An Overview of Multilevel Monte Carlo Techniques for Solving PDEs with Random Coefficients

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Multilevel and Multigrid Workshop, TU Delft

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Contents

PART 1

Classic MLMC

The KU Leuven UQ team

- **NUMA**: numerical analysis and applied mathematics
- 11 professors, about 40 postdocs and PhD students
- Working on UQ:

S. Vandewalle
Professor

P. Robbe
PhD student

A. Van Barel
PhD student

P. Blondeel
PhD student

+ collaborations with prof. D. Nuyens and prof. G. Samaey

Model parametric elliptic PDE

$$-\nabla \cdot a(\boldsymbol{x}, \boldsymbol{y}) \nabla u(\boldsymbol{x}, \boldsymbol{y}) = f(\boldsymbol{x})$$

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- early work
  - [Ghanem, Spanos, 1997]
  - [Babuska, Tempone, Zouraris, 2004]
  - [Babuska, Nobile, Tempone, 2007]
  - and many others
- parametric PDE setting in
  - [Cohen, DeVore, Schwab, 2011]
- recent interest from multilevel/QMC community
  - [Graham, Kuo, Nuyens, Scheichl, Sloan, 2011]
  - [Cliffe, Giles, Scheichl, Teckentrup, 2011]
  - [Kuo, Schwab, Sloan, 2012]
  - [Kuo, Nuyens, 2016]
  - and many others

Example

- $a(\boldsymbol{x}, \boldsymbol{y})$ is derived from a **Gaussian random field** $z(\boldsymbol{x}, \boldsymbol{y})$ with given mean $z_0(\boldsymbol{x})$ and covariance function, e.g.,

$$C(\boldsymbol{x}, \boldsymbol{x}') = \frac{2^{1-\nu}}{\Gamma(\nu)} \left(\sqrt{2\nu} r\right)^{\nu} K_{\nu} \left(\sqrt{2\nu} r\right), \quad r = \frac{\|\boldsymbol{x} - \boldsymbol{x}'\|_2}{\lambda_c}$$

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- Samples can be generated using a **KL expansion**

$$z(\boldsymbol{x}, \boldsymbol{y}) = \sum_{j \geq 1} y_j \sqrt{\theta_j} \psi_j(\boldsymbol{x})$$

where the eigenvalues θ_j and eigenfunctions $\psi_j(\boldsymbol{x})$ satisfy

$$\int_D C(\mathbf{x}, \mathbf{x}') \psi_j(\mathbf{x}') \mathrm{d}\mathbf{x}' = \theta_j \psi_j(\boldsymbol{x})$$

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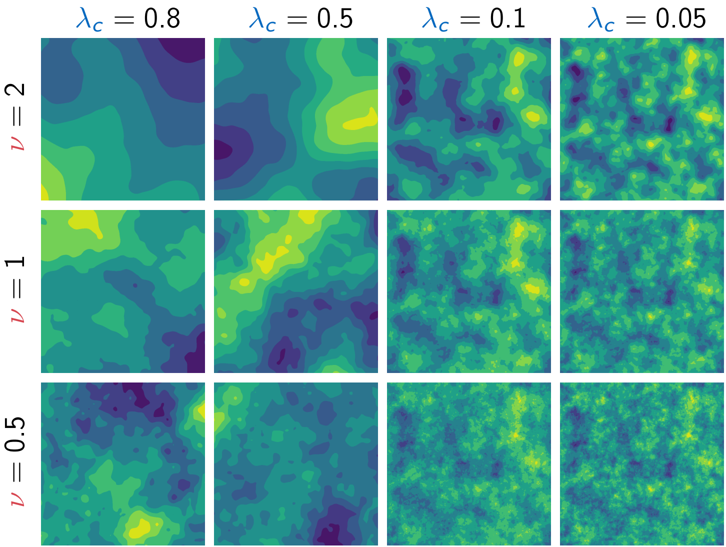
- $a(\boldsymbol{x}, \boldsymbol{y}) = \exp(z(\boldsymbol{x}, \boldsymbol{y}))$ is known as the "*lognormal case*"

Example Gaussian random fields



see GaussianRandomFields.jl

Sampling based methods

- Goal: compute statistics of **quantity of interest**

$$Q = F(u(\boldsymbol{x}, \boldsymbol{y}))$$

quantity of interest is uncertain, denote $F(\boldsymbol{y}) := F(u(\boldsymbol{x}, \boldsymbol{y}))$

