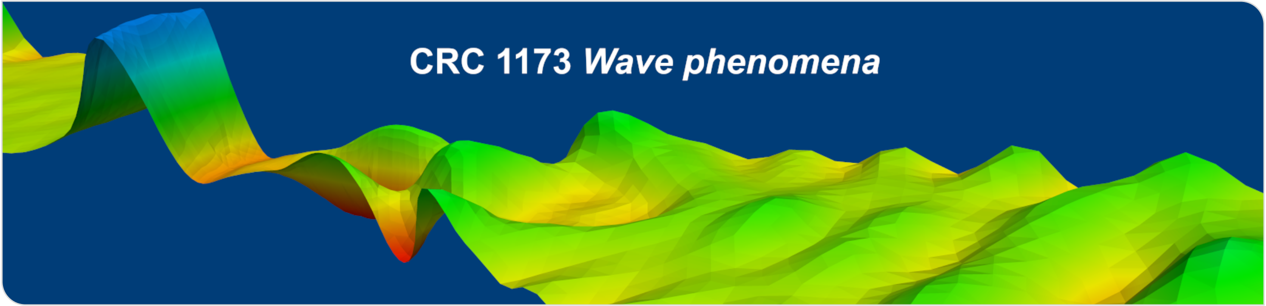
A Fully Parallelized and Budgeted Multi-level Monte Carlo Method

Applications to Acoustic Wave Equations - Parallelization Limits - Automated High-Performance Computing

Niklas Baumgarten, Christian Wieners, Sebastian Krumscheid | 23.10.2023



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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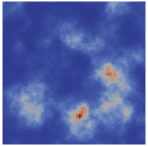

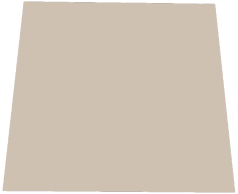

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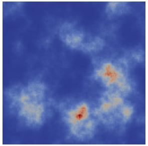

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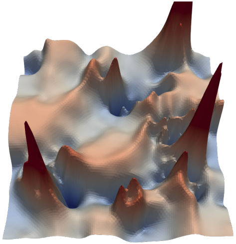

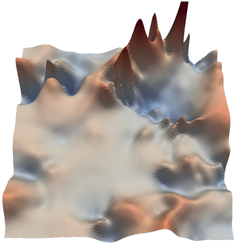

Determine: $$\mathbb{E}[\mathrm{Q}] := \int_\Omega \mathrm{Q}(\omega) \mathrm{d}\mathbb{P} \approx M^{-1} \sum_{m=1}^{M} \mathrm{Q}_\ell(\mathbf{y}^{(m)}) =: \widehat{\mathrm{Q}}_{\ell,M}^{\mathrm{MC}}$$

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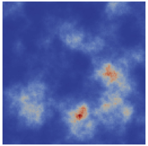

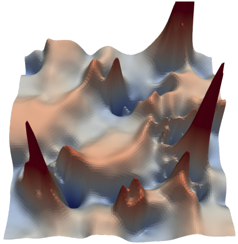

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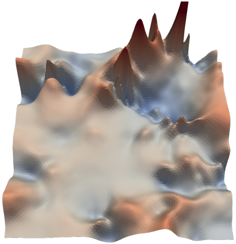
Goal: Find combination of methods to minimize total error

$$\mathrm{err}_{\text{total}} = \mathrm{err}_{\text{input}} + \mathrm{err}_{\text{disc}} + \mathrm{err}_{\text{model}} + \mathrm{err}_{\text{solve}} + \mathrm{err}_{\text{float}} + \mathrm{err}_{\text{bug}} + \dots$$



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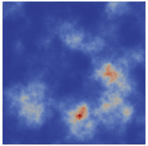

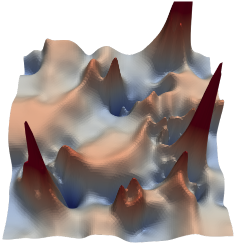

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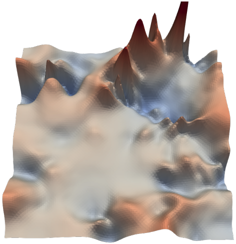

