MultiFidelity UQ sampling for Stochastic Simulations

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Plan of the talk

- Background
- Network Modeling
- Stochastic solvers in Sampling Methods
- Numerical Examples
- Conclusions

Background

Uncertainty Quantification
DoE and DoD deployment activities

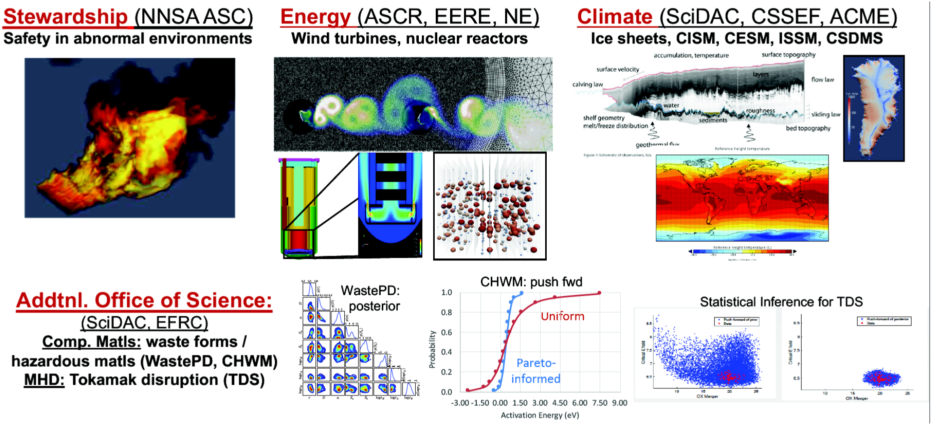

Figure courtesy of Mike Eldred

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

- **Severe** simulations **budget constraints**
- **Significant dimensionality** driven by model complexity

Uncertainty Quantification
Forward Propagation – Why Sampling Methods?

UQ context at a glance:

- **Challenges:** High-dimensionality, non-linearity and possibly non-smooth responses
- **Opportunities:** Rich physics and several discretization levels/models available

Natural candidate:

- **Sampling**-based (MC-like) approaches because they are **non-intrusive**, **robust** and **flexible**...
- **Drawback:** Slow convergence $\mathcal{O}(N^{-1/2}) \rightarrow$ many realizations to build reliable statistics

Goal of MF UQ: **Reducing the computational cost** of obtaining MC reliable statistics

Pivotal idea:

- Simplified (**low-fidelity**) models are **inaccurate** but **cheap**
  - **low-variance** estimates
- **High-fidelity** models are **costly**, but **accurate**
  - **low-bias** estimates

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  - ► **low-variance** estimates
- **High-fidelity** models are **costly**, but **accurate**
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Talk's Contribution: Addressing challenges (and opportunities) introduced by **Stochastic Solvers**

A comment on Stochastic solvers
Examples of Stochastic solvers at Sandia

Q: What do I mean in this presentation with **stochastic solver**?

A: For the sake of this presentation, I mean that in addition to the UQ parameters, the **solver has another source of variability** (that we cannot control)

Few **SNL-relevant examples**:

- **Turbulent flows/Combustion:** the stochasticity is introduced in the time-windowing used for statistics (we cannot integrate long enough)
- **Computer Networks/Cybersecurity:** virtualization of networks that runs real-time on specialized hardware, *i.e.* the status of the hardware produces background noise that cannot be controlled
- **Radiation transport:** MC transport solvers based on the propagation of a finite number of particle histories which need to be averaged to obtain the QoIs
- **GDSA:** stochasticity introduced in the (finite number of random realizations of the) subsurface modeling
- etc.

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Talk's Focus: I'll demonstrate the use of MF UQ for stochastic solvers in the context of **Cybersecurity applications**

Network Modeling

Network models

Simulation vs Emulation: strengths and differences

Simulation: based on deep **understanding of the underlying processes**

- ✔ Fast to **develop**
- ✔ Runs **faster than real-time** since they control the clock
- ✔ Easy to **run in parallel**: neither time-dependent or reliant on virtualized hardware
- ✗ Unable to capture **emergent behaviors**

Emulation: able to **capture unknown or not well-understood behaviors**

- ✔ Runs the **real software** therefore closely resembles a physical testbed
- ✗ Requires **more hardware** and therefore the number of concurrent evaluations are limited

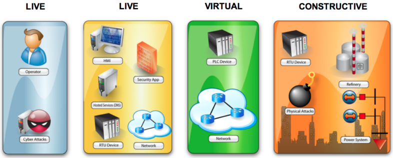


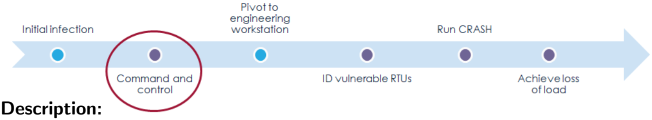
Figure courtesy of David Fritz, SAND2018-3927

Examples of Network modeling at Sandia (Courtesy of David Fritz, SAND2018-3927[1])

- **DevOps:** Ensure operation of new hardware, software, services in high-consequence environments. Detect malfunctions, misconfigurations and malicious consequences
- **Malware:** Understanding of malware through pseudo-in situ execution
- **ICS/SCADA:** Best countermeasures for my IT-connected ICS systems? Can we detect attacks? Can we assess resiliency of the IT-controls over the entire power grids?
- **Nuclear Weapons:** Assure Communication, Command and Control regardless of network state and threats?

