



National
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Multifidelity Uncertainty Quantification in Stochastic Media Transport Problems

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MULTIFIDELITY UQ IN RADIATION TRANSPORT AND STOCHASTIC MEDIA

PLAN OF THE TALK



- MOTIVATION AND BACKGROUND
- MF UQ FOR MC RT (W/ STOCHASTIC MEDIA)
- NUMERICAL RESULTS
- CLOSING REMARKS

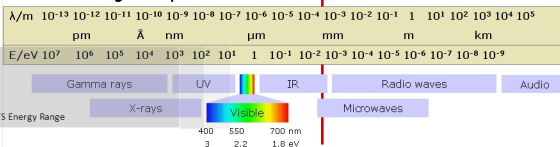
Motivation and background

UNCERTAINTY QUANTIFICATION FOR RADIATION TRANSPORT

CONTEXT AND CHALLENGES



The Electromagnetic Spectrum



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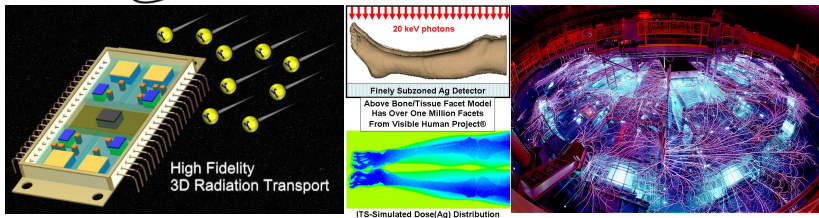


Figure: Courtesy of Brian Franke and Shawn Pautz

High-fidelity state-of-the-art modeling and simulations with HPC

- UQ under **severe** simulations **budget constraints**
- **Significant dimensionality** driven by model complexity

Few considerations on (MF) UQ for MC RT

- MC RT simulations are **expensive** → MF sampling UQ to **reduce the computational cost**
- MF UQ approaches **require correlation** among models
- MC RT are *truly* **stochastic solvers** → significant correlation can be obtained only by **collecting a large number of particle** histories (for accurate MC RT computations $\mathcal{O}(10^3 - 10^9)$)
- The MC RT **cost increases** with # of particle histories → we need to be able to estimate/treat the residual noise

MC RT from the physics/algorithmic perspective:

STEP 1: Use nuclear data to **sample** distance-to-collision event

STEP 2: **Sample** collision events based on cross section values

STEP 3: **Track** particle until it leaves the system

STEP 4: **Evaluate QoIs**, e.g. transmittance (# particles passing through the system)

UNCERTAINTY QUANTIFICATION FOR RADIATION TRANSPORT

FORWARD MF UQ WITH MONTE CARLO RT SOLVERS



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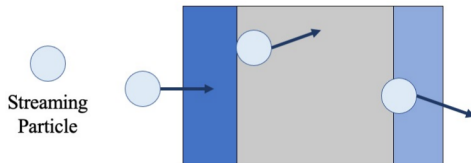


Figure: Courtesy of Kayla Clements.

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MC RT from the UQ perspective:

- **Uncertain parameters**, e.g. cross sections: $\xi \in \Xi \subset \mathbb{R}^d$
- **MC RT (internal) randomness**: $\eta \in H \subset \mathbb{R}^{d'}$
- **Particle histories** are interpreted as elementary events: $f = f(\xi, \eta)$
- **MC RT Qol**: Average of f over the histories for a fixed UQ parameters realization

$$Q(\xi) = \mathbb{E}_\eta [f(\xi, \eta)] \stackrel{MC RT}{\approx} \frac{1}{N_\eta} \sum_{j=1}^{N_\eta} f(\xi, \eta^{(j)}) \stackrel{\text{def}}{=} \tilde{Q}_{N_\eta}(\xi)$$

UQ GOAL: Compute statistics for $Q(\xi)$, e.g. mean $\mathbb{E}[Q]$ and $\text{Var}[Q]$, via sampling

Here, we focus on the MF UQ mean estimator¹

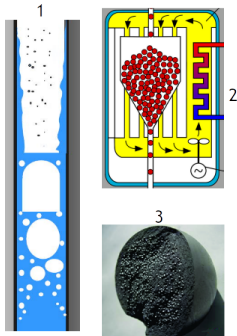
Challenge: $Q(\xi)$ is inaccessible: we can only observe $\tilde{Q}_{N_\eta}(\xi)$

¹Kayla C. Clements, G. Geraci, and Aaron J. Olson. "A Variance Deconvolution Approach to Sampling Uncertainty Quantification for Monte Carlo Radiation Transport Solvers". In: *Computer Science Research Institute Summer Proceedings 2021*. Technical Report SAND2022-0653R. 2021, pp. 293–307.

Stochastic media: materials whose internal structure is treated as random

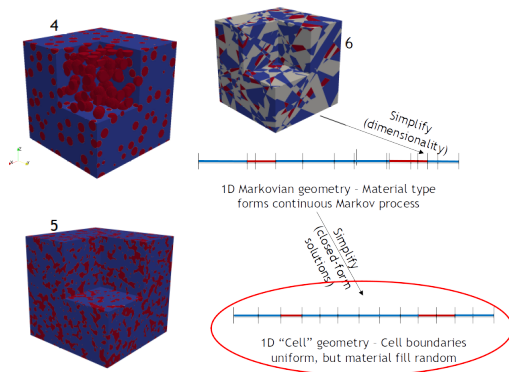
Real-world examples

- Two-phase flow in **Boiling Water Reactor** nuclear power coolant (1)
- **Pebble distribution** in Pebble-Bed nuclear power reactors (2)
- Distribution of **TRISO fuel** particles in Pebble-Bed pebble (3)
- Raleigh-Taylor **instabilities** in Inertial Confinement Fusion reactors
- **Accident scenarios** in various nuclear power reactor cores



Numerical approximations

- Spherical inclusions (4)
- Gaussian process (5)
- Markovian/Poisson (6)





MC RT (+ stochastic media) from the UQ perspective:

- **Uncertain parameters**, e.g. cross sections: $\xi \in \Xi \subset \mathbb{R}^d$
- **MC RT (internal) randomness**: $\eta \in H \subset \mathbb{R}^{d'}$
- **Material arrangements/realizations**: $\omega \in \Omega \subset \mathbb{R}^{d''}$
- **Particle histories** are interpreted as elementary events: $f = f(\xi, \omega, \eta)$
- **MC RT QoI**: Average of f over the histories with fixed UQ parameters realization and **material arrangements**

$$Q(\xi, \omega) = \mathbb{E}_{\eta} [f(\xi, \omega, \eta)] \stackrel{MC RT}{\approx} \frac{1}{N_{\eta}} \sum_{j=1}^{N_{\eta}} f(\xi, \omega, \eta^{(j)}) \stackrel{\text{def}}{=} \tilde{Q}_{N_{\eta}}(\xi, \omega)$$

We are interested in the statistics (i.e. mean) for the following quantity

$$\mathbb{P}_{\mathbb{E}}(\xi) \stackrel{\text{def}}{=} \mathbb{E}_{\omega} [Q(\xi, \omega)] \longrightarrow \boxed{\mathbb{E}_{\xi} [\mathbb{P}_{\mathbb{E}}(\xi)]}$$

MF UQ for MC RT (W/ stochastic media)

We want to compute

$$\mathbb{E}_{\xi} [\mathbb{P}_{\mathbb{E}}] \approx \frac{1}{N_{\xi}} \sum_{i=1}^{N_{\xi}} \mathbb{P}_{\mathbb{E}}(\xi^{(i)})$$

where

$$\mathbb{P}_{\mathbb{E}}(\xi^{(i)}) \stackrel{\text{def}}{=} \mathbb{E}_{\omega} [Q(\xi^{(i)}, \omega)] \approx \frac{1}{N_{\omega}} \sum_{k=1}^{N_{\omega}} Q(\xi^{(i)}, \omega^{(k)})$$

and

$$Q(\xi^{(i)}, \omega^{(k)}) \stackrel{\text{def}}{=} \mathbb{E}_{\eta} [f(\xi^{(i)}, \omega^{(k)}, \eta)] \approx \frac{1}{N_{\eta}} \sum_{j=1}^{N_{\eta}} f(\xi^{(i)}, \omega^{(k)}, \eta^{(j)}) \stackrel{\text{def}}{=} \tilde{Q}_{N_{\eta}}(\xi^{(i)}, \omega^{(k)})$$

Let's now use these definitions in reverse order

$$\mathbb{P}_{\mathbb{E}}(\xi^{(i)}) \approx \frac{1}{N_{\omega}} \sum_{k=1}^{N_{\omega}} \tilde{Q}_{N_{\eta}}(\xi^{(i)}, \omega^{(k)}) \stackrel{\text{def}}{=} \tilde{\mathbb{P}}_{N_{\omega}}^{\mathbb{E}}(\xi^{(i)})$$

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Let's consider a two-model MF UQ estimator

$$\mathbb{E}_{\xi} [\mathbb{P}_{\mathbb{E}}] \approx \left\langle \mathbb{P}_{\mathbb{E}}^{\text{HF}} \right\rangle_{N_{\xi}} + \alpha \left(\left\langle \mathbb{P}_{\mathbb{E}}^{\text{LF}} \right\rangle_{N_{\xi}} - \left\langle \mathbb{P}_{\mathbb{E}}^{\text{LF}} \right\rangle_{\tilde{r}N_{\xi}} \right) \stackrel{\text{def}}{=} \langle \mathbb{P}_{\mathbb{E}} \rangle_{N_{\xi}}^{\text{MF}}$$

The variance of this estimator is²

$$\text{Var} \left[\langle \mathbb{P}_{\mathbb{E}} \rangle_{N_{\xi}}^{\text{MF}} \right] = \text{Var} \left[\left\langle \mathbb{P}_{\mathbb{E}}^{\text{HF}} \right\rangle_{N_{\xi}} \right] \left(1 - \frac{\tilde{r} - 1}{\tilde{r}} \tilde{\rho}^2 \right),$$

where

$$\tilde{r} = \sqrt{\frac{\tilde{\rho}^2}{1 - \tilde{\rho}^2} \frac{\tilde{C}_{\text{HF}}}{\tilde{C}_{\text{LF}}}}$$

Remarks:

- The estimator variance $\text{Var} \left[\left\langle \mathbb{P}_{\mathbb{E}}^{\text{HF}} \right\rangle_{N_{\xi}} \right]$ depends on N_{ξ}, N_{ω} and N_{η}
- All quantities denoted by $\tilde{\cdot}$ are **polluted** by the finite number of samples N_{ω} and N_{η}

²L.W.T. Ng and K. Willcox. "Multifidelity Approaches for Optimization Under Uncertainty". In: *Int. J. Numer. Meth. Engng* 10 (2014), pp. 746–772.

