Hierarchically Accelerated Stochastic Collocation Methods for PDEs with Random Coefficients

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Improving on existing methods

- Stochastic sampling methods for random PDEs are computationally expensive: each sample point corresponds to a PDE solve.

- Traditionally, we try to improve single level methods by reducing the number of samples/solves: Quasi Monte Carlo and importance sampling, (anisotropic) sparse grids, adaptive grids.

Improving on existing methods

- Stochastic sampling methods for random PDEs are computationally expensive: each sample point corresponds to a PDE solve.
- Traditionally, we try to improve single level methods by reducing the number of samples/solves: Quasi Monte Carlo and importance sampling, (anisotropic) sparse grids, adaptive grids.
- Exploit the deterministic hierarchy: For a given accuracy, multilevel methods seek to reduce the complexity by spreading computational cost evenly across several resolutions of the spatial discretization (MLSC - Max Gunzburger's talk)
- Exploit the stochastic hierarchy: Sparse grids with nested grid points provide a natural multilevel hierarchy which we can use to accelerate each PDE solve

Uncertainty Quantification

parameters: $\mathbf{y}(\omega)$, $\omega \in \Omega_{\mathbb{P}}$ $\longrightarrow$ **SPDE model:** $\mathcal{L}(u, \mathbf{y}) = f$ for a.e. $x \in D \subset \mathbb{R}^d$ $\longrightarrow$ quantity of interest $Q[u(\cdot, \mathbf{y})]$

- The parameters $\mathbf{y}(\omega)$ may be affected by uncertainty (experimental data, incomplete description of parameters, unresolved scales, etc.)
- $\mathbf{y} : \Omega \to \Gamma \subset \mathbb{R}^N$ can be assumed to be a random vector with N components, i.e., $\mathbf{y} = (y_1, \ldots, y_N)$, with joint probability density function $\rho(\mathbf{y})$

The solution u is a stochastic function, $u(\cdot, \mathbf{y})$

Goals of forward UQ: Approximate u or some statistical QoI depending on u, i.e.

$$\mathbb{E}[u],\ \mathbb{V}\mathrm{ar}[u],\ \mathbb{P}[u > u_0] = \mathbb{E}[\mathbb{1}_{\{u>u_0\}}]$$

with the minimal computational cost possible.

Model Problem - Linear Elliptic SPDE

Let $(\Omega, \mathcal{F}, P)$ be a complete probability space. Find u such that almost surely, i.e. for P-almost every $\omega \in \Omega$

$$\begin{cases} -\nabla \cdot (a(x,\omega) \cdot \nabla u(x,\omega)) &= f(x,\omega) \quad x \in D, \\ u(x,\omega) &= 0 \quad x \in \partial D. \end{cases} \tag{1}$$

We'll assume that a, f are such that this problem has a unique solution represented in terms of $\mathbf{y} \in \Gamma \subset \mathbb{R}^N$, a finite dimensional random vector.

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- Such a PDE might be used to model ground water flow or current through a random material.
- The methods we'll talk about are not specific to this simple class of problems, but our methods extend, e.g., to non-linear PDEs, and more generally to random PDEs where the solution map $\mathbf{y} \mapsto u(\cdot, \mathbf{y})$ has some analytic regularity.

Monte Carlo Method

Pure random sampling to approximate statistics of the solution:

$$\mathbb{E}(u) = \int_{\Gamma} u(x, \mathbf{y}) \rho(\mathbf{y}) \, d\mathbf{y} \approx \frac{1}{M} \sum_{j=1}^{M} u(x, \mathbf{y}_j)$$

- Most widely used in applications and high (~ 100) dimensional problems
- **Pro:** Simple to implement, easily parallelizable, convergence rate $\mathcal{O}(M^{-1/2})$ is dimension independent, but...
- **Con:** Relatively slow if the solution has some smoothness wrt random parameters

Analytic Regularity

Theorem: [Babuska et al '07,'10, Webster '07]

- Let $\Gamma_n^* = \prod_{\substack{j=1 \\ j \neq n}}^{N} \Gamma_j$, and let $\mathbf{y}_n^*$ denote an arbitrary element of Γ_n^*

$\exists$ constants λ (independent of n), $\gamma_n \geq 0$ and regions $\Sigma_n \equiv \{z \in \mathbb{C}, \ \ \text{dist}(z, \Gamma_n) \leq \gamma_n\}$ in the complex plane for which

$$\max_{\mathbf{y}_n^* \in \Gamma_n^*} \max_{z \in \Sigma_n} \|\nabla u(\cdot, \mathbf{y}_n^*, z)\|_{L^2(D)} \leq \lambda.$$

That is, the solution $u(x, \mathbf{y}_n^*, y_n)$ admits an analytic extension $u(x, \mathbf{y}_n^*, z)$, $z \in \Sigma_n \subset \mathbb{C}$.