[1] http://minimega.org/presentations/gt_2018.slide#7

Command & Control (C2) example
Problem Description



Problem Description:

- **Multi-stage attack** aiming at accessing a **power utility**'s corporate enterprise network
- **Attacker Goal:** pivoting on the industrial control system (ICS) to ultimately **cause load shed**
- **Attacker Perspective:** **Maintaining communication** between C2 host and C2 server
- **Defender Perspective:** Deploying an IDS to **identify/mitigate malicious traffic**

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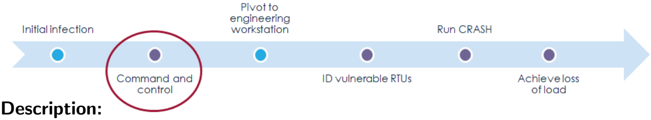

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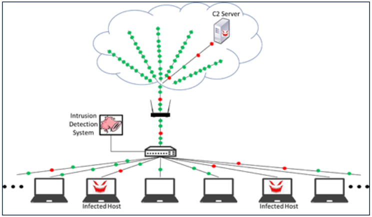

Analysis Scenario:

- One or more hosts with the network have been infected
- **Benign** and **Malicious** traffic co-exist
- The **IDS performs packet inspection** and issues an alert if the content appears suspicious
- Large packet rates make malicious traffic difficult to detect
- **Emotet malware** (banking trojan from 2014) and the Snort IDS

Stochastic solvers in (MF) Sampling Methods

Few **definitions and notation**:

- ξ is the vector of **UQ parameters**
- η is a vector of inaccessible RV that notionally represents the **variability in the solver**
- Every time we run the solver, we get an **elementary realization** $f = f(\xi, \eta)$
- **Running for a fixed $\xi^{(i)}$** multiple times (*replicas*) generates $\left\{ f(\xi^{(i)}, \eta^{(j)}) \right\}_{j=1}^{N_\eta}$
- The QoI for UQ is obtained by **averaging f** (for a fixed ξ):

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

Sampling UQ, *e.g.* mean estimator, is accomplished with **two nested sampling estimators**

$$\mathbb{E}[Q] \approx \frac{1}{N_\xi} \sum_{i=1}^{N_\xi} \tilde{Q}^{(i)} = \frac{1}{N_\xi} \sum_{i=1}^{N_\xi} \left[\frac{1}{N_\eta} \sum_{j=1}^{N_\eta} f(\xi^{(i)}, \eta^{(j)}) \right]$$

Q: How does the noise introduced in the finite averaging over *replicas* propagate in the estimator?

The MC estimator is still *unbiased*...

$$\hat{Q}^{MC} = \frac{1}{N_\xi}\sum_{i=1}^{N_\xi}\left(\frac{1}{N_\eta}\sum_{j=1}^{N_\eta} f(\xi^{(i)},\eta^{(j)})\right) = \frac{1}{N_\xi}\sum_{i=1}^{N_\xi}\tilde{Q}(\xi^{(i)}) \quad \longrightarrow \quad \mathbb{V}ar\left[\hat{Q}^{MC}\right] = \frac{\mathbb{V}ar\left[\tilde{Q}(\xi)\right]}{N_\xi}$$

Law of total variance

$$\mathbb{V}ar\left[\cdot\right] = \mathbb{V}ar\left[\mathbb{E}_\eta\left[\cdot\right]\right] + \mathbb{E}\left[\mathbb{V}ar_\eta\left[\cdot\right]\right],$$

It follows that

$$\begin{aligned}\mathbb{V}ar\left[\tilde{Q}(\xi;\eta)\right] &= \mathbb{V}ar\left[\mathbb{E}_\eta\left[\tilde{Q}(\xi;\eta)\right]\right] + \mathbb{E}\left[\mathbb{V}ar_\eta\left[\tilde{Q}(\xi;\eta)\right]\right] \\ &= \mathbb{V}ar\left[\mathbb{E}_\eta\left[f(\xi,\eta)\right]\right] + \frac{\mathbb{E}\left[\mathbb{V}ar_\eta\left[f(\xi,\eta)\right]\right]}{N_\eta} \\ &= \mathbb{V}ar\left[Q(\xi)\right] + \mathbb{E}\left[\frac{\sigma_\eta^2(\xi)}{N_\eta}\right].\end{aligned}$$

Finally,

$$\mathbb{V}ar\left[\hat{Q}^{MC}\right] = \frac{\mathbb{V}ar\left[\mathbf{Q}(\xi)\right] + \mathbb{E}\left[\frac{\sigma_\eta^2(\xi)}{\mathbf{N}_\eta}\right]}{N_\xi}$$

NOTES:

- The **true variance** is augmented by the (average) **noise** introduced by replicas
- The average **noise** is the average variance of the inner MC estimator

Let's now consider the **control variate** case[2]:

$$\hat{Q}^{CV} = \hat{Q}^{MC}_{HF} + \alpha \left(\hat{Q}^{MC}_{LF} - \mathbb{E}\left[Q^{LF} \right] \right),$$

for which we know a solution that minimizes the estimator cost (for a prescribed variance ε^2).

For the **control variate** case, we need to consider the following **properties**:

- All quantities depend on the **number of replicas**, *i.e.* N^{HF}_{η} and N^{LF}_{η}
- The **correlation** between quantities $\tilde{Q}^{HF}$ and $\tilde{Q}^{LF}$ **increases** by averaging more replicas
- The **computational cost** **increases** with the number of replicas

Q: Can we **optimize** the number of replicas in order to **maximize the efficiency** of the estimator?

[2] This is equivalent to MFMC or ACV with one low-fidelity model

Let's start from the **classical control variate solution** given the quantities $\tilde{Q}^{HF}$ and $\tilde{Q}^{LF}$:

$$\mathbb{V}ar\left[\hat{Q}^{CV}\right] = \frac{\mathbb{V}ar\left[\tilde{Q}^{HF}\right]}{N_\xi}\left(1 - \frac{\tilde{r}-1}{\tilde{r}}\tilde{\rho}^2\right), \quad \text{with} \quad \tilde{r} = \sqrt{\frac{\tilde{\mathcal{C}}_{HF}}{\tilde{\mathcal{C}}_{LF}}\frac{\tilde{\rho}^2}{1-\tilde{\rho}^2}},$$

where we use a **total number of low-fidelity simulations** equal to $\lceil \tilde{r} N_\xi \rceil$.

