

# Recycling Krylov subspace strategies to solve stochastic elliptic equations

Presented by

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# Elliptic equations with random coefficients

- Let  $a(x, \theta)$  be a random coefficient field on a domain  $\Omega$ , and consider the equation

$$\begin{aligned}\nabla \cdot (a(x, \theta) \nabla u(x, \theta)) &= -f(x), \quad x \in \Omega, \quad \theta \in \Theta \\ \mathcal{B}(x, u) &= 0 \quad , \quad x \in \partial\Omega\end{aligned}$$

with deterministic forcing and boundary conditions.

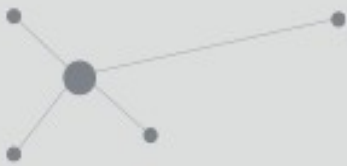
- Moments and other quantities of interest about the solution  $u(x, \theta)$  can be estimated from a sample of random solutions  $\{u^{(s)}(x, \theta)\}_{s=1}^{n_s}$ .

For example, the Monte Carlo (MC) estimator of  $\mathbb{E}[u(x)]$  is given by

$$\bar{u}_{n_s}(x, \theta) := \sum_{s=1}^{n_s} u^{(s)}(x, \theta) / n_s$$

with a sampling error depending on  $n_s$ .

- Reducing the error of an estimator generally requires drawing realizations of a **very large sample of solutions**.



# Sequences of linear systems

- Let's consider a 1D domain. The results presented here are for stationary lognormal coefficient fields  $a(x, \theta)$  such that

$$\log a(x, \theta) \sim G(x, \theta)$$

where  $G$  has 0-mean and a square-exponential covariance

$$\mathbb{E}[G(x)G(x')] = \sigma^2 \exp(-(x - x')^2/2L)$$

with variance  $\sigma^2$  and correlation length  $L$ .

- An estimator of interest is evaluated upon drawing realizations of  $\{a^{(s)}(x)\}_{s=1}^{n_s}$  and solving for  $\{u^{(s)}(x)\}_{s=1}^{n_s}$  such that

$$\partial_x(a(x, \theta)\partial_x u(x, \theta)) = -1, \quad x \in (0, 1)$$

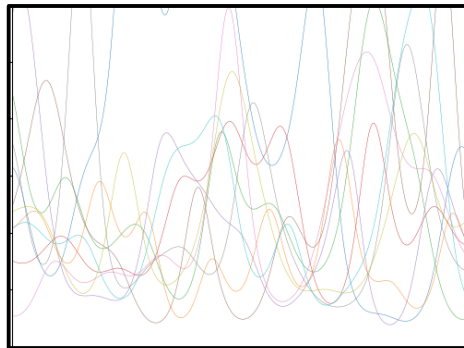
as we let  $u^{(s)}(0) = 0$  and  $\partial_x u^{(s)}(1) = 0$ .

- After discretization into finite elements, a system of the form  $A^{(s)}x^{(s)} = b$  is obtained for each  $a^{(s)}(x)$ , so that the evaluation of the estimator requires to solve a **long sequence of  $n_s$  linear systems**.

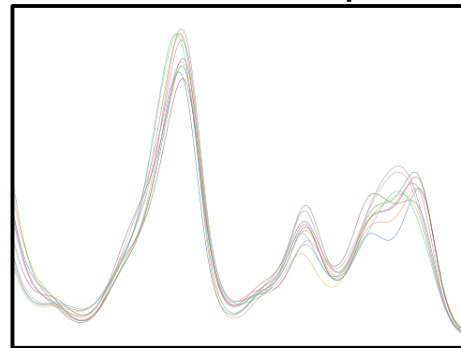
- Questions we want to answer:

- Can we accelerate the iterative resolution of a current system  $A^{(s)}x^{(s)} = b$  by recycling information from the resolution of subsequent systems  $A^{(t < s)}x^{(t < s)} = b$ ?
- If so, does the sampling strategy of the random coefficient field matter?

$\{a^{(s)}(x)\}_{s=1}^{n_s}$  are i.i.d.



$\{a^{(s)}(x)\}_{s=1}^{n_s}$  contains correlated subsequences



VS

- Could we do so efficiently for large problems? Can we speed-up this resolution even when efficient preconditioners are already used?

# Deflation of linear systems with SPD matrices

- Consider the projector  $H = I_n - W(W^T A W)^{-1} W^T A$  with  $W \in \mathbb{R}^{n \times k}$  made of  $k \ll n$  linearly independent vectors.
- A sequence  $\{x_i\}_{i=0}^j$  of approximations of  $x^* := A^{-1}b$  is obtained by

$\hat{\mu}^*$  is the direct solution of the *reduced system*

$$W^T A W \hat{\mu}^* = W^T b$$

$$x_i := \underbrace{W \hat{\mu}^*}_{\mathcal{R}(W)} + \underbrace{H x'_i}_{\mathcal{R}(A W)^\perp}$$

$x'_i$  is an iterative solution of the *deflated system*

$$H^T A x' = H^T b$$

computed by CG( $H^T A, x'_0$ )

- Error bounded by :

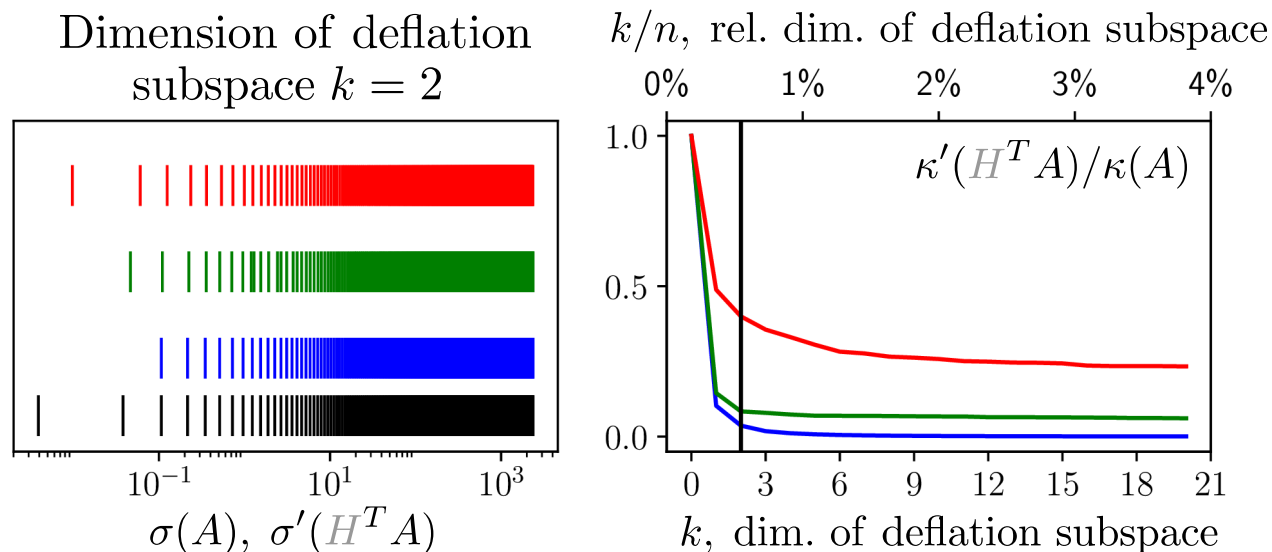
$$\|x^* - x_i\|_A \leq 2\|x^* - x_0\|_A \left( \frac{\sqrt{\kappa'(H^T A)} - 1}{\sqrt{\kappa'(H^T A)} + 1} \right)^i$$

- The lower the conditioning number of the deflated system, the smaller the bound on  $\|x^* - x_i\|_A$ . Ideally, we would pick  $W$  to minimize  $\kappa'(H^T A)$ .

# What part of the spectrum should we deflate?

- A common and efficient way to deflate is to let the columns of  $W$  be eigenvectors of  $A$ .
- Let  $U^{(k)} \in \mathbb{R}^{n \times k}$  contain the  $k$  least dominant eigenvectors of  $A$ . Then,

$$\textcolor{blue}{W} = U^{(k)} \quad \textcolor{green}{W} = U^{(k)} + \delta \textcolor{green}{W} \quad \textcolor{red}{W} = U^{(k)} + \delta \textcolor{red}{W} \quad \|\delta \textcolor{green}{W}\|_2 < \|\delta \textcolor{red}{W}\|_2$$

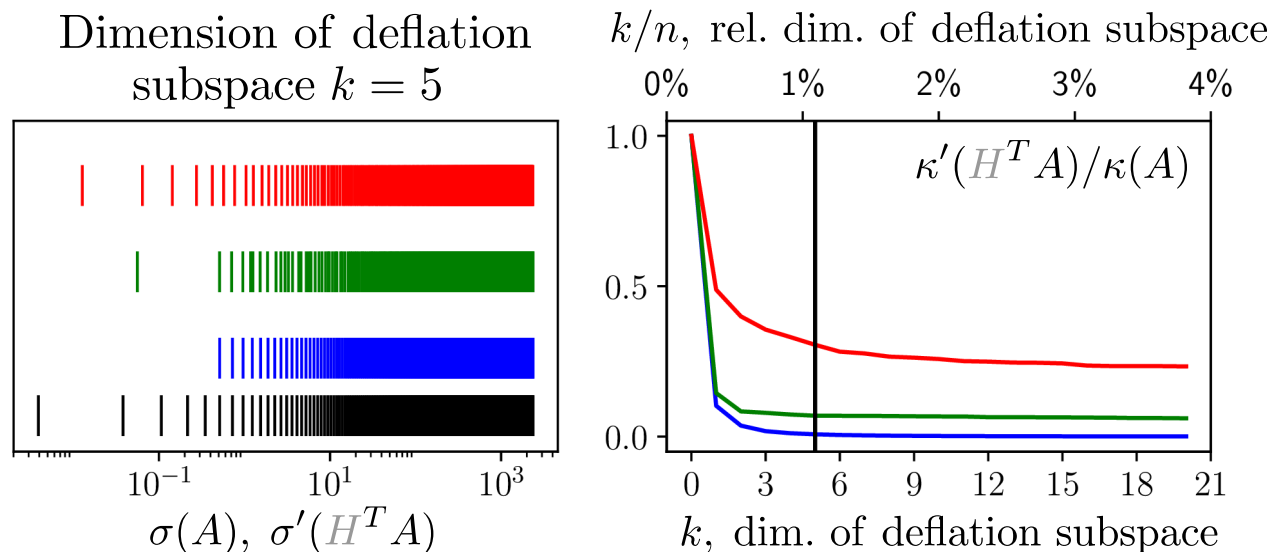


- Letting  $W$  approximate the least dominant eigenvectors of  $A$  significantly improves the conditioning of the system.