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Q: How do we obtain an optimal MF UQ estimator for these problems?

Roadmap

STEP 1: Understand $\text{Var} \left[\left\langle \mathbb{P}_E^{\text{HF}} \right\rangle_{N_\xi} \right]$ dependence on N_ξ, N_ω and N_η

STEP 2: Take into account $\tilde{\rho}^2$ dependence on N_ω and N_η

STEP 3: Introduce cost models \tilde{C}_{HF} and \tilde{C}_{LF}

STEP 4: Take into account \tilde{r} dependence on N_ω and N_η

STEP 5: Quantify MF UQ estimator efficiency w.r.t MC

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$$\text{Var} \left[\tilde{\mathbb{P}}_{N\omega}^E \right] = \underbrace{\text{Var}_{\xi} [\mathbb{P}_E]}_{\text{Parametric variance}} + \underbrace{\mathbb{E}_{\xi} \left[\frac{\text{Var}_{\omega} [Q(\xi, \omega)]}{N_{\omega}} \right]}_{\text{Stochastic media}} + \underbrace{\mathbb{E}_{\xi} \left[\frac{\mathbb{E}_{\omega} [\sigma_{\eta}^2(\xi, \omega)]}{N_{\eta} N_{\omega}} \right]}_{\text{MC RT}}$$

Remarks³

- **Polluted** quantities are the only ones we can **directly measure**
- **Variance deconvolution:** remove noise from polluted variance $\text{Var} \left[\tilde{\mathbb{P}}_{N\omega}^E \right]$
- $\text{Var}_{\omega} [Q(\xi, \omega)]$ is also inaccessible, this requires another variance deconvolution
- MC RT contribution is

$$\sigma_{\eta}^2(\xi, \omega) = \text{Var}_{\eta} [f(\xi, \omega, \eta)]$$

³G. Geraci and Aaron J. Olson. "Deconvolution strategies for efficient parametric variance estimation in stochastic media transport problems". In: *ANS Transactions* (2022), pp. 279–282.

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Link between the polluted correlation $\tilde{\rho}^2$ and ρ^2

$$\tilde{\rho}^2 = \frac{\rho^2}{1 + \tau \rho^2}$$

where

$$\tau = \text{Var}_{\xi} \left[\mathbb{P}_{\text{E}}^{\text{HF}} \right] \gamma_{\text{LF}}(N_{\omega}^{\text{LF}}, N_{\eta}^{\text{LF}}) + \text{Var}_{\xi} \left[\mathbb{P}_{\text{E}}^{\text{LF}} \right] \gamma_{\text{HF}}(N_{\omega}^{\text{HF}}, N_{\eta}^{\text{HF}}) + \gamma_{\text{HF}}(N_{\omega}^{\text{HF}}, N_{\eta}^{\text{HF}}) \gamma_{\text{LF}}(N_{\omega}^{\text{LF}}, N_{\eta}^{\text{LF}})$$

represents the **stochastic solver noise effect**, which decreases ρ^2

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Let's introduce a **cost model**

- We account for the **re-sampling cost**, *i.e.* sampling more time the same configuration is less expensive

- We consider **three nested operations**

- UQ configuration C_ξ
- Stochastic media arrangement C_ω
- Particle histories C_η

- A **single fidelity estimator** will have a total cost of

$$\begin{aligned} C_{tot} &= N_\xi C_\xi + N_\xi (C_\omega N_\omega + C_\eta N_\omega N_\eta) \\ &= N_\xi \bar{C}(N_\omega, N_\eta), \quad \text{where } \bar{C}(N_\omega, N_\eta) = C_\xi + (C_\omega N_\omega + C_\eta N_\omega N_\eta) \end{aligned}$$

- For a **deterministic solver**

$$\bar{C}(1, 1) = C_\xi + C_\omega + C_\eta \stackrel{\text{def}}{=} \mathcal{C}$$

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$$\begin{aligned} C_{tot} &= N_\xi C_\xi + N_\xi (C_\omega N_\omega + C_\eta N_\omega N_\eta) \\ &= N_\xi \bar{C}(N_\omega, N_\eta), \quad \text{where} \quad \bar{C}(N_\omega, N_\eta) = C_\xi + (C_\omega N_\omega + C_\eta N_\omega N_\eta) \end{aligned}$$

- For a **deterministic solver**

$$\bar{C}(1, 1) = C_\xi + C_\omega + C_\eta \stackrel{\text{def}}{=} \mathcal{C}$$

Let's introduce a **cost model**

- We account for the **re-sampling cost**, *i.e.* sampling more time the same configuration is less expensive

- We consider **three nested operations**

- UQ configuration C_ξ
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$$\bar{C}(1, 1) = C_\xi + C_\omega + C_\eta \stackrel{\text{def}}{=} \mathcal{C}$$

Let's introduce a **cost model**

- We account for the **re-sampling cost**, *i.e.* sampling more time the same configuration is less expensive
- We consider **three nested operations**
 - UQ configuration \mathcal{C}_ξ
 - Stochastic media arrangement \mathcal{C}_ω
 - Particle histories \mathcal{C}_η
- A **single fidelity estimator** will have a total cost of

$$\begin{aligned} C_{tot} &= N_\xi \mathcal{C}_\xi + N_\xi (\mathcal{C}_\omega N_\omega + \mathcal{C}_\eta N_\omega N_\eta) \\ &= N_\xi \bar{\mathcal{C}}(N_\omega, N_\eta), \quad \text{where} \quad \bar{\mathcal{C}}(N_\omega, N_\eta) = \mathcal{C}_\xi + (\mathcal{C}_\omega N_\omega + \mathcal{C}_\eta N_\omega N_\eta) \end{aligned}$$

- For a **deterministic solver**

$$\bar{\mathcal{C}}(1, 1) = \mathcal{C}_\xi + \mathcal{C}_\omega + \mathcal{C}_\eta \stackrel{\text{def}}{=} \mathcal{C}$$

Let's introduce a **cost model**

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- A **single fidelity estimator** will have a total cost of

$$\begin{aligned}C_{tot} &= N_\xi C_\xi + N_\xi (C_\omega N_\omega + C_\eta N_\omega N_\eta) \\ &= N_\xi \tilde{C}(N_\omega, N_\eta), \quad \text{where} \quad \tilde{C}(N_\omega, N_\eta) = C_\xi + (C_\omega N_\omega + C_\eta N_\omega N_\eta)\end{aligned}$$

- For a **deterministic solver**

$$\tilde{C}(1, 1) = C_\xi + C_\omega + C_\eta \stackrel{\text{def}}{=} C$$

Let's introduce a **cost model**

- We account for the **re-sampling cost**, *i.e.* sampling more time the same configuration is less expensive
- We consider **three nested operations**
 - UQ configuration C_ξ
 - Stochastic media arrangement C_ω
 - Particle histories C_η

- A **single fidelity estimator** will have a total cost of

$$\begin{aligned} C_{tot} &= N_\xi C_\xi + N_\xi (C_\omega N_\omega + C_\eta N_\omega N_\eta) \\ &= N_\xi \tilde{C}(N_\omega, N_\eta), \quad \text{where} \quad \tilde{C}(N_\omega, N_\eta) = C_\xi + (C_\omega N_\omega + C_\eta N_\omega N_\eta) \end{aligned}$$

- For a **deterministic solver**

$$\tilde{C}(1, 1) = C_\xi + C_\omega + C_\eta \stackrel{\text{def}}{=} \mathcal{C}$$

Roadmap

STEP 1: Understand $\text{Var} \left[\left\langle \mathbb{P}_E^{\text{HF}} \right\rangle_{N_\xi} \right]$ dependence on N_ξ, N_ω and N_η

STEP 2: Take into account $\tilde{\rho}^2$ dependence on N_ω and N_η

STEP 3: Introduce cost models $\tilde{\mathcal{C}}_{\text{HF}}$ and $\tilde{\mathcal{C}}_{\text{LF}}$

STEP 4: Take into account \tilde{r} dependence on N_ω and N_η

STEP 5: Quantify MF UQ estimator efficiency w.r.t MC

Optimal **oversampling ratio**: $\tilde{r} = \sqrt{\frac{\tilde{\rho}^2}{1 - \tilde{\rho}^2} \frac{\tilde{C}_{\text{HF}}}{\tilde{C}_{\text{LF}}}}$

Let's introduce the **polluted terms** $\tilde{\rho}^2$, \tilde{C}_{HF} and \tilde{C}_{LF} (generalization of⁴)

- $\tilde{C}_{\text{HF}} = c_{\xi}^{\text{HF}} + c_{\omega}^{\text{HF}} N_{\omega}^{\text{HF}} + c_{\eta}^{\text{HF}} N_{\eta}^{\text{HF}} = c_{\xi}^{\text{HF}} + c_{\omega, \eta}^{\text{HF}} (N_{\omega}^{\text{HF}}, N_{\eta}^{\text{HF}})$
- $\tilde{C}_{\text{LF}} = c_{\xi}^{\text{LF}} + c_{\omega}^{\text{LF}} N_{\omega}^{\text{LF}} + c_{\eta}^{\text{LF}} N_{\eta}^{\text{LF}} = c_{\xi}^{\text{LF}} + c_{\omega, \eta}^{\text{LF}} (N_{\omega}^{\text{LF}}, N_{\eta}^{\text{LF}})$

$$\tilde{r} = \underbrace{\sqrt{\frac{\rho^2}{1 - \rho^2} \frac{C_{\text{HF}}}{C_{\text{LF}}}}}_{r: \text{unpolluted oversampling ratio}} \underbrace{\sqrt{\frac{1 - \rho^2}{1 - \rho^2 + \tau \rho^2} \frac{1 - \frac{c_{\omega}^{\text{HF}} + c_{\eta}^{\text{HF}}}{C_{\text{HF}}} + \frac{c_{\omega, \eta}^{\text{HF}}}{C_{\text{HF}}}}{1 - \frac{c_{\omega}^{\text{LF}} + c_{\eta}^{\text{LF}}}{C_{\text{LF}}} + \frac{c_{\omega, \eta}^{\text{LF}}}{C_{\text{LF}}}}}}_{R(N_{\omega}^{\text{HF}}, N_{\eta}^{\text{HF}}, N_{\omega}^{\text{LF}}, N_{\eta}^{\text{LF}}): \text{stochastic solver contribution}}$$

⁴G. Geraci, L.P. Swiler, and B.J. Debusschere. "Multifidelity UQ Sampling for Stochastic Simulations". In: *16th U.S. National Congress on Computational Mechanics* (2021).

