A filtered multilevel Monte Carlo method for the estimation of discretized random fields.

Sparse Days 2024

J. Briant[1,2,3], M. Destouches[1], S. Gratton[3,4], S. Gürol[1,2]
P. Mycek[1,2], E. Simon[3,4], A. Weaver[1,2]

[1] Cerfacs, [2] CECI-CNRS, [3] IRIT-CNRS, [4] Université de Toulouse

CERFACS
CENTRE EUROPÉEN DE RECHERCHE ET DE FORMATION AVANCÉE EN CALCUL SCIENTIFIQUE

Table of Contents

Let Y be a random variable whose expectation $\mu = \mathbb{E}[Y]$ we want to estimate. To do so we have access to an ensemble of M realisations of Y and we can compute a Monte Carlo estimator:

$$\hat{\mu} = \frac{1}{M} \sum_{i=1}^{M} Y^{(i)}.$$

Let Y be a random variable whose expectation $\mu = \mathbb{E}[Y]$ we want to estimate. To do so we have access to an ensemble of M realisations of Y and we can compute a Monte Carlo estimator:

$$\hat{\mu} = \frac{1}{M} \sum_{i=1}^{M} Y^{(i)}.$$

But if you have access to ensembles of realisations of different fidelity you may want to try multilevel Monte Carlo methods.

Michael B. Giles, *Multilevel Monte Carlo methods*, Acta Numerica **24** (2015), 259–328 (en), doi : 10.1017/S096249291500001X

Suppose we have different fidelity ensembles (denoted with the subscript ℓ). Then the MLMC estimator of $\mu = \mathbb{E}[Y]$ is:

$$\hat{\mu}_L^{\mathsf{MLMC}} = \hat{\mu}_0^{(0)} + \sum_{\ell=1}^{L} \left(\hat{\mu}_\ell^{(\ell)} - \hat{\mu}_{\ell-1}^{(\ell)} \right)$$

with $\hat{\mu}_\ell^{(\ell')}$ a Monte Carlo estimator based on an $M_{\ell'}$ sample of Y_ℓ.

Suppose we have different fidelity ensembles (denoted with the subscript ℓ). Then the MLMC estimator of $\mu = \mathbb{E}[Y]$ is:

$$\hat{\mu}_L^{\mathsf{MLMC}} = \hat{\mu}_0^{(0)} + \sum_{\ell=1}^{L} \left(\hat{\mu}_\ell^{(\ell)} - \hat{\mu}_{\ell-1}^{(\ell)} \right)$$

with $\hat{\mu}_\ell^{(\ell')}$ a Monte Carlo estimator based on an $M_{\ell'}$ sample of Y_ℓ.

The ensembles used in a correction term are based on the same stochastic inputs.

Table of Contents

We have the different fidelity models f_ℓ each working on an associated grid of size n_ℓ (with $n_L > n_{L-1} > \cdots > n_0$)

$$f_\ell \colon \mathbb{R}^{n_\ell} \mapsto \mathbb{R}^{n_\ell} \quad \ell = 0, \ldots, L.$$

Let $\mathbf{X}_\ell$ be a random vector of size n_ℓ, we denote

$$\mathbf{Y}_\ell := f_\ell(\mathbf{X}_\ell)$$

the random vector, also of size n_ℓ, output of f_ℓ.

We have the different fidelity models f_ℓ each working on an associated grid of size n_ℓ (with $n_L > n_{L-1} > \cdots > n_0$)

$$f_\ell \colon \mathbb{R}^{n_\ell} \mapsto \mathbb{R}^{n_\ell} \quad \ell = 0, \ldots, L.$$

Let $\mathbf{X}_\ell$ be a random vector of size n_ℓ, we denote

$$\mathbf{Y}_\ell := f_\ell(\mathbf{X}_\ell)$$

the random vector, also of size n_ℓ, output of f_ℓ.

We want to estimate $\boldsymbol{\mu} := \mathbb{E}[\mathbf{Y}_L]$ with a MLMC estimator.

