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]
- Motivation for this talk: Move to more general applications, while maintaining usability of many methods.
### Non-intrusive Uncertainty Quantification

<table>
<thead>
<tr>
<th>Method</th>
<th>No UQ</th>
<th>SC</th>
<th>MLMC</th>
<th>MIMC</th>
<th>MLSC</th>
</tr>
</thead>
<tbody>
<tr>
<td>FD</td>
<td>[MNT13; MNT15]</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>FEM</td>
<td>[BW21]</td>
<td>[BNT10; NTW08; FS21]</td>
<td>[CST13; Tec+13]</td>
<td>[HNT16]</td>
<td>[Tec+15]</td>
</tr>
<tr>
<td>DG/FV+TS</td>
<td>[Hoc+15; Boh+21]</td>
<td></td>
<td>[MSŠ12; MSŠ16]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>ST(DG/PG)</td>
<td>[DFW16; Dör+19]</td>
<td></td>
<td>[Bad+21]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Other</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>[JS21]</td>
</tr>
</tbody>
</table>

- **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?
  - 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 \((v, p)(t) = u(t) \in V\)

\[
\begin{align*}
\rho \partial_t v - \nabla p &= f & D \times (0, T) \\
\partial_t p - \kappa \div v &= g & D \times (0, T) \\
(v, p) &= 0 & \partial D \times (0, T) \\
(v, p)(0) &= (v_0, p_0) & D
\end{align*}
\]

where \(V = H(\div; D) \times H_0^1(D) \subset L^2(D, \mathbb{R}^J)\)

- \(\rho, \kappa^{-1} \in L^\infty(D; \mathbb{R}_+) \Rightarrow c(x) = \sqrt{\frac{\kappa(x)}{\rho(x)}} < \infty\)
- \((f, g)(t) = b(t) \in L^2(D; \mathbb{R}^J)\)
- \((v_0, p_0) = u_0 \in L^2(D; \mathbb{R}^J)\)

General setting of linear hyperbolic conservation laws:

\[
M \partial_t u(t) + Au(t) = b(t), \quad t \in (0, T), \quad u(0) = u_0,
\]

where

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

\[
(Av, v)_{0,D} = 0, \quad v \in D(A)
\]

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

\[
\partial_t E(u(t)) = (M \partial_t u(t), u(t))_{0,D} = - (Au(t), u(t))_{0,D} = 0
\]
Random model problem

Random acoustic wave: Search for $u(t): \Omega \rightarrow V$

\[
\begin{align*}
\rho(\omega) \partial_t v(\omega) - \nabla p(\omega) &= f(\omega) & D \times (0, T) \\
\partial_t p(\omega) - \kappa(\omega) \text{div} v(\omega) &= g(\omega) & D \times (0, T) \\
(v, p)(\omega) &= 0 & \partial D \times (0, T) \\
(v, p)(\omega, 0) &= (v_0, p_0)(\omega) & D
\end{align*}
\]

where $\omega \in \Omega$ and

- $\rho, \kappa^{-1} \in L^k(\Omega, L^\infty(D; \mathbb{R}_+)) \Rightarrow c(x) < \infty$ almost surely
- $(f, g)(t) = b(t) \in L^k(\Omega, L^2(D; \mathbb{R}^J))$
- $(v_0, p_0) = u_0 \in L^k(\Omega, L^2(D; \mathbb{R}^J))$
- Further readings [MSŠ16; MS12]

Numerical approximation:

Let $u_h(\omega) = u_\ell(\omega) \in V_\ell$ be an approximation to $u(\omega)$
on level $\ell$ and $Q_\ell(u_\ell(\omega))$ be a quantity of interest of
$u_\ell(\omega)$.

Parametric formulation:

Finite-dimensional noise assumption

$\Rightarrow$ Replace probability space by parametric space

$y = (y_1, \ldots, y_d) \in \Gamma$

and find for all parameters $u(y)$. 

