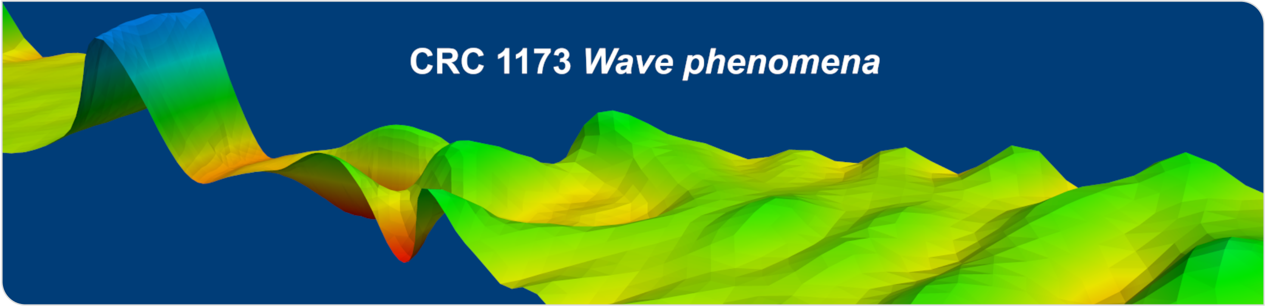
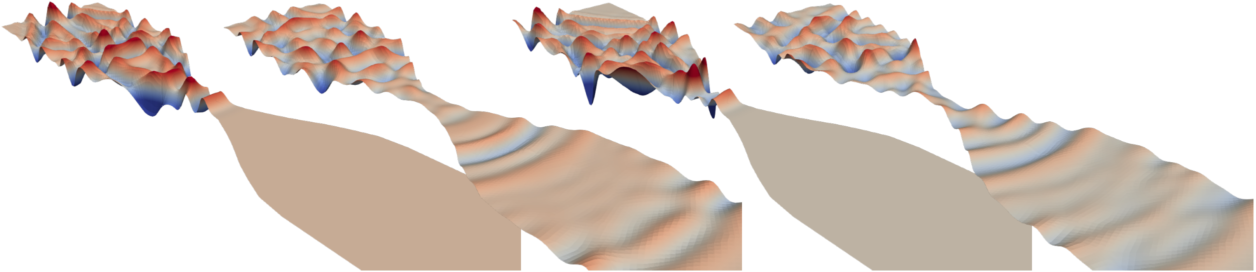
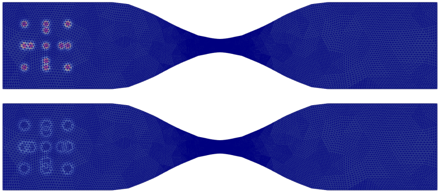
A non-intrusive multilevel Uncertainty Quantification (MLUQ) framework for wave problems with random input data

Niklas Baumgarten | 03.05.2022



Introductory example





- Sparse grid generator `TASMANIAN`: [Sto+13]
- Analyzed for random wave speeds in: [MNT13]
- <u>Motivation for this talk:</u> Move to more general applications, while maintaining usability of many methods.

Non-intrusive Uncertainty Quantification

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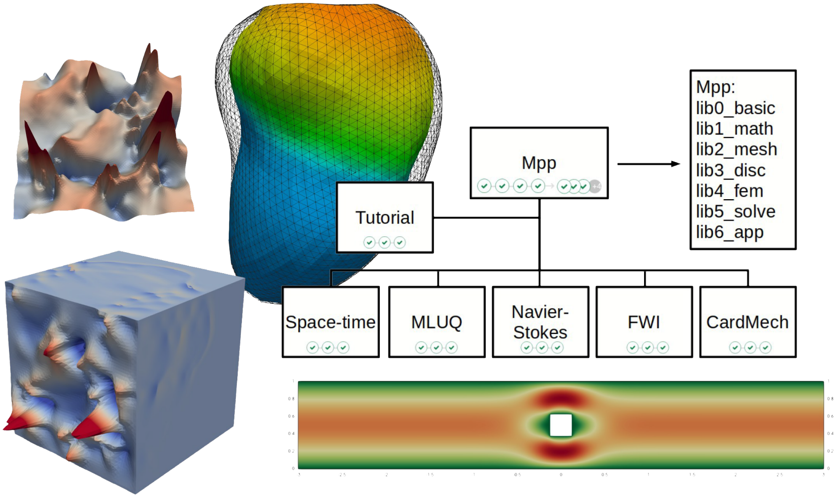
	No UQ	SC	MLMC	MIMC	MLSC
FD		[MNT13; MNT15]			
FEM	[BW21]	[BNT10; NTW08; FS21]	[CST13; Tec+13] [BW21]	[HNT16]	[Tec+15]
DG/FV+TS	[Hoc+15; Boh+21]		[MSŠ12; MSŠ16] [BW21]		
ST(DG/PG)	[DFW16; Dör+19] [Ern18; Zie19]		[Bad+21]		
Other					[JS21]