We have the different fidelity models f_ℓ each working on an associated grid of size n_ℓ (with $n_L > n_{L-1} > \cdots > n_0$)

$$f_\ell \colon \mathbb{R}^{n_\ell} \mapsto \mathbb{R}^{n_\ell} \quad \ell = 0, \ldots, L.$$

Let $\mathbf{X}_\ell$ be a random vector of size n_ℓ, we denote

$$\mathbf{Y}_\ell := f_\ell(\mathbf{X}_\ell)$$

the random vector, also of size n_ℓ, output of f_ℓ.

We want to estimate $\boldsymbol{\mu} := \mathbb{E}[\mathbf{Y}_L]$ with a MLMC estimator.

$\Rightarrow$ Impossible due to the inconsistent dimensions across levels.

$\Rightarrow$ **We need operators to transfer signals from a grid to another one.** Let us choose here linear operators $\mathbf{R}$ and $\mathbf{P}$.

$\Rightarrow$ **We need operators to transfer signals from a grid to another one.** Let us choose here linear operators $\mathbf{R}$ and $\mathbf{P}$.

The 2-level MLMC estimator is:

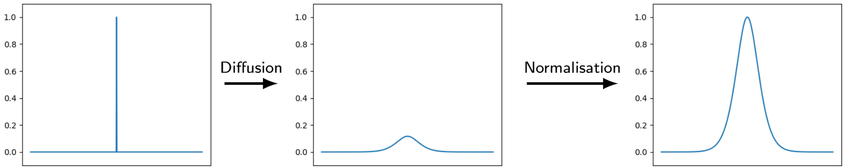
$$\hat{\boldsymbol{\mu}}_1^{\mathsf{MLMC}} = \frac{1}{M_0}\sum_{i=1}^{M_0} \mathbf{P} f_0(\mathbf{R}\mathbf{X}_1^{(0,i)}) + \frac{1}{M_1}\sum_{i=1}^{M_1} f_1(\mathbf{X}_1^{(1,i)}) - \mathbf{P} f_0(\mathbf{R}\mathbf{X}_1^{(1,i)}).$$

Table of Contents

In oceanography, the diffusion equation can be used as a correlation model:

$$\frac{\partial u}{\partial t} = \boldsymbol{\kappa}\Delta u, \quad \text{with } u(x,0) = u_0(x).$$

$\boldsymbol{\kappa}$ is the diffusivity field. A normalisation step is required afterward to regain the lost amplitude.



Let $\mathbf{X} \sim \mathcal{N}(\mathbf{0}_n, \mathbf{I}_n)$ be a random discretized field and f the diffusion model. The normalization coefficients can be estimated using a Monte Carlo method:

$$\hat{\boldsymbol{\mu}} = \frac{1}{M} \sum_{i=1}^{M} f(\mathbf{X}^{(i)}) \circ f(\mathbf{X}^{(i)}),$$

with $\circ$ being the Schur product.

$\Rightarrow$ MLMC estimator should lead to a better estimation.

For this problem the values of the discretized fields are defined at the center of grid cells. The grids are 2D and of size 128×256, 64×128, 32×64 and 16×32. The (very simple) transfer operators chosen for the MLMC estimator have the following stencil

$$\mathbf{R} = \frac{1}{2} \left] \begin{matrix} 1 & & 1 \\ & * & \\ 1 & & 1 \end{matrix} \right[_{h}^{2h} \quad \text{and} \quad \mathbf{P} = \left] \begin{matrix} 1 & & 1 \\ & * & \\ 1 & & 1 \end{matrix} \right[_{2h}^{h} .$$

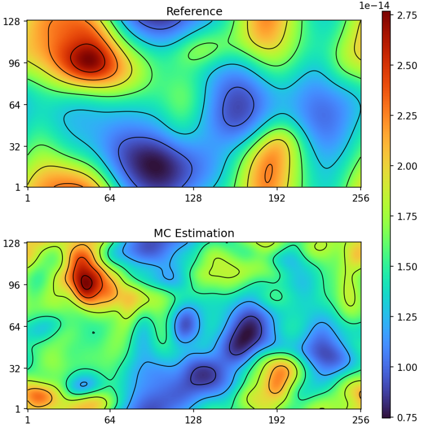


Figure: The exact field of normalisation coefficients computed explicitly for a given diffusivity tensor $\boldsymbol{\kappa}$ and a MC estimation computed from 100 samples.

