Controlling error in multi-level approximations of stochastic PDEs

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Table of contents

- Model problem introduction
- First approach: standard Monte-Carlo
- First approach: error control
- Second approach: multi-level Monte-Carlo
- Second approach: error control
- MLMC Algorithm
- Future work

Table of contents

Model problem introduction

We are interested in a model problem for groundwater flow modelling in porous media.
Let D be a physical domain (of dimension d), f a deterministic data function and a a Matérn Gaussian random field defined on $\Omega \times D$ where $(\Omega, \mathcal{A}, P)$ is some probability space.

Darcy problem [Eigel et al., 2016]

Almost everywhere on Ω,

$$\begin{aligned} -\operatorname{div}(\exp(a)\nabla u) &= f \quad \text{in } D, \\ u &= 0 \quad \text{on } \partial D. \end{aligned} \qquad \text{(Darcy)}$$

Model problem introduction

Recalls on Gaussian random fields

Gaussian random field

Let $(E, \mathcal{B}, m)$ be a measure space. A real valued Gaussian random field G on E is a function

$$\begin{array}{rccc} G: & \Omega \times E & \longrightarrow & \mathbb{R} \\ & (\omega, e) & \longmapsto & G_\omega(e), \end{array}$$

such that for any finite set $\{e_1, \cdots, e_n\} \subset E$, the vector $(G(e_1), \cdots, G(e_n))$, is a Gaussian random vector.
A Gaussian random field is charaterized by μ and Σ resp. its mean and autocovariance functions

$$\begin{array}{rccc} \mu: & E & \longrightarrow & \mathbb{R} \\ & e & \longmapsto & \mathbb{E}\left[G(e)\right], \end{array}$$

$$\begin{array}{rccc} \Sigma: & E \times E & \longrightarrow & \mathbb{R} \\ & (e, e') & \longmapsto & \mathbb{E}\left[(G(e) - \mu(e))(G(e') - \mu(e'))\right]. \end{array}$$

Model problem introduction

Recalls on Gaussian random fields

Gaussian white noise

We call Gaussian white noise on $\mathbb{R}^d$ the gaussian random field

$$\dot{\mathcal{W}} : \Omega \times L^2(\mathbb{R}^d) \longrightarrow \mathbb{R},$$

with zero mean and autocovariance function defined by

$$\begin{array}{rccc} \Sigma_{\dot{\mathcal{W}}} : & L^2(\mathbb{R}^d) \times L^2(\mathbb{R}^d) & \longrightarrow & \mathbb{R} \\ & (v, w) & \longmapsto & \displaystyle\int_{\mathbb{R}^d} vw \, \mathrm{d}x. \end{array}$$

Model problem introduction

Recalls on Gaussian random fields

Matérn random fields

Let us denote Γ the Euler gamma function and $\mathcal{K}_\nu$ the Bessel's modified function of the second kind of parameter ν. A Matérn random field on D is a particular Gaussian random field (on D) with autocovariance function $\mathcal{C}$ defined for x, y in D by

$$\mathcal{C}(x,y) = \frac{\sigma^2}{2^{\nu-1}\Gamma(\nu)}(\kappa r)^\nu \mathcal{K}_\nu(\kappa r),$$

where,

$$r := |x-y|_2, \quad \kappa := \frac{\sqrt{8\nu}}{\lambda},$$

and the non-negative real parameters σ^2, ν and λ denote resp. the marginal variance, smoothness and correlation length of the field.

Model problem introduction

Weak form and quantity of interest

Darcy problem [Eigel et al., 2016]

Almost everywhere on Ω,

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Weak form

Seek u in $L^2(\Omega) \times H_0^1(D)$ such that a.e. in Ω and for every v in $H_0^1(D)$

$$\int_D \exp(a)\nabla u \cdot \nabla v \, \mathrm{d}x = \int_D f v \, \mathrm{d}x. \tag{SPDE}$$

Model problem introduction

Weak form and quantity of interest

We are not interested in the entire solution u but only in the expectation of some linear quantity of interest defined from a deterministic function g by

Quantity of interest

$$\mathbb{E}[Q] := \mathbb{E}[Q(u)] := \int_\Omega \int_D gu \,\mathrm{d}x \,\mathrm{d}P(\omega). \qquad \text{(QoI)}$$

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Goals

- Estimate $\mathbb{E}[Q]$.
- Control the estimation error.

