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SEIT 1386

UM++ Bridge - Accessing FEM-Models and UQ-Methods from M++

A Fully Parallelized and Budgeted MLMC Method - Acoustic Wave Propagation - Client and Server Interface to Umbridge

Niklas Baumgarten, Christian Wieners, Sebastian Krumscheid, Linus Seelinger | 12.12.2023

Model Problem and Investigation Goals

Acoustic wave: Search $(\mathbf{v}, p)\colon \Omega \times \mathcal{D} \times [0, T] \to \mathbb{R}^{D+1}$,

such that $$\begin{cases} \rho(\omega)\partial_t \mathbf{v}(\omega) - \nabla p(\omega) & = & \mathbf{f} & \mathcal{D} \times (0, T] \\ \partial_t p(\omega) - \operatorname{div}(\mathbf{v}(\omega)) & = & g & \mathcal{D} \times (0, T] \\ \mathbf{v} \cdot \mathbf{n} & = & 0 & \Gamma \times (0, T] \\ \mathbf{v}(0) & = & \mathbf{v}_0 & \mathcal{D} \\ p(0) & = & p_0 & \mathcal{D} \end{cases}$$

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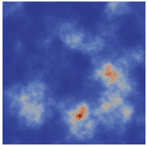

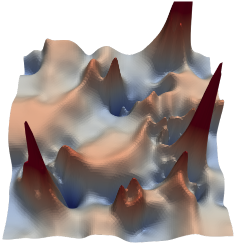

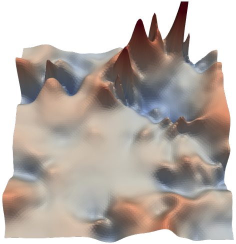

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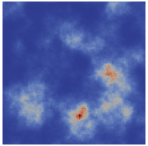
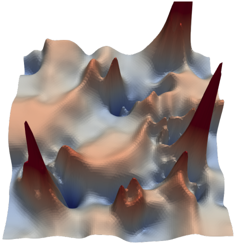
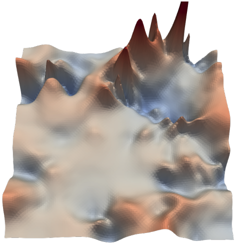




Determine: $\mathbb{E}[\mathrm{Q}] := \int_\Omega \mathrm{Q}(\omega) \mathrm{d}\mathbb{P} \approx M^{-1} \sum_{m=1}^{M} \mathrm{Q}_\ell(\mathbf{y}^{(m)}) =: \widehat{\mathrm{Q}}_{\ell,M}^{\mathrm{MC}}$



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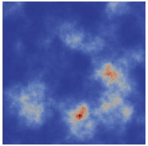

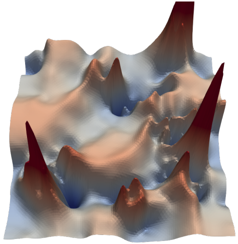

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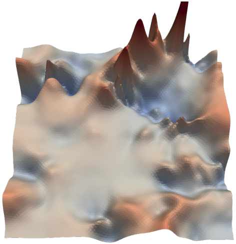

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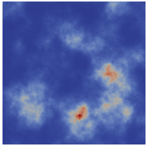

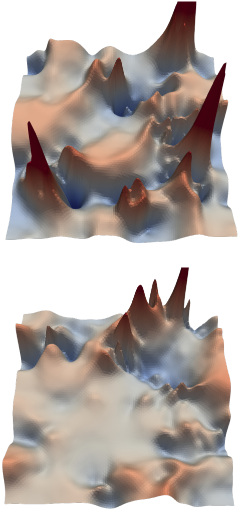

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Constraint: Finite computational capacities (CPUs, time, memory)

$\Rightarrow$ Introduce budget for error minimization and utilize effective parallelization

Multi-level Monte Carlo - Introduction

Assumptions: Let $\alpha, \beta, \gamma > 0$ and

$$|\mathbb{E}[\mathrm{Q}_\ell - \mathrm{Q}]| \lesssim h_\ell^\alpha$$
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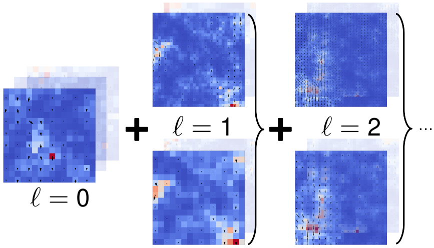

