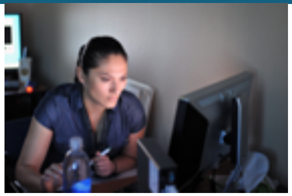
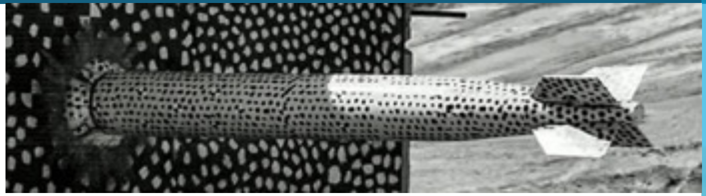
SAND2021-2125 C

Application of Multifidelity Uncertainty Quantification Methods to a Subsurface Transport Model





SIAM CSE21

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UQ for geologic disposal safety assessment (GDSA)

Performance assessment for nuclear waste repository site.

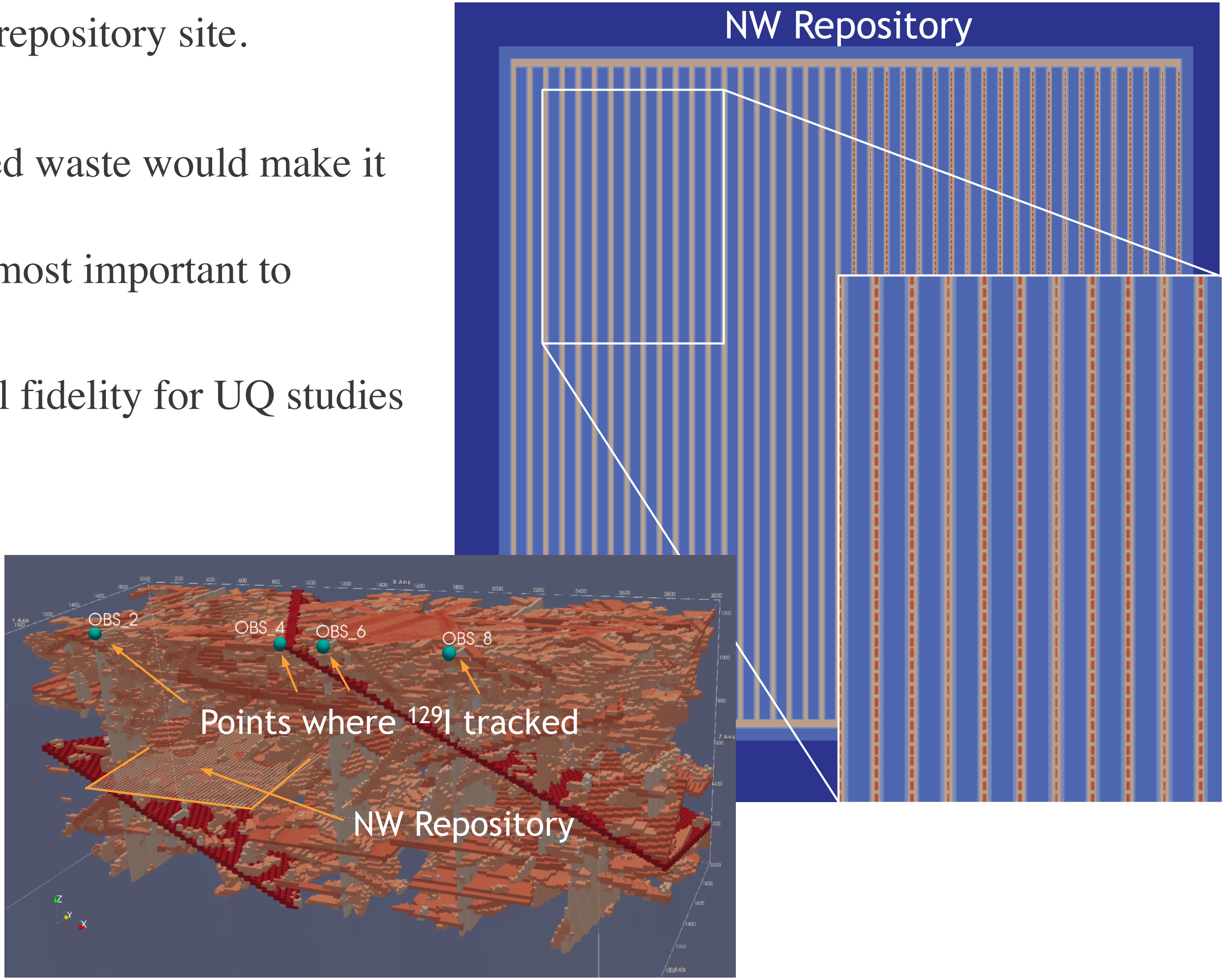
Want to understand things like:

1) probability dangerous levels of leaked waste would make it to a water supply;
2) subsurface/waste storage properties most important to repository performance.

Deploying an unprecedented level of model fidelity for UQ studies in this application area.

Simulations very costly (~1.5 hours on 512 cores per simulation): $\mathcal{O}(1000)$ model evaluations for production UQ studies.

