A multiscale model and variance reduction method for wave propagation in heterogeneous materials

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Motivation

- Metamaterials are heterogeneous materials microscopically engineered to exhibit properties that cannot be found in homogeneous materials.
- Study wave propagation in metamaterials: **photonic bandgap**

**Applications**

- Waveguides, fibers, cavities...
Motivation: Photonic Bandgap

Highly **sensitive** to material properties and geometry **variations**

Accurate simulations are required
Problem statement

Consider the **Helmholtz** equation in 2d

\[- \nabla \cdot (\rho(x) \nabla u) - k^2(x) u = f \quad + \text{B.C.}\]

where \(\rho(x), k^2(x)\) represent material properties

- **Time-harmonic solutions of scalar wave equation**
- **2d Maxwell’s equations for TE and TM polarizations**

\[\text{TE: } u = H_z \quad \text{TM: } u = E_z\]

Wave propagation is considered for **structured** materials

\[\Omega \]

Material 1 \(\rho(x), k^2(x)\)

Material 2 \(\rho(x), k^2(x)\)

\[\Omega = \bigcup_{m=1}^{M} \Omega^m\]

\[\text{piecewise constant}\]
Objectives

Develop methods for robust design of heterogeneous materials to control wave propagation

Simulate wave propagation in structured media

- Wave equation is non-coercive, need high accuracy
- Complex geometries, repeated patterns, mismatch in length scales

Stochastic simulation of wave propagation

- Framework to deal with geometry variations
- Models are expensive: develop surrogates, use control variates
MultiScale continuous Galerkin (MSCG) method

Identify **repeated geometries** in domain

Discretize **subdomains** and **global skeleton**

Local problem

High-order CG discretization

Capture small features

Global problem

Lagrange polynomial for solution on global faces

Capture frequencies on large scale
For every subdomain $\Omega^m$, solve Helmholtz equation

1. Source problem $\bigtriangleup \mathbf{u}_f = \mathbf{f}$

2. Inhomogeneous Dirichlet given by $\varphi_j$, $1 \leq j \leq J$ $\bigtriangleup \mathbf{u}_{\varphi_j} = \mathbf{d}_{\varphi_j}$
On the subdomain level we apply **linearity** and **superposition**

\[ u = u_f + \sum_{j=1}^{J} \lambda_j u_{\varphi_j} \]

The contribution of each subdomain to the global problem is

\[
\begin{align*}
K_{ij} &= u_{\varphi_i}^T A u_{\varphi_j}, \quad 1 \leq i, j \leq J \\
F_i &= u_{\varphi_i}^T f, \quad 1 \leq i \leq J
\end{align*}
\]

Solve the global problem \( K\Lambda = F \)
Simulation of waveguide bends

Photonic crystals are expensive to simulate given the complexity of the geometry.

Subdomain dof

\[ 415 \times 1\text{K} = 0.5\text{M} \]

\[ 320 \times 17\text{K} = 5.4\text{M} \]

Skeleton dof \hspace{1cm} 15\text{K}

MSCG solution in < 3s

Bandgap

\[ \frac{\omega a}{2\pi c} \in [0.42, 0.456] \]

Results for \[ \frac{\omega a}{2\pi c} = 0.454 \]
Reference domain formulation

Reformulate governing equations [Persson et.al. 09] with deformation mapping parametrized by $y$

\[ -\nabla_r \cdot (\rho(x) g G^{-1} G^{-T} \nabla_r u) - k^2(x) u g = f g \]

\[ \nabla \cdot (\rho(x) \nabla u) - k^2(x) u = f \]
MSCG for geometry variations

Analyze response of a structured medium under geometry variations

reference radius

dilation

nonhomogeneous manufacturing errors
modeled with random field

variance and correlation length

uniform r.v.