Monte Carlo and stochastic collocation

**MC estimator:** Draw $\omega^{(m)} \in \Omega$, compute $u_\ell(\omega^{(m)})$

\[
\hat{u}^{\text{MC}}_{\ell,M} = M^{-1} \sum_{m=1}^{M} u_\ell(\omega^{(m)}), \quad \hat{Q}^{\text{MC}}_{\ell,M} = M^{-1} \sum_{m=1}^{M} Q_\ell(\omega^{(m)})
\]

**Mean square error and cost:**

\[
e(\hat{Q}^{\text{MC}}_{\ell,M})^2 = M^{-1} \mathbb{V}[Q_\ell] + e_{\text{Approx.}}
\]

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

\[
C_\epsilon(\hat{Q}^{\text{MC}}_{\ell,M}) \lesssim \epsilon^{-2 - \frac{\gamma}{\alpha}}
\]

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

\[
\hat{u}^{\text{SC}}_{\ell,M} = \sum_{m=1}^{M} w_m u_\ell(y^{(m)}), \quad \hat{Q}^{\text{SC}}_{\ell,M} = \sum_{m=1}^{M} w_m Q_\ell(y^{(m)})
\]

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

\[e \sim C_{\text{Tensor}} M^{-a/d} + e_{\text{Approx.}}\]

- Suffers from curse of dimensionality w.r.t. $d$
Multilevel estimator

- Assumptions: The approximation is convergent
  \[ |E[Q_\ell - Q]| \lesssim h_\ell^\alpha, \quad \alpha > 0 \] (1)

  The cost for one sample is bounded
  \[ C(Q_\ell(\omega^{(m)})) \lesssim h_\ell^{-\gamma}, \quad \gamma > 0 \] (2)

  The variance of \( Q_\ell - Q_{\ell-1} \) decays
  \[ \nabla[Q_\ell - Q_{\ell-1}] \lesssim h_\ell^\beta, \quad \beta > 0 \] (3)

- Idea: Set \( Y_\ell := Q_\ell - Q_{\ell-1}, Y_0 := Q_0 \), compute samples on \( \ell \in \{0, \ldots L\} \), balance \( C_\ell \) and \( M_\ell \)

\[ E[Q_L] = E[Q_0] + \sum_{\ell=1}^{L} E[Q_\ell - Q_{\ell-1}] = \sum_{\ell=0}^{L} E[Y_\ell] \]

- Multilevel estimators: Estimate \( Y_\ell \) with MC / SC

\[ \hat{Y}_{\ell,M_\ell}^{MC} = M_\ell^{-1} \sum_{m=1}^{M_\ell} Y_\ell(\omega^{(m)}) \Rightarrow \hat{Q}_{L,\{M_\ell\}_{\ell=0}}^{MLMC} = \sum_{\ell=0}^{L} \hat{Y}_{\ell,M_\ell}^{MC} \]

- Mean square error and cost for MLMC:

\[ e^2(\hat{Q}_{L,\{M_\ell\}_{\ell=0}}^{MLMC}) = L \sum_{\ell=0}^{L} M_\ell^{-1} \nabla[Y_\ell] + e_{\text{Approx.},} \]

\[ C(\hat{Q}_{L,\{M_\ell\}_{\ell=0}}^{MLMC}) \lesssim \sum_{\ell=0}^{L} M_\ell C_\ell, \]

\[ C_\epsilon(\hat{Q}_{L,\{M_\ell\}_{\ell=0}}^{MLMC}) \lesssim \epsilon^{-2-(\gamma-\beta)/\alpha} \]
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

$$\triangle M_\ell = 1 \implies \mathcal{M}_T$$

$$k \in \mathbb{N}: 2^k \leq \frac{|\mathcal{P}|}{\triangle M_\ell} < 2^{k+1} \implies \left\{ \mathcal{M}_{\mathcal{P}_k}^{(m)} \right\}_{m=1}^{\triangle M_\ell}, \mathcal{P}_k \subset \mathcal{P}, |\mathcal{P}_k| = 2^k$$

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

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 $\gamma^{(m)} \in \Theta_{M_\ell}$:
  - Distribute deterministic samples on $\mathcal{P}$

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

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

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

$$L_\ell^{(m)} \mathbf{u}_\ell^{(m)} = \mathbf{b}_\ell^{(m)} \text{ on } \mathcal{M}_{\mathcal{P}_k}^{(m)}, m = 1, \ldots, M_\ell$$

Further readings: [ŠMS11; Šuk13; Drz+17; BHP21]
Multi-sample system for the model problem and cost restricted implementation