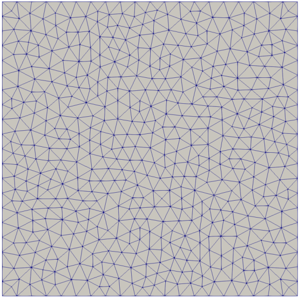
Table of contents

First approach: standard Monte-Carlo

Deterministic discretisation: Finite element method

To discretise our problem we need:

- A mesh (triangulation) $\mathcal{T}_h$ composed by cells denoted T,



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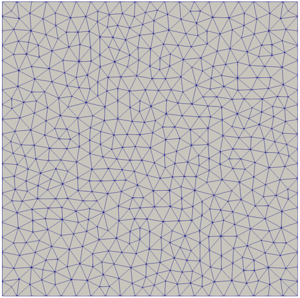

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- A mesh (triangulation) $\mathcal{T}_h$ composed by cells denoted T,
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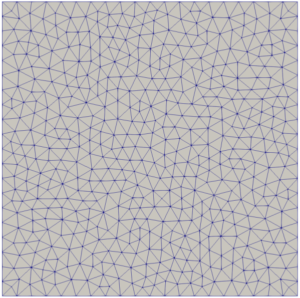
- a finite dimensional space $V_h \subset H_0^1$,



$$V_h := \left\{ v_h \in \mathcal{C}^0(D),\ v_h \in \mathcal{P}^k(T)\ \forall T \in \mathcal{T}_h,\ v_{h|\partial D} = 0 \right\}.$$

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Deterministic discretisation: Finite element method

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Discretisation of the random field

We need to draw a sample from a discretization of the random field a.

- Cholesky decomposition,
  - simple to derive,
  - dense covariance matrix decomposition,

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- Karhunen-Loève decomposition [Matthies, 2008],
  - dense eigenvalue problem to solve or dense covariance matrix decomposition,
  - can be expensive if the random field is not smooth.

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- Karhunen-Loève decomposition [Matthies, 2008],
  - dense eigenvalue problem to solve or dense covariance matrix decomposition,
  - can be expensive if the random field is not smooth.
- SPDE numerical resolution (with FEM) [Whittle, 1954], [Lindgren et al., 2011], [Bolin et al., 2017]
  - reduced computational complexity due to sparse precision matrix,
  - problem similar to the main one,
  - allows to define generalisations of the Matérn field that are still useful in practice,
  - a «straightforward» generalisation to manifolds using Laplace-Beltrami operator.

First approach: standard Monte-Carlo

Discretisation of the random field

Matérn SPDE [Croci et al., 2018]

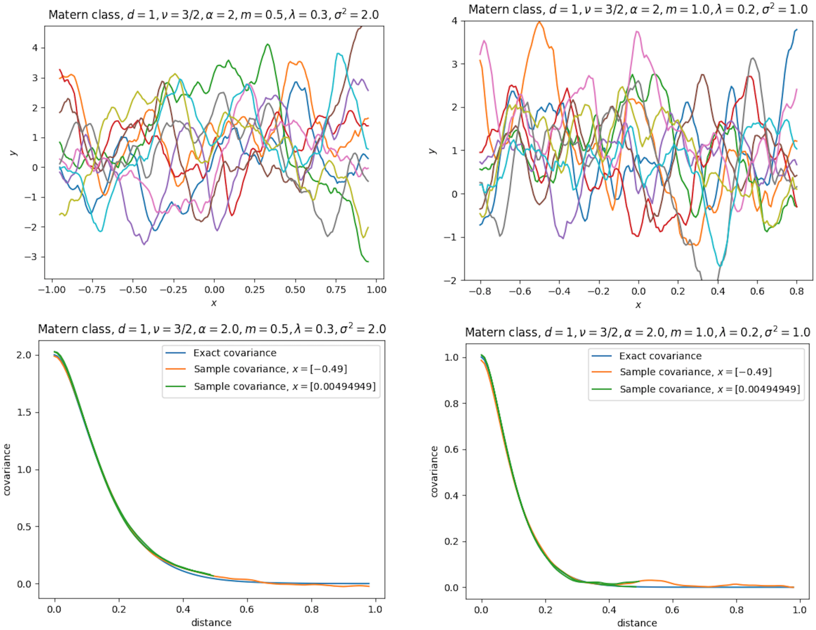
Given a Gaussian white noise $\dot{\mathcal{W}}$ defined on $\mathbb{R}^d$ and real parameters $\kappa > 0$ and $\alpha > d/2$, the solution a of the SPDE

