# A multilevel stochastic gradient algorithm for PDE-constrained optimal control problems under uncertainty

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**Joint work with**: M. Martin (Criteo, Grenoble), S. Krumscheid (RWTH Aachen), P. Tsilifis (EPFL)

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# Outline

1. Problem setting – quadratic optimal control problem
2. Discretization by finite elements + Monte Carlo
3. Deterministic (CG) iterative solvers versus Stochastic Gradient
4. Multilevel stochastic gradient algorithms
5. Conclusions

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- Forward problem

$$\begin{cases} -\mathrm{div}(a(x,\omega)\nabla y(x,\omega)) = g(x) + u(x), & \text{for a.e. } x \in D,\ \omega \in \Omega \\ y(x,\omega) = 0, & \text{for a.e. } x \in \partial D,\ \omega \in \Omega \end{cases} \qquad (*)$$

with $a(\cdot,\omega)$ a random field s.t. $0 < a_{min} \le a(x,\omega) \le a_{max}$, $\forall (x,\omega) \in D \times \Omega$.

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## Optimal control problem

$$\min_{\substack{u \in L^2(D) \\ y \in L^2_{\mathcal{P}}(\Omega; H_0^1(D))}} \tilde{J}(u,y) := \frac{1}{2}\mathbb{E}_\omega[\|y(\cdot,\omega) - y_{target}\|^2] + \frac{\beta}{2}\|u\|^2, \qquad \text{subject to } (*)$$

# Reduced functional

- (Stochastic) Affine solution operator: $y_\omega : L^2(D) \to H_0^1(D)$

$$\forall \omega \in \Omega \quad u \mapsto y_\omega(u), \quad \text{solution of } \begin{cases} -\text{div}(a(\cdot,\omega)\nabla y_\omega(u)) = g + u, & \text{in } D \\ y_\omega(u) = 0, & \text{on } \partial D. \end{cases}$$

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- Reduced functional: $\min_{u \in L^2(D)} J(u)$

$$J(u) = \mathbb{E}_\omega[f(u,\omega)], \qquad f(u,\omega) = \frac{1}{2}\|y_\omega(u) - y_{target}\|^2 + \frac{\beta}{2}\|u\|^2$$

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- Adjoint based gradient computation:

$$\nabla_u f(u,\omega) = \beta u + p_\omega(u), \qquad \nabla_u J(u) = \beta u + \mathbb{E}_\omega[p_\omega(u)]$$

where $p_\omega(u)$ solves the adjoint problem $\forall \omega \in \Omega$

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- Lipschitz and strong convexity properties of $\nabla_u f$: $\forall u_1, u_1 \in L^2(D)$, $\omega \in \Omega$

$$\|\nabla_u f(u_1,\omega) - \nabla_u f(u_2,\omega)\| \le L\|u_1 - u_2\|, \qquad L = \beta + \frac{C_P^4}{a_{min}^2}$$

$$\langle \nabla_u f(u_1,\omega) - \nabla_u f(u_2,\omega), u_1 - u_2\rangle_{L^2(D)} \ge \frac{\ell}{2}\|u_1 - u_2\|^2, \quad \ell = 2\beta$$

# Outline

# Finite dimensional approximation

- Finite Element approximation of the PDE: $\forall u \in L^2(D)$, $\omega \in \Omega$

$$u \mapsto y_\omega^h(u) \quad \text{solves} \quad \int_D a(\cdot,\omega)\nabla y_\omega^h(u)\cdot\nabla v_h = \int_D (g+u)v_h, \quad \forall v_h \in Y_h^r$$

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- Monte Carlo approximation of expectation: $\omega_i \overset{\text{iid}}{\sim} \mathcal{P},\ i = 1,\dots N$

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- Discrete optimal control problem:

$$\min_{u\in L^2(D)} J^{h,N}(u) := \frac{1}{N}\sum_{i=1}^N f^h(u,\omega_i) = \frac{1}{N}\sum_{i=1}^N \left[\frac{1}{2}\|y_{\omega_i}^h(u) - y_{target}\|^2 + \frac{\beta}{2}\|u\|^2\right]$$

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Remark: The unique minimizer $u_\star^{h,N} \in Y_h^r$

