Adaptive multilevel approaches for stochastic partial differential equations

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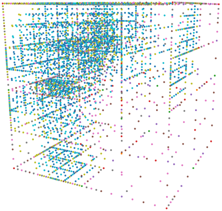
17 November 2016

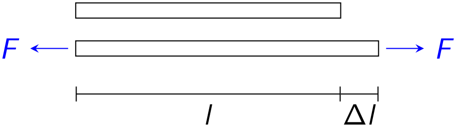


Why stochastics?

- In **engineering problems** the knowledge of certain system describing parameters such as
  - time-dependent environment temperature,
  - time-dependent loading,
  - or spatially-dependent material parameters

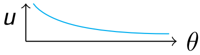
  is **imprecise**.
- Nowadays, civil engineering guidelines account for these uncertainties via the **partial safety factor concept**.
- The **conservative nature** and the **economic viability** of such partial safety factors cannot be ensured without detailed investigation.
- **Stochastic methods** can account for these **uncertainties** in input data and make predictions as to the **probability of outcomes**.

Why stochastics?



$$\begin{aligned} \varepsilon &= \frac{\mathrm{d}u}{\mathrm{d}x} \\ \sigma &= E\varepsilon \\ F &= A\sigma \end{aligned}$$

- Consider the example of a simple one dimensional stretch bar with homogeneous Young's modulus E and constant cross section area A.
- **Deterministic case**: Solving the ODE for one fixed value of the Young's modulus E:
  - $E\frac{\mathrm{d}^2u}{\mathrm{d}x^2} + \boldsymbol{b} = 0$
- **Stochastic case**: Incorporating probabilities accounts for the lack of knowledge resulting in solving the ODE, e.g. for a range of different Young's modulus $E(\theta)$:
  - $E(\theta)\frac{\mathrm{d}^2u}{\mathrm{d}x^2} + \boldsymbol{b} = 0.$



  - The result can be seen as a response surface in the stochastic state space, which can be used for sensitivity analysis.
  - Probability theory provides the tools to investigate the behavior of the stochastic system.

An overview of stochastic methods

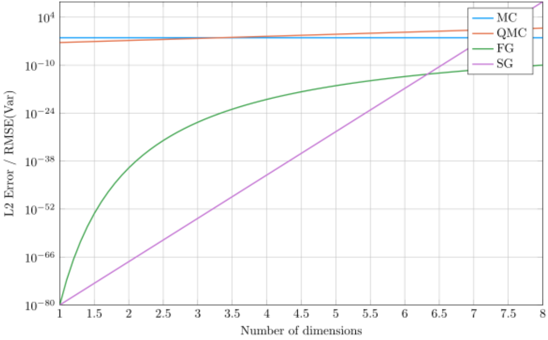
- The **randomized** method, **Monte Carlo integration**:
  - Random number generator, e.g. Mersenne Twister,
  - Convergence independent of number of random dimensions d, smoothness of integrand.
- **Deterministic** methods:
  - **Quasi Monte Carlo** integration (QMC):
    - **Low-discrepancy sequences** for problems with bounded variation in mixed derivatives,
    - Convergence better than Monte Carlo, dimension-dependent.

An overview of stochastic methods

- **Deterministic** methods:
  - **Classical Stochastic Galerkin** (SG):
    - Galerkin projection of the parametric response onto a suitable polynomial basis,
    - Large, sparse system matrix, suitable for dependent random variables.
  - **Classical Stochastic Collocation** (SC):
    - Global or local tensor-product polynomial basis on sparse grids,
    - Interpolation problem, suitable for independent random variables.
- Convergence of SG and SC methods is dependent on NUMBER OF RANDOM DIMENSIONS, SMOOTHNESS OF INTEGRAND.
- Adaptive and multilevel variants exist for many of these methods. (see e.g. Giles, Chernov, Tempone)

The benefit of sparse grids

- Goal: integration and interpolation of multivariate functions with higher-dimensional inputs.
- Full tensor grids suffer from **curse of dimensionality**: $\mathcal{O}(N^{-r/n})$ and therefore fall behind Monte Carlo sampling $\mathcal{O}(N^{-1/2})$ for functions in C^1 when $n > 2$.
- Smolyak's Sparse Grid: $\mathcal{O}(N^{-r}(\log N)^{(n-1)(r+1)})$