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Draw a sufficiently large sample set y^(1), y^(2), ..., y^(N)
for n = 1 to N do
    Compute the random field a(x, y^(n))
    Solve a deterministic PDE using method of choice
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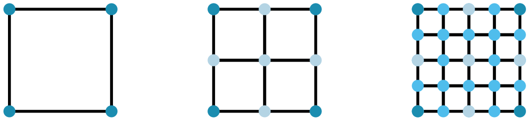
- Example: the Monte Carlo (MC) estimator for E$[Q]$ is

$$\mathcal{Q}^{\mathrm{MC}} = \frac{1}{N} \sum_{n=1}^{N} F(\boldsymbol{y}^{(n)})$$

A hierarchy of coarser grids



$\ell = 0$ $\ell = 1$ $\ell = 2$

- Solution of the PDE (and hence quantity of interest F) is approximated numerically
- Suppose we have a **hierarchy of approximations** F_ℓ, $\ell = 0, \ldots, L$ and $F_\ell \to F$ as $\ell \to \infty$
- Do not compute $\mathrm{E}[F_L]$ by sampling from F_L, but by sampling from the whole hierarchy F_ℓ, $\ell = 0, \ldots, L$

Multilevel Monte Carlo (MLMC)

- Basis is the **telescoping sum**

$$\mathrm{E}[F_L] = \mathrm{E}[F_0] + \sum_{\ell=1}^{L} \mathrm{E}[F_\ell - F_{\ell-1}]$$

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$$\mathcal{Q}_L^{\mathrm{MC}} = \sum_{\ell=0}^{L} \frac{1}{N_\ell} \sum_{n=1}^{N_\ell} \left(F_\ell(\boldsymbol{y}_\ell^{(n)}) - F_{\ell-1}(\boldsymbol{y}_\ell^{(n)}) \right) \quad (F_{-1} := 0)$$

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$$V_\ell := \mathrm{V}[F_\ell - F_{\ell-1}] = \mathrm{V}[F_\ell] + \mathrm{V}[F_{\ell-1}] - 2\mathrm{cov}(F_\ell, F_{\ell-1})$$
$$\ll \mathrm{V}[F_\ell] + \mathrm{V}[F_{\ell-1}]$$

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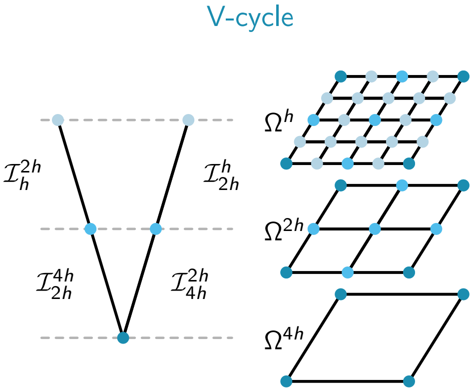
- Most samples will be taken on the coarse grid, where samples are cheap, and only few samples are needed on the finest grid

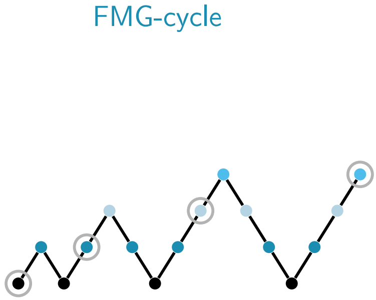
PART 2

Extensions of MLMC

Full Multigrid (FMG)

- **Full Multigrid** can compute a solution to discretization accuracy in $\mathcal{O}(M)$ time, where M is the number of DOF
- FMG also computes free solutions on coarser grids





Multigrid Multilevel Monte Carlo (MG-MLMC)

- Idea is to **recycle** the coarse solutions from the FMG method as coarse samples in the MLMC method
- MG-MLMC estimator [Kumar, Oosterlee, Dwight, 2017]

$$\mathcal{Q}_{L,\text{reuse}}^{\text{MC}} := \sum_{\ell=0}^{L} \left(\frac{1}{\sum_{i=\ell}^{L} N_i} \right) \sum_{k=\ell}^{L} \sum_{n=1}^{N_k} \left(F_\ell(\boldsymbol{y}_k^{(n)}) - F_{\ell-1}(\boldsymbol{y}_k^{(n)}) \right)$$