Stochastic Solvers and sampling methods
Extension to Multifidelity (2/3)

Let's start from the **classical control variate solution** given the quantities $\tilde{Q}^{HF}$ and $\tilde{Q}^{LF}$:

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Q: Can we write this solution such that we **separate the stochastic component** controlled by the number of replicas?

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where we use a **total number of low-fidelity simulations** equal to $\lceil \tilde{r} N_\xi \rceil$.

Q: Can we write this solution such that we **separate the stochastic component** controlled by the number of replicas?

STEP 1: **Re-write the correlation** as

$$\tilde{\rho}^2 = \frac{\left(\mathrm{Cov}\left[\tilde{Q}^{HF}, \tilde{Q}^{LF}\right]\right)^2}{\mathbb{V}ar\left[\tilde{Q}^{HF}\right]\mathbb{V}ar\left[\tilde{Q}^{LF}\right]} \longrightarrow \boxed{\tilde{\rho}^2 = \frac{\rho^2}{1+\rho^2\tilde{\tau}}},$$

$$\text{where} \quad \tilde{\tau} = \frac{\mathbb{V}ar\left[Q^{LF}\right]\frac{\mathbb{E}\left[\sigma^2_{\eta,\mathrm{HF}}\right]}{N_\eta^{\mathrm{HF}}} + \mathbb{V}ar\left[Q^{HF}\right]\frac{\mathbb{E}\left[\sigma^2_{\eta,\mathrm{LF}}\right]}{N_\eta^{\mathrm{LF}}} + \frac{\mathbb{E}\left[\sigma^2_{\eta,\mathrm{HF}}\right]\mathbb{E}\left[\sigma^2_{\eta,\mathrm{LF}}\right]}{N_\eta^{\mathrm{HF}}N_\eta^{\mathrm{LF}}}}{\left(\mathrm{Cov}\left[\tilde{Q}^{HF}, \tilde{Q}^{LF}\right]\right)^2}$$

NOTES:

- $\mathrm{Cov}\left[\tilde{Q}^{HF}, \tilde{Q}^{LF}\right] = \mathrm{Cov}\left[Q^{HF}, Q^{LF}\right]$
- $\mathbb{V}ar\left[\tilde{Q}^{HF}\right] = \mathbb{V}ar\left[Q^{HF}\right] + \mathbb{E}\left[\frac{\sigma_\eta^{2,HF}}{N_\eta}\right]$ (same for the low-fidelity)

STEP 2: **Re-write the cost** as a function of an elementary realization

$$\tilde{\mathcal{C}}_{\mathrm{HF}} = N_\eta^{\mathrm{HF}} \mathcal{C}^{\mathrm{HF}}$$
$$\tilde{\mathcal{C}}_{\mathrm{LF}} = N_\eta^{\mathrm{LF}} \mathcal{C}^{\mathrm{LF}}$$

STEP 3: Finally **write the sample allocation** (for a prescribed variance ε^2)

$$\tilde{r}^\star = \sqrt{\frac{\mathbf{1}-\boldsymbol{\rho}^{\mathbf{2}}}{\mathbf{1}-\boldsymbol{\rho}^{\mathbf{2}}+\boldsymbol{\rho}^{\mathbf{2}}\tilde{\tau}} \frac{\mathbf{N}_\eta^{\mathrm{HF}}}{\mathbf{N}_\eta^{\mathrm{LF}}}} \sqrt{\frac{\rho^2}{1-\rho^2}\frac{\mathcal{C}^{\mathrm{HF}}}{\mathcal{C}^{\mathrm{LF}}}} = \tilde{\mathbf{R}} r^\star$$

$$\tilde{\Lambda} = 1 - \frac{\tilde{R}r^\star - 1}{\tilde{R}r^\star} \frac{\rho^2}{1+\rho^2\tilde{\tau}}$$

$$N_\xi^\star = \frac{\mathbb{V}ar\left[Q^{HF}\right] + \frac{1}{N_\eta^{\mathrm{HF}}}\mathbb{E}\left[\sigma^2_{\eta,\mathrm{HF}}\right]}{\varepsilon^2}\tilde{\Lambda}$$

$$\mathcal{C}_{tot} = N_\xi \tilde{\mathcal{C}}_{\mathrm{HF}} + \tilde{r} N_\xi \tilde{\mathcal{C}}_{\mathrm{LF}} = N_\xi \mathcal{C}^{\mathrm{HF}} \left(N_\eta^{\mathrm{HF}} + \tilde{R} r \frac{\mathcal{C}^{\mathrm{LF}}}{\mathcal{C}^{\mathrm{HF}}} N_\eta^{\mathrm{LF}} \right)$$