- The analyticity of the solution $u(x, \mathbf{y})$ w.r.t. each random direction y_n suggests the use of multivariate **global** polynomial approximation. In cases with less regularity we might turn to the use of **local** basis functions.

Analytic polydisc regularity: [Cohen-DeVore-Schwab 2010, Chkifa-Cohen-DeVore-Schwab 2013, Tran-Trenchea-Webster 2013, Tran-Webster-Zhang 2014]

Spectral Polynomial Methods

- **Stochastic Galerkin:** projection technique, intrusive approach
- **Stochastic collocation:** interpolation technique, non-intrusive approach

$$u_{h,M}^{SL}(x, \mathbf{y}) = \sum_{j=1}^{M} c_j(x)\psi_j(\mathbf{y})$$

pro: convergence can be faster than MC

con: curse of dimensionality

- ψ_j is a linear combination of tensorized 1D global Lagrange nodal basis functions and c_j are determined through $u_h(x, \mathbf{y}_j)$
- Collocation usually beats Galerkin from a point of view of complexity.

Generalized Sparse Grid Interpolation

- Define $\{y_{n,j}^{(l)}\}_{j=1}^{p(l)} \subset \Gamma_n$ to be a set of $p(l)$ points in Γ_n.
- $\{\mathcal{U}_n^{p(l)}\}_{l \in \mathbb{N}} : C^0(\Gamma_n) \to \mathcal{P}_{p(l)-1}(\Gamma_n)$ is the standard one-dimensional Lagrange interpolation operator for $\{y_{n,j}^{(l)}\}_{j=1}^{p(l)} \subset \Gamma_n$.
- $\Delta_n^{p(l)} := \mathcal{U}_n^{p(l)} - \mathcal{U}_n^{p(l-1)}$.
- $g : \mathbb{N}_+^N \to \mathbb{N}$ is strictly increasing and defines the mapping between the multi-index $\mathbf{l}$ and the level L used to construct the sparse grid.

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The *L-th level generalized sparse-grid approximation* of $v \in C^0(\Gamma)$ is given by

$$\mathcal{A}_L^{p,g}[v] = \sum_{g(\mathbf{l})\le L} \bigotimes_{n=1}^{N} \Delta_n^{p(l_n)}[v]$$

$$= \mathcal{A}_{L-1}^{p,g}[v] + \sum_{g(\mathbf{l})=L} \bigotimes_{n=1}^{N} \Delta_n^{p(l_n)}[v]$$

Polynomial Spaces

Choose g and p to construct the SG approximation in a given polynomial space:

$$\mathcal{A}_L^{p,g}[v] = \sum_{g(\mathbf{l}) \leq L} \bigotimes_{n=1}^{N} \Delta_n^{p(l_n)}[v]$$

Polynomial Space	$p(l_n)$	$g(\mathbf{l})$
Tensor product	$p(l_n) = l_n$	$\max_{1 \leq n \leq N}(l_n - 1)$
Total degree	$p(l_n) = l_n$	$\sum_{n=1}^{N}(l_n - 1)$
Hyperbolic cross	$p(l_n) = l_n$	$\prod_{n=1}^{N}(l_n - 1)$
Sparse Smolyak	$p(l_n) = 2^{l_n - 1} + 1,\ l > 1$	$\sum_{n=1}^{N}(l_n - 1)$
Anisotropic Smolyak	$p(l_n) = 2^{l_n - 1} + 1,\ l > 1$	$\sum_{n=1}^{N} \frac{\alpha_n}{\alpha_{\min}}(l_n - 1),\ \boldsymbol{\alpha} \in \mathbb{R}_+^N$

Convergence of Sparse Grid Interpolants

We will use the sparse Smolyak construction, with Clenshaw-Curtis abscissas for $\Gamma_n = [-1, 1]$ and $p(l_n) > 1$:

$$y_{n,j}^{(l_n)} = -\cos\left(\frac{\pi(j-1)}{p(l_n)-1}\right) \quad \text{for } j = 1, \ldots, p(l_n).$$

These choices result in a nested set of multidimensional collocation points.

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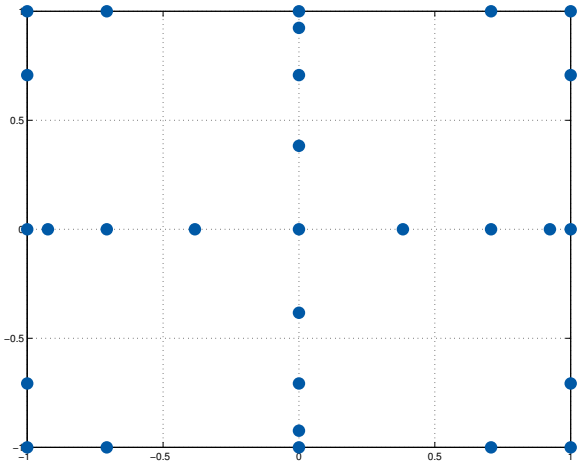
Let $\mathcal{H}_L$—a set of size $\#(\mathcal{H}_L) = M_L$, to be the set of multiD interpolation points