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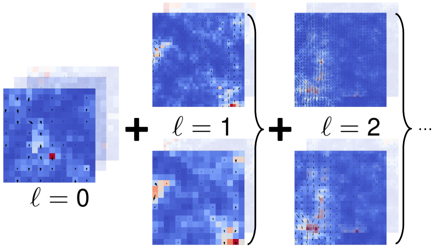

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Epsilon-Cost Theorem: $\exists \{M_\ell\}_{\ell=0}^L$, such that

$$\mathrm{err}_{\mathrm{MSE}} = \sum_{\ell=0}^{L} M_\ell^{-1} \mathbb{V}[\mathrm{Y}_\ell] + (\mathbb{E}[\mathrm{Q}_L - \mathrm{Q}])^2 < \epsilon^2$$

and $\quad \mathrm{T}_\epsilon := \mathrm{C}_\epsilon \lesssim \begin{cases} \epsilon^{-2} & \beta > \gamma \\ \epsilon^{-2-(\gamma-\beta)/\alpha} & \beta < \gamma \end{cases}$

M. Giles. *Multilevel Monte Carlo path simulation.* (2008)

Budgeted Multi-level Monte Carlo - Introduction

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Conjecture: For a feasible and parallel execution, it is

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with $\delta \in \left\{ \frac{1}{2}, \frac{\alpha}{(2\alpha + (\gamma - \beta))} \right\}$ and $\lambda_\mathrm{p} \in [0, 1]$.

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- Decomposition in overlapping subproblems
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Approximated Knapsack Problem:

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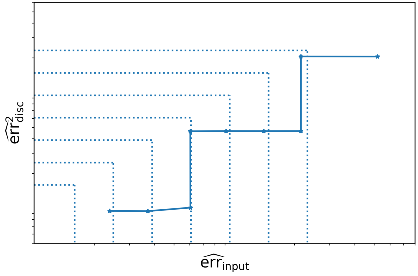
$$\texttt{data} = \left\{ \mathrm{i} \mapsto \left\{ \mathrm{err}_\mathrm{i}, \{M_{\mathrm{i},\ell}\}_{\ell=0}^{L_\mathrm{i}}, \{\widehat{\mathrm{Q}}_{\mathrm{i},\ell}\}_{\ell=0}^{L_\mathrm{i}}, \{\widehat{\mathrm{C}}_{\mathrm{i},\ell}\}_{\ell=0}^{L_\mathrm{i}}, \{\widehat{\mathrm{Y}}_{\mathrm{i},\ell}\}_{\ell=0}^{L_\mathrm{i}}, \dots \right\} \right\}$$

$\texttt{function BMLMC}(\mathrm{B}_0, \{M_{0,\ell}^{\mathrm{init}}\}_{\ell=0}^{L_0})$:

$$\begin{cases} \texttt{for } \ell = L_0, \dots, 0: & \Delta\texttt{data}_{0,\ell} \leftarrow \texttt{MS-FEM}(M_{0,\ell}^{\mathrm{init}}, \mathcal{P}) \\ \texttt{data}_0 \leftarrow \texttt{Welford}(\texttt{data}_{-1}, \Delta\texttt{data}_0) & \texttt{return BMLMC}(\mathrm{B}_0 - \sum_{\ell=0}^{L_0} \mathrm{C}_\ell, \eta \cdot \mathrm{err}_0) \end{cases}$$

$\texttt{function BMLMC}(\mathrm{B}_\mathrm{i}, \epsilon_\mathrm{i})$:

$$\begin{cases} \texttt{if } \mathrm{B}_\mathrm{i} \approx 0: & \texttt{return } \mathrm{err}_{\mathrm{i}-1} \\ \texttt{if } \widehat{\mathrm{err}}_{\texttt{disc}}(\texttt{data}_{\mathrm{i}-1}) \geq \sqrt{1-\theta}\epsilon_\mathrm{i}: & L_\mathrm{i} \leftarrow L_\mathrm{i} + 1 \\ \texttt{if } \widehat{\mathrm{err}}_{\texttt{input}}(\texttt{data}_{\mathrm{i}-1}) \geq \theta\epsilon_\mathrm{i}^2: & \widehat{M}_{\mathrm{i},\ell}^{\mathrm{opt}} \sim \left\lceil (\sqrt{\theta}\epsilon)^{-2} \sqrt{s_{\mathrm{Y}_\ell}^2 / \widehat{\mathrm{C}}_\ell} \right\rceil \\ \texttt{for } \ell = L_\mathrm{i}, \dots, 0: & \Delta M_{\mathrm{i},\ell} \leftarrow \max \left\{ \widehat{M}_{\mathrm{i},\ell}^{\mathrm{opt}} - M_{\mathrm{i}-1,\ell}, 0 \right\} \\ \widehat{\mathrm{C}}_\mathrm{i} \leftarrow \sum_{\ell=0}^{L_\mathrm{i}} \Delta M_{\mathrm{i},\ell} \widehat{\mathrm{C}}_{\mathrm{i}-1,\ell} & \\ \texttt{if } \widehat{\mathrm{C}}_\mathrm{i} = 0: & \texttt{return BMLMC}(\mathrm{B}_\mathrm{i}, \eta \cdot \epsilon_\mathrm{i}) \\ \texttt{if } \widehat{\mathrm{C}}_\mathrm{i} > \mathrm{B}_\mathrm{i}: & \texttt{return BMLMC}(\mathrm{B}_\mathrm{i}, 0.5 \cdot (\epsilon_\mathrm{i} + \epsilon_{\mathrm{i}-1})) \\ \texttt{for } \ell = L_\mathrm{i}, \dots, 0: & \Delta\texttt{data}_{\mathrm{i},\ell} \leftarrow \texttt{MS-FEM}(\Delta M_{\mathrm{i},\ell}, \mathcal{P}) \\ \texttt{data}_\mathrm{i} \leftarrow \texttt{Welford}(\texttt{data}_{\mathrm{i}-1}, \Delta\texttt{data}_\mathrm{i}) & \texttt{return BMLMC}(\mathrm{B}_\mathrm{i} - \sum_{\ell=0}^{L_\mathrm{i}} \mathrm{C}_\ell, \epsilon_\mathrm{i}) \end{cases}$$



M. Giles. *Multilevel Monte Carlo methods.* (2015)

Collier et al. *A continuation multilevel Monte Carlo algorithm.* (2015)

Multi-sample Finite Element Method (MS-FEM)

Problem: Approximate M_ℓ-times a PDE on discretization level ℓ on a fixed set of CPUs $\mathcal{P}$

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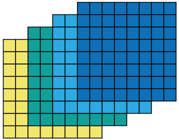

$1 < |\mathcal{P}| \leq M_\ell$

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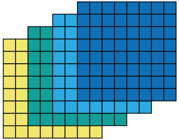
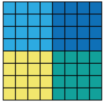


$1 < |\mathcal{P}| \leq M_\ell$



$1 < |\mathcal{P}|$ & $M_\ell = 1$

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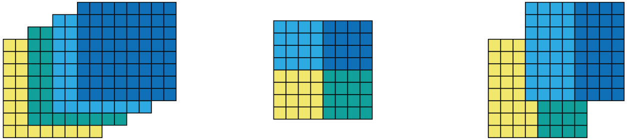

$1 < |\mathcal{P}| \leq M_\ell$ $\quad$ $1 < |\mathcal{P}|$ & $M_\ell = 1$ $\quad$ $1 < M_\ell < |\mathcal{P}|$

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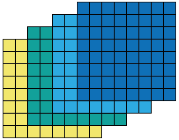

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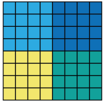

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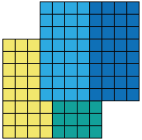

$1 < M_\ell < |\mathcal{P}|$

Minimize Communication: Search $k \in \mathbb{N}_0$, such that

$$2^k \leq \frac{|\mathcal{P}|}{M_\ell} < 2^{k+1} \quad \Rightarrow \quad \mathcal{P} = \bigsqcup_{m=1}^{M_\ell} \mathcal{P}_k^{(m)} \text{ with } \left|\mathcal{P}_k^{(m)}\right| = 2^k$$

