Multifidelity Uncertainty Quantification

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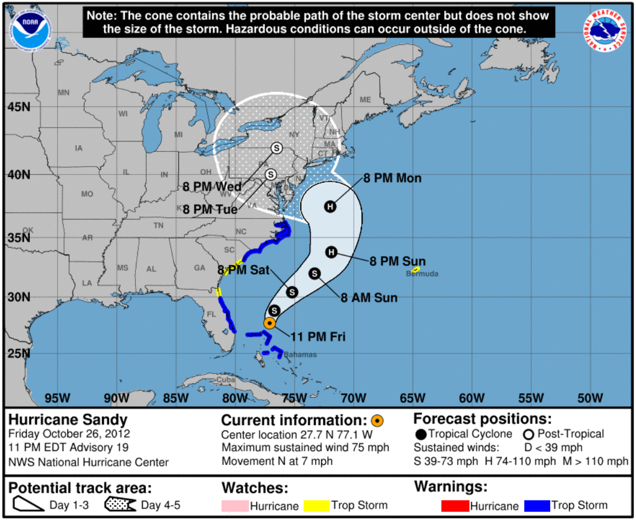
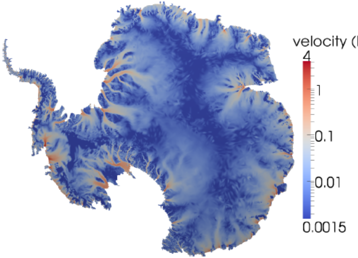
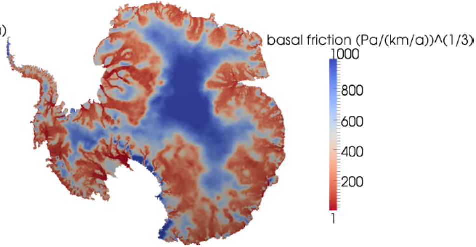
Intro: Uncertainties due to data



[Figure: NOAA]

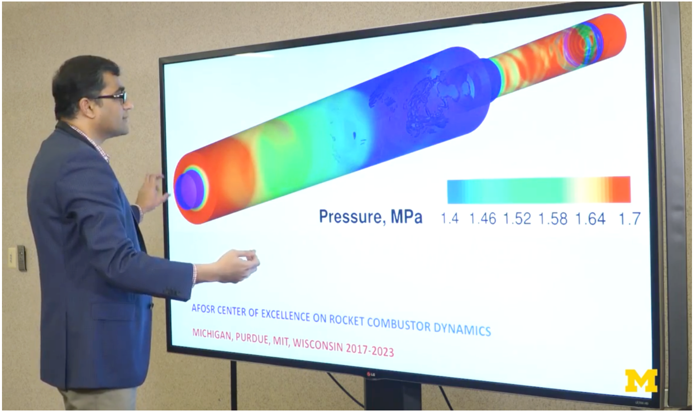
Intro: Uncertainties due to unknown parameters





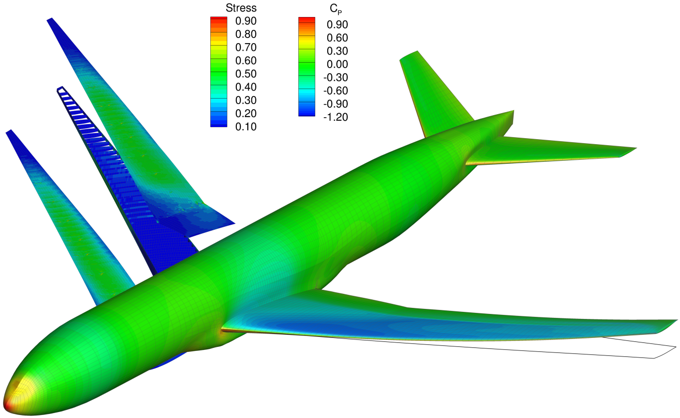
[Figures: Petra, Ghattas, Isaac, Martin, Stadler, et al.]

Intro: No hope to exhaustively model physics



[Figure: University of Michigan]

Intro: Manufacturing variations

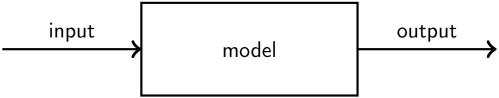


[Kenway, G. K., Martins, J. R., & Kennedy, G. J. (2014). Aerostructural optimization of the Common Research Model configuration. Group (ADODG), 6(7), 8-9.]

Intro: Model

Model of system of interest

- Model describes response of system to inputs, parameters, configurations
- Response typically is a quantity of interest
- Evaluating a model means numerically simulating the model
- Many models given in form of partial differential equations



Mathematical formulation

$$f : \mathcal{D} \to \mathcal{Y}$$

- Input domain $\mathcal{D}$ and output domain $\mathcal{Y}$
- Maps $\boldsymbol{z} \in \mathcal{D}$ input onto $\boldsymbol{y} \in \mathcal{Y}$ output (quantity of interest)

Intro: Model - Navier-Stokes equations

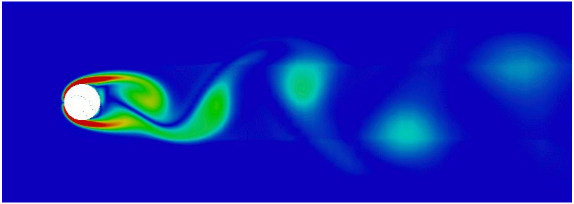
$$\rho \left(\frac{\partial u}{\partial t} + u \cdot \nabla u \right) = -\nabla p + \mu \Delta u + g$$

Examples of inputs

- Density ρ
- Dynamic viscosity μ

Examples of outputs (quantities of interest)

- Velocity at monitoring point
- Average pressure



[Figure: MFIX, NETL, DOE]

Intro: Model - Diffusion-convection-reaction flow

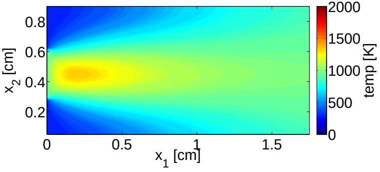
$$\frac{\partial u}{\partial t} = \Delta u - v \nabla u + g(u, \boldsymbol{\mu})$$

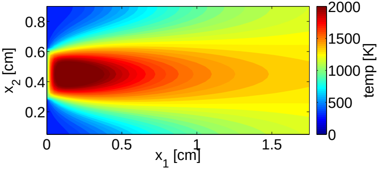
Examples of inputs

- Activation energy and pre-exponential factor (Arrhenius-type reaction)
- Temperature at boundary
- Ratio of fuel and oxidizer

Examples of outputs

- Average temperature in chamber





Intro: Uncertain inputs

Inputs are uncertain

- Measurement errors in boundary conditions
- Manufacturing variations
- Model parameters determined by engineering judgment
- ...

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Mathematically formulate uncertain inputs as random variables

$$Z : \Omega \to \mathcal{D}$$

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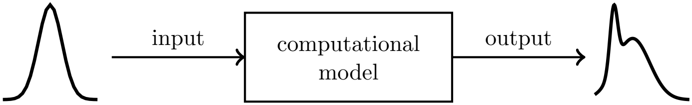
$$Z : \Omega \to \mathcal{D}$$

Quantify effect of uncertainties in inputs on model outputs



Intro: General sampling-based approach to UQ

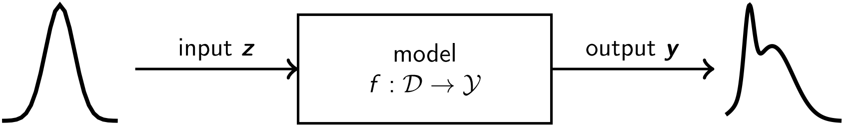
- Take many realizations of input random variable Z

$$\boldsymbol{z}_1, \ldots, \boldsymbol{z}_n \in \mathcal{D}$$

- Evaluate model f at all $\boldsymbol{z}_1, \ldots, \boldsymbol{z}_n$ realizations

$$\boldsymbol{y}_1 = f(\boldsymbol{z}_1), \ldots, \boldsymbol{y}_n = f(\boldsymbol{z}_n)$$

- Estimate statistics (mean, std. deviation, etc) from outputs $\boldsymbol{y}_1, \ldots, \boldsymbol{y}_n$



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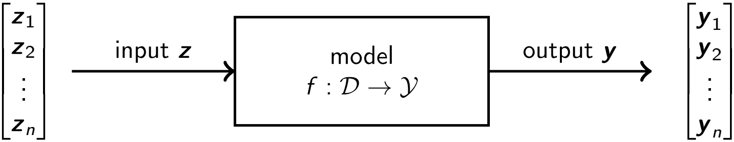

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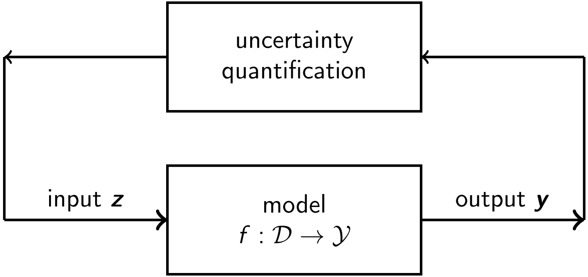

Monte Carlo

[Figure: Martinp1, Wikipedia]

Monte Carlo

- Models treated as black box

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Monte Carlo

- Models treated as black box
- Dimension independent

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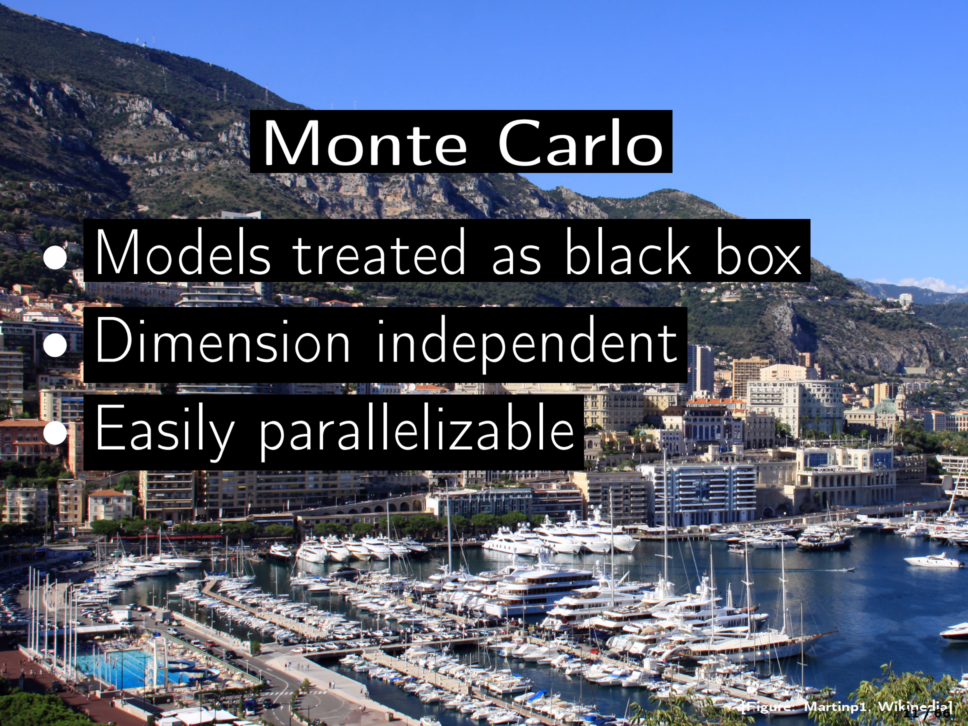
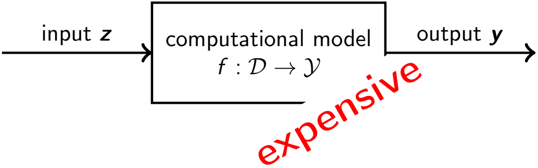
Monte Carlo