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$$\tilde{r}^\star = \sqrt{\frac{1-\rho^2}{1-\rho^2+\rho^2\tilde{\tau}} \frac{N_\eta^{\mathrm{HF}}}{N_\eta^{\mathrm{LF}}}} \sqrt{\frac{\rho^2}{1-\rho^2} \frac{\mathcal{C}^{\mathrm{HF}}}{\mathcal{C}^{\mathrm{LF}}}} = \tilde{R}r^\star \quad \leftarrow \textbf{LF oversampling}$$

$$\tilde{\Lambda} = 1 - \frac{\tilde{R}r^\star - 1}{\tilde{R}r^\star} \frac{\rho^2}{1+\rho^2\tilde{\tau}} \quad \leftarrow \textbf{variance reduction}$$

$$N_\xi^\star = \frac{\mathbb{V}ar\left[Q^{HF}\right] + \frac{1}{N_\eta^{\mathrm{HF}}}\mathbb{E}\left[\sigma^2_{\eta,\mathrm{HF}}\right]}{\varepsilon^2} \tilde{\Lambda} \quad \leftarrow \textbf{HF samples}$$

$$\mathcal{C}_{tot} = N_\xi \tilde{\mathcal{C}}_{\mathrm{HF}} + \tilde{r} N_\xi \tilde{\mathcal{C}}_{\mathrm{LF}} = N_\xi \mathcal{C}^{\mathrm{HF}} \left(N_\eta^{\mathrm{HF}} + Rr \frac{\mathcal{C}^{\mathrm{LF}}}{\mathcal{C}^{\mathrm{HF}}} N_\eta^{\mathrm{LF}} \right) \quad \leftarrow \textbf{Total cost}$$

NOTE: All quantities denoted with $\tilde{\cdot}$ depend on the number of replicas

MF for stochastic solvers

Can we explore the efficiency of the estimator?

The total cost of the MF estimator (for reaching a prescribed variance ε^2) is

$$\mathcal{C}_{tot}^{MF} = \frac{\mathbb{V}ar\left[f^{\mathrm{HF}}\right] + \frac{1}{\mathbf{N}_\eta^{\mathrm{HF}}}\mathbb{E}\left[\sigma^2_{\eta,\mathrm{HF}}\right]}{\varepsilon^2}\mathcal{C}^{\mathrm{HF}}\left(1 - \frac{\tilde{\mathbf{R}}r - 1}{\tilde{\mathbf{R}}r}\frac{\rho^2}{1+\rho^2\tilde{\tau}}\right)\left(\mathbf{N}_\eta^{\mathrm{HF}} + \tilde{\mathbf{R}}r\frac{\mathcal{C}^{\mathrm{LF}}}{\mathcal{C}^{\mathrm{HF}}}\mathbf{N}_\eta^{\mathrm{LF}}\right)$$

Q: How costly would it be to obtain the same accuracy with MC?

$$\mathcal{C}_{MC} = \frac{\mathbb{V}ar\left[f^{\mathrm{HF}}\right] + \frac{1}{N_\eta^{\mathrm{HF}}}\mathbb{E}\left[\sigma^2_{\eta,\mathrm{HF}}\right]}{\varepsilon^2}\tilde{\mathcal{C}}_{\mathrm{HF}} = \frac{\mathbb{V}ar\left[f^{\mathrm{HF}}\right] \frac{1}{N_\eta^{\mathrm{HF}}}\mathbb{E}\left[\sigma^2_{\eta,\mathrm{HF}}\right]}{\varepsilon^2}\mathcal{C}^{\mathrm{HF}}N_\eta^{\mathrm{HF}}$$

Cost ratio:

$$\Theta = \frac{\mathcal{C}_{tot}^{MF}}{\mathcal{C}_{MC}} = \left(1 - \frac{\tilde{R}r - 1}{\tilde{R}r}\frac{\rho^2}{1+\rho^2\tilde{\tau}}\right)\left(1 + \tilde{R}r\frac{\mathcal{C}^{\mathrm{LF}}}{\mathcal{C}^{\mathrm{HF}}}\frac{N_\eta^{\mathrm{LF}}}{N_\eta^{\mathrm{HF}}}\right)$$

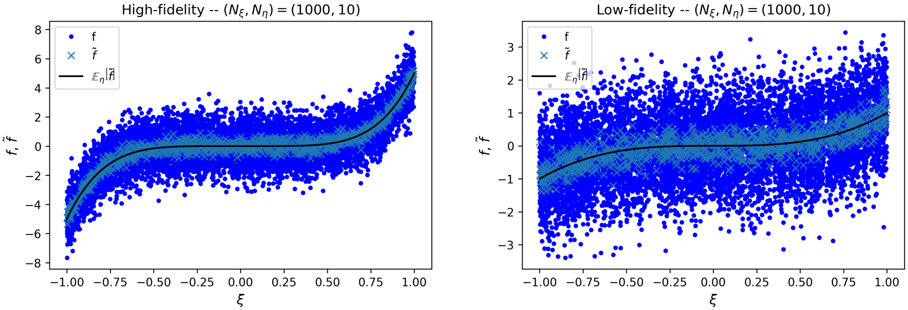
For all these results, in the limit of no noise and $N_\eta^{\mathrm{HF}} = N_\eta^{\mathrm{LF}} = 1$ the original allocation problem is recovered (HINT: $\tau = 0$ and $\tilde{\rho}^2 = \rho^2$...)