$$(\kappa^2 - \Delta)^{\alpha/2} a = \dot{\mathcal{W}},$$

is a Matérn random field defined on $\mathbb{R}^d$ with:

- smoothness $\nu = \alpha - d/2$,
- marginal variance $\sigma^2 = \frac{\Gamma(\nu)}{\Gamma(\nu+d/2)(4\pi)^{d/2}\kappa^{2\nu}}$,
- correlation length $\lambda \simeq \frac{\sqrt{8\nu}}{\kappa}$.

$$(\kappa^2 - \Delta)^{\alpha/2} a = \dot{\mathcal{W}}.$$



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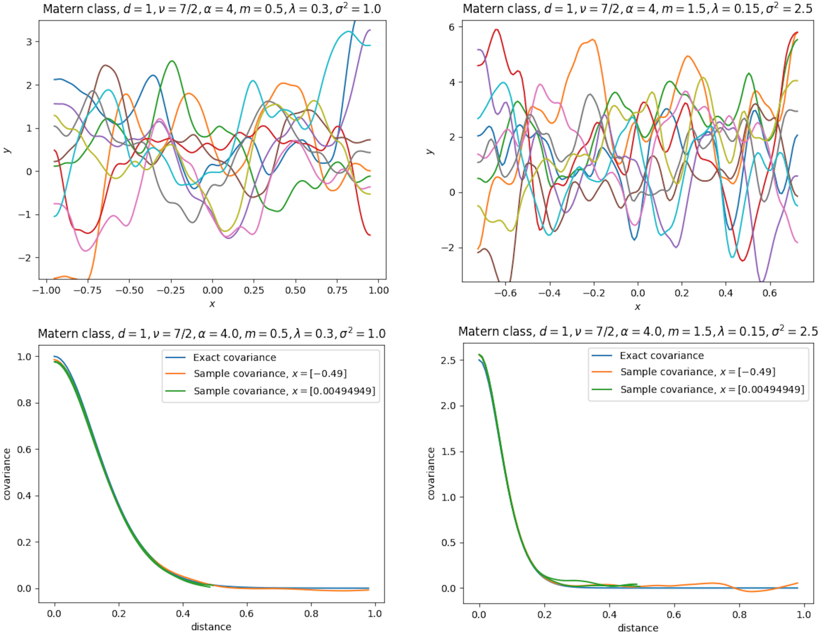

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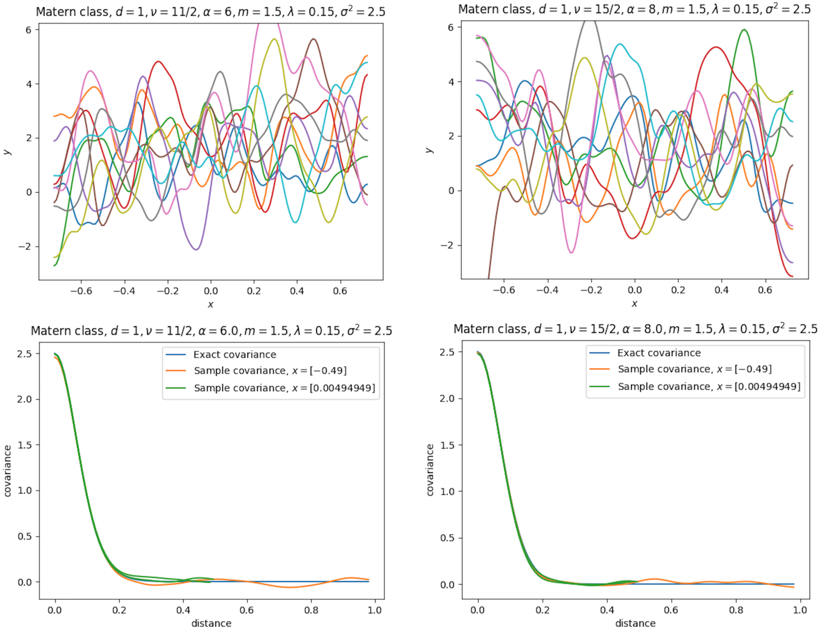