- Question in theory: Which methods converge and what are the stability/regularity constraints?
- Question in application: Which methods do I use, given a certain problem?

$\rightarrow$ The ones which give the most accurate outcome, given that they used the same resources.

- This is joint work with Christian Wieners and Daniele Corallo
  N. Baumgarten, C. Wieners: The parallel finite element system M++ with integrated multilevel preconditioning and MLMC methods. Computers & Mathematics with Applications 2021

Software and project design of `M++`



- Design motivated by mathematical structure
- Knowledge transfer by clean code / design
- FAIR & trustworthy, documented, efficient
- Automated falsification and continuous deployment support by `nhr.kit.edu`

Deterministic model problem

Acoustic wave: Search for $(\mathbf{v}, p)(t) = \mathbf{u}(t) \in V$

$$\begin{cases} \rho\partial_t \mathbf{v} - \nabla p = \mathbf{f} & D \times (0,T) \\ \partial_t p - \kappa \operatorname{div} \mathbf{v} = g & D \times (0,T) \\ (\mathbf{v}, p) = \mathbf{0} & \partial D \times (0,T) \\ (\mathbf{v}, p)(0) = (\mathbf{v}_0, p_0) & D \end{cases},$$

where $V = \mathrm{H}(\operatorname{div}; D) \times \mathrm{H}_0^1(D) \subset \mathrm{L}^2(D, \mathbb{R}^J)$ and

- $\rho, \kappa^{-1} \in \mathrm{L}^\infty(D; \mathbb{R}_+) \;\Rightarrow\; c(\mathbf{x}) = \sqrt{\frac{\kappa(\mathbf{x})}{\rho(\mathbf{x})}} < \infty$
- $(\mathbf{f}, g)(t) = \mathbf{b}(t) \in \mathrm{L}^2(D; \mathbb{R}^J)$
- $(\mathbf{v}_0, p_0) = \mathbf{u}_0 \in \mathrm{L}^2(D; \mathbb{R}^J)$

General setting of linear hyperbolic conservation laws:

$$\underline{M}\partial_t \mathbf{u}(t) + \underline{A}\mathbf{u}(t) = \mathbf{b}(t), \quad t \in (0,T), \quad \mathbf{u}(0) = \mathbf{u}_0,$$

where

- $\underline{M} \in \mathrm{L}^\infty(D; \mathbb{R}^{J \times J})$ uniformly positive and sym.
- $\underline{A}$ linear operator with dense domain in V with

$$(\underline{A}\mathbf{v}, \mathbf{v})_{0,D} = 0, \quad \mathbf{v} \in \mathcal{D}(\underline{A})$$

- The energy $\mathrm{E} = \frac{1}{2}(\mathbf{v}, \mathbf{v})_V$ is conserved, if $\mathbf{b} \equiv \mathbf{0}$

$$\begin{aligned} \partial_t \mathrm{E}(\mathbf{u}(t)) &= (\underline{M}\partial_t \mathbf{u}(t), \mathbf{u}(t))_{0,D} \\ &= -(\underline{A}\mathbf{u}(t), \mathbf{u}(t))_{0,D} = 0 \end{aligned}$$

