University of Stuttgart
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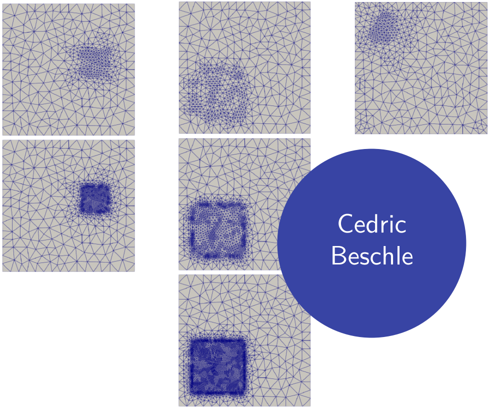

CLMC techniques for elliptic PDEs with random discontinuities

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Joint work with
Andrea Barth

30.06.23

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MCM 2023

Outline

$$u \xrightarrow{\text{adaptive FE}} u_\ell \xrightarrow{\text{q.o.i}} Q_\ell := \mathcal{Q}(u_\ell) \xrightarrow{\text{mean}} \mathbb{E}[Q_\ell] \xrightarrow{\text{(Q)CLMC}} \widehat{Q} \approx \mathbb{E}[\mathcal{Q}_\ell]$$

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Random PDE with discontinuous coefficient and its discretization

Continuous level Monte Carlo (CLMC)

Quasi continuous level Monte Carlo (QCLMC)

Numerical experiments

Random PDE with discontinuous coefficient

Flow through fractured porous media:

- PDE with discontinuous random coefficient
- spatial discontinuities accounting for fractures
- randomness accounting for uncertainties

Simplified model problem

Define

- complete probability space $(\Omega, \mathcal{A}, \mathbb{P})$
- bounded and connected Lipschitz domain $\mathcal{D} \subset \mathbb{R}^2$
- linear random elliptic PDE: Given a and f, let u be the solution to

$$\begin{aligned} -\nabla \cdot (a(\omega, x)\nabla u(\omega, x)) &= f(x) \qquad &\text{in } \Omega \times \mathcal{D}, \\ u(\omega, x) &= 0 \qquad &\text{on } \Omega \times \partial\mathcal{D}. \end{aligned}$$

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Coefficient $a : \Omega \times \mathcal{D} \to \mathbb{R}$:

- random
- discontinuous in space

$\Rightarrow$ interface problem cf. [Babuška, 1970, Teckentrup, Scheichl, Giles and Ullmann, 2013, Barth and Stein, 2018].

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$\Rightarrow$ interface problem cf. [Babuška, 1970, Teckentrup, Scheichl, Giles and Ullmann, 2013, Barth and Stein, 2018].

Remark: Weak solutions $u(\omega) \in H_0^1(\mathcal{D})$ for $\mathbb{P}$-almost all $\omega \in \Omega$ and

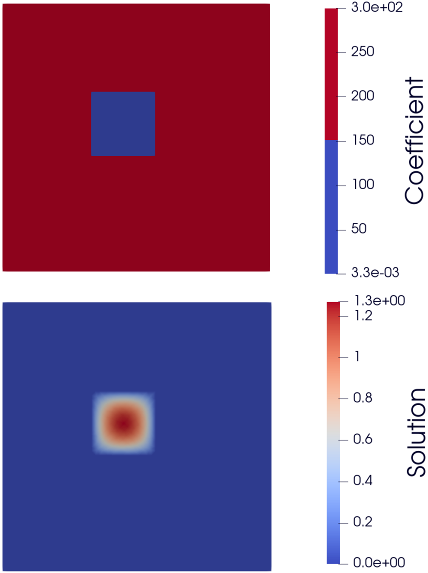
$$\|u\|_{L^p(\Omega; H_0^1)} \leq C(p, P, f, \mathcal{D}) \quad \text{for} \quad 1 \leq p \leq \infty.$$

Sample of Box PDE coefficient and solution

$\mathcal{D} := [0,1]^2$, for $\omega \in \Omega$, blue box:

- random center $\sim \mathcal{U}([0.4, 0.6]^2)$
- random edge length $\sim \mathcal{U}([0.2, 0.3])$
- outside $P \in \mathbb{R}_{>0}$ and inside P^{-1}

Approximation of $u(\omega)$ by $u_\ell(\omega)$ with linear finite elements on a mesh $\mathcal{K}_\ell$.