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- This is a sum of $L+1$ estimators $\mathcal{Y}_\ell$, i.e.,

$$\mathcal{Q}^{\mathrm{MC}}_{L,\mathrm{reuse}} := \sum_{\ell=0}^{L} \mathcal{Y}_\ell,$$

  that are **not independent**
- Accuracy of estimator is controlled using mean-square-error

$$\mathrm{MSE}\left(\mathcal{Q}^{\mathrm{MC}}_{L,\mathrm{reuse}}\right) = \mathrm{V}[\mathcal{Q}^{\mathrm{MC}}_{L,\mathrm{reuse}}] + \mathrm{Bias}\left(\mathcal{Q}^{\mathrm{MC}}_{L,\mathrm{reuse}}\right)^2$$

Obtaining a variance estimate

- Variance of the MG-MLMC estimator is

$$\mathsf{V}[\mathcal{Q}_{L,\text{reuse}}^{\text{MC}}] = \sum_{\ell=0}^{L} \mathsf{V}[\mathcal{Y}_\ell] + 2 \sum_{0 \le \ell < \tau \le L} \text{cov}(\mathcal{Y}_\ell, \mathcal{Y}_\tau)$$

$$= \sum_{\ell=0}^{L} \left(\frac{V_\ell}{\sum_{i=\ell}^{L} N_i} \right) + 2 \sum_{0 \le \ell < \tau \le L} \rho_{\ell\tau} \sqrt{\left(\frac{V_\ell}{\sum_{i=\ell}^{L} N_i} \right) \left(\frac{V_\tau}{\sum_{i=\tau}^{L} N_i} \right)}$$

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- 3 approaches to obtain variance estimates:

1. Bound the covariances using **Cauchy-Schwarz**:
   analytic solution for the optimal number of samples required on each level, but the error bound is too conservative
2. Use the **de-biasing technique** from [Rhee, Glynn, 2015]:
   randomization of the final level L
3. Randomly shifted lattice rules from **Quasi-Monte Carlo**

Quasi-Monte Carlo (QMC)

- A **Quasi-Monte Carlo** method uses well-chosen sample points, as opposed to the random points with Monte Carlo
- A popular choice are **rank-1 lattice rules**

$$\boldsymbol{t}^{(n)} := \frac{n\boldsymbol{z} \bmod N}{N} = \left\{ \frac{n\boldsymbol{z}}{N} \right\}$$

where $\boldsymbol{z} \in \mathbb{Z}_N^s$ is a generating vector and $\{\cdot\}$ denotes mod 1

[1] more details to be found in standard works such as [Dick, Kuo, Sloan, 2013]

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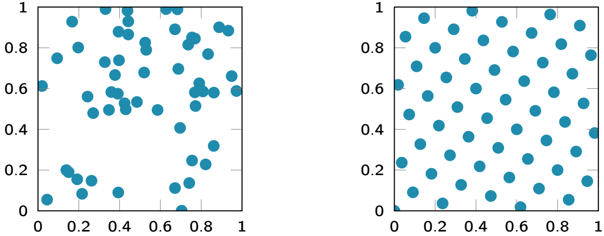
where $\boldsymbol{z} \in \mathbb{Z}_N^s$ is a generating vector and $\{\cdot\}$ denotes mod 1
- Can potentially obtain $\mathcal{O}(1/N)$ convergence, if integrand is *sufficiently smooth and decaying importance of dimensions*[1]



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Random shifting

- Lattice points are chosen deterministically, hence, they are **correlated**
- Solution is **random shifting**:

$$\bar{\mathcal{Q}}^{\mathrm{QMC}}_{L,P,\mathrm{reuse}} := \frac{1}{P}\sum_{p=1}^{P}\sum_{\ell=0}^{L}\left(\frac{1}{\sum_{i=\ell}^{L} N_i}\right)\sum_{k=\ell}^{L}\sum_{n=1}^{N_k}\left(F_\ell(\boldsymbol{y}_{k,p}^{(n)}) - F_{\ell-1}(\boldsymbol{y}_{k,p}^{(n)})\right)$$

where $\boldsymbol{y}_{k,p}^{(n)} := \Phi^{-1}\left(\left\{\boldsymbol{t}_\ell^{(k)} + \boldsymbol{u}_k^{(p)}\right\}\right)$ and $\boldsymbol{u}_k^{(p)} \sim \boldsymbol{U}(0,1)$