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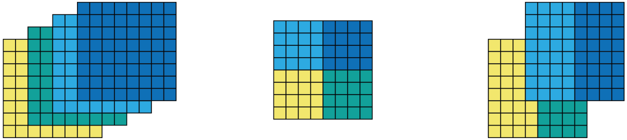


$1 < |\mathcal{P}| \leq M_\ell$ $\quad$ $1 < |\mathcal{P}|$ & $M_\ell = 1$ $\quad$ $1 < M_\ell < |\mathcal{P}|$

Define: Set of FE meshes

$$\mathcal{M}_\mathcal{P} := \left\{ \mathcal{M}_{\mathcal{P}_k}^{(m)} \right\}_{m=1}^{M_\ell}$$

Minimize Communication: Search $k \in \mathbb{N}_0$, such that

$$2^k \leq \frac{|\mathcal{P}|}{M_\ell} < 2^{k+1} \;\Rightarrow\; \mathcal{P} = \bigsqcup_{m=1}^{M_\ell} \mathcal{P}_k^{(m)} \text{ with } \left| \mathcal{P}_k^{(m)} \right| = 2^k$$

MS-FEM: Search for representation of

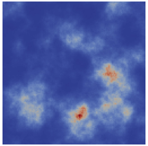
$$(\mathbf{u}_\ell)_{m=1}^{M_\ell} \in \prod_{m=1}^{M_\ell} V_\ell^{(m)}$$

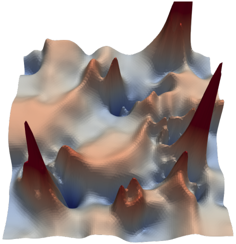
defined on $\mathcal{M}_\mathcal{P}$

Model Problem and Discretization

Acoustic wave: Search $(\mathbf{v}, p)\colon \Omega \times \mathcal{D} \times [0, T] \to \mathbb{R}^{D+1}$,

$$\text{such that} \quad \begin{cases} \rho(\omega)\partial_t \mathbf{v}(\omega) - \nabla p(\omega) & = & \mathbf{f} & \mathcal{D} \times (0, T] \\ \partial_t p(\omega) - \operatorname{div}(\mathbf{v}(\omega)) & = & g & \mathcal{D} \times (0, T] \\ \mathbf{v} \cdot \mathbf{n} & = & 0 & \Gamma \times (0, T] \\ \mathbf{v}(0) & = & \mathbf{v}_0 & \mathcal{D} \\ p(0) & = & p_0 & \mathcal{D} \end{cases}$$



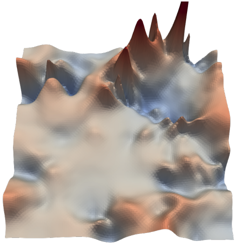


Discontinuous Galerkin (dG): Search for $(\mathbf{v}, p)^\top =: \mathbf{u}_\ell \in V_{\ell,\mathbf{p}}^{\mathrm{dG}}$

$$\mathrm{M}_\ell \partial_t \mathbf{u}_\ell + \mathrm{A}_\ell \mathbf{u}_\ell = \mathbf{b}_\ell \quad \text{and} \quad \mathbf{u}_\ell(0) = \mathbf{u}_{\ell,0}$$

Implicit midpoint-rule (IMPR): Solve for $t_n = n\tau_\ell$ with $\tau_\ell = T/N_\ell^\mathcal{T}$

$$\left(\mathrm{M}_\ell + \frac{\tau_\ell}{2}\mathrm{A}_\ell\right)\mathbf{u}_\ell(t_n) = \left(\mathrm{M}_\ell - \frac{\tau_\ell}{2}\mathrm{A}_\ell\right)\mathbf{u}_\ell(t_{n-1}) + \tau_\ell \mathbf{b}_\ell(t_{n-1/2})$$