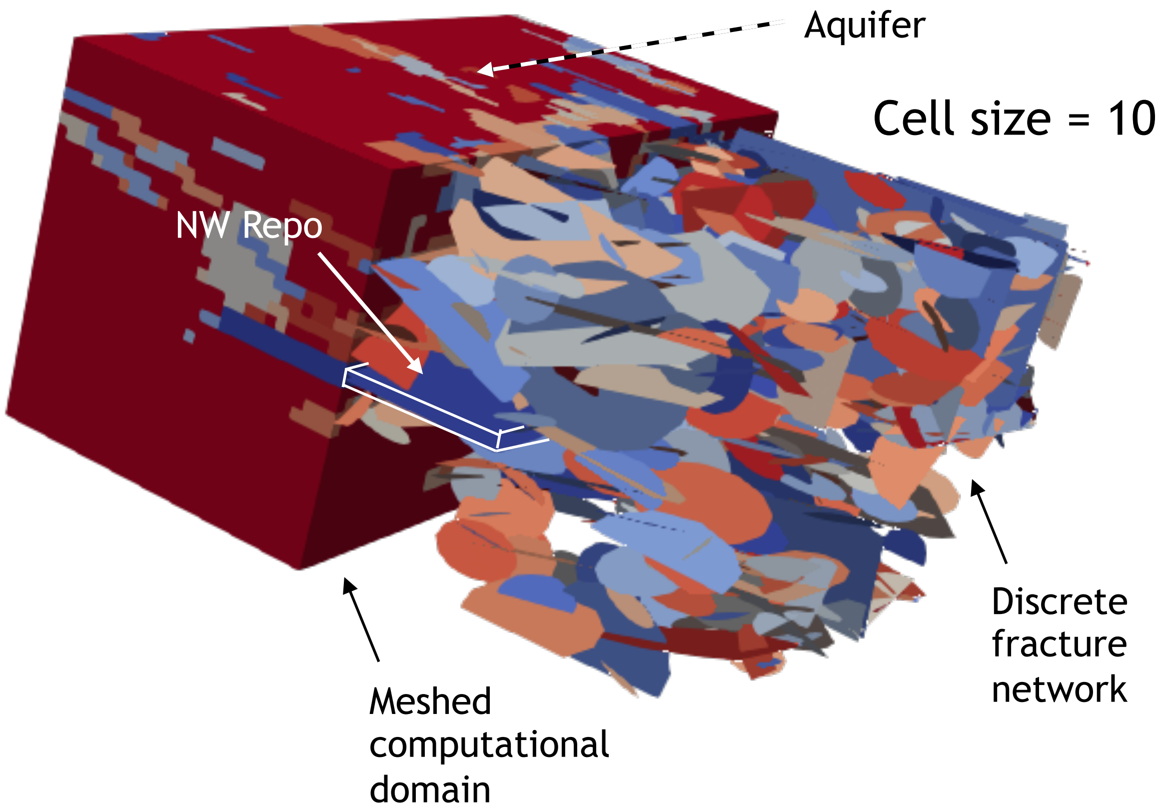
Goal: explore feasibility of using multifidelity polynomial chaos expansion (PCEs) for global sensitivity analysis (GSA) in this problem.

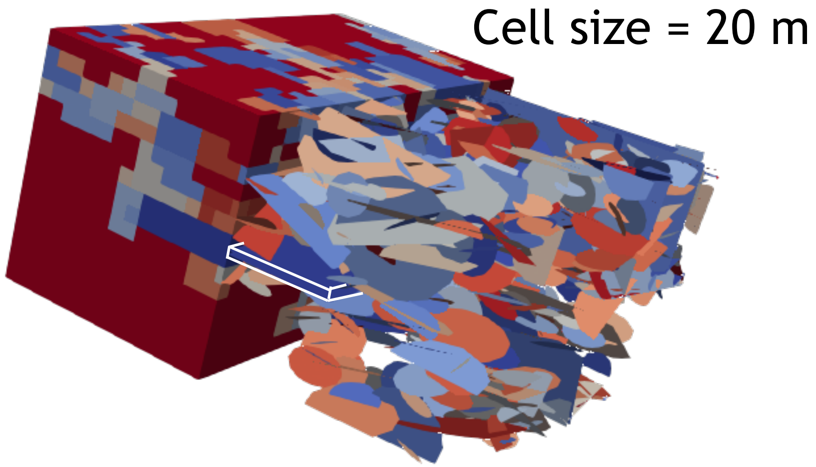


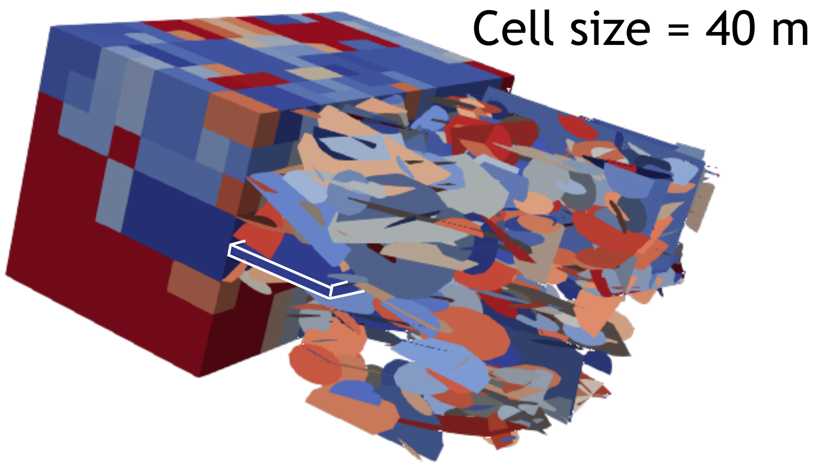
Fractured subsurface uncertainty treatment and model hierarchy

- Can't observe all fractures in subsurface; represent uncertainty using random instantiations of discrete fracture networks (DFNs).

- DFNs mapped to equivalent continuous porous media (ECPMs).
  - Define grid, sweep through cells and map fracture permeability and porosity to equivalent continuum values.