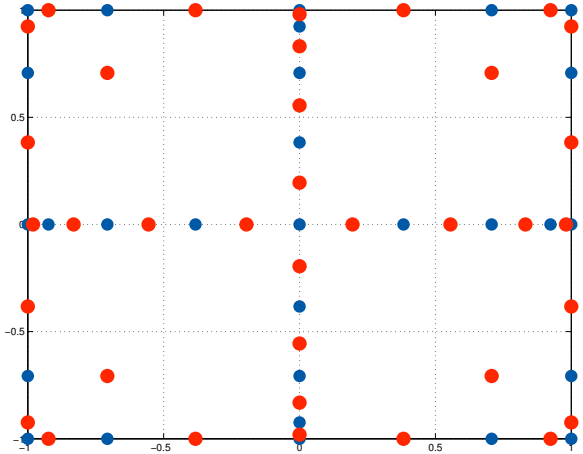
- **Tensor product:** $\mathcal{O}(M_L^{-r/N})$
- **Isotropic sparse grids:** $\mathcal{O}(M_L^{-r/\log(N)})$
  [Smolyak 1963; Nobile-Tempone-Webster 2008]
- **Anisotropic sparse grids:** $\mathcal{O}(M_L^{-r/G(\boldsymbol{\alpha},N)})$
  [Nobile-Tempone-Webster 2008]

Main idea: exploit the stochastic hierarchy

When nested sparse grids are used to construct a global Lagrange interpolant, we can solve the PDE at samples points in a hierarchical order (*i.e.*, proceed level by level), and construct coarse grid solutions at intermediate steps in the construction of the full interpolant.
Since we have to solve a linear system at each collocation sample point, we can use these intermediate solutions to provide strong preconditioners and good initial guesses for the iterative solver.



Solve $A_j \mathbf{c}_j = \mathbf{f}_j$
at all blue points
$\longrightarrow$
Interpolate to
accelerate
solution



Some Previous Work

Gordon, Powell. *Solving Stochastic Collocation with Algebraic Multigrid*

- Compare mean-based, full multigrid, and multigrid + recycled setup for preconditioning SC systems
- They also implement a "nearest neighbor" strategy for initial vectors

Gunzburger, Webster, Zhang. *Stochastic finite element methods for PDEs with random input data*

- Implement acceleration using local basis functions
- No significant additional cost for interpolation

Relationship to multilevel: Multilevel methods reduce the complexity of stochastic sampling methods by balancing errors across a sequence of stochastic and spatial approximations.

$$u_K^{(\mathrm{ML})} = \sum_{k=0}^{K} \mathcal{I}_{L_{K-k}} [u_{h_k} - u_{h_{k-1}}]$$

Construction of fully discrete solution

For a prescribed accuracy $\tau > 0$, the semi-discrete solution $u_h(x, \mathbf{y}_j)$ is approximated by

$$u_h(x, \mathbf{y}_j) = \sum_{i=1}^{N_h} c_{j,i}\varphi_i(x) \approx \widetilde{u}_h(x, \mathbf{y}_j) = \sum_{i=1}^{N_h} \widetilde{c}_{j,i}\varphi_i(x),$$

where

$$\widetilde{\mathbf{c}}_j = (\widetilde{c}_{j,1}, \ldots, \widetilde{c}_{j,N_h})^T$$

is the output of the solver satisfying $\|\mathbf{c}_j - \widetilde{\mathbf{c}}_j\|_{A_j} < \tau$.

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is the output of the solver satisfying $\|\mathbf{c}_j - \widetilde{\mathbf{c}}_j\|_{A_j} < \tau$. Our final approximation is given by :

$$\widetilde{u}_{h,L}(x, \mathbf{y}) := \sum_{j=1}^{M_L} \left(\sum_{i=1}^{N_h} \widetilde{c}_{j,i}\varphi_i(x) \right) \psi_{L,j}(\mathbf{y}).$$

Interpolated initial vectors

Convergence of CG for $A_j \mathbf{c}_j = \mathbf{f}_j$:

$$\|\mathbf{c}_j - \mathbf{c}_j^{(k)}\|_{A_j} \leq 2 \left(\frac{\sqrt{\kappa_j} - 1}{\sqrt{\kappa_j} + 1} \right)^k \|\mathbf{c}_j - \mathbf{c}_j^{(0)}\|_{A_j}$$

Improving the performance of the CG solver is a matter of either improving the condition number κ_j, or improving the initial guess $\mathbf{c}_j^{(0)}$.

