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Lasso Monte Carlo, a Novel Method for High Dimensional Uncertainty Quantification

Zurich PhD Seminar, 27th January 2023

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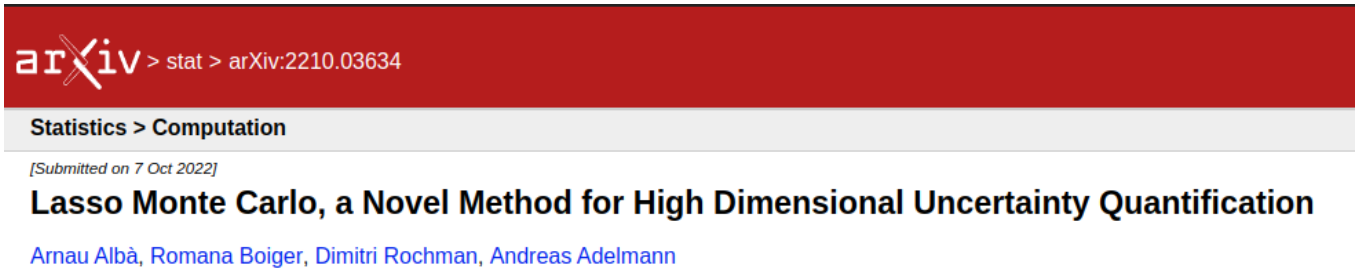
Pre-print available:



Currently under review for SIAM UQ journal.

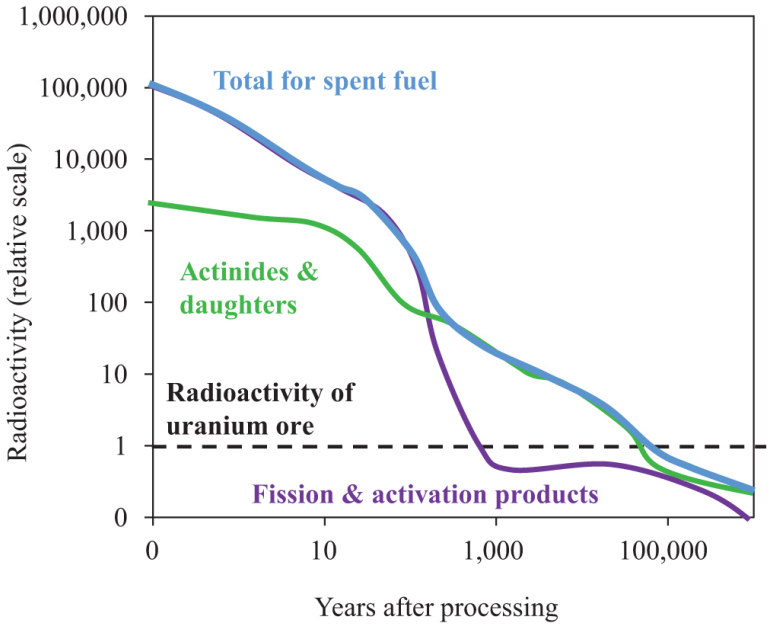
See paper for full proofs, details of algorithm, and citations.

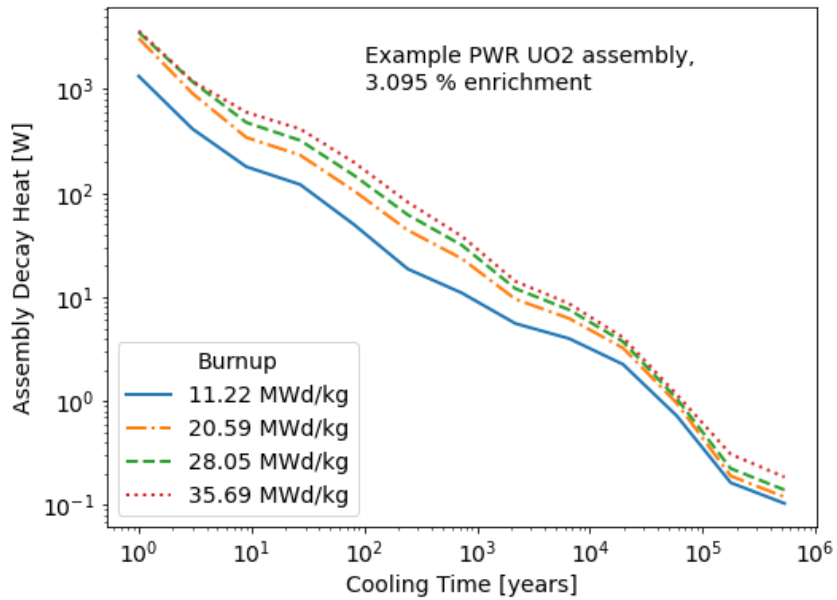
Overview

Motivation: SNF Characterisation

Spent Nuclear Fuel (SNF) remains hazardous for up to a 1 million years, due to:

- Decay Heat
- Isotopic Content
- Criticality





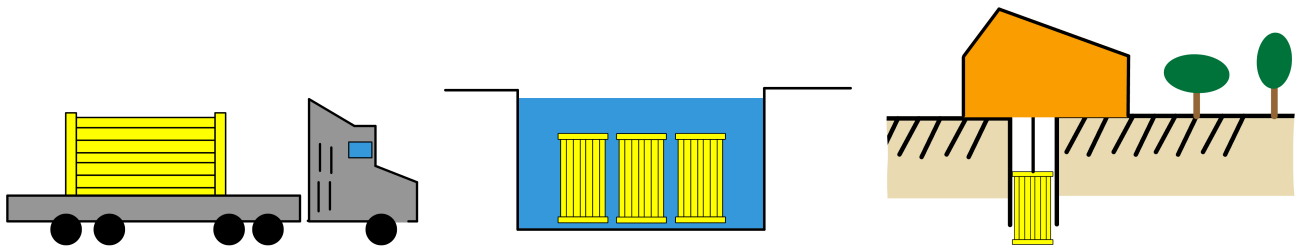
Corkhill, and Hyatt. Nuclear Waste Management. IOP Publishing, 2018

Motivation: SNF Characterisation

Nuclear burnup and criticality simulations are used to characterise spent nuclear fuel:

$$f : \underbrace{\begin{pmatrix} \texttt{Fresh Fuel Parameters} \\ \texttt{Irradiation History} \\ \texttt{Reactor Parameters} \\ \texttt{Nuclear Data} \end{pmatrix}}_{\text{Input with known uncertainty}} \rightarrow \underbrace{\begin{pmatrix} \texttt{Decay Heat} \\ \texttt{Isotopic Content} \\ \texttt{Criticality} \end{pmatrix}}_{\text{Output with unknown uncertainty}}$$

Any uncertainty in outputs will increase the risks and costs of



Transport Storage Disposal

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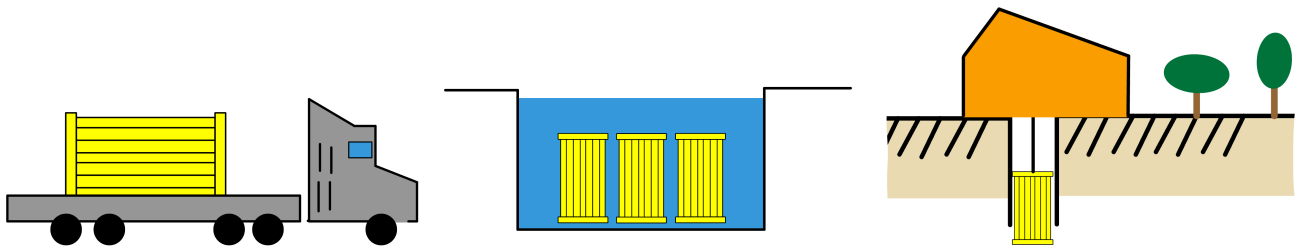

Transport Storage Disposal

Accurate estimation of uncertainty saves money and reduces risks.

Motivation: UQ due to Nuclear Data

More specifically, we are dealing with **high-dimensional** UQ, due to Nuclear Data:

$$f : \underbrace{\text{Nuclear Data}}_{\in \mathbb{R}^{15\,557}} \rightarrow \begin{pmatrix} \texttt{Decay Heat} \\ \texttt{Isotopic Content} \\ \texttt{Criticality} \end{pmatrix}$$

Nuclear data includes:

- Cross-sections
- Fission spectrum
- Fission yield
- Neutron multiplicity

For every isotope and energy.

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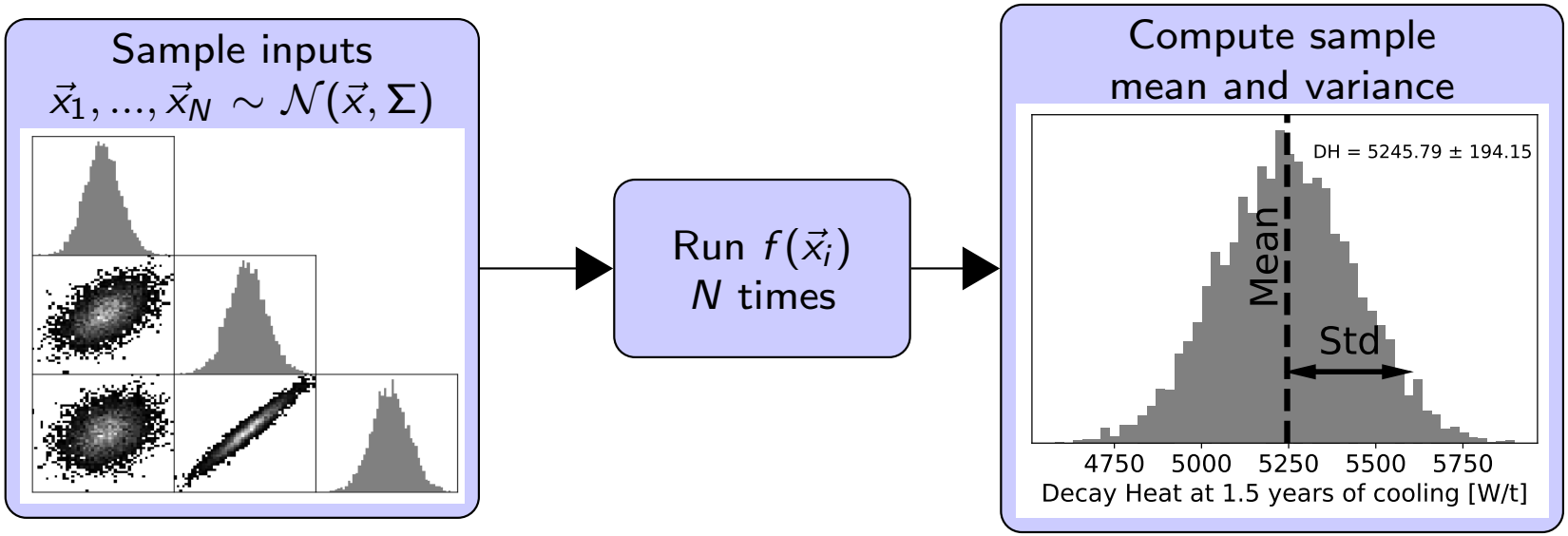
Goal: find an efficient method for high-dimensional UQ.