- Models treated as black box
- Dimension independent
- Easily parallelizable



[Figure: Martinp1, Wikipedia]

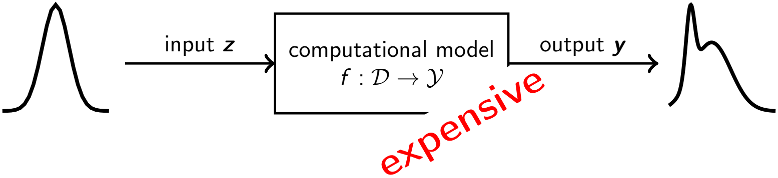
Intro: Challenges of sampling-based UQ



Challenges

- Formulation and modeling of uncertainties
- Models based on PDEs: nonlinear, multi-scale, multi-physics
- Single model solve expensive; repeated solves prohibitive $\Rightarrow$ multifidelity
- Uncertain parameters are of high dimension

Intro: Challenges of sampling-based UQ



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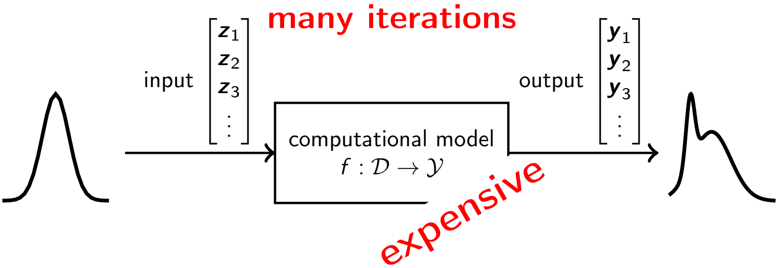

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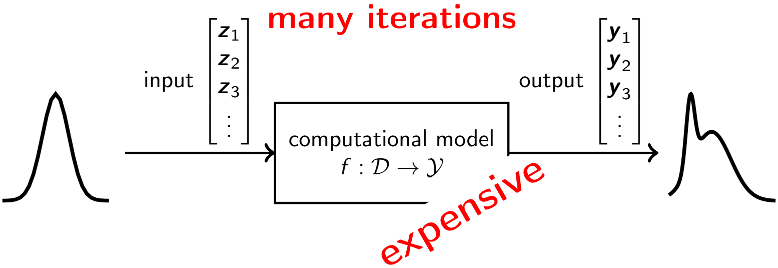

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- Formulation and modeling of uncertainties
- Models based on PDEs: nonlinear, multi-scale, multi-physics
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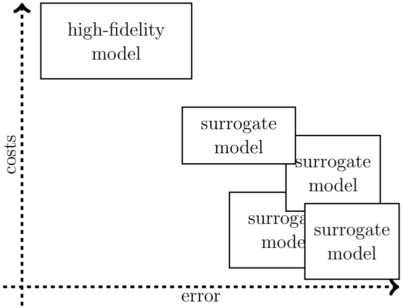
Intro: Opportunity of low-fidelity models

Given is typically a high-fidelity model

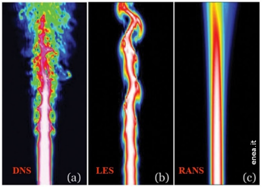
- Large-scale numerical simulation
- Achieves required accuracy
- Computationally expensive

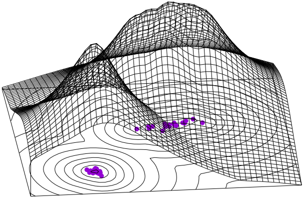


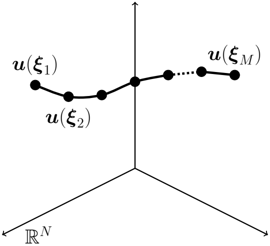
Additionally, often have available or can train low-fidelity models

- Approximate same quantity of interest as high-fidelity model
- Often orders of magnitudes cheaper than high-fidelity model
- Less accurate and typically no accuracy guarantees

Intro: Three types of low-fidelity models







simplified models

- Simplifying physics
- Coarser discretizations
- Linearized models
- Early stopping of iterative solvers

data-fit models

- Fitting model to data of input-output map given by high-fidelity model
- Response surfaces
- Gaussian processes
- Neural networks

reduced models

- Extract important dynamics of full states from *data*
- Approximate high-dimensional states in subspaces
- Restrict solving governing equations to subspaces

Intro: Low-fidelity models

Replace high- with low-fidelity model

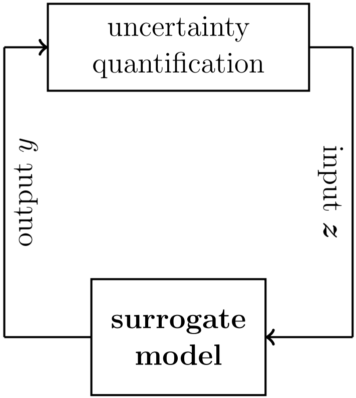
- Costs of outer loop application reduced
- Often orders of magnitude speedups

Low-fidelity model introduces error

- Control with error bounds/estimators*
- Rebuild if accuracy too low
- No guarantees without bounds/estimators

Issues

- Propagation of output error on estimate
- Applications without error control
- Costs of rebuilding a low-fidelity model



Multifidelity: Combine multiple models

Combine high-fidelity and low-fidelity models

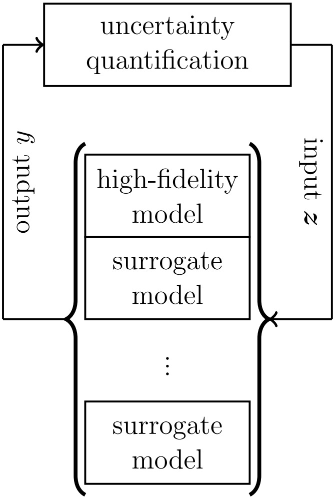
- Leverage low-fidelity models for speedup
- Recourse to high-fidelity for accuracy

Multifidelity speeds up computations

- Balance #solves among models
- Adapt, fuse, filter with low-fidelity models

Multifidelity guarantees high-fidelity accuracy

- Occasional recourse to high-fidelity model
- High-fidelity model is kept in the loop
- Independent of error control of low fidelity



[P., Willcox, Gunzburger, Survey of multifidelity methods in uncertainty propagation, inference, and optimization. SIAM Review, 60(3):550-591, 2018]

Intro: Survey with *many* references

SIAM REVIEW
Vol. 60, No. 3, pp. 550–591

Survey of Multifidelity Methods in Uncertainty Propagation, Inference, and Optimization*

Benjamin Peherstorfer[†]
Karen Willcox[‡]
Max Gunzburger[§]

Abstract. In many situations across computational science and engineering, multiple computational models are available that describe a system of interest. These different models have varying evaluation costs and varying fidelities. Typically, a computationally expensive high-fidelity model describes the system with the accuracy required by the current application at hand, while lower-fidelity models are less accurate but computationally cheaper than the high-fidelity model. Outer-loop applications, such as optimization, inference, and uncertainty quantification, require multiple model evaluations at many different inputs, which often leads to computational demands that exceed available resources if only the high-fidelity model is used. This work surveys multifidelity methods that accelerate the solution of outer-loop applications by combining high-fidelity and low-fidelity model evaluations, where the low-fidelity evaluations arise from an explicit low-fidelity model (e.g., a simplified physics approximation, a reduced model, a data-fit surrogate) that approximates the same output quantity as the high-fidelity model. The overall premise of these multifidelity methods is that low-fidelity models are leveraged for speedup while the high-fidelity model is kept in the loop to establish accuracy and/or convergence guarantees. We categorize multifidelity methods according to three classes of strategies: adaptation, fusion, and filtering. The paper reviews multifidelity methods in the outer-loop contexts of uncertainty propagation, inference, and optimization.

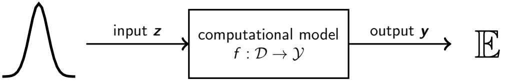
Key words. multifidelity, surrogate models, model reduction, multifidelity uncertainty quantification, multifidelity uncertainty propagation, multifidelity statistical inference, multifidelity optimization

AMS subject classifications. 65-02, 62-02, 49-02

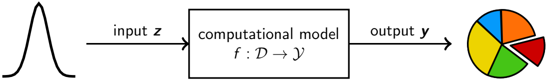
DOI. 10.1137/16M1082469

Uncertainty quantification tasks

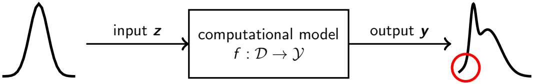
1. Multifidelity uncertainty propagation



2. Multifidelity sensitivity analysis



3. Multifidelity failure probability estimation



4. Other multifidelity uncertainty quantification tasks

Uncertainty quantification tasks

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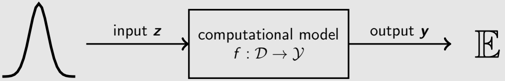

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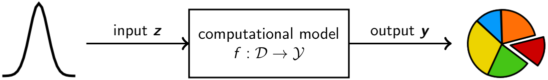

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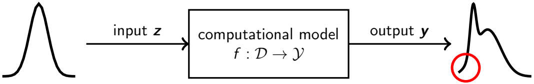


