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Multimodel Methods for Uncertainty Quantification of Repository Systems

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U.S. DEPARTMENT OF ENERGY NNSA National Nuclear Security Administration

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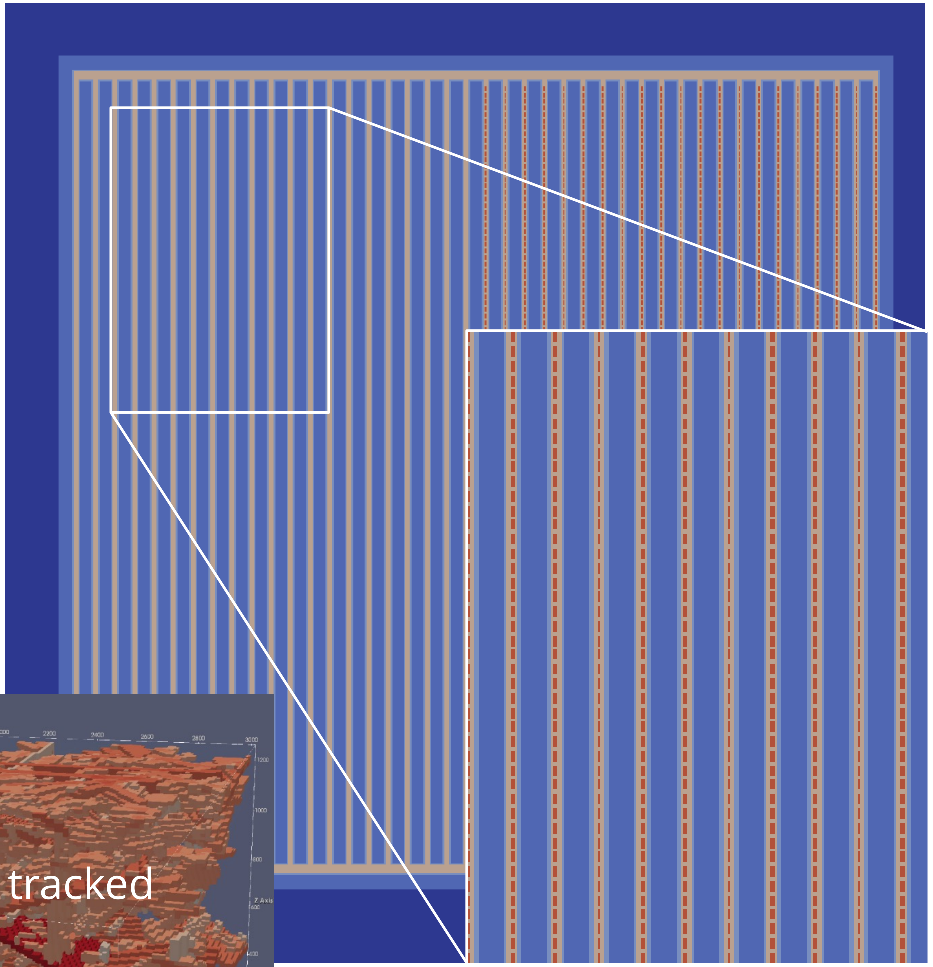
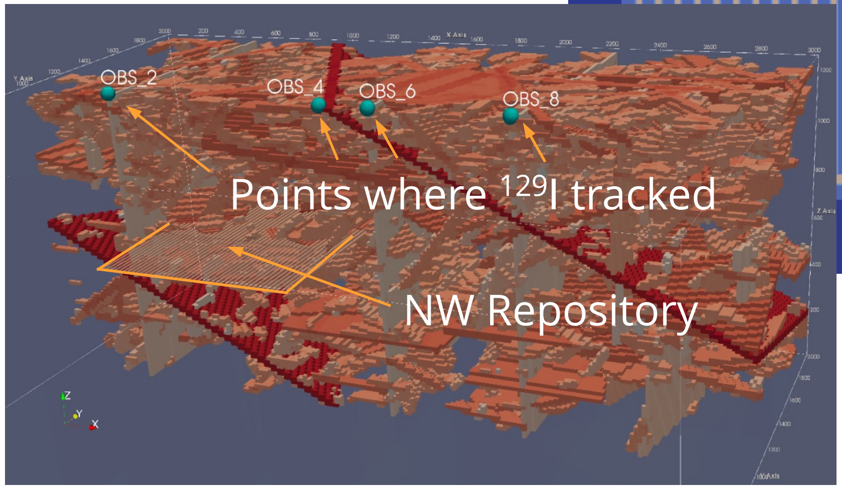
Uncertainty Quantification (UQ) for geologic disposal safety assessment (GDSA)