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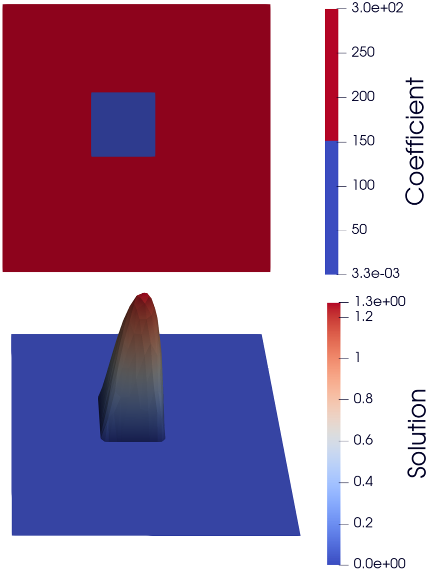
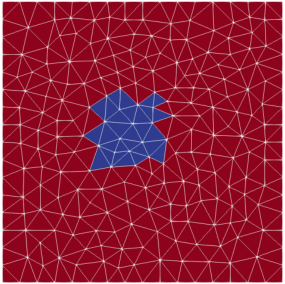
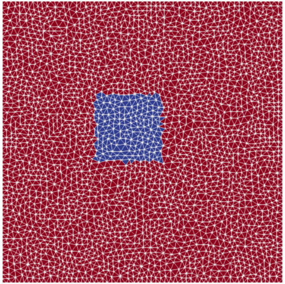
Important: Discontinuous coefficient with large jump:

- flat areas – no refinement
- steep areas – refinement!







Unstructured uniform meshes $\mathcal{K}$

$\downarrow$

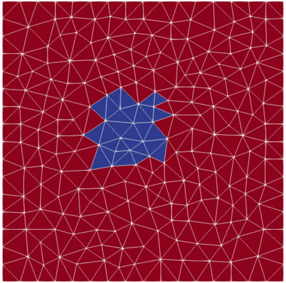
high resolution at the discontinuity

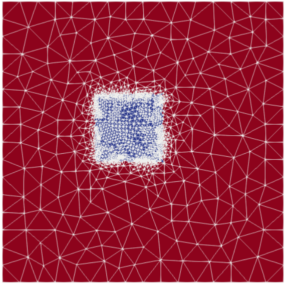
$\downarrow$

overall high resolution

$\downarrow$

high computational cost





Sample adaptive meshes $\mathcal{K}(\omega)$, for $\omega \in \Omega$

$\downarrow$

(goal-oriented) a-posteriori error estimation

$\downarrow$

adaptive refinement

$\downarrow$

high resolution only at the discontinuity

$\downarrow$

lower computational cost

Goal-oriented a-posteriori error estimator for
$\mathcal{Q}(u(\omega)) := \|u(\omega)\|_{H^1(\mathcal{D})}$,
[B. and Barth, '23 (1)].

Outline

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Continuous level Monte Carlo (CLMC)

Continuous level Monte Carlo (CLMC) [Detommaso, Dodwell and Scheichl, 2019]

- generalisation of MLMC
- continuous level of refinement $\ell \in \mathbb{R}_{\geq 0}$
- stochastic process of approximations $(Q(\ell))_{\ell \geq 0} := (\mathcal{Q}(u_\ell))_{\ell \geq 0}$
- random variable $L_r \sim \mathsf{Exp}(r)$ with $r \in \mathbb{R}_{>0}$
- sample-adaptive approximations

Continuous level Monte Carlo (CLMC)

Select

- maximal level $L_{max} \in \mathbb{R}_{>0}$
- sample number $M \in \mathbb{N}$
- $((Q^{(k)}(\ell)_{\ell\geq 0})_{k=1}^{M}$ i.i.d. copies of $Q(\ell)_{\ell\geq 0}$