4. Other multifidelity uncertainty quantification tasks

MFMC: Monte Carlo estimation

High-fidelity ("truth") model, costs $w_1 > 0$

$$f^{(1)} : \mathcal{D} \to \mathcal{Y}$$

Random variable Z, estimate

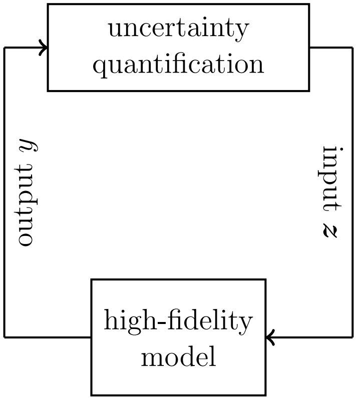
$$s = \mathbb{E}[f^{(1)}(Z)]$$

Monte Carlo estimate of s with real. $z_1, \dots, z_n$

$$\bar{y}_n^{(1)} = \frac{1}{n} \sum_{i=1}^{n} f^{(1)}(z_i)$$

Computational costs

- Many evaluations of high-fidelity model
- Typically $10^3 - 10^6$ evaluations
- Intractable if $f^{(1)}$ expensive



MFMC: Control variates

Given is a random variable A and we want to estimate its mean

$$s_A = \mathbb{E}[A]$$

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Independent and identically distributed (i.i.d.) samples

$$a_1, \dots, a_n$$

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Regular Monte Carlo estimator of s_A

$$\bar{a}_n = \frac{1}{n} \sum_{i=1}^{n} a_i$$

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Regular Monte Carlo estimator of s_A

$$\bar{a}_n = \frac{1}{n} \sum_{i=1}^{n} a_i$$

Unbiased estimator $\mathbb{E}[\bar{a}_n] = s_A$ with mean-squared error (MSE)

$$\mathrm{Var}[\bar{a}_n] = \frac{1}{n^2} \mathrm{Var}\left[\sum_{i=1}^{n} a_i\right] = \frac{\mathrm{Var}[A]}{n}$$

MFMC: Control variates (cont'd)

Additional random variable B with *known* mean $s_B = \mathbb{E}[B]$ and samples

$$b_1, \dots, b_n$$

MFMC: Control variates (cont'd)

Additional random variable B with *known* mean $s_B = \mathbb{E}[B]$ and samples

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Regular Monte Carlo estimator of s_B

$$\bar{b}_n = \frac{1}{n} \sum_{i=1}^{n} b_i$$

MFMC: Control variates (cont'd)

Additional random variable B with *known* mean $s_B = \mathbb{E}[B]$ and samples

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$$\bar{b}_n = \frac{1}{n} \sum_{i=1}^{n} b_i$$

Control variate estimator of s_A that uses samples from A and B

$$\hat{s}_A = \bar{a}_n + \left(s_B - \bar{b}_n\right)$$

MFMC: Control variates (cont'd)

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Control variate estimator of s_A that uses samples from A and B

$$\hat{s}_A = \bar{a}_n + \left(s_B - \bar{b}_n\right)$$

Introduce coefficient $\alpha \in \mathbb{R}$ to balance A and B

$$\hat{s}_A = \bar{a}_n + \alpha \left(s_B - \bar{b}_n\right)$$

Combines n samples of A and n samples of B

[Nelson, 87]

MFMC: Control variates (cont'd)

Control variate estimator

$$\hat{s}_A = \bar{a}_n + \alpha \left(s_B - \bar{b}_n \right)$$

MFMC: Control variates (cont'd)

Control variate estimator

$$\hat{s}_A = \bar{a}_n + \alpha \left(s_B - \bar{b}_n \right)$$

Unbiased estimator of s_A because

$$\mathbb{E}[\hat{s}_A] = \underbrace{\mathbb{E}[\bar{a}_n]}_{=s_A} + \alpha \underbrace{\mathbb{E}[s_B - \bar{b}_n]}_{=0} = s_A$$

MFMC: Control variates (cont'd)

Control variate estimator

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Variance of control variate estimator for optimal* $\alpha \in \mathbb{R}$

$$\mathrm{Var}[\hat{s}_A] = (1 - \rho^2) \frac{\mathrm{Var}[A]}{n} = (1 - \rho^2) \, \mathrm{Var}[\bar{a}_n]$$

- Correlation coefficient $-1 \leq \rho \leq 1$ of A and B
- If $\rho = 0$, same variance as regular Monte Carlo
- If $|\rho| > 0$, lower variance
- The higher correlated, the lower variance of $\hat{s}_A$

MFMC: Multifidelity Monte Carlo Estimation

Estimate expected value

$$s = \mathbb{E}[f^{(1)}(Z)]$$

Low-fidelity models

$$f^{(2)}, f^{(3)}, \dots, f^{(k)} : \mathcal{D} \to \mathcal{Y}$$

Correlation coefficients

$$\rho_2 = \mathrm{Corr}[f^{(1)}, f^{(2)}], \rho_3 = \mathrm{Corr}[f^{(1)}, f^{(3)}], \dots, \rho_k = \mathrm{Corr}[f^{(1)}, f^{(k)}]$$

Costs

$$w_1, w_2, \dots, w_k > 0$$

***No* need to know expected values of low-fidelity models!**

MFMC: Multifidelity Monte Carlo

Reminder: Monte Carlo estimator

$$\bar{y}_n^{(1)} = \frac{1}{n} \sum_{i=1}^{n} f^{(1)}(z_i)$$

Multifidelity Monte Carlo (MFMC) estimator

$$\hat{s} = \underbrace{\bar{y}_{m_{\mathbf{1}}}^{(1)}}_{\text{from HFM}} + \sum_{i=2}^{k} \alpha_i \underbrace{\left(\bar{y}_{m_i}^{(i)} - \bar{y}_{m_{i-\mathbf{1}}}^{(i)} \right)}_{\text{from low-fid. models}}$$

- Monte Carlo estimator

$$\bar{y}_{m_i}^{(i)} = \frac{1}{m_i} \sum_{i=1}^{m_i} f^{(i)}(\boldsymbol{z}_i)$$

- Number of model evaluations $\boldsymbol{m} = [m_1, \ldots, m_k]^T$
- Control variate coefficients $\boldsymbol{\alpha} = [\alpha_2, \ldots, \alpha_k]^T$
- Optimal selection of $\boldsymbol{m}$ and $\boldsymbol{\alpha}$ $\rightarrow$ our code

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MFMC: Recipe 1

Download

`https://github.com/pehersto/mfmc`

Given

- Models $f^{(1)}, f^{(2)}, \ldots, f^{(k)}$
- Computational budget b

Pilot run

- Draw m_0 (≈ 50) realizations of Z
- Evaluate each model $f^{(1)}, f^{(2)}, \ldots, f^{(k)}$ at the m_0 realizations

$$\boldsymbol{Y} = \begin{bmatrix} f^{(1)}(\boldsymbol{z}_1) & f^{(2)}(\boldsymbol{z}_1) & \ldots & f^{(k)}(\boldsymbol{z}_1) \\ \vdots & \vdots & & \vdots \\ f^{(1)}(\boldsymbol{z}_{m_0}) & f^{(2)}(\boldsymbol{z}_{m_0}) & \ldots & f^{(k)}(\boldsymbol{z}_{m_0}) \end{bmatrix}$$

- Estimate computational costs of model evaluations $\boldsymbol{w} = [w_1, \ldots, w_k]^T$

MFMC: Recipe 1 (cont'd)

Determine number of model evaluations

```
[ m, a ] = optiMlevelCorr( Y, w, b )
```

- Number of model evaluations $\boldsymbol{m} = [m_1, m_2, \dots, m_k]^T$
- Coefficients $\boldsymbol{a} = [\alpha_2, \alpha_3, \dots, \alpha_k]^T$

Draw realizations

$$\boldsymbol{z}_1, \boldsymbol{z}_2, \dots, \boldsymbol{z}_{m_k}$$

Evaluate models

$$f^{(i)}(\boldsymbol{z}_1), \dots, f^{(i)}(\boldsymbol{z}_{m_i}), \qquad i = 1, \dots, k$$

Estimate

$$\hat{s} = \underbrace{\bar{y}_{m_1}^{(1)}}_{\text{from HFM}} + \sum_{i=2}^{k} \alpha_i \underbrace{\left(\bar{y}_{m_i}^{(i)} - \bar{y}_{m_{i-1}}^{(i)}\right)}_{\text{from low.-fid. models}}$$

MFMC: Matlab code for Recipe 1

```
modelList = {HFM,LFM1,LFM2,LFM3}; % models
w = [100, 50, 20, 10]'; % costs
budget = 1000*w(1); % total budget
```

MFMC: Matlab code for Recipe 1

```
modelList = {HFM,LFM1,LFM2,LFM3}; % models
w = [100, 50, 20, 10]'; % costs
budget = 1000*w(1); % total budget

mu = drawSamples(50); % pilot samples
for i=1:length(modelList)
  Y(:, i) = modelList{i}(mu);
end
```

MFMC: Matlab code for Recipe 1

```matlab
modelList = {HFM,LFM1,LFM2,LFM3}; % models
w = [100, 50, 20, 10]'; % costs
budget = 1000*w(1); % total budget

mu = drawSamples(50); % pilot samples
for i=1:length(modelList)
  Y(:, i) = modelList{i}(mu);
end

[m, alpha] = optiMlevelCorr(Y, w, budget); % MFMC
```

MFMC: Matlab code for Recipe 1

```matlab
modelList = {HFM,LFM1,LFM2,LFM3}; % models
w = [100, 50, 20, 10]'; % costs
budget = 1000*w(1); % total budget

mu = drawSamples(50); % pilot samples
for i=1:length(modelList)
  Y(:, i) = modelList{i}(mu);
end

[m, alpha] = optiMlevelCorr(Y, w, budget); % MFMC

z = drawSamples(m(end)); % draw realizations
```

MFMC: Matlab code for Recipe 1

```
modelList = {HFM,LFM1,LFM2,LFM3}; % models
w = [100, 50, 20, 10]'; % costs
budget = 1000*w(1); % total budget

mu = drawSamples(50); % pilot samples
for i=1:length(modelList)
  Y(:, i) = modelList{i}(mu);
end

[m, alpha] = optiMlevelCorr(Y, w, budget); % MFMC

z = drawSamples(m(end)); % draw realizations

y = modelList{1}(z(1:m(1), :)); % evaluate HFM
sHat = alpha(1)*mean(y);
```

MFMC: Matlab code for Recipe 1

```
modelList = {HFM,LFM1,LFM2,LFM3}; % models
w = [100, 50, 20, 10]'; % costs
budget = 1000*w(1); % total budget

mu = drawSamples(50); % pilot samples
for i=1:length(modelList)
  Y(:, i) = modelList{i}(mu);
end

[m, alpha] = optiMlevelCorr(Y, w, budget); % MFMC

z = drawSamples(m(end)); % draw realizations

y = modelList{1}(z(1:m(1), :)); % evaluate HFM
sHat = alpha(1)*mean(y);

% evaluate low-fidelity models
for i=2:length(modelList)
  y = modelList{i}(z(1:m(i), :));
  sHat = sHat+alpha(i)*(mean(y)-mean(y(1:m(i-1))));
end
```

MFMC: Recipe 2 (MFMC as post-processing)