First approach: standard Monte-Carlo

Discretisation of the random field

Once we have solved the Matérn SPDE as well as the (FE) problem, we get a sample of the numerical solution u_h and we can compute an approximation of (QoI)

$$Q_h := Q(u_h) = \int_D g u_h \, \mathrm{d}x.$$

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$$Q_h := Q(u_h) = \int_D g u_h \, \mathrm{d}x.$$

Then,

$$\mathbb{E}\left[Q\right] \simeq \mathbb{E}\left[Q_h\right].$$

First approach: standard Monte-Carlo

Stochastic discretisation: Monte Carlo method

Monte Carlo

Let $\left(Q_h^{(n)}\right)_{n=1}^{N}$ be independent random variables in $L^1(\Omega, \mathbb{R})$ of same law than Q_h, then

$$\mathrm{E}_N^{\mathrm{MC}}\left[Q_h\right] := N^{-1} \sum_{n=1}^{N} Q_h^{(n)} \xrightarrow{a.s.} \mathbb{E}\left[Q_h\right].$$

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For N large enough we have,

$$\mathbb{E}\left[Q\right] \simeq \mathbb{E}\left[Q_h\right] \simeq \mathrm{E}_N^{\mathrm{MC}}\left[Q_h\right].$$

First approach: error control

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- **Mean square error:** for a given tolerance ε,

$$\mathbb{E}\left[\left(\mathrm{E}_N^{\mathrm{MC}}\left[Q_h\right] - \mathbb{E}\left[Q\right]\right)^2\right] \quad = \quad \mathrm{Var}\left[\mathrm{E}_N^{\mathrm{MC}}\left[Q_h\right]\right] \quad + \quad \mathbb{E}\left[\mathrm{E}_N^{\mathrm{MC}}\left[Q_h\right] - Q\right]^2$$

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- **Mean square error:** for a given tolerance ε,

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\mathbb{E}\left[\left(\mathrm{E}_N^{\mathrm{MC}}[Q_h] - \mathbb{E}[Q]\right)^2\right] &= \mathrm{Var}\left[\mathrm{E}_N^{\mathrm{MC}}[Q_h]\right] + \mathbb{E}\left[\mathrm{E}_N^{\mathrm{MC}}[Q_h] - Q\right]^2 \\
&= N^{-1}\,\mathrm{Var}[Q] + \mathbb{E}[Q_h - Q]^2
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&= N^{-1}\,\mathrm{Var}[Q] &+& \quad \mathbb{E}[Q_h - Q]^2 \\
&= \text{Variance} &+& \quad \text{FE bias} \\
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&= N^{-1}\,\mathrm{Var}[Q] + \mathbb{E}[Q_h - Q]^2 \\
&= \text{Variance} + \text{FE bias} \\
&\leqslant \varepsilon^2.
\end{aligned}$$

- **Computational cost:** if we assume that $|\mathbb{E}[Q_h - Q]| \leqslant ch^{\alpha}$,

$$\mathrm{Cost}(\mathrm{E}_N^{\mathrm{MC}}[Q_h]) = \mathcal{O}\left(Nh^{-1}\right) = \mathcal{O}(\varepsilon^{-2-\alpha}).$$

Table of contents

Second approach: multi-level Monte-Carlo

Deterministic discretisation: Finite element method

Finite element problem

Let $\mathcal{T}_l$ be a triangulation on D of maximum diameter h_l and $V_l \subset H_0^1$ be a finite dimensional function space. Seek u_l in $L^2(\Omega) \times V_l$ such that almost everywhere in Ω and for any v_l in V_l,

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Quantity of interest

The finite element approximation of (QoI) is given by,

$$\mathbb{E}\left[Q_l\right] := \mathbb{E}\left[Q(u_l)\right] := \int_\Omega \int_D g u_l \, \mathrm{d}x \, \mathrm{d}P(\omega).$$

Second approach: multi-level Monte-Carlo

Stochastic discretisation: Multi-level Monte Carlo method

Multi-level Monte Carlo method is a multi-fidelity method and variance reduction method ([Peherstorfer et al., 2018], [Giles, 2015]).