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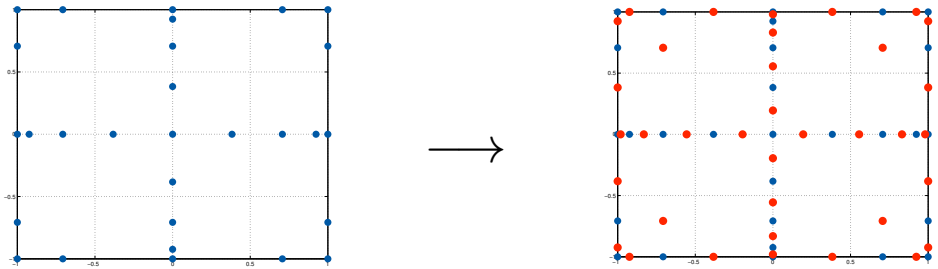

Specifically, assume we have solved for each the vectors $\widetilde{\mathbf{c}}_m$, $m = 1, \ldots, M_{L-1}$. Then for any new point $\mathbf{y}_j \in \Delta\mathcal{H}_L$, a good approximation to $\mathbf{c}_j$ is given by

$$\mathbf{c}_j^{(0)} = \sum_{m=1}^{M_{L-1}} \widetilde{\mathbf{c}}_m \psi_{L-1,m}(\mathbf{y}_j).$$

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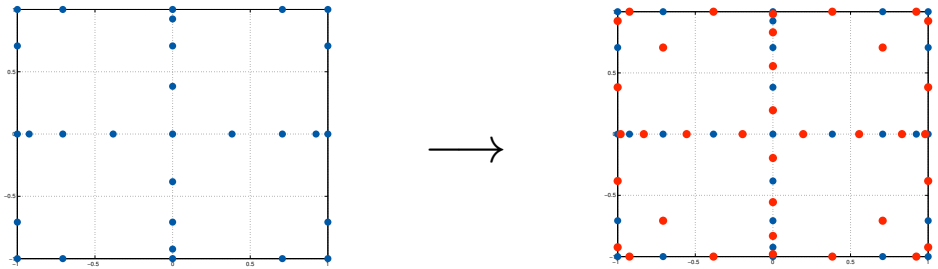

Alternatively, suppose we have constructed strong preconditioners $\mathbf{P}_m$, $m = 1, \ldots, M_{L-1}$. Then for any new point $\mathbf{y}_j \in \Delta\mathcal{H}_L$,

$$\mathbf{P}_j = \sum_{m=1}^{M_{L-1}} \mathbf{P}_m \psi_{L-1,m}(\mathbf{y}_j).$$

The total error $e = u(x, y) - \tilde{u}_{h,M_L}(x, \mathbf{y})$ can be split into

$$\|e\| \leq \underbrace{\|u - u_h\|}_{e_1} + \underbrace{\|u_h - u_{h,M_L}\|}_{e_2} + \underbrace{\|u_{h,M_L} - \tilde{u}_{h,M_L}\|}_{e_3 (\text{solver error})}$$

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Sufficient conditions to achieve overall error $\leq \varepsilon$:

$$\|e_1\| \leq C_1 \, h^s \leq \frac{\varepsilon}{3}$$
$$\|e_2\| \leq C_2(N) \, e^{-\sigma(N)L} \leq \frac{\varepsilon}{3}$$
$$\|e_3\| \leq C_3 \, \Lambda_L \, e_{\text{cg}} \leq \frac{\varepsilon}{3}$$

Here s, $\sigma(N)$ are the convergence rates of the FEM and interpolation methods, Λ_L is the Lebesgue constant, and

$$e_{CG} = \max_{\mathbf{y}_j \in \mathcal{H}_L} \|\mathbf{c}_j - \tilde{\mathbf{c}}_j\|_{A_j}$$

Iteration Estimate: Zero Vectors

Theorem: [Galindo, J, Webster, Zhang]

Given $\varepsilon > 0$, the total number of CG iterations needed to achieve an error $\|u - \tilde{u}_{h,M_L}\| < \varepsilon$ using zero initial vectors is bounded by:

$$K_{zero} \leq \alpha_1(N)\, \varepsilon^{\frac{-\ln 2}{\sigma}} \left\{\alpha_2(N) + \alpha_3 \ln \varepsilon^{-1}\right\}^{N-1} \times \sqrt{\bar{\kappa}} \left\{\ln \varepsilon^{-1} + \ln \Lambda_L + \alpha_4(N)\right\}$$

where $\bar{\kappa} = \max_{\mathbf{y} \in \mathcal{H}_L} \bar{\kappa}(\mathbf{y})$.

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where $\bar{\kappa} = \max_{\mathbf{y} \in \mathcal{H}_L} \bar{\kappa}(\mathbf{y})$.

The first line (in blue) comes from the number of collocation nodes, which we can't affect by our algorithm. The second part comes from the convergence of the CG algorithm, which for fine grid points we can reduce by a log factor (in red).