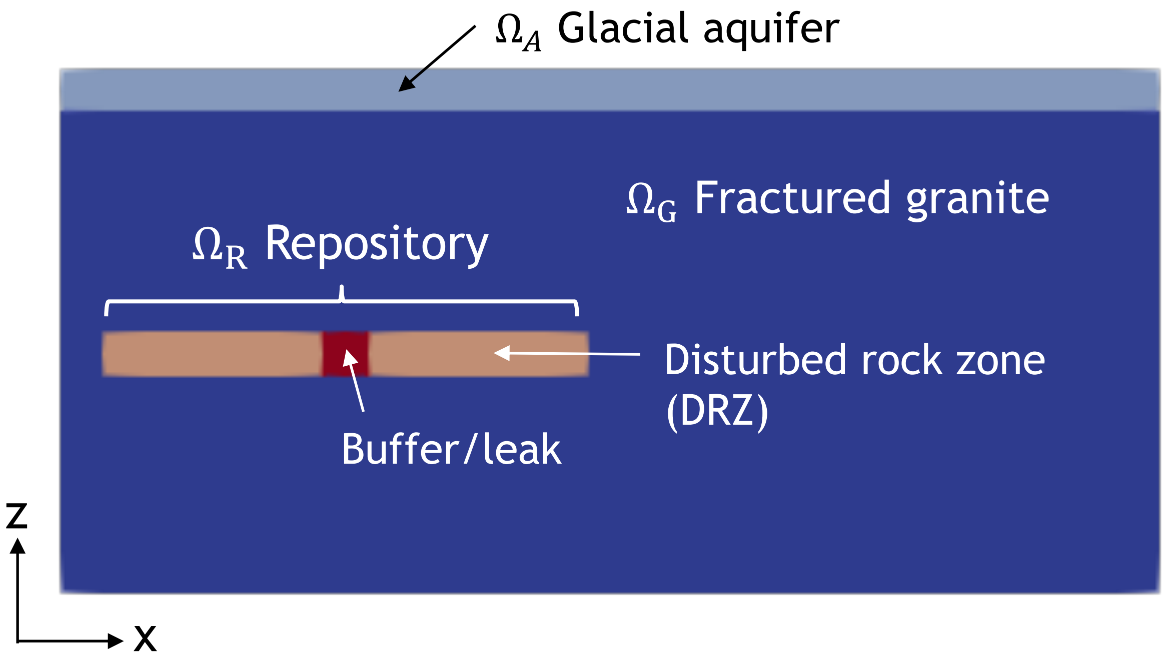




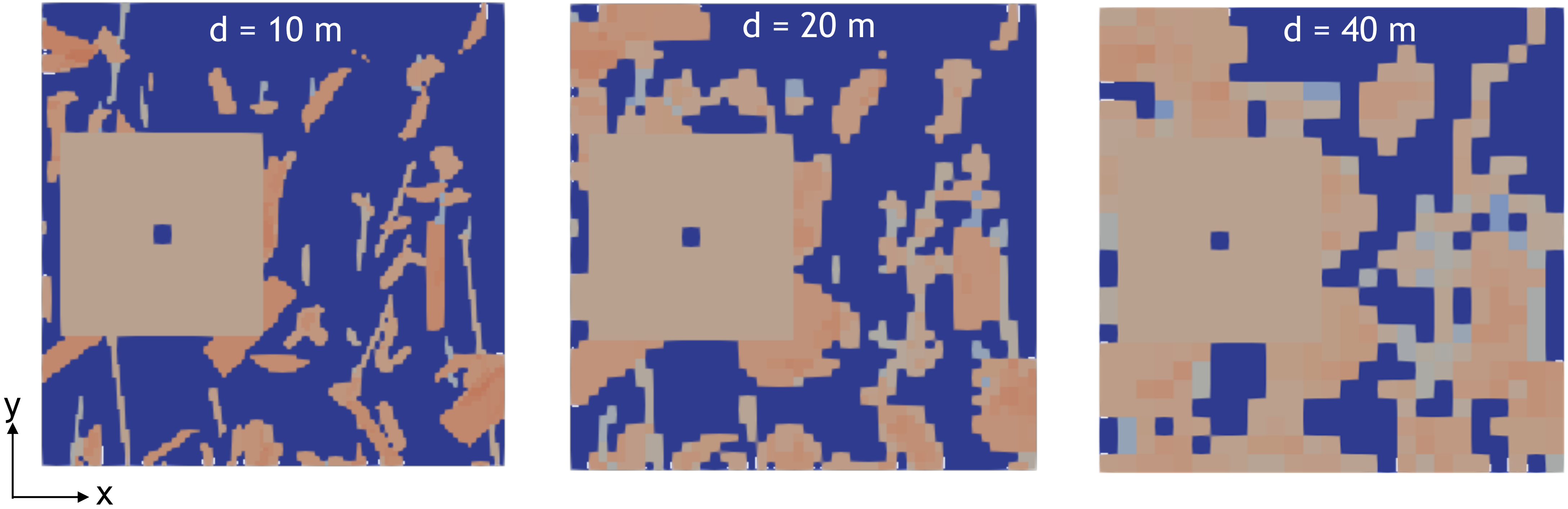
Domains generated using https://dfnworks.lanl.gov.

Simplified crystalline problem

- 1000 x 1000 x 500 m
- 1 waste package in buffer region
- Same underlying DFN statistics as production problem.
- Same QoIs as production problem.

