AGUQ Dortmund
12.3 - 14.3 2018

Bayesian Inversion and Adaptive Low-Rank Tensor Decomposition

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We present a Bayesian inversion method with functional representations of all quantities. The posterior density is given in terms of a polynomial basis, based on an adaptive stochastic Galerkin discretization. The sampling-free approach, using tensor trains, alleviates the curse of dimensionality by hierarchical subspace approximations of the respective low-rank manifolds. All computations are adjusted adaptively based on a posteriori error estimators or indicators. Convergence of the posterior can be shown with respect to the discretization parameters.

Explicit and parametric Bayesian inversion

- applies in **parameter identification** and **upscaling**
- **parametrized** model operator $\Xi \ni y \mapsto G(\mathbf{y}) = \sum_{\mu\in\Lambda} g_\mu(x)\mathbf{P}_\mu(\mathbf{y}), \quad g_\mu = \langle G, \mathbf{P}_\mu\rangle$
- finite measurements $\delta \in \mathbb{R}^K$ of indirect quantity, observed by linear operator $\mathcal{O}$
- prior measure π_0 on parameters y and noise measure $\mathcal{N}(0,\Gamma)$ on measurement error η

Statistical **inverse problem:** Find $\mathbf{y}\in\Xi$ from δ s.t. $\delta = (\mathcal{O}\circ G)(\mathbf{y}) + \eta, \quad \eta\sim\mathcal{N}(0,\Gamma)$
Bayes' theorem yields existence of posterior measure π_δ in functional representation [1]:

$$\frac{\mathrm{d}\pi_\delta}{\mathrm{d}\pi_0}(\mathbf{y}) = \mathbb{E}_{\pi_\delta}[1]^{-1}\exp\left(-\frac{1}{2}\langle\delta - (\mathcal{O}\circ G)(\mathbf{y}), \Gamma^{-1}(\delta - (\mathcal{O}\circ G)(\mathbf{y}))\rangle\right) = \sum_{\mu\in\Lambda'} \alpha_\mu \mathbf{P}_\mu(\mathbf{y}).$$

Model reduction: Tensor formats

- **high dimensional** problem, curse of dimensionality: $O\left(n^M\right)$
- **HT/TT** allows for polynomial complexity: $O(r^2 M n)$ via

$$\mathbf{U}[x_1,\dots,x_M] = \sum_{\mathbf{k}}^{\mathbf{r}} \prod_{m=1}^{M} U_m[k_{m-1}, x_m, k_m]$$

- **Features**:
  - + separation of variables and closedness of rank $\mathbf{r}$ manifold,
  - − indirect access to tensor elements by **hierarchical basis**
- **Creation** by tensor recovery/reconstruction [2] or cross-approximation

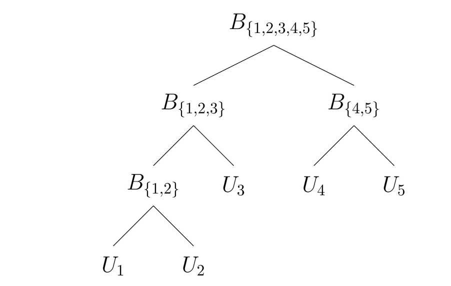


Figure: dimension partition tree

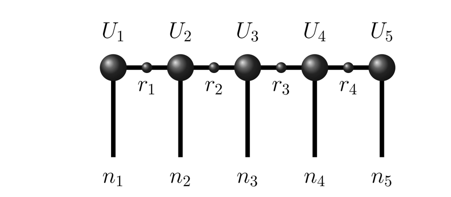


Figure: schematical tensor train (TT) tree of order 5 with subspaces, dimensions, ranks

Adaptive Stochastic Galerkin FEM using Tensor Trains

- random coefficient, parametrized and represented in functional/extended tensor train format