Given

- Model evaluations

$$f^{(i)}(\boldsymbol{z}_1), \dots, f^{(i)}(\boldsymbol{z}_{m_i}), \qquad i = 1, \dots, k$$

- Model evaluation costs $w_1, \dots, w_k$

Pilot samples

- Use the first $m_0 \ll m_1$ samples to form

$$\boldsymbol{Y} = \begin{bmatrix} f^{(1)}(\boldsymbol{z}_1) & f^{(2)}(\boldsymbol{z}_1) & \dots & f^{(k)}(\boldsymbol{z}_1) \\ \vdots & \vdots & & \vdots \\ f^{(1)}(\boldsymbol{z}_{m_0}) & f^{(2)}(\boldsymbol{z}_{m_0}) & \dots & f^{(k)}(\boldsymbol{z}_{m_0}) \end{bmatrix}$$

- Derive coefficients

```
[ ~, a ] = optiMlevelCorr( Y, w, b )
```

Estimate

$$s = \underbrace{\bar{y}^{(1)}_{m_1}}_{\text{from HFM}} + \sum_{i=2}^{k} \alpha_i \underbrace{\left(\bar{y}^{(i)}_{m_i} - \bar{y}^{(i)}_{m_{i-1}}\right)}_{\text{from low.-fid. models}}$$

MFMC: Recipe 2 (MFMC as post-processing)

Given

- Model evaluations

$$f^{(i)}(\boldsymbol{z}_1), \dots, f^{(i)}(\boldsymbol{z}_{m_i}), \qquad i = 1, \dots, k$$

- Model evaluation costs $w_1, \dots, w_k$

Pilot samples

- Use the first $m_0 \ll m_1$ samples to form

$$\boldsymbol{Y} = \begin{bmatrix} f^{(1)}(\boldsymbol{z}_1) & f^{(2)}(\boldsymbol{z}_1) & \dots & f^{(k)}(\boldsymbol{z}_1) \\ \vdots & \vdots & & \vdots \\ f^{(1)}(\boldsymbol{z}_{m_0}) & f^{(2)}(\boldsymbol{z}_{m_0}) & \dots & f^{(k)}(\boldsymbol{z}_{m_0}) \end{bmatrix}$$

- Derive coefficients

```
[ ~, a ] = optiMlevelCorr( Y, w, b )
```

Estimate

$$s = \underbrace{\bar{y}^{(1)}_{m_1}}_{\text{from HFM}} + \sum_{i=2}^{k} \alpha_i \underbrace{\left(\bar{y}^{(i)}_{m_i} - \bar{y}^{(i)}_{m_{i-1}}\right)}_{\text{from low.-fid. models}}$$

MFMC: AeroStruct: Problem setup

Coupled aero-structural wing analysis

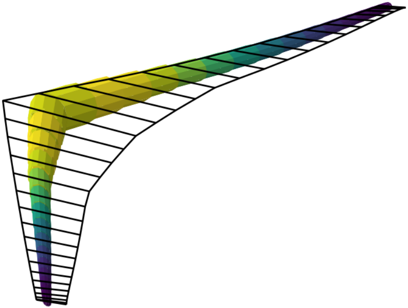
- Uncertain are angle of attack, air density, Mach number
- Estimate expected fuel burn

High-fidelity model $f^{(1)}$

- OpenAeroStruct code
- Vortex-lattice method
- 6 DoF 3-dim spatial beam model
- Used with default configuration

Low-fidelity models

- Spline interpolants on equidistant grid
- Low-fidelity model $f^{(2)}$ from 343 points
- Low-fidelity model $f^{(3)}$ from 125 points



[Jasa, J. P., Hwang, J. T., and Martins, J. R. R. A., "Open-source coupled aerostructural optimization using Python," Structural and Multidisciplinary Optimization, 2018.]

https://github.com/johnjasa/OpenAeroStruct/

MFMC: AeroStruct: Distribution of work

Model properties

model	evaluation costs [s]	offline costs [s]	correlation coefficient
high-fid. $f^{(1)}$	1.61×10^{-1}	-	-
low-fid. $f^{(2)}$	1.23×10^{-7}	55.382	9.9552×10^{-1}
low-fid. $f^{(3)}$	1.21×10^{-7}	20.183	9.9192×10^{-1}

Number of model evaluations

	Monte Carlo	MFMC with $f^{(1)}, f^{(2)}$		MFMC with $f^{(1)}, f^{(3)}$	
online costs [s]	#evals $f^{(1)}$	#evals $f^{(1)}$	#evals $f^{(2)}$	#evals $f^{(1)}$	#evals $f^{(3)}$
7.99×10^{0}	50	4.90×10^{1}	4.48×10^{5}	4.90×10^{1}	5.97×10^{5}
1.61×10^{1}	100	9.90×10^{1}	8.95×10^{5}	9.90×10^{1}	1.19×10^{6}
8.07×10^{1}	500	4.96×10^{2}	4.48×10^{6}	4.95×10^{2}	5.97×10^{6}
1.61×10^{2}	1000	9.93×10^{2}	8.95×10^{6}	9.90×10^{2}	1.19×10^{7}
8.07×10^{2}	5000	4.97×10^{3}	4.48×10^{7}	4.95×10^{3}	5.97×10^{7}

MFMC trades high-fidelity evaluations for low-fidelity evaluations

- The high-fidelity model evaluations guarantee unbiased
- The low-fidelity model evaluations help to reduce the variance
- The balance is optimal with respect to the mean-squared error

MFMC: AeroStruct: Distribution of work

Model properties

model	evaluation costs [s]	offline costs [s]	correlation coefficient
high-fid. $f^{(1)}$	1.61×10^{-1}	-	-
low-fid. $f^{(2)}$	1.23×10^{-7}	55.382	9.9552×10^{-1}
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Number of model evaluations

	Monte Carlo	MFMC with $f^{(1)}, f^{(2)}$		MFMC with $f^{(1)}, f^{(3)}$	
online costs [s]	#evals $f^{(1)}$	#evals $f^{(1)}$	#evals $f^{(2)}$	#evals $f^{(1)}$	#evals $f^{(3)}$
7.99×10^{0}	50	4.90×10^{1}	4.48×10^{5}	4.90×10^{1}	5.97×10^{5}
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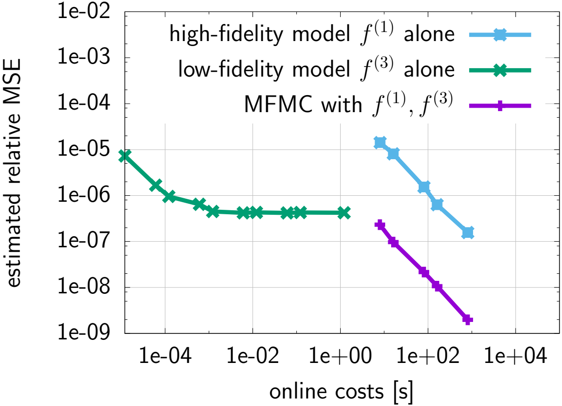
8.07×10^{1}	500	4.96×10^{2}	4.48×10^{6}	4.95×10^{2}	5.97×10^{6}
1.61×10^{2}	1000	9.93×10^{2}	8.95×10^{6}	9.90×10^{2}	1.19×10^{7}
8.07×10^{2}	5000	4.97×10^{3}	4.48×10^{7}	4.95×10^{3}	5.97×10^{7}

MFMC trades high-fidelity evaluations for low-fidelity evaluations

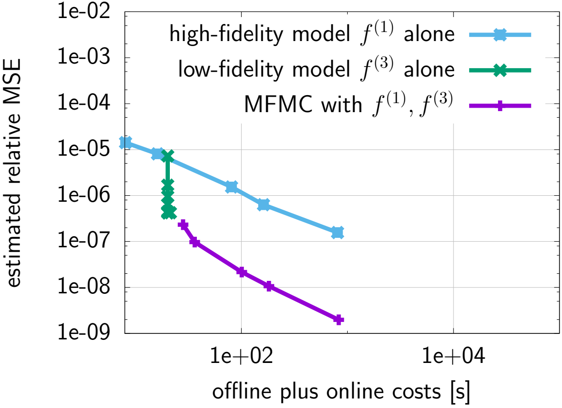
- The high-fidelity model evaluations guarantee unbiased
- The low-fidelity model evaluations help to reduce the variance
- The balance is optimal with respect to the mean-squared error

MFMC: AeroStruct: Speedup results



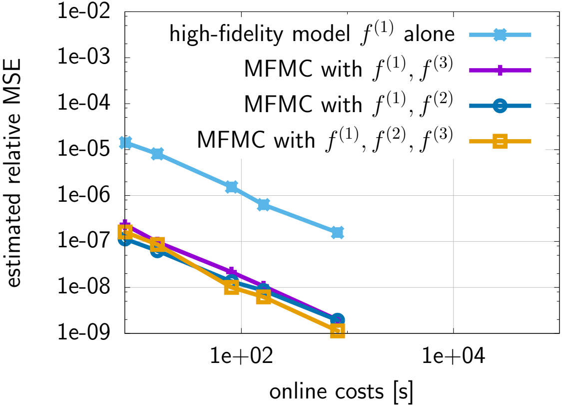
- Low-fidelity model alone leads to biased estimators
- MFMC achieves speedup of about two order of magnitude

MFMC: AeroStruct: Speedup with offline costs



- Constructing low-fidelity models incurs offline costs
- In this example, offline costs low compared to savings

MFMC: AeroStruct: Combining all three models



- Model $f^{(2)}$ and $f^{(3)}$ are similar with respect to costs/correlations
- Adding model $f^{(2)}$ has little effect

MFMC: Plate

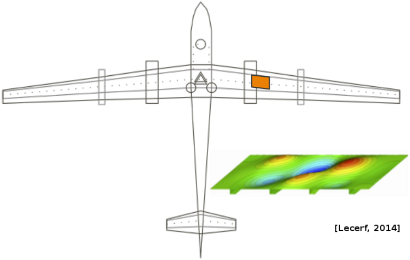
Locally damaged plate in bending

- Inputs: nominal thickness, load, damage
- Output: maximum deflection of plate
- **Only distribution of inputs known**
- Estimate **expected** deflection

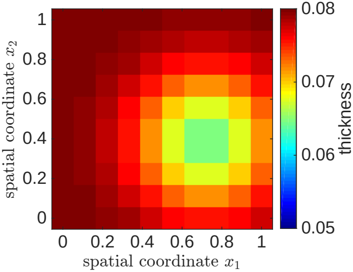
Six models

- High-fidelity model: FEM, 300 DoFs
- Reduced model: POD, 10 DoFs
- Reduced model: POD, 5 DoFs
- Reduced model: POD, 2 DoFs
- Data-fit model: linear interp., 256 pts
- Support vector machine: 256 pts