# Optimality conditions

primal pbs: $\int_D a(\cdot,\omega_i)\nabla y^h_{\omega_i}\cdot\nabla v_h = \int_D (g+u^{h,N})v_h, \quad \forall v_h\in Y^r_h,\ i=1,\dots,N,$

adjoint pbs: $\int_D a(\cdot,\omega_i)\nabla v_h\cdot\nabla p^h_{\omega_i} = \int_D (y^h_{\omega_i}-y_{tar})v_h, \quad \forall v_h\in Y^r_h,\ i=1,\dots,N,$

sensitivity: $\int_D (\beta u^{h,N}+\frac{1}{N}\sum_{i=1}^{N} p^h_{\omega_i})v_h = 0 \quad \forall v_h\in Y^r_h.$

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## Algebraic system

$$\left[\begin{array}{ccc|ccc|c} A_1 & & & & & & -M \\ & \ddots & & & & & \vdots \\ & & A_N & & & & -M \\ \hline -M & & & A_1^T & & & \\ & \ddots & & & \ddots & & \\ & & -M & & & A_N^T & \\ \hline & & & M & \cdots & M & \beta NM \end{array}\right] \left[\begin{array}{c} \mathbf{y}_1 \\ \vdots \\ \mathbf{y}_N \\ \hline \mathbf{p}_1 \\ \vdots \\ \mathbf{p}_N \\ \hline \mathbf{u} \end{array}\right] = \left[\begin{array}{c} \mathbf{g} \\ \vdots \\ \mathbf{g} \\ \hline -\mathbf{y}_{tar} \\ \vdots \\ -\mathbf{y}_{tar} \\ \hline \mathbf{0} \end{array}\right]$$

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- Several appraoches can be used to solve this coupled system
  [Kouri-Heinkenschloss-eal 2013], [VanBarel-Vandewalle 2018], [Borzì-vonWinckel 2011]

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- Eliminating $(\mathbf{y}_1, \ldots, \mathbf{y}_N)$ and $(\mathbf{p}_1, \ldots, \mathbf{p}_N)$ and introducing the block matrices

$$\mathcal{A} = \begin{bmatrix} A_1 & & \\ & \ddots & \\ & & A_N \end{bmatrix}, \quad \mathcal{M} = \begin{bmatrix} M & & \\ & \ddots & \\ & & M \end{bmatrix}, \quad \mathbb{1} = \begin{bmatrix} Id \\ \vdots \\ Id \end{bmatrix}$$

leads to a reduced system $\mathcal{G}\mathbf{u} = \boldsymbol{\xi}$ with matrix

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EPFL

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- The matrix $\mathcal{G}$ is spd and $Cond(\mathcal{G}) = O(\beta^{-1})$ indep. of $h$ and $N$.
- Reduced system can be solved efficiently by e.g. conjugate gradient. Denoting $u_j^{h,N}$ the $j$-th iterate

$$\|u_\star^{h,N} - u_j^{h,N}\| \leq C\rho^j, \qquad \rho = \frac{\sqrt{Cond(\mathcal{G})} - 1}{\sqrt{Cond(\mathcal{G})} + 1}$$

# Deterministic approach

Use standard (deterministic) iterative method (e.g. CG) to solve the fully discrete system

- Error splitting assuming smooth solutions $y_\omega(u_\star), p_\omega(u_\star) \in H^{r+1}(D)$

$$\mathbb{E}[\|u_\star - u_j^{h,N}\|^2] \leq \underbrace{C_1 \rho^{2j}}_{\text{CG error}} + \underbrace{\frac{C_2}{N}}_{\text{MC error}} + \underbrace{C_3 h^{2r+2}}_{\text{FE error}}$$

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- Complexity analysis. Balancing errors contributions: $\rho^j \sim N^{-\frac{1}{2}} \sim h^{r+1} \sim tol$

$$Work(tol) \lesssim \underbrace{tol^{-2}}_{\text{MC}} \underbrace{tol^{-\frac{\gamma d}{r+1}}}_{\text{FE}} \underbrace{\log tol^{-1}}_{\text{solver}}$$

# Stochastic gradient (Robbins-Monro)

Instead of introducing upfront the Monte Carlo approximation and then solve the discrete problem by a deterministic iterative solver, we could apply a stochastic gradient method to the continuous problem (non-discrete in probability)

$$\begin{aligned} u_{j+1}^h &= u_j^h - \tau_j \nabla_u f^h(u_j^h, \omega_j) \\ &= (1 - \tau_j \beta) u_j^h - \tau_j p_{\omega_j}^h(u_j^u) \end{aligned} \qquad \omega_j \overset{\text{iid}}{\sim} \mathcal{P}$$

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**Proposition** [Martin-Nobile-Krumscheid 2018]

Assuming $y_\omega(u_\star), p_\omega(u_\star) \in H^{r+1}(D)$, for any $\alpha \in \mathbb{R}_+$ and $\tau_0 > \frac{1}{2\beta}$ there exist $D_1, D_2 > 0$ independent of $j$ and $h$ s.t.