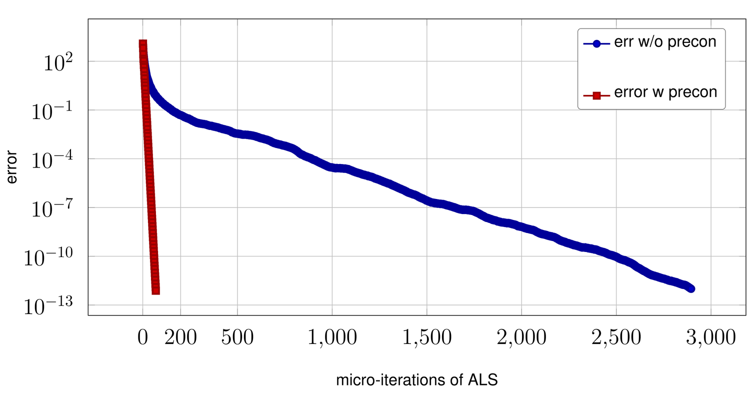
$$a(x,\mathbf{y}) = \sum_{\mathbf{k}}^{\mathbf{r}} \sum_{i=1}^{N_a} A_0[i,k_0]\varphi_i(x) \prod_{m=1}^{M} \sum_{\mu_m=1}^{n_m} A_m[k_{m-1},\mu_m,k_m] P_{\mu_m}(y_m), \quad (P_{\mu_m})_{\mu_m} \text{ polynomial basis}$$

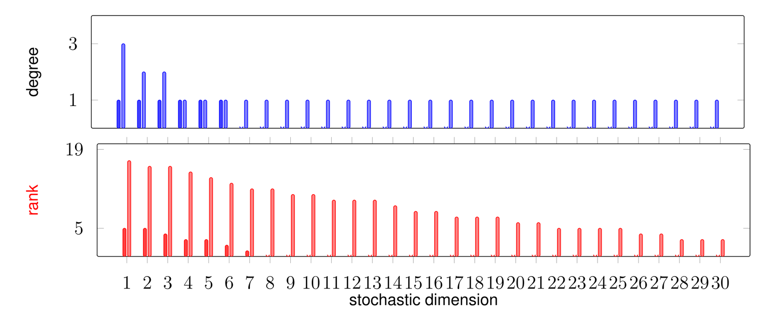
- weak PDE formulation obtained using tensor train operators and system solved by preconditioned ALS

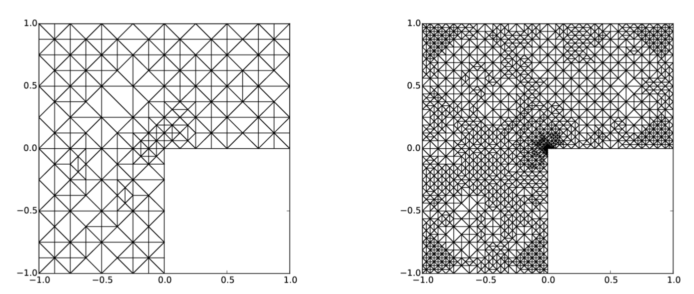
$$\mathcal{A}(u_N, v) := \mathbb{E}\left[\langle u_N, v\rangle_a\right] = \mathbb{E}\left[\langle f, v\rangle\right], \quad \forall v\in\mathcal{V}_N, \quad u_N \text{ Galerkin solution}$$

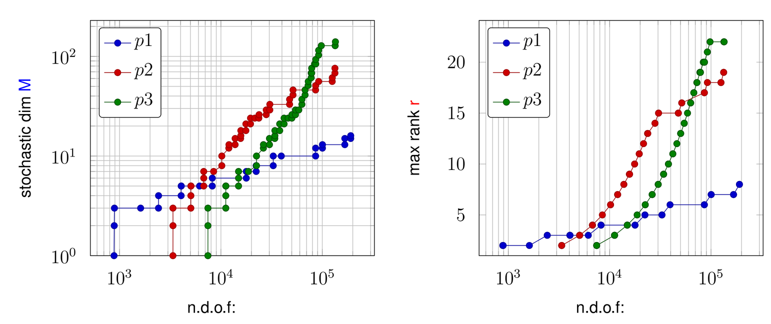
- A-posteriori adaptivity in *physical mesh*, *stochastic polynomial space* and choice of *rank* $\mathbf{r}$, see [3]