Iteration Estimate: Accelerated Case

Theorem: [Galindo, J, Webster, Zhang]

Given $\varepsilon > 0$, the total number of CG iterations needed to achieve an error $\|u - \tilde{u}_{h,M_L}\| < \varepsilon$ using the hierarchically accelerated stochastic collocation algorithm is bounded by:

$$K_{acc} \leq \alpha_1(N)\, \varepsilon^{\frac{-\ln 2}{\sigma}} \left\{\alpha_2(N) + \alpha_3 \ln \varepsilon^{-1}\right\}^{N-1} \times \sqrt{\bar{\kappa}} \left\{\ln \Lambda_L + \alpha_5(N)\right\}$$

where $\bar{\kappa} = \max_{\mathbf{y} \in \mathcal{H}_L} \bar{\kappa}(\mathbf{y})$.

To perform this method, we incur an addition cost of interpolation (and preconditioning).

Example 1: **Local** Basis for Sparse Grid SC

Consider the 2D Poisson equation with random diffusivity and forcing term, i.e.,

$$\begin{cases} -\nabla \cdot (a(x,\mathbf{y})\nabla u(x,\mathbf{y})) &= f(x,\mathbf{y}) \quad [0,1]^2 \times \Gamma \\ u(\mathbf{x},\mathbf{y}) &= 0 \quad \text{on } \partial D \times \Gamma \end{cases}$$

where a and f are the nonlinear functions of the random vector $\mathbf{y}$ given by

$$a(x,\mathbf{y}) = 0.1 + \exp\left[y_1 \cos(\pi x_1) + y_2 \sin(\pi x_2)\right],$$

and

$$f(x,\mathbf{y}) = 10 + \exp\left[y_3 \cos(\pi x_1) + y_4 \sin(\pi x_2)\right],$$

- y_n, $n = 1,2,3,4$, are i. i. d. random variables following the uniform distribution $U([-1,1])$
- The quantity of interest is the mean value of the solution over $D \times \Gamma$, i.e.

$$\text{QoI} = \mathbb{E}\left[\int_D u(x,\mathbf{y})dx\right]$$

Computational savings: Local Basis

Gunzburger, Webster, Zhang. **Stochastic finite element methods for PDEs with random input data**, 2014 *Acta Numerica*

Table: The computational savings of the local SG with hierarchical acceleration

Basis type	Error	# SG points	hSGSC cost	hSGSC+acceleration	
				cost	saving
Linear	1.0e-2	377	13,841	7,497	45.8%
	1.0e-3	1,893	81,068	38,670	52.2%
	1.0e-4	7,777	376,287	167,832	55.3%
Quadratic	1.0e-3	701	29,874	11,877	60.2%
	1.0e-4	2,285	110,744	36,760	66.8%
	1.0e-5	6,149	329,294	100,420	69.5%
Cubic	1.0e-4	1,233	59,344	23,228	60.8%
	1.0e-5	3,233	172,845	57,777	66.5%
	1.0e-6	7,079	415,760	129,433	68.8%

Example 2: Global Basis w/ Error Balancing

We consider a 1D Poisson equation with random diffusivity term:

$$\nabla \cdot (a(x, \mathbf{y}) \nabla u(x, \mathbf{y})) = 10 \text{ in } [0, 1] \times \Gamma$$
$$u(x, \mathbf{y}) = 0 \text{ on } \partial D \times \Gamma$$

with

$$a(x, \mathbf{y}) = 1 + \exp\left\{\exp^{-1/8}(y_1 \cos \pi x + y_2 \sin \pi x + y_3 \cos 2\pi x + y_4 \sin 2\pi x)\right\}$$

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Error	#SG Pts	CG iters	CG + acc	% Savings
1×10^{-2}	137	29,355	22,219	24.3
5×10^{-3}	401	180,087	90,300	49.9
1×10^{-3}	1105	2,072,625	696,935	66.4
5×10^{-4}	2929	11,253,264	2,217,615	80.3
1×10^{-4}	7537	118,429,119	16,204,912	86.3

Table: Iterations and savings between the hierarchically acclerated SG method and the zero vector method