Simple Monte Carlo UQ

1. 

2. Compute sample mean and variance

$$\mu_N = \frac{1}{N}\sum_{i=1}^{N} f(\boldsymbol{x}_i)\,, \quad \sigma_N^2 = \frac{1}{N-1}\sum_{i=1}^{N}\left(f(\boldsymbol{x}_i) - \sum_{j=1}^{N}\frac{f(\boldsymbol{x}_j)}{N}\right)^2 .$$

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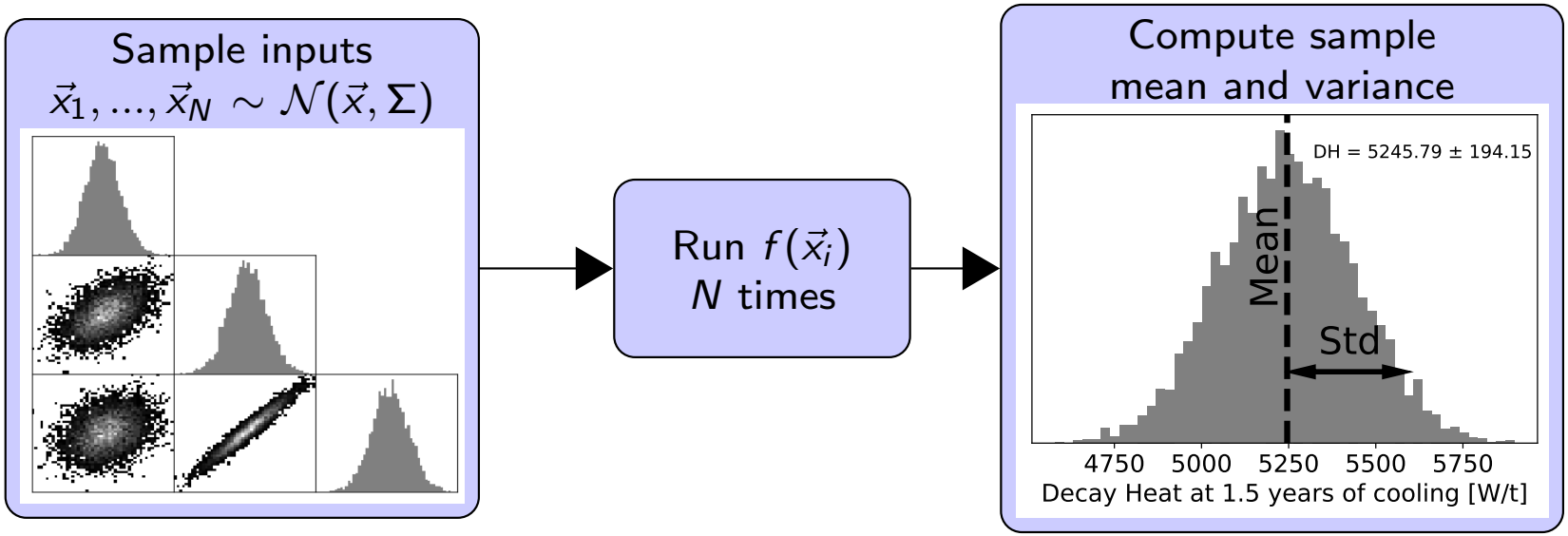
1. 

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Simple MC is **unbiased**, but **slow** (MSE $= \mathcal{O}\left(\frac{1}{N}\right)$):

$$\lim_{N\to\infty}\mu_N = \mathbb{E}[f]\,, \quad \text{since MSE}\left(\mu_N - \mathbb{E}[f]\right) = \frac{\mathrm{Var}[f]}{N}\,,$$

$$\lim_{N\to\infty}\sigma_N^2 = \mathrm{Var}[f]\,, \quad \text{since MSE}\left(\sigma_N^2 - \mathrm{Var}[f]\right) = \frac{1}{N}\left(m_4[f] - \frac{N-3}{N-1}\mathrm{Var}^2[f]\right) .$$

Simple Monte Carlo UQ

Simple MC is the currently used method for nuclear data UQ [Rochman et al., 2018]:

- MSE $= \mathcal{O}\left(\frac{1}{N}\right)$, i.e. many simulations required!
- For SNF characterisation $N \sim 1000$.
- Each simulation lasts a few hours.
- Expecting > 12000 fuel assemblies in Switzerland.
- $\Rightarrow$ millions of CPU hours $\Rightarrow$ **MC UQ is too slow!**

UQ with Surrogate Models

A more modern approach: Surrogate models (e.g. PCE [Frey and Adelmann, 2021], NNs [Fiorina et al., 2020, Solans et al., 2021]):

2. Train a surrogate model $\widetilde{f} \sim f$, that is **fast to evaluate**.
3. Run surrogate M times to obtain samples $\widetilde{f}(\boldsymbol{z}_1), \widetilde{f}(\boldsymbol{z}_2), ..., \widetilde{f}(\boldsymbol{z}_M)$, with $Z \sim \mathcal{N}(\boldsymbol{x}, \Sigma)$.
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- Converges very fast, since M can be large
- Training $\widetilde{f}$ requires a big training set, at least $N_{tr} > d$ (*curse of dimensionality*).
- Estimates are biased since

$$\text{MSE}\left(\widetilde{\mu}_M - \mathbb{E}[f]\right) = \mathbb{E}^2\left[\widetilde{f} - f\right] + \frac{\text{Var}\left[\widetilde{f}\right]}{M},$$

$$\text{MSE}\left(\widetilde{\sigma}^2_M - \text{Var}[f]\right) = \left(\text{Var}[f] - \text{Var}[\widetilde{f}]\right)^2 + \frac{1}{M}\left(m_4[\widetilde{f}] - \frac{M-3}{M-1}\text{Var}^2[\widetilde{f}]\right).$$

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In summary: simple MC and surrogate models are inadequate for high-dimensional UQ.

Lasso Monte Carlo

Lasso Monte Carlo (LMC) is a new technique that combines two existing methods:

- Multilevel Monte Carlo (MLMC) [Giles, 2008, Krumscheid et al., 2020]
- Lasso regression [Tibshirani, 1996]

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- Multilevel Monte Carlo (MLMC) [Giles, 2008, Krumscheid et al., 2020] $\Rightarrow$ Combine models of different fidelities into an **unbiased estimator**.
- Lasso regression [Tibshirani, 1996] $\Rightarrow$ Train surrogate models with **small training sets**.

Two-level MC

Let

- f be the true, expensive model, that we evaluate N times: $f(\boldsymbol{x}_1), f(\boldsymbol{x}_2), ..., f(\boldsymbol{x}_N)$.
- $\widetilde{f}$ a cheap, biased, surrogate model, that we evaluate $N + M$ times, with $M \gg N$: $\widetilde{f}(\boldsymbol{x}_1), \widetilde{f}(\boldsymbol{x}_2), ..., \widetilde{f}(\boldsymbol{x}_N)$, and $\widetilde{f}(\boldsymbol{z}_1), \widetilde{f}(\boldsymbol{z}_2), ..., \widetilde{f}(\boldsymbol{z}_M)$.

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Then the estimators are

$$\mu_{N,M} = \frac{1}{M}\sum_{i=1}^{M} \widetilde{f}(\boldsymbol{z}_i) + \frac{1}{N}\sum_{i=1}^{N} f(\boldsymbol{x}_i) - \widetilde{f}(\boldsymbol{x}_i) = \widetilde{\mu}_M + \mu_N - \widetilde{\mu}_N \,,$$

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$$\sigma^2_{N,M} = \widetilde{\sigma}^2_M + \sigma^2_N - \widetilde{\sigma}^2_N \,.$$

- Estimators are unbiased
- More accurate than simple MC μ_N, σ^2_N (under certain conditions of f).

Two-level MC

Common usage of MLMC:

1. Gather a training set $\boldsymbol{x}_1, f(\boldsymbol{x}_1)$, $\boldsymbol{x}_2, f(\boldsymbol{x}_2)$, ..., $\boldsymbol{x}_{N_{tr}}, f(\boldsymbol{x}_{N_{tr}})$.
2. Train a surrogate model $\widetilde{f} \sim f$, that is **fast to evaluate**.
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4. Evaluate f N times, to obtain $f(\boldsymbol{x}_1), f(\boldsymbol{x}_2), ..., f(\boldsymbol{x}_N)$.
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- Unbiased.
- More accurate than simple MC for a given N.
- However, bottleneck is still generating the training set N_{tr} (especially in high-dimensional cases).

Choosing Surrogate Model

Surrogate model that can be trained with a small training set $N_{tr} \ll d$?