\[ r \rightarrow r + \delta r = r + r \left( 1 + y_1 \sqrt{\lambda_0} + \sum_{d=1}^{D} \sqrt{\lambda_d} (y_{2d} \sin \theta d + y_{2d+1} \cos \theta d) \right) \]

Nanogaps of Al$_2$O$_3$ on gold substrate

[Yoo et al. 2016]
Stochastic simulation of waveguide

- Radius of rods modeled with 15 r.v. (90% energy)
- Relative radius perturbation $|\delta r|/r < 0.05$
- Independent realizations of errors for each rod

no longer capitalize repetition of subdomains
Develop an accurate surrogate efficient to evaluate

- Proper orthogonal decomposition [Sirovich 87]
- Reduced basis method [Noor et al. 80, Rozza et al. 08,...]

Reduced basis for multiscale CG and geometry parameters

✓ RB for each type of subdomain [Huynh et al. 13]
✓ Empirical interpolation [Barrault et al. 04] for parameter dependent mapping $G(y)$

\[
\mathbf{A}(y)\mathbf{u}_{\varphi_j} = \mathbf{d}_{\varphi_j}(y)
\]

\[
\sum_{q=1}^{Q} \sigma_q(y) \mathbf{A}_q \mathbf{u}_{\varphi_j} = \sum_{q=1}^{Q} \sigma_q(y) \mathbf{d}_{q,\varphi_j}
\]
Reduced basis for MSCG (2/2)

✓ For each Dirichlet BC $\varphi_j$, compute snapshots sampling $y$

✓ **Single** RB $Z$ compressing snapshots for all Dirichlet BC $\varphi_j$, $1 \leq j \leq J$

$$u_{\varphi_j}^N = Zc_j$$

✓ Linear system with **multiple** RHS

$$\sum_{q=1}^{Q} \sigma_q(y) Z^\dagger A_q Z c_j = \sum_{q=1}^{Q} \sigma_q(y) Z^\dagger d_{q,\varphi_j}$$

✓ RB approximation to local contribution to stiffness matrix

$$K_{ij}^N = \sum_{q=1}^{Q} \sigma_q(y) c_j^\dagger Z^\dagger A_q Z c_j, \quad 1 \leq i, j \leq J$$
Combine **high-fidelity solver** with one (or multiple) **low-fidelity models**

- Multilevel MC [Giles 08]
- Multifidelity MC [Ng et al. 12]
- RB control variate [Boyaval 12]

Exploit statistical correlation: **reduce variance** in estimates

Use **reduced basis** as low-fidelity model

**Model and variance reduction method** [Vidal-Codina 15]

Output $s$ as a functional of the solution of stochastic PDE

\[
E[s] = E[s - s_N] + E[s_N]
\]

\[
E_{M_0, M_1}[s] = E_{M_1}[s - s_N] + E_{M_0}[s_N]
\]

- **Variance reduction** (statistical correlation)
- **Model reduction** (cheaper output evaluation)
Choose $N_1 < N_2 < \ldots < N_L$ and define $L$-MVR estimator

\[
E_{M_0,\ldots,M_L}[s] = E_{M_0}[s_{N_1}] + \sum_{\ell=1}^{L-1} E_{M_\ell}[s_{N_{\ell+1}} - s_{N_\ell}] + E_{M_L}[s - s_{N_L}]
\]

For i.i.d. samples between levels, we apply the central limit theorem

\[
\lim_{M_0 \to \infty} \ldots \lim_{M_L \to \infty} \Pr\left(\left|E[s] - E_{M_0,\ldots,M_L}[s]\right| \leq \Delta_E\right) = \text{erf}\left(\frac{a}{\sqrt{2}}\right), \quad \forall a \geq 0
\]

obtain \textit{a posteriori} sampling error estimates

\[
\Delta_E = a \sqrt{\frac{V_{M_0}[s_{N_1}]}{M_0} + \sum_{\ell=1}^{L-1} \frac{V_{M_\ell}[s_{N_{\ell+1}} - s_{N_\ell}]}{M_\ell} + \frac{V_{M_L}[s - s_{N_L}]}{M_L}}
\]