Clenshaw-Curtis Grid

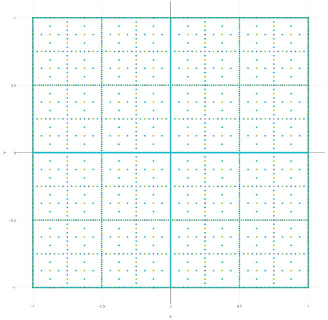


Figure: 3329 points

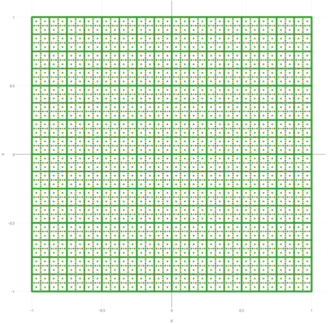
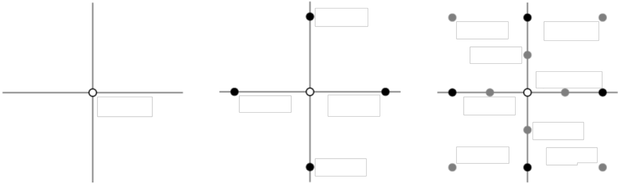


Figure: 32769 Points

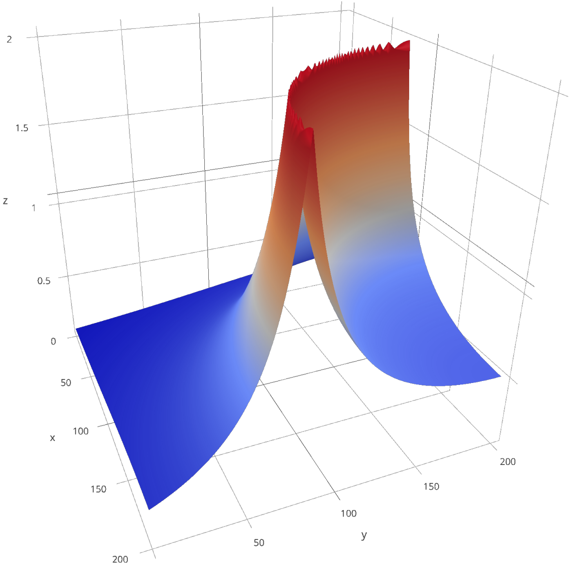
Sparse-grid construction

- Each collocation point on level l spawns at most $2n$ collocation points on level $l+1$:



- Construction admits k-**ary tree structure** with $k = 2n$ (at most $2n$ children per node).
- Multiple parents may spawn the same child, points are kept **unique using multi-indices** of the form $\boldsymbol{m}^{\boldsymbol{i}}$.
- Linear hierarchical basis functions provide adaptivity and a hierarchical surplus.
- **Distributed-memory implementation** (out-of-core) in julia using cooperative multi-tasking and dictionary datastructures.
- For a **MATLAB implementation** see the excellent **spinterp package** (Klimke, A. and Wohlmuth, B., 2005).