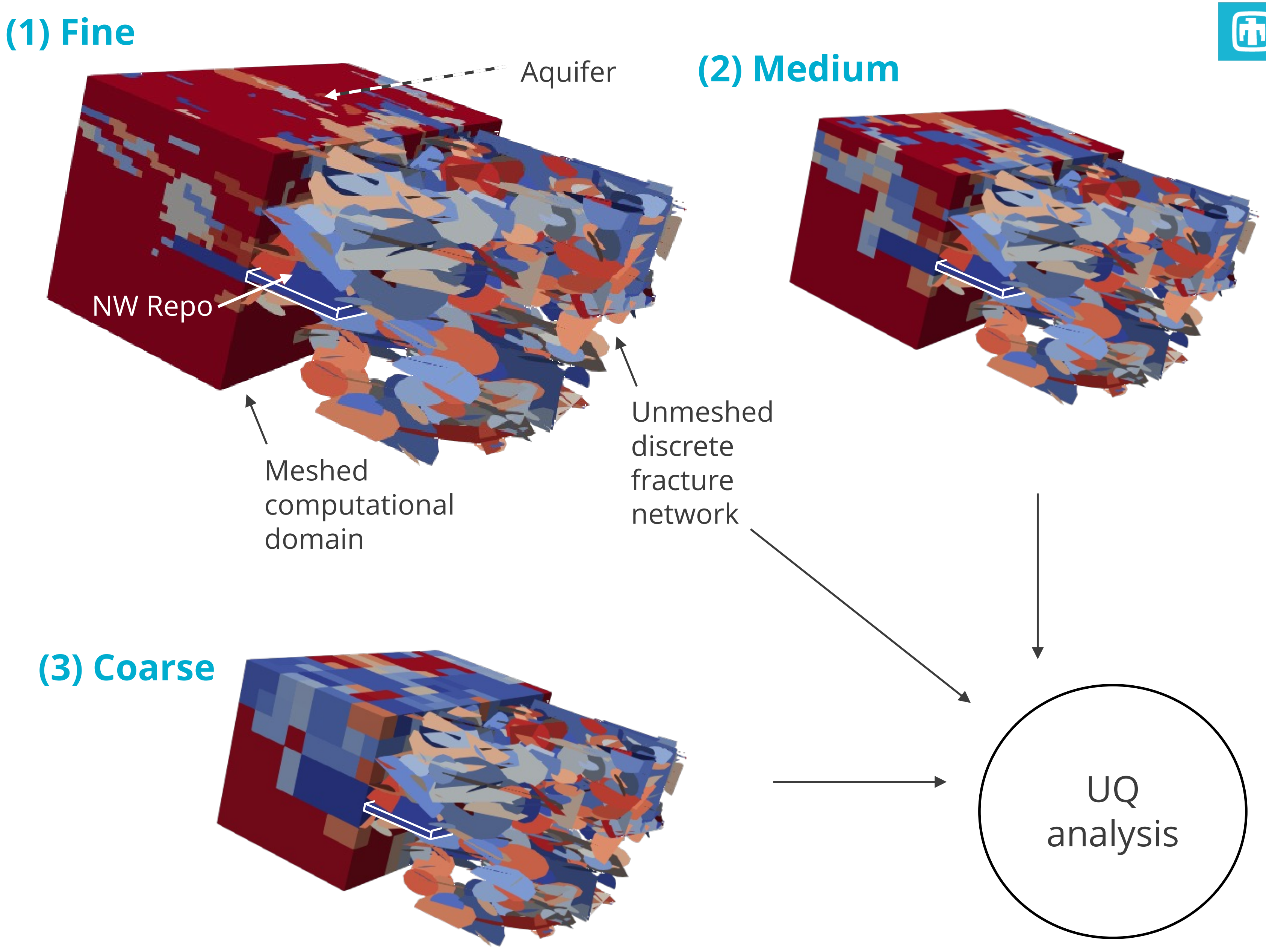
GDSA workflow at Sandia is deploying an unprecedented level of model fidelity for UQ studies in this application area.