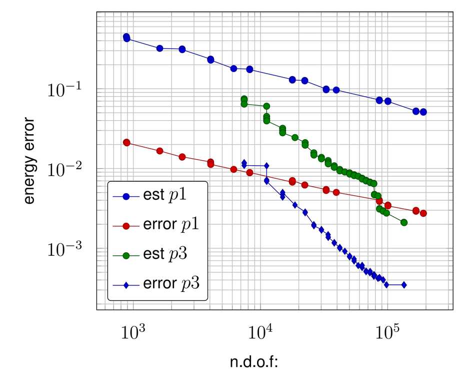
$$\|u - w_N\|_{\mathcal{A}}^2 \lesssim \mathrm{est}_{\mathrm{all}}(w_N) := \left(\mathrm{est}_{\mathrm{det}}(w_N) + \mathrm{est}_{\mathrm{param}}(w_N) + \mathrm{est}_{\mathrm{disc}}(w_N)\right)^2 + \mathrm{est}_{\mathrm{disc}}(w_N)^2$$











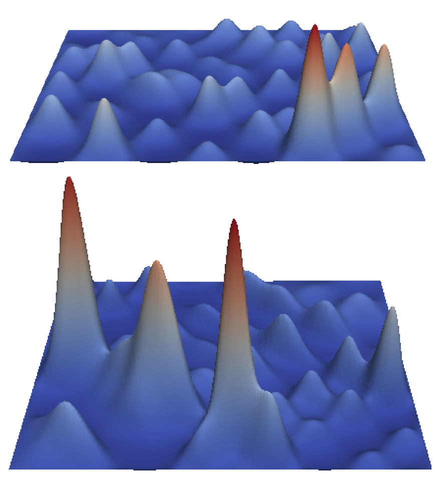


Figure: Realisation of coefficient

forward

Darcy flow model

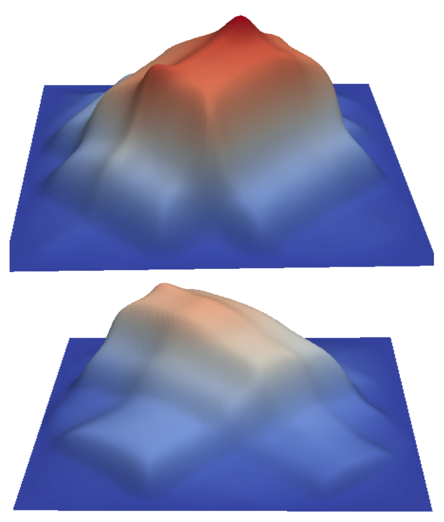


Figure: Realisation of solution

measurement

fit to model

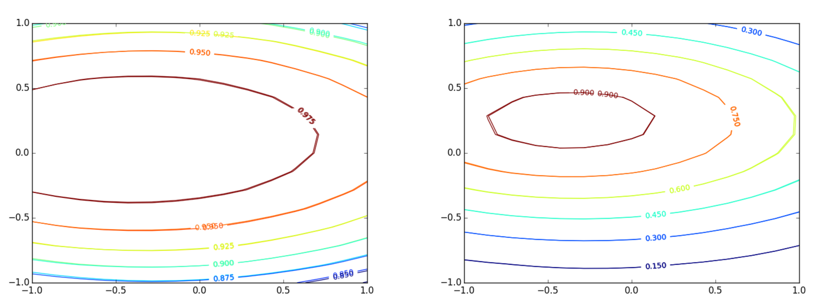


Figure: marginal density esimtation of parameter for various measurements

Sampling free Bayesian inversion using Tensor Trains

- explicit forward solver yields **surrogate model** in TT format

$$G^{N,M}(x,\mathbf{y}) = \sum_{i=1}^{N}\sum_{\mu\in\Lambda_M} U[i,\boldsymbol{\mu}]\varphi_i(x) P_{\boldsymbol{\mu}}(\mathbf{y})$$

- approximation of **Bayesian potential** in closed TT form by exact and *anisotropic* interpolation

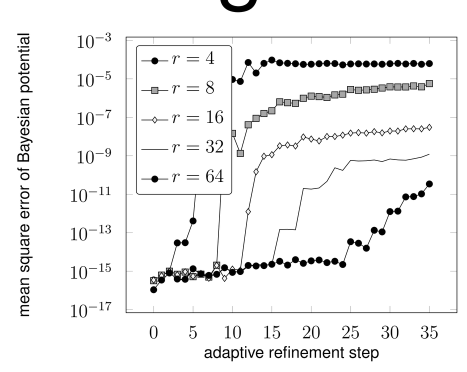


Figure: Rank dependency of Bayesian potential.