Constraint: Finite computational capacities (CPUs, time, memory)

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

Multi-level Monte Carlo - Introduction

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

$$
\begin{aligned}
|\mathbb{E}[\mathrm{Q}_\ell - \mathrm{Q}]| &\lesssim h_\ell^{\alpha} \\
\mathbb{V}[\mathrm{Q}_\ell - \mathrm{Q}_{\ell-1}] &\lesssim h_\ell^{\beta} \\
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Idea: Telescoping sum with $\mathrm{Y}_0 \coloneqq \mathrm{Q}_0, \mathrm{Y}_\ell \coloneqq \mathrm{Q}_\ell - \mathrm{Q}_{\ell-1}$

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

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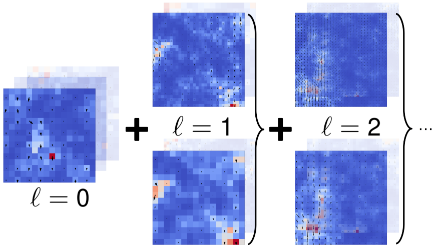

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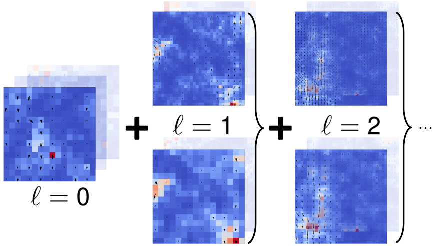

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Epsilon-Cost Theorem: $\exists \{M_\ell\}_{\ell=0}^L$, such that

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

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

Goal: Replace accuracy ϵ by budget $|\mathcal{P}| \cdot \mathrm{T_B} =: \mathrm{B} > 0$ measured in $[\mathrm{B}] = \#$CPU $\cdot$ hours

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- Often no a priori knowledge about α, β and γ
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Knapsack Problem:

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such that $$\sum_{\ell=0}^{L} \sum_{m=1}^{M_\ell} \mathrm{C}_\ell(\mathbf{y}^{(m)}) \leq \mathrm{B}$$

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Karlsruhe Institute of Technology

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

Baumgarten et al. *A Fully Parallelized and Budgeted MLMC Method.* arXiv Preprint (2023)

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Dynamic Programming (DP):

- Decomposition in overlapping subproblems
- Solve subproblems with optimal strategy
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Approximated Knapsack Problem:

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Budgeted Multi-level Monte Carlo - Algorithm

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

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

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

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

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

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

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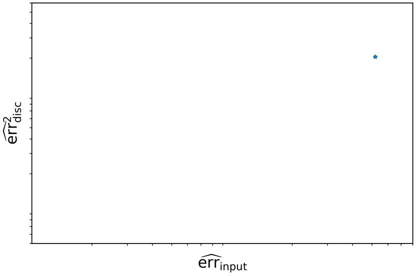

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Budgeted Multi-level Monte Carlo - Algorithm

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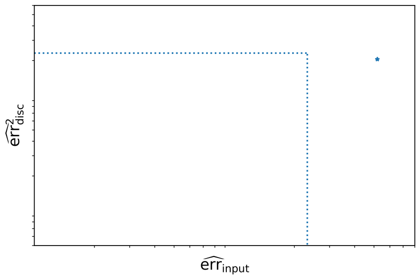

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Budgeted Multi-level Monte Carlo - Algorithm

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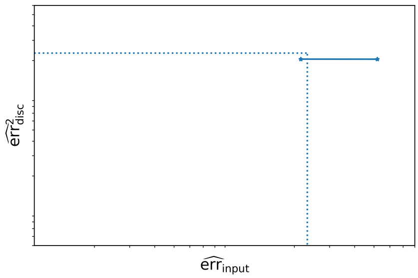

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Budgeted Multi-level Monte Carlo - Algorithm

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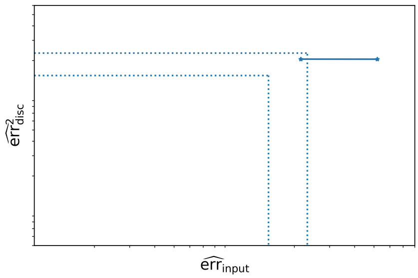