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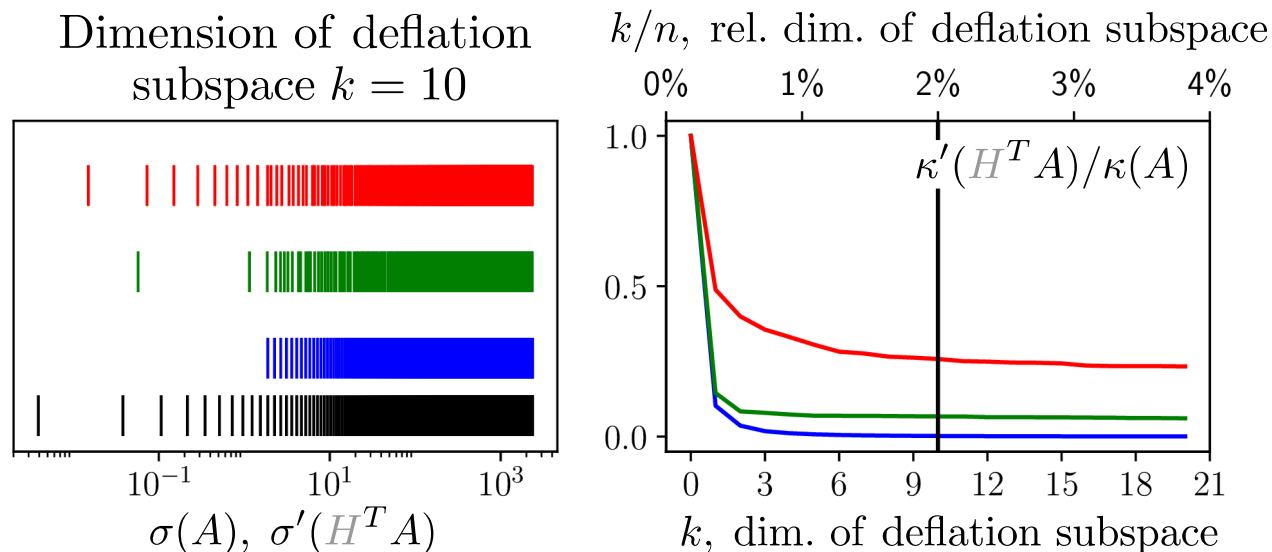


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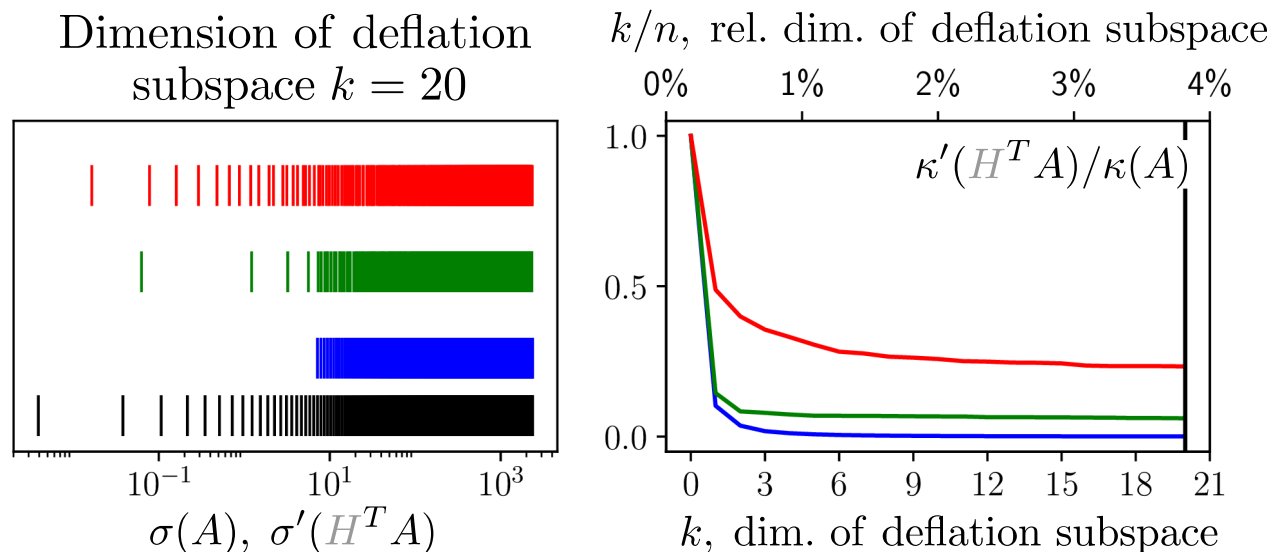
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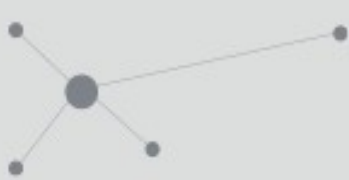
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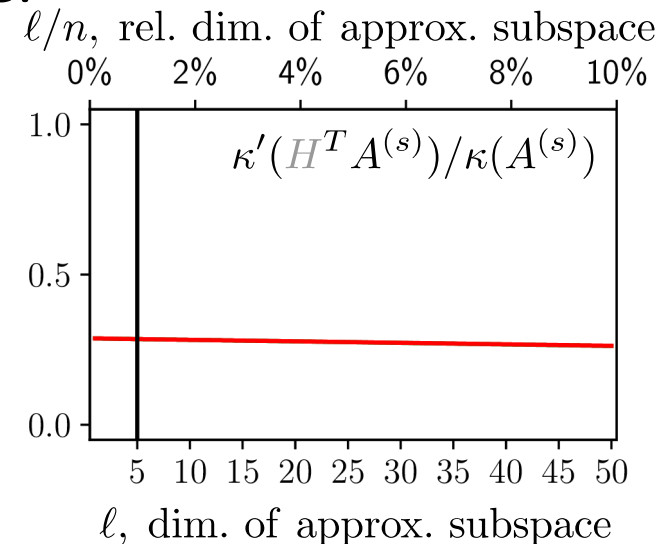
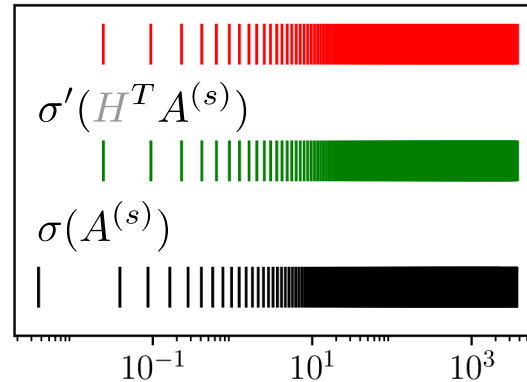
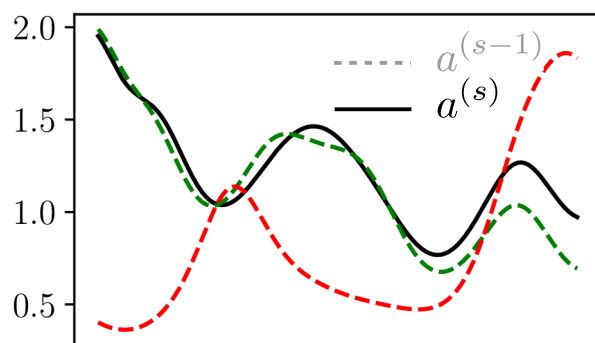
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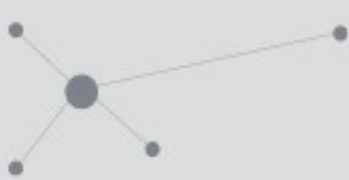
# Effect of similarity between sampled fields on quality of deflation

- Deflate  $A^{(s)}$  with approximate eigenvectors contained in  $\mathcal{R}(W^{(s-1)}) \oplus \mathcal{K}_\ell(A^{(s-1)}, r_0)$ . Effect of relation between  $A^{(s-1)}$  and  $A^{(s)}$  on the deflation process?
- Let  $a^{(s)}$  be the coefficient field of  $A^{(s)}$ , and consider different fields  $a^{(s-1)}$  of  $A^{(s-1)}$ . For  $W^{(s-1)} = \emptyset$ , we observe:

Dimension of deflation subspace  $k = 1$



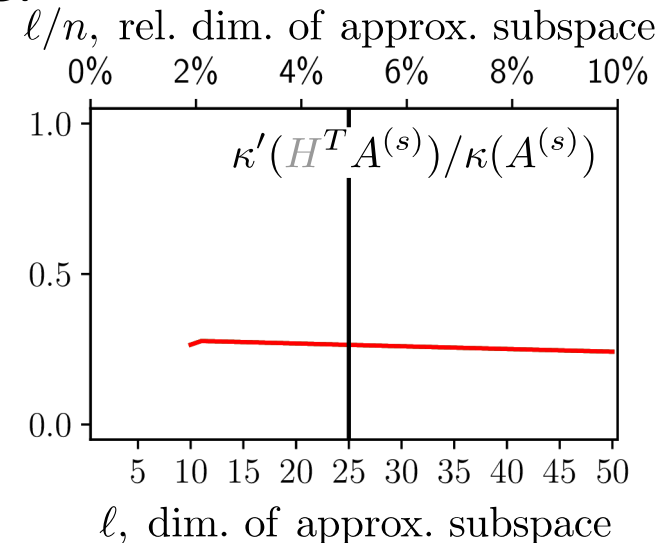
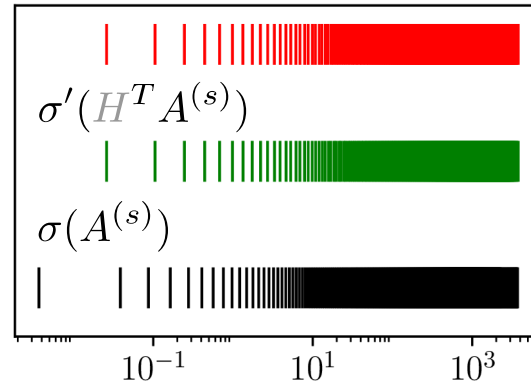
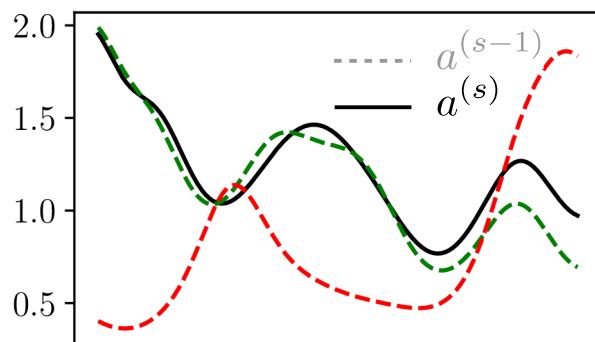
- Similarity between the fields has no effect,
- The dimension of the approximation subspace has no effect.