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Lasso regression technique fits a sparse linear model:

$$\widetilde{f}(\boldsymbol{x}) = \boldsymbol{\beta} \cdot \boldsymbol{x}, \quad \text{with } \boldsymbol{\beta} \text{ sparse,}$$

by minimising loss function

$$\mathcal{L}(\boldsymbol{\beta}) = \underbrace{\frac{1}{2}\sum_{i=1}^{N_{tr}} \left(f(\boldsymbol{x}_i) - \boldsymbol{\beta} \cdot \boldsymbol{x}_i\right)^2}_{\text{OLS loss}} + \underbrace{\lambda ||\boldsymbol{\beta}||_1}_{\text{Regularisation term}},$$

with $\lambda > 0$ a chosen regularisation constant.

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with $\lambda > 0$ a chosen regularisation constant.

- Lasso can be trained for small training sets, without overfitting.

Lasso Monte Carlo

Two-level MC + Lasso:

1. Gather small set $\boldsymbol{x}_1, f(\boldsymbol{x}_1)$, $\boldsymbol{x}_2, f(\boldsymbol{x}_2)$, ..., $\boldsymbol{x}_{N_{tr}}, f(\boldsymbol{x}_{N_{tr}})$.
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Reuse the same set for training!

Lasso Monte Carlo

LMC algorithm:

1. Evaluate f N times: $\boldsymbol{x}_1, f(\boldsymbol{x}_1)$, $\boldsymbol{x}_2, f(\boldsymbol{x}_2)$, ..., $\boldsymbol{x}_N, f(\boldsymbol{x}_N)$.
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- Unbiased.
- Faster (or equal) convergence than simple MC for a given N.
- Surrogate model trained *for free* (no extra simulations required).
- Note: this version of LMC omits some steps (splitting and averaging), see full algorithm in paper.