~1.5 hours on 512 cores per simulation)
$\mathcal{O}(1000)$ model evaluations for current UQ studies



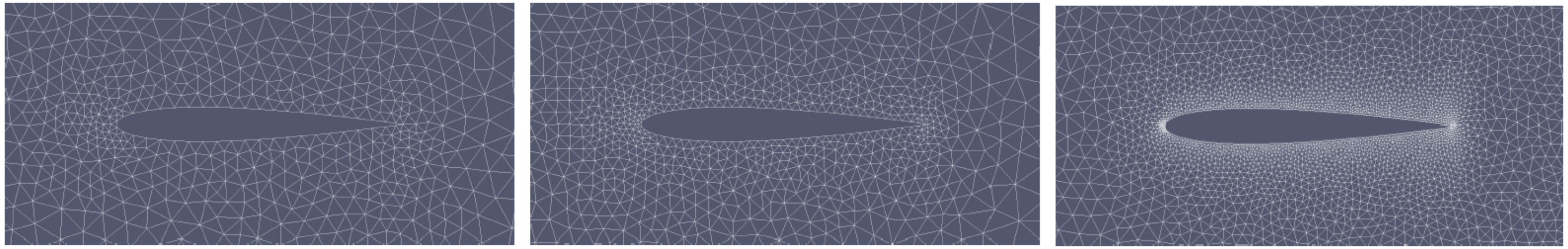
Multimodel methods can make UQ studies more efficient.

Idea: exploit lower-fidelity, cheaper models to lower cost for same accuracy

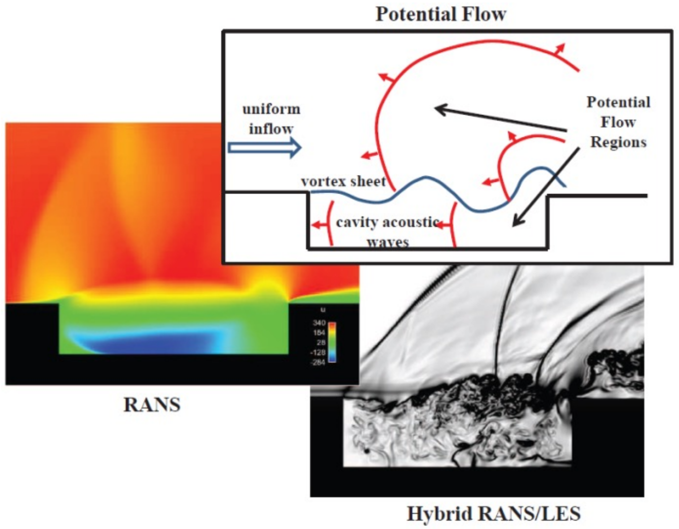


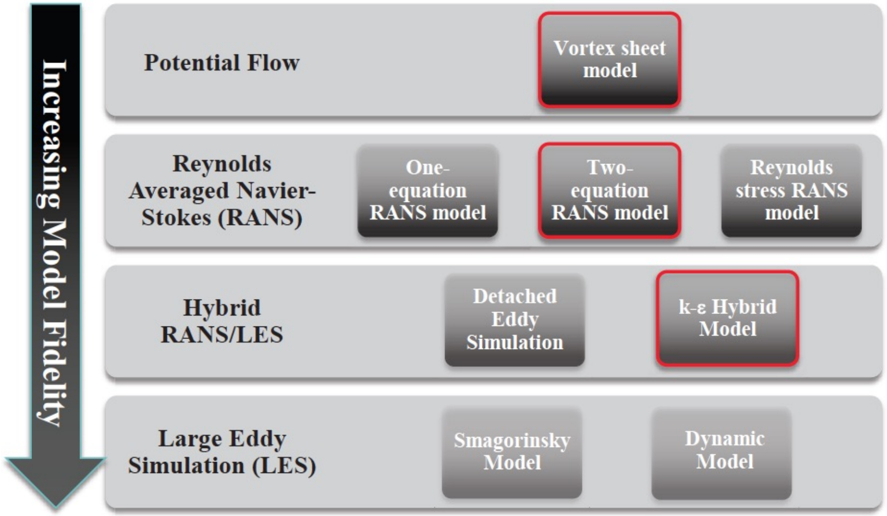
Idea: exploit lower-fidelity, cheaper models to lower cost for same accuracy