Known function with singularity



Interpolant on Clenshaw-Curtis grid

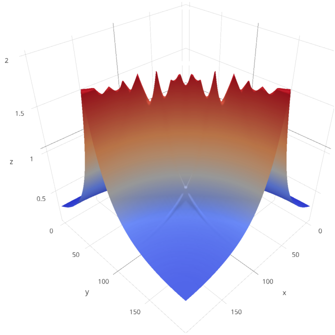


Figure: 3329 points

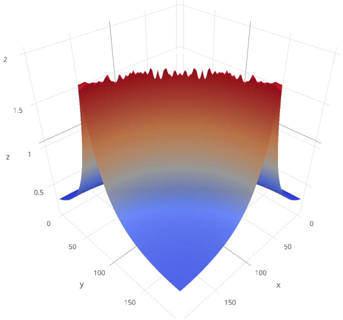
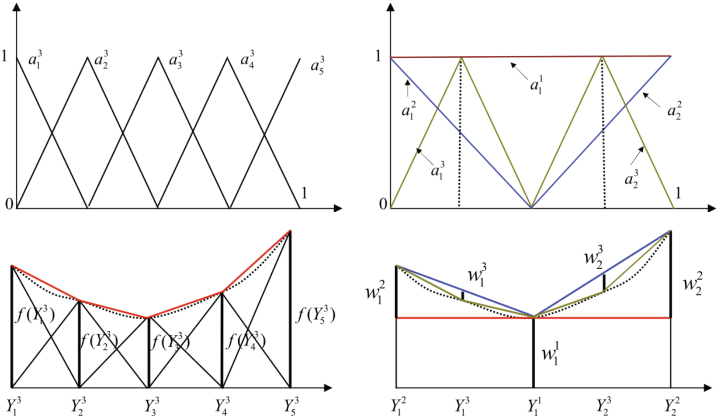


Figure: 32769 Points

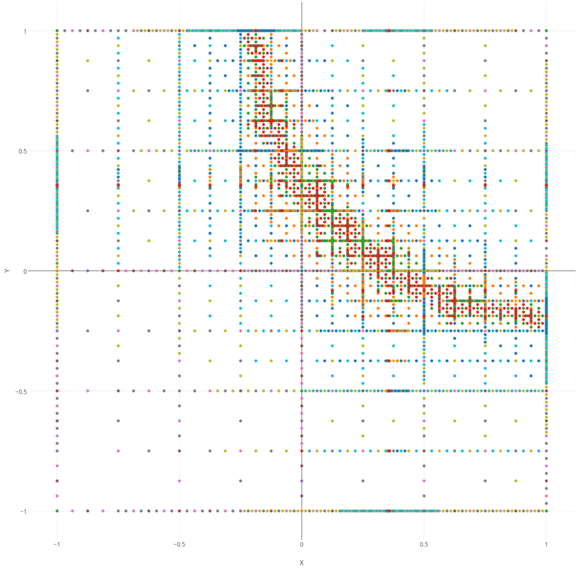
Nodal vs. hierarchical basis in 1D



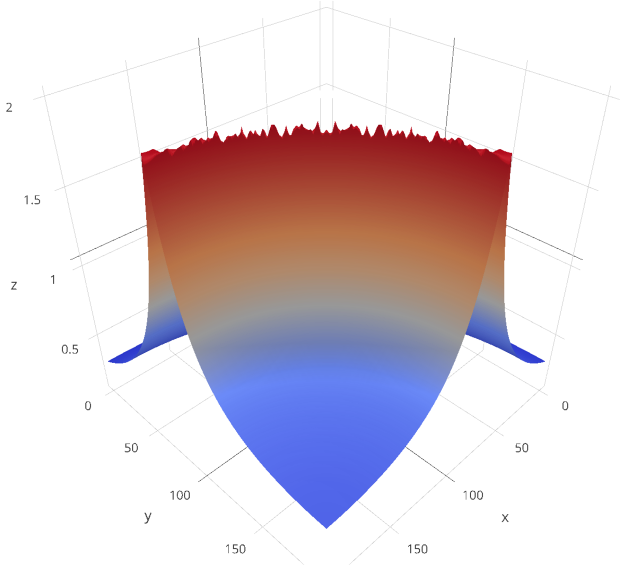
Ma, X., Zabaras, N.: J. Comp. Phys. (2009)

- $f = f(Y_1^3)a_1^3 + f(Y_2^3)a_2^3 + f(Y_3^3)a_3^3 + f(Y_4^3)a_4^3 + f(Y_5^3)a_5^3$
- $f = w_1^1 a_1^1 + w_1^2 a_1^2 + w_2^2 a_2^2 + w_1^3 a_1^3 + w_2^3 a_2^3$