Roadmap

STEP 1: Understand $\text{Var} \left[\left\langle \mathbb{P}_E^{\text{HF}} \right\rangle_{N_\xi} \right]$ dependence on N_ξ, N_ω and N_η

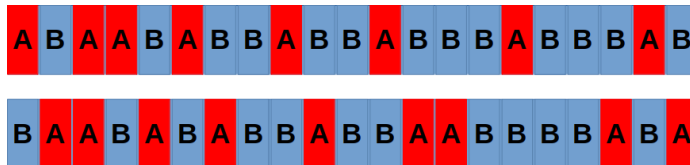
STEP 2: Take into account $\tilde{\rho}^2$ dependence on N_ω and N_η

STEP 3: Introduce cost models $\tilde{\mathcal{C}}_{\text{HF}}$ and $\tilde{\mathcal{C}}_{\text{LF}}$

STEP 4: Take into account \tilde{r} dependence on N_ω and N_η

STEP 5: Quantify MF UQ estimator efficiency w.r.t MC

Numerical results



- 1D slab, neutral particle, **absorption-only** mono-energetic steady state radiation transport
- Normally incident beam with unitary magnitude
- **Random cross sections** ($m = A, B$): $\Sigma_{t,m}(\xi_m) = \Sigma_{t,m}^0 + \Sigma_{t,m}^\Delta \xi_m$, where $\xi_A, \xi_B \sim \mathcal{U}(-1, 1)$
- The **QoI** is the **transmittance**

Analytical solution:

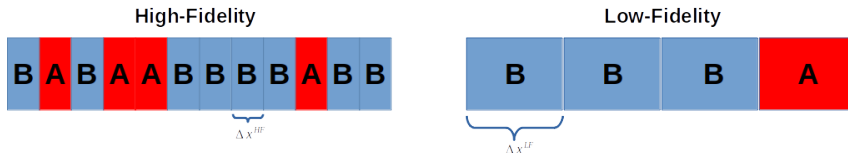
Transmittance: $T(\xi, \omega) = \exp[-\tau(\xi, \omega)]$, where

Slab optical thickness: $\tau(\xi, \omega) = \Delta x (N_A(\omega)\Sigma_{t,A}(\xi_A) + N_B(\omega)\Sigma_{t,B}(\xi_B))$

NOTE: $N_A(\omega) \sim \mathcal{B}(N_{tot}, P_A)$, where $N_A(\omega) + N_B(\omega) = N_{tot}$

1D MC RT FOR STOCHASTIC MEDIA WITH UNCERTAIN PROPERTIES

MULTIFIDELITY ANALYSIS SCENARIO



Material	$\Sigma_{t,m}^0$ [cm ⁻¹]	$\Sigma_{t,m}^\Delta$ [cm ⁻¹]	p_m
A	1.0	0.95	0.3
B	0.4	0.25	0.7

TABLE: Material properties

Model	N_{tot}	Δx [cm]	C_ξ	C_ω	C_η	C
HF	50	1.0	1.0	0.5	0.01	1.51
LF	10	5.0	0.02	0.01	0.001	0.031

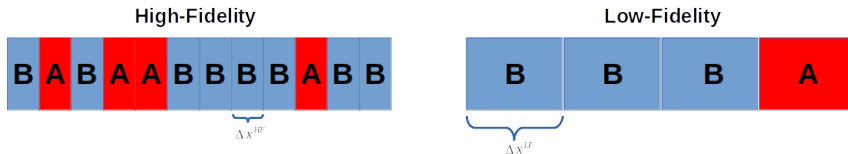
TABLE: Model configuration – $C_{HF}/C_{LF} = 48.71$

Two analysis scenarios:

- First – HF dataset assigned, i.e. N_ω^{HF} and N_η^{HF} are assigned
- Second – Stochastic media configurations assigned for both models, i.e. N_ω^{HF} and N_ω^{LF} are assigned

1D MC RT FOR STOCHASTIC MEDIA WITH UNCERTAIN PROPERTIES

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Material	$\Sigma_{t,m}^0$ [cm ⁻¹]	$\Sigma_{t,m}^\Delta$ [cm ⁻¹]	p_m
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TABLE: Model configuration – $C_{HF}/C_{LF} = 48.71$

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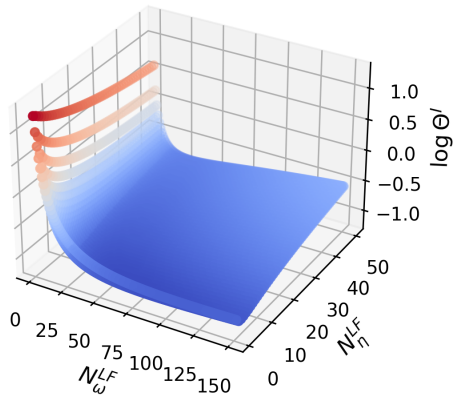
NUMERICAL RESULTS

COST REDUCTION COMPARED TO MC (3D VIEW)



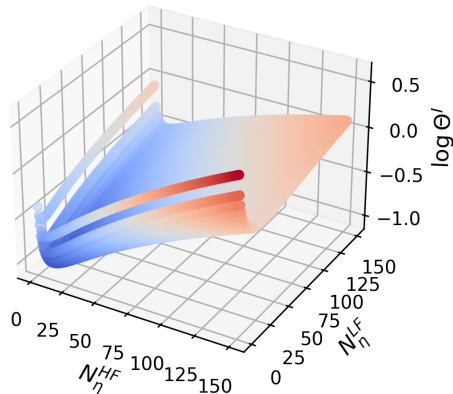
Scenario 1: HF dataset assigned – $N_{\omega}^{HF} = 10$ and $N_{\eta}^{HF} = 15$

$$\Theta^I \text{ -- } (N_{\omega}^{HF}, N_{\eta}^{HF}) = (10, 15)$$



Scenario 2: Stoch media assigned – $N_{\omega}^{HF} = 10$ and $N_{\omega}^{LF} = 25$

$$\Theta^I \text{ -- } (N_{\omega}^{HF}, N_{\omega}^{LF}) = (10, 25)$$

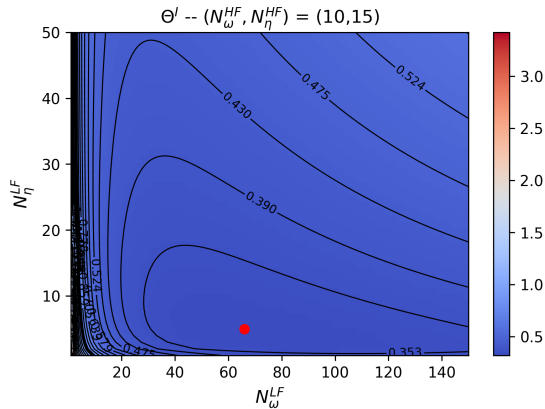


NUMERICAL RESULTS

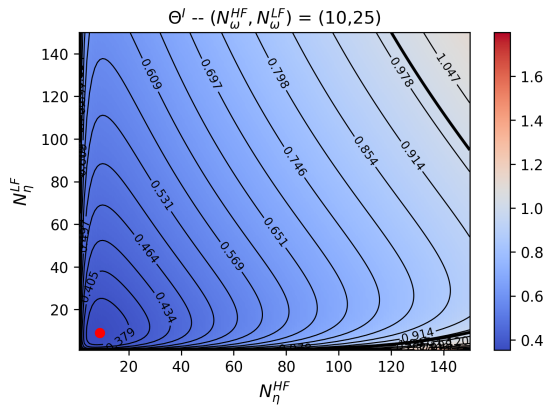
COST REDUCTION COMPARED TO MC (CONTOUR PLOT)



Scenario 1: HF dataset assigned – $N_{\omega}^{\text{HF}} = 10$ and $N_{\eta}^{\text{HF}} = 15$



Scenario 2: Stoch media assigned – $N_{\omega}^{\text{HF}} = 10$ and $N_{\omega}^{\text{LF}} = 25$





Closing remarks



Summary

- Radiation transport methods can **benefit from MF UQ**
- Deploying **MF UQ for stochastic solvers** is more **challenging** than for deterministic solvers
- Stochastic **noise needs to be optimally controlled** to preserve MF UQ performance

Talk's contributions

- Formulation for **MF UQ applied to MC RT** problems
- **Stochastic media** effect explicitly included
- Cost model extended to include **re-sampling cost**
- **Verification** exact solution for MF UQ with **binary mixing**

Next steps

- Extension to a realistic deployment (**from pilot samples** to statistics estimation)
- Extension to **multiple models** (e.g. leveraging Approximate Control Variate⁵, etc.)
- Extension to **high-order statistics**

⁵A. Gorodetsky et al. "A generalized approximate control variate framework for multifidelity uncertainty quantification". In: *Journal of Computational Physics* 408 (2020).

THANKS!



Acknowledgements

- Kayla Clements (Oregon State University and SNL)
- Bryan Reuter and Tim Wildey (SNL)

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Kayla C. Clements, G. Geraci, and Aaron J. Olson. "A Variance Deconvolution Approach to Sampling Uncertainty Quantification for Monte Carlo Radiation Transport Solvers". In: *Computer Science Research Institute Summer Proceedings 2021*. Technical Report SAND2022-0653R. 2021, pp. 293–307.



G. Geraci and Aaron J. Olson. "Deconvolution strategies for efficient parametric variance estimation in stochastic media transport problems". In: *ANS Transactions* (2022), pp. 279–282.



G. Geraci, L.P. Swiler, and B.J. Debusschere. "Multifidelity UQ Sampling for Stochastic Simulations". In: *16th U.S. National Congress on Computational Mechanics* (2021).



A. Gorodetsky et al. "A generalized approximate control variate framework for multifidelity uncertainty quantification". In: *Journal of Computational Physics* 408 (2020).



L.W.T. Ng and K. Willcox. "Multifidelity Approaches for Optimization Under Uncertainty". In: *Int. J. Numer. Meth. Engng* 10 (2014), pp. 746–772.