Lasso Monte Carlo

An actual code example:

```
>>> from sklearn.linear_model import LassoCV, Lasso
>>> from LMC.classLMC import LassoMC

>>> lmc = LassoMC(regressor = Lasso(lambda = 0.02),
                  random_state = seed, verbose = True,
                  validation_method = '5Fold')
>>> N = 150; M = 6000
>>> Xs = get_inputs(N)
>>> ys = [my_simulation(x) for x in Xs]
>>> Zs = get_inputs(M)
>>> lmc.get_single_estimate(Xtrain = Xs,
                            ytrain = ys,
                            Xtest = Zs)
Ntr = 150 labelled samples, Ntest = 6000 unlabelled samples
MC estimates: 5234.470666666667 +- 174.65316984757996
LMC estimates: 5246.745253371253 +- 192.6719429998857
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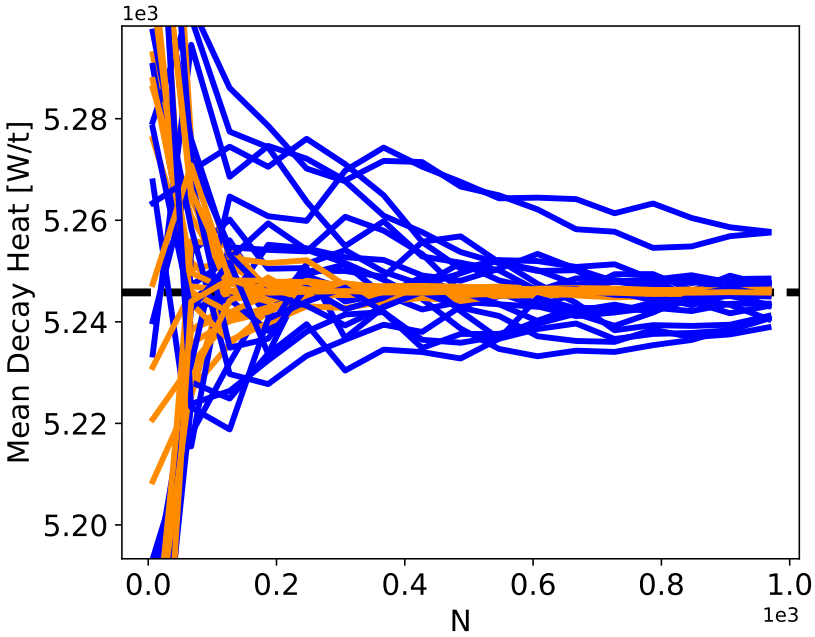
Most expensive step of the algorithm

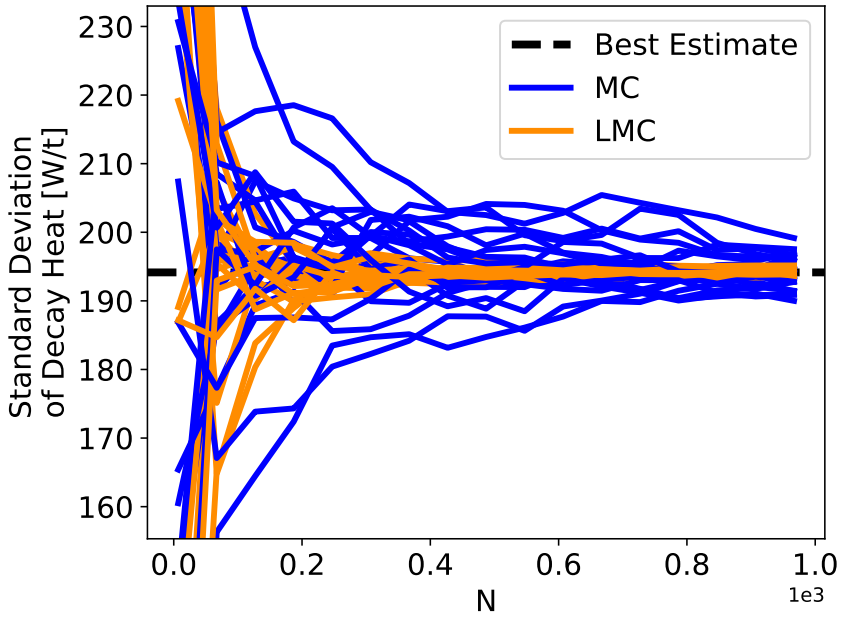
SNF Characterisation

$$f : \mathbb{R}^{15\,557} \rightarrow \mathbb{R}$$

$$\text{Nuclear Data} \mapsto \text{Decay Heat}$$

Plots show increasing N, and fixed $M = 6000$.





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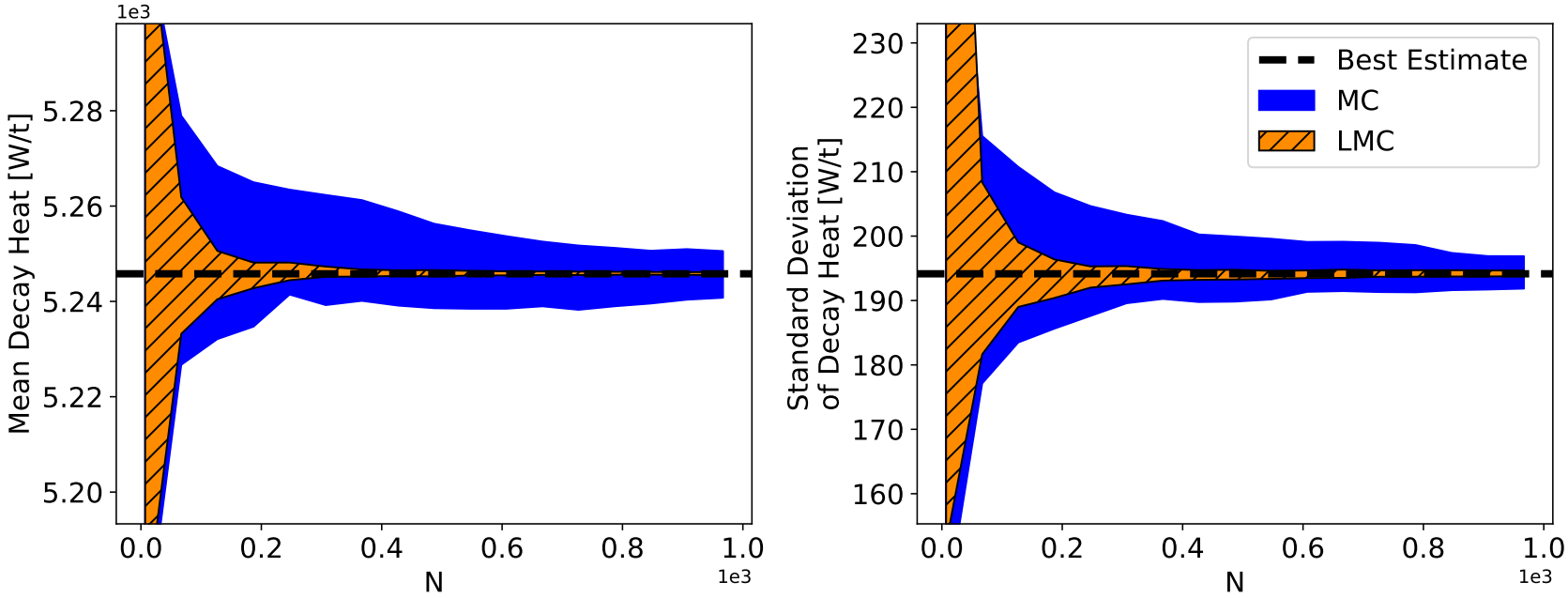

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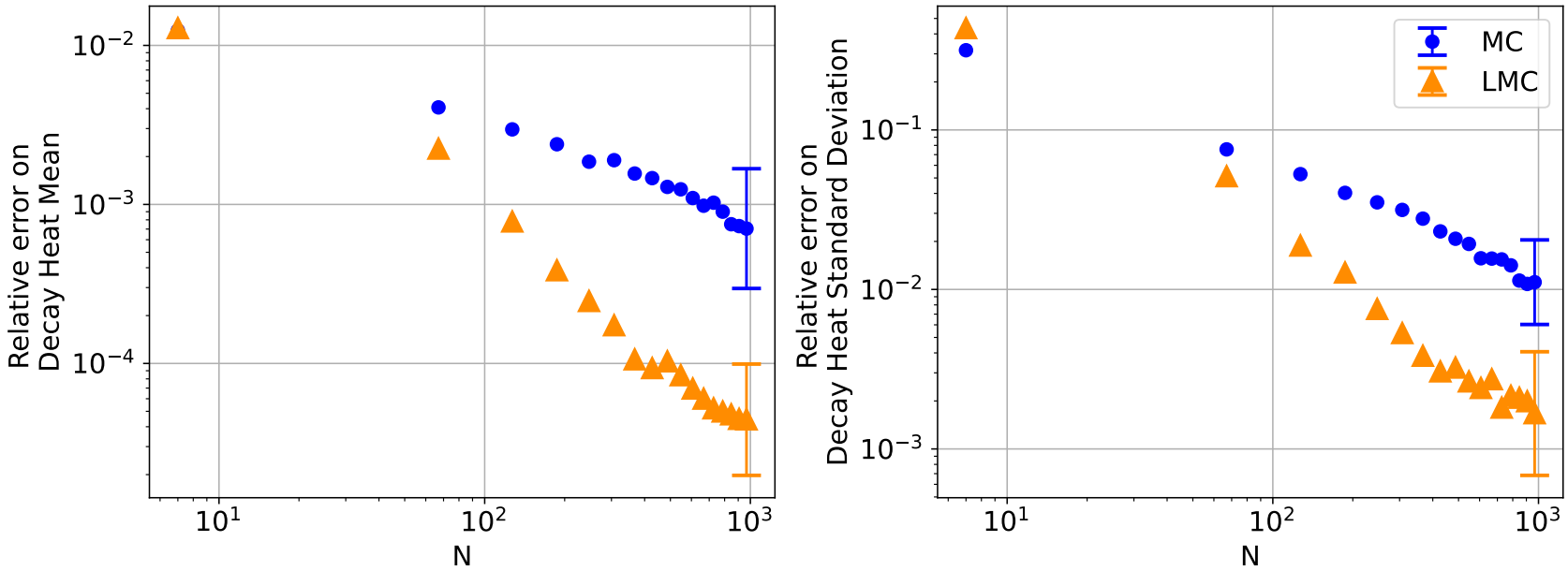


To obtain a 1% error in estimations, simple MC requires $N = 1000$ expensive simulations f, while LMC requires $N = 200$. I.e. **5 times speedup thanks to LMC**.

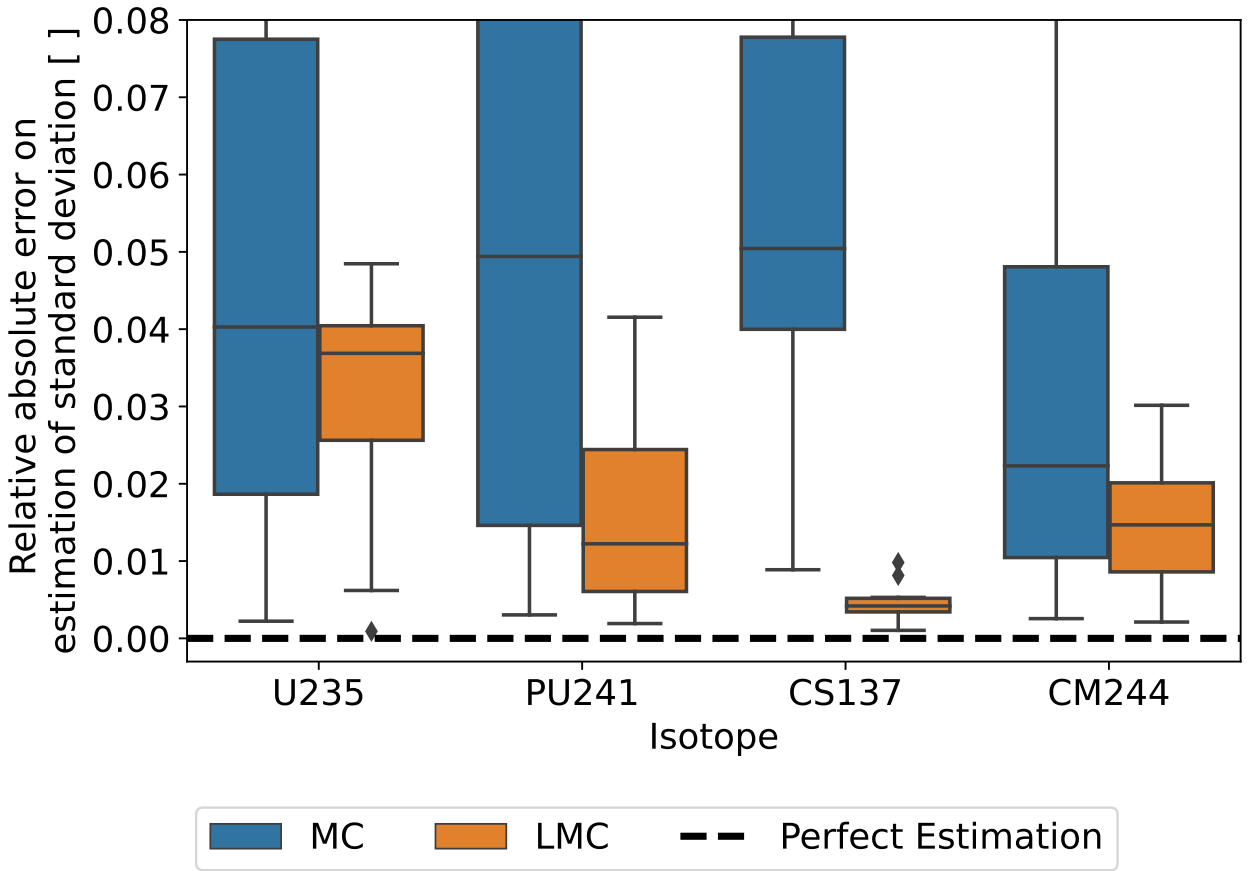
SNF Characterisation

Fixed $N = 150$ and $M = 6000$.

$$f : \mathbb{R}^{15\,557} \rightarrow \mathbb{R}$$