CLMC estimator for the expectation $\mathbb{E}(\mathcal{Q} - Q_0)$:

$$\widehat{Q}_{L_{max}}^{\mathsf{CLMC}} := \frac{1}{M}\sum_{k=1}^{M}\int_0^{\min\{L_{max},L_r^{(k)}\}} \frac{1}{\mathbb{P}(L_r \geq \ell)}\left(\frac{\mathrm{d}Q}{\mathrm{d}\ell}\right)^{(k)}(\ell)\mathrm{d}\ell$$

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$$= \frac{1}{M} \sum_{k=1}^{M} \int_0^{L_{max}} e^{r\ell} \left(\frac{\mathrm{d}Q}{\mathrm{d}\ell} \right)^{(k)} (\ell) \mathbb{1}_{[0, L_r^{(k)}]}(\ell) \mathrm{d}\ell.$$

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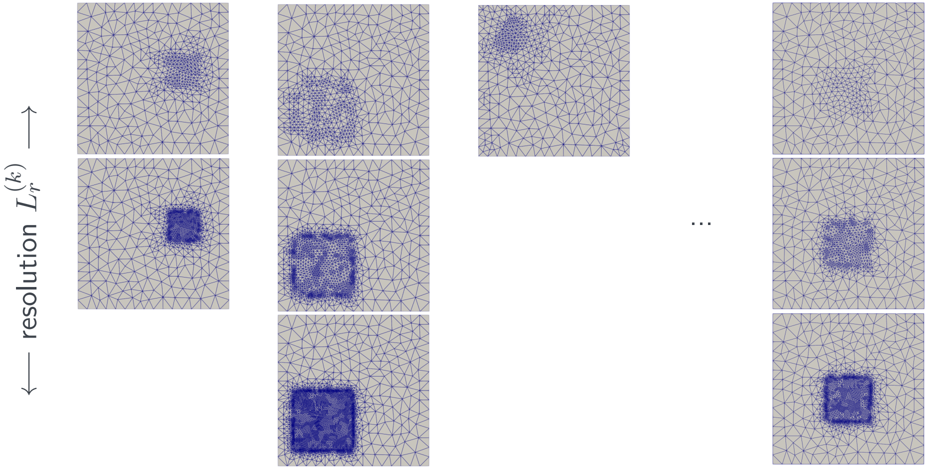
Denote by $(Q_j^{(k)})_{j \geq 1}$ a sequence of approximations at level $(\ell_j^{(k)})_{j \geq 1}$. Then define via linear interpolation

$$\left(\frac{\mathrm{d}Q}{\mathrm{d}\ell} \right)^{(k)} (\ell) := \frac{Q_j^{(k)} - Q_{j-1}^{(k)}}{\ell_j^{(k)} - \ell_{j-1}^{(k)}} \quad \text{for} \quad \ell \in (\ell_{j-1}^{(k)}, \ell_j^{(k)}).$$

$\longleftarrow$ M samples $\longrightarrow$



$L_r^{(1)} = 2$ $L_r^{(2)} = 3$ $L_r^{(3)} = 1$ $L_r^{(M)} = 3$

Outline

Random PDE with discontinuous coefficient and its discretization

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Numerical experiments

Motivation: Quasi continuous level Monte Carlo

$$\widehat{Q}^{\mathsf{CLMC}}_{L_{max}} := \frac{1}{M}\sum_{k=1}^{M}\int_0^{L_{max}} e^{r\ell}\left(\frac{\mathrm{d}Q}{\mathrm{d}\ell}\right)^{(k)}(\ell)\mathbb{1}_{[0,L_r^{(k)}]}(\ell)\mathrm{d}\ell.$$

Approximation of the tail distribution

$$e^{-r\ell} = \mathbb{P}(L \geq \ell) = \mathbb{E}(\mathbb{1}_{[0,L_r]}(\ell)) \approx \frac{1}{M}\sum_{k=1}^{M}\mathbb{1}_{[0,L_r^{(k)}]}(\ell) \quad \text{for all} \quad \ell \in [0,\infty).$$

$\Rightarrow$ Generate $(L_r^{(k)}; k = 1, \ldots, M)$ as a deterministic quasi random sequence.