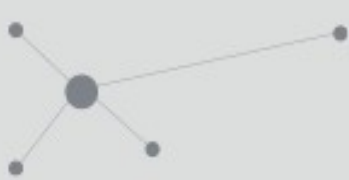
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Dimension of deflation subspace  $k = 10$



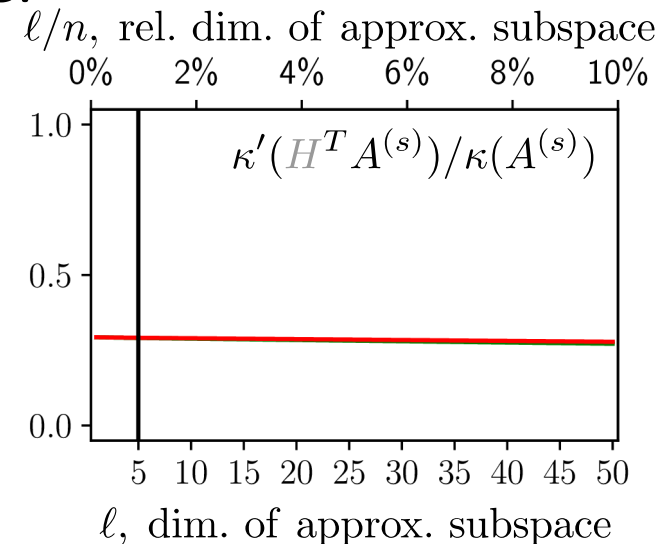
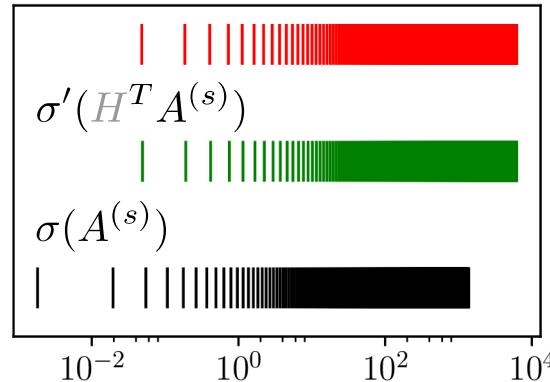
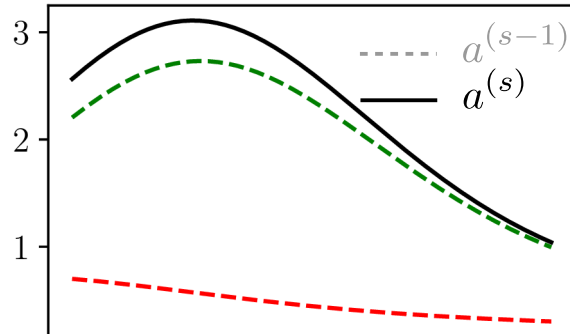
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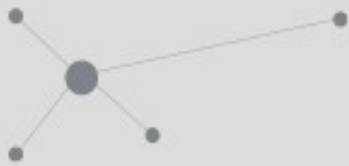
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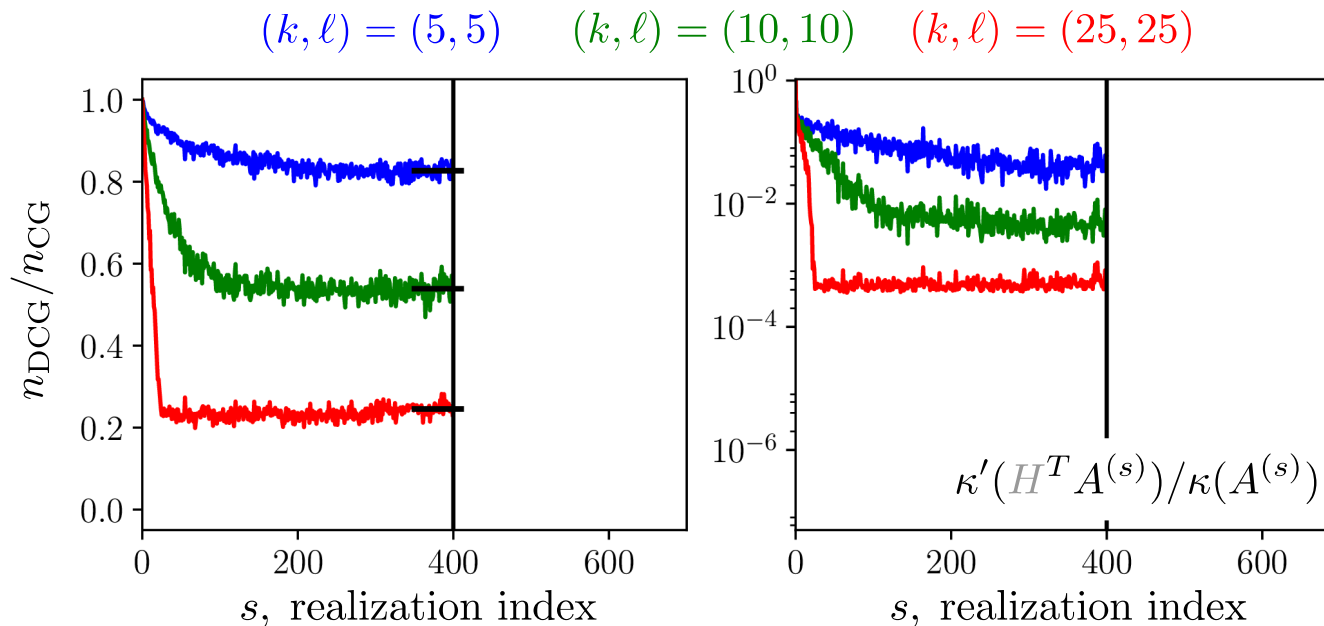


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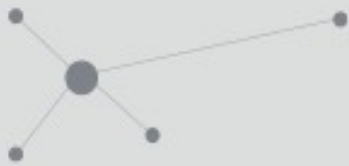


# Solving a MC sampled sequence of systems $A^{(s)}x^{(s)} = b$ by deflated CG

- Deflate current system with approximate eigenvectors  $W^{(s)} := [w_1^{(s)}, \dots, w_k^{(s)}]$  of  $A^{(s)}$  built by harmonic Ritz analysis in  $\mathcal{R}(W^{(s-1)}) \oplus \mathcal{K}_\ell(A^{(s-1)}, r_0)$ .
- Considering different dimensions  $k$  of deflation subspaces, we observe:



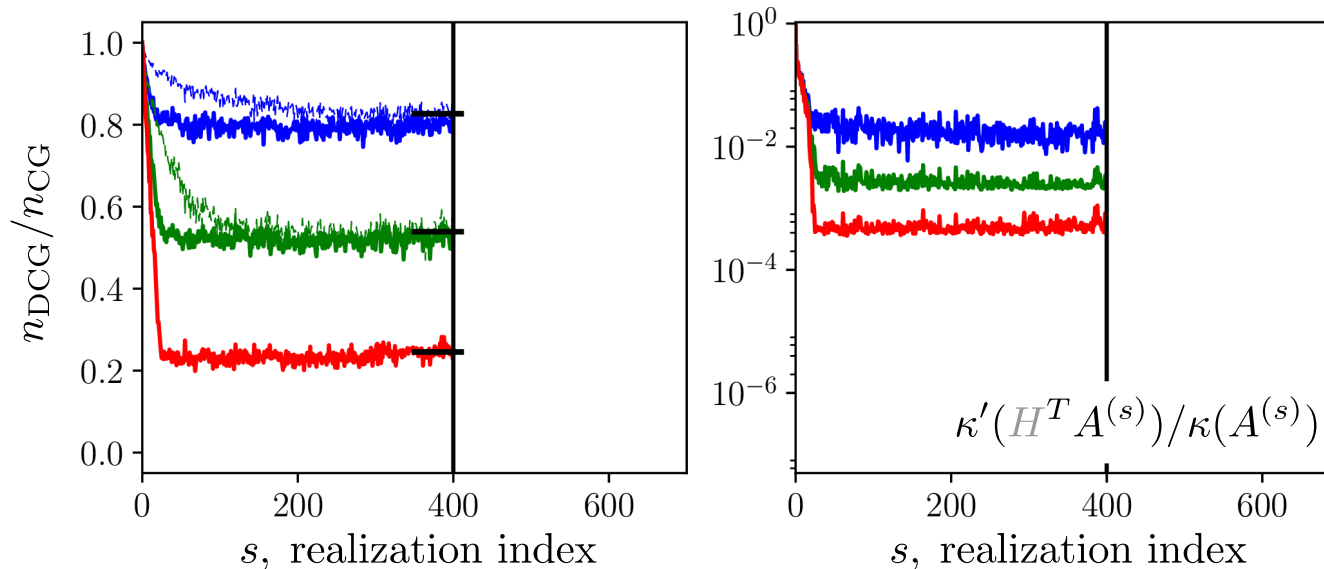
an asymptotic gain of iterations over CG which strongly depends on  $k$ .



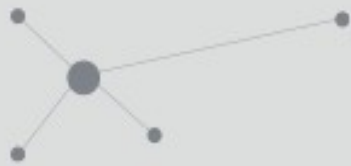
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- Increasing the dimension  $\ell$  of the approximation subspaces used for the harmonic Ritz analysis, we observe:

$(k, \ell) = (5, 25)$      $(k, \ell) = (10, 25)$      $(k, \ell) = (25, 25)$

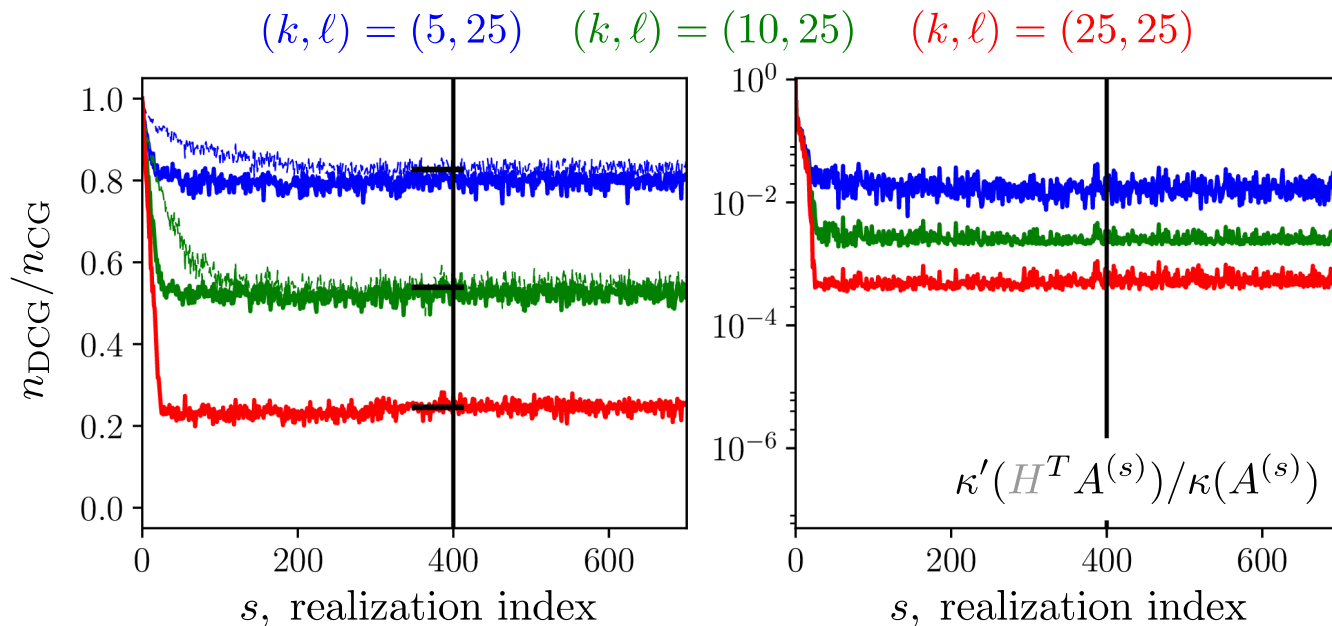


a faster gain of iterations over CG, still to the same asymptotic speed-up.