- **exponential** of TT tensor by Runge-Kutta method
- convergence in **Hellinger** distance

$$d_{Hell}(\pi_\delta, \pi_{\delta,L,\tau}^{N,M}) = \mathcal{E}\left(N, M, L, \sigma, \tau\right) \to 0$$

FEM error — truncation error — interpolation nodes — tensor approx. — Runge-Kutta time step

- functional representation of **posterior density**

$$\frac{\mathrm{d}\pi_{\delta,L,\tau}^{N,M}}{\mathrm{d}\pi_0}(\mathbf{y}) = \sum_{\boldsymbol{\mu}\in\Lambda'_M} \Pi[\boldsymbol{\mu}]\mathbf{P}_{\boldsymbol{\mu}}(\mathbf{y})$$

- fast access to Q.o.I., e.g. the mean
- **posterior** as new **prior**

Inverse scattering: Helmholtz problem

Consider two random **media** $D_1(\omega), D_2(\omega)$, $D_1(\omega)\cup D_2(\omega) = \mathbb{R}^d$ separated by **interface** $\Gamma(\omega)$.
Transmission and **reflection** problem for plane-wave incidence and known material parameters given by transformed Helmholtz equation

$$\begin{cases} -\nabla\cdot(a(\Gamma(\omega),\cdot)\nabla q) - \kappa^2(\Gamma(\omega),\cdot)q = 0 \text{ in } \mathbb{R}^d \\ \text{boundary condition} \\ \text{radiation condition}\end{cases}$$

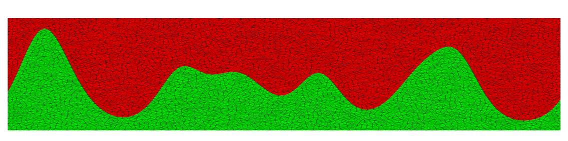


Figure: triangulation of 2D interface

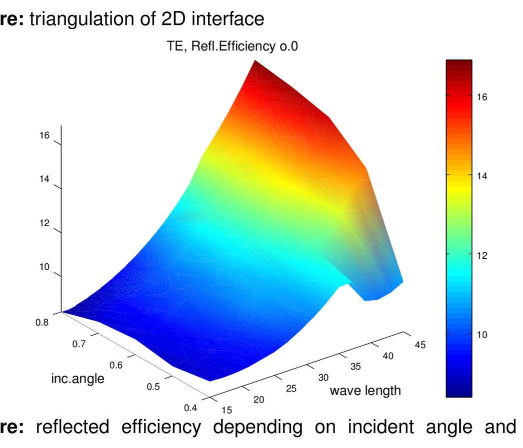


Figure: reflected efficiency depending on incident angle and wave

Outlook and references

Adaptive functional representation combined with hierarchical model reduction:

- Statistical parameter identification for shape reconstruction in scattering applications
- Reconstruction of shapes of blood-cells from measured reflection intensities (with PTB)

[1] M. Eigel, M. Marschall, R. Schneider, "Sampling-free Bayesian inversion with adaptive hierarchical tensor representations", Inverse Problems, Feburary 2018
[2] M. Eigel, J. Neumann, R. Schneider, S. Wolf, "Non-intrusive tensor reconstruction for high dimensional random PDEs", WIAS Preprint 2444
[3] M. Eigel, M. Marschall, M. Pfeffer, R. Schneider, "Adaptive stochastic Galerkin FEM for lognormal coefficients in hierarchical tensor representation", in preparation

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Funding

Coorperation