Random model problem

Random acoustic wave: Search for $\mathbf{u}(t)\colon \Omega \to V$

$$
\begin{cases}
\rho(\omega)\partial_t \mathbf{v}(\omega) - \nabla p(\omega) = \mathbf{f}(\omega) & D \times (0, T) \\
\partial_t p(\omega) - \kappa(\omega) \operatorname{div} \mathbf{v}(\omega) = g(\omega) & D \times (0, T) \\
(\mathbf{v}, p)(\omega) = \mathbf{0} & \partial D \times (0, T) \\
(\mathbf{v}, p)(\omega, 0) = (\mathbf{v}_0, p_0)(\omega) & D
\end{cases},
$$

where $\omega \in \Omega$ and

- $\rho, \kappa^{-1} \in \mathrm{L}^k(\Omega, \mathrm{L}^\infty(D; \mathbb{R}_+)) \;\Rightarrow\; c(\mathbf{x}) < \infty$ a.s.
- $(\mathbf{f}, g)(t) = \mathbf{b}(t) \in \mathrm{L}^k(\Omega, \mathrm{L}^2(D; \mathbb{R}^J))$
- $(\mathbf{v}_0, p_0) = \mathbf{u}_0 \in \mathrm{L}^k(\Omega, \mathrm{L}^2(D; \mathbb{R}^J))$
- Further readings [MSŠ16; MS12]

Numerical approximation:

Let $\mathbf{u}_h(\omega) = \mathbf{u}_\ell(\omega) \in V_\ell$ be an approximation to $\mathbf{u}(\omega)$ on level ℓ and $\mathrm{Q}_\ell(\mathbf{u}_\ell(\omega))$ be a quantity of interest of $\mathbf{u}_\ell(\omega)$.

Parametric formulation:

Finite-dimensional noise assumption

$\Rightarrow$ Replace probability space by parametric space

$$\underline{y} = (y_1, \dots, y_d) \in \Gamma$$

and find for all parameters $\mathbf{u}(\underline{y})$.

Monte Carlo and stochastic collocation

MC estimator: Draw $\omega^{(m)} \in \Omega$, compute $\mathbf{u}_\ell(\omega^{(m)})$

$$\widehat{\mathbf{u}}^{\mathrm{MC}}_{\ell,M} = M^{-1} \sum_{m=1}^{M} \mathbf{u}_\ell(\omega^{(m)}), \quad \widehat{\mathrm{Q}}^{\mathrm{MC}}_{\ell,M} = M^{-1} \sum_{m=1}^{M} \mathrm{Q}_\ell(\omega^{(m)})$$

Mean square error and cost:

$$e(\widehat{\mathrm{Q}}^{\mathrm{MC}}_{\ell,M})^2 = \underbrace{M^{-1}\mathbb{V}[\mathrm{Q}_\ell]}_{\text{Estimator error}} + e_{\mathrm{Approx.}}$$

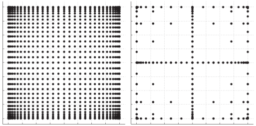
The cost $\mathrm{C}(\widehat{\mathrm{Q}}^{\mathrm{MC}}_{\ell,M}) \lesssim M \cdot N_\ell^\gamma$ for $e(\widehat{\mathrm{Q}}^{\mathrm{MC}}_{\ell,M})^2 < \epsilon^2$ is

$$\mathrm{C}_\epsilon(\widehat{\mathrm{Q}}^{\mathrm{MC}}_{\ell,M}) \lesssim \epsilon^{-2-\frac{\gamma}{\alpha}}$$

SC estimator: $\{\underline{y}^{(m)}\}_{m=1}^{M} \subset \Gamma$, compute $\mathbf{u}_\ell(\underline{y}^{(m)})$

$$\widehat{\mathbf{u}}^{\mathrm{SC}}_{\ell,M} = \sum_{m=1}^{M} w_m \mathbf{u}_\ell(\underline{y}^{(m)}), \quad \widehat{\mathrm{Q}}^{\mathrm{SC}}_{\ell,M} = \sum_{m=1}^{M} w_m \mathrm{Q}_\ell(\underline{y}^{(m)})$$

Collocation points: $\Theta_M = \{\underline{y}^{(m)}\}_{m=1}^{M} \subset \Gamma$ is tensor grid or Smolyak sparse grid



- $e \sim C_{\mathrm{Tensor}} M^{-a/d} + e_{\mathrm{Approx.}}$
- Suffers from curse of dimensionality w.r.t. d

Multilevel estimator

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- Assumptions: The approximation is convergent

$$|\mathbb{E}[\mathrm{Q}_\ell - \mathrm{Q}]| \lesssim h_\ell^\alpha, \quad \alpha > 0 \tag{1}$$