Discretization



Modeling assumptions





There are two classes of multimodel methods

Sampling-based

- Multilevel Monte Carlo (MLMC) [1]
- Multifidelity Monte Carlo (MFMC) [2]
- Approximate Control Variates (ACV) [3]
- Multilevel Best Linear Unbiased Estimate (MLBLUE) [4]

Surrogate-based

- Multifidelity Gaussian Processes [5]
- Multifidelity Polynomial Chaos Expansions [6]
- Multilevel/multi-index stochastic collocation [7,8]
- MFNets[9]

There are two classes of multimodel methods

Sampling-based

- Unbiased
- Performance independent of number of parameters, output smoothness
- Theoretical development has focused on functions of moments
  - More work needed for efficient estimation of CDFs, tail probabilities, calibration

Surrogate-based

- Build once, use for multiple UQ tasks (forward propagation, SA, calibration)
- Can exploit relationships that sampling-based can't (e.g. sparsity in discrepancy between two models)
- Same weaknesses as their single-fidelity counterparts: e.g. GPs, PCEs can't handle 100s of inputs, discontinuous model outputs.

Sampling-based methods

$$\widehat{M}(\theta) = \frac{1}{N}\sum_{i=1}^{N} M\left(\theta^{(i)}\right), \qquad \theta^{(i)} \sim p(\theta)\ \mathrm{i.i.d.}$$

$$\mathbb{V}\left[\widehat{M}\right] = \frac{\mathbb{V}[M]}{N}$$

Sampling-based methods – control variates

$$M_1(\theta) \qquad c_1 = \frac{C_1}{C} \ll 1 \qquad \mathrm{corr}(\mathrm{M}, \mathrm{M}_1) = \rho$$

$$\widehat{M}_{CV}(\theta) = \widehat{M}(\theta) + \alpha\left(\widehat{M}_1(\theta) - \mathbb{E}[M_1]\right)$$

$$\mathbb{E}\left[\widehat{M}_{CV}(\theta)\right] = \mathbb{E}[M]$$ ← Unbiased

$$\mathbb{V}\left[\widehat{M}_{CV}(\theta)\right] = \frac{1}{N}\left(\mathbb{V}[M] + \alpha^2\mathbb{V}[M_1] + 2\alpha\mathrm{Cov}[M, M_1]\right)$$

$$\alpha^* = \min_{\alpha} \mathbb{V}\left[\widehat{M}_{CV}(\theta)\right] = -\frac{\mathrm{Cov}[M, M_1]}{\mathbb{V}[M_1]}$$

$$\mathbb{V}\left[\widehat{M}_{CV}(\theta)\right] = \frac{\mathbb{V}[M]}{N}(1 - \rho^2)$$ ← $\rho^2 \approx 1 \rightarrow$ orders of magnitude reduction in variance

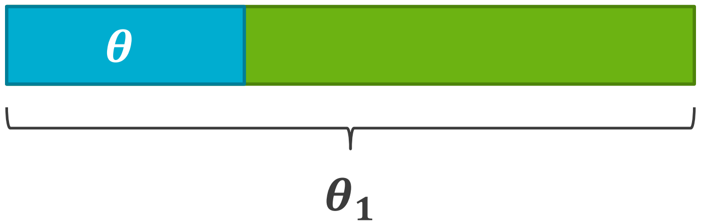
Sampling-based methods – beyond control variates

$$\widehat{M}_{CV}(\theta) = \widehat{M}(\theta) + \alpha\left(\widehat{M}_1(\theta) - \mathbb{E}[M_1]\right)$$

Have to estimate this too

Multifidelity Monte Carlo [2]:

$$\widehat{M}_{MFMC} = \widehat{M}(\boldsymbol{\theta}) + \alpha\left(\widehat{M_1}(\boldsymbol{\theta}) - \widehat{M_1}(\boldsymbol{\theta}_1)\right)$$



$$\alpha^* = -\frac{\rho\sqrt{\mathbb{V}[M]}}{\sqrt{\mathbb{V}[M_1]}}$$

$$r_1^* = \sqrt{\frac{\mathrm{Cost}(M)\rho^2}{\mathrm{Cost}(M_1)(1-\rho^2)}} \qquad N_1 = \lceil r_1 N \rceil$$

$$\mathbb{V}\left[\widehat{M}_{MFMC}\right] = \frac{\mathbb{V}[M]}{N}\left(1 - \rho^2\left(\frac{r_1 - 1}{r_1}\right)\right)$$

