

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



CRC 1173 *Wave phenomena*

Model Problem and Investigation Goals

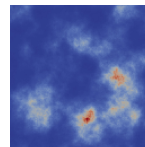
Acoustic wave: Search $(\mathbf{v}, p): \Omega \times \mathcal{D} \times [0, T] \rightarrow \mathbb{R}^{D+1}$,

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

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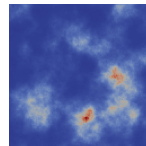
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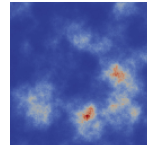


Determine: $\mathbb{E}[Q] := \int_{\Omega} Q(\omega) d\mathbb{P} \approx M^{-1} \sum_{m=1}^M Q_{\ell}(\mathbf{y}^{(m)}) =: \hat{Q}_{\ell, M}^{\text{MC}}$

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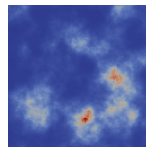
Goal: Find combination of methods to minimize total error

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

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

⇒ Introduce budget for error minimization and utilize effective parallelization

Multi-level Monte Carlo - Introduction

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

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

$$\mathbb{V}[Q_\ell - Q_{\ell-1}] \lesssim h_\ell^\beta$$

$$C(Q_\ell(\mathbf{y}^{(m)})) \lesssim h_\ell^{-\gamma}$$

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

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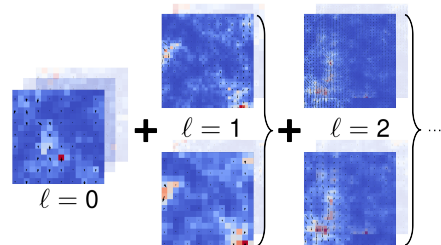
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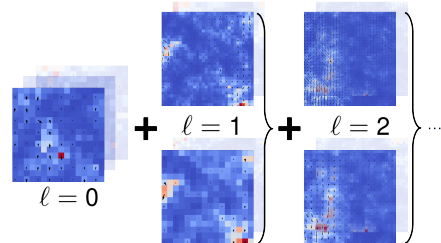
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Epsilon-Cost Theorem: $\exists \{M_\ell\}_{\ell=0}^L$, such that

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

$$\text{and } T_\epsilon := C_\epsilon \lesssim \begin{cases} \epsilon^{-2} & \beta > \gamma \\ \epsilon^{-2 - (\gamma - \beta)/\alpha} & \beta < \gamma \end{cases}$$

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

Budgeted Multi-level Monte Carlo - Introduction

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

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$$\min_{(L, \{M_\ell\}_{\ell=0}^L)} \text{err}_{\text{MSE}} = \sum_{\ell=0}^L M_\ell^{-1} \mathbb{V}[Y_\ell] + (\mathbb{E}[Q_L - Q])^2$$

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

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Conjecture: For a feasible and parallel execution, it is

$$\epsilon \lesssim \underbrace{(1 - \lambda_p) \cdot T_B^{-\delta}}_{=: \epsilon_s} + \underbrace{\lambda_p (|\mathcal{P}| \cdot T_B)^{-\delta}}_{=: \epsilon_p}$$

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

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

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Approximated Knapsack Problem:

$$\min_{(L, \{M_\ell\}_{\ell=0}^L)} \sum_{\ell=0}^L M_\ell^{-1} s_{Y_\ell}^2 + \left(\widehat{\text{err}}_{\text{disc}}(\widehat{Y}_\ell, \widehat{\alpha}) \right)^2$$

such that
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Budgeted Multi-level Monte Carlo - Algorithm

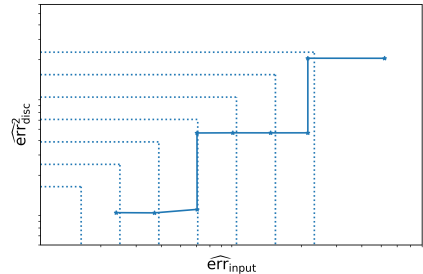
$$\text{data} = \left\{ i \mapsto \left\{ \text{err}_i, \{M_{i,\ell}\}_{\ell=0}^{L_i}, \{\widehat{Q}_{i,\ell}\}_{\ell=0}^{L_i}, \{\widehat{C}_{i,\ell}\}_{\ell=0}^{L_i}, \{\widehat{Y}_{i,\ell}\}_{\ell=0}^{L_i}, \dots \right\} \right\}$$