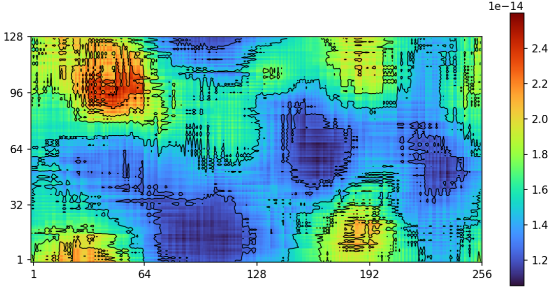


Figure: 4 levels MLMC estimation computed with the same budget as a 100 samples MC.

⇒ When looking at the total MSE of the MLMC it is much better than the MC estimator.

Table of Contents

Why performing a spectral analysis ?

- Total MSE is a scalar error $\Rightarrow$ limited for estimation of discretized fields;
- Is the error different among the scales ?
- Explaining the interferences on the MLMC estimation;
- Understanding the effects of the restriction operator $\mathbf{R}$ and the prolongation operator $\mathbf{P}$.

To conduct such an analysis we consider a Hartley basis $\mathbf{H}$ of the spectral space.

When restricting a high frequency signal to a coarse grid where it cannot be represented it will appear as a low frequency signal.
$\Rightarrow$ **Error brought on the low frequencies (aliasing).**

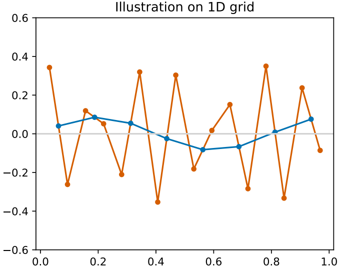


Figure: The 13th column of $\mathbf{H}$ on a grid of size 16 (orange), and its restriction on a grid of size 8 (blue).

When prolongating a signal, another high frequency term will appear.
$\Rightarrow$ **Bad estimation of high frequencies.**

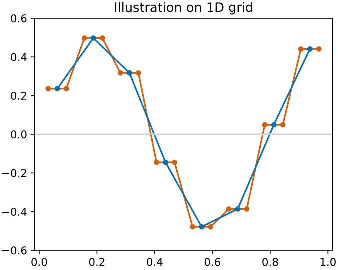
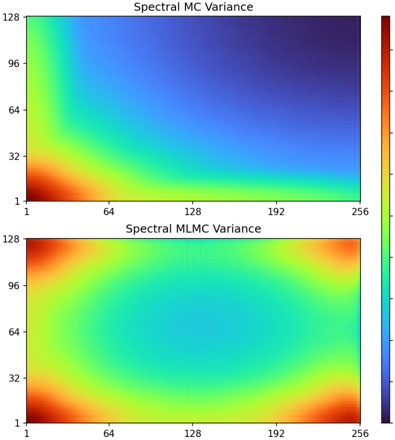
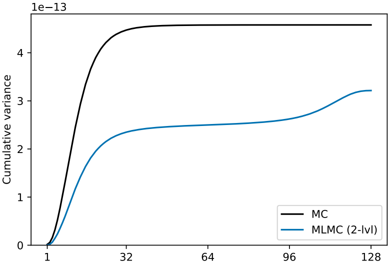


Figure: The 2nd column of $\mathbf{H}$ on a grid of size 8 (blue), and its prolongation on a grid of size 16 (orange).



(a) Spectral decomposition of the variance of MC and MLMC estimators



(b) Cumulative variance of MLMC

Table of Contents

Idea: filtering the high frequencies when transferring discretized fields from a grid to another with smoother operators. A second-order Shapiro filter with the following stencil for example:

$$\frac{1}{4}\begin{pmatrix} 1/16 & 1/8 & 1/16 \\ 1/8 & 1/4 & 1/8 \\ 1/16 & 1/8 & 1/16 \end{pmatrix}.$$

If we denote $\mathbf{S}$ the smoother operator used we would have:

$$\mathbf{Y} = \mathbf{S}\mathbf{P} f_0(\mathbf{R}\mathbf{S}\mathbf{X}).$$

Ralph Shapiro, *Smoothing, filtering, and boundary effects*, Reviews of Geophysics **8** (1970), no. 2, 359–387 (en), doi: 10.1029/RG008i002p00359

