



Adaptive Stochastic Galerkin FEM with Hierarchical Tensor Representations

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Elliptic BVP with $u(x, y) \in \mathcal{V} := \mathcal{X} \otimes \mathcal{Y} := H_0^1(D) \otimes L_\pi^2(\Gamma)$

$$-\nabla \cdot (a(x, y) \nabla u(x, y)) = f(x) \quad \text{in } D \times \Gamma \quad \text{and} \quad u(x)|_{\partial D} = 0$$

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on Lipschitz $D \subset \mathbb{R}^d$. Expansion of random field a

$$a(x, y) = a_0 + \sum_{m=1}^{\infty} a_m(x) y_m$$

with independent and uniformly distributed random variables

$$y = (y_m)_{m=1}^{\infty} \in \Gamma := [-1, 1]^{\infty}, \quad \pi = \bigotimes_{m=1}^{\infty} \pi_m$$

$$(UEC) \quad \sum_{m=1}^M \left\| \frac{a_m}{a_0} \right\|_{L^\infty(D)} < 1, \quad a_0 > 0, \quad a_0, a_0^{-1} \in L^\infty(D)$$

Discretisation with (i) P_k conforming FEM in \mathcal{X}
and (ii) orthogonal polynomials in \mathcal{Y}

- \rightarrow very high dimensional coupled system
(*curse of dimensionality* w.r.t. parameter dimensions)
- reduction of computational complexity necessary
- some approaches:
 - sampling or interpolation
 - a priori or a posteriori adaptivity
 - model order reduction (RBM, low-rank tensors)

Piecewise **polynomials of degree p** on mesh \mathcal{T} of D
 \rightarrow FEM space $\mathcal{X}_p(\mathcal{T}) := \text{span}\{\varphi_i\}_{i=0}^{N-1} \subset \mathcal{X}$

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Tensorised **Legendre polynomials**

$$\mu \in \mathcal{F} := \{\mu \in \mathbb{N}_0^\infty : |\text{supp } \mu| < \infty\} : P_\mu(y) := \prod_{m \in \text{supp } \mu} P_{\mu_m}(y_m)$$

→ $(P_\mu)_{\mu \in \mathcal{F}}$ is orthonormal basis of $\mathcal{Y} := L^2_\pi(\Gamma) = \bigotimes_{m=1}^\infty L^2_{\pi_m}(\Gamma_m)$

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(Finite) **index set $\Lambda \subset \mathcal{F}$** determines discrete approximation

$u_N \in \mathcal{V}_N := \mathcal{X}_p \otimes \text{span}\{P_\mu\}_{\mu \in \Lambda} \subset \mathcal{V}$

$$\rightarrow u_N(x, y) = \sum_{\mu \in \Lambda} u_{N,\mu}(x) P_\mu(y), \quad (u_{N,\mu})_{\mu \in \Lambda} \in \prod_{\mu \in \Lambda} \mathcal{X}_p(\mathcal{T})$$

where coefficients $u_{N,\mu}$ are s.t.

$$\mathbb{E}_\pi[\langle u_N, v \rangle_A] = \mathbb{E}_\pi[\langle f, v \rangle] \quad (v \in \mathcal{V}_N)$$

Define operators

$$A = \sum_{m=0}^{\infty} A_m \quad \text{and} \quad A_m v := -\nabla \cdot (a_m \nabla v)$$

with

$$A : v \mapsto -\nabla \cdot (a(x, y) \nabla v).$$

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Expansion $u(x, y) = \sum_{\mu \in \mathcal{F}} u_{\mu}(x) P_{\mu}(y)$ holds with

$$A_0 u_{\mu} + \sum_{m=1}^{\infty} A_m (\beta_{\mu_m+1} u_{\mu+\epsilon_m} + \beta_{\mu_m} u_{\mu-\epsilon_m}) = f \delta_{\mu 0} \quad (\mu \in \Lambda)$$

due to $y_m P_{\mu}(y) = \beta_{\mu_m+1} P_{\mu+\epsilon_m}(y) + \beta_{\mu_m} P_{\mu-\epsilon_m}(y)$.

Assume we can determine important stochastic modes.

→ Construct as small a set $\Lambda \subset \mathcal{F}$ as possible.