Computed Cost

A Metric for Computational Cost

Zero Vectors: $Cost_{\text{zero}} = C_D N_h K_{\text{zero}}$

Acceleration: $Cost_{\text{acc}} = C_D N_h K_{\text{acc}} + Cost_{\text{int}}$

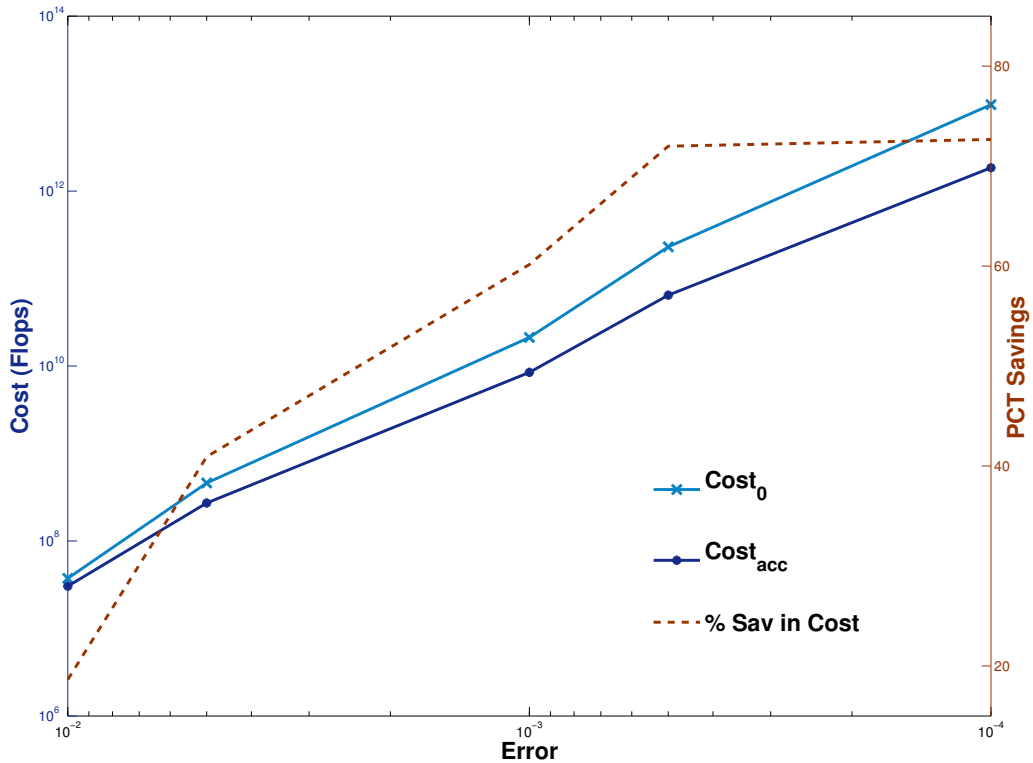

Figure: Cost (left axis) and percent savings (right axis) in flops of the hierarchically accelerated SG method versus the zero vector method.

Example 3: Global Basis w/ Interpolated Preconditioners

Let $\mathbf{x} = (x_1, x_2)$ and consider the following linear elliptic SPDE:

$$\begin{cases} -\nabla \cdot (a(x_1, \mathbf{y}(\omega)) \nabla u(\mathbf{x}, \mathbf{y}) &= \cos(x_1)\sin(x_2) & [0,1]^2 \times \Gamma \\ u(\mathbf{x}, \mathbf{y}) &= 0 & \text{on } \partial D \times \Gamma \end{cases}$$

The diffusion coefficient is a 1d random field (varies only in x_1) and is $a(x_1, \mathbf{y}) = 0.5 + \exp\{\gamma(x_1, \mathbf{y})\}$, where γ is a truncated random field with correlation length R and covariance

$$Cov[\gamma](x_1, \tilde{x}_1) = \exp\left(-\frac{(x_1 - \tilde{x}_1)^2}{R^2}\right), \quad \forall (x_1, \tilde{x}_1) \in [0,1]$$

$$\gamma(x_1, \mathbf{y}) = 1 + y_1(\omega)\left(\frac{\sqrt{\pi}R}{2}\right)^{1/2} + \sum_{n=2}^{N} \beta_n \, \varphi_n(x_1) \, y_n(\omega)$$

$$\beta_n := \left(\sqrt{\pi}R\right)^{1/2} e^{\frac{-\left(\lfloor \frac{n}{2} \rfloor \pi R\right)^2}{8}}, \quad \varphi_n(x_1) := \begin{cases} \sin\left(\lfloor \frac{n}{2} \rfloor \pi x_1\right), & \text{if } n \text{ even}, \\ \cos\left(\lfloor \frac{n}{2} \rfloor \pi x_1\right), & \text{if } n \text{ odd} \end{cases}$$

- $\mathbb{E}[y_n] = 0$ and $\mathbb{E}[y_n y_m] = \delta_{nm}$ for $n, m \in \mathbb{N}_+$ and iid in $U(-\sqrt{3}, \sqrt{3})$