Similar estimators for the \textbf{variance}
Robust design of photonic slab

✓ Silicon slab on triangular lattice with air holes
✓ TE polarization, solve for $H_z$
✓ Output $s$ is optical power at outlet
Computational domain and subproblem selection

Subdomain #1 (optimization)

✓ Develop RB for geometry and frequency
✓ Lagrange polynomial of order 10

18K dof
\[ p = 2 \]

Subdomain #2

18K dof
\[ p = 2 \]

Subdomain #3

1K dof
\[ p = 2 \]

Subdomain #4

1K dof
\[ p = 2 \]
Shape optimization at discrete frequencies

✓ Optimize radius of holes to maximize transmission [NLOPT-Johnson 10]

\[ \max_{\theta} s \quad \text{where} \quad r_i = r_0(1 + \theta_i), \quad \theta_i \in \mathbb{E} \]

✓ Replace CG for RB on optimization subdomains: speedup $\sim 150$

![Output convergence graph](image-url)

![Power spectrum comparison](image-url)
Shape optimization for range of frequencies

Objective function

\[ s^* = \max_{\theta} E_\omega [s] - \gamma \sqrt{V_\omega [s]} \]
Robust shape optimization for range of frequencies

\[ \hat{s} = \max_{\theta} E_{g,\omega}[s] - \gamma \sqrt{V_{g,\omega}[s]} \rightarrow \text{MVR to approximate statistics} \]

✓ **Robust design** guarantees lower performance degradation
✓ **MVR replaces expensive MSCG simulations for cheaper RB simulations**
Conclusions

Multiscale model and variance reduction method for wave propagation in heterogeneous materials

✓ Multiscale CG exploits repeated patterns in domain

✓ Develop RB for geometry variations at the subdomain level

✓ Combine MSCG and RB on a multilevel estimator of output statistics

✓ Ideal for stochastic simulation and robust design of structured materials
Thanks for your attention

Questions?
\[ \mathcal{W}_h = \{ w \in L^2(\Omega) : w \in C^0(\Omega^m), w|_T \in \mathcal{P}^{p^m}(T), \forall T \in \mathcal{T}_h^m, 1 \leq m \leq M \}, \]

\[ \mathcal{W}_h^m = \{ w \in C^0(\Omega^m), w|_T \in \mathcal{P}^{p^m}(T), \forall T \in \mathcal{T}_h^m \}, \]

\[ M_h = \{ \mu \in L^2(\partial \Omega^m : \Omega^m \in \mathcal{T}_h) : \mu|_{\partial \Omega^m} = w|_{\partial \Omega^m}, w \in \mathcal{W}_h \}, \]

\[ V_h = \{ \nu \in C^0(\mathcal{F}_f) : \nu|_f \in \mathcal{P}^{p^f}(f), \forall f \in \mathcal{F}_f \} \]

\[ \mathcal{F}_f = \{ f_i, 1 \leq i \leq \sum_{\ell=1}^{L} \mathcal{N}^\ell \} \]
Introduce auxiliary variable $\mathbf{q}_h$ approximating the flux, with $[\mathbf{q}_h \cdot \mathbf{n}]$ the normal component.

Seek $(u_h, \lambda_h, \mathbf{q}_h) \in W_h \times V_h(u_D) \times M_h$

$$
(q_h, \nabla w)_\Omega - (k^2 u_h, w)_\Omega - \sum_{m=1}^{M} \langle q_h \cdot n, w \rangle_{\partial \Omega^m} = (f, w)_\Omega
$$