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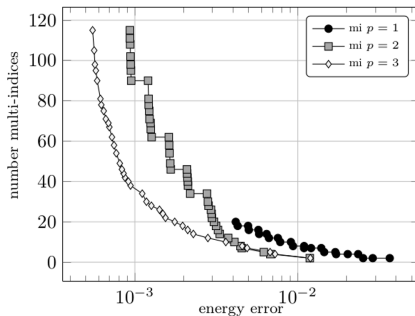
→ Construct as small a set $\Lambda \subset \mathcal{F}$ as possible.

- operator construction *on the fly*
- separate meshes per stochastic dimension [EGSZ1]
- single mesh higher-order FEM [EGSZ2]

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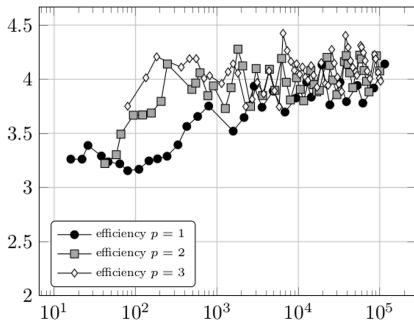
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- guaranteed error control [EM]



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- still choose set adaptively¹
 - number dimensions M
 - anisotropic polynomial degrees d_1, \dots, d_M
- however: employ full tensor set

$$\Lambda := \{(\mu_1, \dots, \mu_M, 0, \dots) \in \mathcal{F} \mid \mu_m = 0, \dots, d_m - 1; m = 1, \dots, M\}$$

which grows exponentially in M (curse of dimensionality)

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→ tensor structure of problem has to be exploited

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Stochastic solution field can be written as

$$u_N(x, y) = \sum_{i=0}^{N-1} \sum_{\mu \in \Lambda} U(i, \mu) \varphi_i(x) P_\mu(y)$$

with coefficient tensor $U \in \mathbb{R}^{N \times d_1 \times \dots \times d_M}$ determined by

$$A(U) := \left(\sum_{m=0}^M A_m \right) (U) = F$$

where

$$A_m = K_m \otimes I \otimes \dots \otimes B_m \otimes \dots \otimes I$$
$$F = f \otimes e_1 \otimes \dots \otimes e_1$$

Problem has a natural tensor structure

$$A_m(i, \mu, j, \nu) = \int_D a_m(x) \nabla \varphi_i \cdot \nabla \varphi_j \, dx \int_{-1}^1 P_{\mu_1} P_{\nu_1} \, dy_1 \cdots \\ \cdots \int_{-1}^1 y_m P_{\mu_m} P_{\nu_m} \, dy_m \cdots \int_{-1}^1 P_{\mu_M} P_{\nu_M} \, dy_M$$

→ high-order tensor representations

$$A_m = K_m \otimes I \otimes \dots \otimes B_m \otimes \dots \otimes I$$


with

$$K_m(i, j) = \int_D a_m(x) \nabla \varphi_i \cdot \nabla \varphi_j \, dx \\ B_m(\mu_m, \nu_m) = \int_{-1}^1 y_m P_{\mu_m} P_{\nu_m} \, dy_m$$

For the tensor

$$U \in \mathbb{R}^{N \times d_1 \times \dots \times d_M}, \quad U(i, \mu) = \mathcal{U}(i_0, i_1, \dots, i_M)$$

we obtain the **TT representation** (SVD separated decomposition)

$$\underbrace{\mathcal{U}(i_0, i_1, \dots, i_M)}_{=\mu} = \sum_{k_1=1}^{r_1} \cdots \sum_{k_M=1}^{r_M} U_0(i_0, k_1) U_1(k_1, i_1, k_2) \cdots U_M(k_M, i_M)$$


$$= U_0(i_0) U_1(i_1) \cdots U_M(i_M)$$

i.e. a “separation of variables” with $U_m \in \mathbb{R}^{r_m \times d_m \times r_{m+1}}$ and $U_m(i_m) \in \mathbb{R}^{r_m \times r_{m+1}}$.