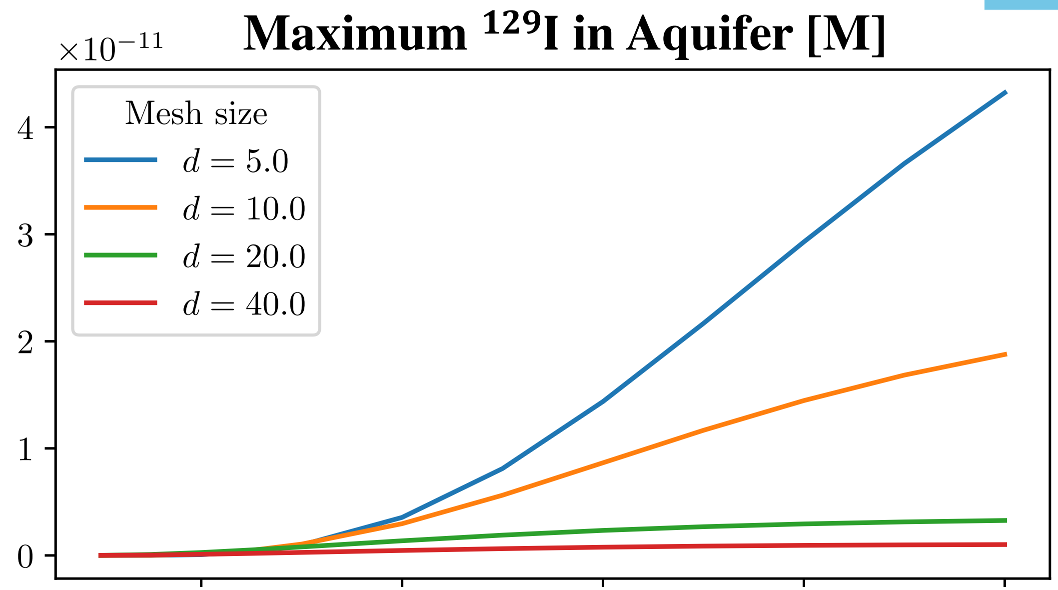


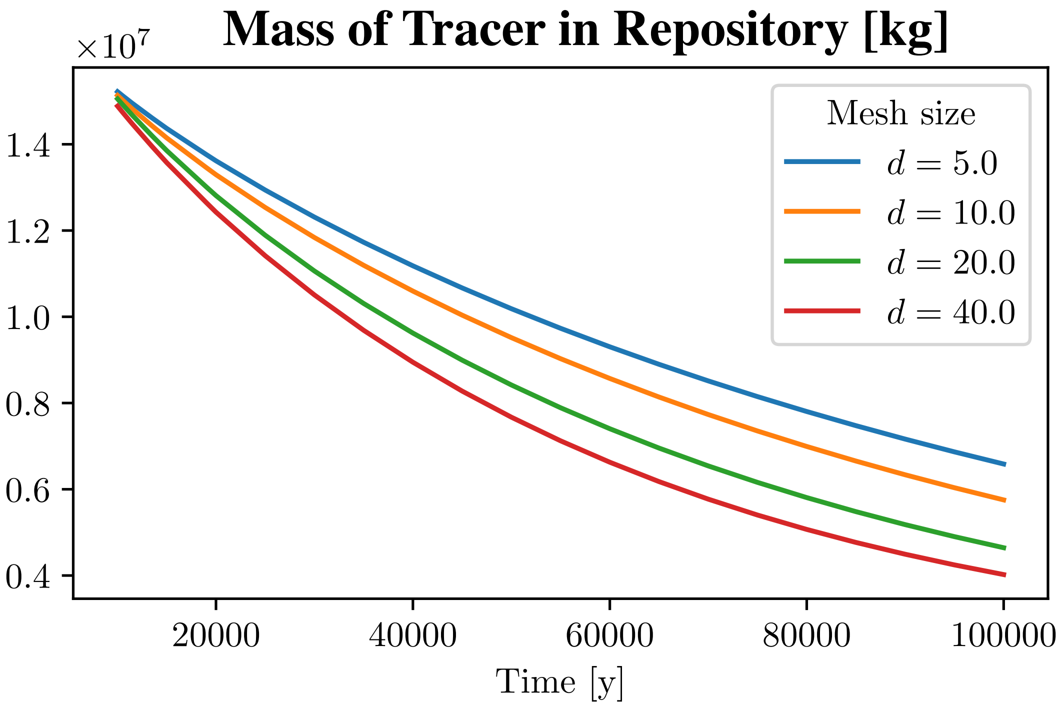
K_{xx} view from above:



Challenge: mesh dependence of quantities of interest (QoIs)

- Behavior of several QoIs converges as mesh is refined, but some do not.
- Max ^{129}I concentration in aquifer affected significantly by numerical diffusion/dispersion.
  - No correlation in location of max across meshes.
  - Some derived quantities depend on location of max.
- Mass in repository affected by increased flow from false connections in coarse mesh.
- Using the finest mesh we can afford.





Multifidelity Polynomial Chaos Expansion (MF PCE) for GSA

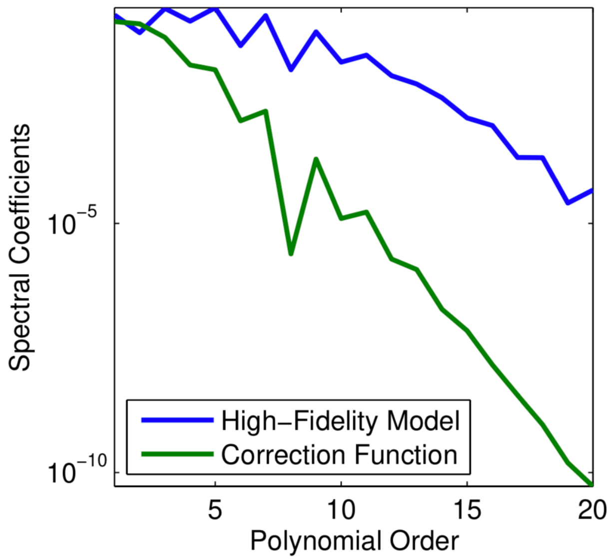
- Discrepancy-based, hierarchical multifidelity PCE (Ng, Eldred 2012).
- MF PCE coefficients can be recombined and used to compute Sobol indices in postprocessing (Sudret 2008).
- (R – model response; P – PCE expansion):