$$
u_h = P_{W_h}^m(\lambda_h), \quad \text{on } \mathcal{F}_f$$

$$
\langle [q_h \cdot n], v \rangle_{\mathcal{F}_f} = \langle g_N, v \rangle
$$

for all $(w, v) \in W_h \times V_h(0)$

- Enforce continuity of the normal component of the flux across interfaces
- Uniqueness of solution can be proved
Seek \((u^f_h|_{\Omega^m}, u^\eta_h|_{\Omega^m}) \in \mathcal{W}^{m}_h(0) \times \mathcal{W}^{m}_h(\eta)\)

\[
\begin{align*}
(\rho\nabla_{\chi} u^f_h, \nabla_{\chi} w)_{\Omega^m} - (k^2 u^f_h, w g)_{\Omega^m} &= (f, w g)_{\Omega^m}, \quad \forall w \in \mathcal{W}^{m}_h(0), \\
(\rho\nabla_{\chi} u^\eta_h, \nabla_{\chi} w)_{\Omega^m} - (k^2 u^\eta_h, w g)_{\Omega^m} &= 0, \quad \forall w \in \mathcal{W}^{m}_h(0)
\end{align*}
\]

Applying \textit{linearity} and \textit{superposition} we have \(u_h = u^f_h + u^\lambda_h\) and the Lagrange multipliers \(\lambda_h \in V_h(u_D)\) satisfy

\[
(\rho\nabla_{\chi} u^\lambda_h, \nabla_{\chi} u^\mu_h)_{\Omega} - (k^2 u^\lambda_h, u^\mu_h g)_{\Omega} = (f, u^\mu_h g)_{\Omega} + \langle g_N, \mu \rangle_{\Omega_N}, \quad \forall \mu \in V_h(0)
\]
For each subdomain
\[ \mathbf{A}^m \mathbf{u}_f^m = \mathbf{f}^m \quad \text{for BC} \quad \varphi = \{ \varphi_i \}_{i=1}^{N_m} \]
\[ \mathbf{A}^m \mathbf{u}_{\varphi_i}^m = \mathbf{A}_{\varphi_i}^m \]

Assemble the elementary global matrices
\[ \mathbf{K}_{ij}^m = (\mathbf{u}_{\varphi_i}^m)^T \mathbf{A}^m \mathbf{u}_{\varphi_j}^m, \quad 1 \leq i, j \leq N_m \]
\[ \mathbf{F}_i^m = (\mathbf{u}_{\varphi_i}^m)^T \mathbf{f}^m + \mathbf{g}_i^m, \quad 1 \leq i \leq N_m \]

Solve the global problem \[ \mathbf{K} \Lambda = \mathbf{F} \] where \[ \lambda_h = \sum_{i=1}^{N} \Lambda_i \varphi_i \]

Recover the solution at each subdomain
\[ \mathbf{u}^m = \mathbf{u}_f^m + \sum_{i=1}^{N_m} \Lambda_i \mathbf{u}_{\varphi_i}^m \]
Weak formulation for the Dirichlet problem

\[
\left( \rho G \nabla \times u_h^\eta, \nabla \times w \right)_{\Omega^m} - (k^2 u_h^\eta, w g)_{\Omega^m} = 0, \quad \forall w \in W_h^m(0)
\]

Approximate geometry quantities using DEIM

\[
\sum_{q=1}^{Q} \sigma_q(y) (\phi^G_q \rho \nabla \times u_h^\eta, \nabla \times w)_{\Omega^m} - \sum_{q=1}^{Q'} \sigma'_q(y) (k^2 u_h^\eta, w \phi^g_q)_{\Omega^m} = 0, \quad \forall w \in W_h^m(0)
\]

Develop a single RB with POD for all possible BC. The RB solution is

\[
\sum_{q=1}^{Q} \sigma_q(y) (\phi^G_q \rho \nabla \times u_N^{\phi_i}, \nabla \times w)_{\Omega^m} - \sum_{q=1}^{Q'} \sigma'_q(y) (k^2 u_N^{\phi_i}, w \phi^g_q)_{\Omega^m} = 0, \quad \forall w \in W_N^m(0)
\]