For $u_N = \sum_{i=0}^{N-1} \sum_{\mu \in \Lambda} U(i, \mu) \varphi_i P_\mu \in \mathcal{V}_N$,

$$U(i, \mu_1, \dots, \mu_M) = \sum_{k_1=1}^{r_1} \cdots \sum_{k_{M+1}=1}^{r_{M+1}} U_0(i, k_1) \prod_{m=1}^M U_m(k_m, \mu_m, k_{m+1}).$$

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Expectation is determined by

$$\begin{aligned} \mathbb{E}(u_N) &= \int_{\Gamma} u_N(y) \, d\pi(y) \\ &= \sum_{i=0}^{N-1} \sum_{\mu \in \Lambda} U(i, \mu) \varphi_i \prod_{m=1}^M \int_{-1}^1 P_{\mu_m}(y_m) \, d\pi(y_m) \\ &= \sum_{i=0}^{N-1} U(i, 1, \dots, 1) \varphi_i. \end{aligned}$$

Thm. [EGSZ]: Energy error bound w.r.t. some $w_N \in \mathcal{V}_p(\Lambda; \mathcal{T})$ and Galerkin approximation $u_N \in \mathcal{V}_p(\Lambda; \mathcal{T})$ of exact solution u

$$\|w_N - u\|_{\mathcal{A}} \lesssim \underbrace{\eta(w_N, \Lambda, \mathcal{T})}_{\text{approximation}} + \underbrace{\zeta(w_N, \partial\Lambda)}_{\text{tail}} + \underbrace{\|w_N - u_N\|_{\mathcal{A}}}_{\text{consistency}}$$

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with estimators

$$\eta_{\mu}(w_N)^2 := \sum_{T \in \mathcal{T}} \eta_{\mu, T}(w_N)^2 + \sum_{S \in \mathcal{S}} \eta_{\mu, S}(w_N)^2$$

$$\eta_{\mu, T}(w_N) := h_T \|a_0^{-1/2} (f \delta_{\mu 0} + \nabla \cdot \sigma_{\mu}(w_N))\|_{L^2(T)}$$

$$\eta_{\mu, S}(w_N) := h_S^{1/2} \|a_0^{-1/2} \llbracket \sigma_{\mu}(w_N) \rrbracket_S\|_{L^2(S)}$$

$$\zeta_{\nu}(w_N) := \sum_{m=1}^{\infty} \left\| \frac{a_m}{a_0} \right\|_{L^{\infty}(D)} \left(\beta_{\nu_m+1} \|w_{N, \nu+\epsilon_m}\|_{\mathcal{X}} + \beta_{\nu_m} \|w_{N, \nu-\epsilon_m}\|_{\mathcal{X}} \right)$$

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$$\|w_N - u\|_{\mathcal{A}} \lesssim \eta(w_N, \Lambda, \mathcal{T}) + \zeta(w_N, \partial\Lambda) + \|w_N - u_N\|_{\mathcal{A}}$$

adaptive algorithm (single iteration)

- evaluate solution w_N in TT format by ALS
- evaluate error bounds $\eta(u_N, \Lambda, \mathcal{T})$ and $\zeta(u_N, \partial\Lambda)$
- **spatial** refinement if η dominates \rightarrow **refine mesh** \mathcal{T}
- **stochastic** refinement if ζ dominates \rightarrow **enlarge active set** Λ
- **tensor upgrade** if consistency error dominates
 \rightarrow **increase TT rank**

All estimators (approximation, tail, algebraic) can be evaluated efficiently in TT format, e.g.,

$$\begin{aligned}
 \sum_{\mu \in \Lambda} \eta_{\mu, T}(w_N)^2 &:= \sum_{\mu \in \Lambda} h_T^2 \|a_0^{-1/2} (f \delta_{\mu 0} + \nabla \cdot \sigma_{\mu}(w_N))\|_{L^2(T)}^2 \\
 &= \sum_{\mu \in \Lambda} h_T^2 \langle f \delta_{\mu 0} + \nabla \cdot \sigma_{\mu}(w_N), a_0^{-1} (f \delta_{\mu 0} + \nabla \cdot \sigma_{\mu}(w_N)) \rangle_T \\
 &= h_T^2 (\langle f \delta_{\mu 0}, a_0^{-1} f \rangle_T + 2 \langle f \delta_{\mu 0}, a_0^{-1} \nabla \cdot \sigma_0(w_N) \rangle_T \\
 &\quad + \sum_{\mu \in \Lambda} \langle \nabla \cdot \sigma_{\mu}(w_N), a_0^{-1} \nabla \cdot \sigma_{\mu}(w_N) \rangle_T)
 \end{aligned}$$