Circulant Embedding: Sample from log-normally distributed material density ρ

Numerical Experiments - Covariance Function

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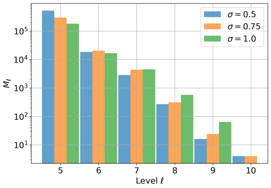
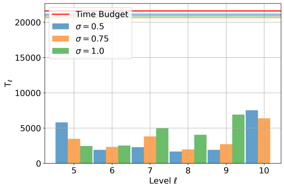
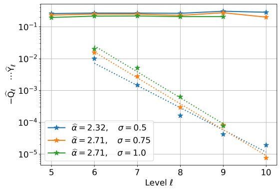
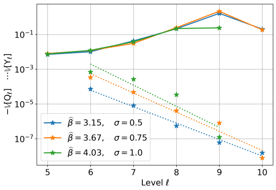
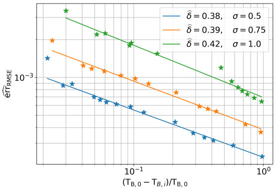
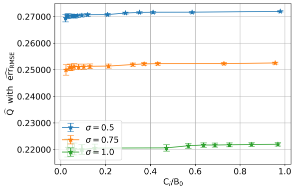












Covariance Function:

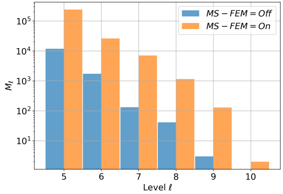
$$\mathrm{Cov}(\mathbf{x}_1, \mathbf{x}_2) = \sigma^2 \exp\left(- \left\| \left(\frac{\mathbf{x}_1 - \mathbf{x}_2}{\lambda} \right) \right\|_2^\nu \right)$$

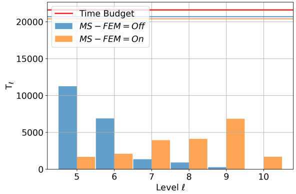
with $\lambda = 0.15$, $\nu = 1.8$ and $\sigma \in \{0.5, 0.75, 1.0\}$

Numerical Experiments - Parallelization

1st Experiment:

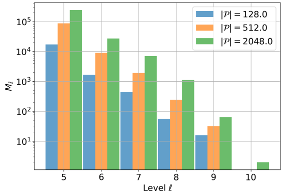
- Solver parallelization vs. MS-FEM with fixed $\mathrm{B} = 2048 \cdot 6\mathrm{h}$

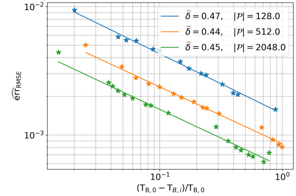




2nd Experiment:

- Weak scaling measurement with $\mathrm{T_B} = 6\mathrm{h}$ on $|\mathcal{P}| \in \{128, 512, 2048\}$





Recall of Algorithm & Umbridge Client Interface

$$\texttt{data} = \left\{ \mathrm{i} \mapsto \left\{ \mathrm{err}_\mathrm{i}, \{M_{\mathrm{i},\ell}\}_{\ell=0}^{L_\mathrm{i}}, \{\widehat{\mathrm{Q}}_{\mathrm{i},\ell}\}_{\ell=0}^{L_\mathrm{i}}, \{\widehat{\mathrm{C}}_{\mathrm{i},\ell}\}_{\ell=0}^{L_\mathrm{i}}, \{\widehat{\mathrm{Y}}_{\mathrm{i},\ell}\}_{\ell=0}^{L_\mathrm{i}}, \dots \right\} \right\}$$

$\texttt{function BMLMC}(\mathrm{B}_0, \{M^{\text{init}}_{0,\ell}\}_{\ell=0}^{L_0})$:

$$\begin{cases} \texttt{for } \ell = L_0, \dots, 0: & \Delta\texttt{data}_{0,\ell} \leftarrow \texttt{MS-FEM}(M^{\text{init}}_{0,\ell}, \mathcal{P}) \\ \texttt{data}_0 \leftarrow \texttt{Welford}(\texttt{data}_{-1}, \Delta\texttt{data}_0) & \texttt{return BMLMC}(\mathrm{B}_0 - \sum_{\ell=0}^{L_0} \mathrm{C}_\ell, \eta \cdot \mathrm{err}_0) \end{cases}$$

