E}$ Experimental Observations

<u>Bayesian Update of Governing Physics</u>

$$p(\boldsymbol{\varphi} | \boldsymbol{E}, \boldsymbol{\Sigma}_{\boldsymbol{E}}) \propto \underbrace{p(\boldsymbol{E} | \boldsymbol{\varphi}, \boldsymbol{\Sigma}_{\boldsymbol{E}})} \, p(\boldsymbol{\varphi})$$

Likelihood computed using GP models extracted from simulations

<u>Physics-Based Models</u>

Build Gaussian Process models trained to simulation datasets produced by executing physics-based models by adaptive sampling of input domain for maximizing fidelity of extracted GP.

Process-Structure: $p(\boldsymbol{\mu} | \boldsymbol{\mathcal{P}}, \boldsymbol{\varphi}, \boldsymbol{\Sigma}_{\boldsymbol{\mathcal{P}}}, \boldsymbol{\Sigma}_{\boldsymbol{\varphi}})$

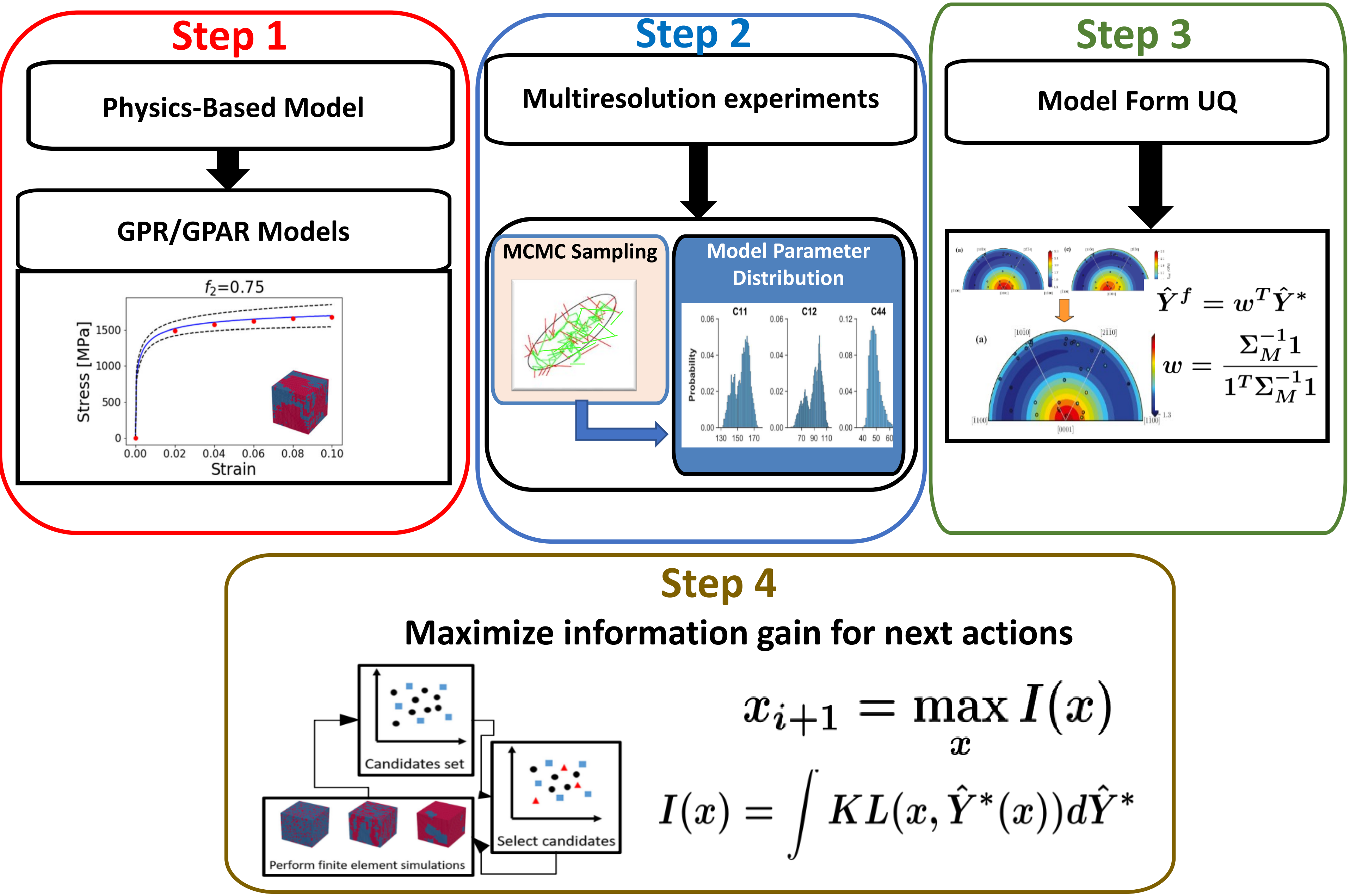
Structure-Property: $p(P | \boldsymbol{\mu}, \boldsymbol{\varphi}, \boldsymbol{\Sigma}_{\boldsymbol{\mu}}, \boldsymbol{\Sigma}_{\boldsymbol{\varphi}})$