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- Sample variance is used as an estimate for the variance

$$\mathbb{V}[\bar{\mathcal{Q}}^{\text{QMC}}_{L,P,\text{reuse}}] \approx \frac{1}{P(P-1)}\sum_{p=1}^{P}\left(\mathcal{Q}^{\text{QMC}}_{L,p,\text{reuse}} - \bar{\mathcal{Q}}^{\text{QMC}}_{L,P,\text{reuse}}\right)^2$$

Cost analysis

- Under the assumptions that

  (1) $|\mathrm{E}[Q_L - Q]| \leq c_\alpha h_L^\alpha$,

  (2) $V_\ell \leq c_\beta h_{\ell-1}^\beta$,

  (3) $C_\ell \leq c_\gamma h_\ell^{-\gamma}$, and

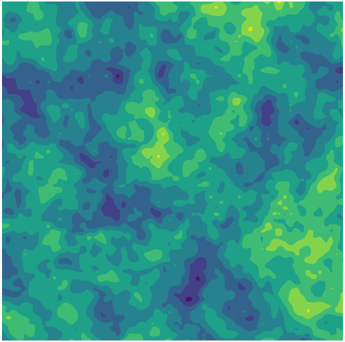
  (4) $\mathrm{V}[\bar{\mathcal{Y}}_\ell] \leq c_\lambda N_\ell^{-1/\lambda} V_\ell$.

  we can show that

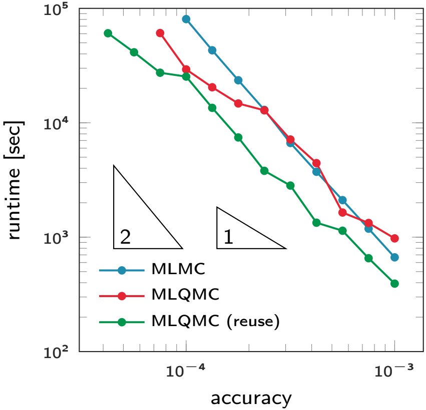
$$\mathrm{cost}(\bar{\mathcal{Q}}^{\mathrm{QMC}}_{L,P,\mathrm{reuse}}) = \left(1 - \left(s^{-(\beta+\gamma)}\right)^{\frac{\lambda}{\lambda+1}}\right) \mathrm{cost}(\bar{\mathcal{Q}}^{\mathrm{QMC}}_{L,P})$$

- This means that the sample reuse is more efficient when
  - The variance of the difference decays slowly (small β)
  - The lattice rule has good performance (small λ)

Numerical results

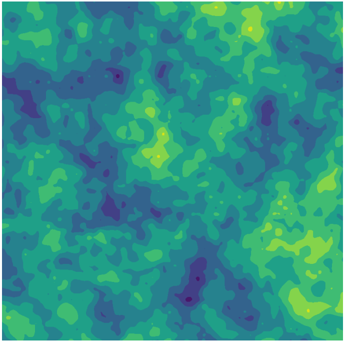


$\lambda = 0.1$, $\nu = 0.5$
3500 KL terms



speedup vs MLMC:
- ~1.34 with MLQMC
- ~2.59 with MLQMC (reuse)

Numerical results



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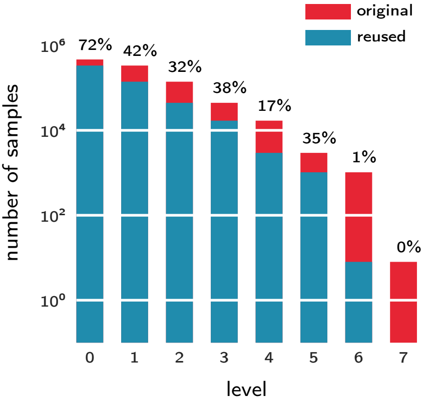
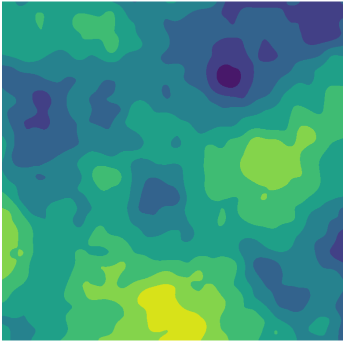
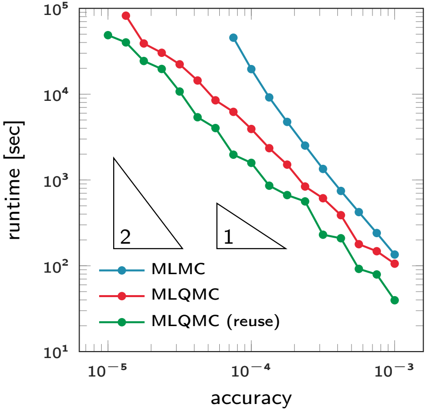