The cost for one sample is bounded

$$\mathrm{C}(\mathrm{Q}_\ell(\omega^{(m)})) \lesssim h_\ell^{-\gamma}, \quad \gamma > 0 \tag{2}$$

The variance of $\mathrm{Q}_\ell - \mathrm{Q}_{\ell-1}$ decays

$$\mathbb{V}[\mathrm{Q}_\ell - \mathrm{Q}_{\ell-1}] \lesssim h_\ell^\beta, \quad \beta > 0 \tag{3}$$

- Idea: Set $\mathrm{Y}_\ell := \mathrm{Q}_\ell - \mathrm{Q}_{\ell-1}$, $\mathrm{Y}_0 := \mathrm{Q}_0$, compute samples on $\ell \in \{0, \dots L\}$, balance C_ℓ and M_ℓ

$$\mathbb{E}[\mathrm{Q}_L] = \mathbb{E}[\mathrm{Q}_0] + \sum_{\ell=1}^{L} \mathbb{E}[\mathrm{Q}_\ell - \mathrm{Q}_{\ell-1}] = \sum_{\ell=0}^{L} \mathbb{E}[\mathrm{Y}_\ell]$$

- Multilevel estimators: Estimate Y_ℓ with MC / SC

$$\widehat{\mathrm{Y}}_{\ell,M_\ell}^{\mathrm{MC}} = M_\ell^{-1} \sum_{m=1}^{M_\ell} \mathrm{Y}_\ell(\omega^{(m)}) \quad \Rightarrow \quad \widehat{\mathrm{Q}}_{L,\{M_\ell\}_{\ell=0}^L}^{\mathrm{MLMC}} = \sum_{\ell=0}^{L} \widehat{\mathrm{Y}}_{\ell,M_\ell}^{\mathrm{MC}}$$

- Mean square error and cost for MLMC:

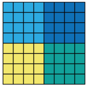
$$e(\widehat{\mathrm{Q}}_{L,\{M_\ell\}_{\ell=0}^L}^{\mathrm{MLMC}})^2 = \underbrace{\sum_{\ell=0}^{L} M_\ell^{-1} \mathbb{V}[\mathrm{Y}_\ell]}_{\text{Estimator error}} + e_{\mathrm{Approx.}},$$

$$\mathrm{C}(\widehat{\mathrm{Q}}_{L,\{M_\ell\}_{\ell=0}^L}^{\mathrm{MLMC}}) \lesssim \sum_{\ell=0}^{L} M_\ell \mathrm{C}_\ell,$$

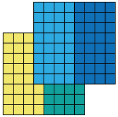
$$\mathrm{C}_\epsilon(\widehat{\mathrm{Q}}_{L,\{M_\ell\}_{\ell=0}^L}^{\mathrm{MLMC}}) \lesssim \epsilon^{-2-(\gamma-\beta)/\alpha}$$

Integrated parallelization for ML estimators and multi-sample systems

ML estimator parallelization: Let $\mathcal{P}$ be the set of processes and $\triangle M_\ell$ be the required sample amount

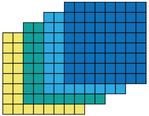


$$\triangle M_\ell = 1 \quad \Rightarrow \quad \mathcal{M}_{\mathcal{P}}$$



$$k \in \mathbb{N}\colon 2^k \leq \frac{|\mathcal{P}|}{\triangle M_\ell} < 2^{k+1} \quad \Rightarrow$$

$$\left\{\mathcal{M}^{(m)}_{\mathcal{P}_k}\right\}_{m=1}^{\triangle M_\ell}, \quad \mathcal{P}_k \subset \mathcal{P}, \quad |\mathcal{P}_k| = 2^k$$



$$\triangle M_\ell \geq |\mathcal{P}| \;\Rightarrow\; \left\{\mathcal{M}^{(m)}_{\{P\}}\right\}_{m=1}^{|\mathcal{P}|}, \quad P \in \mathcal{P}$$

Classic parallelization approaches:

- FE parallelization on discretized domain D:
  Distribute $\mathcal{M} = \{\mathcal{V}, \mathcal{K}, \mathcal{F}, \mathcal{E}\}$ on $\mathcal{P}$
- Parallelization over $\omega^{(m)} \in \Omega$ or $\underline{y}^{(m)} \in \Theta_{M_\ell}$:
  Distribute deterministic samples on $\mathcal{P}$