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Budgeted Multi-level Monte Carlo - Algorithm

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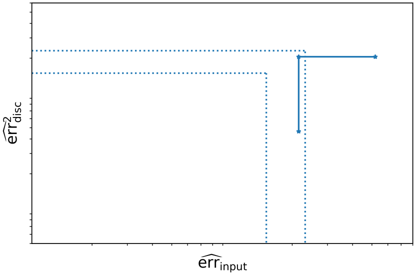

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Budgeted Multi-level Monte Carlo - Algorithm

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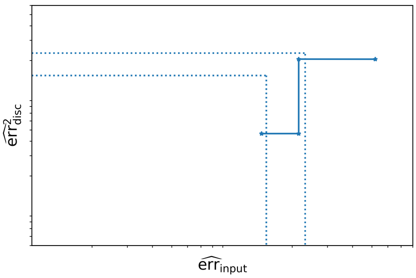

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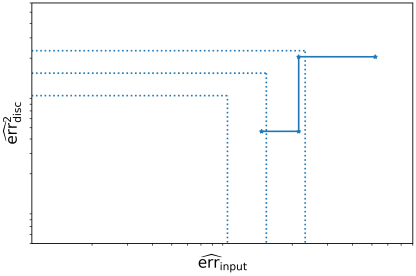

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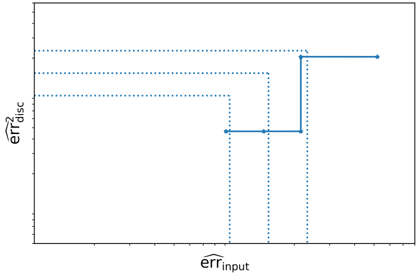
$$\begin{cases} \texttt{if } \mathrm{B}_\mathrm{i} \approx 0: & \texttt{return } \mathrm{err}_{\mathrm{i}-1} \\ \texttt{if } \widehat{\mathrm{err}}_{\texttt{disc}}(\texttt{data}_{\mathrm{i}-1}) \geq \sqrt{1-\theta}\,\epsilon_\mathrm{i}: & L_\mathrm{i} \leftarrow L_\mathrm{i} + 1 \\ \texttt{if } \widehat{\mathrm{err}}_{\texttt{input}}(\texttt{data}_{\mathrm{i}-1}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



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

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

Budgeted Multi-level Monte Carlo - Algorithm

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

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

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

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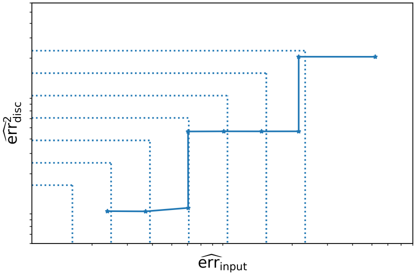

M. Giles. *Multilevel Monte Carlo methods.* (2015)

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

Multi-sample Finite Element Method (MS-FEM)

Karlsruhe Institute of Technology

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

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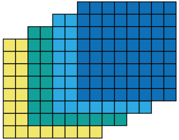

$1 < |\mathcal{P}| \leq M_\ell$

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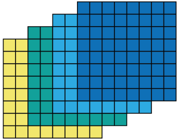

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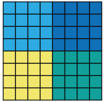

$1 < |\mathcal{P}|$ & $M_\ell = 1$

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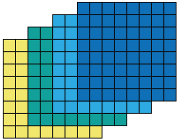

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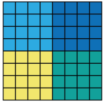

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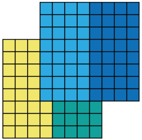

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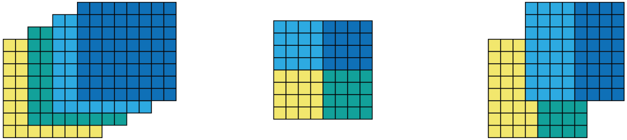

$1 < |\mathcal{P}| \leq M_\ell$ $\quad$ $1 < |\mathcal{P}|$ & $M_\ell = 1$ $\quad$ $1 < M_\ell < |\mathcal{P}|$