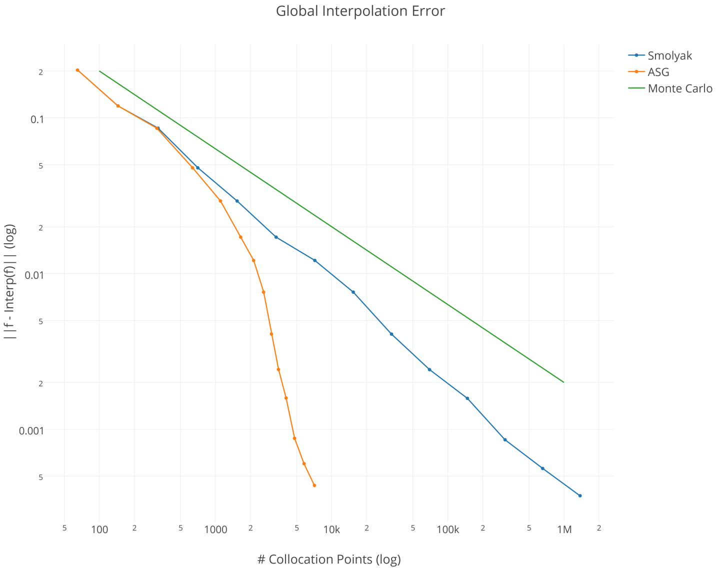
Adaptive sparse grid, 3488 points



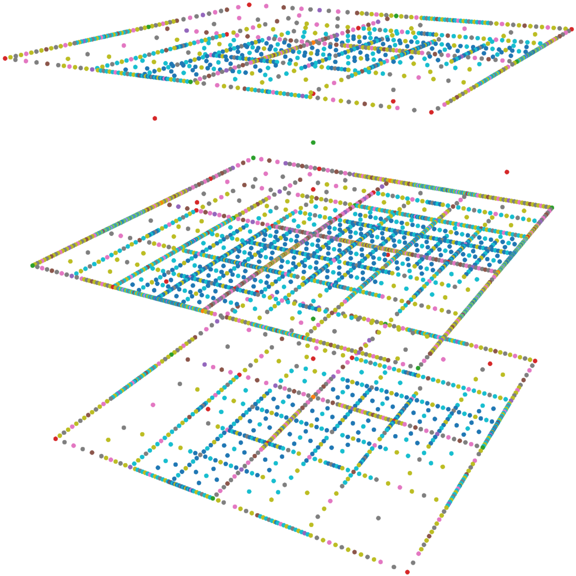
Adaptive interpolant, 3488 points



Global interpolation error



Dealing with anisotropy



Deterministic two-bar contact problem

- One dimensional **mixed elasticity problem**, compliance law & conservation of momentum:

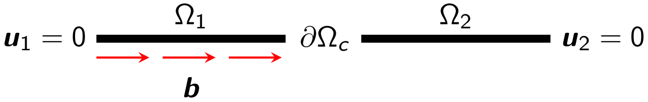
$$E^{-1}\boldsymbol{\sigma} = -\boldsymbol{\delta}\boldsymbol{u} \quad \text{and} \quad \mathbf{d}\boldsymbol{\sigma} + \boldsymbol{b} = 0 \quad \text{on } \Omega \quad + \text{ BC}\,,$$

  where $\boldsymbol{\sigma} \in \Lambda^0$, $\boldsymbol{u}, \boldsymbol{b} \in \Lambda^1$, $\mathbf{d} : \Lambda^k \to \Lambda^{k+1}$, $\boldsymbol{\delta} : \Lambda^{k+1} \to \Lambda^k$, Ω oriented, simply-connected.
- In one dimension, the elasticity problem is analogous to the **Hodge Laplacian** for $k = 1$.
- **Weak form** of equilibrium (single body), via Leibniz product rule, Stokes' theorem:

$$\begin{aligned} \langle \boldsymbol{\tau}, E^{-1}\boldsymbol{\sigma} \rangle_\Omega + \langle \mathbf{d}\boldsymbol{\tau}, \boldsymbol{u} \rangle_\Omega &= \langle \mathrm{tr}\boldsymbol{\tau}, \mathrm{tr}\boldsymbol{u} \rangle_{\partial\Omega} \\ \langle \boldsymbol{v}, \mathbf{d}\boldsymbol{\sigma} \rangle_\Omega &= -\langle \boldsymbol{v}, \boldsymbol{b} \rangle_\Omega\,. \end{aligned}$$

- FEEC (Arnold, Falk, Winther, 2006) discretization of polynomial order r: $\boldsymbol{\tau}, \boldsymbol{\sigma} \in \mathcal{P}_r^- \Lambda^0$ (Lagrange), $\boldsymbol{v}, \boldsymbol{u} \in \mathcal{P}_r^- \Lambda^1$ (discontinuous Galerkin).