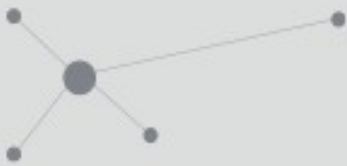


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- After stopping the update of the deflation subspace, we observe

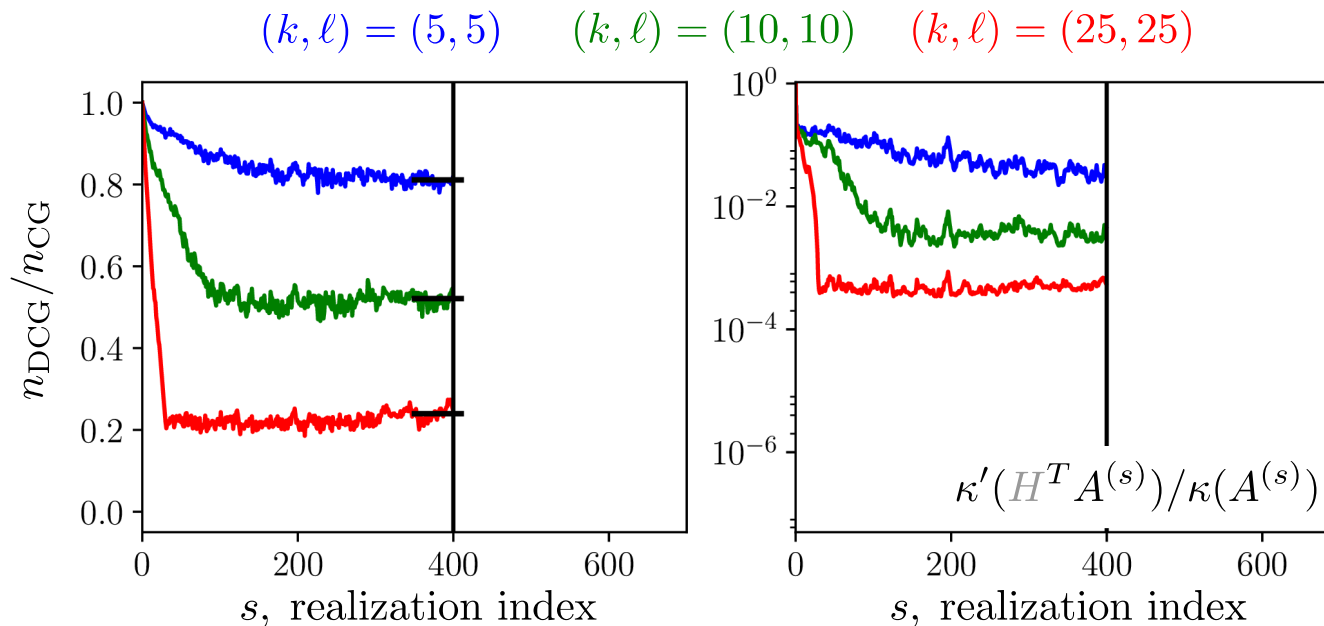


the relative gain of iteration is preserved.



# Solving a MCMC sampled sequence of systems $A^{(s)}x^{(s)} = b$ by deflated CG

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- When sampling the fields of coefficients by Markov Chain Monte Carlo,

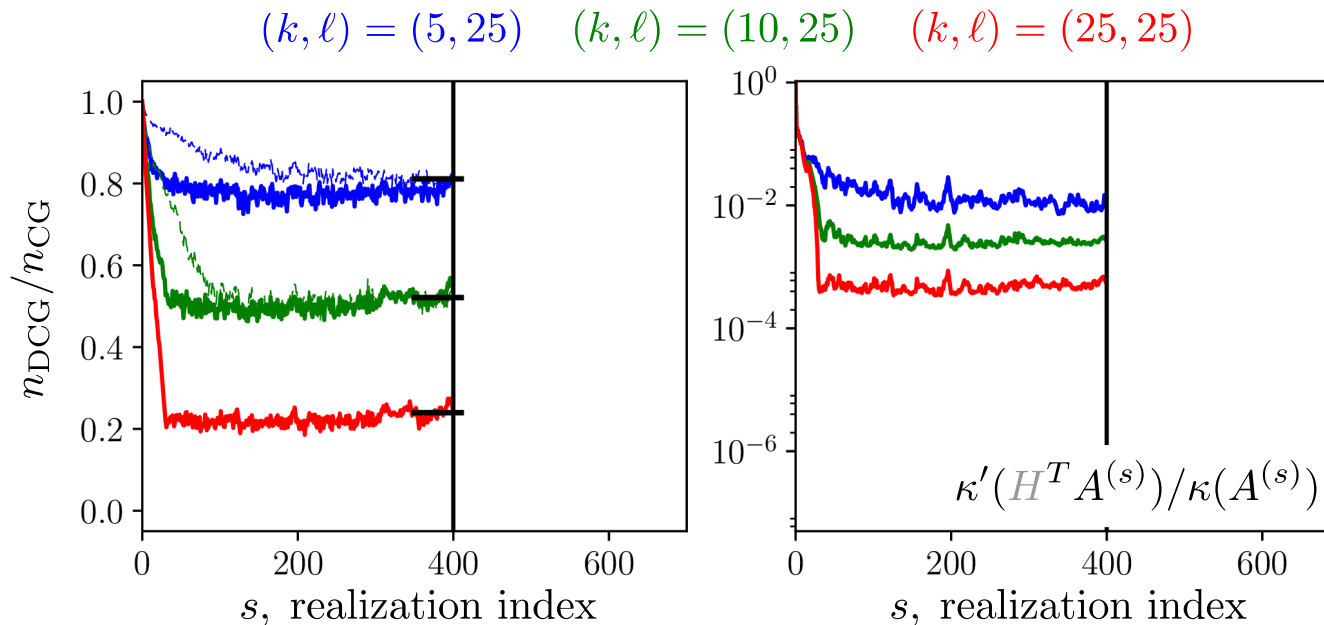


a similar behavior is observed.



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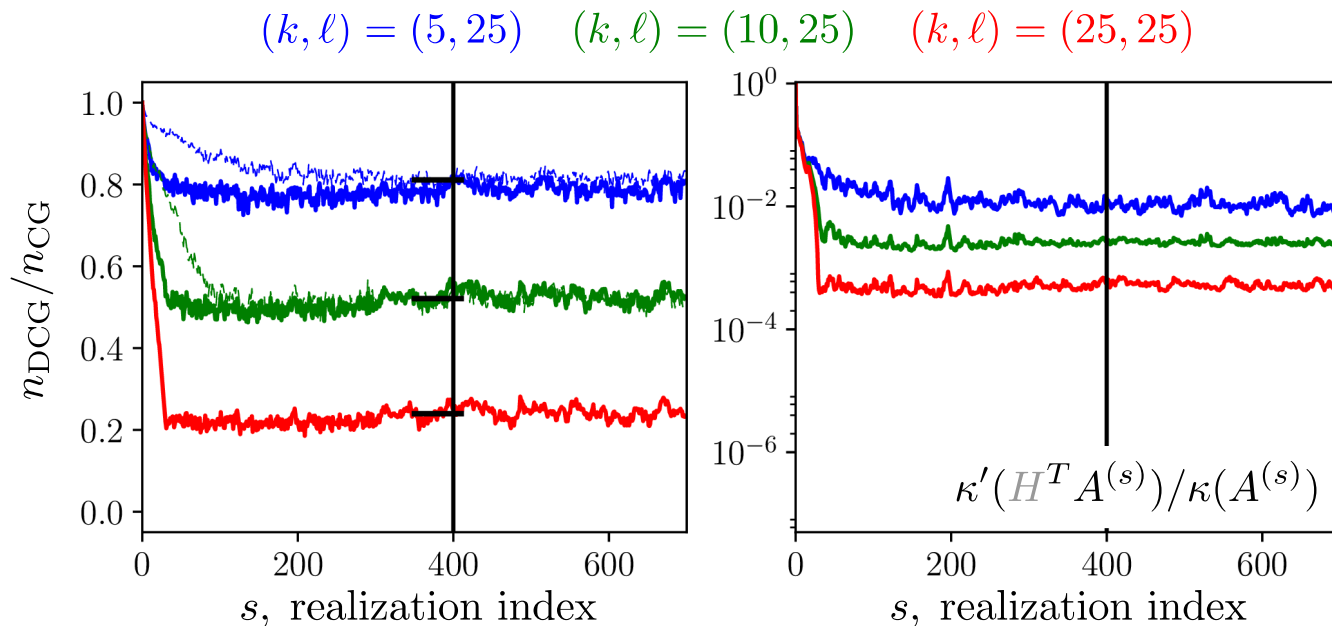
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- When sampling the fields of coefficients by Markov Chain Monte Carlo,



a similar behavior is observed.

# Deflation and preconditioning of SPD systems

- Consider a preconditioner  $M = LL^T$ . Let  $\dot{A} := L^{-1}AL^{-T}$  and define the projector  $\dot{H} = I_n - \dot{W}(\dot{W}^T \dot{A} \dot{W})^{-1} \dot{W}^T \dot{A}$  with  $k \ll n$  linearly independent vectors  $[\dot{w}_1, \dots, \dot{w}_k] =: \dot{W}$ .
- A sequence  $\{x_i\}_{i=0}^j$  of approximations of  $x^* := A^{-1}b$  is obtained by

$\hat{\mu}^*$  is the direct solution of a *reduced system*

$$x_i := L^{-T}(\dot{W} \hat{\mu}^* + \dot{H} x'_i)$$

$x'_i$  is an iterative solution of the *deflated system*  
 $\dot{H}^T \dot{A} x' = \dot{H}^T L^{-1}b$

- Error bounded by  $\|x^* - x_i\|_A \leq 2\|x^* - x_0\|_A \left( \frac{\sqrt{\kappa'(\dot{H}^T \dot{A})} - 1}{\sqrt{\kappa'(\dot{H}^T \dot{A})} + 1} \right)^i$
- Two heuristics are considered for the choice of  $\dot{W}$  :

- (1) Deflated Preconditioned CG (DPCG)
- (2) Preconditioned Deflated CG (PDCG)