2D example: Iterations vs Level

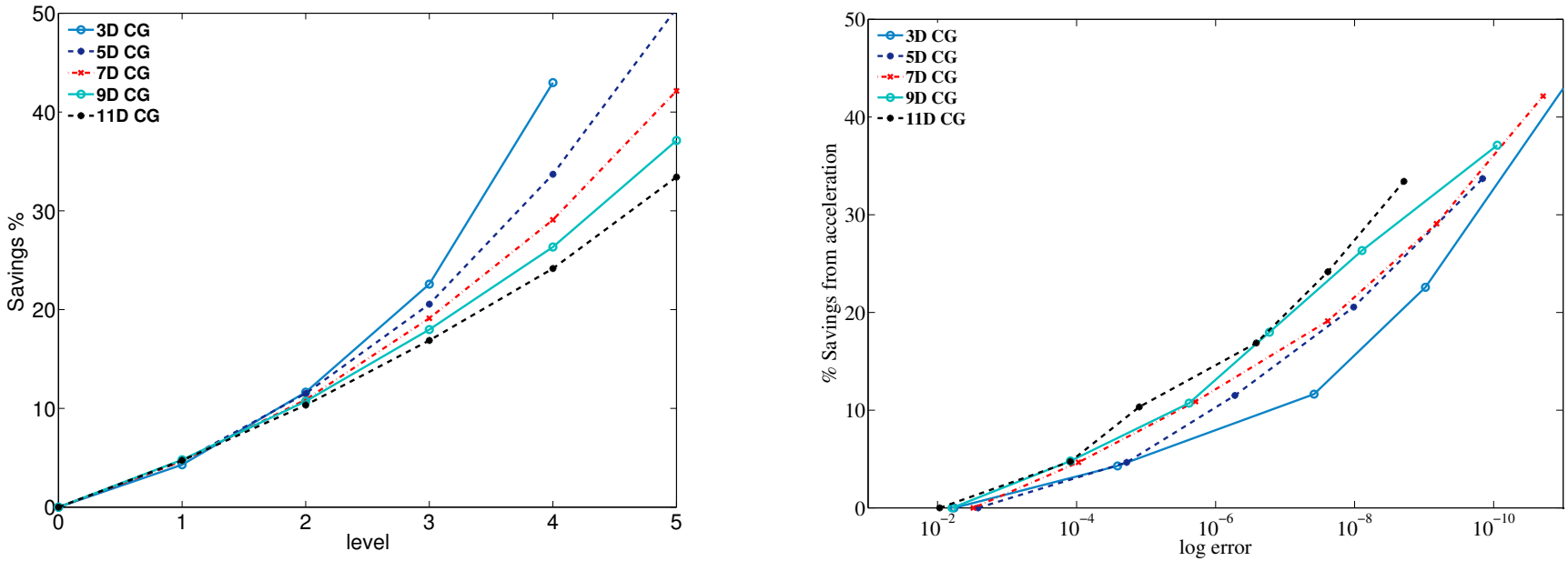

Figure: Percentage reduction in CG iterations per level (left) and vs error (right) with $N = 3, 5, 7, 9, 11$ and 13 and for correlation length $R_c = 1/2$

Preconditioning

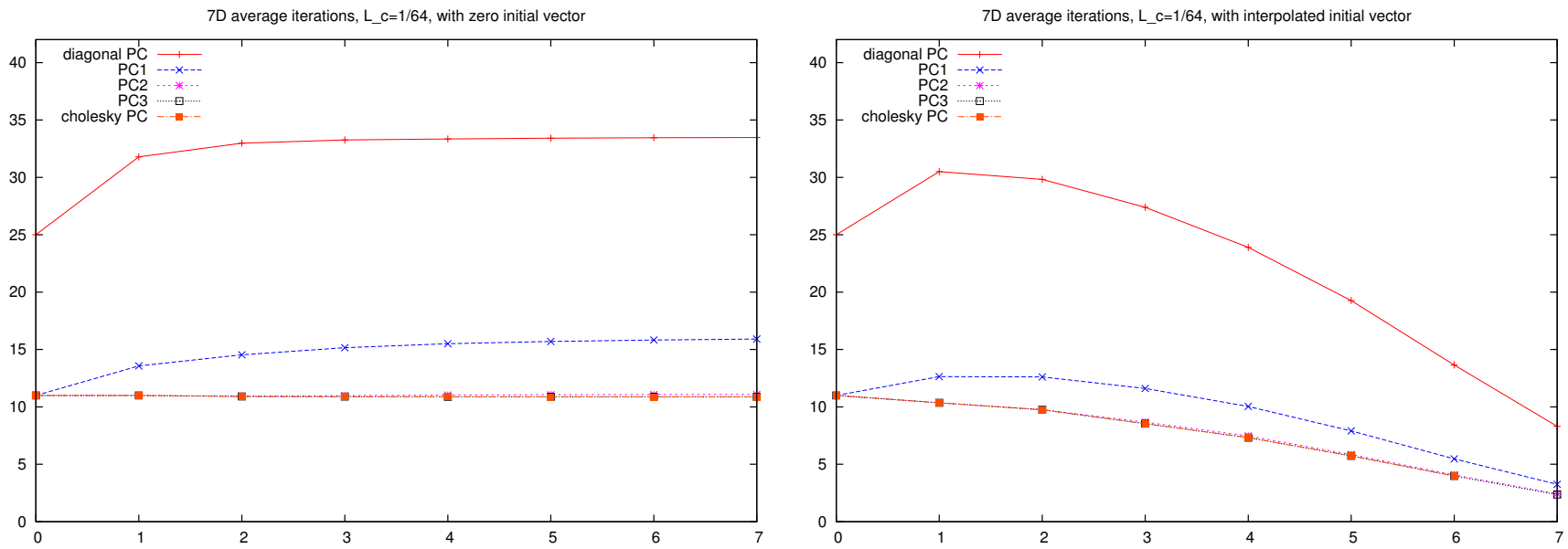

Figure: Average CG iterations per level for $N = 7$ for $L = 1/64$, with zero initial vectors (left) and with accelerated initial vectors(right), for preconditioning options: diagonal preconditioner, 1-3 level interepolated incomplete Cholesky preconditioner, and fully locally adapted incomplete Cholesky preconditioner