Numerical Examples

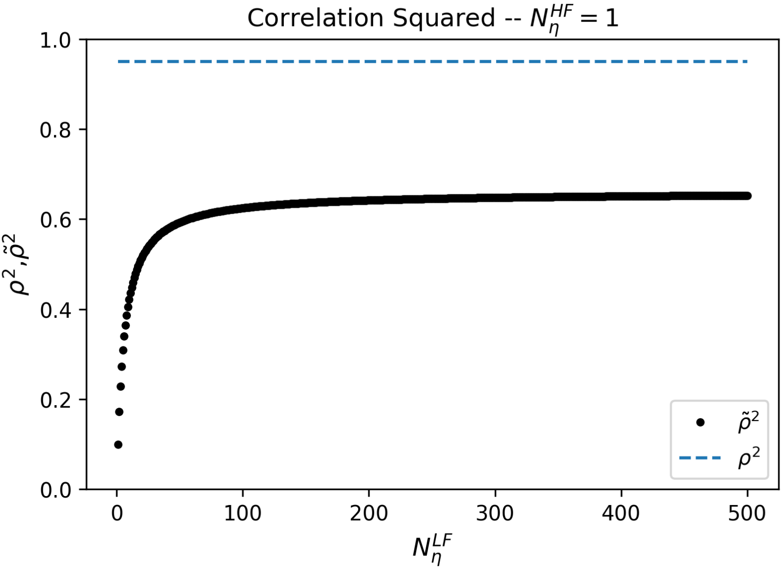
Analytical Verification

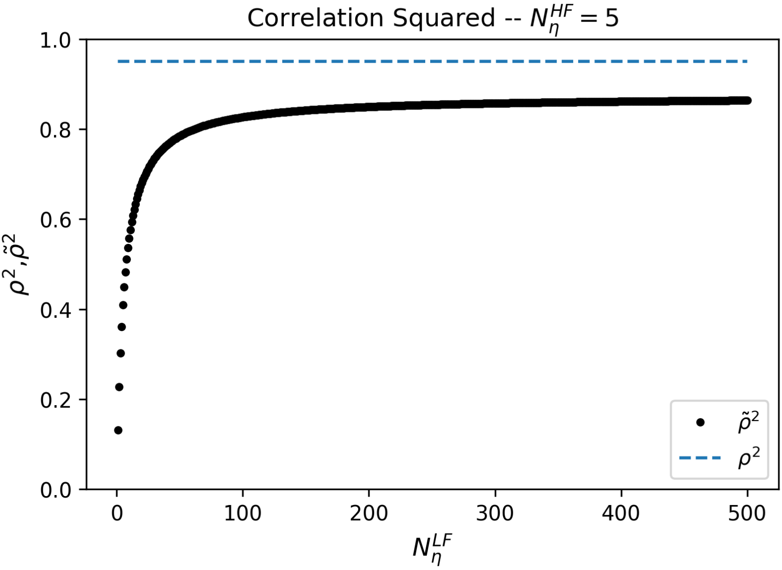
Verification Test Case
Problem Definition

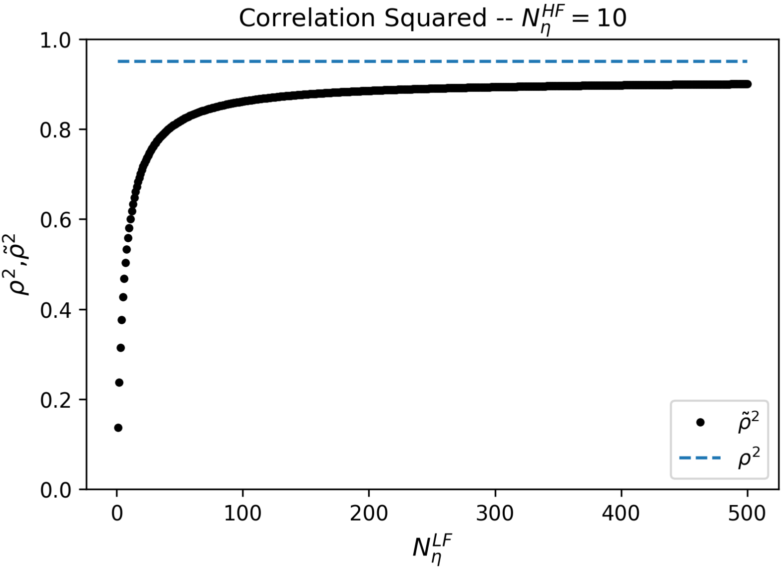
- Stochastic Parameter: $\xi \sim \mathcal{U}(-1, 1)$
- $f_{\text{HF}} = 5\xi^5 + \eta_{\text{HF}}$ where $\eta_{\text{HF}} \sim \mathcal{N}(0, \sigma_{\eta,\text{HF}} = 1)$
- $f_{\text{LF}} = \xi^3 + \eta_{\text{LF}}$ where $\eta_{\text{LF}} \sim \mathcal{N}(0, \sigma_{\eta,\text{LF}} = 0.9)$

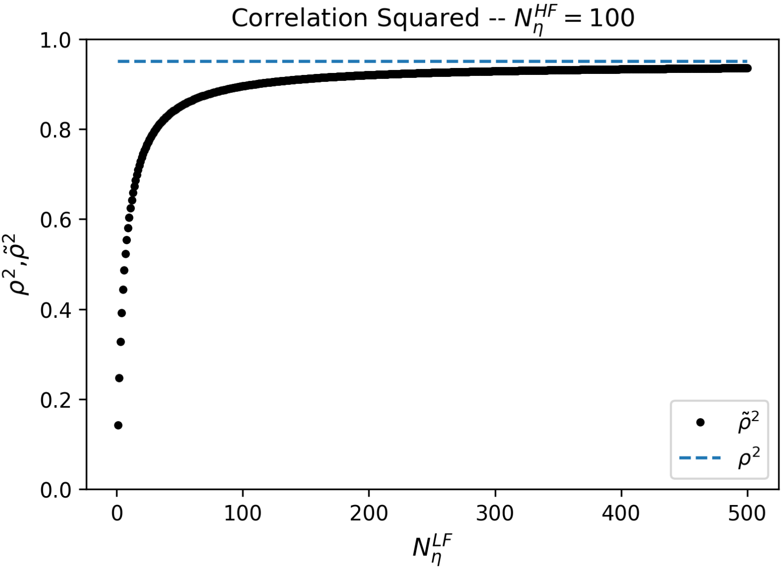


Q: Can we explore the **effect of the number of replicas on the correlation**?
A: The polluted correlation $\tilde{\rho}^2$ is expected to approach ρ^2 for $(N_\eta^{HF}, N_\eta^{LF}) \to \infty$