for $w_N = \sum_{i=0}^{N-1} \sum_{\mu \in \Lambda} W(i, \mu) \varphi_i P_{\mu} \in \mathcal{V}_N(\Lambda; \mathcal{T})$ with numerical flux

$$\sigma_{\mu}(w_N) = a_0 \nabla w_{N, \mu} + \sum_{m=1}^M a_m \nabla (\beta_{\mu_m+1} w_{N, \mu+\epsilon_m} + \beta_{\mu_m} w_{N, \mu-\epsilon_m})$$

On any $T \in \mathcal{T}$,

$$\begin{aligned} & \sum_{\mu \in \Lambda} \langle \nabla \cdot \sigma_{\mu}(w_N), a_0^{-1} \nabla \cdot \sigma_{\mu}(w_N) \rangle \\ &= \sum_{m_1, m_2=0}^M \sum_{i, j=0}^{N-1} \langle \nabla \cdot (a_{m_1} \nabla \varphi_i), a_0^{-1} \nabla \cdot (a_{m_2} \nabla \varphi_j) \rangle_T \sum_{\mu \in \Lambda} W^{m_1}(i, \mu) W^{m_2}(j, \mu) \end{aligned}$$

with TT tensors $W^m := [I_0 \otimes I_1 \otimes \cdots \otimes B_m \otimes \cdots \otimes I_M](W)$.

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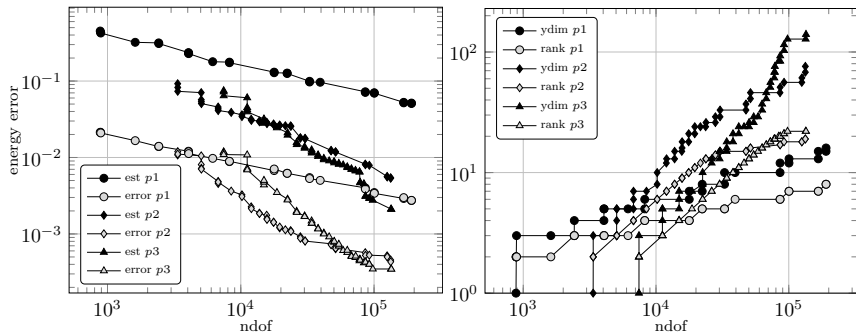
$$\begin{aligned} & \sum_{\mu \in \Lambda} \langle \nabla \cdot \sigma_{\mu}(w_N), a_0^{-1} \nabla \cdot \sigma_{\mu}(w_N) \rangle \\ &= \sum_{m_1, m_2=0}^M \sum_{i, j=0}^{N-1} \langle \nabla \cdot (a_{m_1} \nabla \varphi_i), a_0^{-1} \nabla \cdot (a_{m_2} \nabla \varphi_j) \rangle_T \sum_{\mu \in \Lambda} W^{m_1}(i, \mu) W^{m_2}(j, \mu) \end{aligned}$$

with TT tensors $W^m := [I_0 \otimes I_1 \otimes \cdots \otimes B_m \otimes \cdots \otimes I_M](W)$.

Another low-rank decomposition yields

$$= \sum_{m_1, m_2=0}^M \sum_{k_1=1}^{r_1} \langle \nabla \cdot (a_{m_1} \sum_{i=0}^{N-1} \nabla \varphi_i V^{m_1, m_2}(i, k_1)), a_0^{-1} \nabla \cdot (a_{m_2} \sum_{j=0}^{N-1} \nabla \varphi_j) W_0(j, k_1) \rangle_T.$$