F-discrepancy

Let $F : B \to \mathbb{R}$ be a CDF.
For a given point set $P := \{y_1, ..., y_M\}$ the F-discrepancy is defined as

$$D_{F,P} := \sup_{y \in B} \left| \frac{1}{M} \sum_{k=1}^{M} \mathbb{1}_{\{y_k \leq y\}} - F(y) \right|,$$

cf. [Fang, Wang and Bentler, 1994].

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cf. [Fang, Wang and Bentler, 1994].

If F is continuous with continuous inverse, then

$$D_{F,P} = D_M^*(P).$$

The same holds true for the TDF, since $T = 1 - F$.

Quasi random numbers and F-discrepancy

Lemma (*B. and Barth, '23 (2)*)

Let $L_r \sim$ Exp(r) for some $r > 0$ and

$$L_r^{(k)} = -\frac{\ln(1 - x^{(k)})}{r}$$

from a $[0, 1)$-uniform quasi random Sobol sequence, cf. [Sobol, 1967] and [Owen, 1998], $x^{(k)}$ for $k = 1, \ldots, M$ and $M \in \mathbb{N}$. Then,

$$\sup_{x \in [0,\infty)} \left| \frac{1}{M} \sum_{m=1}^{M} \mathbb{1}_{[0, L_r^{(k)}]}(x) - e^{-rx} \right| \leq C M^{-1},$$

for $C > 0$ independent of M,

Cf. [Dick and Pillichshammer, 2014] for the convergence rate.

F-discrepancy convergence, for $L_r = \mathbf{Exp}(1.3)$

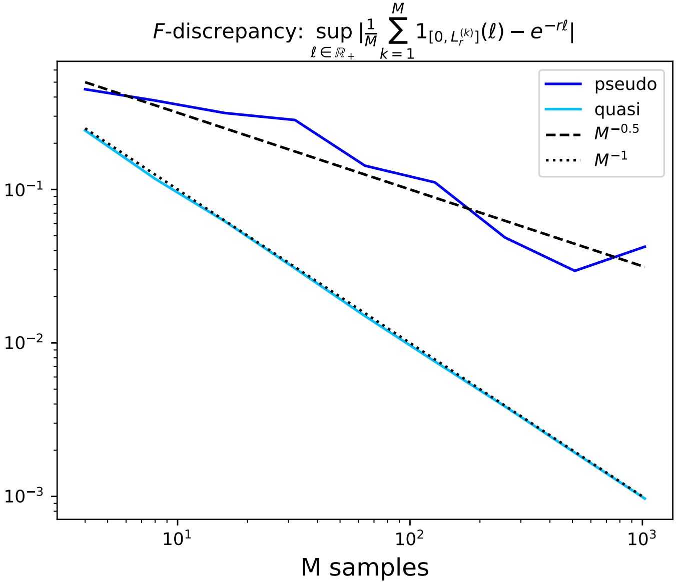
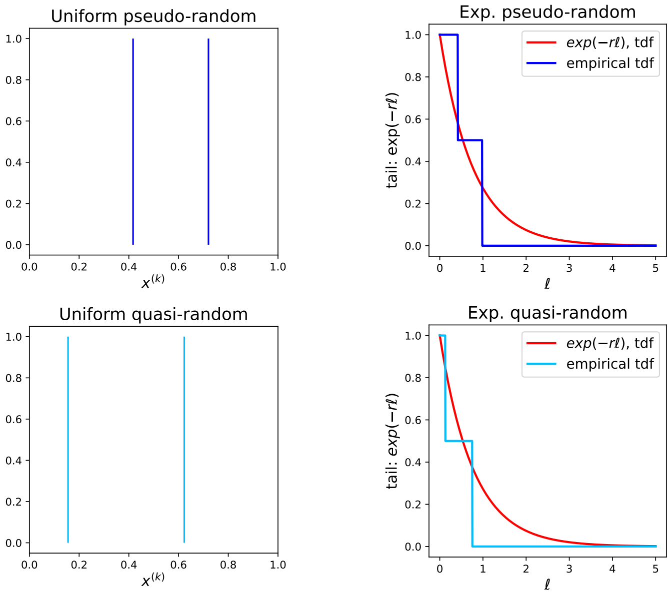