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

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

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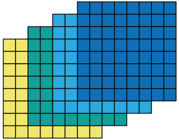

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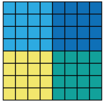

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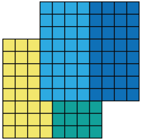


$1 < M_\ell < |\mathcal{P}|$

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

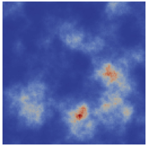
$$(\mathbf{u}_\ell)_{m=1}^{M_\ell} \in \prod_{m=1}^{M_\ell} V_\ell^{(m)}$$

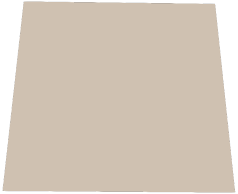
defined on $\mathcal{M}_{\mathcal{P}}$

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 $\tau_\ell = T/N_\ell^T$

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

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

Experimental Setup via Continuous Delivery (CD)

Goal: Find combination of methods for minimal error

$$\mathrm{err}_{\text{total}} = \mathrm{err}_{\text{input}} + \mathrm{err}_{\text{disc}} + \mathrm{err}_{\text{model}} + \mathrm{err}_{\text{bug}} + \dots$$

under computational constraint

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under computational constraint

Default Budget: $\mathrm{B} = |\mathcal{P}| \cdot \mathrm{T}_{\mathrm{B}} = 1024 \cdot 6\text{h}$

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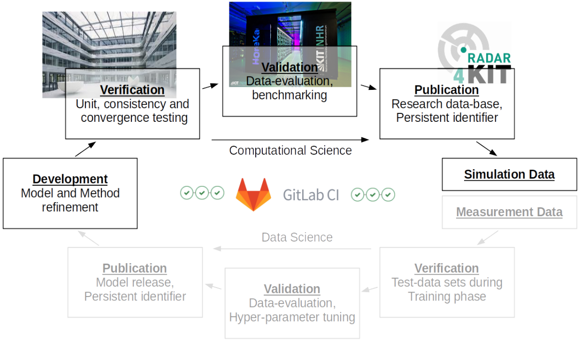
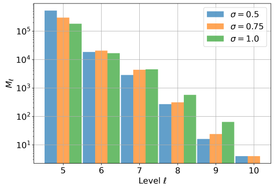
Default Budget: $\mathrm{B} = |\mathcal{P}| \cdot \mathrm{T}_{\mathrm{B}} = 1024 \cdot 6\text{h}$

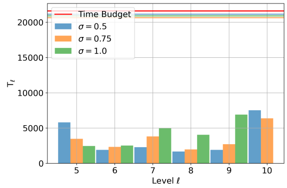
Automated High-Performance Computing:

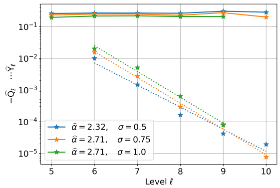
- Code verification
- Model and method comparison
- Data collection and postprocessing

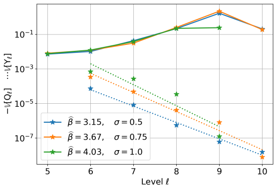


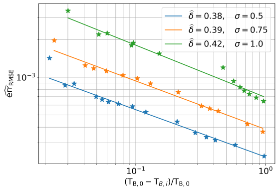
Numerical Experiments - Covariance Function

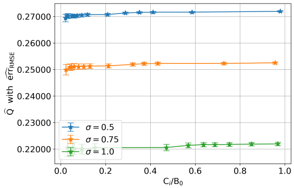












Covariance Function:

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

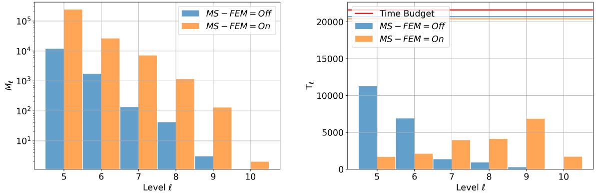
with $\lambda = 0.15$, $\nu = 1.8$ and $\sigma \in \{0.5, 0.75, 1.0\}$