Multi-sample FE space: Def. $V_\ell^{\mathcal{P}} = \prod_{\mathcal{P}_k \in \mathcal{P}} V_\ell^{\mathcal{P}_k}$ with

$$V_\ell^{\mathcal{P}_k} = \left\{\mathbf{v}_\ell \in V_\ell(D;\mathbb{R}^J)\colon\ \mathbf{v}_\ell|_K \in V_\ell(K;\mathbb{R}^J),\ \forall K \in \mathcal{K}_{\mathcal{P}_k}\right\}$$

Multi-sample system: Search for $(\mathbf{u}_\ell)_{m=1}^{M_\ell} \in V_\ell^{\mathcal{P}}$, s.t.

$$\underline{L}_\ell^{(m)} \mathbf{u}_\ell^{(m)} = \mathbf{b}_\ell^{(m)} \quad \text{on} \quad \mathcal{M}^{(m)}_{\mathcal{P}_k}, \qquad m = 1, \dots, M_\ell$$

Further readings: [ŠMS11; Šuk13; Drz+17; BHP21]

Multi-sample system for the model problem and cost restricted implementation

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Multi-sample dG-sys.: Search for $(\mathbf{u}_\ell(t))_{m=1}^{M_\ell} \in V_{\ell,p}^{\mathrm{dG},\mathcal{P}}$

$$\underline{M}_\ell^{(m)} \partial_t \mathbf{u}_\ell^{(m)}(t) + \underline{A}_\ell^{(m)} \mathbf{u}_\ell^{(m)}(t) = \mathbf{b}_\ell^{(m)}(t), \quad t \in (0, T),$$

where $V_{\ell,p}^{\mathrm{dG},\mathcal{P}} = \prod_{\mathcal{P}_k \in \mathcal{P}} V_{\ell,k,p}^{\mathrm{dG}}$:

- Considers computational resources
- Spans adaptively in spacial & stochastic domain
- Fully algebraic system decoupled for each sample, mildly coupled on spatial domain
- Parallel preconditioning and time-integration
- Applicable to arbitrary FE-space: E.g.

$$V_{\ell,p}^{\mathrm{dG}} = \left\{ \mathbf{v}_\ell \in \mathrm{L}^2(D; \mathbb{R}^J) \colon \mathbf{v}_\ell|_K \in \mathbb{P}_p(K; \mathbb{R}^J), \forall K \in \mathcal{K} \right\}$$

Classic ML estimator implementation:

- Requires a-priori knowledge about α, β, γ and hidden constants in (1), (2), (3).

Implementation with post estimation:

- $M_\ell = \left\lceil 2\epsilon^{-2} \sqrt{\frac{\mathbb{V}[\mathrm{Y}_\ell]}{\mathrm{C}_\ell}} \left(\sum_{\ell=0}^{L} \sqrt{\mathbb{V}[\mathrm{Y}_\ell] \mathrm{C}_\ell} \right) \right\rceil$
- Richardson-extrapolation to find L

Cost restricted implementation:

- Total computational budget B^0 is given, $\eta < 1$

```
while B^i > 0:
    Q^i, C^i <- MLMC(ε^i)
    ε^{i+1} <- η ε^i,   B^{i+1} <- B^i - C^i,   i <- i + 1
```

Discontinuous Galerkin (DG) discretization with time stepping and space-time methods

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Semi-discrete system: Search for $\mathbf{u}_\ell(t) \in V_{\ell,p}^{\mathrm{dG}}$

$$\underline{M}_\ell \partial_t \mathbf{u}_\ell(t) + \underline{A}_\ell \mathbf{u}_\ell(t) = \mathbf{b}_\ell(t), \quad t \in (0, T),$$

where $\underline{M}_\ell, \underline{A}_\ell \in \mathcal{L}(V_{\ell,p}^{\mathrm{dG}}, V_{\ell,p}^{\mathrm{dG}})$:

- $\underline{M}_\ell$ is block-diagonal and positive definite
- $\underline{A}_\ell$ is non-symmetric stiffness matrix
- Stability, consistency, convergence see [Hoc+15]

Implicit time-stepping:

$$\mathbf{u}^{n+1} = \Phi_n \left(-\tau \underline{M}_\ell^{-1} \underline{A}_\ell \right) \mathbf{u}^n, \quad n = 0, 1, \ldots,$$