<u>Sequential Design of Physical Experiments</u>

Decide on the next experiment that is likely to produce the largest information gain in updating the governing physics.

$$\textit{Final Property Estimation} = \int \boxed{P(\boldsymbol{\mu}(\boldsymbol{\mathcal{P}}, \boldsymbol{\varphi}), \boldsymbol{\varphi})} \, \boxed{p(\boldsymbol{\varphi})} \, d\boldsymbol{\varphi}$$

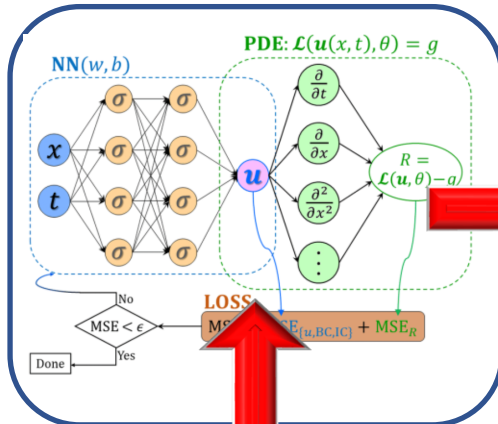
Task 1: Foundational Four-Step Bayesian Framework



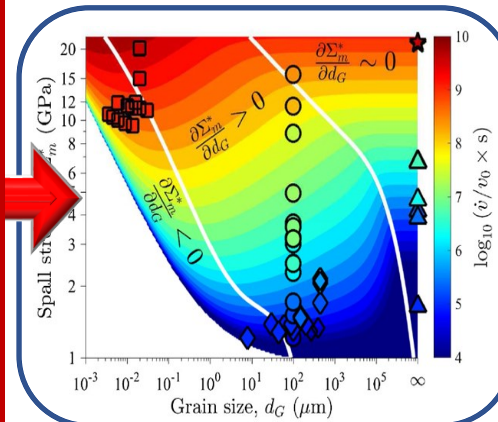
Task 2: Integration of Physics-based Constraints

Modify Step 1 and/or Step 2 of the Bayesian framework in Task 1 to constrain the models with physics-based priors

