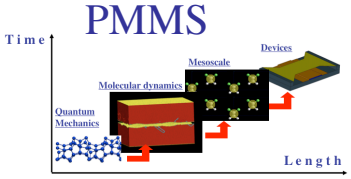
Optimal orchestration of high-fidelity simulations in multiscale materials models

Ale Strachan (strachan@purdue.edu)

School of Materials Engineering
Birck Nanotechnology Center
Purdue University



Objective

- Develop, implement and demonstrate an *uncertainty quantification-based orchestrator* for multi-fidelity and multi-scale simulations of materials.

- Determine when and where high-fidelity simulations are more critically needed to maximize their impact in terms of increasing the accuracy of the predicted quantity of interest (QoI).

PURDUE UNIVERSITY

Problem statement

The result of the simulation is a function of input parameters $\{P_i\}$ and a functional of constitutive functions $\{f_i\}$

$$Q = Q\left(\left\{P_i\right\}, \left\{f_i\left(z_i; Q_i\right)\right\}\right)$$

Assume constitutive models f_i can be replaced with a higher fidelity, but computationally costly, simulation: g_i

When and where (value of its independent variable) to run the high-fidelity model?

PURDUE UNIVERSITY

Functional uncertainty quantification

- Quantity of interest: $Q = Q\left(\left\{P_i\right\}, \left\{f_i\left(z_i; Q_i\right)\right\}\right)$

- Functional (Frechet) derivatives
  - Quantifies how the QoI depends on the constitutive function
  - It depends on the independent variable

$$\delta Q = \int \frac{\delta Q[f]}{\delta f(z)} \delta f(z) dz$$

$$\frac{\delta Q[f]}{\delta f(z)}(z_0) = \lim_{\varepsilon \to 0} \frac{Q[f(z) + \varepsilon \delta(z - z_0)] - Q[f(z)]}{\varepsilon}$$

PURDUE UNIVERSITY

Functional uncertainty quantification

1. Uncertainty quantification:

$$\Delta Q_{UQ} = \int \left| \frac{\delta Q[f]}{\delta f(z)} \right| \Delta f(z)\, dz$$

2. Error correction:

Functional sensitivity

$$\Delta Q_{Corr} = \int \frac{\delta Q[f]}{\delta f(z)} \underline{\left(g(z) - f(z)\right)} dz$$

Functional discrepancy

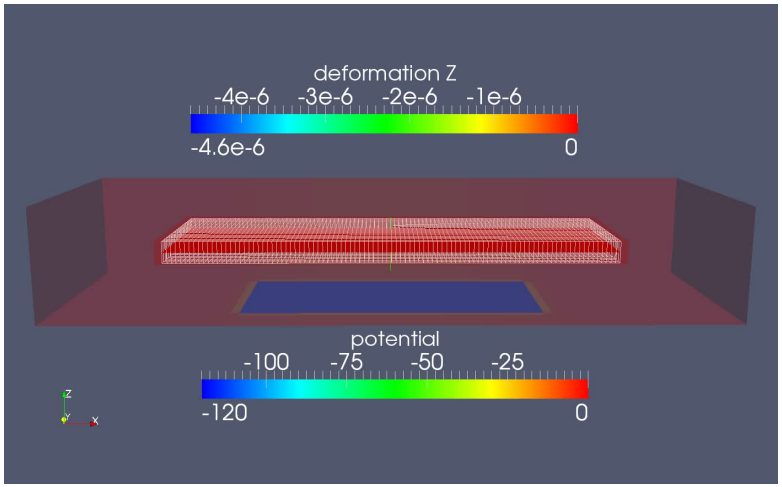
3. Ranking high-fidelity simulations

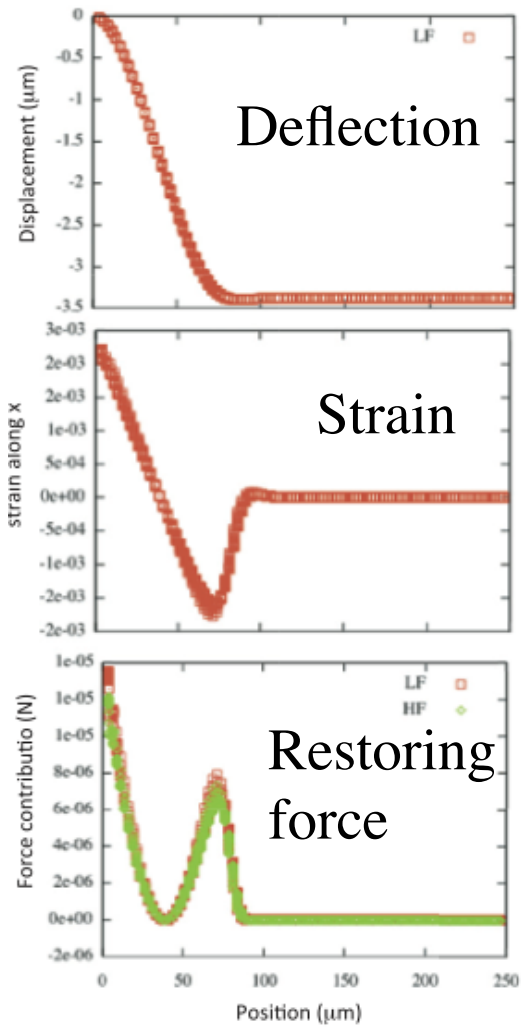
$$\left| \frac{\delta Q[f]}{\delta f(z)} \left(g(z) - f(z)\right) \right|$$