$$\text{Nuclear Data} \mapsto \text{Isotopic Content}$$

Predicting different quantities gives different improvements. But **LMC is always equal or better than simple MC**.

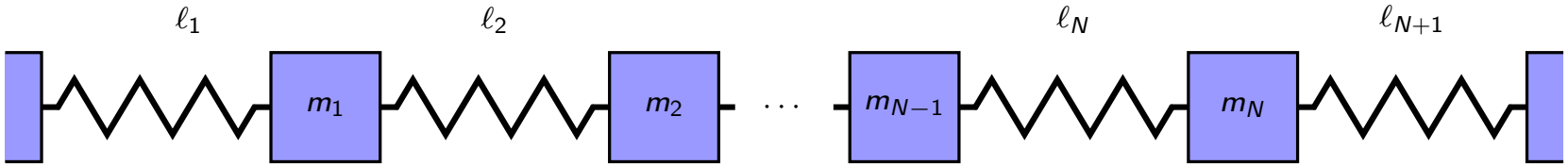


FPUT Oscillator

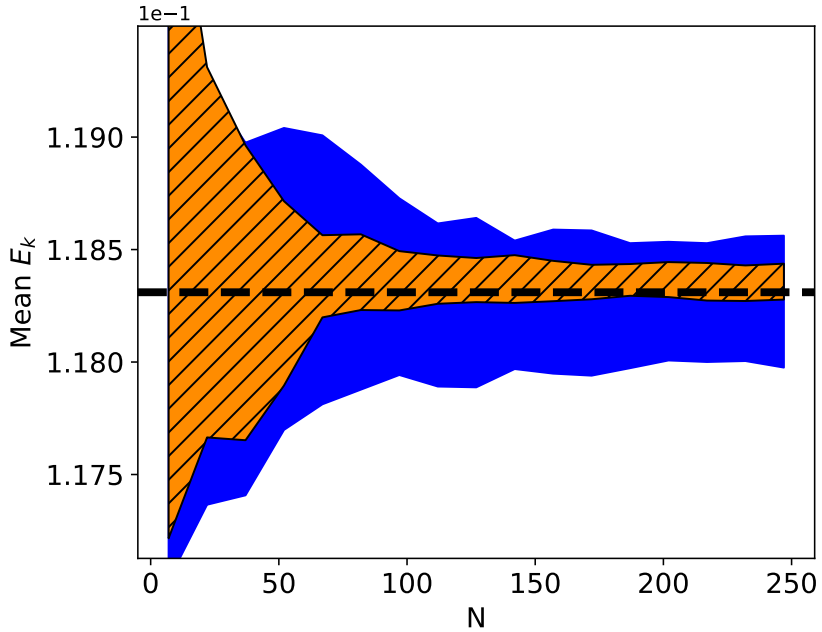
Let there be a chain of nonlinear oscillators

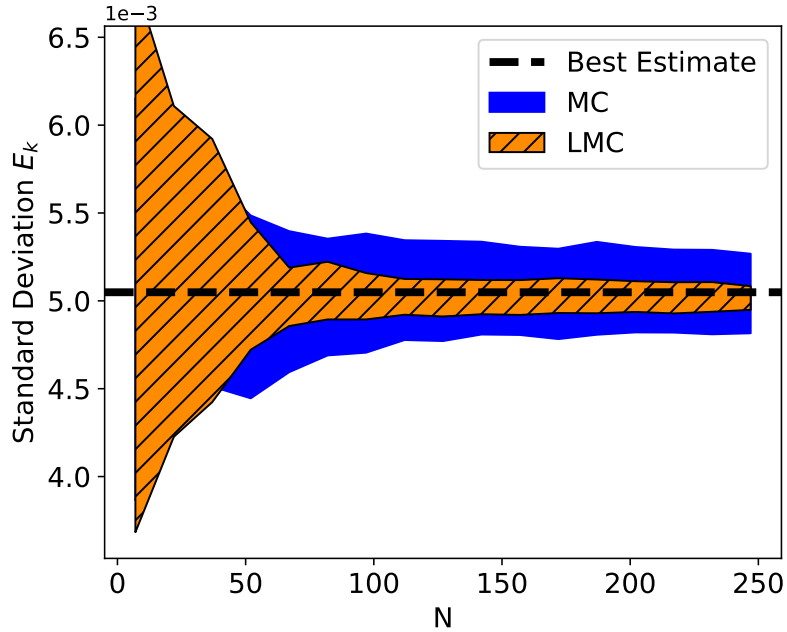
$$\ddot{x}_j = k_j \left(\ell_{j+1} - \ell_j\right) + \alpha k_j (\ell_{j+1}^2 - \ell_j^2)\,, \quad \forall j = 1, 2, ..., N\,,$$

with appropriate boundary conditions.



Consider an uncertainty in the spring constants $k_1, k_2, ..., k_N$, and nonlinear term α, with $N = 40$. What is the uncertainty in E_{kin}?





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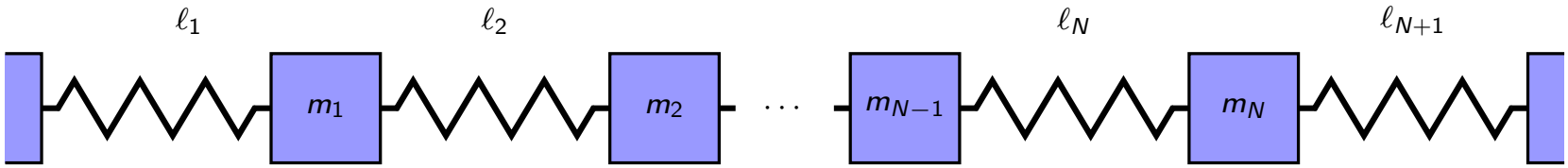
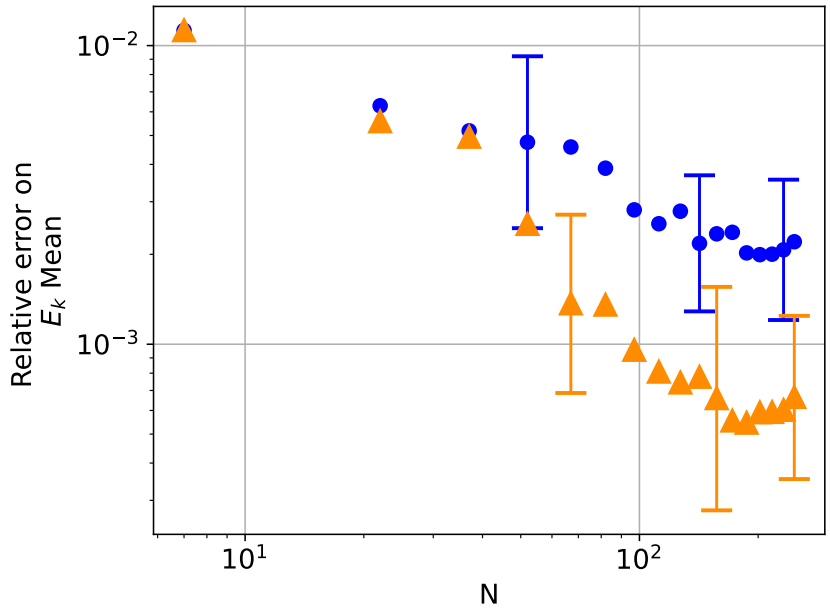
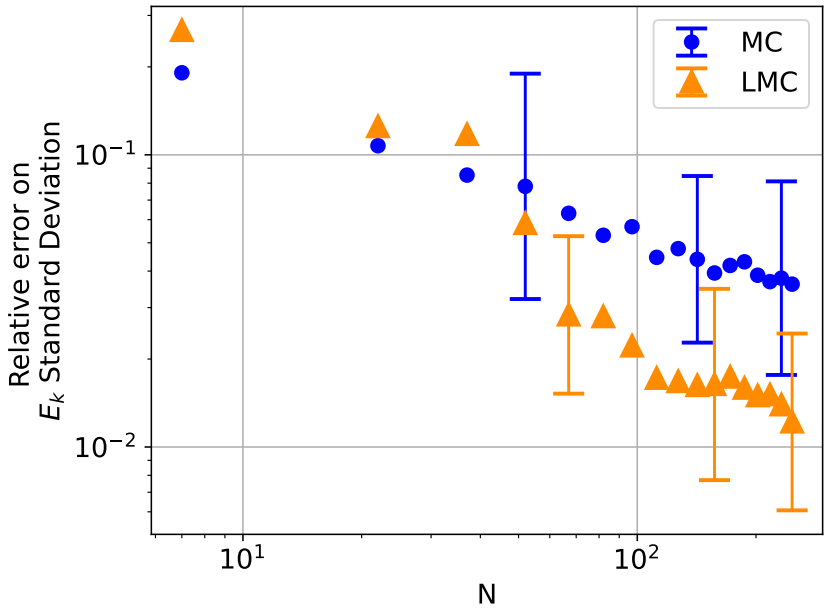
$$\ddot{x}_j = k_j \left(\ell_{j+1} - \ell_j\right) + \alpha k_j (\ell_{j+1}^2 - \ell_j^2)\,, \quad \forall j = 1, 2, ..., N\,,$$

with appropriate boundary conditions.



Consider an uncertainty in the spring constants $k_1, k_2, ..., k_N$, and nonlinear term α, with $N = 40$. What is the uncertainty in E_{kin}?



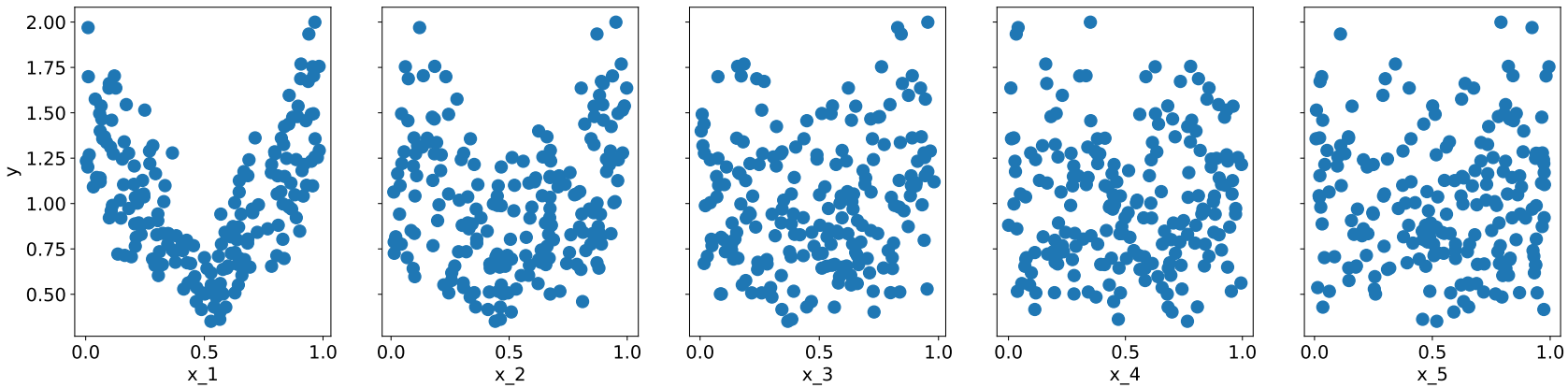


Sobol Function

$$\begin{cases} f(\boldsymbol{x}) = \prod_{i=1}^{d} \frac{|4x_i - 2| + c_i}{1 + c_i}, \\ \text{with } \boldsymbol{c} = (1, 2, 5, 10, 20, 50, 100, 200, 500, 500, ..., 500)\,, \end{cases}$$

with $d = 400$, and $\boldsymbol{X} \sim U[0,1]^d$.