Numerical Experiments - Parallelization

Karlsruhe Institute of Technology

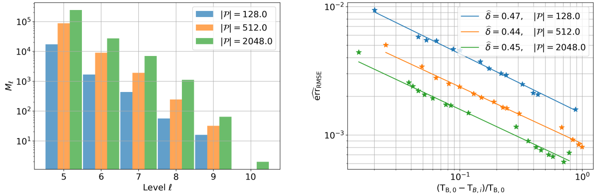
1st Experiment:

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



2nd Experiment:

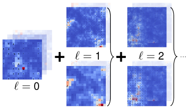
- Weak scaling measurement with $T_B = 6h$ on $|\mathcal{P}| \in \{128, 512, 2048\}$

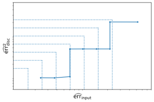


Conclusion and Outlook

Conclusion:

- Budgeted Multi-level Monte Carlo (BMLMC)





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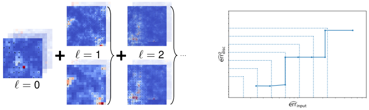

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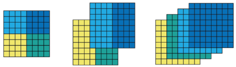

Conclusion and Outlook

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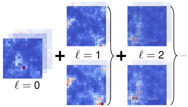

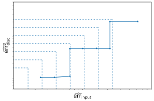

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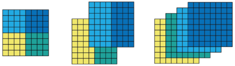
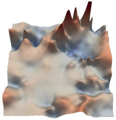
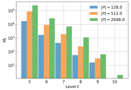
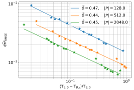


- Acoustic Wave Simulations in Random Media



Conclusion and Outlook

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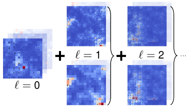

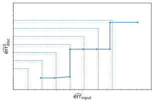

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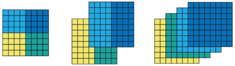

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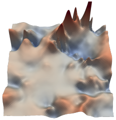

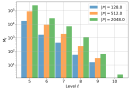

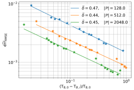

Further Work:

- 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 3.3.0.* (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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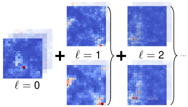
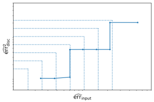
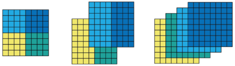
- Budgeted Multi-level Monte Carlo (BMLMC)

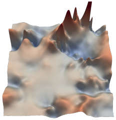


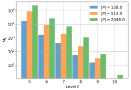


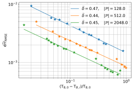
- Multi-Sample Finite Element Method (MS-FEM)



- Acoustic Wave Simulations in Random Media







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 3.3.0.* (2023)

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

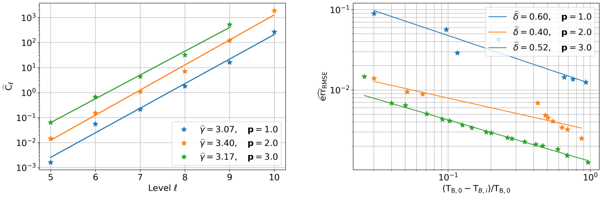
In Progress / Outlook / Interests:

- Interfaces: Umbridge & Ginkgo
- (B)MLSC, (B)MLQMC, (B)MIMC
- Implementation of $\widehat{\mathbf{u}}_L$ in Mpp 3.3.1
- SGD/ADAM for Optimal Control
- Bayesian Inverse UQ via SMC

Numerical Experiments - Method Comparison

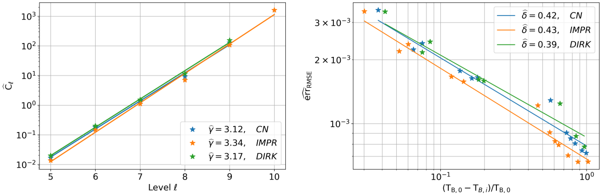
1st Experiment:

- Polynomial degree $\mathbf{p} \in \{1, 2, 3\}$ of $V_{\ell,\mathbf{p}}^{\mathrm{dG}}$