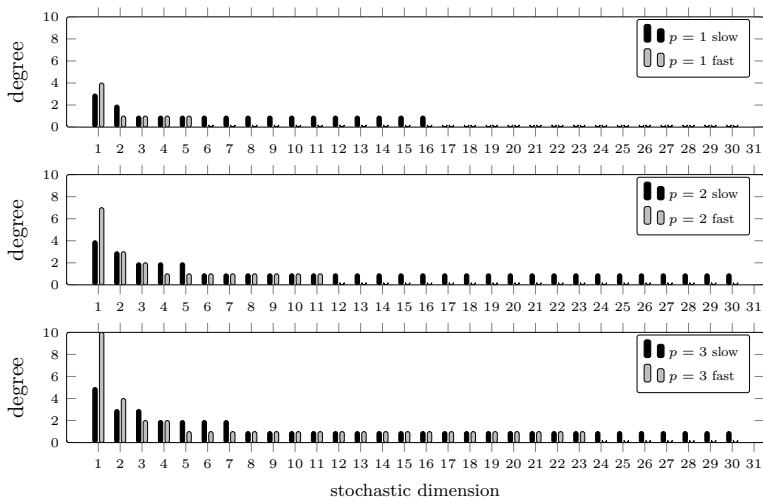
All other estimator terms can be treated similarly.



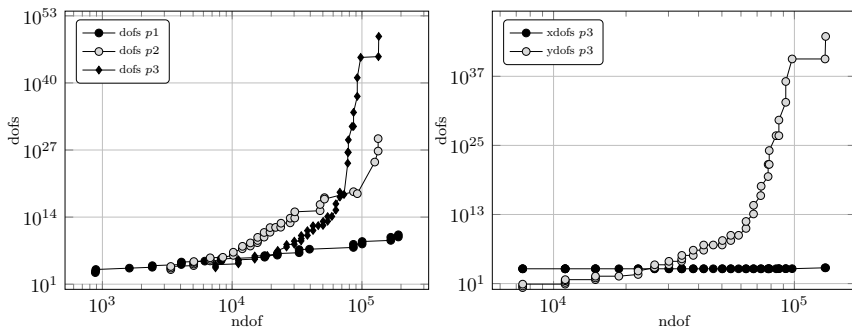
(estimator, energy error (left) and stochastic dimensions, TT rank (right))

With random coefficient $a(x, y) := a_0 + \sum_{m=1}^{\infty} a_m(x) y_m$

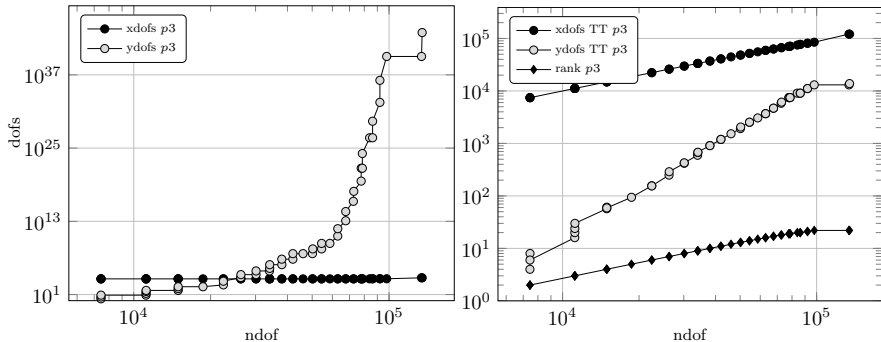
$$a_m(x) := \alpha m^{-2} \cos(2\pi\beta_1(m)x_1) \cos(2\pi\beta_2(m)x_2)$$



(anisotropic gpc degrees per stochastic dimension)



(full overall problem size (left) and dofs of χ and \mathcal{Y} (right))



(dofs of \mathcal{X} and \mathcal{Y} (left) and in TT format (right))

[EPS] E, M. Pfeffer and R. Schneider,

Adaptive stochastic Galerkin FEM with hierarchical tensors (2015).

[EM] E and C. Merdon,

Local higher-order equilibration for guaranteed error control in adaptive stochastic Galerkin FEM (2014).

[EGSZ2] E, C.J. Gittelsohn, C. Schwab and E. Zander,

Convergent higher-order adaptive stochastic Galerkin FEM (2014).

[EGSZ1] E, C.J. Gittelsohn, C. Schwab and E. Zander,

Adaptive stochastic Galerkin FEM (2014).