Correlation Squared -- $N_\eta^{HF} = 1$
1.0
0.8
0.6
0.4
0.2
0.0
$\rho^2, \tilde{\rho}^2$
0
100
200
300
400
500
N_η^{LF}
$\tilde{\rho}^2$
ρ^2


Correlation Squared -- $N_\eta^{HF} = 5$
1.0
0.8
0.6
0.4
0.2
0.0
$\rho^2, \tilde{\rho}^2$
0
100
200
300
400
500
N_η^{LF}
$\tilde{\rho}^2$
ρ^2

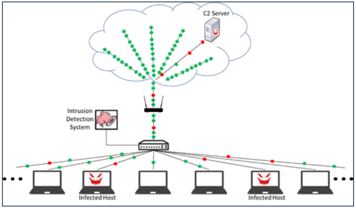

Correlation Squared -- $N_\eta^{HF} = 10$
1.0
0.8
0.6
0.4
0.2
0.0
$\rho^2, \tilde{\rho}^2$
0
100
200
300
400
500
N_η^{LF}
$\tilde{\rho}^2$
ρ^2



Correlation Squared -- $N_\eta^{HF} = 100$
1.0
0.8
0.6
0.4
0.2
0.0
$\rho^2, \tilde{\rho}^2$
0
100
200
300
400
500
N_η^{LF}
$\tilde{\rho}^2$
ρ^2

Cybersecurity – Command and Control (C2)

Command & Control (C2) example
Multifidelity UQ Analysis Scenario



Computer Models:

- **High-Fidelity** is a performed via a **Emulation-Based model**:
  - Set of Virtual Machines (VMs) running **full operating systems on virtualized hardware**
  - `minimega` (SNL) tool for launching and managing VMs
  - SCORCH (SNL) automated scenario orchestration framework
  - Background traffic is present in the system (it introduces stochastic behavior)
  - **Runtime:** 162 s
- **Low-Fidelity** is a performed via a **math model**:
  - **Probabilistic and discrete-time** representation for both traffic and IDS
  - **Runtime:** 0.001 s
  - **Cost ratio** $\mathcal{C}^{HF}/\mathcal{C}^{LF}$ is very high (162×10^3)

Parameters Varied in Experiment	Units	Value	Distribution
Aggregate Benign traffic rate in packets/sec	Packets per sec	100-3000	Continuous log-uniform
Fraction of benign packets with emotet signatures.	No Units	1e-5 to 8e-4	Log-uniform
Aggregate Malware traffic rate in packets/sec	Packets per sec	10-20	Uniform
Fraction of malware packets with emotet signatures	No units	0.01-0.025	Uniform
RAM assigned to the 1 CPU running SNORT	Mbytes	128, 256, 512, 1024	Discrete with equal probability

Command & Control example
Numerical Approach

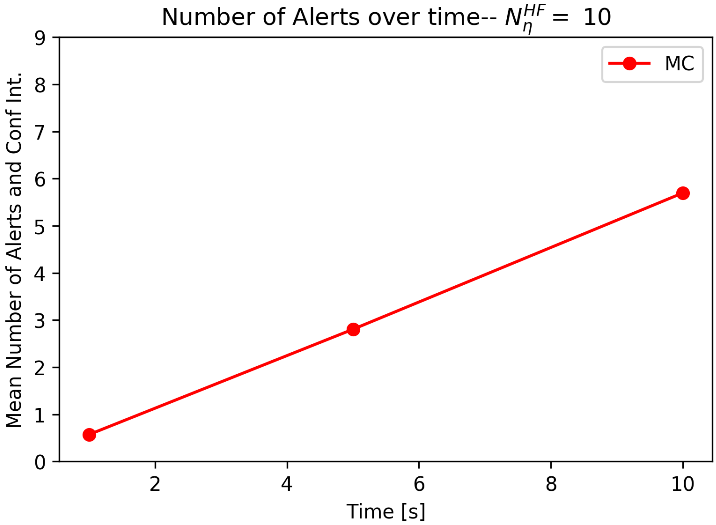
Numerical Study:

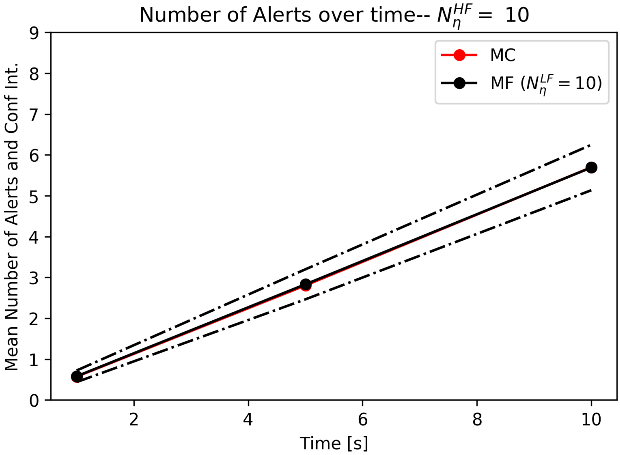
- We have a pilot set of $(N_\xi, N_\eta^{HF}) = (40, 10)$ for both model
  - From pilot samples we can estimate $\rho^2 = \rho^2(\tilde{\tau}, \tilde{\rho})$
  - $\mathbb{V}ar\left[Q^{HF}\right] = \mathbb{V}ar\left[Q^{HF}\right]\left(\mathbb{V}ar\left[\tilde{Q}^{HF}\right], N_\eta^{HF}\right)$ and $\mathbb{V}ar\left[Q^{LF}\right] = \mathbb{V}ar\left[Q^{LF}\right]\left(\mathbb{V}ar\left[\tilde{Q}^{LF}\right], N_\eta^{LF}\right)$
- We want to **build the most optimal MF estimator given the HF runs**, *i.e.* we need to optimize the total number of LF simulations (and the number of replicas)