function BMLMC($B_0, \{M_{0,\ell}^{\text{init}}\}_{\ell=0}^{L_0}$):

$$\left\{ \begin{array}{ll} \text{for } \ell = L_0, \dots, 0: & \Delta \text{data}_{0,\ell} \leftarrow \text{MS-FEM}(M_{0,\ell}^{\text{init}}, \mathcal{P}) \\ \text{data}_0 \leftarrow \text{Welford}(\text{data}_{-1}, \Delta \text{data}_0) & \text{return BMLMC}(B_0 - \sum_{\ell=0}^{L_0} C_{\ell}, \eta \cdot \text{err}_0) \end{array} \right.$$

function BMLMC(B_i, ϵ_i):

$$\left\{ \begin{array}{ll} \text{if } B_i \approx 0: & \text{return err}_{i-1} \\ \text{if } \widehat{\text{err}}_{\text{disc}}(\text{data}_{i-1}) \geq \sqrt{1 - \theta} \epsilon_i: & L_i \leftarrow L_i + 1 \\ \text{if } \widehat{\text{err}}_{\text{input}}(\text{data}_{i-1}) \geq \theta \epsilon_i^2: & \widehat{M}_{i,\ell}^{\text{opt}} \sim \left[(\sqrt{\theta} \epsilon)^{-2} \sqrt{S_{Y_{i,\ell}}^2 / \widehat{C}_{i,\ell}} \right] \\ \text{for } \ell = L_i, \dots, 0: & \Delta M_{i,\ell} \leftarrow \max \left\{ \widehat{M}_{i,\ell}^{\text{opt}} - M_{i-1,\ell}, 0 \right\} \\ \widehat{C}_i \leftarrow \sum_{\ell=0}^{L_i} \Delta M_{i,\ell} \widehat{C}_{i-1,\ell} & \\ \text{if } \widehat{C}_i = 0: & \text{return BMLMC}(B_i, \eta \cdot \epsilon_i) \\ \text{if } \widehat{C}_i > B_i: & \text{return BMLMC}(B_i, 0.5 \cdot (\epsilon_i + \epsilon_{i-1})) \\ \text{for } \ell = L_i, \dots, 0: & \Delta \text{data}_{i,\ell} \leftarrow \text{MS-FEM}(\Delta M_{i,\ell}, \mathcal{P}) \\ \text{data}_i \leftarrow \text{Welford}(\text{data}_{i-1}, \Delta \text{data}_i) & \text{return BMLMC}(B_i - \sum_{\ell=0}^{L_i} C_{\ell}, \epsilon_i) \end{array} \right.$$



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

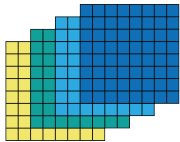
Collier et al. *A continuation multilevel Monte Carlo algorithm*. (2015)

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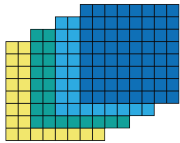
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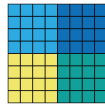
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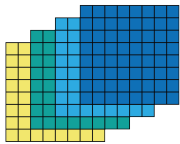
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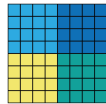
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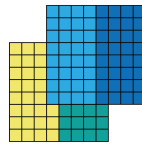
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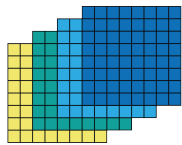
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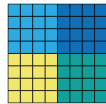
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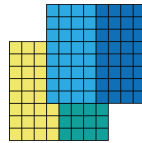
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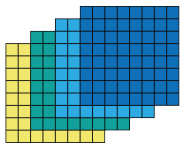
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Minimize Communication: Search $k \in \mathbb{N}_0$, such that

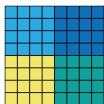
$$2^k \leq \frac{|\mathcal{P}|}{M_\ell} < 2^{k+1} \Rightarrow \mathcal{P} = \bigsqcup_{m=1}^{M_\ell} \mathcal{P}_k^{(m)} \text{ with } |\mathcal{P}_k^{(m)}| = 2^k$$

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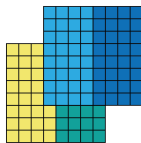
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Define: Set of FE meshes

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

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MS-FEM: Search for representation of