~$3 \cdot 10^6$ samples on a 4×4 grid
~$2 \cdot 10^2$ samples on a 512×512 grid

Numerical results



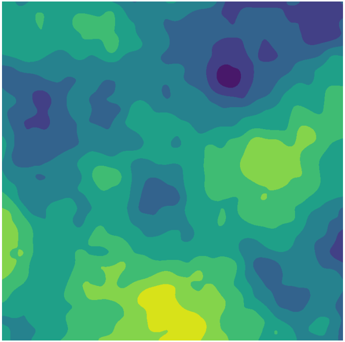
$\lambda = 0.3$, $\nu = 1$
1000 KL terms



speedup vs MLMC:

~3.17 with MLQMC
~7.82 with MLQMC (reuse)

Numerical results



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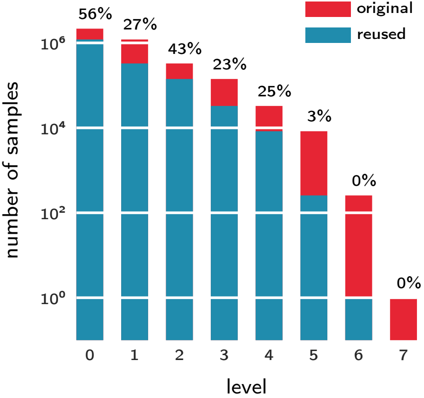
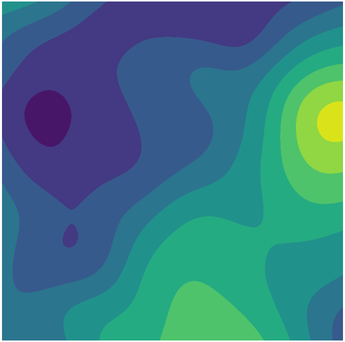
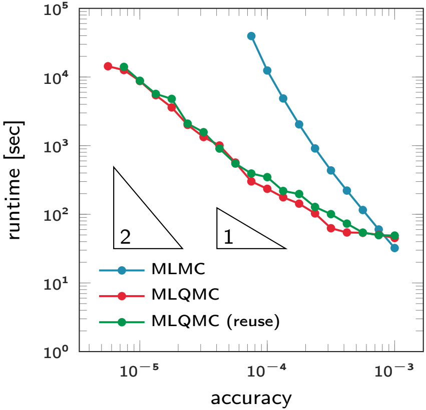


~$2 \cdot 10^7$ samples on a 4×4 grid
~$2 \cdot 10^1$ samples on a 512×512 grid

Numerical results



$\lambda = 0.5$, $\nu = 2$
100 KL terms

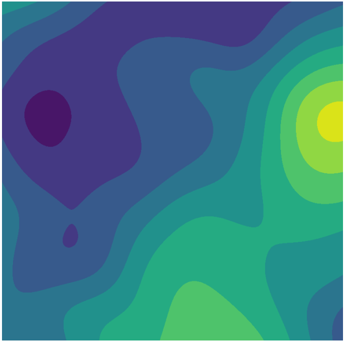


speedup vs MLMC:

~41.93 with MLQMC

~36.94 with MLQMC (reuse)

Numerical results



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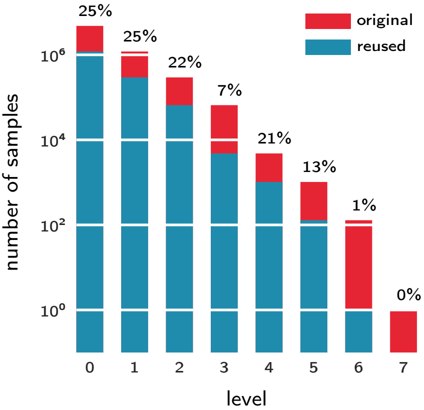