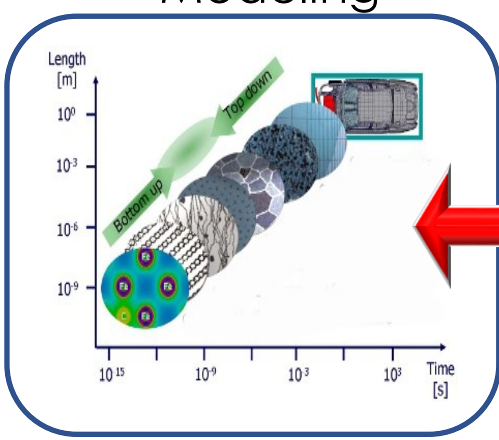
Physics-Aware Surrogates



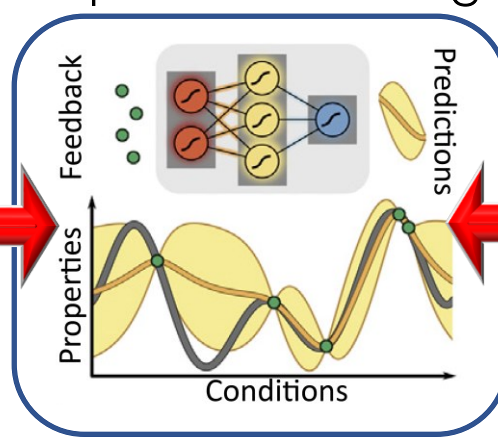
Mechanism Maps



Multi-Scale Modeling

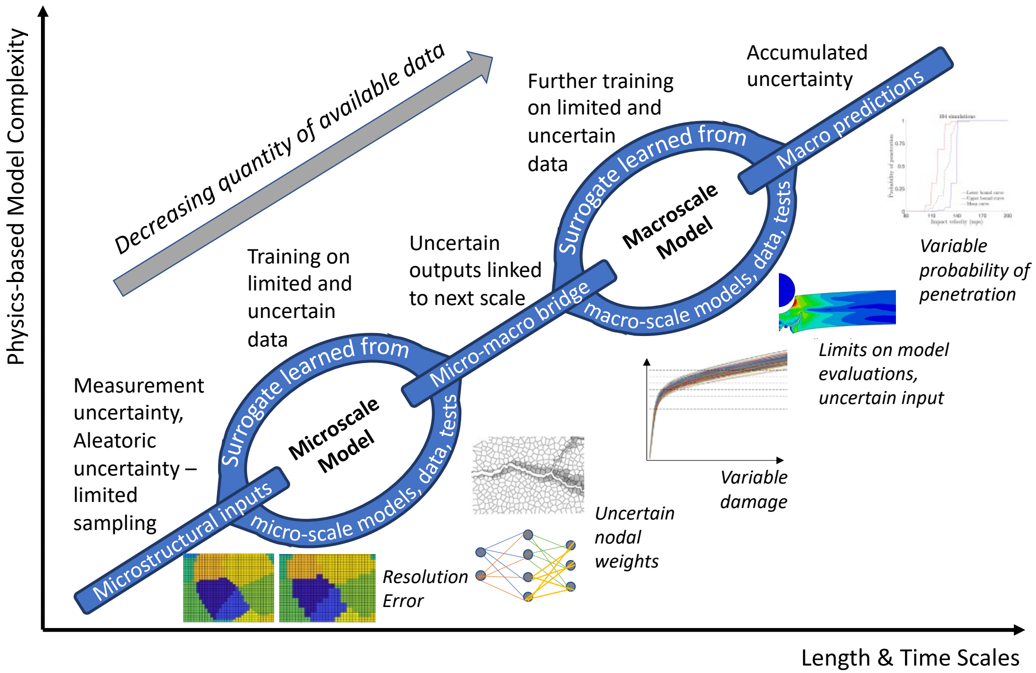


Bayesian Experimental Design



High Strain Rate Experiments

Task 3: Analysis of uncertainty propagation through chained surrogate models



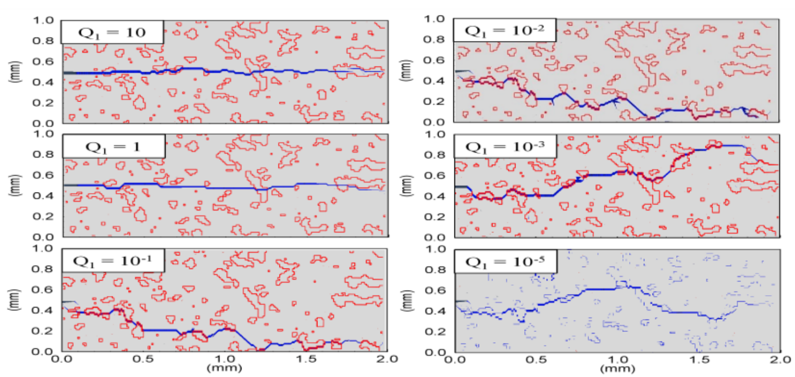
- Develop tools for ranking and learning multiscale physics controlling material responses
- Evaluate and demonstrate workflows for efficiency and accuracy
- Focus on models in our related tasks
  - Dynamic energy dissipation & fracture resistance in multiphase polycrystalline ceramics
  - High-throughput and automated Ashby-style maps for ballistic performance
- Compare Bayesian surrogates to probabilistic prediction from simulations, at both micro- and macro-scale