BACKUP SLIDES

$$\mathbb{V}ar \left[\left\langle \mathbb{P}_{\mathbb{E}}^{\text{HF}} \right\rangle_{N_{\xi}} \right] = \mathbb{V}ar \left[\frac{1}{N_{\xi}} \sum_{i=1}^{N_{\xi}} \tilde{\mathbb{P}}_{N_{\omega}}^{\mathbb{E}, \text{HF}}(\xi^{(i)}) \right] = \frac{1}{N_{\xi}} \textcolor{red}{\mathbb{V}ar} \left[\tilde{\mathbb{P}}_{N_{\omega}}^{\mathbb{E}, \text{HF}} \right]$$

Law-of-total variance

$$\textcolor{red}{\mathbb{V}ar} \left[\tilde{\mathbb{P}}_{N_{\omega}}^{\mathbb{E}, \text{HF}} \right] = \mathbb{V}ar_{\xi} \left[\mathbb{E}_{\eta, \omega} \left[\tilde{\mathbb{P}}_{N_{\omega}}^{\mathbb{E}, \text{HF}} \right] \right] + \mathbb{E}_{\xi} \left[\textcolor{teal}{\mathbb{V}ar}_{\eta, \omega} \left[\tilde{\mathbb{P}}_{N_{\omega}}^{\mathbb{E}, \text{HF}} \right] \right]$$

By applying, once again, the law-of-total variance we get

$$\textcolor{teal}{\mathbb{V}ar}_{\eta, \omega} \left[\tilde{\mathbb{P}}_{N_{\omega}}^{\mathbb{E}} \right] = \frac{\mathbb{V}ar_{\omega} [Q(\xi, \omega)]}{N_{\omega}} + \frac{\mathbb{E}_{\omega} \left[\sigma_{\eta}^2(\xi, \omega) \right]}{N_{\omega} N_{\eta}}$$

which leads to the final estimator variance

$$\textcolor{red}{\mathbb{V}ar} \left[\tilde{\mathbb{P}}_{N_{\omega}}^{\mathbb{E}} \right] = \mathbb{V}ar_{\xi} [\mathbb{P}_{\mathbb{E}}] + \mathbb{E}_{\xi} \left[\frac{\mathbb{V}ar_{\omega} [Q(\xi, \omega)]}{N_{\omega}} \right] + \mathbb{E}_{\xi} \left[\frac{\mathbb{E}_{\omega} \left[\sigma_{RT, N_{\eta}}^2(\xi, \omega) \right]}{N_{\omega}} \right]$$

$$\mathbb{V}ar \left[\left\langle \mathbb{P}_{\mathbb{E}}^{\text{HF}} \right\rangle_{N_{\xi}} \right] = \mathbb{V}ar \left[\frac{1}{N_{\xi}} \sum_{i=1}^{N_{\xi}} \tilde{\mathbb{P}}_{N_{\omega}}^{\mathbb{E}, \text{HF}}(\xi^{(i)}) \right] = \frac{1}{N_{\xi}} \mathbb{V}ar \left[\tilde{\mathbb{P}}_{N_{\omega}}^{\mathbb{E}, \text{HF}} \right]$$

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$$\mathbb{V}ar \left[\tilde{\mathbb{P}}_{N_{\omega}}^{\mathbb{E}} \right] = \mathbb{V}ar_{\xi} [\mathbb{P}_{\mathbb{E}}] + \mathbb{E}_{\xi} \left[\frac{\mathbb{V}ar_{\omega} [Q(\xi, \omega)]}{N_{\omega}} \right] + \mathbb{E}_{\xi} \left[\frac{\mathbb{E}_{\omega} \left[\sigma_{RT, N_{\eta}}^2(\xi, \omega) \right]}{N_{\omega}} \right]$$

$$\mathbb{V}ar \left[\left\langle \mathbb{P}_{\mathbb{E}}^{\text{HF}} \right\rangle_{N_{\xi}} \right] = \mathbb{V}ar \left[\frac{1}{N_{\xi}} \sum_{i=1}^{N_{\xi}} \tilde{\mathbb{P}}_{N_{\omega}}^{\mathbb{E}, \text{HF}}(\xi^{(i)}) \right] = \frac{1}{N_{\xi}} \textcolor{red}{\mathbb{V}ar} \left[\tilde{\mathbb{P}}_{N_{\omega}}^{\mathbb{E}, \text{HF}} \right]$$

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$$\textcolor{red}{\mathbb{V}ar} \left[\tilde{\mathbb{P}}_{N_{\omega}}^{\mathbb{E}, \text{HF}} \right] = \mathbb{V}ar_{\xi} \left[\mathbb{E}_{\eta, \omega} \left[\tilde{\mathbb{P}}_{N_{\omega}}^{\mathbb{E}, \text{HF}} \right] \right] + \mathbb{E}_{\xi} \left[\textcolor{teal}{\mathbb{V}ar}_{\eta, \omega} \left[\tilde{\mathbb{P}}_{N_{\omega}}^{\mathbb{E}, \text{HF}} \right] \right]$$

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which leads to the final estimator variance

$$\textcolor{red}{\mathbb{V}ar} \left[\tilde{\mathbb{P}}_{N_{\omega}}^{\mathbb{E}} \right] = \textcolor{green}{\mathbb{V}ar}_{\xi} [\mathbb{P}_{\mathbb{E}}] + \mathbb{E}_{\xi} \left[\frac{\mathbb{V}ar_{\omega} [Q(\xi, \omega)]}{N_{\omega}} \right] + \mathbb{E}_{\xi} \left[\frac{\mathbb{E}_{\omega} \left[\sigma_{RT, N_{\eta}}^2(\xi, \omega) \right]}{N_{\omega}} \right]$$

$$\tilde{\rho}^2 = \frac{\text{Cov}^2\left(\tilde{\mathbb{P}}_{N_\omega}^{\text{E,HF}}, \tilde{\mathbb{P}}_{N_\omega}^{\text{E,LF}}\right)}{\text{Var}\left[\tilde{\mathbb{P}}_{N_\omega}^{\text{E,HF}}\right] \text{Var}\left[\tilde{\mathbb{P}}_{N_\omega}^{\text{E,LF}}\right]}$$

Properties:

- **Law-of-total covariance:** $\text{Cov}\left[\tilde{\mathbb{P}}_{N_\omega}^{\text{E,HF}}, \tilde{\mathbb{P}}_{N_\omega}^{\text{E,LF}}\right] = \mathbb{E}_\xi \left[\text{Cov}_{\omega, \eta} \left[\tilde{\mathbb{P}}_{N_\omega}^{\text{E,HF}}, \tilde{\mathbb{P}}_{N_\omega}^{\text{E,LF}} \right] \right] + \text{Cov}_\xi \left[\mathbb{E}_{\xi, \omega} \left[\tilde{\mathbb{P}}_{N_\omega}^{\text{E,HF}} \right], \mathbb{E}_{\xi, \omega} \left[\tilde{\mathbb{P}}_{N_\omega}^{\text{E,LF}} \right] \right]$
- All **estimators are unbiased**, e.g. $\mathbb{E}_\omega \left[\tilde{\mathbb{P}}_{N_\omega}^{\text{E,HF}} \right] = \mathbb{P}_\text{E}^{\text{HF}}$
- ω and η for HF and LF variables are independent

$$\tilde{\rho}^2 = \frac{\left(\text{Cov}_\xi \left[\mathbb{P}_\text{E}^{\text{HF}}, \mathbb{P}_\text{E}^{\text{LF}} \right] \right)^2}{\left(\text{Var}_\xi \left[\mathbb{P}_\text{E}^{\text{HF}} \right] + \gamma_{\text{HF}}(N_\omega^{\text{HF}}, N_\eta^{\text{HF}}) \right) \left(\text{Var}_\xi \left[\mathbb{P}_\text{E}^{\text{LF}} \right] + \gamma_{\text{LF}}(N_\omega^{\text{LF}}, N_\eta^{\text{LF}}) \right)}$$

$$\gamma_{\text{HF}} = \mathbb{E}_\xi \left[\frac{\text{Var}_\omega \left[Q^{\text{HF}}(\xi, \omega) \right]}{N_\omega^{\text{HF}}} \right] + \mathbb{E}_\xi \left[\frac{\mathbb{E}_\omega \left[\sigma_\eta^2(\xi, \omega) \right]}{N_\omega^{\text{HF}} N_\eta^{\text{HF}}} \right]$$

$$\gamma_{\text{LF}} = \mathbb{E}_\xi \left[\frac{\text{Var}_\omega \left[Q^{\text{LF}}(\xi, \omega) \right]}{N_\omega^{\text{LF}}} \right] + \mathbb{E}_\xi \left[\frac{\mathbb{E}_\omega \left[\sigma_\eta^2(\xi, \omega) \right]}{N_\omega^{\text{LF}} N_\eta^{\text{LF}}} \right]$$

$$\tilde{\rho}^2 = \frac{\text{Cov}^2(\tilde{\mathbb{P}}_{N_\omega}^{\text{E},\text{HF}}, \tilde{\mathbb{P}}_{N_\omega}^{\text{E},\text{LF}})}{\text{Var}[\tilde{\mathbb{P}}_{N_\omega}^{\text{E},\text{HF}}] \text{Var}[\tilde{\mathbb{P}}_{N_\omega}^{\text{E},\text{LF}}]}$$

Properties:

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- ω and η for HF and LF variables are independent

$$\tilde{\rho}^2 = \frac{(\text{Cov}_\xi[\mathbb{P}_\text{E}^{\text{HF}}, \mathbb{P}_\text{E}^{\text{LF}}])^2}{(\text{Var}_\xi[\mathbb{P}_\text{E}^{\text{HF}}] + \gamma_{\text{HF}}(N_\omega^{\text{HF}}, N_\eta^{\text{HF}})) (\text{Var}_\xi[\mathbb{P}_\text{E}^{\text{LF}}] + \gamma_{\text{LF}}(N_\omega^{\text{LF}}, N_\eta^{\text{LF}}))}$$

$$\gamma_{\text{HF}} = \mathbb{E}_\xi \left[\frac{\text{Var}_\omega[Q^{\text{HF}}(\xi, \omega)]}{N_\omega^{\text{HF}}} \right] + \mathbb{E}_\xi \left[\frac{\mathbb{E}_\omega[\sigma_\eta^2(\xi, \omega)]}{N_\omega^{\text{HF}} N_\eta^{\text{HF}}} \right]$$

$$\gamma_{\text{LF}} = \mathbb{E}_\xi \left[\frac{\text{Var}_\omega[Q^{\text{LF}}(\xi, \omega)]}{N_\omega^{\text{LF}}} \right] + \mathbb{E}_\xi \left[\frac{\mathbb{E}_\omega[\sigma_\eta^2(\xi, \omega)]}{N_\omega^{\text{LF}} N_\eta^{\text{LF}}} \right]$$