Filtered MLMC (F-MLMC) estimation

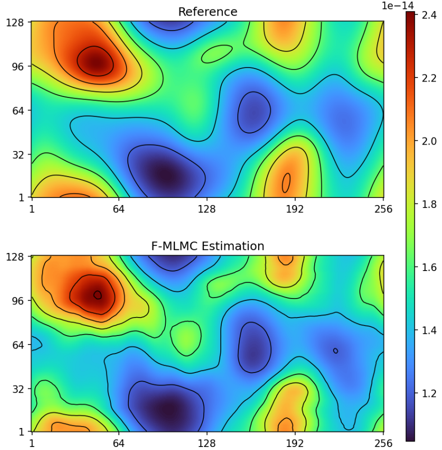
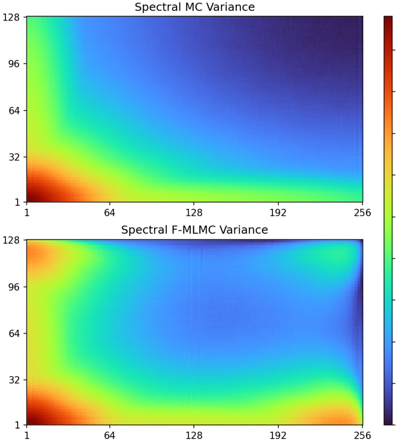
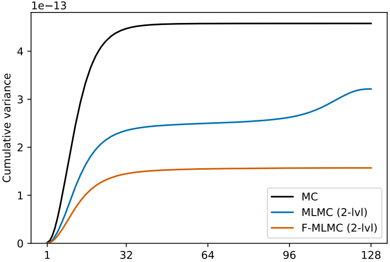


Figure: The exact normalization coefficients and a 4-levels F-MLMC estimation computed with the same budget as a 100 samples MC.

Filtered MLMC (F-MLMC) estimation



(a) Spectral decomposition of the variance of MC and F-MLMC estimators



(b) Cumulative variance of MC, MLMC and F-MLMC estimator

Table of Contents

Two estimators tested:

- the MLMC estimator with $\mathbf{Y}_\ell = \mathbf{P} f_\ell(\mathbf{R}\mathbf{X})$.
- the F-MLMC estimator with $\mathbf{Y}_\ell = \mathbf{S}\mathbf{P} f_\ell(\mathbf{R}\mathbf{S}\mathbf{X})$,

The F-MLMC can reach much lower variance.

$\Rightarrow$ Results depends a lot on chosen $\mathbf{P}$ and $\mathbf{R}$.

Two estimators tested:

- the MLMC estimator with $\mathbf{Y}_\ell = \mathbf{P} f_\ell(\mathbf{R}\mathbf{X})$.
- the F-MLMC estimator with $\mathbf{Y}_\ell = \mathbf{S}\mathbf{P} f_\ell(\mathbf{R}\mathbf{S}\mathbf{X})$,

The F-MLMC can reach much lower variance.

$\Rightarrow$ Results depends a lot on chosen $\mathbf{P}$ and $\mathbf{R}$.

Problematic

How can one choose the best $\mathbf{P}$ and $\mathbf{R}$ (or the smoothing operator $\mathbf{S}$) such that the variance of the MLMC estimator is minimized ?

Problematic

How can one choose the best $\mathbf{P}$ and $\mathbf{R}$ (or the smoothing operator $\mathbf{S}$) such that the variance of the MLMC estimator is minimized ?

- Testing different smoothing operators (2nd order Shapiro, 4th order Shapiro, iterative Shapiro, ...).
- Choosing the operators based on their order compared to the order of the models f_ℓ.
- Using estimators similar to the Multilevel Best Linear Unbiased Estimator (MBLUE).