$\texttt{function BMLMC}(\mathrm{B}_\mathrm{i}, \epsilon_\mathrm{i})$:

$$\begin{cases} \texttt{if } \mathrm{B}_\mathrm{i} \approx 0: & \texttt{return } \mathrm{err}_{\mathrm{i}-1} \\ \texttt{if } \widehat{\mathrm{err}}_{\texttt{disc}}(\texttt{data}_{\mathrm{i}-1}) \geq \sqrt{1-\theta}\epsilon_\mathrm{i}: & L_\mathrm{i} \leftarrow L_\mathrm{i} + 1 \\ \texttt{if } \widehat{\mathrm{err}}_{\texttt{input}}(\texttt{data}_{\mathrm{i}-1}) \geq \theta\epsilon_\mathrm{i}^2: & \widehat{M}^{\text{opt}}_{\mathrm{i},\ell} \sim \left\lceil (\sqrt{\theta}\epsilon)^{-2} \sqrt{s^2_{\mathrm{Y}_\ell} / \widehat{\mathrm{C}}_\ell} \right\rceil \\ \texttt{for } \ell = L_\mathrm{i}, \dots, 0: & \Delta M_{\mathrm{i},\ell} \leftarrow \max\left\{ \widehat{M}^{\text{opt}}_{\mathrm{i},\ell} - M_{\mathrm{i}-1,\ell}, 0 \right\} \\ \widehat{\mathrm{C}}_\mathrm{i} \leftarrow \sum_{\ell=0}^{L_\mathrm{i}} \Delta M_{\mathrm{i},\ell} \widehat{\mathrm{C}}_{\mathrm{i}-1,\ell} & \\ \texttt{if } \widehat{\mathrm{C}}_\mathrm{i} = 0: & \texttt{return BMLMC}(\mathrm{B}_\mathrm{i}, \eta \cdot \epsilon_\mathrm{i}) \\ \texttt{if } \widehat{\mathrm{C}}_\mathrm{i} > \mathrm{B}_\mathrm{i}: & \texttt{return BMLMC}(\mathrm{B}_\mathrm{i}, 0.5 \cdot (\epsilon_\mathrm{i} + \epsilon_{\mathrm{i}-1})) \\ \texttt{for } \ell = L_\mathrm{i}, \dots, 0: & \Delta\texttt{data}_{\mathrm{i},\ell} \leftarrow \texttt{MS-FEM}(\Delta M_{\mathrm{i},\ell}, \mathcal{P}) \\ \texttt{data}_\mathrm{i} \leftarrow \texttt{Welford}(\texttt{data}_{\mathrm{i}-1}, \Delta\texttt{data}_\mathrm{i}) & \texttt{return BMLMC}(\mathrm{B}_\mathrm{i} - \sum_{\ell=0}^{L_\mathrm{i}} \mathrm{C}_\ell, \epsilon_\mathrm{i}) \end{cases}$$

```cpp
#ifdef UMBRIDGE_CLIENT
    umbridge::HTTPModel client(
        "http://localhost:4242", "forward"
    );
#else
  std::unique_ptr<PDESolver> pdeSolver =
    CreatePDESolverUnique(slEstmConf.pdeSolvConf.
          WithCommSplit(commSplit));
#endif
// Only code snippet, more stuff happening here
#ifdef UMBRIDGE_CLIENT
    fineSolution.Q = client.Evaluate(input);
    if (!slEstmConf.onlyFine)
        coarseSolution.Q = client.Evaluate(input);
#else
    // Solves PDE for several samples in parallel
    fineSolution = pdeSolver->Run(input);
    if (!slEstmConf.onlyFine)
        coarseSolution = pdeSolver->Run(input);
#endif
// Only code snippet, more stuff happening here
```

Umbridge Server Interface & M++

```cpp
#include "AcousticPDESolver"
#include "umbridge.h"

class AcousticPDESolver4Umbridge : public AcousticPDESolver, public umbridge::Model {
public:
  explicit AcousticPDESolver4Umbridge(const PDESolverConfig &conf)
      : AcousticPDESolver(conf), umbridge::Model("forward") {}

  std::vector<std::size_t> GetInputSizes(const json &config_json) const override {
    return {static_cast<unsigned long>(GetProblem().StochasticDimension())};
  }

  std::vector<std::size_t> GetOutputSizes(const json &config_json) const override {
    return {1}; // Always one since only a QoI is returned
  }

  std::vector<std::vector<double>> Evaluate(const std::vector<std::vector<double>> &
        inputs, json json_config) override {
    PPM->Broadcast(inputs); // WIP
    GetProblem().SetSample(inputs);
    return {{Run().Q}};
  }
};
```