Best sampling-based method depends on model ensemble

$$\mathbb{V}[\hat{M}_{MFMC}] = \frac{\mathbb{V}[M]}{N}\left(1 - \rho^2\left(\frac{r_1 - 1}{r_1}\right)\right)$$

$$r_1 = \sqrt{\frac{\text{Cost}(M)\rho^2}{\text{Cost}(M_1)(1 - \rho^2)}}$$

Each method combines models and samples differently.

Which one performs best is a nonintuitive function of model costs and correlations.

In practice model costs and correlations have to be estimated through a pilot study.

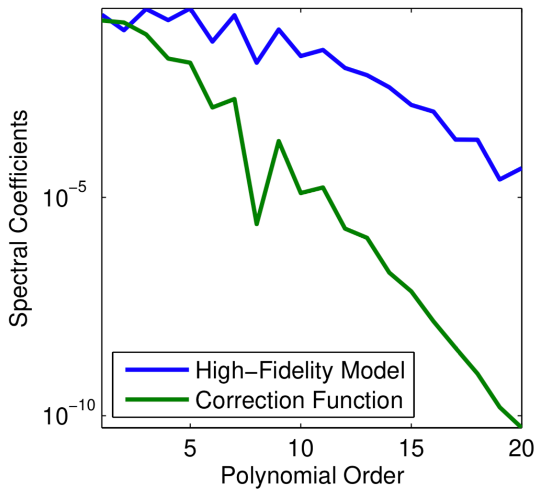
Dakota can project performance of each method so the user can select the best one for their problem. Methods currently implemented:

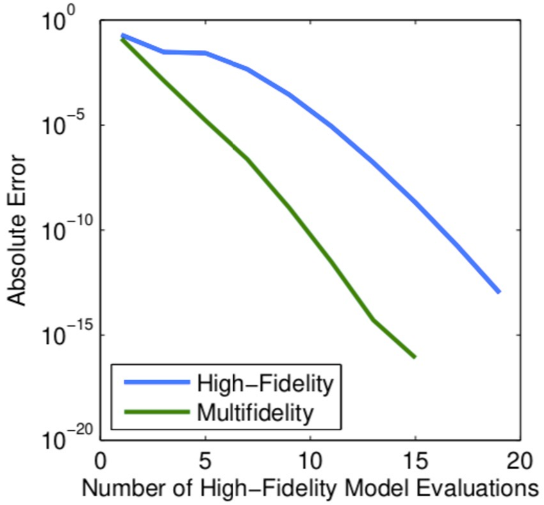
- MLMC
- MFMC
- MLCV
- ACV-MF
- ACV-IS

DAKOTA

Surrogate-based methods

Single-fidelity surrogate: $M(\theta) \approx f(\theta)$





Images courtesy of [6]

Hierarchical surrogates

$$M_1(\theta) \approx f_1(\theta)$$

$$M(\theta) - M_1(\theta) \approx f_\Delta(\theta)$$

$$M(\theta) \approx f_1(\theta) + f_\Delta(\theta)$$

More computationally efficient if need fewer samples to resolve discrepancy vs original high-fidelity model.