Function is symmetric around $x = 0.5$, so a Lasso fit model will be flat, **i.e. worst-case scenario, LMC will be equally accurate as simple MC**.

However we can instead fit a modified Lasso model $\widetilde{f}(\boldsymbol{x}) = \boldsymbol{\beta} \cdot \boldsymbol{\phi}(\boldsymbol{x})$, with $\boldsymbol{\phi}(\boldsymbol{x}) = |x - 0.5|$.



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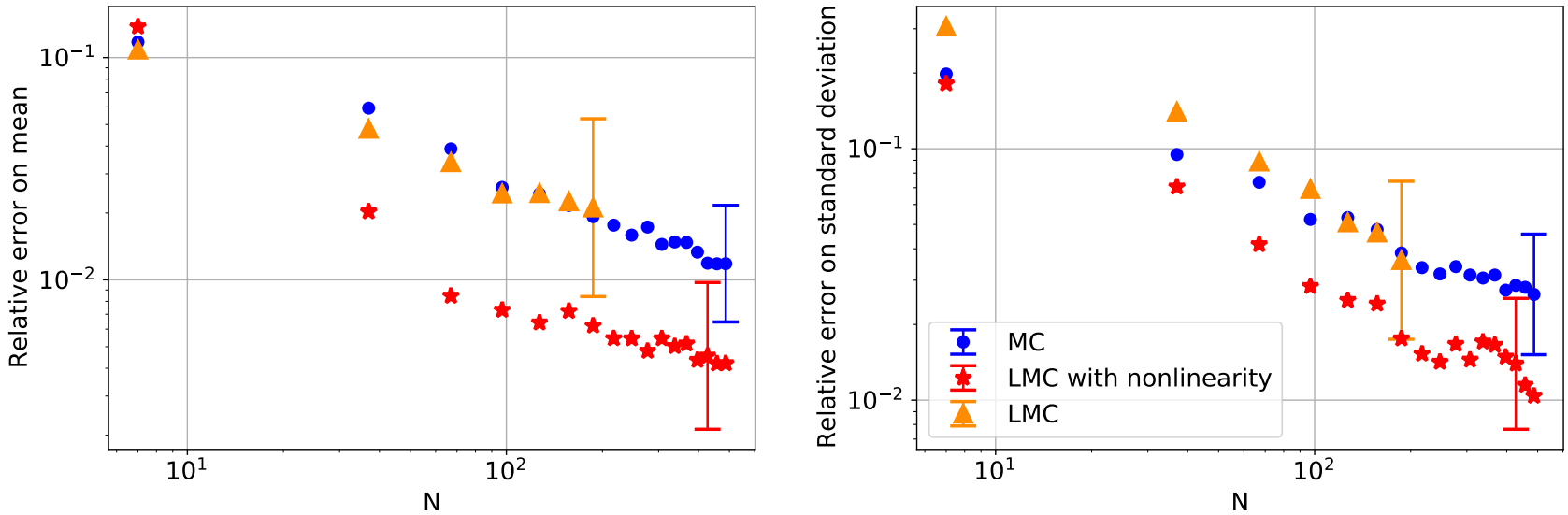
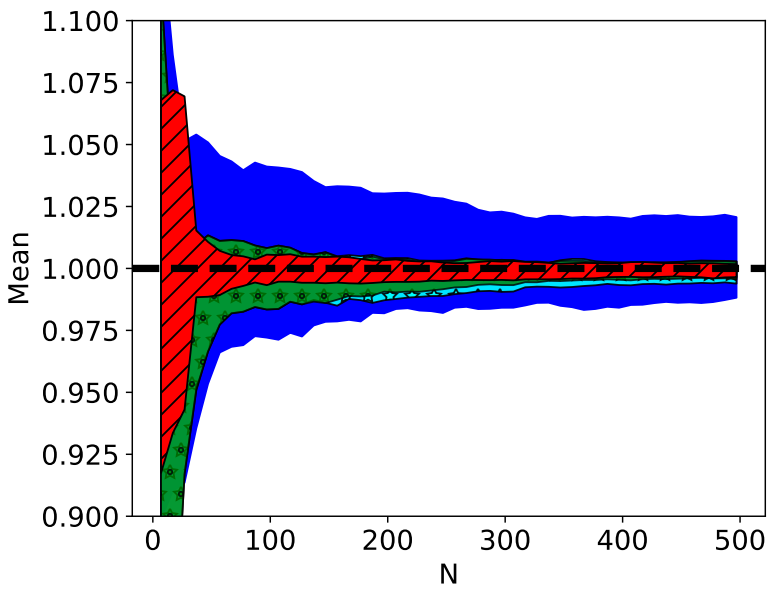
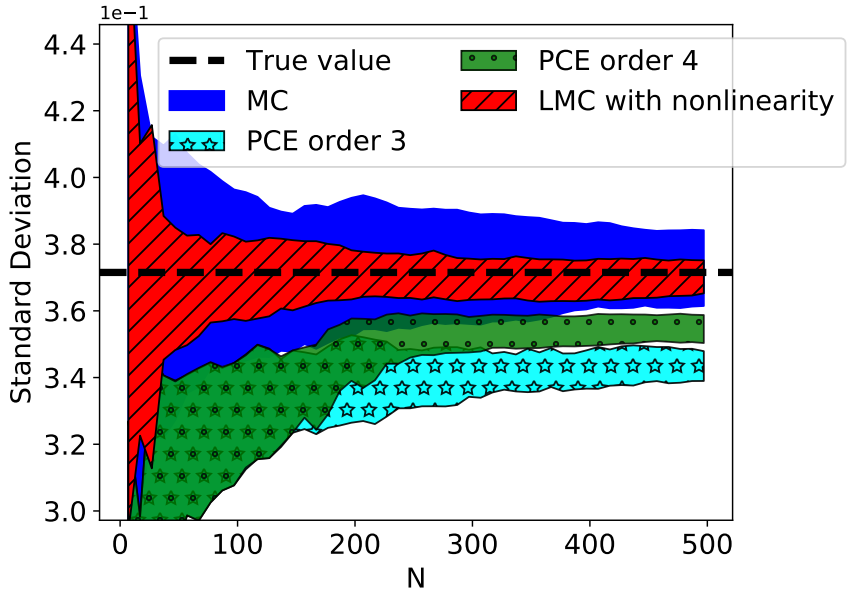


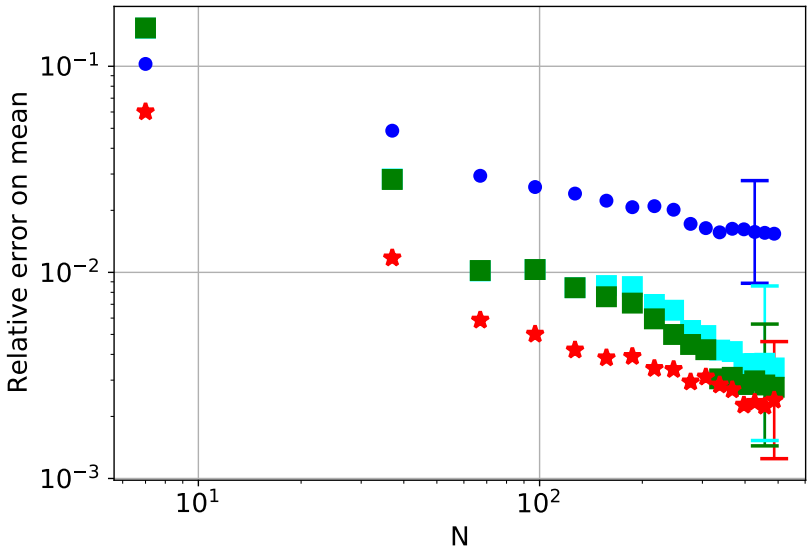
Any kind of surrogate could be used in LMC, **as long as it is strongly regularised**.

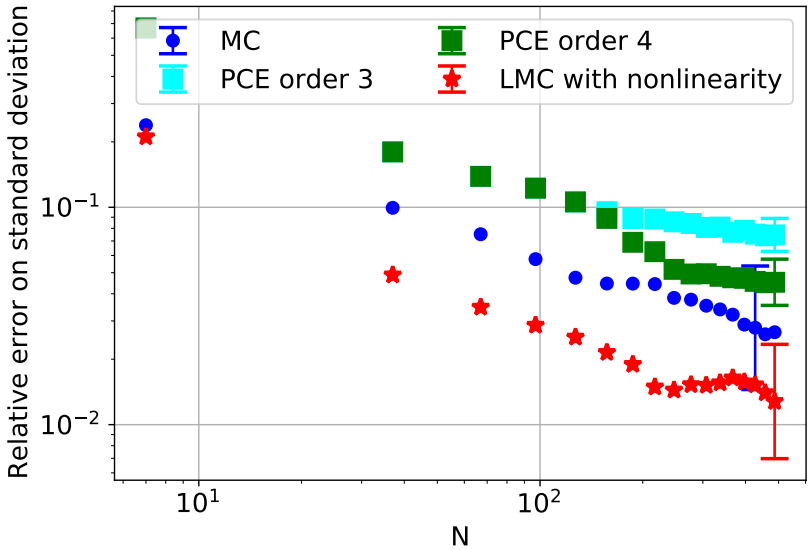
Comparison to PCE

Use the Sobol function, with input dimension $d = 8$ (higher dimensions are too slow to handle with Chaospy library).









Conclusions and Further Work

- LMC converges up to **5 times faster than simple MC**! I.e. same results with 20% of the computing resources.
- LMC is advantageous for a variety of nonlinear problems, **including UQ for spent nuclear fuel**.
- Given a set of simulations $\boldsymbol{x}_1, f(\boldsymbol{x}_1)$, $\boldsymbol{x}_2, f(\boldsymbol{x}_2)$, ..., $\boldsymbol{x}_N, f(\boldsymbol{x}_N)$, the LMC estimates can be obtained without any extra simulations.
- Could in principle be used with any surrogate model, as long as it is regularised

- The speedup is not constant, it's very dependent on f.
- Unfortunately, theoretical guarantee of faster convergence is conditioned on:
  - mild conditions on f