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Complexity: $Work(tol) \lesssim tol^{-2} tol^{-\frac{\gamma d}{r+1}}$ (no log terms !)

# Numerical results

**Optimal control problem**:

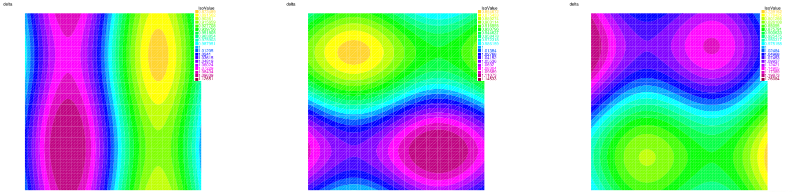
$$\min_{u \in L^2(D)} \frac{1}{2} \mathbb{E}_\omega \left[ \| y_\omega(u) - y_{target} \|^2 \right] + \frac{\beta}{2} \| u \|^2$$

$$\text{subject to} \quad \begin{cases} -\text{div}(a(\cdot,\omega) \nabla y_\omega(u)) = g + u & \text{in } D \\ y_\omega(u) = 0 & \text{on } \partial D \end{cases}$$

**Problem parameters**

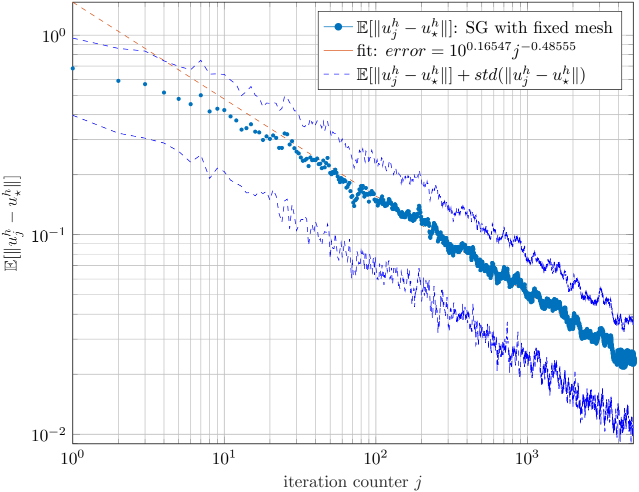
$$D = (0,1)^2, \quad g = 1, \quad y_{target}(x_1, x_2) = \sin(\pi x) \sin(\pi y), \quad \beta = 10^{-4}$$

$$a(x_1, x_2, \boldsymbol{\xi}) = 1 + \exp\{\theta(\xi_1 \cos(1.1\pi x_1) + \xi_2 \cos(1.2\pi x_1) + \xi_3 \sin(1.3\pi x_2) + \xi_4 \sin(1.4\pi x_2))\}$$



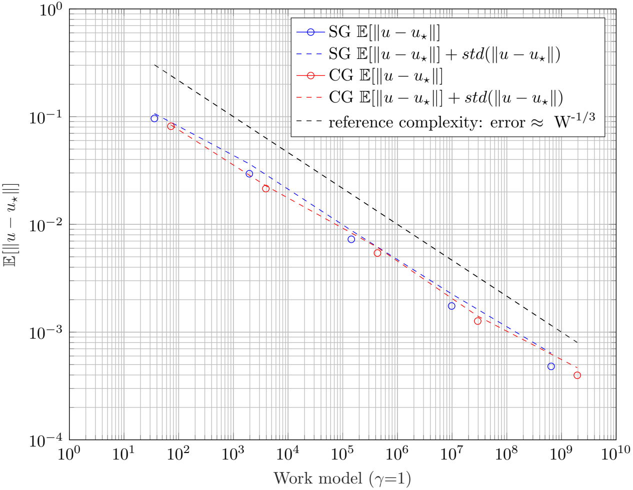

*three realization of the random coefficient*

# Numerical results – SG convergence




*Mean $L^2$ error as a function of iteration counter, estimated by sample average over 100 independent realizations. Fixed mesh size $h = 2^{-4}$ – $\mathbb{P}_1$ finite elements.*

# Numerical results – complexity of CG versus SG




*Complexity plot for CG and SG (average over 20 repetitions)*

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**Idea**: In the Stochastic Gradient algorithm, replace the single evaluation $\nabla_u f^h(u_j, \omega_j)$ by a multilevel approx. of the expectation [Heinrich 1998], [Giles 2008]