# Solving a sampled sequence of systems by DPCG or PDCG with exact eigenvectors

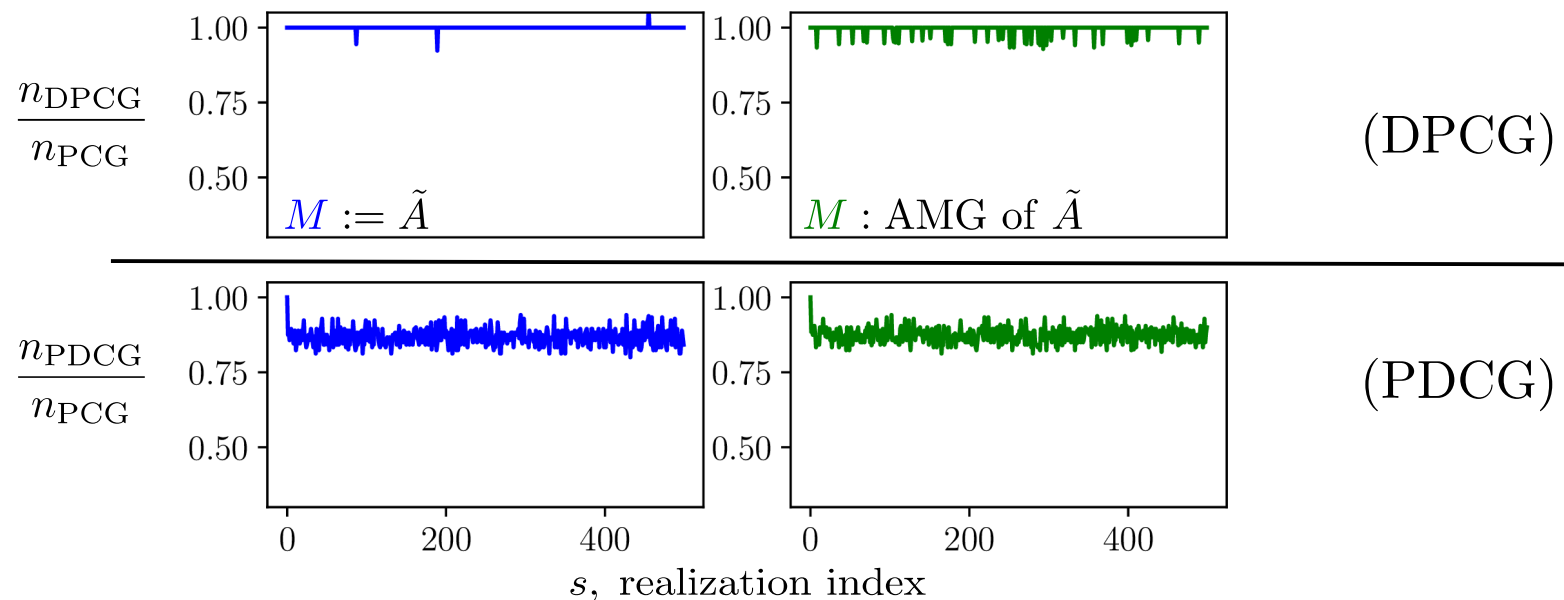
- Consider two preconditioners :

(1)  $M := \tilde{A} \implies n_{\text{PCG}}/n_{\text{CG}} = 2.8\%$  on average

(2)  $M$  : AMG of  $\tilde{A} \implies n_{\text{PCG}}/n_{\text{CG}} = 3.1\%$  on average

and compare their relative performance with DPCG and PDCG.

- Considering a relative dimension of deflation subspace  $k/n = 0.4\%$  , i.e.  $k = 2$  :



# Solving a sampled sequence of systems by DPCG or PDCG with exact eigenvectors

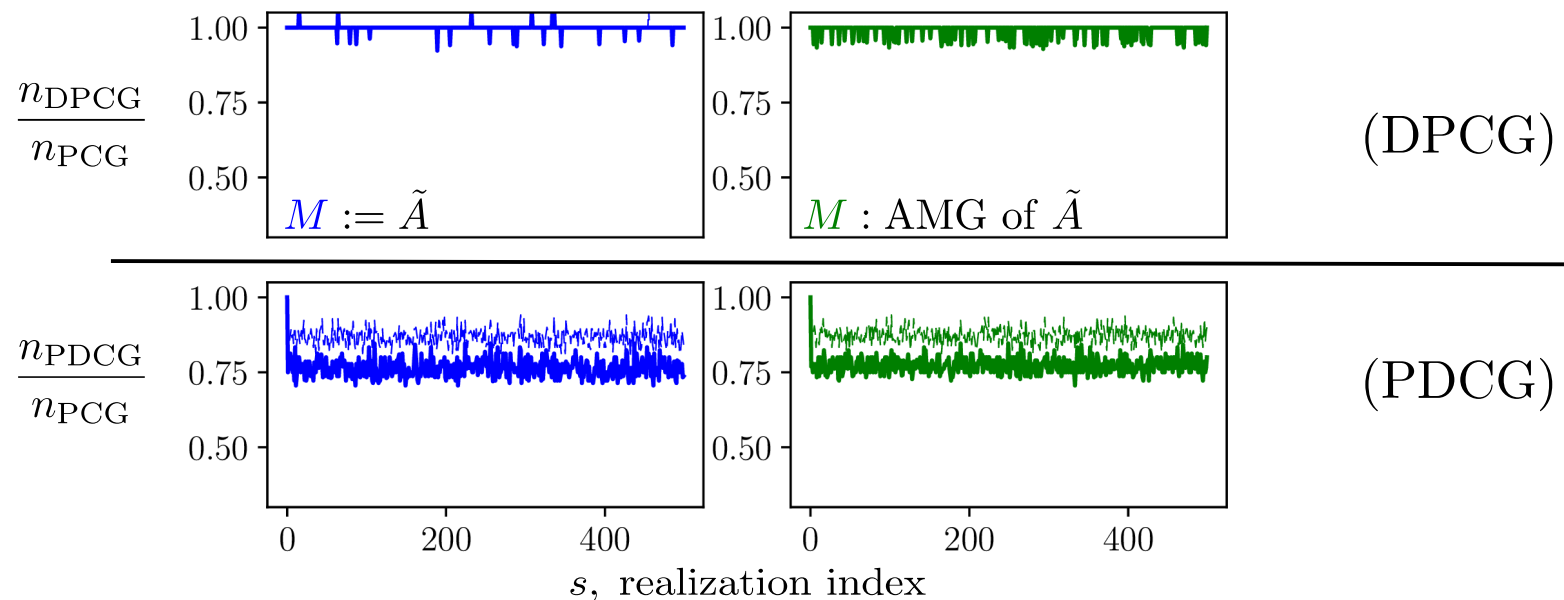
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# Solving a sampled sequence of systems by DPCG or PDCG with exact eigenvectors

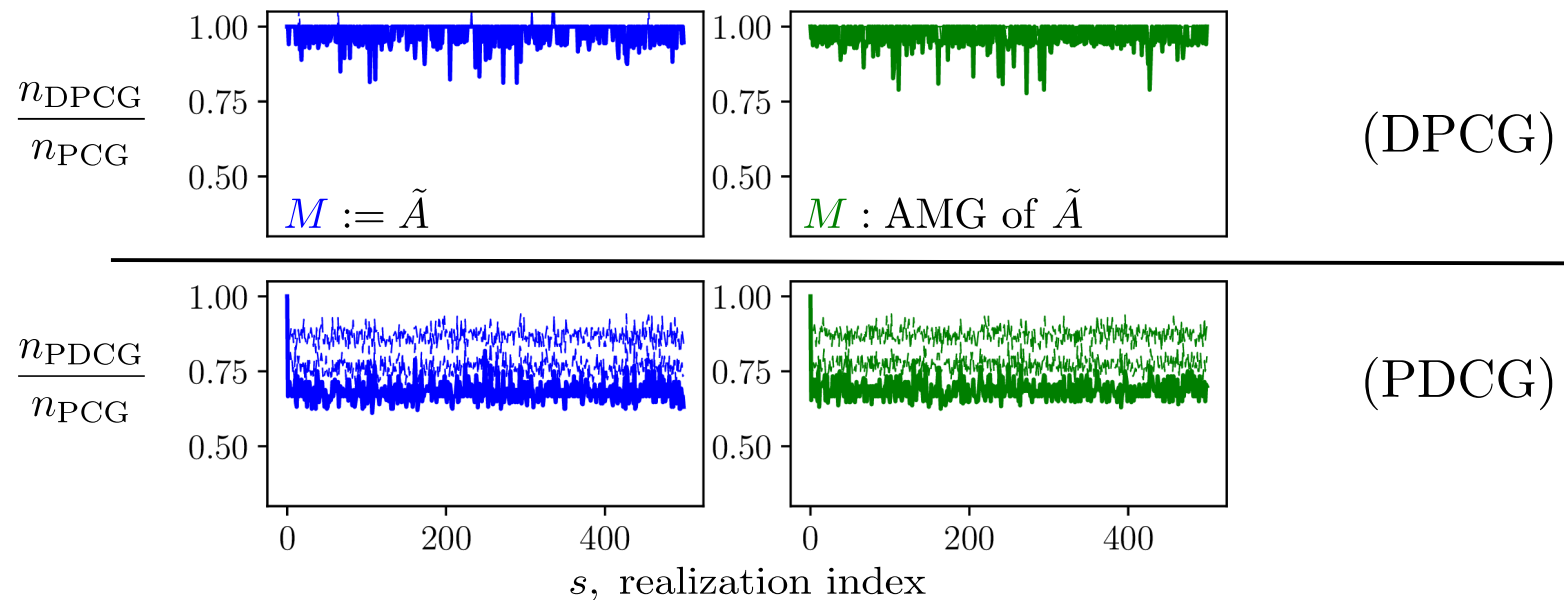
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- Considering a relative dimension of deflation subspace  $k/n = 8\%$  , i.e.  $k = 40$  :



# Solving a sampled sequence of systems by DPCG or PDCG with exact eigenvectors

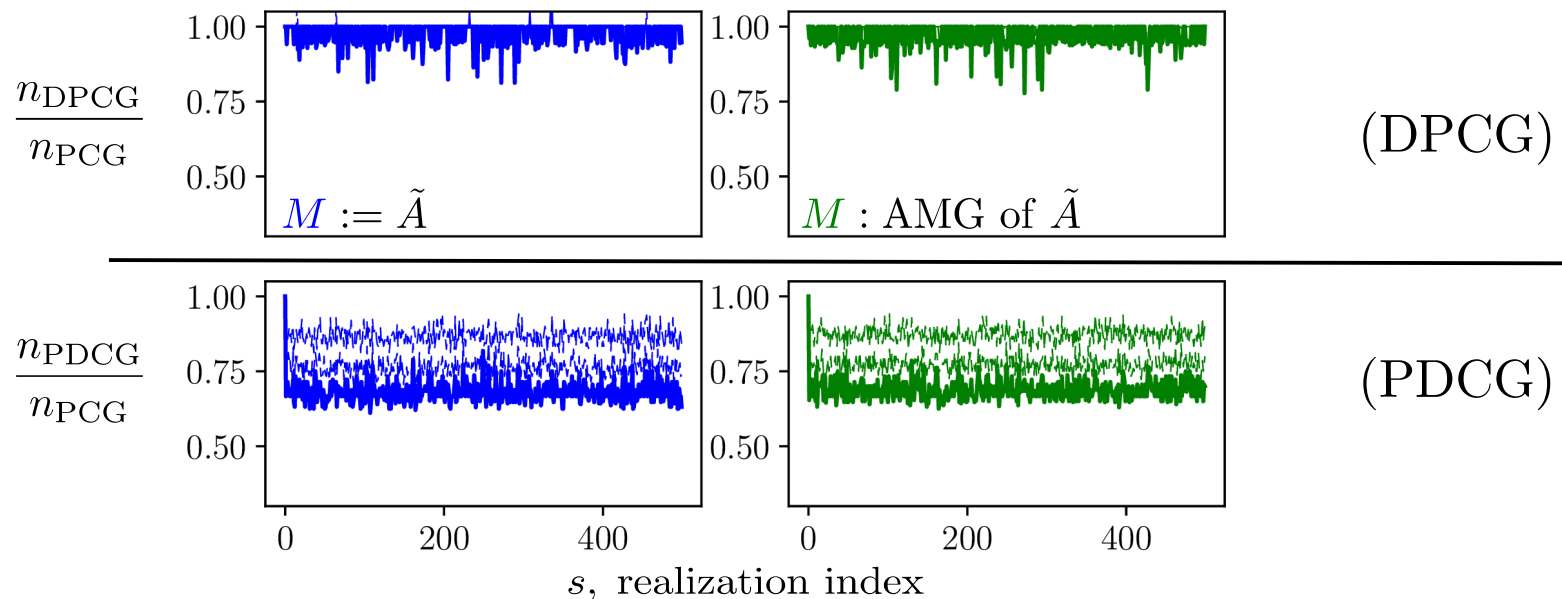
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and compare their relative performance with DPCG and PDCG.