  - an optimal choice of regularisation parameter λ (chosen empirically so far).


Thank you for your attention.
Questions?

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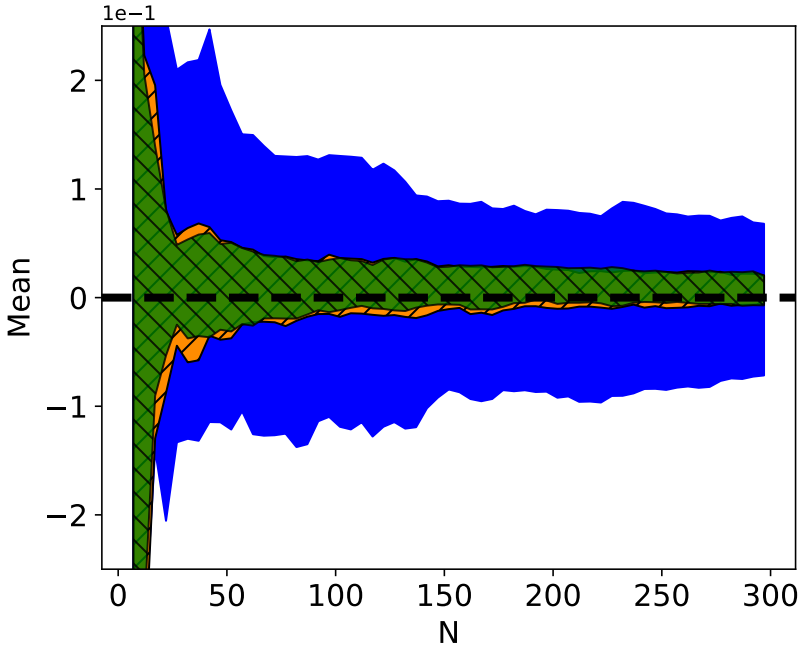
Extra Slides

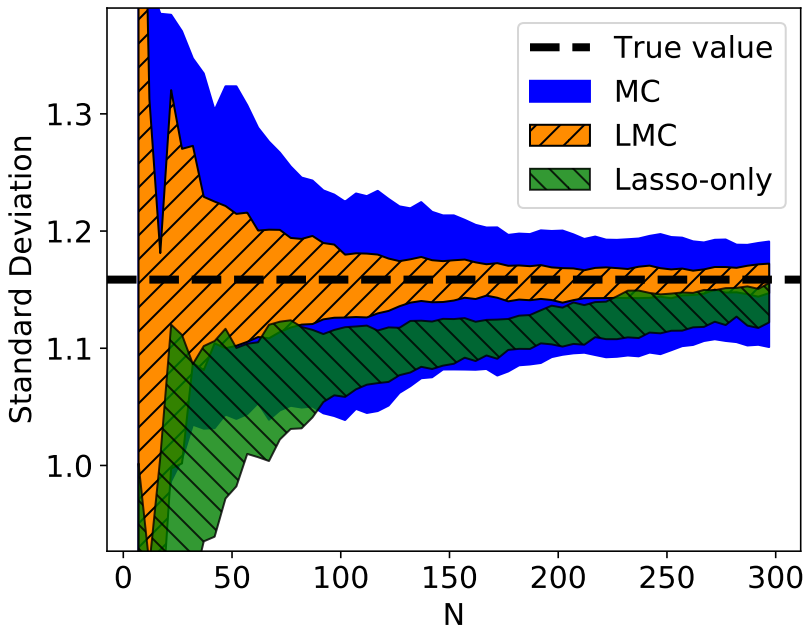
Linear Function

Let f be a linear function with a large input dimension $d = 400$:

$$\begin{cases} f(\boldsymbol{x}) = \boldsymbol{\alpha} \cdot \boldsymbol{x}, \\ \text{with } \boldsymbol{\alpha} = \left(1, \frac{1}{2}, \frac{1}{5}, \frac{1}{10}, \frac{1}{20}, \frac{1}{50}, \frac{1}{100}, \frac{1}{100}, \ldots, \frac{1}{100}\right), \end{cases}$$

with $\dim(\boldsymbol{\alpha}) = 400$ and with a normally distributed input $X \sim \mathcal{N}(0, I_d)$.





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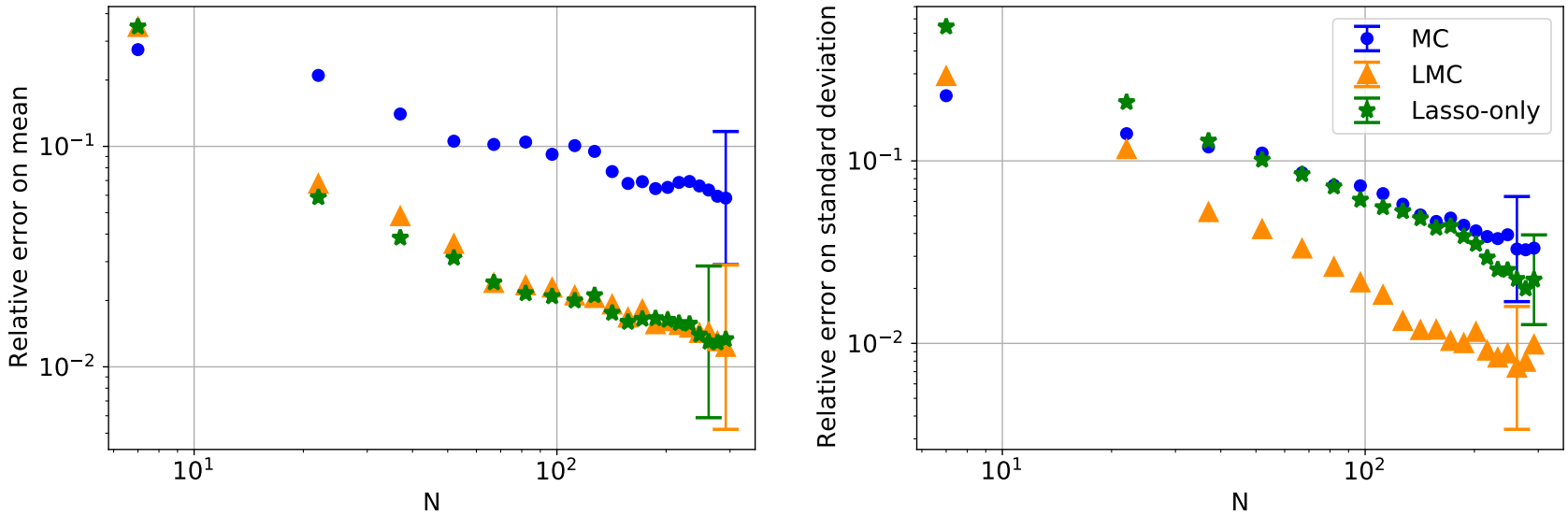
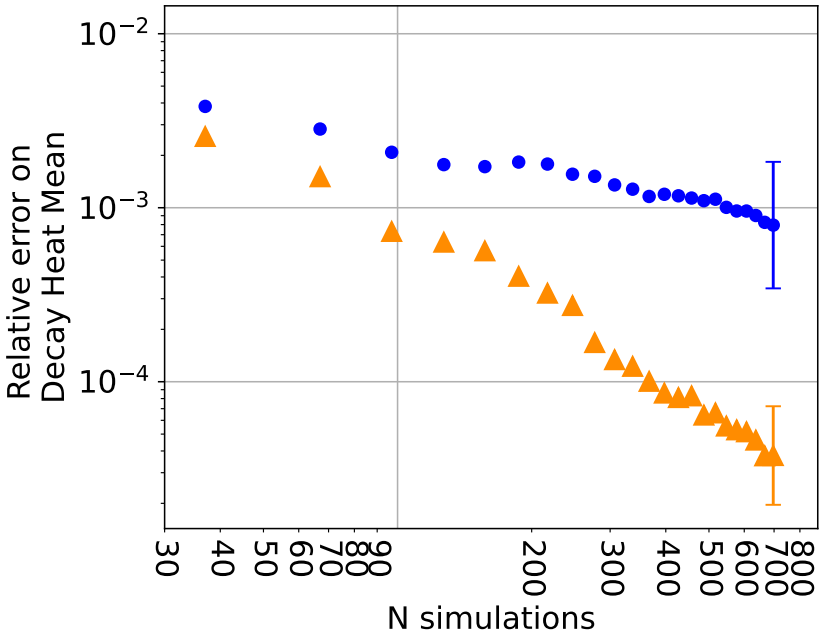
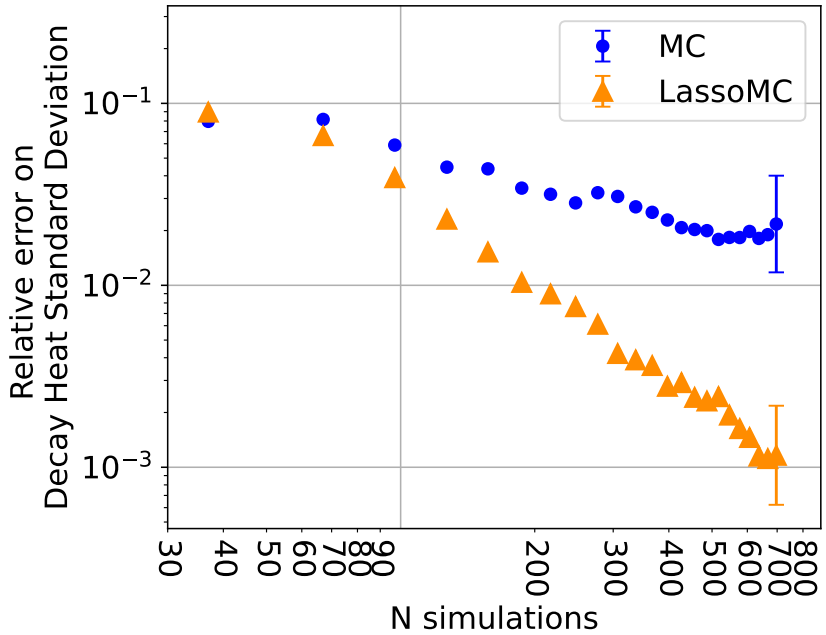


Results

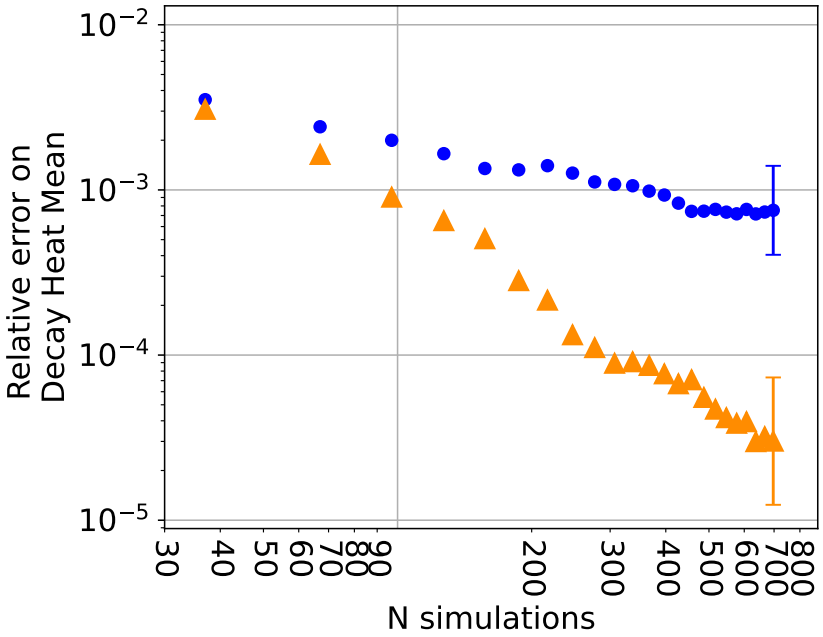
Decay heat prediction at 30 years of cooling:

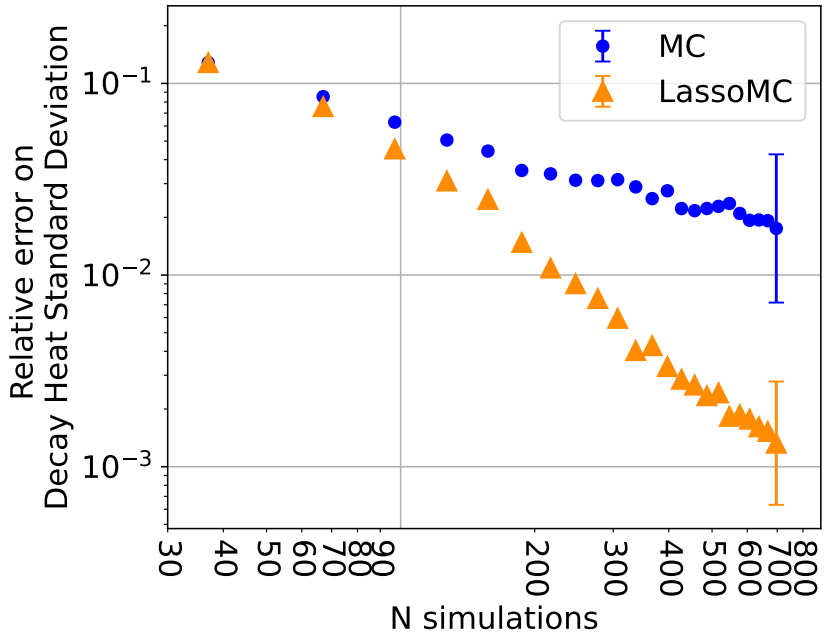




Results

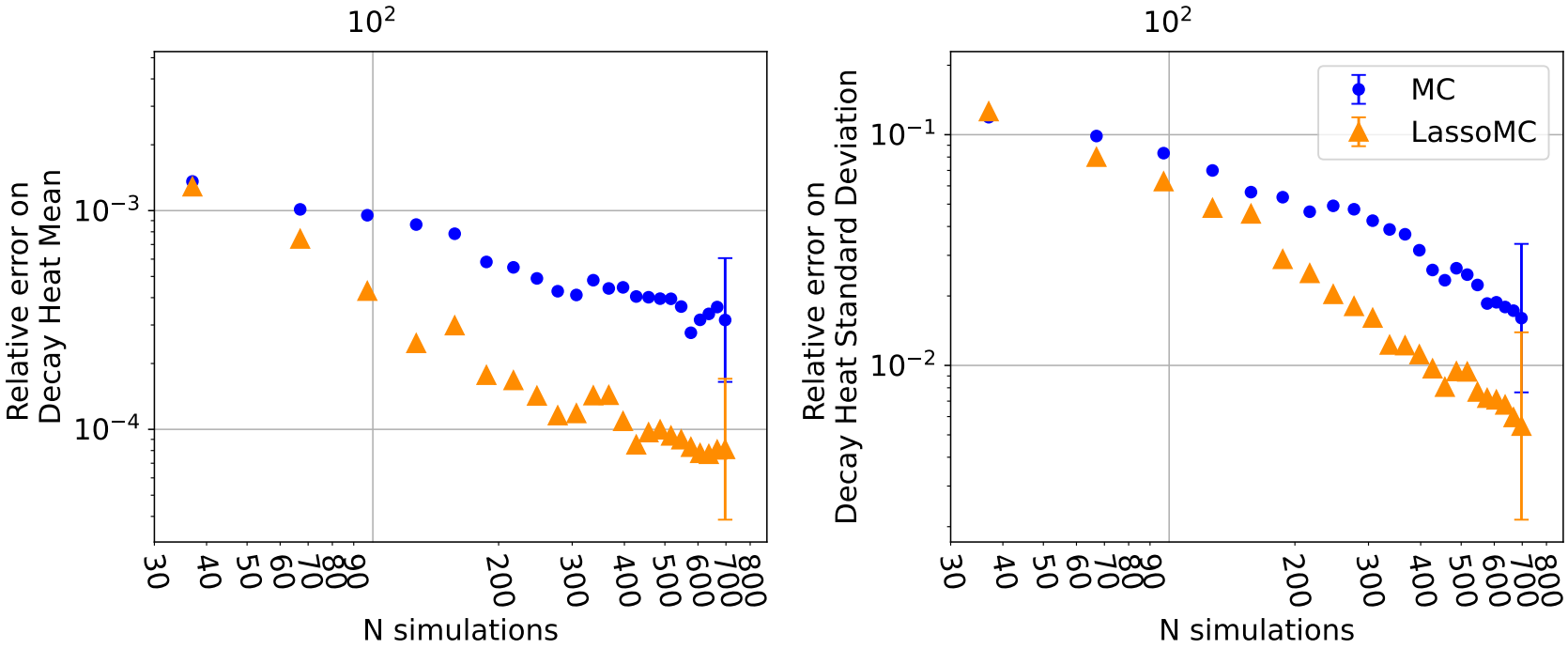
Decay heat prediction at 50 years of cooling:





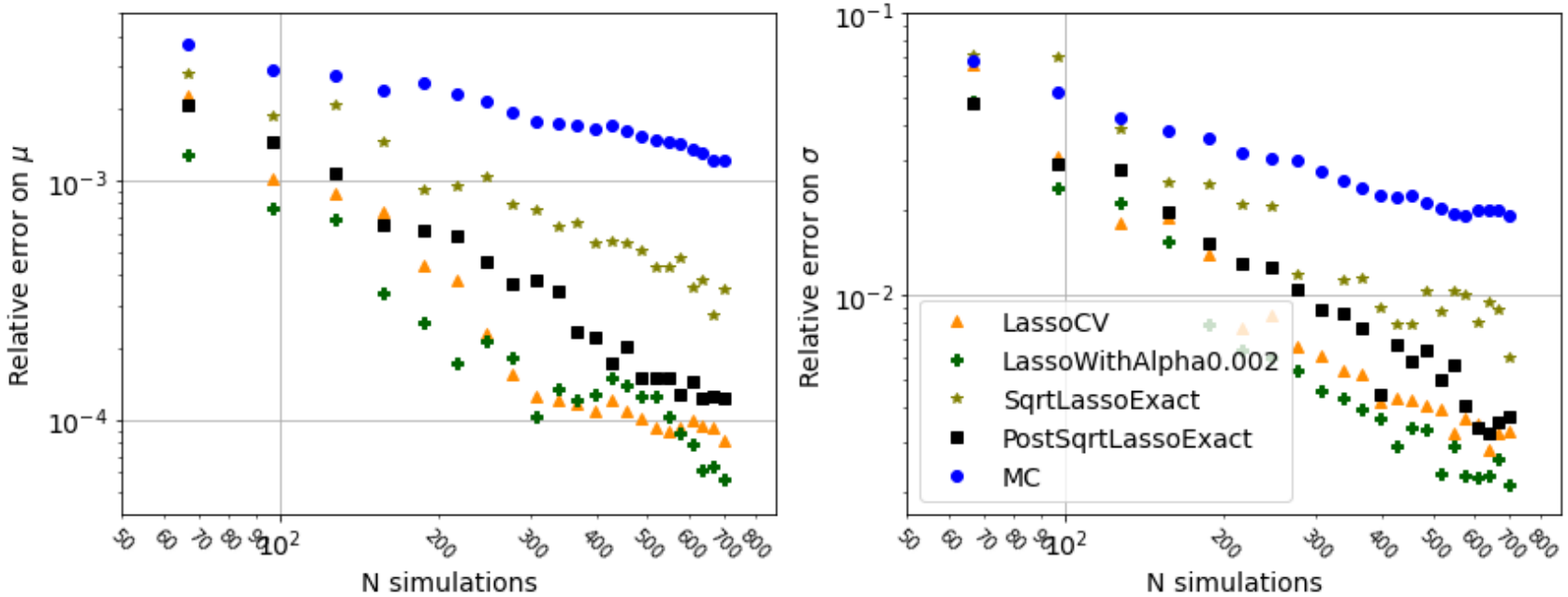
Results

U235 concentration at discharge



Lasso versions

Other versions of Lasso regression



Full LMC Algorithm

Require: the probability distribution of the input of $f(\boldsymbol{x})$, the training sets $\{\boldsymbol{x}_1, ...\boldsymbol{x}_N\}$ and $\{\boldsymbol{z}_1, ...\boldsymbol{z}_M\}$

Ensure: $N \ll M$