Nonhierarchical surrogates

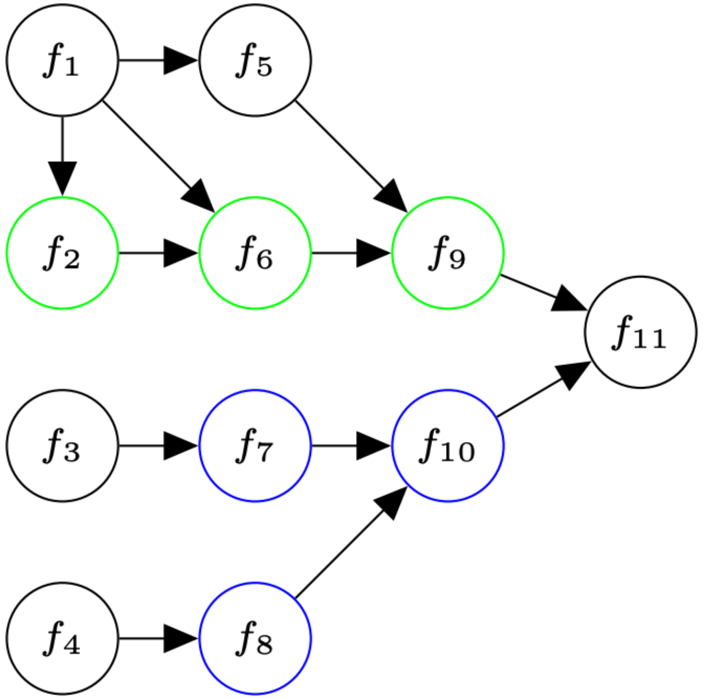
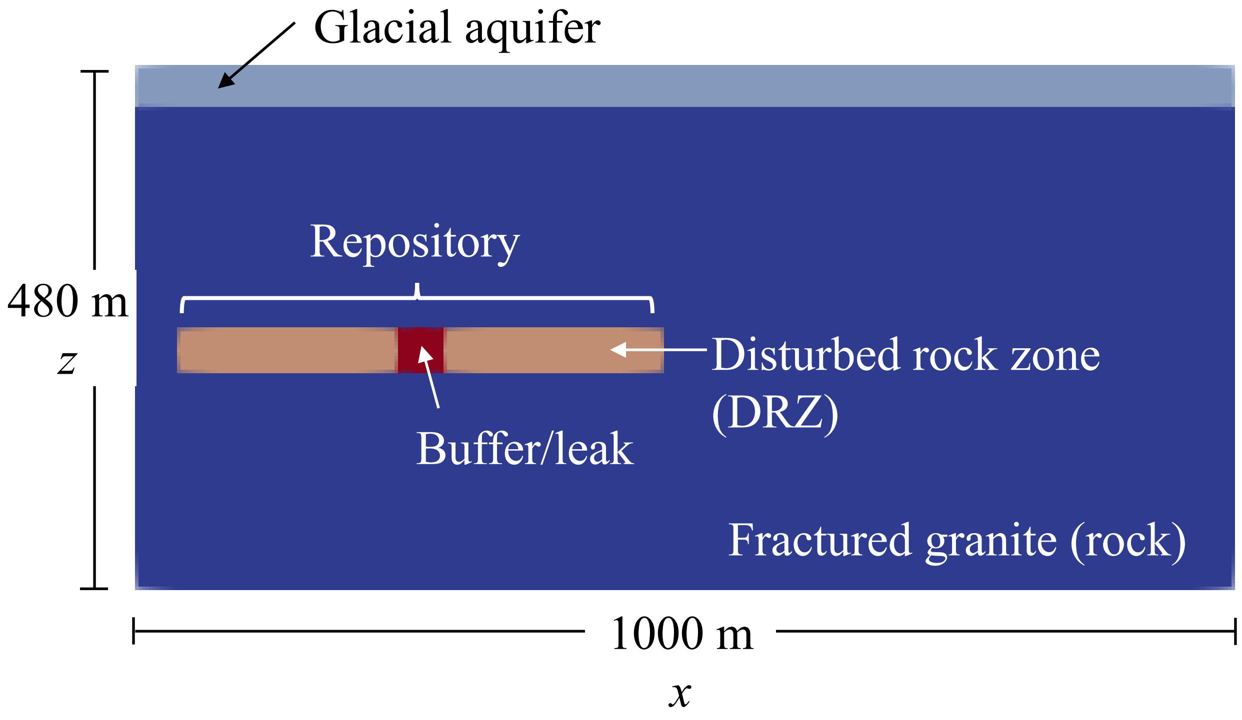
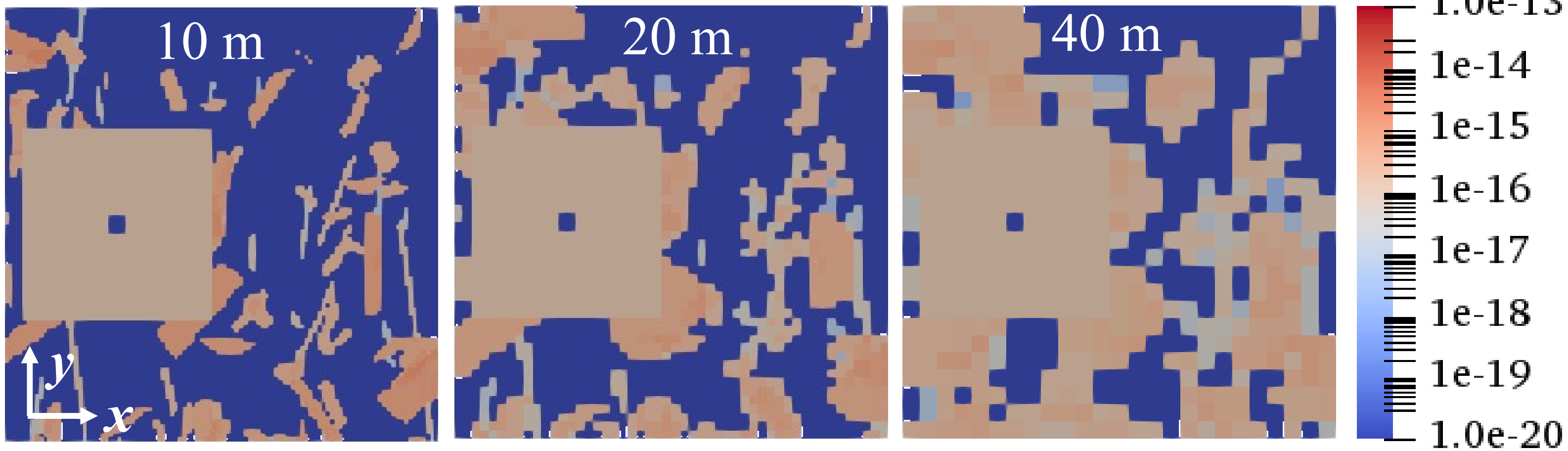