Φ_n being a rational stability function:

- A-stable method to avoid random CFL

Weak formulation in space-time: Search for $\mathbf{u} \in V$

$$(\mathbf{u}, \underline{L}^* \mathbf{w})_Q = (\mathbf{b}, \mathbf{w})_Q + (\mathbf{u}_0, \mathbf{w}(0))_D, \quad \forall \mathbf{w} \in W$$

with $Q := D \times [0, T]$. Discr. $[0, T]$ with $\mathcal{I}$, search in:

$$V_{\ell,p,q}^{\text{ST-dG}} = \Big\{ \mathbf{v}_\ell \in \mathrm{L}^2([0, T]; \mathrm{L}^2(D; \mathbb{R}^J)) : \\ \mathbf{v}_\ell|_{K,I} \in \mathbb{P}_p(K; \mathbb{R}^J) \otimes \mathbb{P}_q(I; \mathbb{R}^J), \\ \forall K \in \mathcal{K}, \forall I \in \mathcal{I} \Big\}$$

- Resulting in huge linear system
- Assume $\mathbf{u} \in H^s(Q)$ with $s \geq 1$, then

$$\| (\mathbf{u}_\ell - \mathbf{u})(T) \|_D \lesssim h^{s-1/2}$$

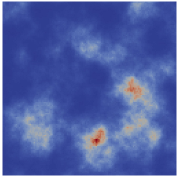
- Further readings [Ban+21; Zie19]

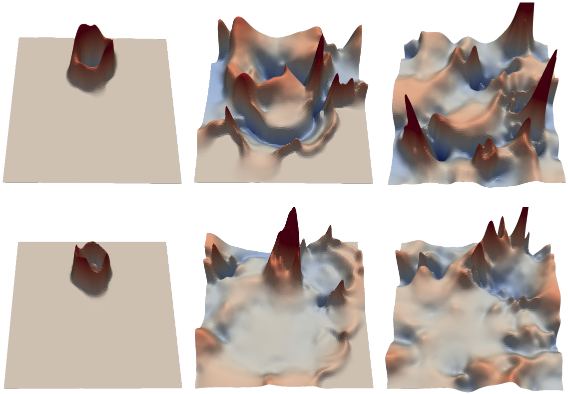
Experimental setup for stochastic acoustic model

Deterministic input: Initial conditions $(\mathbf{v}_0, p_0) = (\mathbf{0}, 0)$, $\kappa(\mathbf{x}) \equiv 1$, $\mathbf{f} \equiv \mathbf{0}$ and $g(t, \mathbf{x}) = g_1(t) g_2(\mathbf{x})$

Stochastic input: Log-normal field for $\rho(\omega, \mathbf{x})$ with

$$\mathrm{Cov}(x_1, x_2) = \sigma^2 \exp\left(- \|x_1 - x_2\|_2^s / \lambda^s\right)$$





Methods and hardware:

- 3^{rd} order DIRK + $V_{\ell,p=1}^{\mathrm{dG}}$ + MLMC on $|\mathcal{P}| = 128$
- Used $V_{\ell,p=1,q=1}^{\mathrm{ST\text{-}dG}}$ + MLMC on $|\mathcal{P}| = 512$

Output: $\widehat{\mathrm{Q}}_{L,\{M_\ell\}_{\ell=0}^L}^{\mathrm{MLMC}}$ in region of interest and $\widehat{\mathbf{u}}_{L,\{M_\ell\}_{\ell=0}^L}^{\mathrm{MLMC}}$

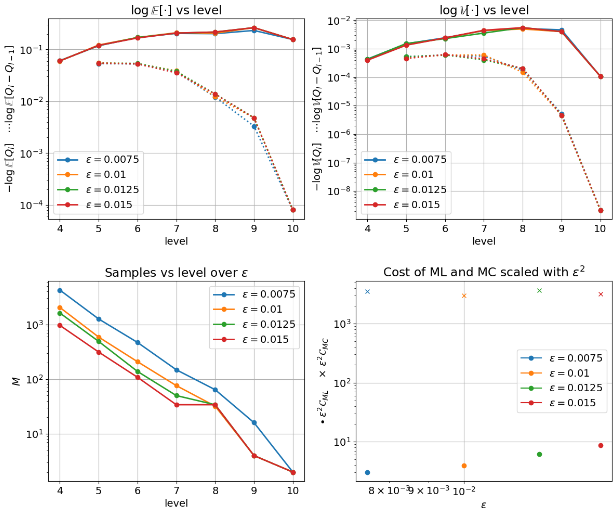
Numerical results - convergence in L^2 in region of interest