Illustration of tail approximation



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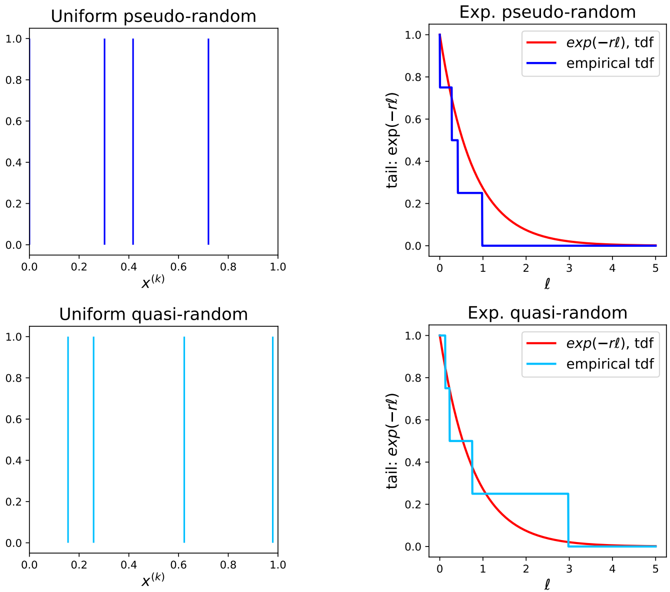

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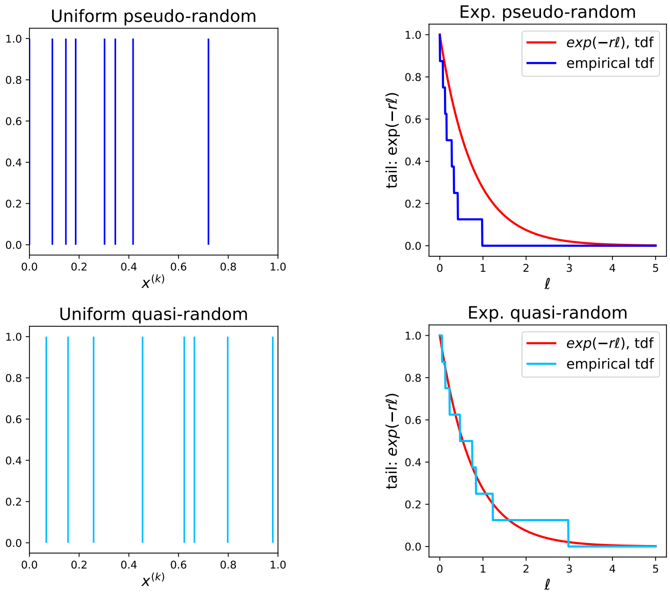

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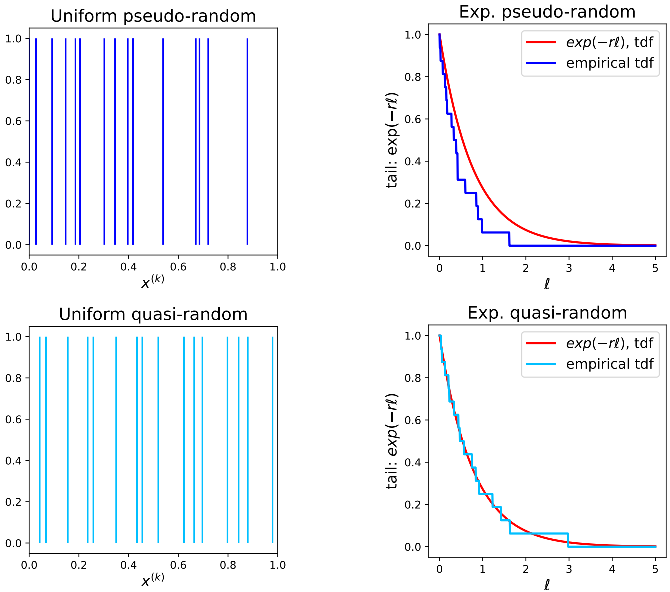