Var, corr, and costs est. from 100 samples

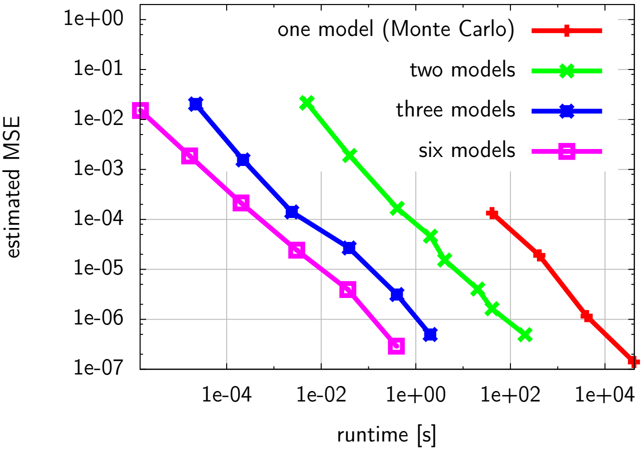


(a) wing panel



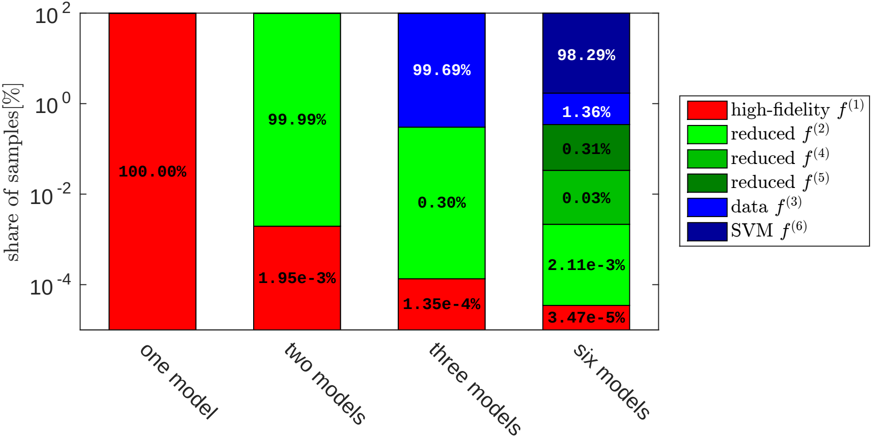
(b) damaged plate

MFMC: Plate: Combining many models



- Largest improvement from "single $\rightarrow$ two" and "two $\rightarrow$ three"
- Adding yet another reduced/SVM model reduces variance only slightly

MFMC: Plate: #evals of models



- MFMC distributes #evals among models depending on corr/costs
- Number of evaluation changes exponentially between models
- Highest #evals in data-fit models (cost ratio $w_1/w_6 \approx 10^6$)

MFMC: Multi-fidelity Monte Carlo in the wild

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Multifidelity prediction in wildfire spread simulation: Modeling, uncertainty quantification and sensitivity analysis

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[b] Center for Turbulence Research, Stanford University, Stanford, CA, 94305, USA
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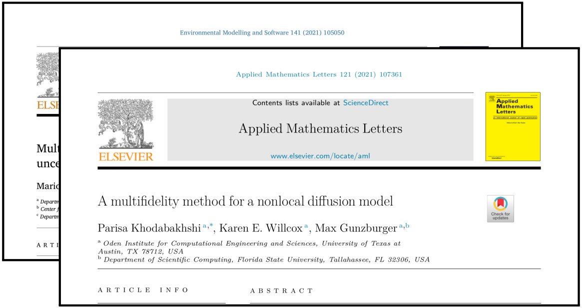
ARTICLE INFO

ABSTRACT

MFMC: Multi-fidelity Monte Carlo in the wild



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A multifidelity method for a nonlocal diffusion model

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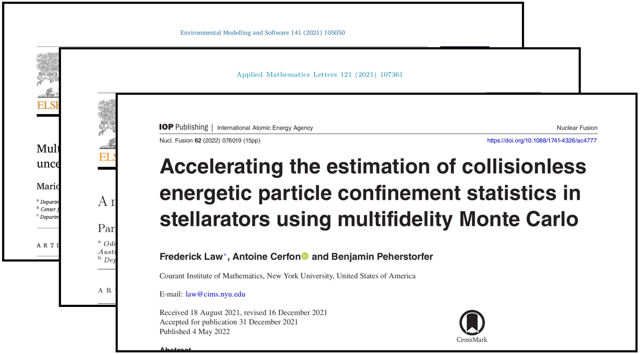

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Nucl. Fusion **62** (2022) 076019 (15pp) https://doi.org/10.1088/1741-4326/ac4777

Accelerating the estimation of collisionless energetic particle confinement statistics in stellarators using multifidelity Monte Carlo

Frederick Law*, **Antoine Cerfon** and **Benjamin Peherstorfer**

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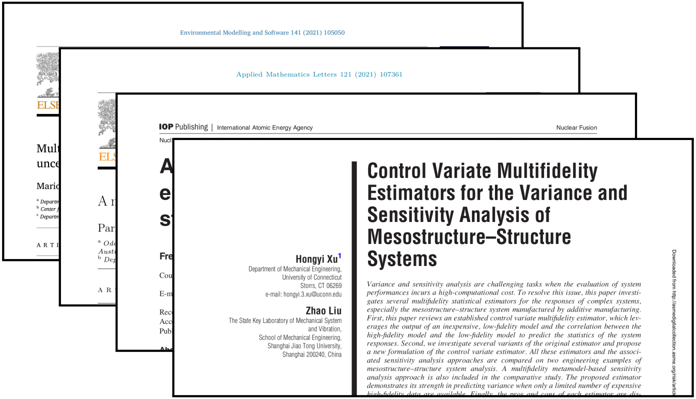
CrossMark

Abstract

MFMC: Multi-fidelity Monte Carlo in the wild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Control Variate Multifidelity Estimators for the Variance and Sensitivity Analysis of Mesostructure–Structure Systems

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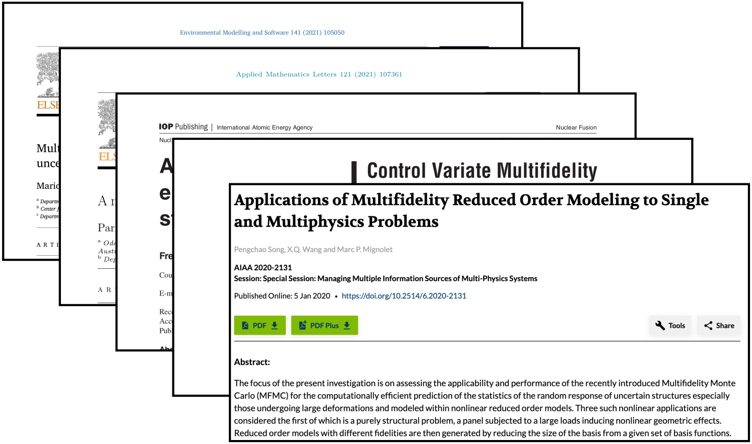
Variance and sensitivity analysis are challenging tasks when the evaluation of system performances incurs a high-computational cost. To resolve this issue, this paper investigates several multifidelity statistical estimators for the responses of complex systems, especially the mesostructure–structure system manufactured by additive manufacturing. First, this paper reviews an established control variate multifidelity estimator, which leverages the output of an inexpensive, low-fidelity model and the correlation between the high-fidelity model and the low-fidelity model to predict the statistics of the system responses. Second, we investigate several variants of the original estimator and propose a new formulation of the control variate estimator. All these estimators and the associated sensitivity analysis approaches are compared on two engineering examples of mesostructure–structure system analysis. A multifidelity metamodel-based sensitivity analysis approach is also included in the comparative study. The proposed estimator demonstrates its strength in predicting variance when only a limited number of expensive

MFMC: Multi-fidelity Monte Carlo in the wild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Control Variate Multifidelity

Applications of Multifidelity Reduced Order Modeling to Single and Multiphysics Problems

Pengchao Song, X.Q. Wang and Marc P. Mignolet

AIA 2020-2131

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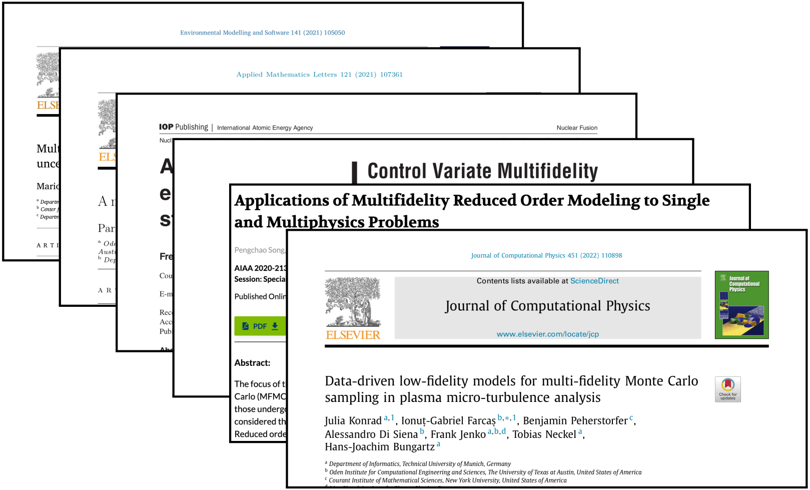
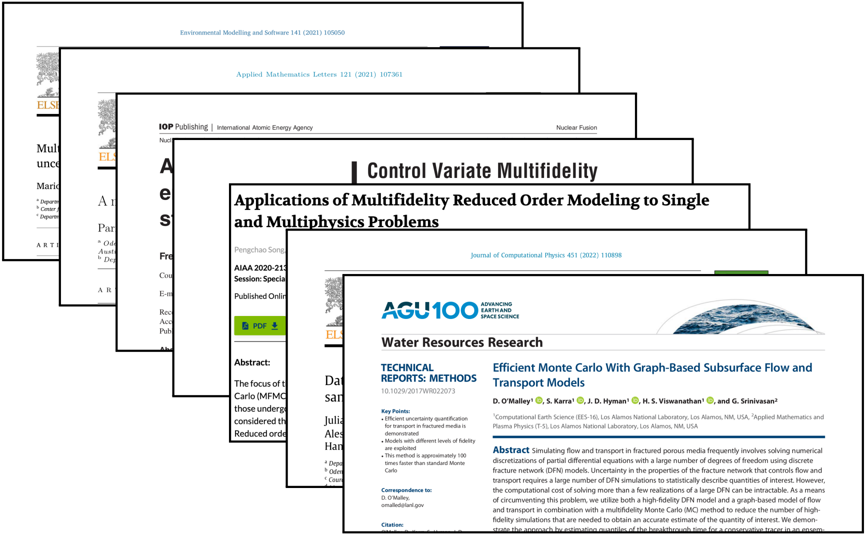
Abstract:

The focus of the present investigation is on assessing the applicability and performance of the recently introduced Multifidelity Monte Carlo (MFMC) for the computationally efficient prediction of the statistics of the random response of uncertain structures especially those undergoing large deformations and modeled within nonlinear reduced order models. Three such nonlinear applications are considered the first of which is a purely structural problem, a panel subjected to a large loads inducing nonlinear geometric effects. Reduced order models with different fidelities are then generated by reducing the size of the basis from a given set of basis functions.