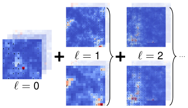
https://gitlab.kit.edu/kit/mpp/mpp

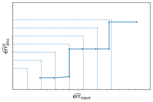
```
src/
  lib0_basic/
  lib1_math/
  lib2_mesh/
  ...
  lib6_app/      ← Umbridge Server
  lib7_uq/       ← Umbridge Client
CMakeLists.txt
Dockerfile
.gitlab-ci.yml ← CI for Images (WIP)
```

Conclusion and Outlook

Conclusion:

- Budgeted Multi-level Monte Carlo (BMLMC)





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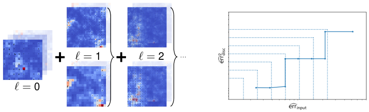

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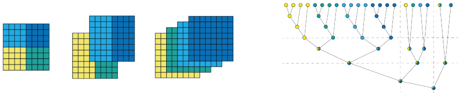

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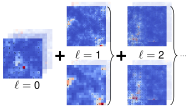

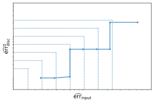

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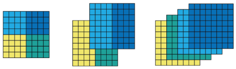
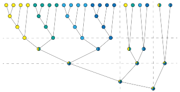
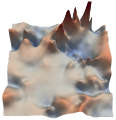
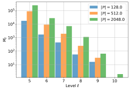
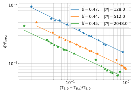




- Acoustic Wave Simulations in Random Media







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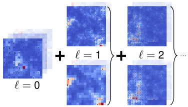

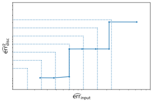

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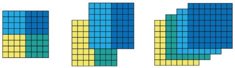

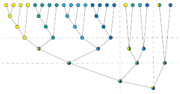

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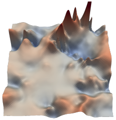

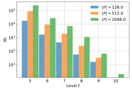

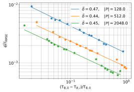

Further Work:

- Other PDEs with various FE&UQ methods

N. Baumgarten. *A Fully Parallelized and Budgeted Multi-level Monte Carlo Framework for Partial Differential Equations: From Mathematical Theory to Automated Large-Scale Computations.* (2023)

Baumgarten, Wieners. *The parallel finite element system M++ with integrated multilevel preconditioning and multilevel Monte Carlo methods.* (2021)

- FEM-Software M++ & Main Source of Talk

Wieners, Corallo, Schneiderhan, Stengel, Lindner, Rheinbay, Baumgarten. *Mpp 3.2.0.* (2023)

Baumgarten et al. *A Fully Parallelized and Budgeted Multi-level Monte Carlo Method and the Application to Acoustic Waves.* arXiv Preprint (2023)

Conclusion and Outlook

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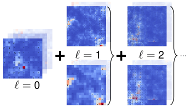

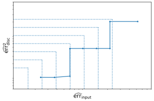

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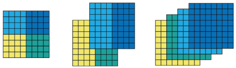

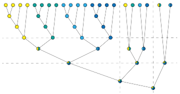

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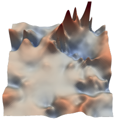

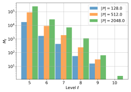

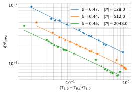

Further Work:

- Other PDEs with various FE&UQ methods

  N. Baumgarten. *A Fully Parallelized and Budgeted Multi-level Monte Carlo Framework for Partial Differential Equations: From Mathematical Theory to Automated Large-Scale Computations.* (2023)

  Baumgarten, Wieners. *The parallel finite element system M++ with integrated multilevel preconditioning and multilevel Monte Carlo methods.* (2021)

- FEM-Software M++ & Main Source of Talk

  Wieners, Corallo, Schneiderhan, Stengel, Lindner, Rheinbay, Baumgarten. *Mpp 3.2.0.* (2023)

  Baumgarten et al. *A Fully Parallelized and Budgeted Multi-level Monte Carlo Method and the Application to Acoustic Waves.* arXiv Preprint (2023)

In Progress / Outlook / Interests:

- Interface to Umbridge
- (B)MLSC, (B)MLQMC, (B)MIMC
- Implementation of $\widehat{\mathbf{u}}_L$ in Mpp 3.2.1
- SGD/ADAM for Optimal Control
- Bayesian Inverse UQ via SMC