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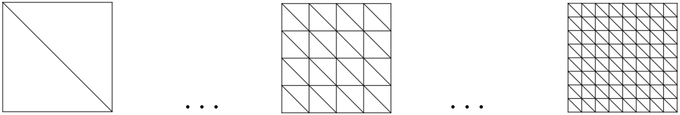

u_0 $\quad\dots\quad$ u_l $\quad\dots\quad$ u_L

$$Q(u_0) =: Q_0 \qquad Q(u_l) =: Q_l \qquad Q(u_L) =: Q_L$$

Less precise	$\longrightarrow$	More precise
Less expensive	$\longrightarrow$	More expensive

Second approach: multi-level Monte-Carlo

Stochastic discretisation: Multi-level Monte Carlo method

$$\mathbb{E}[Q] \quad \approx \quad \mathbb{E}[Q_L]$$

Second approach: multi-level Monte-Carlo

Stochastic discretisation: Multi-level Monte Carlo method

$$\begin{aligned}\mathbb{E}[Q] &\approx \mathbb{E}[Q_L] \\ &= \mathbb{E}[Q_0] + \sum_{l=1}^{L} \mathbb{E}[Q_l - Q_{l-1}]\end{aligned}$$

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$$\wr \qquad \wr$$

$$
\mathrm{E}_L^{\mathrm{ML}}[Q_L] := N_0^{-1} \sum_{n=1}^{N_0} Q_0^{(n)} + \sum_{l=1}^{L} N_l^{-1} \sum_{n=1}^{N_l} \left(Q_l^{(n)} - Q_{l-1}^{(n)} \right)
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&= \mathrm{E}_{N_0}^{\mathrm{MC}}[Q_0] + \sum_{l=1}^{L} \mathrm{E}_{N_l}^{\mathrm{MC}}[Q_l - Q_{l-1}] .
\end{aligned}
$$

Second approach: multi-level Monte-Carlo

Stochastic discretisation: Multi-level Monte Carlo method

Let us rewrite the MLMC estimator by defining

$$Y_l := \begin{cases} Q_0, & l = 0, \\ Q_l - Q_{l-1}, & l > 0. \end{cases}$$

Then,

$$\mathrm{E}_L^{\mathrm{ML}}\left[Q_L\right] := \sum_{l=0}^{L} \mathrm{E}_{N_l}^{\mathrm{MC}}\left[Y_l\right].$$

Second approach: multi-level Monte-Carlo

Stochastic discretisation: Multi-level Monte Carlo method

Lvl	Mesh	Precision & Comp. cost	[Samples]	$\xrightarrow{N^{-1}\sum}$	MC estimator
0		Low	$\left[Y_0^{(1)},\ Y_0^{(2)},\ \cdots,\ Y_0^{(N_0-1)},\ Y_0^{N_0}\right]$	$\xrightarrow{{N_0}^{-1}\sum}$	$\mathrm{E}_{N_0}^{\mathrm{MC}}\left[Y_0\right]$
$\vdots$					
l		Mid	$\left[Y_l^{(1)},\cdots,Y_l^{(N_l-1)},Y_l^{(N_l)}\right]$	$\xrightarrow{{N_l}^{-1}\sum}$	$\mathrm{E}_{N_l}^{\mathrm{MC}}\left[Y_l\right]$
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$$\mathrm{E}_L^{\mathrm{ML}}[Q_L]$$

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L		High	$\left[Y_L^{(1)},\cdots,Y_L^{(N_L)}\right]$	$\xrightarrow{{N_L}^{-1}\sum}$	$\mathrm{E}^{\mathrm{MC}}_{N_L}[Y_L]$

How to choose these parameters ?