MFMC: Multi-fidelity Monte Carlo in the wild

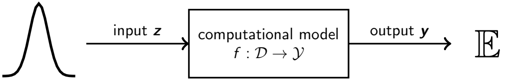


MFMC: Multi-fidelity Monte Carlo in the wild

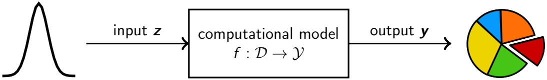


Uncertainty quantification tasks

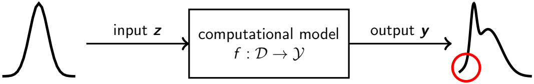
1. Multifidelity uncertainty propagation



2. Multifidelity sensitivity analysis



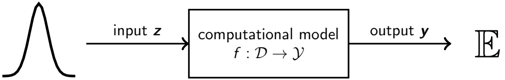
3. Multifidelity failure probability estimation



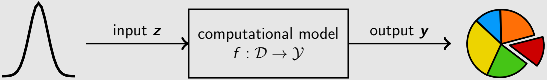
4. Other multifidelity uncertainty quantification tasks

Uncertainty quantification tasks

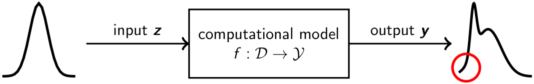
1. Multifidelity uncertainty propagation



2. Multifidelity sensitivity analysis

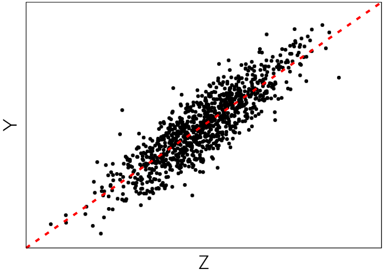


3. Multifidelity failure probability estimation

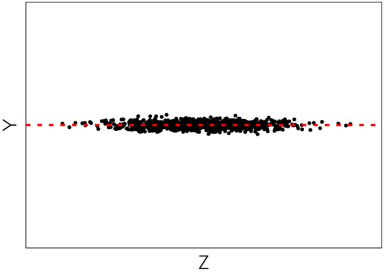


4. Other multifidelity uncertainty quantification tasks

MFGSA: Sensitivity analysis



Y is sensitive to Z



Y is *not* sensitive to Z

Sensitivity analysis

- Determine which inputs influence output most
- Can sample Y as a black box for inputs Z and need to determine what components of $Z = [Z_1, \dots, Z_d]^T$ influence Y most

MFGSA: Sensitivity analysis in engineering

Risk communication for decision-making

- Determine if one can rely on model output or if "noise"
- Communicate to upstream decision-making which inputs are critical

Feedback to improve model

- Determine which inputs need to be sampled carefully
- Prioritize effort on reducing uncertainty
- Modify model with respect to sensitive inputs

Model reduction and dimensionality reduction

- Focus on important inputs and ignore ineffective inputs
- Derive surrogate models that depend on important inputs only

MFGSA: Variance-based global sensitivity analysis

- Input $Z = [Z_1, \dots, Z_d]^T \in \mathcal{D}$ is a random *vector*
- Output of model $Y = f^{(1)}(Z_1, \dots, Z_d)$ is sensitive to inputs
- Measure sensitivity with variance
- Main effect sensitivity
$$S_i = \frac{\mathrm{Var}[\mathbb{E}[Y|Z_i]]}{\mathrm{Var}[Y]}$$
- Main sensitivity indices are normalized
$$\sum_{i=1}^{d} S_i = 1\,, \qquad S_i \in [0, 1]$$

MFGSA: Multifidelity estimation

Estimation of sensitivity indices

- Estimate variance instead of expected value

$$S_i = \frac{\mathrm{Var}[\mathbb{E}[Y|Z_i]]}{\mathrm{Var}[Y]}$$

- Requires estimating variance for all d inputs $Z = [Z_1, \dots, Z_d]$

Multifidelity estimation

- Given are low-fidelity models $f^{(2)}, \dots, f^{(k)}$
- Similarly to MFMC, exploit correlations

$$\rho_2 = \mathrm{Corr}[f^{(1)}, f^{(2)}], \rho_3 = \mathrm{Corr}[f^{(1)}, f^{(3)}], \dots, \rho_k = \mathrm{Corr}[f^{(1)}, f^{(k)}]$$

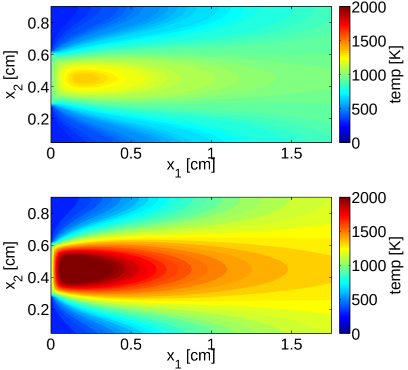
- Estimator has similar structure as estimator for expected values

MFGSA: Premixed flame

Inputs to model are

- Parameters of Arrhenius reaction
- Temperatures at boundary
- Ratio of fuel and oxidizer
- Activation Energy

Output is maximum temperature in chamber



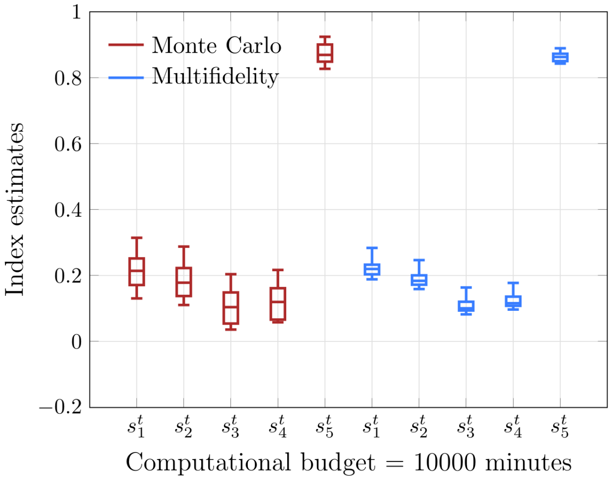
Models

- Model based on finite differences serves as high-fidelity model
- Model with lower fidelity derived with proper orthogonal decomposition

Code available on GitHub

`https://github.com/elizqian/mfgsa`

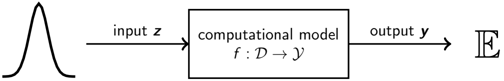
MFGSA: Premixed flame: Results



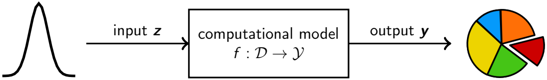
- Monte Carlo too inaccurate for ranking inputs
- Multi-fidelity Monte Carlo allows ranking of inputs

Uncertainty quantification tasks

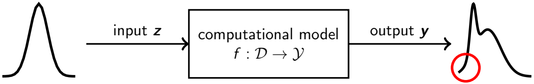
1. Multifidelity uncertainty propagation



2. Multifidelity sensitivity analysis



3. Multifidelity failure probability estimation



4. Other multifidelity uncertainty quantification tasks

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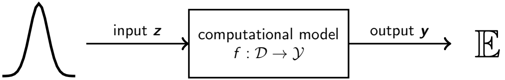

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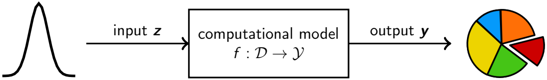

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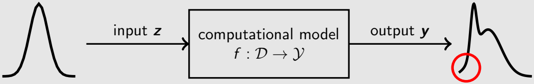


4. Other multifidelity uncertainty quantification tasks

MFIS: Failure probabilities

System described by high-fidelity model $f^{(1)} : \mathcal{D} \to \mathcal{Y}$

- Input $\boldsymbol{z} \in \mathcal{Z}$
- Output $\boldsymbol{y} \in \mathcal{Y}$
- Costs of one high-fidelity model evaluation $w_1 > 0$

Define indicator function

$$I^{(1)}(\boldsymbol{z}) = \begin{cases} 1\,, & f^{(1)}(\boldsymbol{z}) < 0 \\ 0\,, & \text{else}\,. \end{cases}$$

Indicator function $I^{(1)}(\boldsymbol{z}) = 1$ signals *failure* for input $\boldsymbol{z}$

Given random variable Z, estimate failure probability

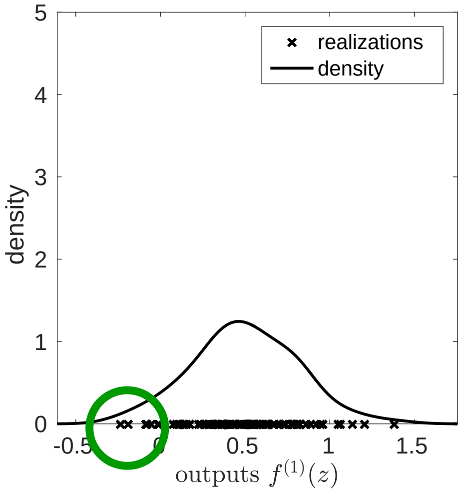
$$P_f = \mathbb{E}_p[I^{(1)}(Z)]$$

MFIS: Rare event simulation

- Monte Carlo estimator of P_f using $m \in \mathbb{N}$ realizations

$$P_f^{\mathrm{MC}} = \frac{1}{m} \sum_{i=1}^{m} I^{(1)}(\boldsymbol{z}_i)$$

- If P_f small, then only few realizations with $f^{(1)}(\boldsymbol{z}) < 0$
- Require (very) large m to obtain Monte Carlo estimator with acceptable accuracy $\rightarrow$ expensive



MFIS: Rare event simulation is challenging

Costs of rare event simulation grow inverse proportional to P_f

- Monte Carlo estimation of P_f with m realizations

$$P_f^{\text{MC}} = \frac{1}{m} \sum_{i=1}^{m} I^{(1)}(\boldsymbol{z}_i)$$

- Relative mean-squared error (MSE) of P_f^{MC}

$$e(P_f^{\text{MC}}) = \mathbb{E}_p \left[\left(\frac{P_f^{\text{MC}} - P_f}{P_f} \right)^2 \right] = \frac{\text{Var}_p \left[I^{(1)}(Z) \right]}{P_f^2 m} = \frac{1 - P_f}{P_f m}$$