- Considering a relative dimension of deflation subspace  $k/n = 8\%$  , i.e.  $k = 40$  :



Deflating with the AMG preconditioner works as well as with the median operator,

# Solving a sampled sequence of systems by DPCG or PDCG with exact eigenvectors

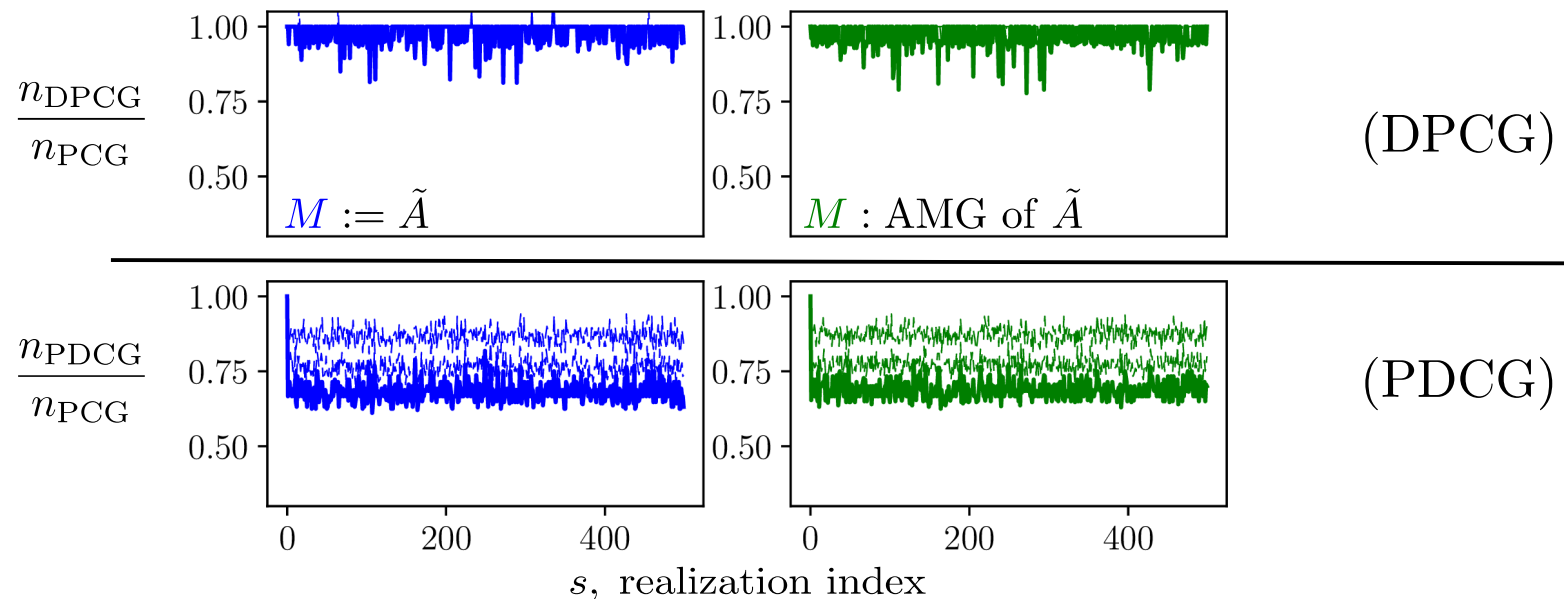
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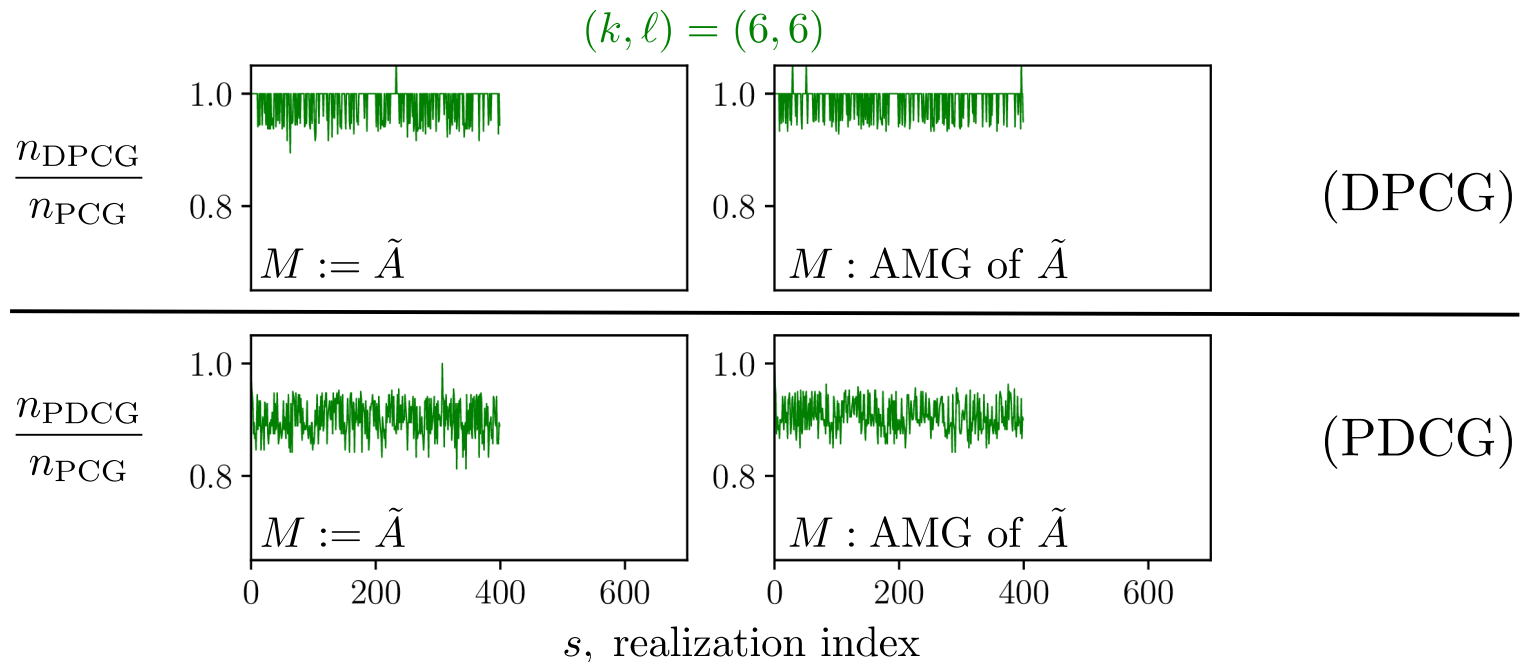


Deflating before preconditioning (PDCG) works better than the opposite (DPCG).



# Solving a sampled sequence of systems by DPCG or PDCG with approximate eigenvectors

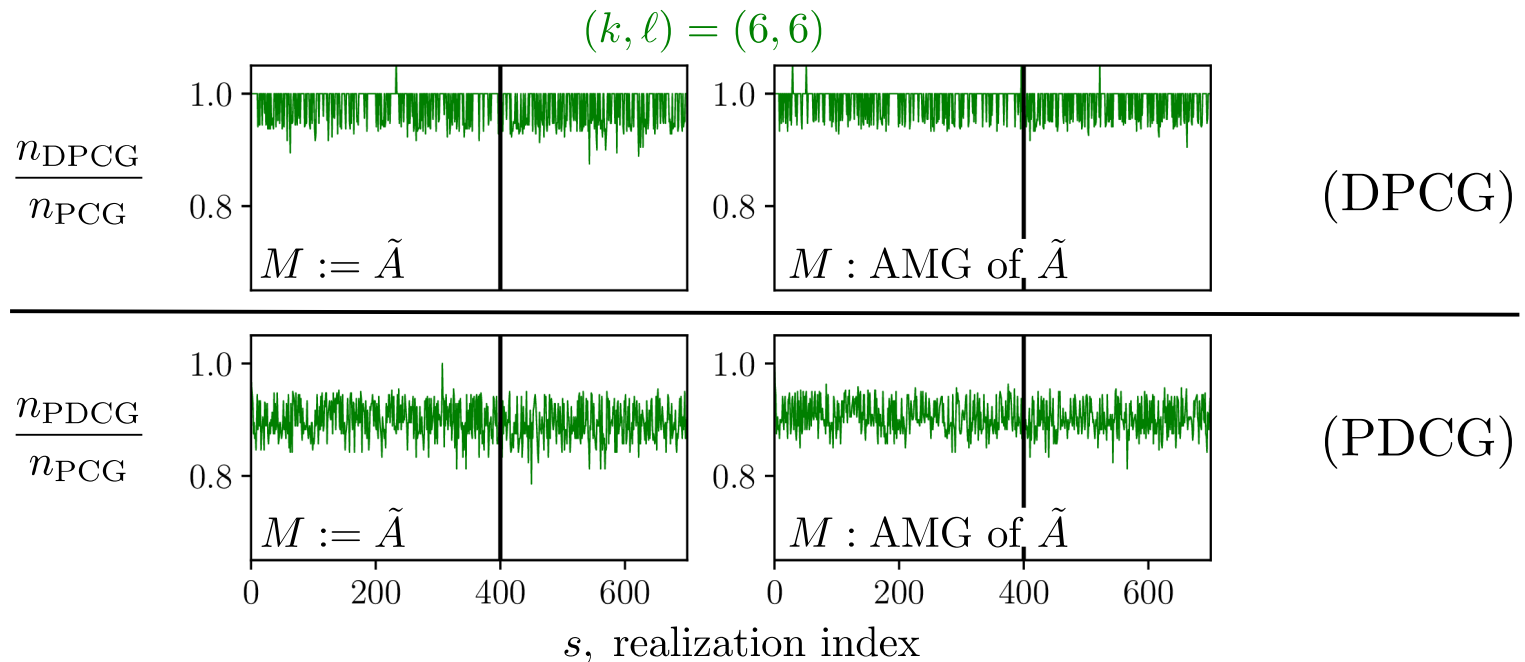
- Deflate current system with approximate eigenvectors  $\dot{W}^{(s)} := [\dot{w}_1^{(s)}, \dots, \dot{w}_k^{(s)}]$  of  $L^{-1}A^{(s)}L^{-T}$  (DPCG), or  $L^T A^{(s)}L^{-T}$  (PDCG), obtained by harmonic Ritz analysis in an approximation subspace of dimension  $(k + \ell)$  obtained while solving the precedent system  $A^{(s-1)}x^{(s-1)} = b$ .
- Sampling the coefficient fields by Monte Carlo (MC), we obtain:



The asymptotic speed-up is quickly reached. PDCG still yields a greater acceleration than DPCG. The AMG preconditioner is as good as the median.