1: Compute the labels $f(\boldsymbol{x}_1), ..., f(\boldsymbol{x}_N)$ from the training set.
2: Compute the simple MC estimates μ_N, σ_N^2 with the labelled training set, using the simple MC estimators.
3: Do an S-fold split on the training set to obtain S smaller training sets $T_1, T_2, ..., T_S$ of size $N\frac{S-1}{S}$ each, and S correction sets $C_1, C_2, ..., C_S$ of size $n := \frac{N}{S}$ each. Each training set T_i does not overlap with its corresponding correction set C_i.
4: **for** $\mathrm{s} = 1 \dots S$ **do**
5: Fit a Lasso model $\widetilde{f}_\mathrm{s}$ on training set T_s.
6: Use the surrogate model to compute the labels of the surrogate set $\widetilde{f}_\mathrm{s}(\boldsymbol{z}_1), \widetilde{f}_\mathrm{s}(\boldsymbol{z}_2), ..., \widetilde{f}_\mathrm{s}(\boldsymbol{z}_M)$, and the C_s correction set $\widetilde{f}_\mathrm{s}\left(\boldsymbol{x}_{n(\mathrm{s}-1)+1}\right), f_\mathrm{s}\left(\boldsymbol{x}_{n(\mathrm{s}-1)+2}\right), ..., \widetilde{f}_\mathrm{s}\left(\boldsymbol{x}_{n\mathrm{s}}\right)$.
7: Combine the n labels from the correction set and the M from the surrogate set to compute the two-level estimators $(\mu_{n,M})_\mathrm{s}$ and $(\sigma^2_{n,M})_\mathrm{s}$.
8: **end for**
9: Compute the LMC mean and variance, by averaging out the estimations of each split

$$M_{N,M} = \frac{1}{S}\sum_{\mathrm{s}=1}^{S}\left(\mu_{n,M}\right)_\mathrm{s}, \quad \text{and} \quad \Sigma^2_{N,M} = \frac{1}{S}\sum_{\mathrm{s}=1}^{S}\left(\sigma^2_{n,M}\right)_\mathrm{s}.$$