Software:

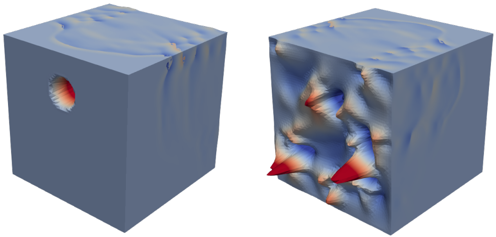
- `https://git.scc.kit.edu/mpp/mpp`
- `https://git.scc.kit.edu/mpp/mluq`

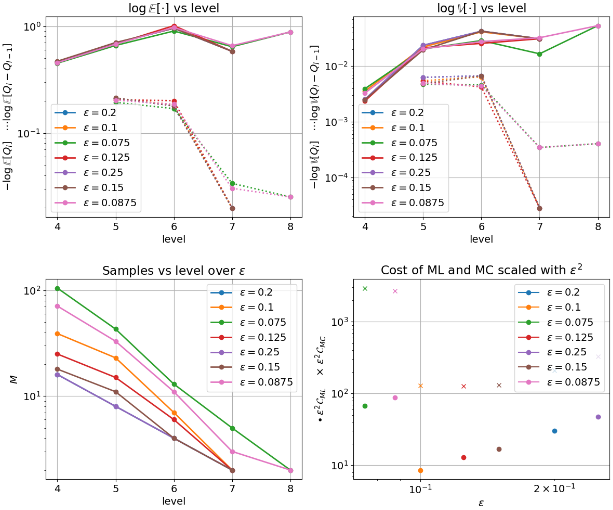
Further ideas and outlook:

- Cost restricted implementation
- Apply to visco-acoustic, visco-elastic or Maxwell systems [Hoc+15]
- Regularity investigations like in [Tec+13; BW21] and in L^1
- Post smoothing, higher moments, cost statistics
- Pick up ideas from MLSC for NLS [JS21]



Numerical results - proof of concept for space-time





Further ideas and outlook:

- Multilevel preconditioning [DFW16; Dör+19]
- Apply p, q - adaptivity [Zie19]
- Cut out space-time cone [Ern18]
- Matrix-free implementation [KK19]
- Combining MIMC [HNT16] with space-time

Outlook and Conclusion

Conclusion:

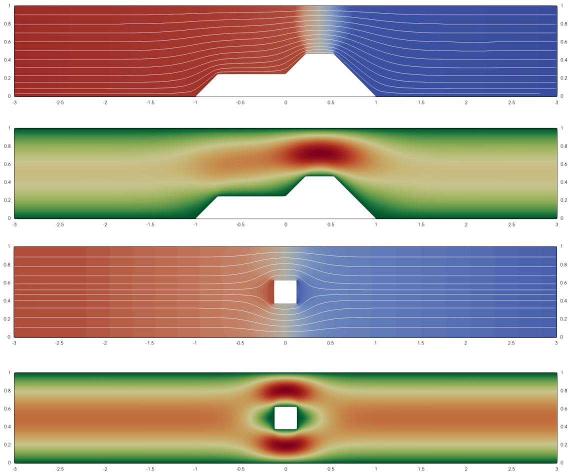
- Acoustic wave equation with random coefficients
- Integrated estimator parallelization leading to a multi-sample system
- Comparison of implicit time-stepping schemes and space-time discretizations with MLMC

Further ideas:

- Cost restricted implementation for rigorous benchmarking
- Use stochastic collocation for comparison
- Employ UQ methods in other `M++` applications

Interval arithmetic existence proof of the Navier-Stokes equation

$$
\begin{aligned}
-\Delta u + \mathrm{Re}[(u \cdot \nabla)u + (u \cdot \nabla)\Gamma + (\Gamma \cdot \nabla)u + \nabla p] &= g \quad \text{in } \Omega \\
\operatorname{div} u &= 0 \quad \text{in } \Omega \\
u &= 0 \quad \text{on } \partial\Omega
\end{aligned}
$$



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