# Solving a sampled sequence of systems by DPCG or PDCG with approximate eigenvectors

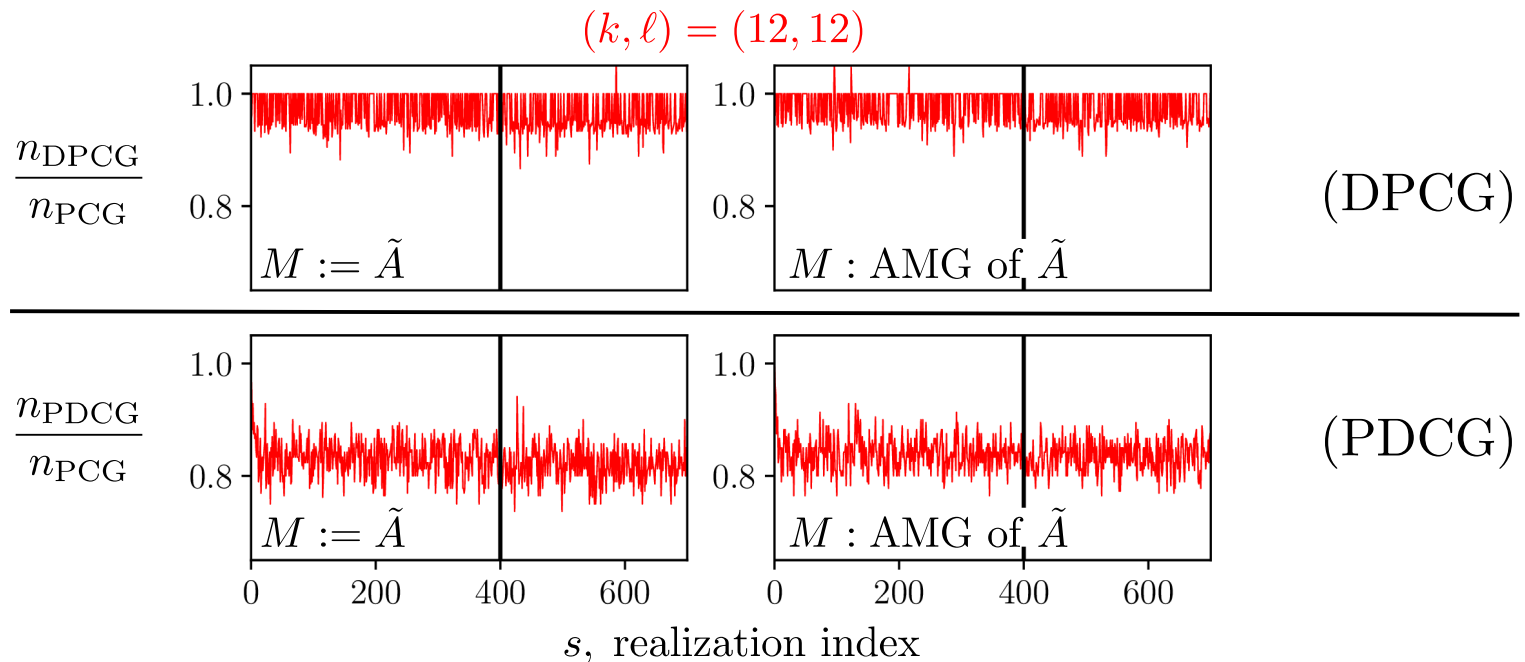
- Deflate current system with approximate eigenvectors  $\dot{W}^{(s)} := [\dot{w}_1^{(s)}, \dots, \dot{w}_k^{(s)}]$  of  $L^{-1}A^{(s)}L^{-T}$  (DPCG), or  $L^T A^{(s)}L^{-T}$  (PDCG), obtained by harmonic Ritz analysis in an approximation subspace of dimension  $(k + \ell)$  obtained while solving the precedent system  $A^{(s-1)}x^{(s-1)} = b$ .
- Sampling the coefficient fields by Monte Carlo (MC), we obtain:



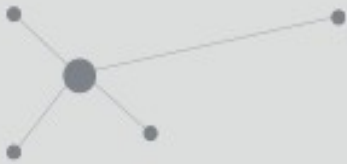
Similarly as for the non-preconditioned case, the deflation subspace need not be updated to preserve the asymptotic speed-up.

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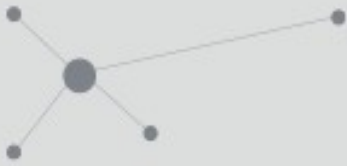


a similar behavior is observed when increasing the dimension of the deflation subspace.



# Conclusions

- Deflation is a low-cost solution to accelerate the iterative resolution of sequences of linear systems which arise when evaluating estimators based on solutions of random elliptic equations
- The sampling strategy of the random field has little impact on the quality of the deflation
- Once a stable iteration gain is reached, there is no need to keep updating the deflation subspace
- Using an adequate deflation heuristic allows to reach iteration gains over PCG when paired with preconditioners based on a median operator
- Even when using a preconditioner whose parallel application is known to be more scalable than the median operator itself

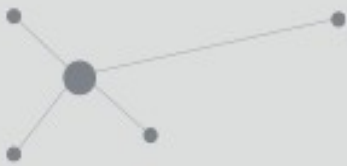


# Perspectives

- 2D problems
- Domain decomposition
- Parallel implementation



Thank you



# Eigenvector approximation

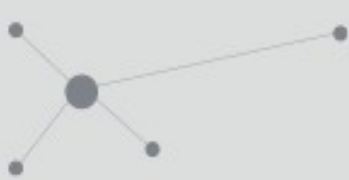
- Least dominant eigenvectors of  $A^{(s)}$  are commonly approximated with harmonic Ritz vectors  $w$  in some subspace  $\mathcal{S}^{(s)}$  s.t.

$$A^{(s)}w - \theta w \perp A^{(s)}\mathcal{S}^{(s)}$$

- If a basis  $Z^{(s)} \in \mathbb{R}^{n \times m}$  of  $\mathcal{S}^{(s)}$  is available, the Ritz vector  $w = Z^{(s)}\hat{w}$  is obtained by solving the  $m$ -dimensional generalized eigenvalue problem

$$(A^{(s)}Z^{(s)})^T A^{(s)}Z^{(s)}\hat{w} = \theta Z^{(s)T} A^{(s)}Z^{(s)}\hat{w}$$

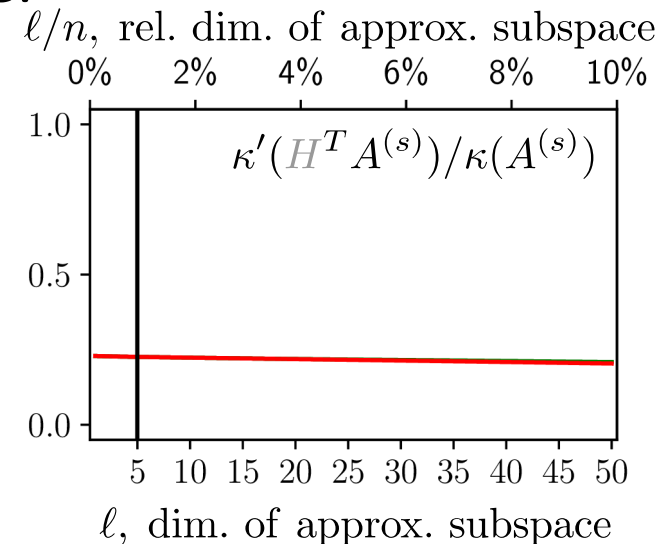
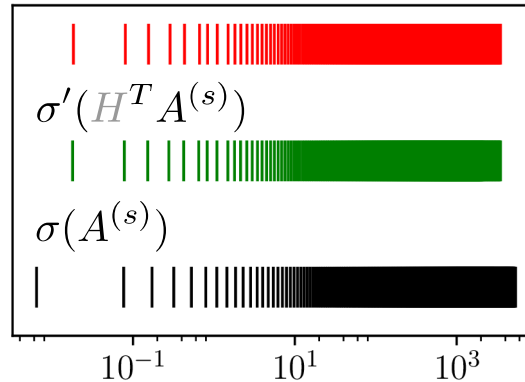
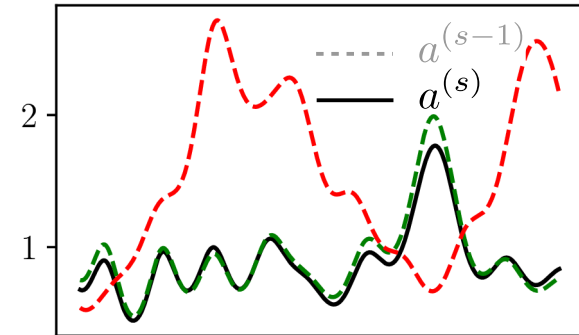
- Note that upon generating some iterates  $\{x_i\}_{i=0}^{\ell}$  to solve  $A^{(s-1)}x^{(s-1)} = b$ , a basis is constructed for  $\mathcal{R}(W^{(s-1)}) \oplus \mathcal{K}_{\ell}(A^{(s-1)}, r_0)$
- Therefore, the system  $A^{(s)}x^{(s)} = b$  can be deflated with a basis  $W^{(s)}$  made of Harmonic Ritz vectors of  $A^{(s)}$  in  $\mathcal{R}(W^{(s-1)}) \oplus \mathcal{K}_{\ell}(A^{(s-1)}, r_0)$ .



# Effect of similarity between sampled fields on quality of deflation

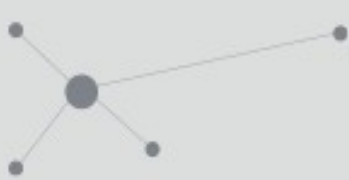
- Deflate  $A^{(s)}$  with approximate eigenvectors contained in  $\mathcal{R}(W^{(s-1)}) \oplus \mathcal{K}_\ell(A^{(s-1)}, r_0)$ . Effect of relation between  $A^{(s-1)}$  and  $A^{(s)}$  on the deflation process?
- Let  $a^{(s)}$  be the coefficient field of  $A^{(s)}$ , and consider different fields  $a^{(s-1)}$  of  $A^{(s-1)}$ . For  $W^{(s-1)} = \emptyset$ , we observe:

Dimension of deflation subspace  $k = 1$



- Similarity between the fields has no effect,
- The dimension of the approximation subspace has no effect.