Task 4: Dynamic Fracture Toughness and Energy Dissipation of Ceramics

Microscale Fracture and Energy Dissipation Mechanism Tracking $\Rightarrow$ Microstructure-Macroscale Fracture Toughness and Energy Dissipation Relations

Crack propagation

Explicit resolution of microstructure, transgrnular and intergranular fraction, internal friction, dissipation, temperature increase, and thermal effects



Fracture toughness

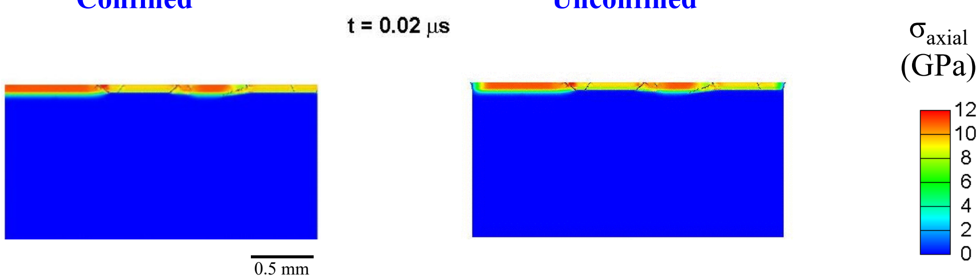
Dynamic *J*-integral, driving force & resistance tracking

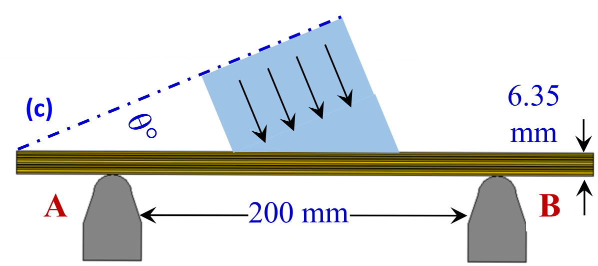
$$K_{IC} = \sqrt{\frac{\bar{E}}{1-\bar{\nu}^2}\xi\left(\mathrm{Q}, s, f\right)\left(\Phi_{in}H_{in} + \Phi_m H_m + \Phi_p H_p\right)}$$

$$E = \int\left(\int_{S_{int}} \boldsymbol{f}\cdot\boldsymbol{v}dS\right)dt + \int\left(\int_V \boldsymbol{\sigma} : \boldsymbol{D}^{inel} dV\right)dt$$