Cost ratio w.r.t. MC for same estimator variance ε_{target}^2

• MF UQ cost allocation

$$N_{\xi}^{MF} = \frac{\text{Var} \left[\tilde{\varepsilon}_{N_{\omega}}^{2, HF} \right] (N_{\omega}^{HF}, N_{\eta}^{HF})}{\varepsilon_{target}^2} \left(1 - \frac{rR - 1}{rR} \frac{\rho^2}{1 + \tau \rho^2} \right)$$

$$C_{tot}^{MF} = N_{\xi}^{MF} \tilde{C}_{HF} + N_{\xi}^{MF} rR \tilde{C}_{LF}$$

$$= N_{\xi}^{MF} C_{HF} \left(\left(1 - \frac{C_{\omega}^{HF} + C_{\eta}^{HF}}{C_{HF}} + \frac{C_{\omega, \eta}^{HF}}{C_{HF}} \right) + rR \frac{C_{LF}}{C_{HF}} \left(1 - \frac{C_{\omega}^{LF} + C_{\eta}^{LF}}{C_{LF}} + \frac{C_{\omega, \eta}^{LF}}{C_{LF}} \right) \right)$$

• MC cost allocation

$$N_{\xi}^{MC} = \frac{\text{Var} \left[\tilde{\varepsilon}_{N_{\omega}}^{2, HF} \right] (N_{\omega}^{HF}, N_{\eta}^{HF})}{\varepsilon_{target}^2}$$

$$C_{tot}^{MC} = N_{\xi}^{MC} \tilde{C}_{HF} = N_{\xi}^{MC} C_{HF} \left(1 - \frac{C_{\omega}^{HF} + C_{\eta}^{HF}}{C_{HF}} + \frac{C_{\omega, \eta}^{HF}}{C_{HF}} \right)$$

Cost ratio w.r.t. MC for same estimator variance ε_{target}^2

• **MF UQ** cost allocation

$$N_{\xi}^{MF} = \frac{\text{Var} \left[\tilde{\mathbb{P}}_{N_{\omega}}^{\mathbb{E}, \text{HF}} \right] (N_{\omega}^{\text{HF}}, N_{\eta}^{\text{HF}})}{\varepsilon_{target}^2} \left(1 - \frac{rR - 1}{rR} \frac{\rho^2}{1 + \tau \rho^2} \right)$$

$$C_{tot}^{MF} = N_{\xi}^{MF} \tilde{C}_{\text{HF}} + N_{\xi}^{MF} rR \tilde{C}_{\text{LF}}$$

$$= N_{\xi}^{MF} C_{\text{HF}} \left(\left(1 - \frac{C_{\omega}^{\text{HF}} + C_{\eta}^{\text{HF}}}{C_{\text{HF}}} + \frac{C_{\omega, \eta}^{\text{HF}}}{C_{\text{HF}}} \right) + rR \frac{C_{\text{LF}}}{C_{\text{HF}}} \left(1 - \frac{C_{\omega}^{\text{LF}} + C_{\eta}^{\text{LF}}}{C_{\text{LF}}} + \frac{C_{\omega, \eta}^{\text{LF}}}{C_{\text{LF}}} \right) \right)$$

• **MC** cost allocation

$$N_{\xi}^{MC} = \frac{\text{Var} \left[\tilde{\mathbb{P}}_{N_{\omega}}^{\mathbb{E}, \text{HF}} \right] (N_{\omega}^{\text{HF}}, N_{\eta}^{\text{HF}})}{\varepsilon_{target}^2}$$

$$C_{tot}^{MC} = N_{\xi}^{MC} \tilde{C}_{\text{HF}} = N_{\xi}^{MC} C_{\text{HF}} \left(1 - \frac{C_{\omega}^{\text{HF}} + C_{\eta}^{\text{HF}}}{C_{\text{HF}}} + \frac{C_{\omega, \eta}^{\text{HF}}}{C_{\text{HF}}} \right)$$

Cost ratio w.r.t. MC for same estimator variance ε_{target}^2

• **MF UQ** cost allocation

$$N_{\xi}^{MF} = \frac{\text{Var} \left[\tilde{\mathbb{P}}_{N_{\omega}}^{\mathbb{E}, \text{HF}} \right] (N_{\omega}^{\text{HF}}, N_{\eta}^{\text{HF}})}{\varepsilon_{target}^2} \left(1 - \frac{rR - 1}{rR} \frac{\rho^2}{1 + \tau \rho^2} \right)$$

$$C_{tot}^{MF} = N_{\xi}^{MF} \tilde{C}_{\text{HF}} + N_{\xi}^{MF} rR \tilde{C}_{\text{LF}}$$

$$= N_{\xi}^{MF} C_{\text{HF}} \left(\left(1 - \frac{C_{\omega}^{\text{HF}} + C_{\eta}^{\text{HF}}}{C_{\text{HF}}} + \frac{C_{\omega, \eta}^{\text{HF}}}{C_{\text{HF}}} \right) + rR \frac{C_{\text{LF}}}{C_{\text{HF}}} \left(1 - \frac{C_{\omega}^{\text{LF}} + C_{\eta}^{\text{LF}}}{C_{\text{LF}}} + \frac{C_{\omega, \eta}^{\text{LF}}}{C_{\text{LF}}} \right) \right)$$

• **MC** cost allocation

$$N_{\xi}^{MC} = \frac{\text{Var} \left[\tilde{\mathbb{P}}_{N_{\omega}}^{\mathbb{E}, \text{HF}} \right] (N_{\omega}^{\text{HF}}, N_{\eta}^{\text{HF}})}{\varepsilon_{target}^2}$$

$$C_{tot}^{MC} = N_{\xi}^{MC} \tilde{C}_{\text{HF}} = N_{\xi}^{MC} C_{\text{HF}} \left(1 - \frac{C_{\omega}^{\text{HF}} + C_{\eta}^{\text{HF}}}{C_{\text{HF}}} + \frac{C_{\omega, \eta}^{\text{HF}}}{C_{\text{HF}}} \right)$$

First analysis scenario – same averaging for HF

$$\Theta \stackrel{\text{def}}{=} \frac{C_{tot}^{MF}(N_{\xi}^{MF}, N_{\omega}^{HF}, N_{\eta}^{HF}, N_{\omega}^{LF}, N_{\eta}^{LF})}{C_{tot}^{MC}(N_{\xi}^{MC}, N_{\omega}^{HF}, N_{\eta}^{HF})} = \left(1 - \frac{rR-1}{rR} \tilde{\rho}^2\right) \left(1 + rR \frac{C_{LF}}{C_{HF}} \frac{1 - \frac{C_{\omega}^{LF} + C_{\eta}^{LF}}{C_{LF}} + \frac{C_{\omega, \eta}^{LF}}{C_{LF}}}{1 - \frac{C_{\omega}^{HF} + C_{\eta}^{HF}}{C_{HF}} + \frac{C_{\omega, \eta}^{HF}}{C_{HF}}}\right)$$

Second analysis scenario – $N_{\omega}^{HF} = 1$ and $N_{\eta}^{HF} = 1$ for MC

$$\begin{aligned} \Theta_I &\stackrel{\text{def}}{=} \frac{C_{tot}^{MF}(N_{\xi}^{MF}, N_{\omega}^{HF}, N_{\eta}^{HF}, N_{\omega}^{LF}, N_{\eta}^{LF})}{C_{tot}^{MC}(N_{\xi}^{MC}, N_{\omega}^{HF} = 1, N_{\eta}^{HF} = 1)} \\ &= \frac{\text{Var} \left[\tilde{P}_{N_{\omega}}^{\omega, HF} \right] (N_{\omega}^{HF}, N_{\eta}^{HF})}{\text{Var} \left[\tilde{P}_{N_{\omega}}^{\omega, HF} \right] (N_{\omega}^{HF} = 1, N_{\eta}^{HF} = 1)} \left(1 - \frac{rR-1}{rR} \tilde{\rho}^2\right) \left(1 - \frac{C_{\omega}^{HF} + C_{\eta}^{HF}}{C_{HF}} + \frac{C_{\omega, \eta}^{HF}}{C_{HF}}\right) \left(1 + rR \frac{C_{LF}}{C_{HF}} \frac{1 - \frac{C_{\omega}^{HF} + C_{\eta}^{HF}}{C_{HF}} + \frac{C_{\omega, \eta}^{HF}}{C_{HF}}}{1 - \frac{C_{\omega}^{LF} + C_{\eta}^{LF}}{C_{LF}} + \frac{C_{\omega, \eta}^{LF}}{C_{LF}}}\right) \\ &= \frac{\text{Var}_{\xi} \left[\mathbb{P}_{\xi}^{HF} \right] + \mathbb{E}_{\xi} \left[\frac{\text{Var}_{\omega} [Q_{\eta}^{HF}(\xi, \omega)]}{N_{\omega}^{HF}} \right] + \mathbb{E}_{\xi} \left[\frac{\mathbb{E}_{\omega} [\sigma_{\eta}^2(\xi, \omega)]}{N_{\omega}^{HF} N_{\eta}^{HF}} \right]}{\text{Var}_{\xi} \left[\mathbb{P}_{\xi}^{HF} \right] + \mathbb{E}_{\xi} [\text{Var}_{\omega} [Q_{\eta}^{HF}(\xi, \omega)]] + \mathbb{E}_{\xi} [\mathbb{E}_{\omega} [\sigma_{\eta}^2(\xi, \omega)]]} \left(1 - \frac{C_{\omega}^{HF} + C_{\eta}^{HF}}{C_{HF}} + \frac{C_{\omega, \eta}^{HF}}{C_{HF}}\right) \Theta \end{aligned}$$