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

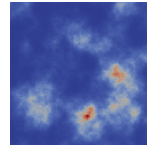
defined on $\mathcal{M}_{\mathcal{P}}$

Model Problem and Discretization

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

such that

$$\left\{ \begin{array}{ll} \rho(\omega) \partial_t \mathbf{v}(\omega) - \nabla p(\omega) & = \mathbf{f} \quad \mathcal{D} \times (0, T] \\ \partial_t p(\omega) - \operatorname{div}(\mathbf{v}(\omega)) & = g \quad \mathcal{D} \times (0, T] \\ \mathbf{v} \cdot \mathbf{n} & = 0 \quad \Gamma \times (0, T] \\ \mathbf{v}(0) & = \mathbf{v}_0 \quad \mathcal{D} \\ \rho(0) & = \rho_0 \quad \mathcal{D} \end{array} \right.$$



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

$$M_\ell \partial_t \mathbf{u}_\ell + A_\ell \mathbf{u}_\ell = \mathbf{b}_\ell \quad \text{and} \quad \mathbf{u}_\ell(0) = \mathbf{u}_{\ell,0}$$

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

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

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

Experimental Setup via Continuous Delivery (CD)

Goal: Find combination of methods for minimal error

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

under computational constraint

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under computational constraint

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

Experimental Setup via Continuous Delivery (CD)

Goal: Find combination of methods for minimal error

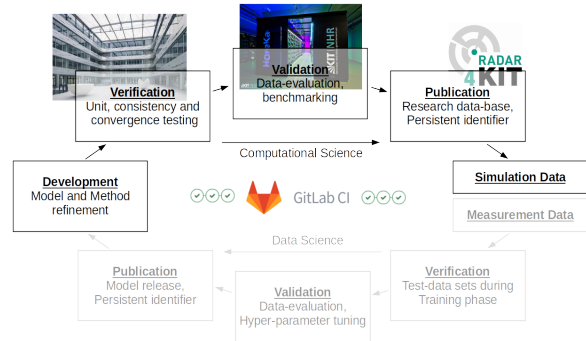
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under computational constraint

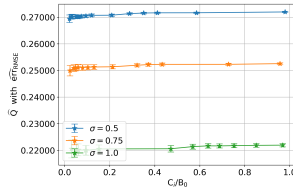
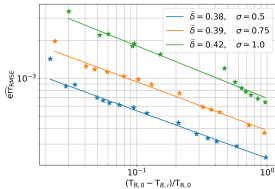
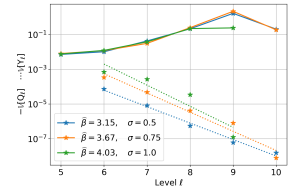
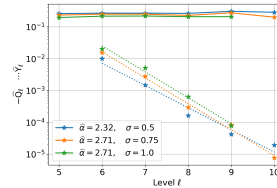
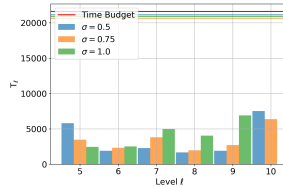
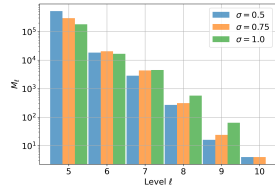
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Automated High-Performance Computing:

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



Numerical Experiments - Covariance Function



Covariance Function:

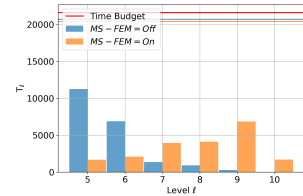
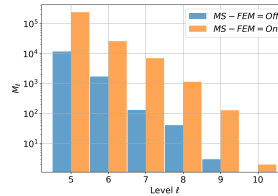
$$\text{Cov}(\mathbf{x}_1, \mathbf{x}_2) = \sigma^2 \exp \left(- \left\| \left(\frac{\mathbf{x}_1 - \mathbf{x}_2}{\lambda} \right) \right\|_2^\nu \right)$$

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

Numerical Experiments - Parallelization

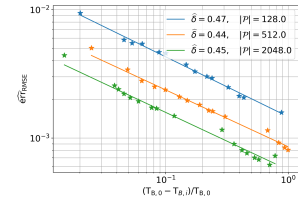
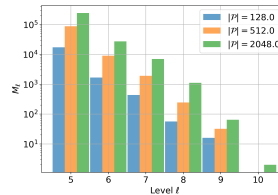
1st Experiment:

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



2nd Experiment:

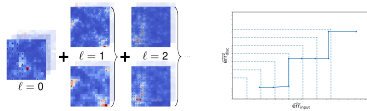
- Weak scaling measurement with $T_B = 6h$ on $|\mathcal{P}| \in \{128, 512, 2048\}$