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- $\vec{N} = (N_0, \ldots, N_L)$ controls the variance of the estimator (MC error)

$$\mathbb{V}ar\left[\mathbb{E}^{MLMC}_{L,\vec{N}}[\nabla_u f(u_j, \cdot)]\right] = \sum_{\ell=0}^{L} \frac{\mathbb{V}ar\left[\nabla_u f^{h_\ell}(u_j, \cdot) - \nabla_u f^{h_{\ell-1}}(u_j, \cdot)\right]}{N_\ell}$$

# Multilevel stochastic gradient algorithm – first version

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\begin{aligned}
u_{j+1} &= u_j - \tau_j \mathbb{E}^{MLMC}_{L_j,\vec{N}_j}[\nabla_u f(u_j,\cdot)] \\
&= (1-\tau_j\beta)u_j - \tau_j \sum_{\ell=0}^{L_j} \frac{1}{N_{\ell,j}} \sum_{i=1}^{N_{\ell,j}} \left[ p^{h_\ell}(u_j,\omega_j^{(i,\ell)}) - p^{h_{\ell-1}}(u_j,\omega_j^{(i,\ell)}) \right]
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Learning rate $\tau_j = \frac{\tau_0}{j+\alpha}$. Notice that $\forall j, \;\; u_{j+1} \in Y^r_{h_{L_j}}$

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Similar approach proposed in [Dereich-MuellerGronbach 2015] for abstract optimization problem. Different working assumptions but similar results.

# Convergence analysis

- Bias term $\varepsilon_j = \left\| \mathbb{E}[\nabla_u f^{h_{L_j}}(u_\star, \cdot) - \nabla_u f(u_\star, \cdot)] \right\|$
- Variance term $\sigma_j^2 = \mathbb{E}\left[ \left\| \mathbb{E}^{MLMC}_{L_j, \vec{N}_j}[\nabla_u f(u_\star, \cdot)] - \mathbb{E}[\nabla_u f^{h_{L_j}}(u_\star, \cdot)] \right\|^2 \right]$

**Proposition** [Martin-Nobile-Tsilifis 2019]

There exist $\lambda, \mu > 0$ independent of $h$ and $j$ such that

$$\mathbb{E}[\|u_{j+1} - u_\star\|^2] \leq c_j \mathbb{E}[\|u_j - u_\star\|^2] + \lambda \tau_j^2 \sigma_j^2 + \mu \tau_j \varepsilon_j^2$$

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Square bias should decrease faster than variance !

# Compexity analysis: optimal bias/variance decrease

Take $\tau_0 > \frac{1}{\beta}$ and $\eta > 2$

$$\varepsilon_j^2 \sim (j+\alpha)^{1-\eta} \qquad \Longrightarrow \qquad L_j \sim \frac{\eta-1}{2r+2}\log(j+\alpha)$$

$$\sigma_j^2 \sim (j+\alpha)^{2-\eta} \qquad \Longrightarrow \qquad N_{\ell,j} \sim 2^{-\ell\frac{2r+2+\gamma d}{2}}(j+\alpha)^{\eta-2}$$

**Proposition** [Martin-Nobile-Tsilifis 2019]

The work to achieve a mean squared error $\mathbb{E}[\|u_j - u_\star\|^2] = O(tol^2)$ is bounded by

$$Work(tol) \lesssim \begin{cases} tol^{-2}, & 2r+2 > \gamma d, \quad \eta \geq 2 + \frac{\gamma d}{2r+2-\gamma d}, \quad \tau_0 > \frac{\eta-1}{\beta} \\ tol^{-2(1+\frac{1}{\tau_0\beta})}|\log tol|^{3+\frac{1}{\tau_0\beta}}, & 2r+2 = \gamma d, \quad \eta = \tau_0\beta + 1 \\ tol^{-2(\frac{\gamma d}{2r+2}+\frac{1}{\tau_0\beta})}|\log tol|^{\frac{\gamma d}{2r+2}+\frac{1}{\tau_0\beta}}, & 2r+2 < \gamma d, \quad \eta = \tau_0\beta + 1 \end{cases}$$

# Multilevel stochastic gradient algorithm – second version

The multilevel Stochastic Gradient algorithm (MLSG) is in between a Stochastic Gradient and a Full gradient: at each iteration, we compute an approximation $\mathbb{E}^{MLMC}_{L,\vec{N}}[\nabla_u f(u_j,\cdot)]$ of increasing accuracy ($\varepsilon_j, \sigma_j \to 0$ as $j \to \infty$).