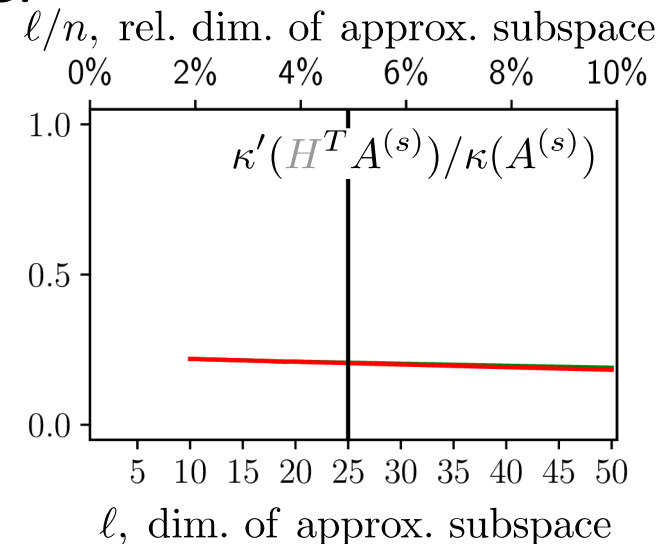
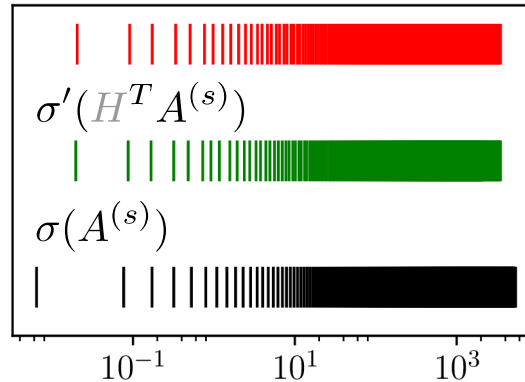
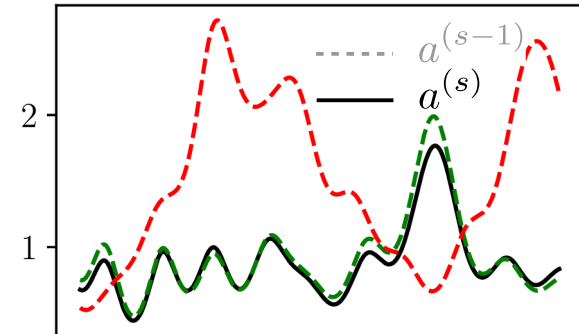




# Effect of similarity between sampled fields on quality of deflation

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Dimension of deflation subspace  $k = 10$



- Similarity between the fields has no effect,
- The dimension of the approximation subspace has no effect.

# DPCG vs PDCG

- Consider a preconditioner  $M = LL^T$ . Let  $\dot{A} := L^{-1}AL^{-T}$  and define the projector  $\dot{H} = I_n - \dot{W}(\dot{W}^T \dot{A} \dot{W})^{-1} \dot{W}^T \dot{A}$  with  $k \ll n$  linearly independent vectors  $[\dot{w}_1, \dots, \dot{w}_k] =: \dot{W}$ .
- A sequence  $\{x_i\}_{i=0}^j$  of approximations of  $x^* := A^{-1}b$  is obtained by

$$x_i := L^{-T}(\dot{W}\hat{\mu}^* + \dot{H}x'_i) \quad \text{where}$$

$x'_i$  is an iterative solution of the **deflated system**  
 $\dot{H}^T \dot{A} x' = \dot{H}^T L^{-1} b$

- Error bounded by  $\|x^* - x_i\|_A \leq 2\|x^* - x_0\|_A \left( \frac{\sqrt{\kappa'(\dot{H}^T \dot{A})} - 1}{\sqrt{\kappa'(\dot{H}^T \dot{A})} + 1} \right)^i$
- Let  $W := L^{-T} \dot{W}$  so that

$$\dot{H}^T \dot{A} = L^{-1} H^T A L^{-T}$$

- (1) Let  $\dot{W}$  be eigenvectors of  $\dot{A}$   
 $\implies W$  are eigenvectors of  $M^{-1}A$

DPCG

- (2) Let  $W$  be eigenvectors of  $A$   
 $\implies \dot{W}$  are eigenvectors of  $L^T A L^{-T}$

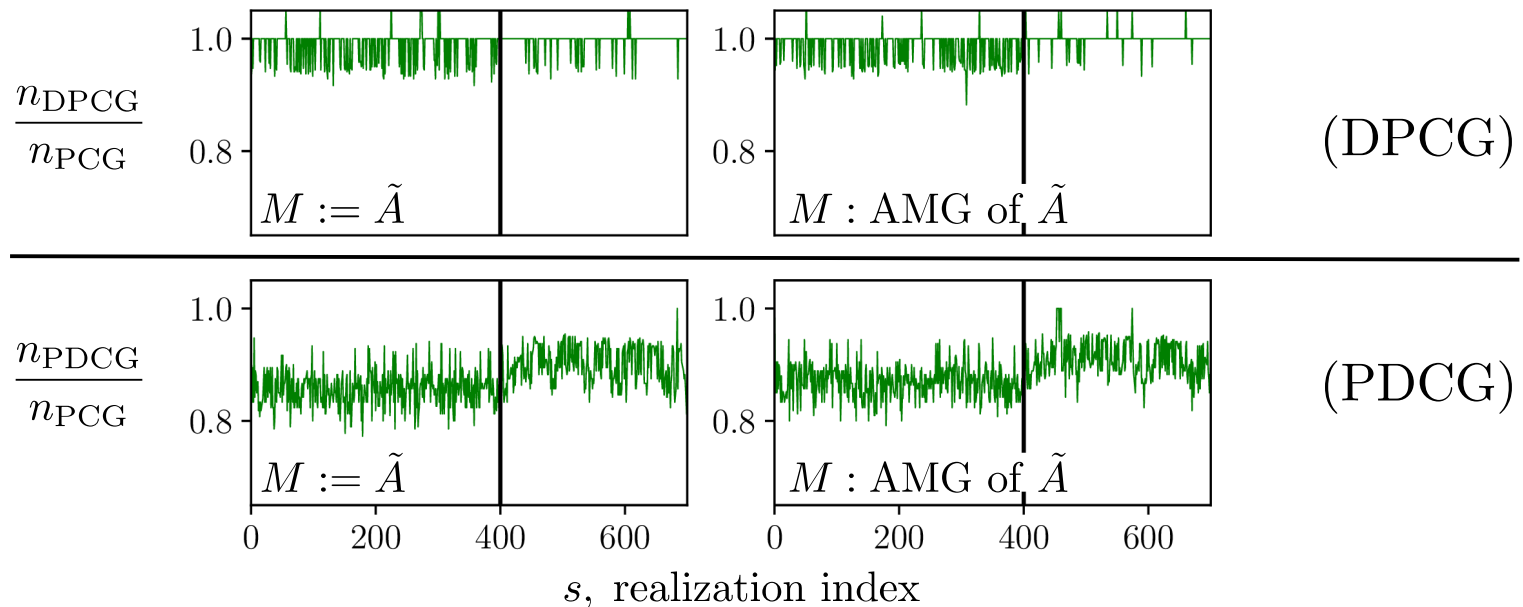
PDCG

- Two approaches :

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- Sampling the coefficient fields by Markov chain Monte Carlo, we obtain:

$$(k, \ell) = (6, 6)$$

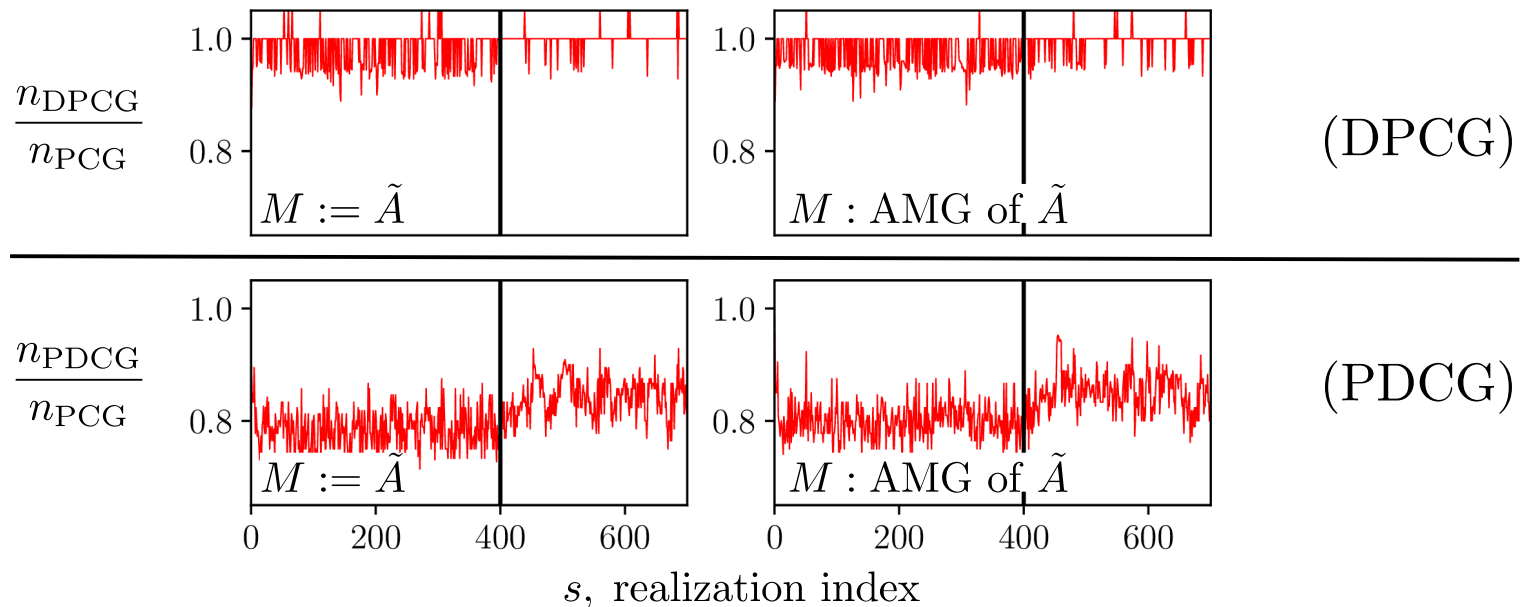


Interrupting the deflation subspace update while sampling by MCMC causes a slight deterioration in the quality of the deflation.

# Solving a sampled sequence of systems by DPCG or PDCG with approximate eigenvectors

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- Sampling the coefficient fields by Markov chain Monte Carlo, we obtain:

$(k, \ell) = (12, 12)$



Interrupting the deflation subspace update while sampling by MCMC causes a slight deterioration in the quality of the deflation.