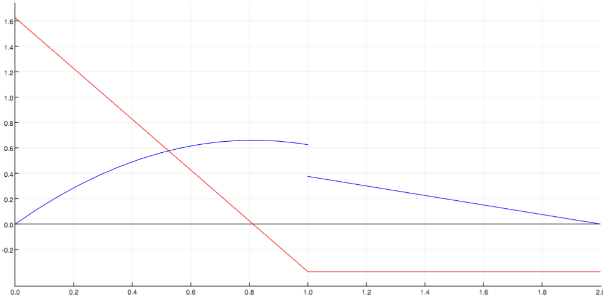
Deterministic two-bar contact problem



- Incorporation of contact with initial gap $\boldsymbol{g}_0$:

$$(1) \quad \boldsymbol{\sigma}_1 = \boldsymbol{\sigma}_2 \quad \text{and} \quad (2) \quad \boldsymbol{u}_2 = \boldsymbol{u}_1 - \boldsymbol{g}_0 \quad \text{on} \quad \partial\Omega_c \,,$$

  when $\boldsymbol{u}_1 > \boldsymbol{g}_0$ in the single-body problem for bar one.
- Impose condition (1) strongly, condition (2) weakly.



Random Field Representation

- Given a **probability space** $(\Omega, \mathcal{F}, \mathbb{P})$, where
  - Ω is a sample space,
  - a set of events $\mathcal{F}$ (also called the σ-algebra associated with Ω) and
  - the probability measure $\mathbb{P} : \mathcal{F} \to \mathbb{R}$,
- A **random element** is defined by the mapping $X : \Omega \to \mathbb{K}$, $\theta \in \Omega$, where
  - X is a *random variable*, if $\mathbb{K} = \mathbb{R}$,
  - X is a *random vector*, if $\mathbb{K}$ is a vector space or
  - X is a *stochastic process*, if $\mathbb{K}$ is a function space.
- A **random field** $H(\mathbf{x}, \theta)$ is a stochastic process, where $\mathbf{x} \in M \subset \mathbb{R}^d$ is a spatial variable.

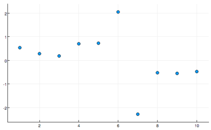


Figure: Realization of a random vector

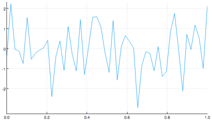
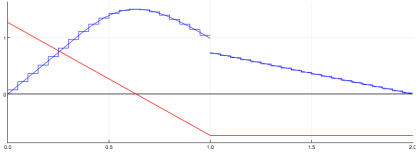


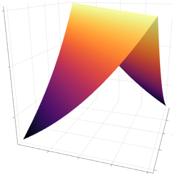
Figure: Realization of a random process



Discretizing the random field

- Let $H(\mathbf{x}, \theta)$ be a square integrable, zero mean random field with a autocorrelation function K.

- The **autocorrelation function** $K : D \times D \to \mathbb{R}$ is defined through $K(\mathbf{x}_1, \mathbf{x}_2) = \mathbb{E}[H(\mathbf{x}_1, \theta)H((\mathbf{x}_2, \theta))]$, for example the Gaussian covariance function $K(\mathbf{x}_1, \mathbf{x}_2) = \sigma^2 e^{-\frac{|\mathbf{x}_1 - \mathbf{x}_2|}{l_c}}$.