Multi-sample dG-sys.: Search for \( (u_\ell(t))_{m=1}^{M_\ell} \in V^{dG,P}_\ell,p \)

\[
\begin{align*}
M_\ell^{(m)} \partial_t u_\ell^{(m)}(t) + A_\ell^{(m)} u_\ell^{(m)}(t) &= b_\ell^{(m)}(t), & t \in (0, T),
\end{align*}
\]

where \( V^{dG,P}_\ell,p = \prod_{p_k \in P} V^{dG}_{\ell,k,p} \):
- 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.

\[
V^{dG}_\ell,p = \{ v_\ell \in L^2(D; \mathbb{R}^J) : v_\ell|_K \in \mathbb{P}_p(K; \mathbb{R}^J), \forall K \in \mathcal{K} \}
\]

Classic ML estimator implementation:
- Requires a-priori knowledge about \( \alpha, \beta, \gamma \) and hidden constants in (1), (2), (3).

Implementation with post estimation:
- \[
M_\ell = \left[ 2\epsilon^2 \sqrt{\frac{\mathbb{V}[Y_\ell]}{C_\ell}} \left( \sum_{\ell=0}^{L} \sqrt{\mathbb{V}[Y_\ell]} C_\ell \right) \right]
\]
- Richardson-extrapolation to find \( L \)

Cost restricted implementation:
- Total computational budget \( B^0 \) is given, \( \eta < 1 \)
  
  while \( B^i > 0 \):

\[
Q^i, C^i \leftarrow \text{MLMC}(\epsilon^i) \quad \epsilon^{i+1} \leftarrow \eta \epsilon^i, \quad B^{i+1} \leftarrow B^i - C^i, \quad i \leftarrow i + 1
\]

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

Semi-discrete system: Search for \( u_\ell(t) \in V_{\ell,p}^{dG} \)

\[
M_\ell \partial_t u_\ell(t) + A_\ell u_\ell(t) = b_\ell(t), \quad t \in (0, T),
\]

where \( M_\ell, A_\ell \in \mathcal{L}(V_{\ell,p}^{dG}, V_{\ell,p}^{dG}) \):
- \( M_\ell \) is block-diagonal and positive definite
- \( A_\ell \) is non-symmetric stiffness matrix
- Stability, consistency, convergence see [Hoc+15]

Implicit time-stepping:

\[
u^{n+1} = \Phi_n \left( -\tau M_\ell^{-1} A_\ell \right) u^n, \quad n = 0, 1, \ldots,
\]

\( \Phi_n \) being a rational stability function:
- A-stable method to avoid random CFL

Weak formulation in space-time: Search for \( u \in V \)

\[
(u, L^* w)_Q = (b, w)_Q + (u_0, w(0))_D, \quad \forall w \in W
\]

with \( Q := D \times [0, T] \). Discr. \([0, T]\) with \( I \), search in:

\[
V_{\ell,p,q}^{ST-dG} = \{ v_\ell \in L^2([0, T]; L^2(D; \mathbb{R}^J)) : v_\ell |_{K,I} \in P_p(K; \mathbb{R}^J) \otimes P_q(I; \mathbb{R}^J), \quad \forall K \in \mathcal{K}, \forall I \in \mathcal{I} \}
\]

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

\[
\| (u_\ell - u)(T) \|_D \lesssim h^{s-1/2}
\]

- Further readings [Ban+21; Zie19]
Deterministic input: Initial conditions \((v_0, p_0) = (0, 0)\), \(\kappa(x) \equiv 1\), \(f \equiv 0\) and \(g(t, x) = g_1(t)g_2(x)\)

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

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

Methods and hardware:
- 3\textsuperscript{rd} order DIRK + \(V_{\ell,p=1}^{dG}\) + MLMC on \(|\mathcal{P}| = 128\)
- Used \(V_{\ell,p=1,q=1}^{\text{ST-dG}}\) + MLMC on \(|\mathcal{P}| = 512\)

Output: \(\hat{Q}_{LMC \{\ell\}, \{M_{\ell}\}_{\ell=0}}^{LMC}\) in region of interest and \(\hat{u}_{LMC \{\ell\}, \{M_{\ell}\}_{\ell=0}}^{LMC}\)
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]
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

\[-\Delta u + \text{Re}\left((u \cdot \nabla)u + (u \cdot \nabla)\Gamma + (\Gamma \cdot \nabla)u + \nabla p\right) = g \quad \text{in } \Omega\]

\[\text{div } u = 0 \quad \text{in } \Omega\]

\[u = 0 \quad \text{on } \partial \Omega\]