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- If one takes $L_j = \infty$, $\forall j$, then the estimator is unbiadsed. Unfortunately, we were not able to prove convergence with this setting.
- Alternatively, decrease the bias as $\varepsilon_j^2 \sim (j+\alpha)^{1-\eta}$

# Compexity analysis of RMLSG: optimal bias decrease

**Proposition** [Martin-Nobile-Tsilifis 2019]

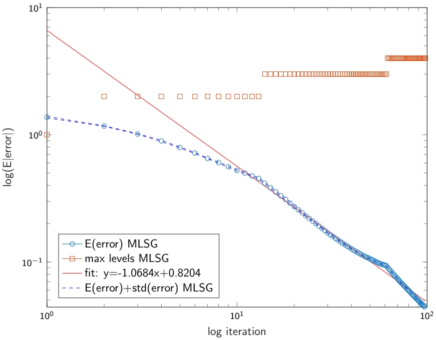
Assume $2r + 2 > \gamma d$ and take $\eta = 2$, $\tau_0 > \frac{1}{\beta}$. Then, the expected work to achieve a mean squared error $\mathbb{E}[\|u_j - u_\star\|^2] = O(tol^2)$ is

$$\mathbb{E}[Work(tol)] \lesssim tol^{-2}$$

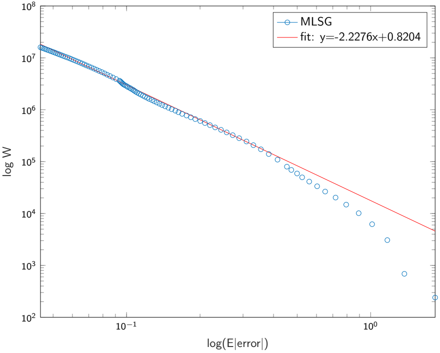
and

$$\frac{\sqrt{\mathbb{V}ar\left[Work(tol)\right]}}{\mathbb{E}\left[Work(tol)\right]} \lesssim tol^{\frac{3(2r+2)-\gamma d}{2(2r+2)}} \xrightarrow{tol \to 0} 0$$

# Numerical results – MLSG complexity



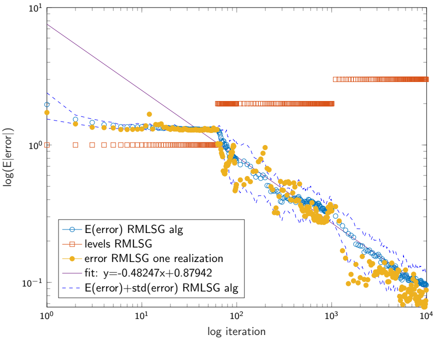

*Mean error vs iteration counter*




*Cost W versus mean error*

(average over 10 repetitions)

# Numerical results – RMLSG complexity

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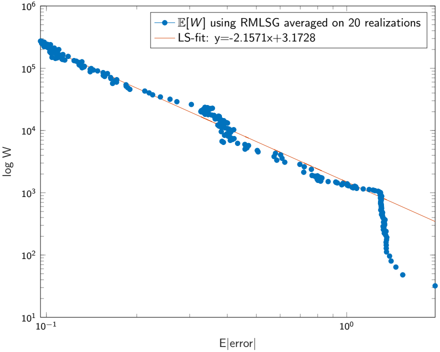


*Cost W versus mean error*

(average over 20 repetitions)

# Outline

1. Problem setting – quadratic optimal control problem
2. Discretization by finite elements + Monte Carlo
3. Deterministic (CG) iterative solvers versus Stochastic Gradient
4. Multilevel stochastic gradient algorithms
5. Conclusions

# Conclusions and future work

- We have analyzed and compared several algorithms to solve a PDE constrained quadratic optimal control problem. Our outcome is that, in the context of a Monte Carlo approximation, the Stochastic gradient algorithm has a slighly better complexity than a deterministic solver such as CG. The multilevel versions, on the other hand, has a substantially better complexity.

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- Extension of the results to more involved risk measures (other than expectation) is in progress.
- In the case on only few random variables, a deterministic quadrature (e.g. full tensor or sparse quadrature) may be more accurate than Monte Carlo. In this case, Stochastic Gradient algorithms can still be effective if properly modified (see SAG / SAGA versions).
  Analysis available in [Martin-Nobile 2018].

# Thank you for your attention!

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in preparation

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