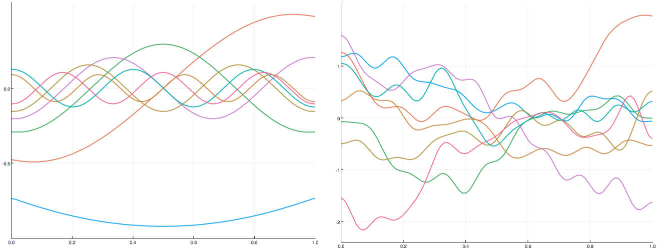
- We obtain the **eigenvalues** λ_k and eigenfunctions f_k by solving the homogeneous **Fredholm integral equation** of the second kind $\int_D K(\mathbf{x}_1, \mathbf{x}_2)\, f_k(\mathbf{x}_2)\, \mathrm{d}\mathbf{x}_2 = \lambda_k f_k(\mathbf{x}_1)$.

- The infinite sum over the **orthogonal eigenfunctions** represents the random field $H(\mathbf{x}, \theta) = \sum_{k=1}^{\infty} \sqrt{\lambda_k}\, \xi_k(\theta)\, f_k(\mathbf{x})$, where $\xi_k(\theta)$ **is the** k**-th random parameter (standard-normally distributed)**.

- Truncating the sum after the M-th term $H(\mathbf{x}, \theta) = \sum_{k=1}^{M} \sqrt{\lambda_k}\, \xi_k(\theta)\, f_k(\mathbf{x})$ results in an **approximate representation of the random field**.

Discretizing the random field

- The Fredholm integral equation is solved numerically by means of a Galerkin procedure.
- The Galerkin projection results in the system $\sum_{j=1}^{J} K_{ij} f_{jk} = \sum_{j=1}^{J} \sum_{l=1}^{M} N_{ij} f_{jl} \Lambda_{lk}$, where $\Lambda_{lk} = \delta_{lk} \lambda_k$
- or in matrix notation: $\mathbf{Kf} = \mathbf{Nf\Lambda}$.
- This is a generalized algebraic eigenvalue problem, which can be solved for the eigenvalues $\mathbf{\Lambda}$ and the eigenvektors $\mathbf{f}$.
- The eigenfunction f_k is approximated by $f_k(\mathbf{x}) \approx \sum_{j=1}^{J} f_{jk} N_j(\mathbf{x})$



Stochastic two-bar contact problem

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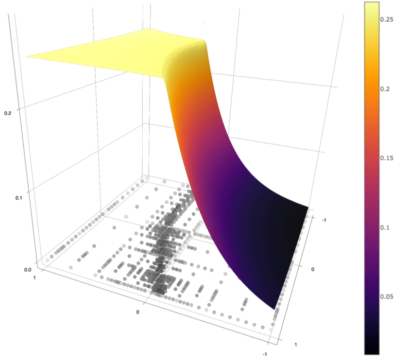
Tip end displacement, interpretation of results:

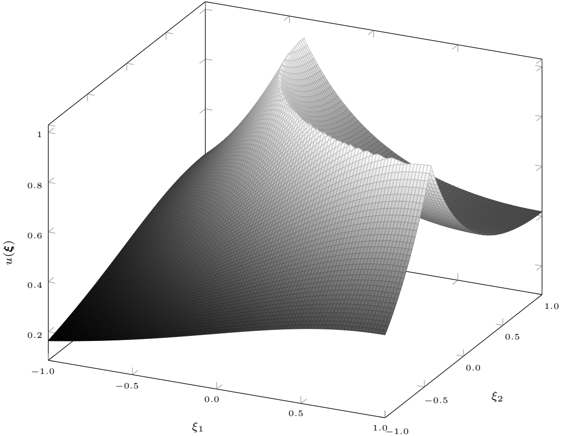
- Body force $\boldsymbol{b} = 0.25\,\mathrm{d}x^1$, initial gap $\boldsymbol{g}_0 = 0.25\,\mathrm{d}x^1$
- The first eigenfunction is negative and the distribution is lognormal, i.e. ξ_1 increases as stiffness E_1 decreases over the whole length of Ω_1. $E_2 = 50$, $\mathbb{E}(E_1) = 1$.