Image courtesy of [9]



Parameter	Description	Distribution
rateUNF	Waste form bulk dissolution rate [yr^{-1}]	$\log\mathcal{U}[10^{-8}, 10^{-6}]$
kGlacial	Glacial aquifer permeability [m^2]	$\log\mathcal{U}[10^{-15}, 10^{-13}]$
permDRZ	DRZ permeability [m^2]	$\log\mathcal{U}[10^{-19}, 10^{-16}]$
permBuffer	Buffer permeability [m^2]	$\log\mathcal{U}[10^{-20}, 10^{-17}]$
pBuffer	Buffer porosity	$\mathcal{U}[0.3, 0.5]$
wpBreachTime	Waste package breach time [yr]	$\mathcal{U}[2500,10000]$

k_{xx} [m^2] at z = 240 m



Mesh size [m]	Core time [s]	Relative cost
10	9822.8	1.0
20	329.7	3.36e-2
40	22.0	2.24e-3

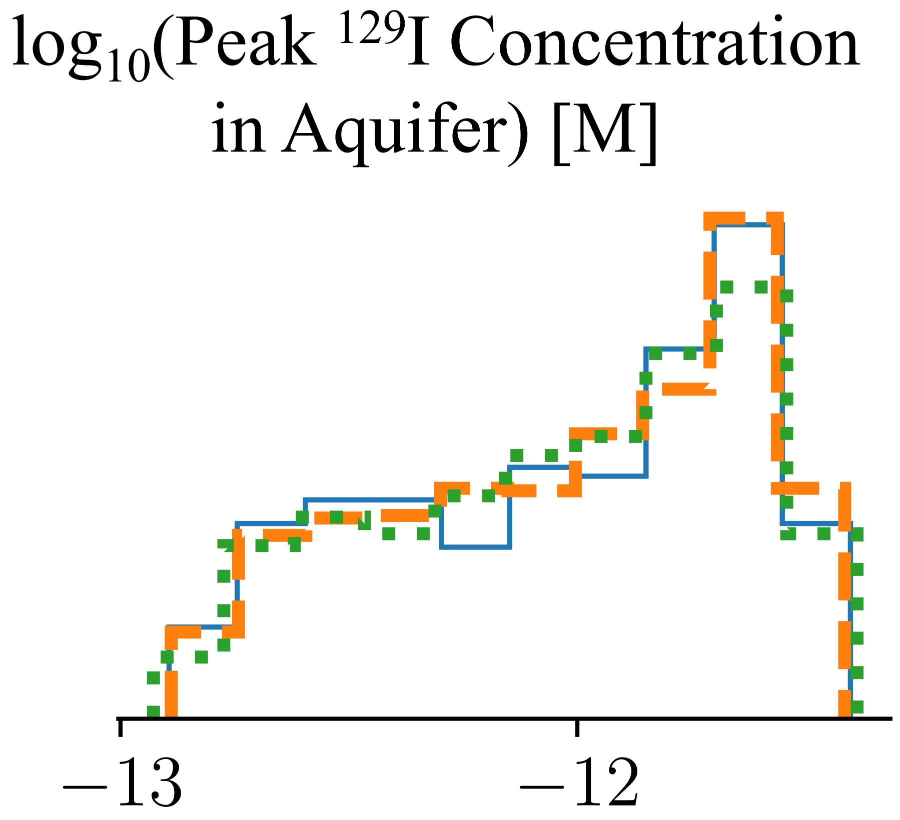
QoI: $\log_{10}$ Peak ^{129}I concentration