First analysis scenario – same averaging for HF

$$\Theta \stackrel{\text{def}}{=} \frac{C_{tot}^{MF}(N_{\xi}^{MF}, N_{\omega}^{HF}, N_{\eta}^{HF}, N_{\omega}^{LF}, N_{\eta}^{LF})}{C_{tot}^{MC}(N_{\xi}^{MC}, N_{\omega}^{HF}, N_{\eta}^{HF})} = \left(1 - \frac{rR-1}{rR} \tilde{\rho}^2\right) \left(1 + rR \frac{C_{LF}}{C_{HF}} \frac{1 - \frac{C_{\omega}^{LF} + C_{\eta}^{LF}}{C_{LF}} + \frac{C_{\omega, \eta}^{LF}}{C_{LF}}}{1 - \frac{C_{\omega}^{HF} + C_{\eta}^{HF}}{C_{HF}} + \frac{C_{\omega, \eta}^{HF}}{C_{HF}}}\right)$$

Second analysis scenario – $N_{\omega}^{HF} = 1$ and $N_{\eta}^{HF} = 1$ for MC

$$\begin{aligned} \Theta_I &\stackrel{\text{def}}{=} \frac{C_{tot}^{MF}(N_{\xi}^{MF}, N_{\omega}^{HF}, N_{\eta}^{HF}, N_{\omega}^{LF}, N_{\eta}^{LF})}{C_{tot}^{MC}(N_{\xi}^{MC}, N_{\omega}^{HF} = 1, N_{\eta}^{HF} = 1)} \\ &= \frac{\text{Var} \left[\tilde{P}_{N_{\omega}}^{E, HF} \right] (N_{\omega}^{HF}, N_{\eta}^{HF})}{\text{Var} \left[\tilde{P}_{N_{\omega}}^{E, HF} \right] (N_{\omega}^{HF} = 1, N_{\eta}^{HF} = 1)} \left(1 - \frac{rR-1}{rR} \tilde{\rho}^2\right) \left(1 - \frac{C_{\omega}^{HF} + C_{\eta}^{HF}}{C_{HF}} + \frac{C_{\omega, \eta}^{HF}}{C_{HF}}\right) \left(1 + rR \frac{C_{LF}}{C_{HF}} \frac{1 - \frac{C_{\omega}^{HF} + C_{\eta}^{HF}}{C_{HF}} + \frac{C_{\omega, \eta}^{HF}}{C_{HF}}}{1 - \frac{C_{\omega}^{LF} + C_{\eta}^{LF}}{C_{LF}} + \frac{C_{\omega, \eta}^{LF}}{C_{LF}}}\right) \\ &= \frac{\text{Var}_{\xi} \left[P_E^{HF} \right] + \mathbb{E}_{\xi} \left[\frac{\text{Var}_{\omega} [Q_{\omega}^{HF}(\xi, \omega)]}{N_{\omega}^{HF}} \right] + \mathbb{E}_{\xi} \left[\frac{\mathbb{E}_{\omega} [\sigma_{\eta}^2(\xi, \omega)]}{N_{\omega}^{HF} N_{\eta}^{HF}} \right]}{\text{Var}_{\xi} \left[P_E^{HF} \right] + \mathbb{E}_{\xi} [\text{Var}_{\omega} [Q_{\omega}^{HF}(\xi, \omega)]] + \mathbb{E}_{\xi} [\mathbb{E}_{\omega} [\sigma_{\eta}^2(\xi, \omega)]]} \left(1 - \frac{C_{\omega}^{HF} + C_{\eta}^{HF}}{C_{HF}} + \frac{C_{\omega, \eta}^{HF}}{C_{HF}}\right) \Theta \end{aligned}$$

1D MC RT FOR STOCHASTIC MEDIA WITH UNCERTAIN PROPERTIES

SUMMARY OF THE UQ EXACT SOLUTION (1/2)



- Derived all terms needed for **closed-form variance** $\text{Var}_\xi [\mathbb{P}_E]$
- MF UQ analysis required $\text{Cov}_\xi [\mathbb{P}_E^{\text{HF}}, \mathbb{P}_E^{\text{LF}}]$ (to evaluate the correlation)

Summary of the Cov derivation

- QoI in closed-form as function of $N_A(\omega)$

$$\mathbb{P}_E^{\text{HF}} = \mathbb{E}_\omega [T^{\text{HF}}] = \exp \left[-N_{\text{tot}}^{\text{HF}} \Delta x \Sigma_{t,B}^{\text{HF}}(\xi_B) \right] \mathbb{E}_\omega \left[N_A^{\text{HF}}(\omega) \Delta x \overbrace{\left(\Sigma_{t,A}^0 - \Sigma_{t,B}^0 + \Sigma_{t,A}^{\Delta} \xi_A - \Sigma_{t,B}^{\Delta} \xi_B \right)}^{F(\xi_A, \xi_B) = F_0 + F_{\Delta}(\xi_A, \xi_B)} \right]$$

- Leverage the probability mass function of $N_A(\omega)$

$$\begin{aligned} \mathbb{E}_\omega \left[N_A(\omega) \Delta x F(\xi_A, \xi_B) \right] &= \sum_{x=0}^{N_{\text{tot}}^{\text{HF}}} \frac{N_{\text{tot}}^{\text{HF}}!}{x!(N_{\text{tot}}^{\text{HF}} - x)!} p_A^x (1 - p_A)^{N_{\text{tot}}^{\text{HF}} - x} \exp \left[-x \Delta x F(\xi_A, \xi_B) \right] \\ &= \sum_{x=0}^{N_{\text{tot}}} B_\omega(x) \exp \left[-x \Delta x F_{\Delta}(\xi_A, \xi_B) \right] \end{aligned}$$

- Evaluate statistics, e.g. the expected value

$$\mathbb{E}_\xi \left[\mathbb{P}_E^{\text{HF}} \right] = \exp \left[-N_{\text{tot}}^{\text{HF}} \Delta x \Sigma_{t,B}^0 \right] \left(\sum_{x=0}^{N_{\text{tot}}^{\text{HF}}} B_\omega(x) (x) \frac{\sinh \left[x \Delta x \Sigma_{t,A}^{\Delta} \right]}{x \Delta x \Sigma_{t,A}^{\Delta}} \frac{\sinh \left[N_{\text{tot}}^{\text{HF}} \Delta x \Sigma_{t,B}^{\Delta} \left(1 - \frac{x}{N_{\text{tot}}^{\text{HF}}} \right) \Delta x \Sigma_{t,A}^{\Delta} \right]}{N_{\text{tot}}^{\text{HF}} \Delta x \Sigma_{t,B}^{\Delta} \left(1 - \frac{x}{N_{\text{tot}}^{\text{HF}}} \right) \Delta x \Sigma_{t,A}^{\Delta}} \right)$$

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$$\begin{aligned} \mathbb{E}_\omega \left[N_A(\omega) \Delta x^{\text{HF}} F(\xi_A, \xi_B) \right] &= \sum_{x=0}^{N_{\text{tot}}^{\text{HF}}} \frac{N_{\text{tot}}^{\text{HF}}!}{x!(N_{\text{tot}}^{\text{HF}} - x)!} p_A^x (1 - p_A)^{N_{\text{tot}}^{\text{HF}} - x} \exp \left[-x \Delta x^{\text{HF}} F(\xi_A, \xi_B) \right] \\ &= \sum_{x=0}^{N_{\text{tot}}} B_\omega(x) \exp \left[-x \Delta x^{\text{HF}} F_\Delta(\xi_A, \xi_B) \right] \end{aligned}$$

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$$\mathbb{E}_\xi [\mathbb{P}_E^{\text{HF}}] = \exp \left[-N_{\text{tot}} \Delta x \Sigma_{t,B}^0 \right] \left(\sum_{x=0}^{N_{\text{tot}}^{\text{HF}}} B_\omega(x) (x) \frac{\sinh \left[x \Delta x^{\text{HF}} \Sigma_{t,A}^\Delta \right]}{x \Delta x^{\text{HF}} \Sigma_{t,A}^\Delta} \frac{\sinh \left[N_{\text{tot}}^{\text{HF}} \Delta x^{\text{HF}} \Sigma_{t,B}^\Delta \left(1 - \frac{x}{N_{\text{tot}}^{\text{HF}}} \right) \Delta x^{\text{HF}} \Sigma_{t,A}^\Delta \right]}{N_{\text{tot}}^{\text{HF}} \Delta x^{\text{HF}} \Sigma_{t,B}^\Delta \left(1 - \frac{x}{N_{\text{tot}}^{\text{HF}}} \right) \Delta x^{\text{HF}} \Sigma_{t,A}^\Delta} \right),$$



$$\text{Cov}_\xi \left[\mathbb{P}_E^{\text{HF}}, \mathbb{P}_E^{\text{LF}} \right] = \mathbb{E}_\xi \left[\mathbb{P}_E^{\text{HF}} \mathbb{P}_E^{\text{LF}} \right] - \mathbb{E}_\xi \left[\mathbb{P}_E^{\text{HF}} \right] \mathbb{E}_\xi \left[\mathbb{P}_E^{\text{LF}} \right]$$