Optimization Solutions:

1. MF estimator given $N_\eta^{LF} = 10$: the total number of LF runs is $\lceil \tilde{R}(10, 10)\, r^\star \rceil \times 10$
2. MF estimator with optimal N_η^{LF}:
$$\underset{N_\eta^{LF}}{\operatorname{argmin}}\, \Theta$$
The total number of LF runs is $\lceil \tilde{R}(10, N_\eta^{LF,\star})\, r^\star \rceil \times N_\eta^{LF,\star}$
3. MF estimator with $N_\eta^{LF} = 10$ but total cost equal to **[2]**: $\lceil \tilde{R}(10, N_\eta^{LF,\star})\, \mathbf{r} \rceil \times N_\eta^{LF,\star}$
4. MC with equivalent cost (of **[2]** and **[3]**)

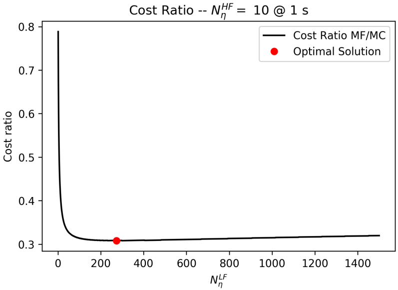
We consider three temporal locations, *i.e.* 1, 5, 10 s → **select the most restrictive condition** (highest number of LF runs)

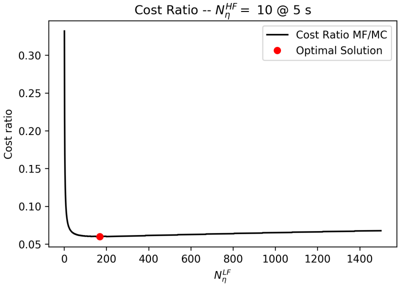

Number of Alerts over time-- $N_{\eta}^{HF} =$ 10
MC
Mean Number of Alerts and Conf Int.
Time [s]
0
1
2
3
4
5
6
7
8
9
2
4
6
8
10

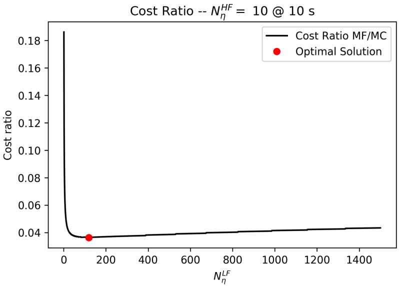


Estimator	N_ξ	$\tilde{r}$	N_η^{LF}	$\tilde{\Lambda}$ $t = 1$s	$t = 5$s	$t = 10$s	$N_\xi^{HF,eq}$
MF	40	1762.34	10	0.425	0.091	0.050	41

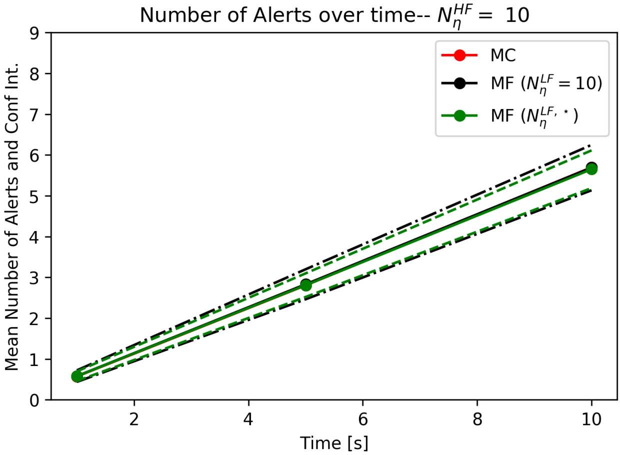
Command & Control example
Optimizing Number of Replicas







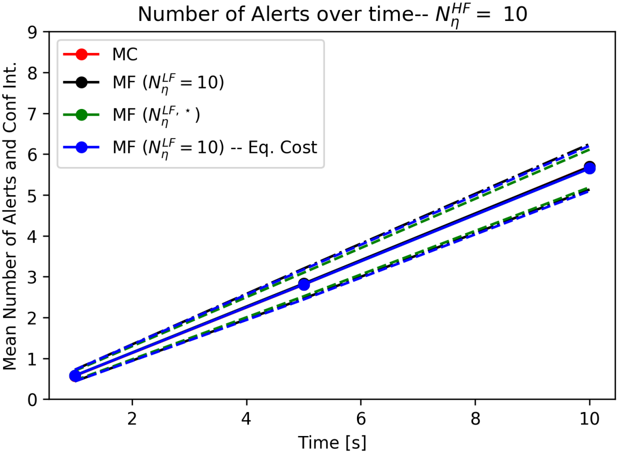
Solving N_η^{LF} for the minimum cost ratio, i.e. maximum MF efficiency



Estimator	N_ξ	$\tilde{r}$	N_η^{LF}	$\tilde{\Lambda}$ $t = 1$s	$t = 5$s	$t = 10$s	$N_\xi^{HF,eq}$
MF	40	1762.34	10	0.425	0.091	0.050	41
MF ($N_\eta^{LF,\star}$)	40	421	274	0.297	0.056	0.034	43