$$\mathrm{E}^{\mathrm{ML}}_{L}[Q_L]$$

Second approach: error control

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Mean square error

$$\mathbb{E}\left[Q\right] \approx \mathbb{E}\left[Q_L\right] \approx \mathrm{E}_L^{\mathrm{ML}}\left[Q_L\right].$$

Second approach: error control

Mean square error

$$\mathbb{E}\left[Q\right] \approx \mathbb{E}\left[Q_L\right] \approx \mathrm{E}_L^{\mathrm{ML}}\left[Q_L\right].$$

- **Mean square error:** given a tolerance ε,

$$\begin{aligned}
\mathbb{E}\left[\left(\mathrm{E}_L^{\mathrm{ML}}\left[Q_L\right]-\mathbb{E}\left[Q\right]\right)^2\right] &= \mathrm{Var}\left[\mathrm{E}_L^{\mathrm{ML}}\left[Q_L\right]\right] + \mathbb{E}\left[\mathrm{E}_L^{\mathrm{ML}}\left[Q_L\right]-Q\right]^2 \\
&= \sum_{l=0}^{L} N_l^{-1}\,\mathrm{Var}\left[Y_l\right] + \mathbb{E}\left[Q_L - Q\right]^2 \\
&= \text{Variance} + \text{FE bias} \\
&\leqslant \varepsilon^2.
\end{aligned}$$

Theorem [Giles, 2008], [Giles, 2015]

If there exist independent estimators Y_l based on N_l Monte Carlo samples, and positives constants $\alpha,\ \beta,\ \gamma,\ c_1,\ c_2,\ c_3$ such that $\alpha \geqslant \frac{1}{2}\min(\beta,\gamma)$ and

1/ $|\mathbb{E}[Q_l - Q]| \leqslant c_1 h_l^\alpha$,

2/ $V_l := \mathrm{Var}[Y_l] \leqslant c_2 N_l^{-1} h_l^\beta$,

3/ C_l, the computational complexity of Y_l is bounded by $C_l \leqslant c_3 N_l h_l^{-\gamma}$,

then for any tolerance $\varepsilon < \mathrm{e}^{-1}$ there exist an integer L and a sequence of integers $(N_l)_{l=0}^L$ for which we achieve the mean square error bound

$$\mathbb{E}\left[\left(\mathrm{E}_L^{\mathrm{ML}}[Q_L] - \mathbb{E}[Q]\right)^2\right] < \varepsilon^2.$$

Moreover there exists a constant $c_4 > 0$ such that the overall computational complexity C of the MLMC estimator is bounded by

$$C \leqslant \begin{cases} c_4\varepsilon^{-2}, & \beta > \gamma, \\ c_4\varepsilon^{-2}\ln(\varepsilon)^2, & \beta = \gamma, \\ c_4\varepsilon^{-2-(\gamma-\beta)/\alpha}, & \beta < \gamma. \end{cases}$$

Theorem [Giles, 2008], [Giles, 2015]

If there exist independent estimators Y_l based on N_l Monte Carlo samples, and positives constants $\alpha,\ \beta,\ \gamma,\ c_1,\ c_2,\ c_3$ such that $\alpha \geqslant \frac{1}{2}\min(\beta,\gamma)$ and

1/ $|\mathbb{E}[Q_l - Q]| \leqslant c_1 h_l^{\alpha}$,

2/ $V_l := \mathrm{Var}[Y_l] \leqslant c_2 N_l^{-1} h_l^{\beta}$,

3/ C_l, the computational complexity of Y_l is bounded by $C_l \leqslant c_3 N_l h_l^{-\gamma}$,

then for any tolerance $\varepsilon < \mathrm{e}^{-1}$ there exist an integer L and a sequence of integers $(N_l)_{l=0}^{L}$ for which we achieve the mean square error bound

$$\mathbb{E}\left[\left(\mathrm{E}_L^{\mathrm{ML}}[Q_L] - \mathbb{E}[Q]\right)^2\right] < \varepsilon^2.$$

Moreover there exists a constant $c_4 > 0$ such that the overall computational complexity C of the MLMC estimator is bounded by

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Second approach: error control