$$\begin{aligned} \mathbb{E}_\xi \left[\mathbb{P}_E^{\text{HF}} \mathbb{P}_E^{\text{LF}} \right] &= \exp \left[-\Sigma_{t,B}^0 \left(N_{tot}^{\text{HF}} \Delta x^{\text{HF}} + N_{tot}^{\text{LF}} \Delta x^{\text{LF}} \right) \right] \left(\sum_{x=0}^{N_{tot}^{\text{LF}}} B_\omega^{\text{HF}}(x) B_\omega^{\text{LF}}(x) \frac{\sinh \left[x \left(\Delta x^{\text{HF}} + \Delta x^{\text{LF}} \right) \Sigma_{t,A}^\Delta \right]}{x \left(\Delta x^{\text{HF}} + \Delta x^{\text{LF}} \right) \Sigma_{t,A}^\Delta} \right. \\ &\quad \cdot \frac{\sinh \left[\left((x - N_{tot}^{\text{HF}}) \Delta x^{\text{HF}} + (x - N_{tot}^{\text{LF}}) \Delta x^{\text{LF}} \right) \Sigma_{t,B}^\Delta \right]}{\left((x - N_{tot}^{\text{HF}}) \Delta x^{\text{HF}} + (x - N_{tot}^{\text{LF}}) \Delta x^{\text{LF}} \right) \Sigma_{t,B}^\Delta} \\ &\quad + \sum_{x=0}^{N_{tot}^{\text{LF}}} \sum_{\substack{y=0 \\ y \neq x}}^{N_{tot}^{\text{LF}}} B_\omega^{\text{HF}}(x) B_\omega^{\text{LF}}(y) \frac{\sinh \left[\left(x \Delta x^{\text{HF}} + y \Delta x^{\text{LF}} \right) \Sigma_{t,A}^\Delta \right]}{\left(x \Delta x^{\text{HF}} + y \Delta x^{\text{LF}} \right) \Sigma_{t,A}^\Delta} \frac{\sinh \left[\left((x - N_{tot}^{\text{HF}}) \Delta x^{\text{HF}} + (y - N_{tot}^{\text{LF}}) \Delta x^{\text{LF}} \right) \Sigma_{t,B}^\Delta \right]}{\left((x - N_{tot}^{\text{HF}}) \Delta x^{\text{HF}} + (y - N_{tot}^{\text{LF}}) \Delta x^{\text{LF}} \right) \Sigma_{t,B}^\Delta} \\ &\quad \left. + \sum_{x=0}^{N_{tot}^{\text{LF}}} \sum_{y=N_{tot}^{\text{LF}}+1}^{N_{tot}^{\text{HF}}} B_\omega^{\text{LF}}(x) B_\omega^{\text{HF}}(y) \frac{\sinh \left[\left(x \Delta x^{\text{LF}} + y \Delta x^{\text{HF}} \right) \Sigma_{t,A}^\Delta \right]}{\left(x \Delta x^{\text{LF}} + y \Delta x^{\text{HF}} \right) \Sigma_{t,A}^\Delta} \frac{\sinh \left[\left((x - N_{tot}^{\text{LF}}) \Delta x^{\text{LF}} + (y - N_{tot}^{\text{HF}}) \Delta x^{\text{HF}} \right) \Sigma_{t,B}^\Delta \right]}{\left((x - N_{tot}^{\text{LF}}) \Delta x^{\text{LF}} + (y - N_{tot}^{\text{HF}}) \Delta x^{\text{HF}} \right) \Sigma_{t,B}^\Delta} \right) \end{aligned}$$

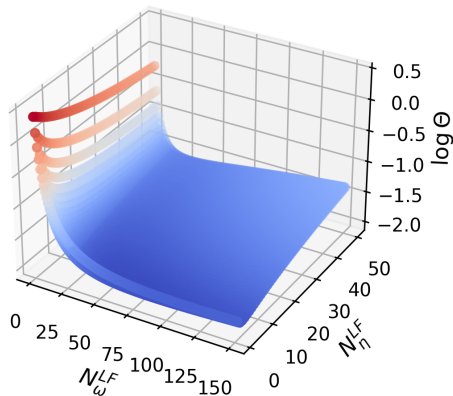
NUMERICAL RESULTS

SCENARIO 1: HF DATASET ASSIGNED - $N_{\omega}^{HF} = 10$ AND $N_{\eta}^{HF} = 15$ - COST RATIO (1/2)

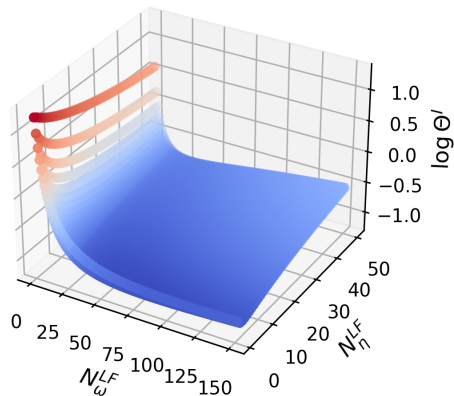


Scenario 1

$\Theta -- (N_{\omega}^{HF}, N_{\eta}^{HF}) = (10, 15)$

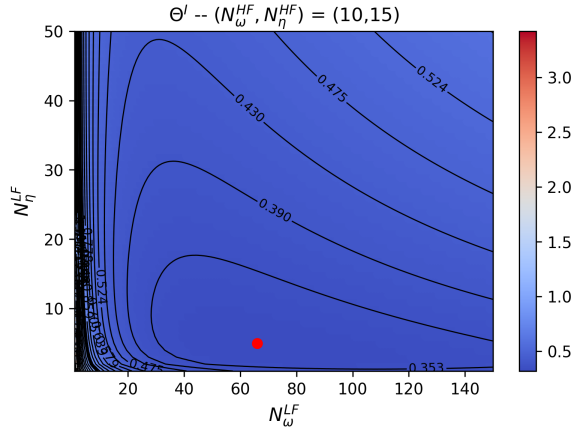
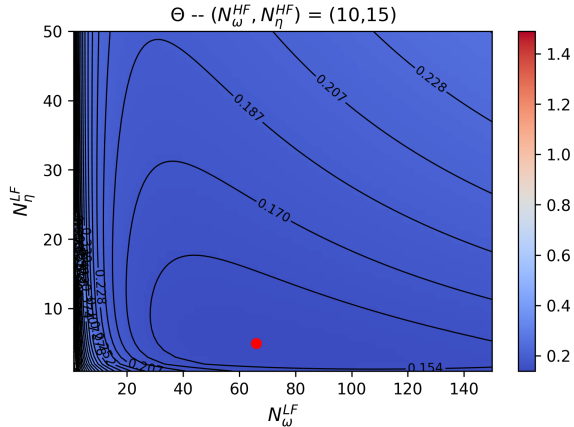


$\Theta' -- (N_{\omega}^{HF}, N_{\eta}^{HF}) = (10, 15)$



NUMERICAL RESULTS

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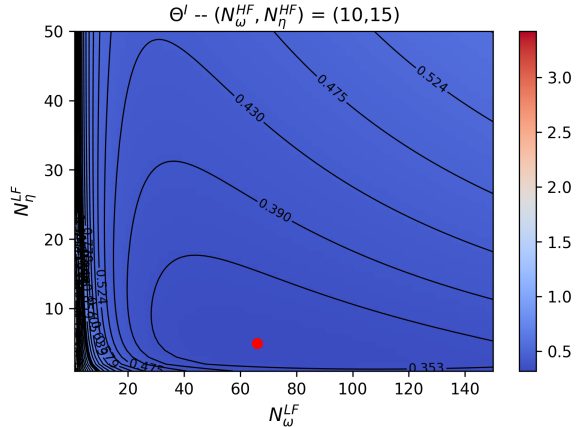
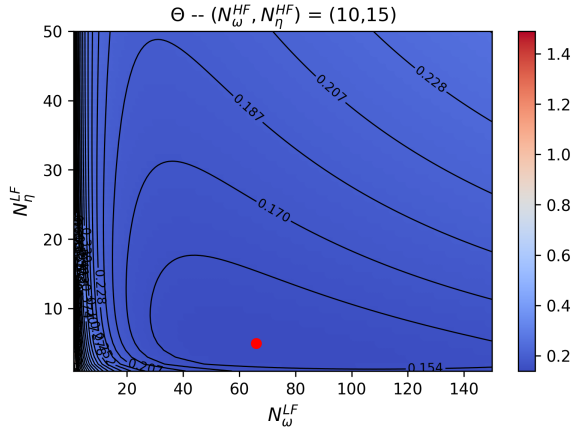


$$\Theta^I = \underbrace{\frac{\text{Var}_{\xi} [\mathbf{P}_{\mathbf{E}}^{\text{PHF}}] + \mathbb{E}_{\xi} \left[\frac{\text{Var}_{\omega} [Q_{\eta}^{\text{HF}}(\xi, \omega)]}{N_{\omega}^{\text{HF}}} \right] + \mathbb{E}_{\xi} \left[\frac{\mathbb{E}_{\omega} [\sigma_{\eta}^2(\xi, \omega)]}{N_{\omega}^{\text{HF}} N_{\eta}^{\text{HF}}} \right]}{\text{Var}_{\xi} [\mathbf{P}_{\mathbf{E}}^{\text{PHF}}] + \mathbb{E}_{\xi} [\text{Var}_{\omega} [Q^{\text{HF}}(\xi, \omega)]] + \mathbb{E}_{\xi} [\mathbb{E}_{\omega} [\sigma_{\eta}^2(\xi, \omega)]]} \left(1 - \frac{C_{\omega}^{\text{HF}} + C_{\eta}^{\text{HF}}}{C_{\text{HF}}} + \frac{C_{\omega, \eta}^{\text{HF}}}{C_{\text{HF}}} \right) \Theta$$

Constant for this test case (> 1)

NUMERICAL RESULTS

SCENARIO 1: HF DATASET ASSIGNED - $N_{\omega}^{\text{HF}} = 10$ AND $N_{\eta}^{\text{HF}} = 15$ - COST RATIO (1/2)



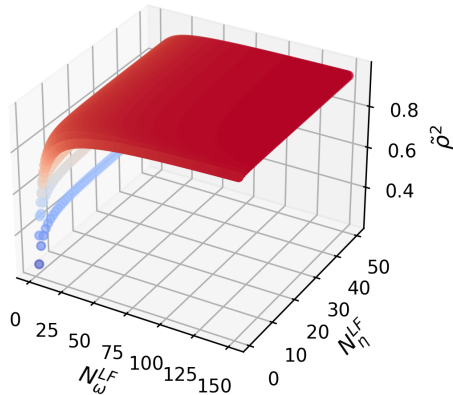
$$\Theta^I = \frac{\text{Var}_{\xi} [\mathbb{P}_{\text{E}}^{\text{HF}}] + \mathbb{E}_{\xi} \left[\frac{\text{Var}_{\omega} [Q^{\text{HF}}(\xi, \omega)]}{N_{\omega}^{\text{HF}}} \right] + \mathbb{E}_{\xi} \left[\frac{\mathbb{E}_{\omega} [\sigma_{\eta}^2(\xi, \omega)]}{N_{\omega}^{\text{HF}} N_{\eta}^{\text{HF}}} \right]}{\underbrace{\text{Var}_{\xi} [\mathbb{P}_{\text{E}}^{\text{HF}}] + \mathbb{E}_{\xi} [\text{Var}_{\omega} [Q^{\text{HF}}(\xi, \omega)]] + \mathbb{E}_{\xi} [\mathbb{E}_{\omega} [\sigma_{\eta}^2(\xi, \omega)]]}_{\text{Constant for this test case } (> 1)}} \left(1 - \frac{C_{\omega}^{\text{HF}} + C_{\eta}^{\text{HF}}}{C_{\text{HF}}} + \frac{C_{\omega, \eta}^{\text{HF}}}{C_{\text{HF}}} \right) \Theta$$