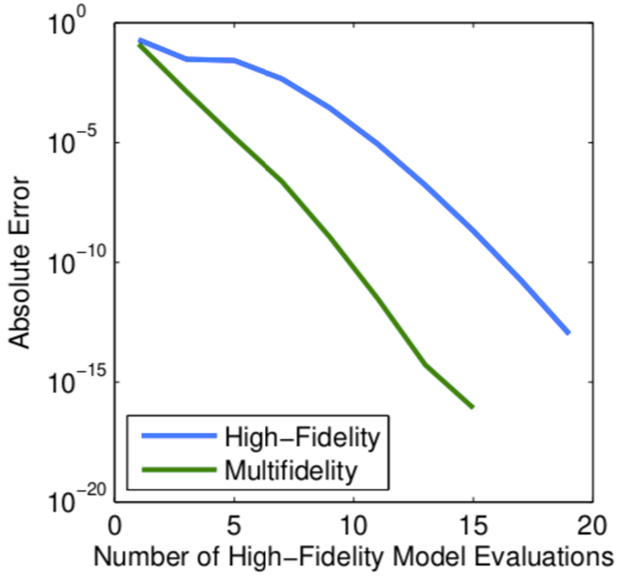
$$\begin{aligned} R_{10} &= R_{10} + (R_{20} - R_{20}) + (R_{40} - R_{40}) \\ &= R_{40} + (R_{20} - R_{40}) + (R_{10} - R_{20}) \\ &\approx P_{40} + (P_{20-40} + P_{10-20}) \end{aligned}$$

- If spectral content of $P_{10-20} \ll P_{10}$, need fewer 10 m evaluations to derive accurate expansion of R_{10}.
- In this case using a recursive approach to construct discrepancy PCE:

$$P_{20-40} \approx R_{20} - P_{40} \text{ rather than } \mathrm{P}_{20-40} \approx R_{20} - R_{40}.$$

- Random (MC) sampling + coefficients estimated with regression + cross validation for PCE order.
- Sampling and PCE construction performed with Dakota.





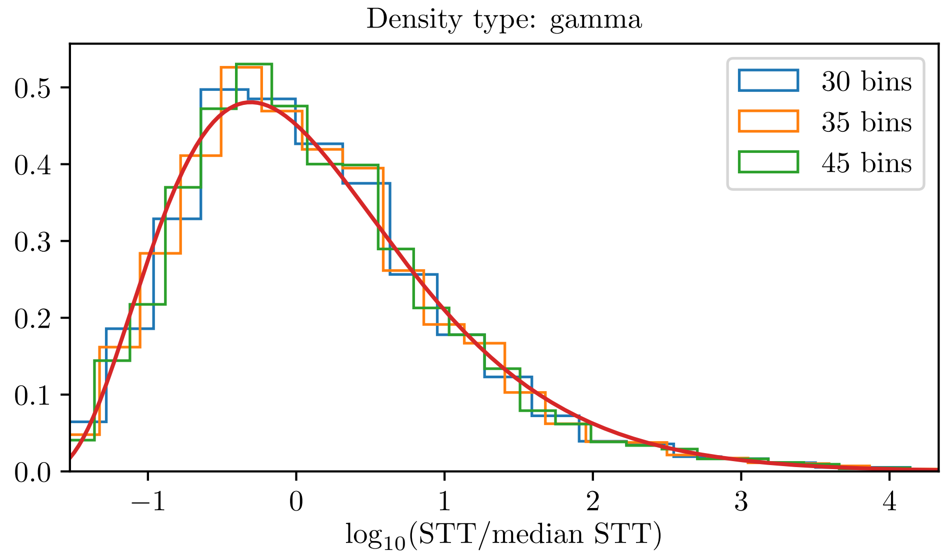
Characterizing subsurface uncertainty

- How do subsurface properties affect quantities of interest through GSA?
  - Can't impose subsurface properties directly-–have to compute them after generating a DFN.

- Compute proxy variables based on graph/network representation of each DFN (fractures = nodes, intersections = edges)
- Looked for proxy variables that were correlated with QoIs.
  - Number intersections with repository (NIwR)
  - Average degree (average number of intersections a fracture is part of)
  - Shortest travel time (STT) between repo and aquifer (rough approx. based on fracture area and pressure differentials)

- **These are derived quantities and therefore can't be prescribed by adaptive algorithms**; use regression.
  - Fitted analytical distributions for proxy variables from ~3000 sample DFNs.
  - Augment build point input space with proxy variables for each DFN

- **This is the first time we have been able to account for subsurface variability in GSA**
  - However, these are only proxies and cannot completely capture the induced variance from subsurface.



Preliminary multifidelity PCE study with subsurface uncertainty

- Each sample model evaluation was generated with a different DFN (different subsurface instantiation)
  - Input parameter space augmented with proxy variables
  - Constructed regression PCE over augmented input space

- Constructed PCE with 828 samples from 10 m model for comparison

- Hand-selected number of samples at d = 10, 20, and 40 for preliminary studies.

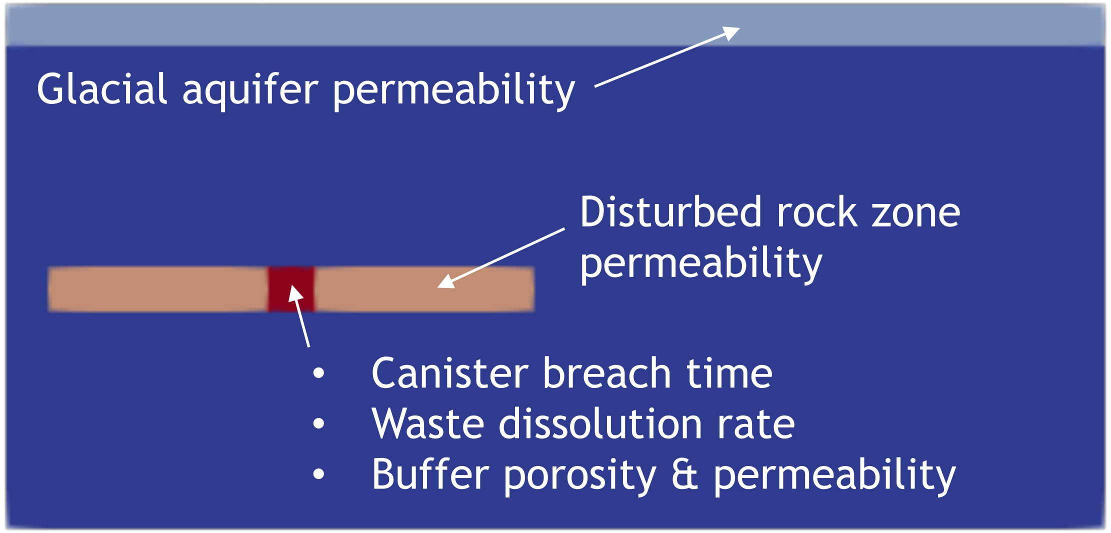
- Interested in potential benefits of augmenting small number of high-fidelity (HF) samples with samples from coarser meshes.