Stochastic error control

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Using the expressions of $(N_l)_{l=0}^{L}$ computed in Giles' theorem, we can write

$$C \leqslant 2\varepsilon^{-2} \left(\sum_{l=0}^{L} \sqrt{V_l C_l} \right)^2$$

$$\leqslant 2\varepsilon^{-2} \left(\sum_{l=0}^{L} h_l^{\frac{\beta-\gamma}{2}} \right)^2$$

MLMC Algorithm

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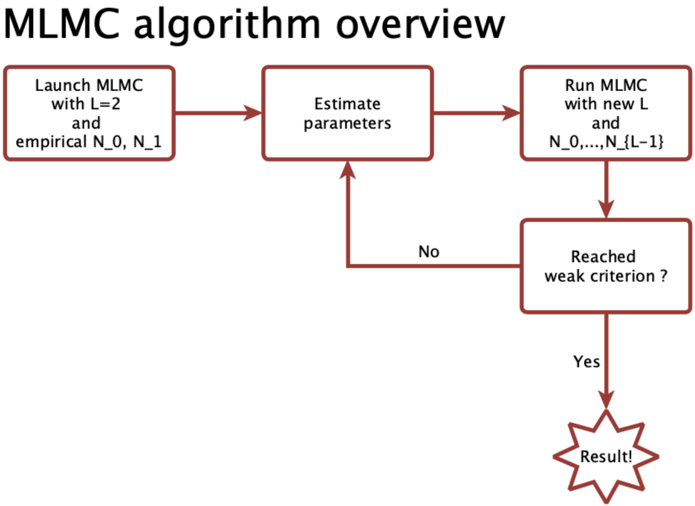
MLMC Algorithm



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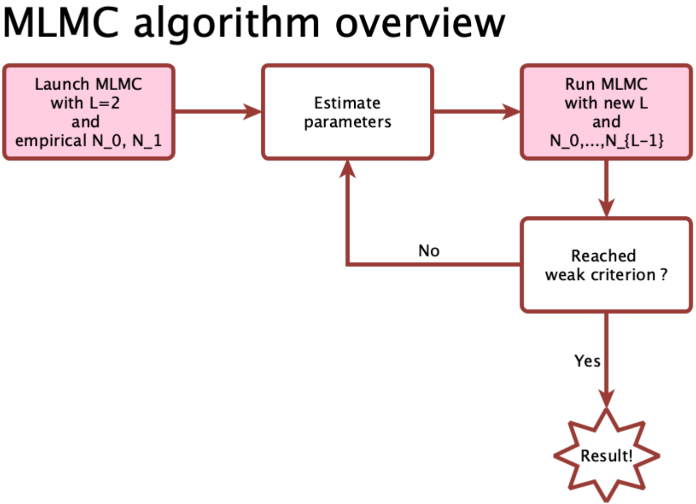

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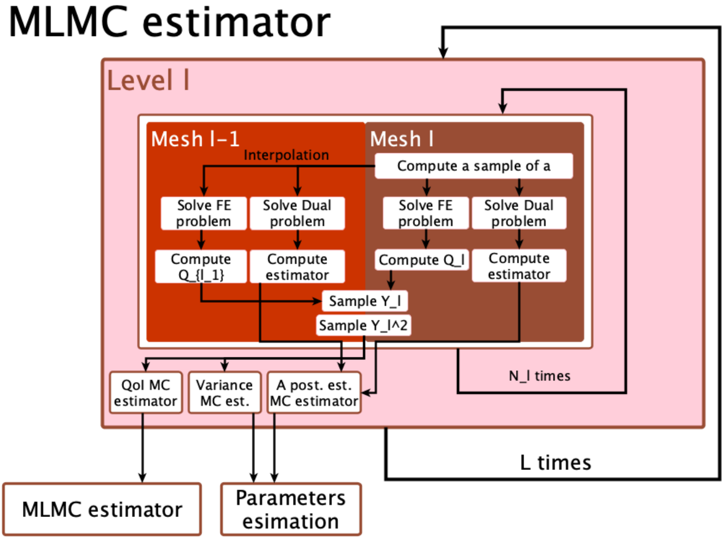

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- If neither a) or b) are satisfied, idem.

Future work

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- try random field data with non-homogeneous correlation length and random region of smaller correlation length.

Acknowledgement

Thank you for your attention!

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