NUMERICAL RESULTS

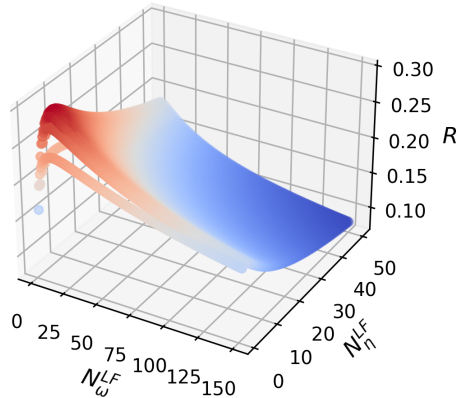
SCENARIO 1: HF DATASET ASSIGNED - $N_{\omega}^{\text{HF}} = 10$ AND $N_{\eta}^{\text{HF}} = 15$ - CORRELATION/ALLOCATION



$$\tilde{\rho}^2 \text{ -- } (N_{\omega}^{\text{HF}}, N_{\eta}^{\text{HF}}) = (10, 15)$$



$$R \text{ -- } (N_{\omega}^{\text{HF}}, N_{\eta}^{\text{HF}}) = (10, 15)$$



$$r \approx 54.32$$

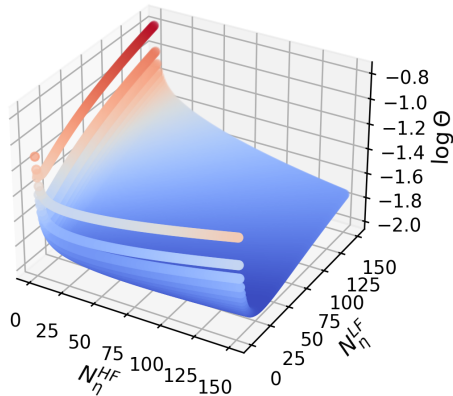
NUMERICAL RESULTS

SCENARIO 2: STOCHASTIC MEDIA ASSIGNED - $N_{\omega}^{HF} = 10$ AND $N_{\omega}^{LF} = 25$ - COST RATIO (1/2)

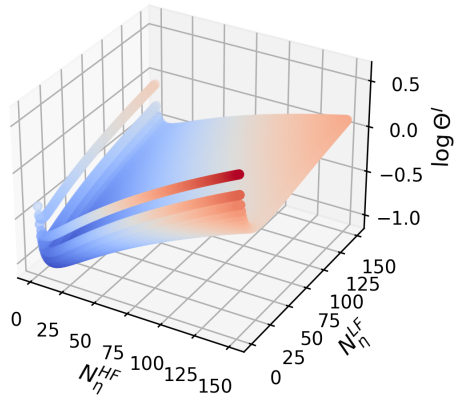


Scenario 2

$\Theta -- (N_{\omega}^{HF}, N_{\omega}^{LF}) = (10, 25)$

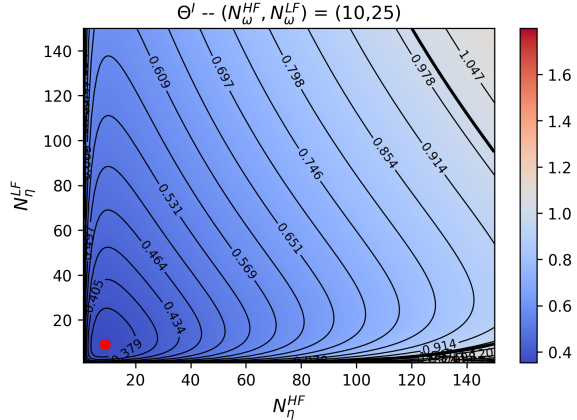
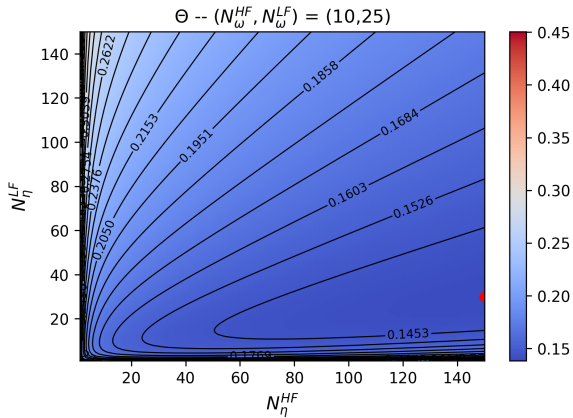


$\Theta' -- (N_{\omega}^{HF}, N_{\omega}^{LF}) = (10, 25)$



NUMERICAL RESULTS

SCENARIO 2: STOCHASTIC MEDIA ASSIGNED - $N_\omega^{\text{HF}} = 10$ AND $N_\omega^{\text{LF}} = 25$ - COST RATIO (1/2)

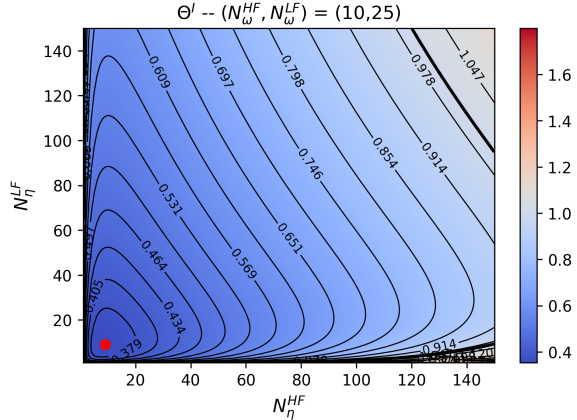
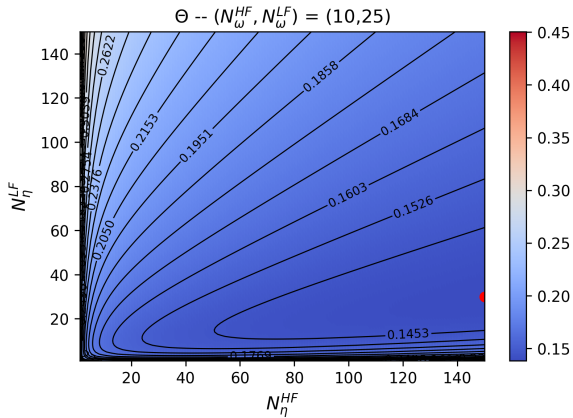


$$\Theta^I = \underbrace{\frac{\text{Var}_\xi [\mathbf{P}_E^{\text{HF}}] + \mathbb{E}_\xi \left[\frac{\text{Var}_\omega [Q_\omega^{\text{HF}}(\xi, \omega)]}{N_\omega^{\text{HF}}} \right] + \mathbb{E}_\xi \left[\frac{\mathbb{E}_\omega [\sigma_\eta^2(\xi, \omega)]}{N_\omega^{\text{HF}} N_\eta^{\text{HF}}} \right]}{\text{Var}_\xi [\mathbf{P}_E^{\text{HF}}] + \mathbb{E}_\xi [\text{Var}_\omega [Q_\omega^{\text{HF}}(\xi, \omega)]] + \mathbb{E}_\xi [\mathbb{E}_\omega [\sigma_\eta^2(\xi, \omega)]]} \left(1 - \frac{C_\omega^{\text{HF}} + C_\eta^{\text{HF}}}{C_{\text{HF}}} + \frac{C_{\omega, \eta}^{\text{HF}}}{C_{\text{HF}}} \right) \Theta$$

Increases with N_η^{HF}

NUMERICAL RESULTS

SCENARIO 2: STOCHASTIC MEDIA ASSIGNED - $N_\omega^{\text{HF}} = 10$ AND $N_\omega^{\text{LF}} = 25$ - COST RATIO (1/2)



$$\Theta^I = \underbrace{\frac{\text{Var}_\xi [\mathbb{P}_E^{\text{HF}}] + \mathbb{E}_\xi \left[\frac{\text{Var}_\omega [Q^{\text{HF}}(\xi, \omega)]}{N_\omega^{\text{HF}}} \right] + \mathbb{E}_\xi \left[\frac{\mathbb{E}_\omega [\sigma_\eta^2(\xi, \omega)]}{N_\omega^{\text{HF}} N_\eta^{\text{HF}}} \right]}{\text{Var}_\xi [\mathbb{P}_E^{\text{HF}}] + \mathbb{E}_\xi [\text{Var}_\omega [Q^{\text{HF}}(\xi, \omega)]] + \mathbb{E}_\xi [\mathbb{E}_\omega [\sigma_\eta^2(\xi, \omega)]]} \left(1 - \frac{C_\omega^{\text{HF}} + C_\eta^{\text{HF}}}{C_{\text{HF}}} + \frac{C_{\omega, \eta}^{\text{HF}}}{C_{\text{HF}}} \right) \Theta$$

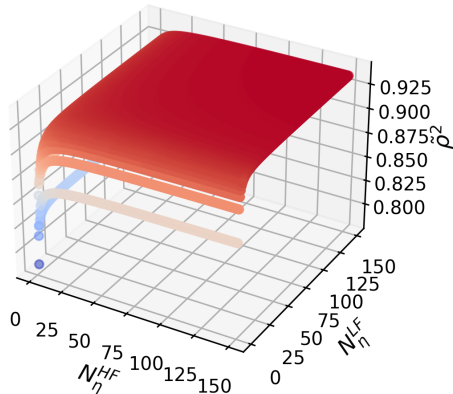
Increases with N_η^{HF}

NUMERICAL RESULTS

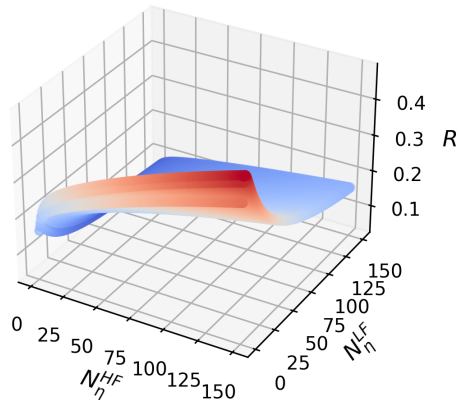
SCENARIO 2: STOCHASTIC MEDIA ASSIGNED - $N_{\omega}^{\text{HF}} = 10$ AND $N_{\omega}^{\text{LF}} = 25$ - CORRELATION/ALLOCATION



$$\tilde{\rho}^2 \text{ -- } (N_{\omega}^{\text{HF}}, N_{\omega}^{\text{LF}}) = (10, 25)$$



$$R \text{ -- } (N_{\omega}^{\text{HF}}, N_{\omega}^{\text{LF}}) = (10, 25)$$



$$r \approx 54.32$$