Conclusion and Outlook

Conclusion:

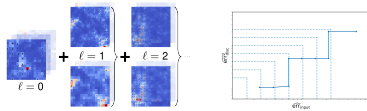
- Budgeted Multi-level Monte Carlo (BMLMC)



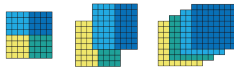
Conclusion and Outlook

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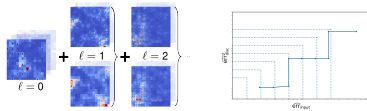
- Multi-Sample Finite Element Method (MS-FEM)



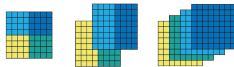
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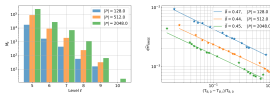
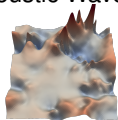
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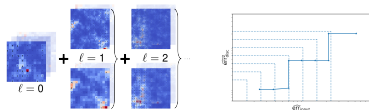
- Acoustic Wave Simulations in Random Media



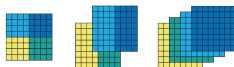
Conclusion and Outlook

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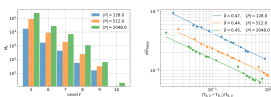
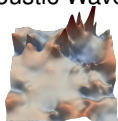
- Budgeted Multi-level Monte Carlo (BMLMC)



- 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

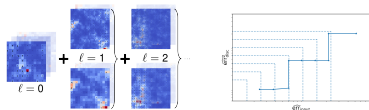
Wieners, Corallo, Schneiderhan, Stengel, Lindner, Rheinbay, Baumgarten. *Mpp 3.3.0*. (2023)

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

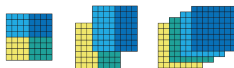
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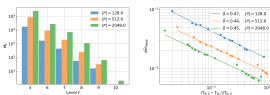
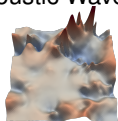
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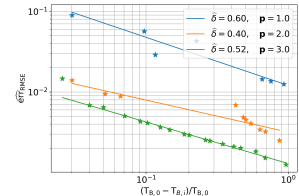
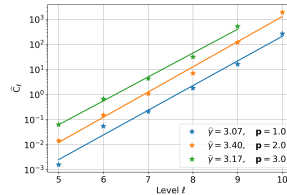
In Progress / Outlook / Interests:

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

Numerical Experiments - Method Comparison

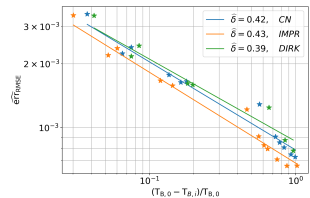
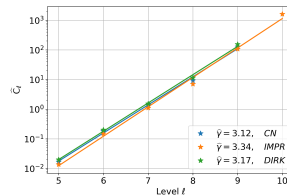
1st Experiment:

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



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 $T_B = 6\text{h}$
- Variable amount of processing units

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

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- Assume λ_p is fixed for a fixed η , then

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

can be estimated with

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

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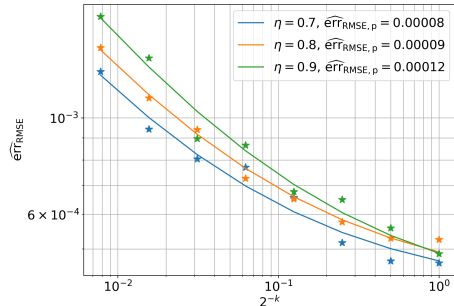
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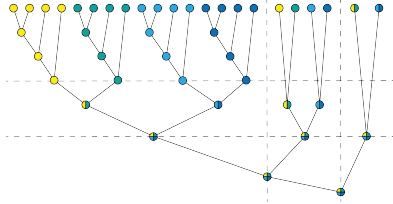
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Budgeted Multi-level Monte Carlo - Optimality Principle