Daniel Schaden and Elisabeth Ullmann, *On Multilevel Best Linear Unbiased Estimators*, SIAM/ASA Journal on Uncertainty Quantification **8** (2020), no. 2, 601–635

The WMLMC estimator is

$$\hat{\boldsymbol{\mu}}_L^{\mathsf{WMLMC}} = \beta_0 \hat{\boldsymbol{\mu}}_0^{(0)} + \sum_{\ell=1}^{L} \left(\beta_\ell \hat{\boldsymbol{\mu}}_\ell^{(\ell)} - \beta_{\ell-1} \hat{\boldsymbol{\mu}}_{\ell-1}^{(\ell)} \right)$$

where $\{\beta_\ell\}_{\ell=0}^{L}$ are scalar weights with $\beta_L = 1$ (for the unbiasedness constraint).

A formula to find the optimal weights $\{\beta_\ell\}_{\ell=0}^{L}$ that minimize the variance of the estimator is known.

Vincent Lemaire and Gilles Pagès, *Multilevel Richardson–Romberg extrapolation*, Bernoulli **23** (2017), no. 4A, 2643–2692

If we impose $\mathbf{P} = \alpha \mathbf{R}^{\mathrm{T}}$, by linearity, the F-MLMC estimator can be written

$$\hat{\boldsymbol{\mu}}_L^{\text{F-MLMC}} = \alpha^L \hat{\boldsymbol{\mu}}_0^{(0)} + \sum_{\ell=1}^{L} \left(\alpha^{L-\ell} \hat{\boldsymbol{\mu}}_\ell^{(\ell)} - \alpha^{L-\ell+1} \hat{\boldsymbol{\mu}}_{\ell-1}^{(\ell)} \right).$$

$\Rightarrow$ It is a WMLMC estimator with weights $\{\alpha^{L-\ell}\}_{\ell=0}^{L}$.

If we impose $\mathbf{P} = \alpha \mathbf{R}^{\mathrm{T}}$, by linearity, the F-MLMC estimator can be written

$$\hat{\boldsymbol{\mu}}_L^{\text{F-MLMC}} = \alpha^L \hat{\boldsymbol{\mu}}_0^{(0)} + \sum_{\ell=1}^{L} \left(\alpha^{L-\ell} \hat{\boldsymbol{\mu}}_\ell^{(\ell)} - \alpha^{L-\ell+1} \hat{\boldsymbol{\mu}}_{\ell-1}^{(\ell)} \right).$$

$\Rightarrow$ It is a WMLMC estimator with weights $\{\alpha^{L-\ell}\}_{\ell=0}^{L}$.

Using the formulas to find the optimal weights will give us the optimal α used to define $\mathbf{P}$. Previously, we used $\alpha = 1/\sqrt{2}$.

Poids optimaux $\{\beta_\ell\}_{\ell=0}^{L}$ de l'estimateur WMLMC						
ℓ	$1/\sqrt{2}^{5-\ell}$	$L=1$	$L=2$	$L=3$	$L=4$	$L=5$
0	0.1768	/	/	/	/	0.1727
1	0.25	/	/	/	0.2497	0.2525
2	0.3536	/	/	0.3538	0.3558	0.3565
3	0.5	/	0.5000	0.5005	0.5013	0.5015
4	0.7071	0.7043	0.7060	0.7067	0.7072	0.7073
5	1	1	1	1	1	1

Table: Optimal weights $\{\beta_\ell\}_{\ell=0}^{L}$ obtained by the WMLMC estimator. The first column is the weights $\{\alpha^{L-\ell}\}_{\ell=0}^{L}$ used previously for the F-MLMC.

Table of Contents

- In many geoscience applications, we want to estimate the expectation of a random discretized fields and the different fidelity levels come from grids of different resolution;
- MLMC for random discretized fields estimation usually requires grid transfer operators;
- The small scales are not well-estimated and introduce errors all across the spectrum;
- **A smoothing step is essential to improve the accuracy of the estimation.**
- Some estimators may help in choosing the optimal operators (the WMLMC for example).

Thank you for your attention !

Contact: jeremy.briant@irit.fr

Thank you for your attention !

Contact: jeremy.briant@irit.fr

Preprint article : Jérémy Briant, Paul Mycek, Mayeul Destouches, Olivier Goux, Serge Gratton, Selime Gürol, Ehouarn Simon, and Anthony T. Weaver, *A filtered multilevel Monte Carlo method for estimating the expectation of discretized random fields*, November 2023