Parametric ODE problem

$$\frac{\mathrm{d}u}{\mathrm{d}t} + \left(|2-(\xi_1-1)^2-(\xi_2-1)^2| + \delta\right) u = 1,$$
IC: $u(t=0,\boldsymbol{\xi}) = 0$, regularization $\delta = 10^{-1}$

Analytical solution $u(t,\boldsymbol{\xi}) = \frac{1-\exp\left(-t\left(|2-(\xi_1-1)^2-(\xi_2-1)^2|+\delta\right)\right)}{|2-(\xi_1-1)^2-(\xi_2-1)^2|+\delta}$



From Single- to Multilevel

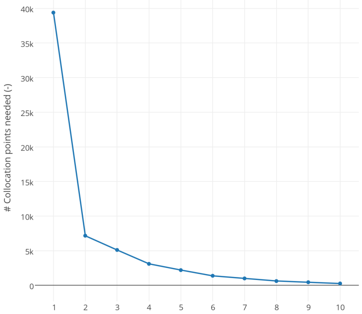
$$\frac{\mathrm{d}u}{\mathrm{d}t} + \left(\left|2 - (\xi_1 - 1)^2 - (\xi_2 - 1)^2\right| + \delta\right) u = 1$$

Forward Euler integration

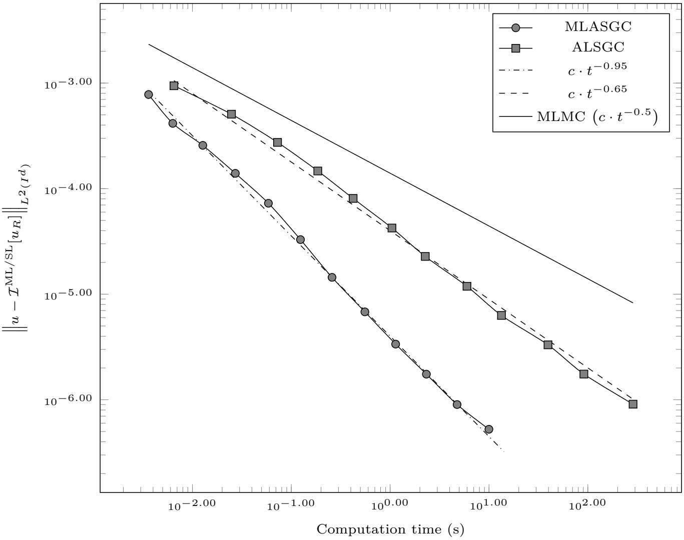
$\Delta t_r = 30^{-1} \cdot 2^{-r}$ time-steps for level $r = 1, 2, \ldots, R-1, R$

$$\mathcal{I}^{\mathrm{ML}}[u_R] = \mathcal{I}^{\mathrm{SL}}[u_1] + \sum_{r=1}^{R} \mathcal{I}^{\mathrm{SL}}[u_r - u_{r-1}] \qquad \lim_{r\to\infty} \mathbb{V}[u_r - u_{r-1}] \to 0$$

No. of collocation points required for computing the level correction to achieve a cumulative local stochastic error of $\varepsilon < 10^{-5}$ for u_R:



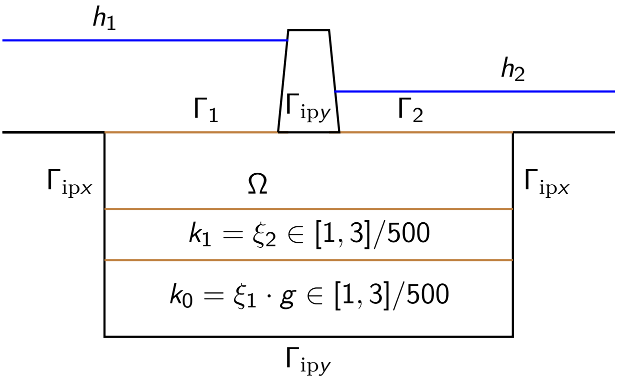
Benchmark of the ODE problem



2D benchmark problem

2D Darcy flow

- $\text{div}(-k\,\text{grad}\,h) = 0$ on $\Omega = [-1,1]^2$, $\boldsymbol{v} = -k\,\text{grad}\,h$
- Dirichlet BC: $h_1 = 1.0$ on Γ_1 and $h_2 = 0.5$ on Γ_2
- Neumann BC: $v_x = 0$ on $\Gamma_{\text{ip}x}$, $v_y = 0$ on $\Gamma_{\text{ip}y}$
- $k = k_1$ on $[-1,1] \times [-0.25, 0.25]$, smooth transition between $y = \pm 0.25$ and ± 0.5, $k = k_0$ elsewhere