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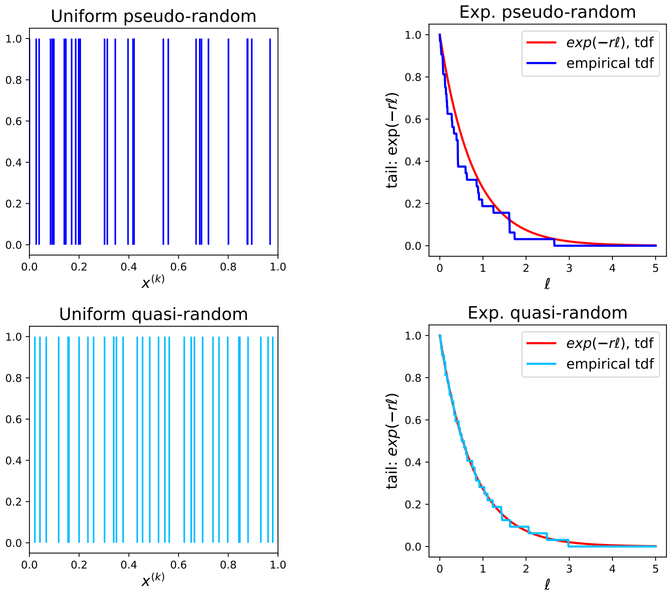

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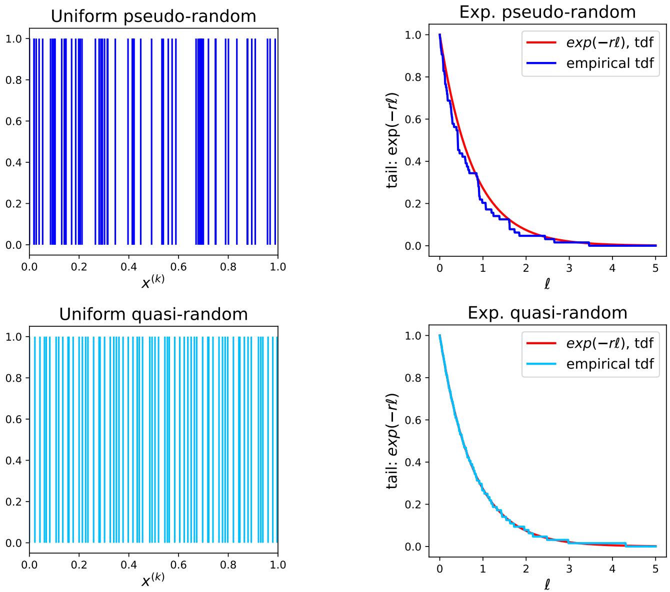

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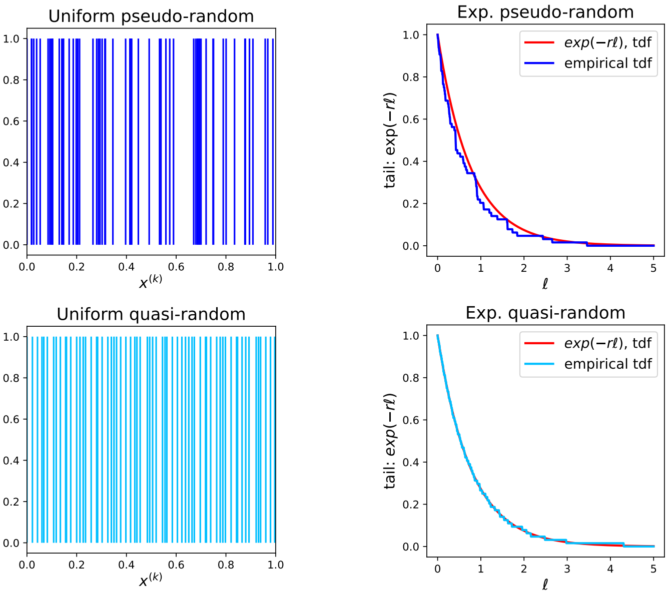

Remark:
$\mathrm{Exp}(r)$ in (Q)CLMC is always one-dimensional.
$\Downarrow$
No additional cost to generate the quasi random numbers.