Energy dissipation under different loading conditions

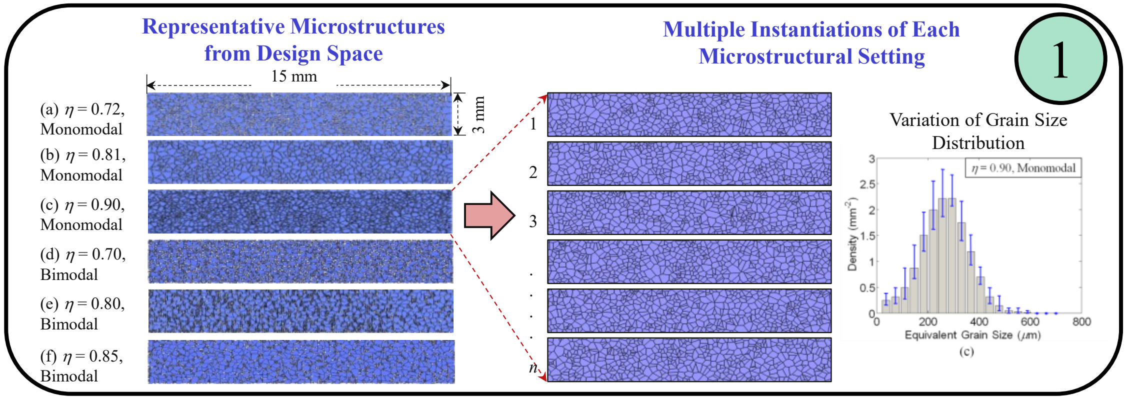
Confined **Unconfined**



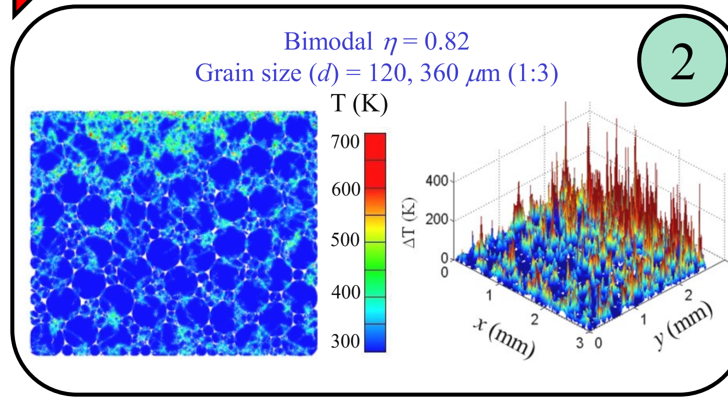


Task 4: Dynamic Fracture Toughness and Energy Dissipation of Ceramics – Microstructure Design

Experimentally-informed Design of statistically equivalent microstructure sample sets (SEMSS)