- Generated single-fidelity PCE with 18 HF samples.

- Generated multifidelity PCE augmenting HF samples with 828 samples from d = 20, d = 40.

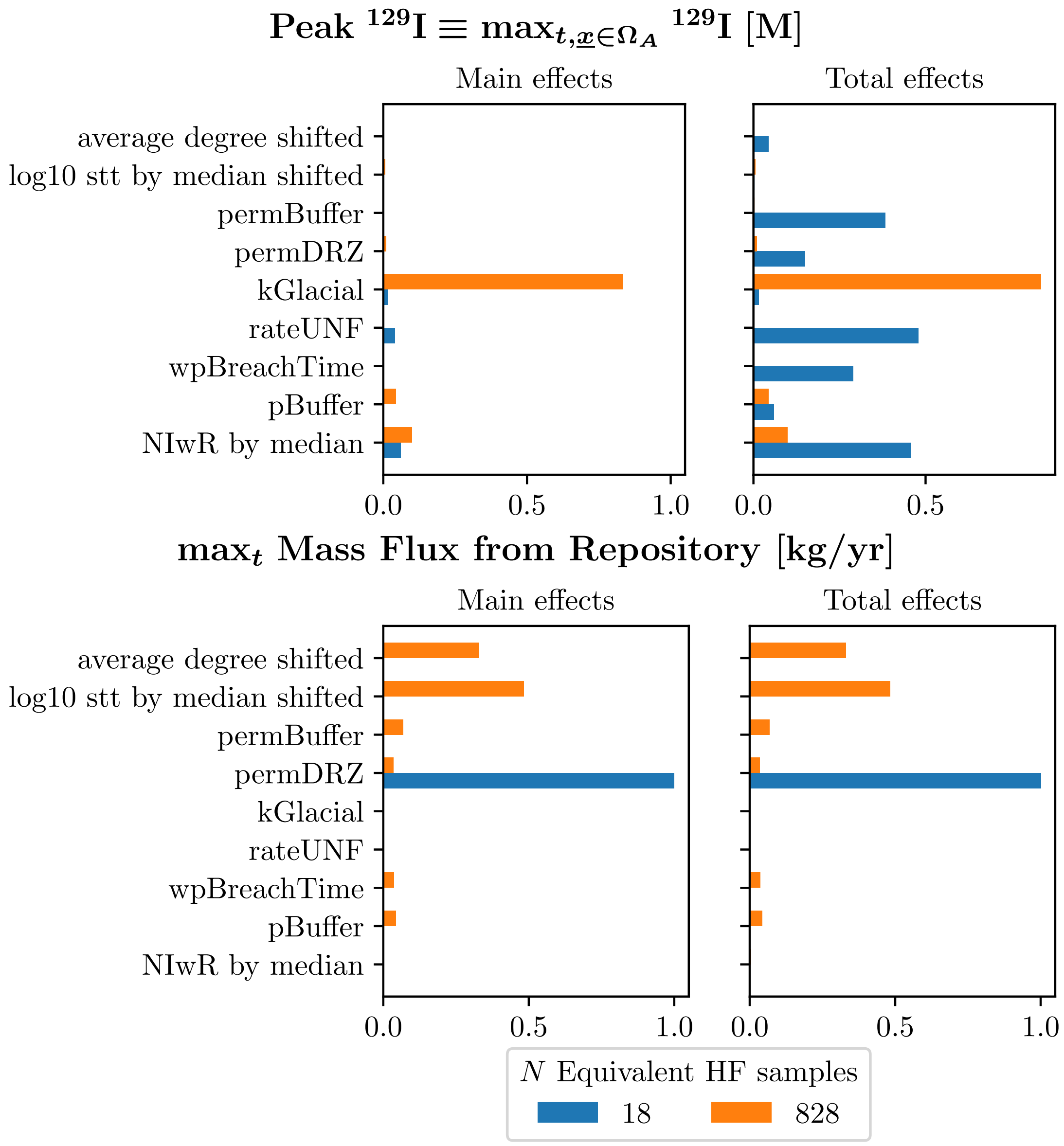
	d = 10	d = 20	d = 40
N samples	18	828	828
Relative costs	1	0.02	0.006

Uncertain parameters:

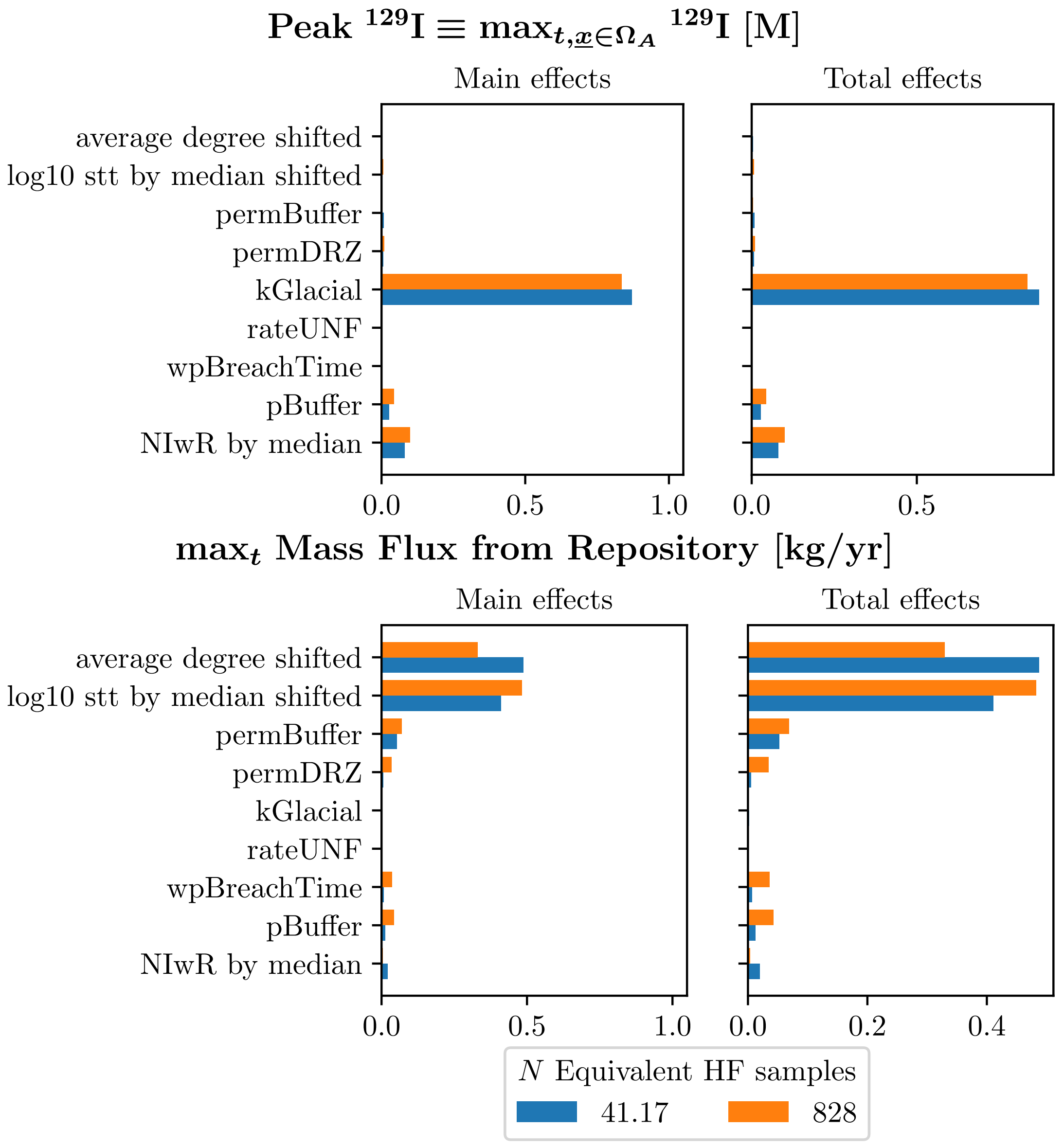


For all but the QOIs depending on location of peak ^{129}I, estimation of Sobol indices was drastically improved with the multifidelity PCE.