Quasi continuous level Monte Carlo (QCLMC)

Recently developed in [B. and Barth, '23 (1)] and analysed in [B. and Barth, '23 (2)]. Select

- deterministic quasi random sequence $L_r^{(k)}$ mimicing an exponential distribution Exp(r), $r > 0$
- maximal level $L_{max} := \min\{\max_{k\in(1,\ldots,M)} L_r^{(k)}, L\}$, where $L \in \mathbb{R}_{>0}$

QCLMC estimator for the expectation $\mathbb{E}(\mathcal{Q} - Q_0)$:

$$\widehat{Q}^{\mathsf{QCLMC}}_{L_{max}} := \frac{1}{M}\sum_{k=1}^{M}\int_0^{L_{max}} e^{r\ell}\left(\frac{\mathrm{d}Q}{\mathrm{d}\ell}\right)^{(k)}(\ell)\mathbb{1}_{[0,L_r^{(k)}]}(\ell)\mathrm{d}\ell.$$

Complexity Theorem (QCLMC)

Theorem (*B. and Barth, '23 (2)*)

Suppose there exist positive constants α, β, γ, c_1, c_2, c_3, with $\beta < 4\alpha$, such that for any $\ell > 0$:

$$\mathbb{E}\left[\frac{dQ}{d\ell}\right] \leq c_1 e^{-\alpha\ell} \quad \text{and} \quad \mathbb{V}\left[\frac{dQ}{d\ell}\right] \leq c_2 e^{-\beta\ell} \quad \text{and} \quad \mathcal{C}(\ell) \leq c_3 e^{\gamma\ell}.$$

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Further, let $(L_r^{(k)}; k = 1, \ldots, M)$ be a deterministic quasi random sequence obtained by inverse transformation, and let $r \in [\min\{\beta, 2\alpha, \gamma\}, \max\{\min\{\beta, 2\alpha\}, \gamma\}]$.

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Further, let $(L_r^{(k)}; k = 1, \dots, M)$ *be a deterministic quasi random sequence obtained by inverse transformation, and let* $r \in [\min\{\beta, 2\alpha, \gamma\}, \max\{\min\{\beta, 2\alpha\}, \gamma\}]$. *Then, there exist* $L \in \mathbb{R}_{>0}$ *and* $M \in \mathbb{N}$, *such that for any* $\varepsilon \in (0, \frac{1}{e})$ *and* $\bar{C} > 0$ *independent of* M *and* ε

$$MSE^{QCLMC} \leq \varepsilon^2 \quad \text{and} \quad \mathcal{C}[\widehat{Q}^{QCLMC}_{L_{max}}] \leq \bar{C}\varepsilon^{-2-\max\{0, \frac{\gamma - \min\{\beta, 2\alpha\}}{\alpha}\}} |\ln(\varepsilon)|^{\delta_{r,\min\{\beta,2\alpha\}} + \delta_{r,\gamma}},$$

where $L_{max} = \min\{L, \max_{k \in (1,\dots,M)} L_r^{(k)}\}$ *and* δ *is the Dirac function.*

Outline

Convergence experiments

We choose

$$\mathcal{Q}(u(\omega)) := \|u(\omega)\|_{H^1(\mathcal{D})}.$$

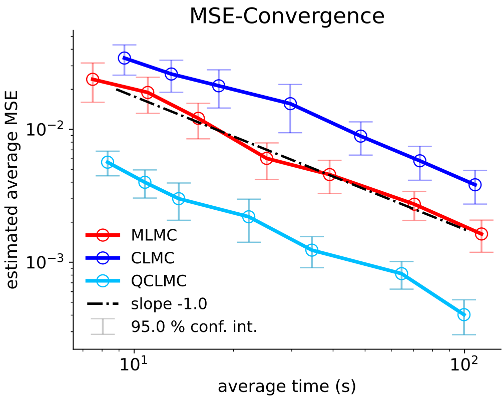
Comparison - time to MSE performance:

- CLMC on sample adaptive meshes, $\alpha \approx 1$, $\beta \approx 2.3$, $\gamma \approx 1$
- QCLMC on sample adaptive meshes
- MLMC on unstructured uniform meshes, $\alpha \approx 0.5$, $\beta \approx 1.4$, $\gamma \approx 1$

  [Barth, Schwab and Zollinger, 2011]
  [Cliffe, Giles, Scheichl and Teckentrup, 2011]
  [Teckentrup, Scheichl, Giles and Ullmann, 2013]
  [Haji-Ali, Nobile, von Schwerin and Tempone, 2016]

Time to MSE performance - box coefficient

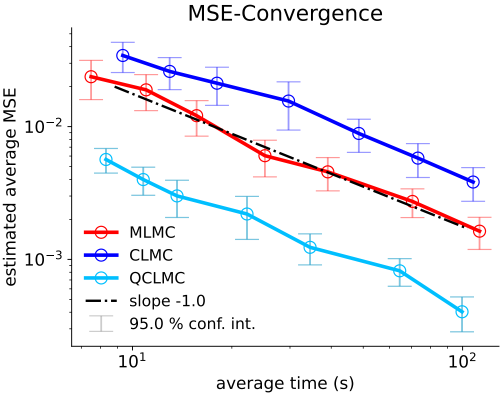
$P = 300$



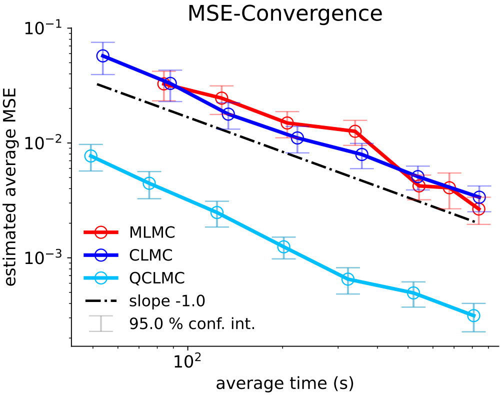
MSE: $\varepsilon^2 \in \{0.04,\ 0.025,\ 0.016,\ 0.01,\ 0.007,\ 0.004,\ 0.003\}$, [B. and Barth, '23 (1)].

Time to MSE performance - box coefficient

$P = 300$



$P = 1000$



MSE: $\varepsilon^2 \in \{0.04, 0.025, 0.016, 0.01, 0.007, 0.004, 0.003\}$, [B. and Barth, '23 (1)].

Summary and conclusion

Random discontinuous coefficient in PDE: negative effect on

- regularity of pathwise weak solution
- pathwise convergence rate on standard meshes (MLMC)

$\Rightarrow$ better use adaptive meshes (CLMC)

New QCLMC estimator

- much better tail estimate for $L_r \sim \text{Exp}(r)$
- variance reduction

Summary and conclusion

Numerical experiments:

- CLMC should outperform MLMC as solution samples have distinct areas with high error contributions
- pseudo random numbers for sampling $L_r \sim \text{Exp}(r)$ renders it worse than MLMC

$\Rightarrow$ QCLMC outperforms both methods

Outlook:

- apply QCLMC to random Burgers equation (discontinuous solutions)
- develop improved automatic stopping criterion for QCLMC

Preprints of submitted work

(1) C. A. Beschle, A. Barth: Quasi Continuous Level Monte Carlo for Random Elliptic PDEs, in MCQMC 2022 Proc., submitted 2023, `https://doi.org/10.48550/arXiv.2303.08694`.

(2) C. A. Beschle, A. Barth: Quasi Continuous Level Monte Carlo, in ESAIM M2AN - Special issue - To commemorate Assyr Abdulle, submitted 2023, `https://doi.org/10.48550/arXiv.2305.15949`.

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