Numerical benchmark problem

Discretization

- $\mathcal{Q}_1\Lambda^0(\Box_2)$ linear quadrilaterals
- $4 \cdot 2^{\alpha_1}$ elements in x-direction, $\alpha_1 \in [1, 6]$
- $4 \cdot 2^{\alpha_2}$ elements in y-direction, $\alpha_2 \in [1, 6]$

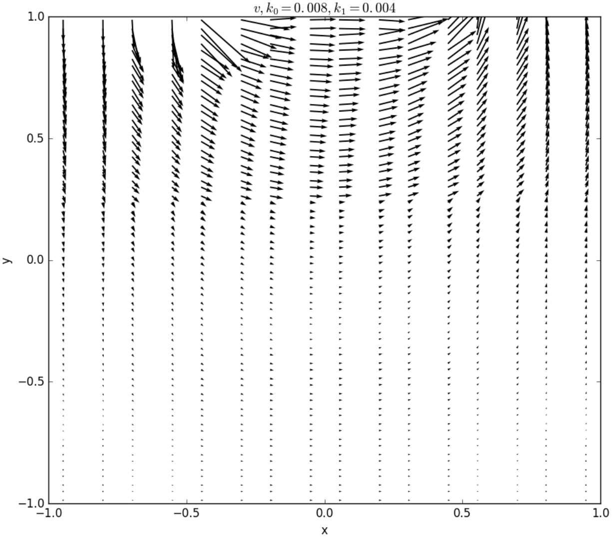
We're interested in the solution field h as the QOI:

$$\mathcal{I}^{\mathrm{MI}}[h_R] = \mathcal{I}^{\mathrm{SL}}[h_{(1,\dots,1)}] + \sum_{\boldsymbol{\alpha} \in \mathcal{A}} \mathcal{I}^{\mathrm{SL}}[\Delta_{\boldsymbol{\alpha}} h]$$

$$\Delta_{\boldsymbol{\alpha}} h = \Delta_n(\dots(\Delta_2(\Delta_1 h_{\boldsymbol{\alpha}}))) \qquad \Delta_i h_{\boldsymbol{\alpha}} = h_{\boldsymbol{\alpha}} - h_{\boldsymbol{\alpha}-\boldsymbol{e}_i}$$

How to compute $\Delta_i h_{\boldsymbol{\alpha}} = h_{\boldsymbol{\alpha}} - h_{\boldsymbol{\alpha}-\boldsymbol{e}_i}$?
Consistent interpolation is exact as meshes are nested.

Interpolated result



Conclusion

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- Adaptive sparse grid techniques:
  - Suitable for moderately high dimensional inputs,
  - Multidimensional interpolation, sensitivity analysis, and integration of arbitrary computational result datatypes,
  - Distributed memory parallel computing.
- Elementary examples were demonstrated, including problems of reduced regularity.
- Multiple deterministic discretizations can be used in a Multilevel/-index Adaptive Sparse Grid Collocation scheme, which can reduce the cost of computation.
- A look to the future:
  - implement MISC knapsack heuristic[1],
  - hierarchical wavelet basis (for stability)[2].

---

[1] Haji-Ali, A.-L. et al.: preprint arXiv:1508.07467 (2015)

[2] Gunzburger, M. et al.: Comp. Sci. Eng. (2014)

Outlook

What we are working on:

- Solving stochastic problems using adaptive techniques
  - mesomechanical contact dynamics of rolling tires on rough road surfaces, and
  - detailed long-term bone-implant interaction and ingrowth problems
- using the Finite Element Exterior Calculus as a deterministic framework for structure-preserving discretization