- For constant m, the rel. MSE increases inverse proportional to P_f
- A small failure probability P_f needs to be compensated with a large number of samples m
- Example: For $P_f = 10^{-5}$ need $m \approx 10^7$ to achieve $e(P_f^{\text{MC}}) \leq 10^{-2}$

Challenge

costs per sample + number of samples

MFIS: Rare events in aerospace engineering

Rare event simulation

- Failure probability estimation
- Reliability engineering

Risk assessment

- Communicate to upstream decision-making
- Mitigate catastrophic events

Risk-averse optimization

- Deliver baseline performance outside nominal operating conditions
- Take into account dynamics at limit states

MFIS: Importance sampling

- Importance sampling (IS) creates biasing density q to put more weight on failure events

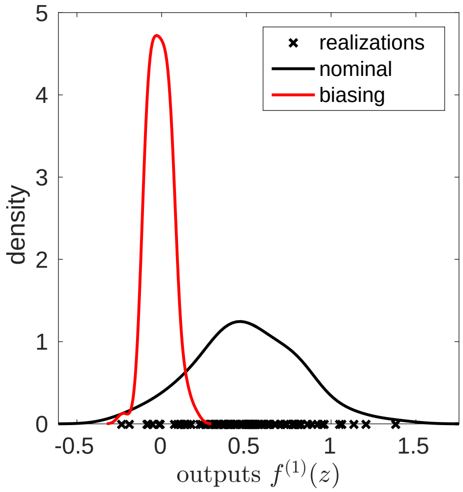
- Let $\hat{Z}$ be the corresponding random variable

- Introduce the weight function

$$r(\boldsymbol{z}') = \frac{p(\hat{\boldsymbol{z}})}{q(\hat{\boldsymbol{z}})}$$

- Reformulate failure probability

$$P_f = \mathbb{E}_p[I^{(1)}(Z)] = \mathbb{E}_q[I^{(1)}(\hat{Z})r(\hat{Z})]$$



MFIS: Multifidelity importance sampling

step 1
construction of
biasing distribution

step 2
estimation of
failure probability

MFIS: Multifidelity importance sampling

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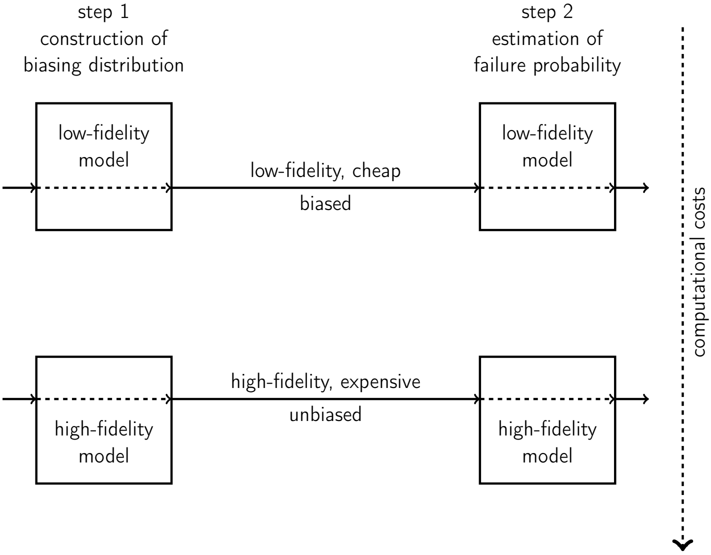

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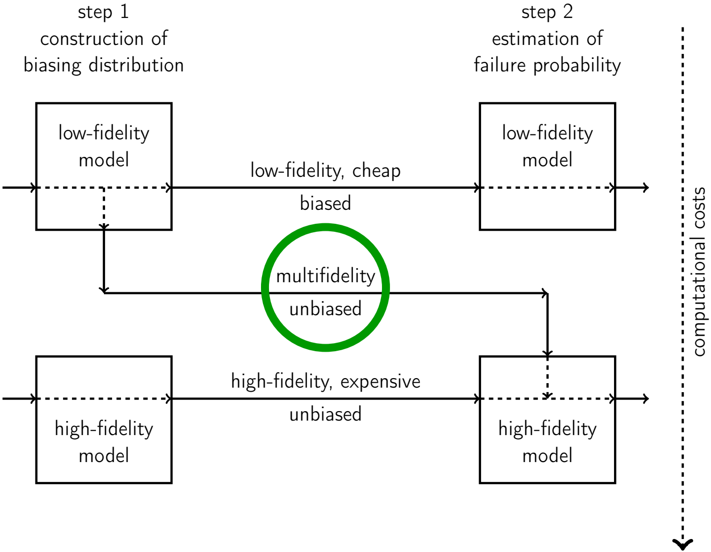

MFIS: Recipe 3

Step 1: Construct biasing distribution using low-fidelity model $f^{(2)}$

- Evaluate $f^{(2)}$ at (many) realizations $\boldsymbol{z}_1, \dots, \boldsymbol{z}_n$ of Z
- Fit mixture model q (biasing) to realizations $\rightarrow$ `scikit-learn`, Matlab

$$\{\boldsymbol{z}_i \,|\, I^{(2)}(\boldsymbol{z}_i) = 1\,, i = 1, \dots, n\}$$

- Derive random variable $\hat{Z}$ with density q

Step 2: Estimate P_f with high-fidelity model $f^{(1)}$

$$P_f^{\mathrm{MFIS}} = \frac{1}{m} \sum_{i=1}^{m} \; I^{(1)}(\hat{\boldsymbol{z}}_i) \quad \frac{p(\hat{\boldsymbol{z}}_i)}{q(\hat{\boldsymbol{z}}_i)}$$

Multifidelity estimator P_f^{MFIS} is unbiased

$$P_{f^{(1)}} = \mathbb{E}_q[P_f^{\mathrm{MFIS}}]$$

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high-fidelity model
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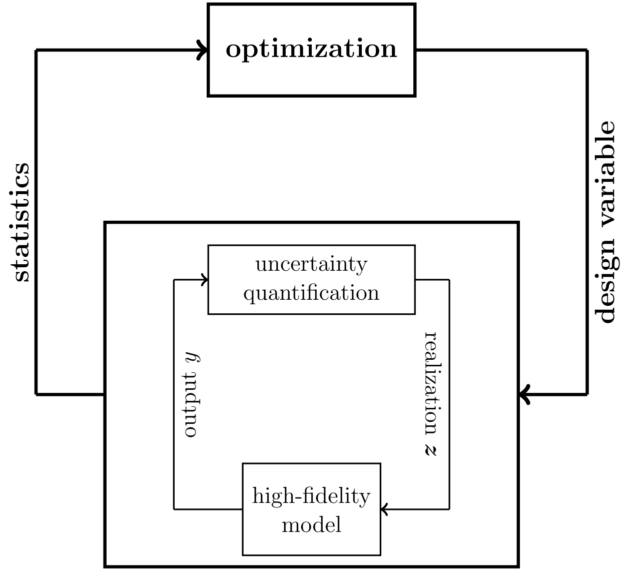
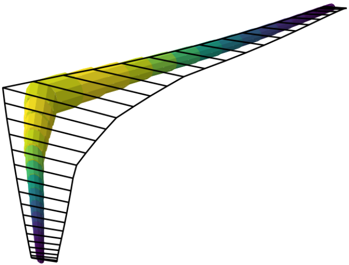
MFIS: Optimization for risk-averse designs



MFIS: Risk-averse design of wing

Consider baseline wing definition in OpenAeroStruct

- Design variables are thickness and position of control points
- Uncertain flight conditions (angle of attack, air density, Mach number)
- Output is fuel burn



Minimize fuel burn at limit states

$$\min_{\boldsymbol{x} \in \mathcal{X}} \mathbb{E}[f^{(1)}(\boldsymbol{x}, Z) \mid f^{(1)}(\boldsymbol{x}, Z) \leq \beta]$$

Derive a data-fit surrogate at current design $\boldsymbol{x}$

- Take a $3 \times 3 \times 3$ equidistant grid in stochastic domain
- Evaluate high-fidelity model at those 27 points at current design $\boldsymbol{x}$
- Derive linear interpolant of output

Apply multifidelity pre-conditioned cross-entropy method

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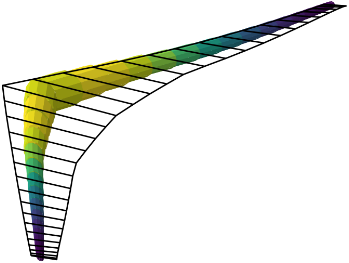

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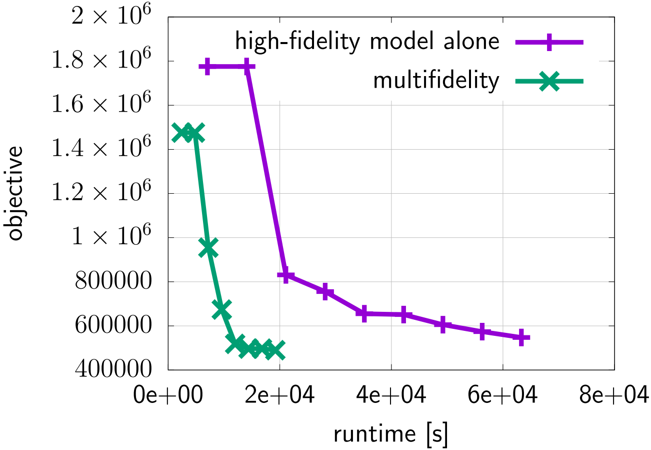

Uncertainty quantification tasks

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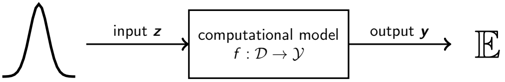

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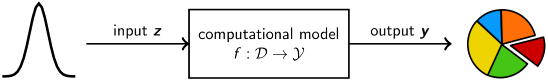

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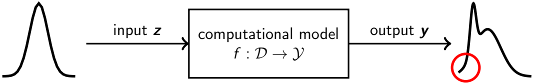

4. Other multifidelity uncertainty quantification tasks

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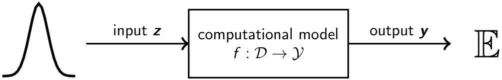

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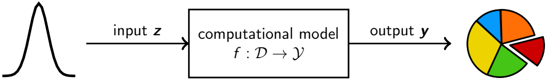

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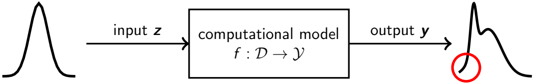

4. Other multifidelity uncertainty quantification tasks

Outlook: Inverse problems

physics-based model

?