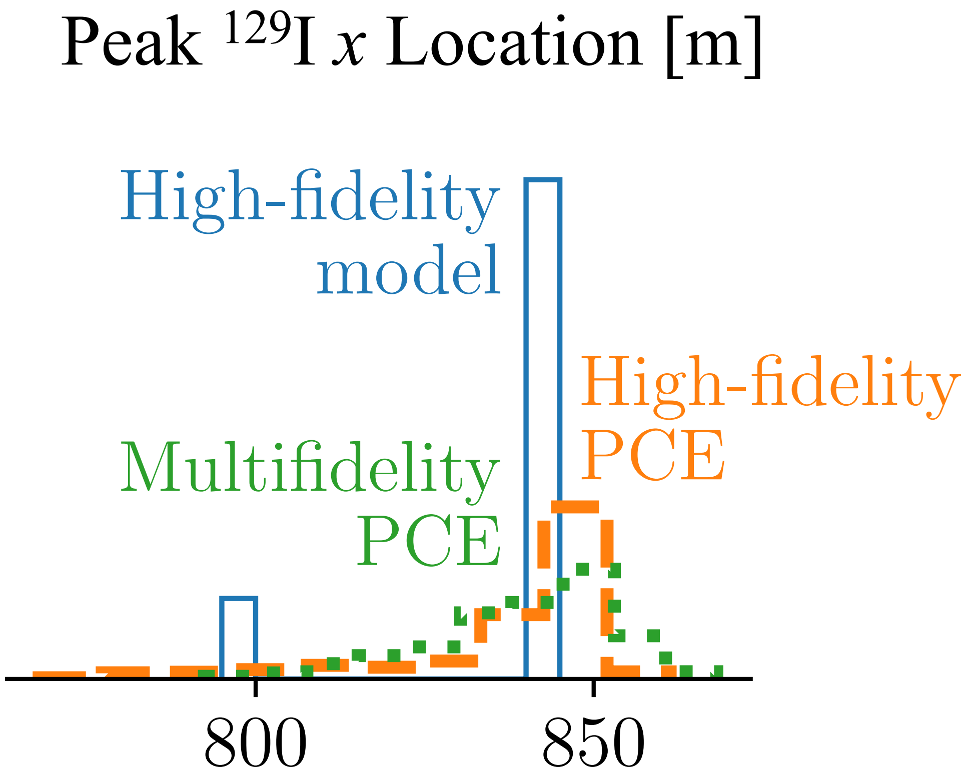
Multimodel methods projected to be almost 2 orders of magnitude more accurate for same cost

Method	Projected estimator variance	Projected MC variance / Projected variance
Monte Carlo	1.78e-3	1.0
Multilevel	1.22e-4	15.7
Multifidelity	2.21e-5	80.6
ACV MF	2.85e-5	62.5

25 pilot samples, equivalent cost of 100 HF evaluations

Multifidelity polynomial chaos expansion (PCE) exhibits same challenges for discontinuous outputs as standard PCE





MF PCE was constructed at equivalent cost of ~22 high-fidelity model evaluations.

- Which method is best depends on model ensemble, goals of analysis

- Multimodel methods can significantly decrease the computational burden of uncertainty analyses (nominally by orders of magnitude)

- More information on pros and cons discussed methods in conference paper

Thanks!

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