~$7 \cdot 10^7$ samples on a 4×4 grid
~$2 \cdot 10^1$ samples on a 512×512 grid

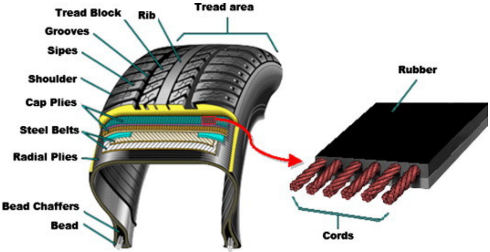
PART 3

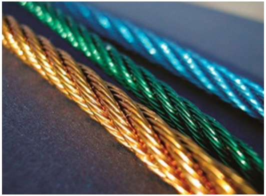
Application: Wire drawing and Bekaert

Bekaert

BEKAERT
better together

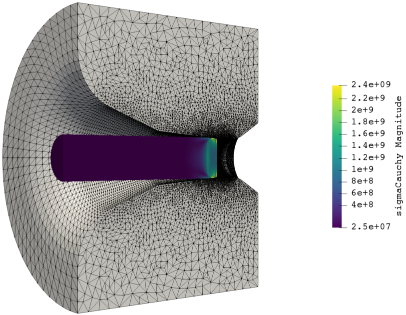
- Belgian company, est. 1880
- Steel wire transformation and coatings
- 30.000 people in 120 countries
- Physical Modelling Team

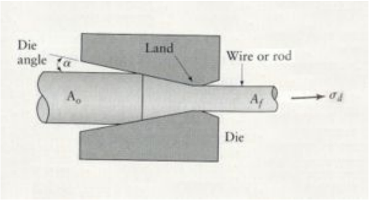




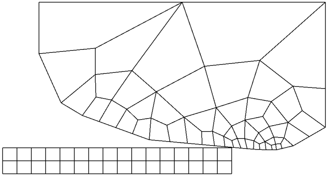
Wire drawing test case

- 2d axisymmetric geometry with die and wire
- **22 uncertainties**: geometrical, physical, process-related. . .
- Quantity of interest: drawing force, stress distribution after several drawing passes

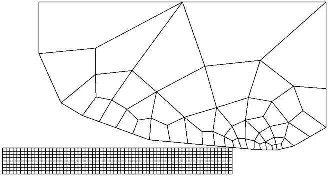




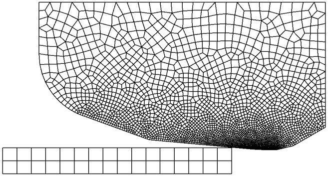
Selection of coarse approximations



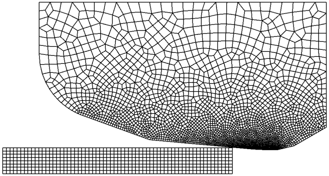
(0,0)



(0,2)

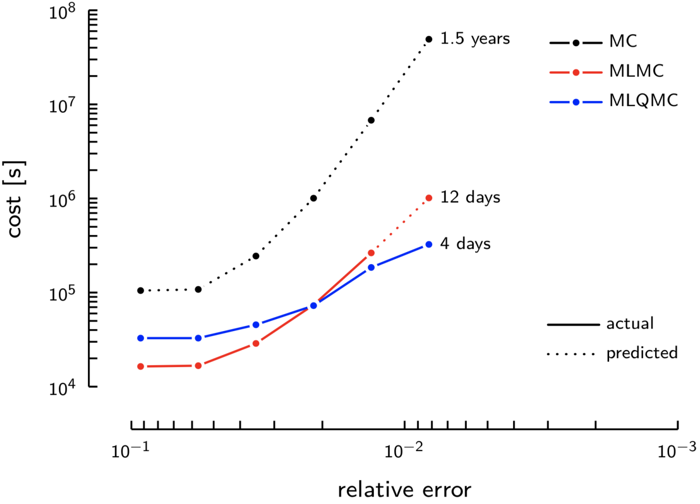


(3,0)



(3,2)

Results



10^8
10^7
10^6
10^5
10^4
cost [s]
1.5 years
12 days
4 days
MC
MLMC
MLQMC
actual
predicted
10^{-1}
10^{-2}
10^{-3}
relative error

Conclusions

- **MLMC** is an efficient **variance reduction** technique
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Thank you for your attention