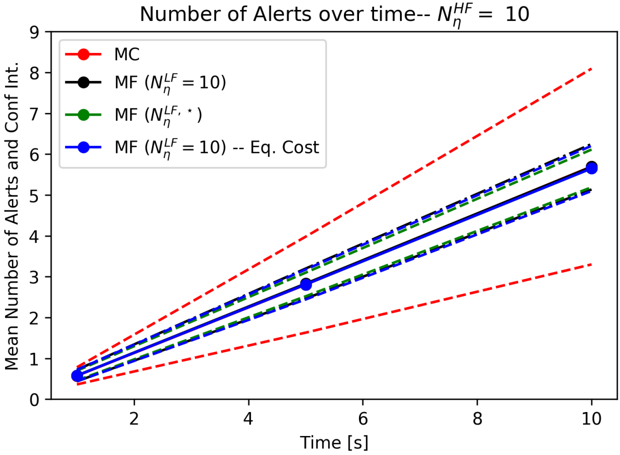
Command & Control example

Comparing Optimization Strategies – 99.7% Confidence Interval



Estimator	N_ξ	$\tilde{r}$	N_η^{LF}	$\tilde{\Lambda}$ $t = 1$s	$t = 5$s	$t = 10$s	$N_\xi^{HF,eq}$
MF	40	1762.34	10	0.425	0.091	0.050	41
MF ($N_\eta^{LF,\star}$)	40	421	274	0.297	0.056	0.034	43
MF ($\mathcal{C}_{eq}$)	40	11536.8	10	0.424	0.090	0.049	43

Command & Control example
Comparing Optimization Strategies – 99.7% Confidence Interval

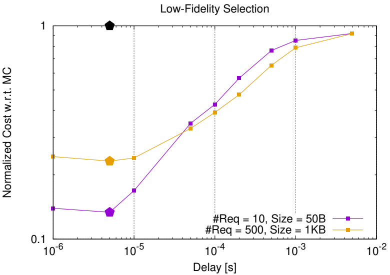


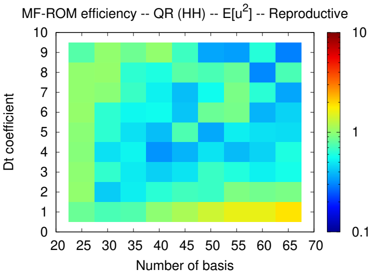
Estimator	N_ξ	$\tilde{r}$	N_η^{LF}	$\tilde{\Lambda}$ $t = 1$s	$t = 5$s	$t = 10$s	$N_\xi^{HF,eq}$
MF	40	1762.34	10	0.425	0.091	0.050	41
MF ($N_\eta^{LF,\star}$)	40	421	274	0.297	0.056	0.034	43
MF ($\mathcal{C}_{eq}$)	40	11536.8	10	0.424	0.090	0.049	43
MC	43	-	-	-	-	-	43

Conclusions

Is something similar arising in other contexts?

- This problem can be interpreted as an instance of a **Model Tuning** problem for MF
- **Model Tuning** in this context means that you could have additional parameters non-shared among models that you could consider hyper-parameters for tuning by increasing the correlation among models, and hopefully the MF estimator efficiency
- For instance, you could select the best spatial resolution of a LF model, the 'optimal' RANS coefficients in a LES-RANS MF problem, etc.
- In a **Model Tuning** exercise you can only optimize LF model parameters





Summary:

- **Stochastic Solvers** are widely used for several computational applications
- UQ with Sampling-based methods needs to **incorporate the noise** introduced by these solvers
- We demonstrated that the **number of replicas can be optimized** for maximizing the MF estimator efficiency

Work-in-Progress:

- Maximizing the MF efficiency is a Model Tuning exercise (more on this in Mike Eldred's talk)
- Extension to ACV (or similar approaches) is possible (and possibly more interesting)

(Incomplete) list of references:

CV Pasupathy, R., Taaffe, M., Schmeiser, B. W. & Wang, W., Control-variate estimation using estimated control means. *IIE Transactions*, **44**(5), 381–385, 2012

MFMC Ng, L.W.T. & Willcox, K. Multifidelity Approaches for Optimization Under Uncertainty. *Int. J. Numer. Meth. Engng* 100, no. 10, pp. 746772, 2014.

MFMC Peherstorfer, B., Willcox, K. & Gunzburger, M., Optimal Model Management for Multifidelity Monte Carlo Estimation. *SIAM J. Sci. Comput*. 38(5), A3163A3194.

ACV A.A. Gorodetsky, G. Geraci, M.S. Eldred & J.D. Jakeman, A Generalized Framework for Approximate Control Variates. *Journal of Computational Physics*, 2020.

CompNetw G. Geraci, J. Crussell, L.P. Swiler & B.J. Debusschere, Exploration of multifidelity UQ sampling strategies for computer network applications. *International Journal for Uncertainty Quantification*, Vol. 11(1), 2021.

MF-ROM P. Blonigan, G. Geraci, F. Rizzi, M.S. Eldred, Towards an integrated and efficient framework for leveraging reduced order models for multifidelity uncertainty quantification. *AIAA SciTech 2020*, 2020.

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Why are we interested in network models?

- Network **operators**: understand the potential impacts of changes **before implementing** them
- Network **designers**: understand trade-offs **before** network **creation**

Network modeling refers to:

- **Simulation:** similar to their physics-modeling counterparts and they are **based on a deep understanding of the underlying processes** to simulate network components and interactions in software
- **Emulation:** run the real software on virtualized hardware thus it is able to **capture unknown or not well-understood behaviors**

Examples of Network modeling at Sandia (Courtesy of David Fritz, SAND2018-3927[3])

- **DevOps:** Ensure operation of new hardware, software, services in high-consequence environments. Predictive analysis to detect malfunctions, misconfigurations and malicious consequences
- **Malware:** Understanding of malware through pseudo-in situ execution
- **ICS/SCADA:** Under uncertain threats, what are the best countermeasures for my IT-connected ICS systems? Can we detect attacks? Can we assess resiliency of the IT-controls over the entire power grids?
- **Nuclear Weapons:** Can we assure Communication, Command and Control regardless of network state and threats?

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[3] http://minimega.org/presentations/gt_2018.slide#7