Example 4: $-\nabla(a \cdot \nabla u) + F(u) = f$

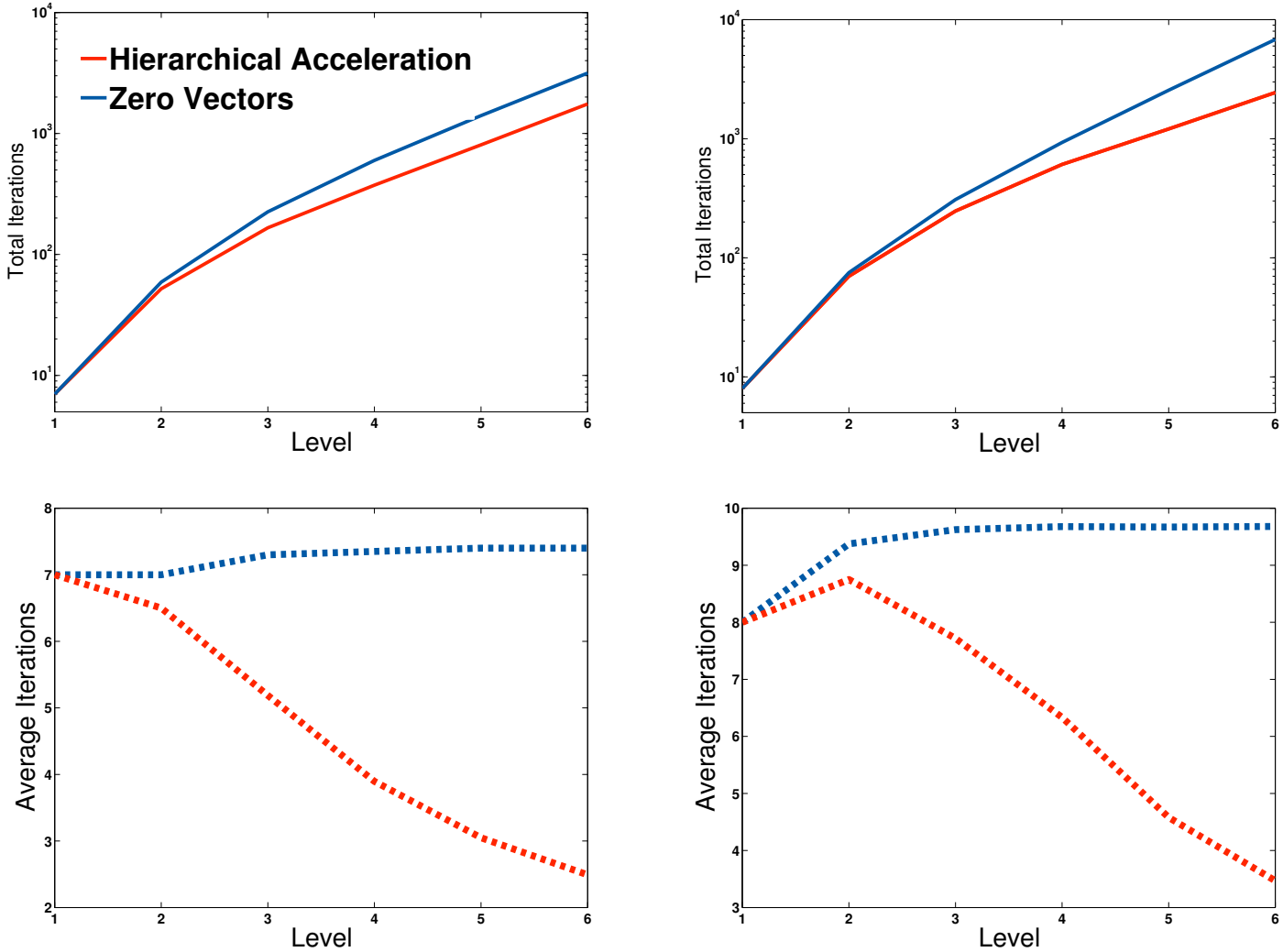

Figure: Total (top) and average (bottom) number of Newton iterations with $F(u) = u * u'$ (left) and $F(u) = u^5$ (right)

Remarks

- Acceleration works together with preconditioning to speed up solvers.
- Especially effective for more complicated or non-linear PDEs
- Improves efficiency of iterative solvers even with the additional cost of interpolation

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