data

inputs

$$\boxed{y} = \boxed{f}(\boxed{z}) + \epsilon$$

noise and model bias

Bayesian inference of parameters z from data y

- Parameters represented as random variable $\boldsymbol{z}$ with prior $p(\boldsymbol{z})$
- Define likelihood $p(\boldsymbol{y}|\boldsymbol{z})$ of data $\boldsymbol{y}$ using model f
- Update distribution of $\boldsymbol{z}$ ("infer") with Bayes' rule

$$\underbrace{p(\boldsymbol{z}|\boldsymbol{y})}_{\text{posterior}} \propto \underbrace{p(\boldsymbol{y}|\boldsymbol{z})}_{\text{likelihood}} \underbrace{p(\boldsymbol{z})}_{\text{prior}}$$

Outlook: Inverse problems (cont'd)

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Posterior provides complete description of uncertainties in z

- Input to future simulations for *predictions with quantified uncertainties*
- Explore posterior to *reduce uncertainties in future predictions*

Sampling posterior $p(\boldsymbol{z}|\boldsymbol{y})$

- Evaluate posterior expectation for function g

$$\mathbb{E}[g] = \int g(\boldsymbol{z}) p(\boldsymbol{z}|\boldsymbol{y}) \mathrm{d}\boldsymbol{z}$$

- Samples required as inputs in upstream simulations
- Explore posterior to decide where to take new data points
- Estimate quantiles

Making sampling tractable $\Rightarrow$ **multifidelity**

Outlook: Inverse problems (cont'd)

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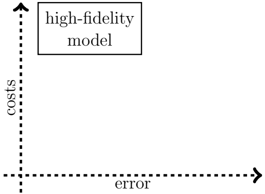

Traditional model reduction is separate from multifidelity computations

- Measures error w.r.t. HFM output while outer-loop result is goal
- Ignores that surrogates are used together with other information sources
- While approximating HFM can be hard, supporting HFM might be easy

$\Rightarrow$ **Need for model reduction that targets multifidelity**

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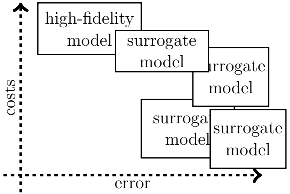

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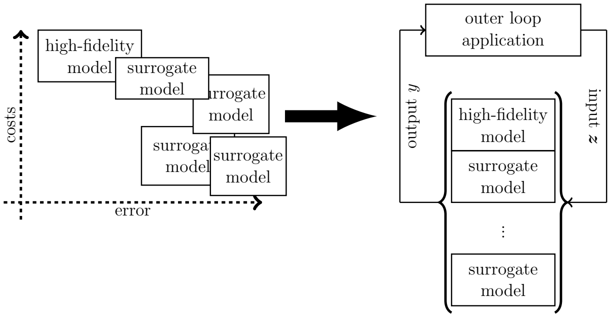

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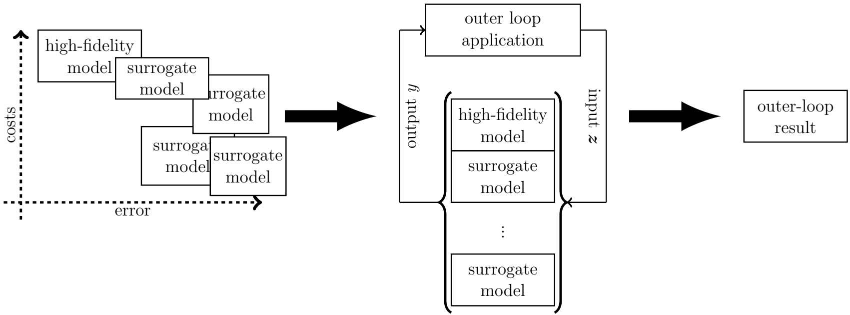

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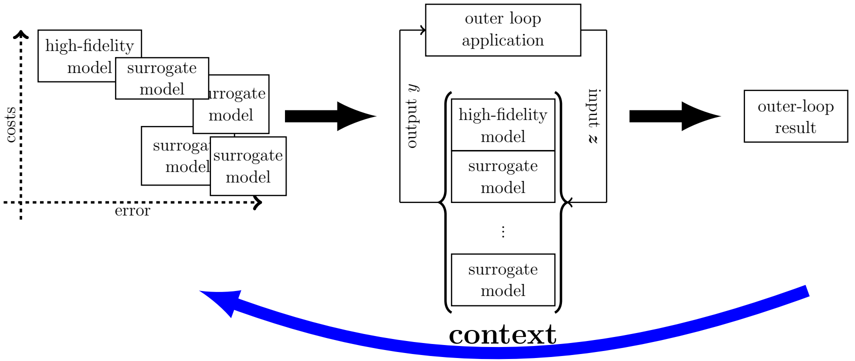

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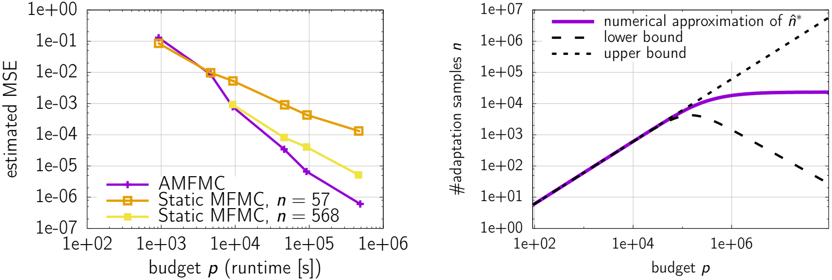

Adapt surrogate models - but not too much

- Adapting surrogate models towards multifidelity is beneficial
- Crude, cheap surrogates can have better costs/benefit ratio
- Proved for MFMC that optimal amount to spend on learning surrogates is bounded

[P.: *Multifidelity Monte Carlo estimation with adaptive low-fidelity models*. SIAM/ASA Journal on Uncertainty Quantification, 2019.]

Summary: Multi-fidelity uncertainty quantification

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Embarrassingly parallel; just as regular Monte Carlo

- Evaluations of low- and high-fidelity models can often be decoupled
- Applicable as post-processing step (re-use databases of past simulations)

Survey with *many* references

SIAM REVIEW
Vol. 60, No. 3, pp. 550–591

Survey of Multifidelity Methods in Uncertainty Propagation, Inference, and Optimization*

Benjamin Peherstorfer[†]
Karen Willcox[‡]
Max Gunzburger[§]

Abstract. In many situations across computational science and engineering, multiple computational models are available that describe a system of interest. These different models have varying evaluation costs and varying fidelities. Typically, a computationally expensive high-fidelity model describes the system with the accuracy required by the current application at hand, while lower-fidelity models are less accurate but computationally cheaper than the high-fidelity model. Outer-loop applications, such as optimization, inference, and uncertainty quantification, require multiple model evaluations at many different inputs, which often leads to computational demands that exceed available resources if only the high-fidelity model is used. This work surveys multifidelity methods that accelerate the solution of outer-loop applications by combining high-fidelity and low-fidelity model evaluations, where the low-fidelity evaluations arise from an explicit low-fidelity model (e.g., a simplified physics approximation, a reduced model, a data-fit surrogate) that approximates the same output quantity as the high-fidelity model. The overall premise of these multifidelity methods is that low-fidelity models are leveraged for speedup while the high-fidelity model is kept in the loop to establish accuracy and/or convergence guarantees. We categorize multifidelity methods according to three classes of strategies: adaptation, fusion, and filtering. The paper reviews multifidelity methods in the outer-loop contexts of uncertainty propagation, inference, and optimization.

Key words. multifidelity, surrogate models, model reduction, multifidelity uncertainty quantification, multifidelity uncertainty propagation, multifidelity statistical inference, multifidelity optimization

AMS subject classifications. 65-02, 62-02, 49-02

DOI. 10.1137/16M1082469

Further reading on methods covered in this talk

[1] L. W. T. Ng and K. Willcox.
Multifidelity approaches for optimization under uncertainty.
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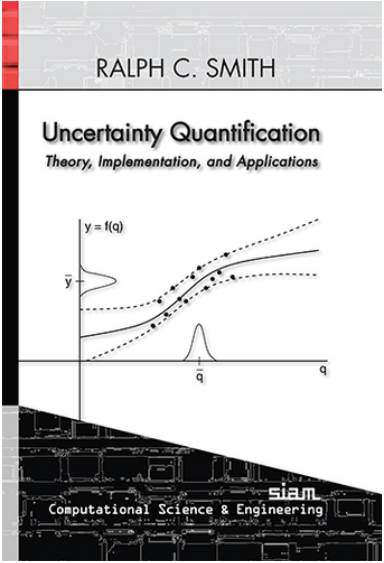
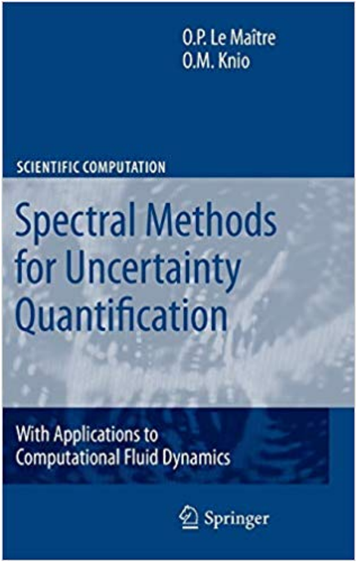
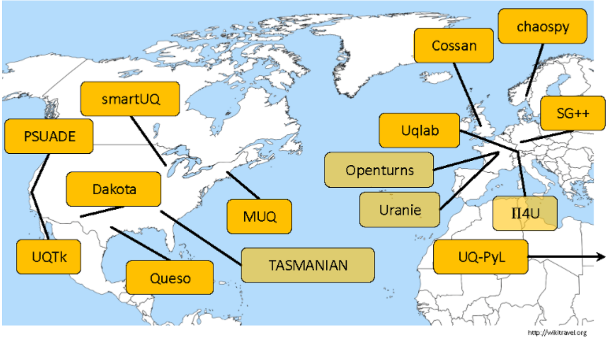
Books on uncertainty quantification





Software

Software for uncertainty quantification



[Figure: Pflüger et al., 2016]

Software with explicit multifidelity support

DAKOTA
Explore and predict with confidence.

https://dakota.sandia.gov/

MFMC

https://github.com/pehersto/mfmc

Summary: Multi-fidelity uncertainty quantification

Wide applicability; integrates well with machine-learning surrogates

- Applicable to *general* low-fidelity models such as response surfaces, coarse-grid approximations, linearized models, neural-network models

Accuracy guarantees; even if errors of low-fidelity models unknown

- High-fidelity model stays in the loop; same accuracy guarantees as using high-fidelity model only
- Useful in real-world applications, where typically error control for low-fidelity models such as neural-network models is unavailable

Nonintrusive technique; *no* re-implementation of codes necessary

- Applicable in a black-box fashion; no in-depth insight in code/implementation/theory necessary

Embarrassingly parallel; just as regular Monte Carlo

- Evaluations of low- and high-fidelity models can often be decoupled
- Applicable as post-processing step (re-use databases of past simulations)