Single-fidelity PCE, HF model

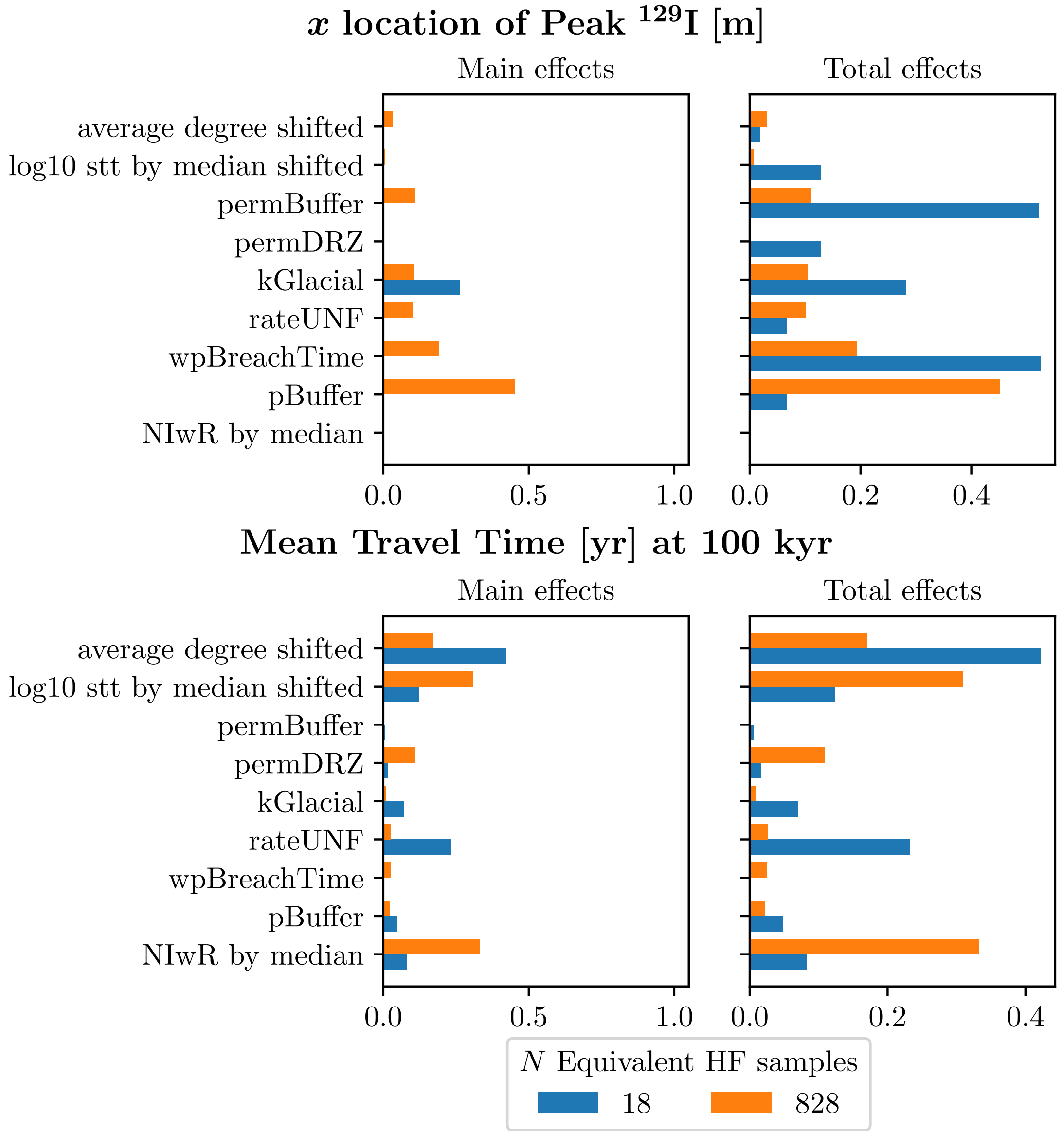


Multifidelity PCE

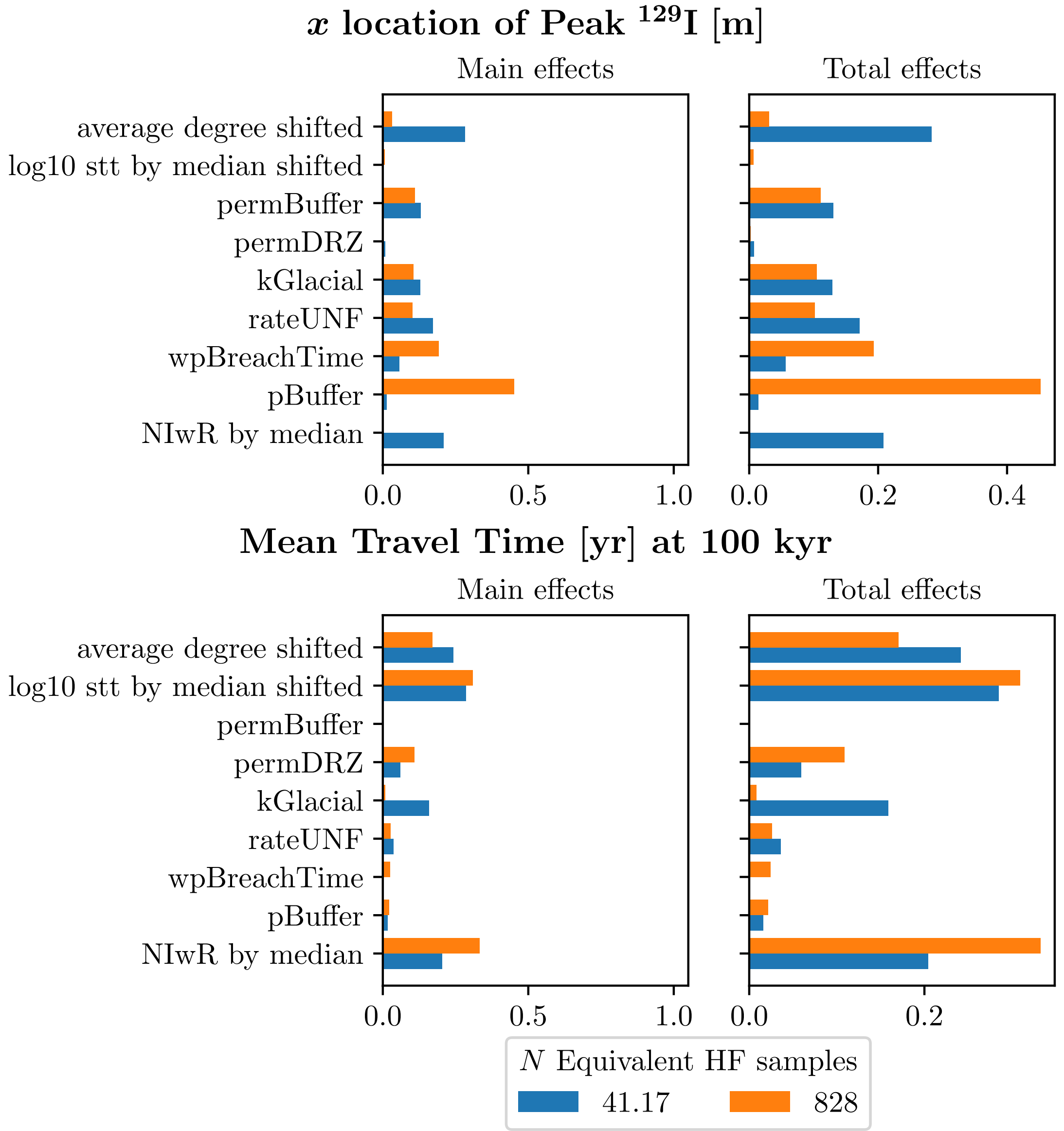


For QOIs depending on location of peak ^{129}I, multifidelity PCE Sobol indices were not significantly improved.

Single-fidelity PCE, HF model



Multifidelity PCE



Takeaways/future directions

- Overall, these results show there is promise in pursuing MF PCE for GSA in this problem.

- However, performance for QoIs depending significantly max ^{129}I location was poor.
  - Most important QoIs for performance assessment not fully settled yet; some of these QoIs may not factor into eventual performance assessment.

- Need to determine reasonable model hierarchy and reasonable QoIs.

- Challenge: how to take advantage of adaptive algorithms/optimize sample profiles in presence of proxy variables?
  - Optimal sample allocations for multifidelity approximation of Sobol indices with PCE – see Michael Merritt's talk later in the session!