2nd Experiment:

- Diagonal implicit Runge-Kutta (DIRK)
- Implicit midpoint-rule (IMPR)
- Crank-Nicolson (CN)



Numerical Experiments - Verification of Conjecture

Weak Scaling Experiments:

- Fixed time budget $\mathrm{T_B} = 6\mathrm{h}$
- Variable amount of processing units

$$|\mathcal{P}| \in \left\{ 2^{-k} \, |\mathcal{P}_{\mathsf{max}}| \, : \, |\mathcal{P}_{\mathsf{max}}| = 8192, \, k = 0, \dots, 7 \right\}$$

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$$\epsilon \lesssim (1 - \lambda_{\mathrm{p}}) \cdot \mathrm{T_B}^{-\delta} + \lambda_{\mathrm{p}} (|\mathcal{P}| \cdot \mathrm{T_B})^{-\delta}$$

can be estimated with

$$\widehat{\mathrm{err}}_{\mathrm{RMSE},k} = \widehat{\mathrm{err}}_{\mathrm{RMSE,s}} + \widehat{\mathrm{err}}_{\mathrm{RMSE,p}} \cdot 2^{k\widehat{\delta}}$$

Numerical Experiments - Verification of Conjecture

Karlsruhe Institute of Technology

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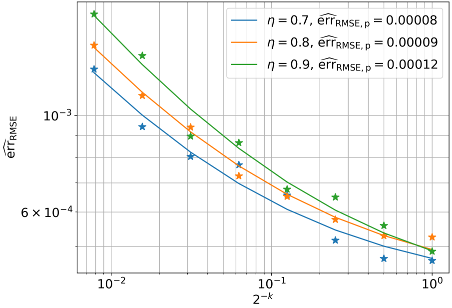
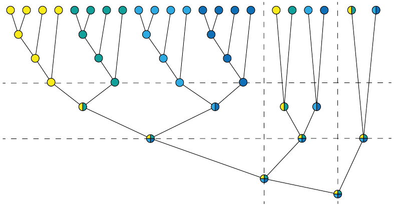


Budgeted Multi-level Monte Carlo - Optimality Principle

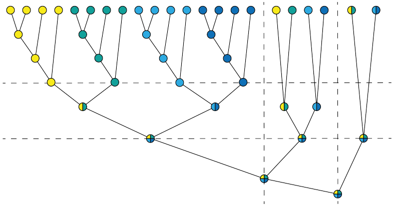


Welford's Update Algorithm:

function Welford$(\text{data}_A, \text{data}_B)$:

$$
\begin{cases}
M_{AB,\ell} & \leftarrow \quad M_{B,\ell} + M_{A,\ell} \\
\delta_{AB,\ell} & \leftarrow \quad \widehat{\mathrm{Q}}_{B,\ell} - \widehat{\mathrm{Q}}_{A,\ell} \\
\widehat{\mathrm{Q}}_{AB,\ell} & \leftarrow \quad \widehat{\mathrm{Q}}_{A,\ell} + \frac{M_{B,\ell}}{M_{AB,\ell}} \delta_{AB,\ell} \\
S_{\mathrm{Q}_2,AB,\ell} & \leftarrow \quad S_{\mathrm{Q}_2,A,\ell} + S_{\mathrm{Q}_2,B,\ell} + \frac{M_{A,\ell} M_{B,\ell}}{M_{AB,\ell}} \delta^2_{AB,\ell} \\
s^2_{\mathrm{Q}_{AB,\ell}} & \leftarrow \quad (M_{AB,\ell} - 1)^{-1} S_{\mathrm{Q}_2,AB,\ell} \\
\texttt{return} & \quad \{M_{AB,\ell}, \widehat{\mathrm{Q}}_{AB,\ell}, S_{\mathrm{Q}_2,AB,\ell}, \dots\}_{\ell=0}^{L_{\mathrm{i}}}
\end{cases}
$$

Budgeted Multi-level Monte Carlo - Optimality Principle



Reward Function: Compute with Welford's Update Algorithm

$$\Delta \mathrm{err}_{\mathsf{MSE}} \colon \mathcal{S} \times \mathcal{A} \to \mathbb{R}$$

with $\mathtt{data}_{\mathtt{i}-1} \in \mathcal{S}$ and $\{\Delta M_{\mathtt{i},\ell}\}_{\ell=0}^{L_{\mathtt{i}}} \in \mathcal{A}$.