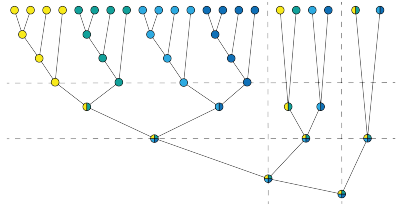


Welford's Update Algorithm:

function Welford(data_A, data_B):

$$\begin{cases}
 M_{AB,\ell} & \leftarrow M_{B,\ell} + M_{A,\ell} \\
 \delta_{AB,\ell} & \leftarrow \widehat{Q}_{B,\ell} - \widehat{Q}_{A,\ell} \\
 \widehat{Q}_{AB,\ell} & \leftarrow \widehat{Q}_{A,\ell} + \frac{M_{B,\ell}}{M_{AB,\ell}} \delta_{AB,\ell} \\
 S_{Q_{2,AB},\ell} & \leftarrow S_{Q_{2,A},\ell} + S_{Q_{2,B},\ell} + \frac{M_{A,\ell} M_{B,\ell}}{M_{AB,\ell}} \delta_{AB,\ell}^2 \\
 s_{Q_{AB},\ell}^2 & \leftarrow (M_{AB,\ell} - 1)^{-1} S_{Q_{2,AB},\ell} \\
 \text{return} & \{M_{AB,\ell}, \widehat{Q}_{AB,\ell}, S_{Q_{2,AB},\ell}, \dots\}_{\ell=0}^{L_i}
 \end{cases}$$

Budgeted Multi-level Monte Carlo - Optimality Principle



Reward Function: Compute with Welford's Update Algorithm

$$\Delta \text{err}_{\text{MSE}} : \mathcal{S} \times \mathcal{A} \rightarrow \mathbb{R}$$

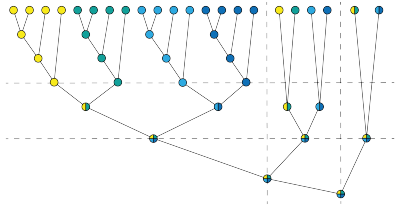
with $\text{data}_{i-1} \in \mathcal{S}$ and $\{\Delta M_{i,\ell}\}_{\ell=0}^{L_i} \in \mathcal{A}$.

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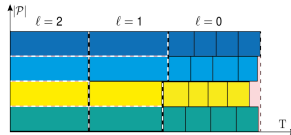
Bellman Equation: Estimation of final MSE

$$\widehat{\text{err}}_{\text{MSE}}^{\text{final}} = \widehat{\text{err}}_{\text{MSE}}^{\text{init}} - \widehat{\text{err}}_{\text{MSE}}(B_i, \epsilon_0)$$

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

$$\widehat{\text{err}}_{\text{MSE}}(B_i, \epsilon_i) = \max_{\{\Delta M_{i,\ell}\}_{\ell=0}^{L_i} \text{ s.t. } \widehat{C}_i < B_i} \left\{ \Delta \text{err}_{\text{MSE}}(\text{data}_{i-1}, \{\Delta M_{i,\ell}\}_{\ell=0}^{L_i}) + \widehat{\text{err}}_{\text{MSE}}\left(B_i - \sum_{\ell=0}^{L_i} C_{i,\ell}, \eta \cdot \epsilon_i\right) \right\}$$

Budgeted Multi-level Monte Carlo - Parallelization Bias

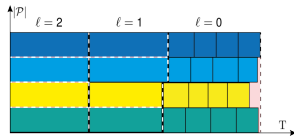


Recall: For a parallel BMLMC execution, it holds

$$\epsilon \lesssim \underbrace{(1 - \lambda_p) \cdot T_B^{-\delta}}_{=:\epsilon_s} + \underbrace{\lambda_p (|\mathcal{P}| \cdot T_B)^{-\delta}}_{=:\epsilon_p}$$

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

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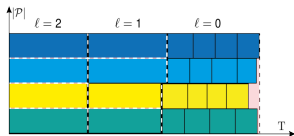
with $\delta \in \left\{ \frac{1}{2}, \frac{\alpha}{(2\alpha + (\gamma - \beta))} \right\}$ and $\lambda_p \in [0, 1]$.

Ansatz: Inverted ϵ -Cost for feasible execution

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$$\lambda_p = 1: \epsilon \lesssim (|\mathcal{P}| \cdot T_B)^{-\delta} = C_\epsilon^{-\delta}$$

Budgeted Multi-level Monte Carlo - Parallelization Bias



Gustafson's Law: Consider hypothetical speedup

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

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

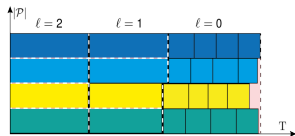
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Additional error reduction by utilizing $|\mathcal{P}|$ units

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Algorithmic Requirements:

Large $L_i \rightarrow$ FE parallelization

Large $M_{i,\ell} \rightarrow$ Sample parallelization

Unknown $M_{i,\ell} \rightarrow$ Dynamic load distribution

Usage of data \rightarrow Distributed state machine