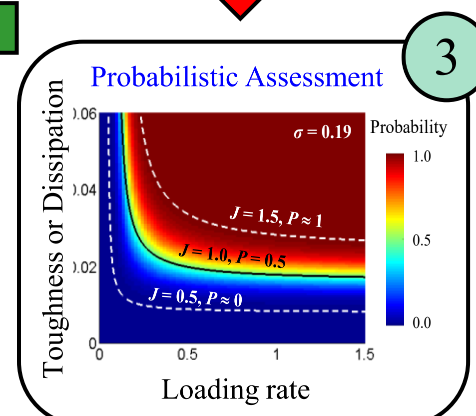


Physics-based simulations with SEMSS

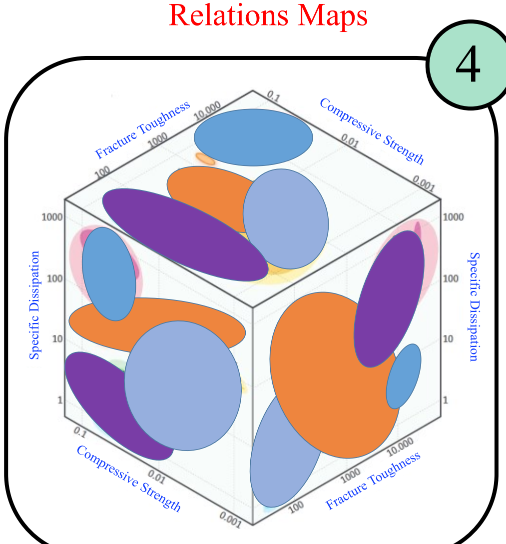


Property assessment

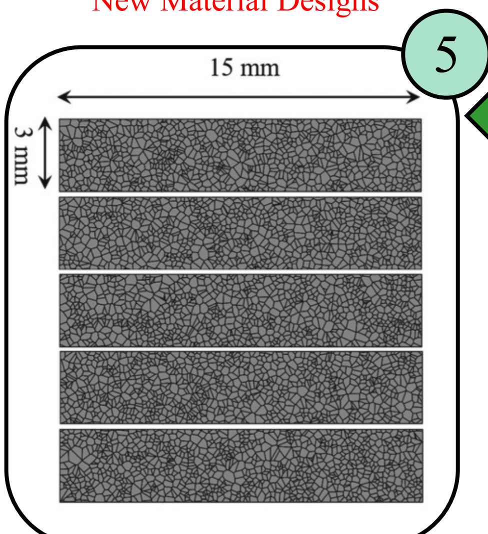
Data-driven ML



Material-Property Relations Maps

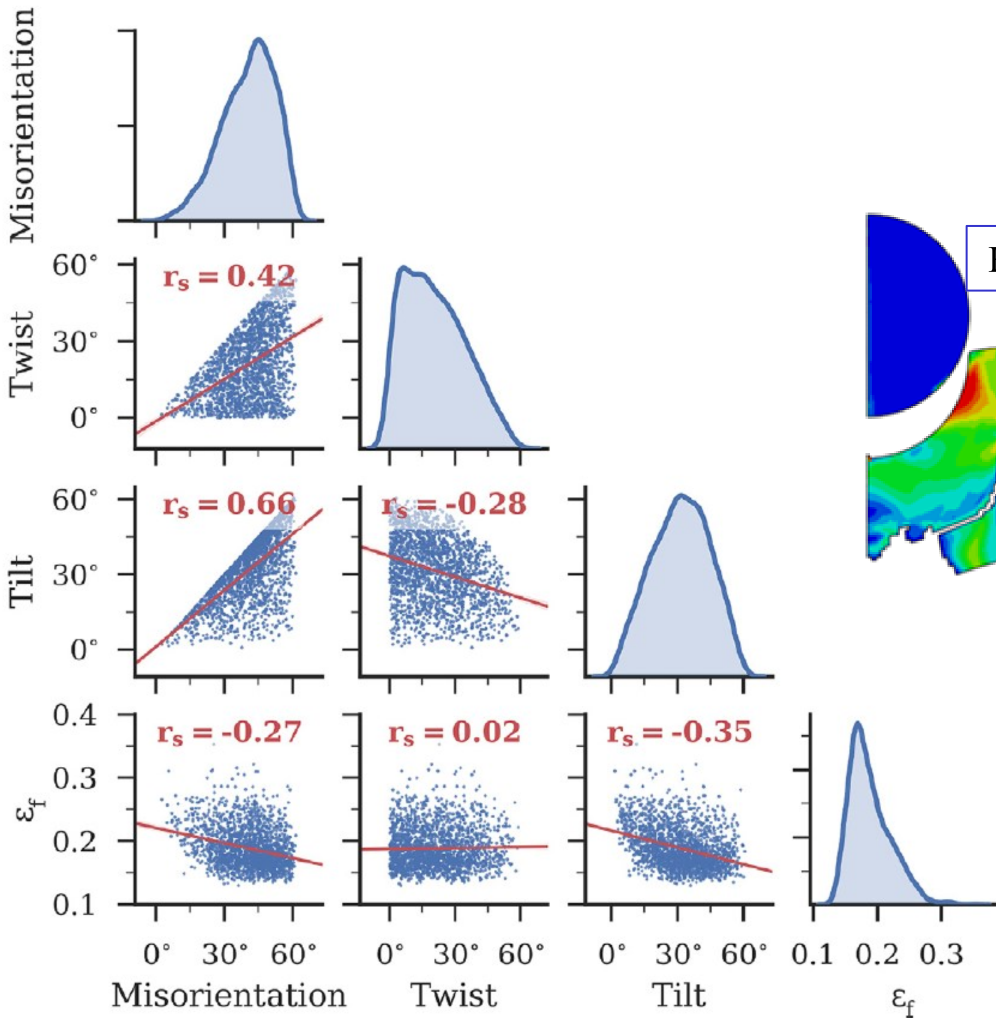


New Material Designs



Task 5: Ashby-style maps for ballistic performance

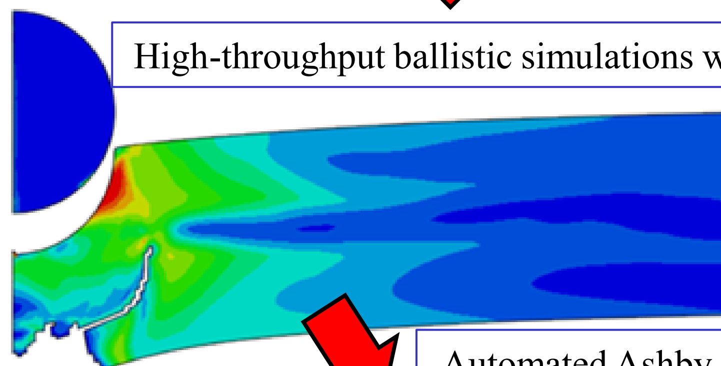
Our existing databases of mesoscale calculations



Automated calibration of Johnson-Cook parameters

$$\varepsilon_f = d_1 + d_2 \exp\left(d_3 \frac{\sigma_m}{\sigma_{eq}}\right)$$

High-throughput ballistic simulations with J-C parameters



Automated Ashby-style Diagrams