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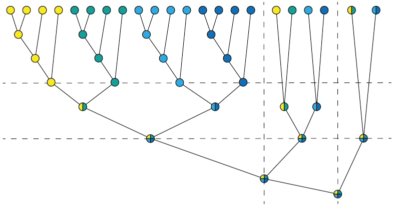

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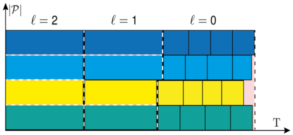
Bellman Equation: Estimation of final MSE

$$\widehat{\mathrm{err}}^{\mathsf{final}}_{\mathsf{MSE}} = \widehat{\mathrm{err}}^{\mathsf{init}}_{\mathsf{MSE}} - \widehat{\mathrm{err}}_{\mathsf{MSE}}(\mathrm{B}_{\mathtt{i}}, \epsilon_0)$$

for $\eta \in (0, 1)$ with

$$\widehat{\mathrm{err}}_{\mathsf{MSE}}(\mathrm{B}_{\mathtt{i}}, \epsilon_{\mathtt{i}}) = \max_{\substack{\{\Delta M_{\mathtt{i},\ell}\}_{\ell=0}^{L_{\mathtt{i}}} \\ \text{s.t. } \widehat{\mathrm{C}}_{\mathtt{i}} < \mathrm{B}_{\mathtt{i}}}} \Big\{ \Delta\mathrm{err}_{\mathsf{MSE}}(\mathtt{data}_{\mathtt{i}-1}, \{\Delta M_{\mathtt{i},\ell}\}_{\ell=0}^{L_{\mathtt{i}}}) + \widehat{\mathrm{err}}_{\mathsf{MSE}}\Big(\mathrm{B}_{\mathtt{i}} - \sum_{\ell=0}^{L_{\mathtt{i}}} \mathrm{C}_{\mathtt{i},\ell},\, \eta \cdot \epsilon_{\mathtt{i}}\Big) \Big\}$$

Budgeted Multi-level Monte Carlo - Parallelization Bias



Recall: For a parallel BMLMC execution, it holds

$$\epsilon \lesssim \underbrace{(1-\lambda_{\mathrm{p}}) \cdot \mathrm{T}_{\mathrm{B}}^{-\delta}}_{=:\epsilon_{\mathrm{s}}} + \underbrace{\lambda_{\mathrm{p}}(|\mathcal{P}| \cdot \mathrm{T}_{\mathrm{B}})^{-\delta}}_{=:\epsilon_{\mathrm{p}}}$$

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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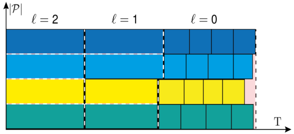

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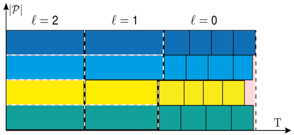

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Gustafson's Law: Consider hypothetical speedup

$$S := \frac{T_{\epsilon,s}}{T_{\epsilon,p}} = \frac{\lambda_s + \lambda_p\,|\mathcal{P}|^{-\delta}}{\lambda_s+\lambda_p} = (1-\lambda_p) + \lambda_p\,|\mathcal{P}|^{-\delta}$$

Additional error reduction by utilizing $|\mathcal{P}|$ units

$$\epsilon \lesssim S \cdot T_B^{-\delta}$$

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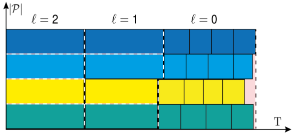

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Algorithmic Requirements:

Large L_i $\longrightarrow$ FE parallelization
Large $M_{i,\ell}$ $\longrightarrow$ Sample parallelization
Unknown $M_{i,\ell}$ $\longrightarrow$ Dynamic load distribution
Usage of `data` $\longrightarrow$ Distributed state machine