PURDUE UNIVERSITY

Example: force on a cantilever beam

RF-MEMS Switch





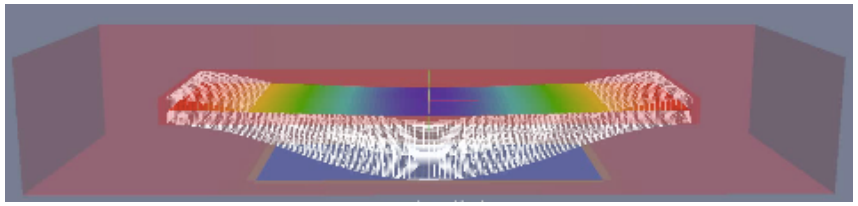
QoI: elastic restoring force when the switch is closed

$$F = \int_{A_0} h_0 \left[\frac{\partial \sigma_{11}(r_1, r_2)}{\partial r_1} \frac{\partial w(r_1, r_2)}{\partial r_1} + \frac{\partial \sigma_{22}(r_1, r_2)}{\partial r_2} \frac{\partial w(r_1, r_2)}{\partial r_2} \right] \mathrm{d}r_1 \, \mathrm{d}r_2.$$

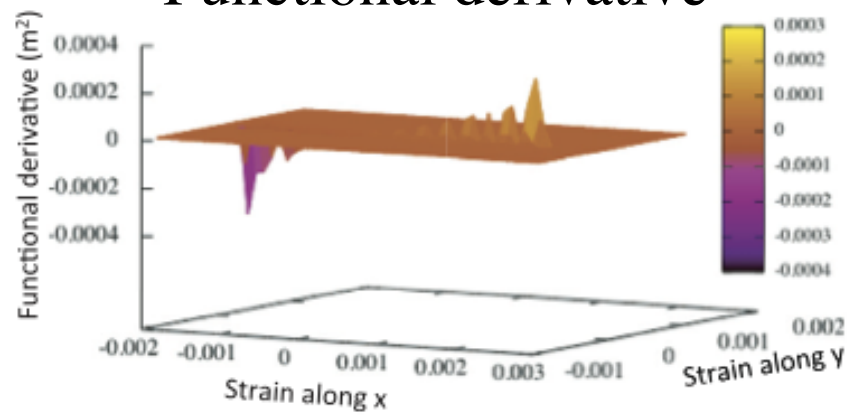
Constitutive law for refinement: stress-strain relationship

Strachan, Mahadevan, Hombal, Sun, Modelling Simul. Mater. Sci. Eng. 21 (2013) 065009

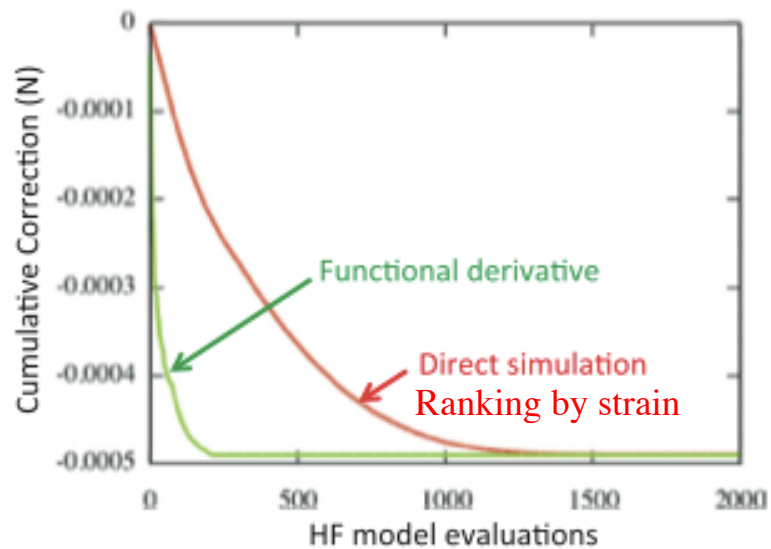
Example: force on a cantilever beam



Functional derivative



Correction as a function of number of evaluation of the high-fidelity model



Strachan, Mahadevan, Hombal, Sun, Modelling Simul. Mater. Sci. Eng. 21 (2013) 065009