Approximate the elementary global matrix

\[
K_{ij}^m \approx \sum_{q=1}^{Q} \sigma_q(y) (\phi^G_q \rho \nabla \times u_N^{\phi_j}, \nabla \times u_N^{\phi_i})_{\Omega^m} - \sum_{q=1}^{Q'} \sigma'_q(y) (k^2 u_N^{\phi_j}, u_N^{\phi_i} \phi^g_q)_{\Omega^m}
\]
Empirical interpolation of mapping

\[
\sum_{q=1}^{Q} \sigma_q(y) A_q^m u_{\varphi_i}^m = \varphi_i
\]

POD basis with all possible Dirichlet BC \( \Phi = \{\zeta_1, \ldots, \zeta_N\} \)

\[
\rightarrow \quad u_{\varphi_i}^m = \Phi c_i
\]

Galerkin projection to compute coefficients

\[
\sum_{q=1}^{Q} \sigma_q(y) \Phi^T A_q^m \Phi c_i = \Phi^T \varphi_i
\]

Approximate global elementary matrix

\[
K_{ij}^m \approx \sum_{q=1}^{Q} \sigma_q(y) c_i^T \Phi^T A_q^m \Phi c_j, \quad 1 \leq i, j \leq N_m
\]

\[
F_i^m \approx c_i^T \Phi^T f^m + g_i^m, \quad 1 \leq i \leq N_m
\]
Contribution #2: Reduced basis for HDG

Reduced basis for hybridizable discontinuous Galerkin method

\[ \begin{align*}
\mathbf{q} - \nabla u &= 0 \quad \mathbf{x} \in \Omega \\
-\nabla \cdot (\rho \mathbf{q}) + k^2 u &= f \quad \mathbf{x} \in \Omega \\
\rho \mathbf{q} \cdot \mathbf{n} + \nu u &= g \quad \mathbf{x} \in \partial\Omega
\end{align*} \]

In [158] we propose a new weak formulation

- Approximate only \( u_h, \hat{u}_h \) by setting \( \mathbf{q}_h(u_h, \hat{u}_h) \) → RB projection
- Retain affine parametric dependence of \( \rho, k^2, \nu \)
- Solve a system with global variables \( \hat{u}_h \) only
Hybridizable Discontinuous Galerkin (HDG) method

### Helmholtz equation

\[
\begin{align*}
\mathbf{q} - \nabla u &= 0 \quad \mathbf{x} \in \Omega \\
-\nabla \cdot (\rho \mathbf{q}) + k^2 u &= f \quad \mathbf{x} \in \Omega \\
\rho \mathbf{q} \cdot \mathbf{n} + \nu u &= g \quad \mathbf{x} \in \partial \Omega
\end{align*}
\]

### Why HDG?

- High order approximations
- Low dispersion (irregular grids)
- Solve for reduced DOF problem

### HDG solution

Block diagonal

\[
\begin{bmatrix}
A & B & -C \\
W & D & -E \\
N & -E^* & M
\end{bmatrix}
\begin{bmatrix}
\mathbf{Q} \\
\mathbf{U} \\
\hat{\mathbf{U}}
\end{bmatrix}
= 
\begin{bmatrix}
0 \\
F \\
G
\end{bmatrix}
\]

- Solve for global DOF \( \mathbf{T} \hat{\mathbf{U}} = \mathbf{R} \) (Schur complement)
- Recover local DOF \( \mathbf{Q}, \mathbf{U} \) element-wise
Projection for RB with HDG

\[ \mathbf{q} - \nabla u = 0 \quad \mathbf{x} \in \Omega \]
\[ -\nabla \cdot (\rho \mathbf{q}) + k^2 u = f \quad \mathbf{x} \in \Omega \]
\[ \rho \mathbf{q} \cdot \mathbf{n} + \nu u = g \quad \mathbf{x} \in \partial \Omega \]

Which DOF should we use to parametrize snapshot \( \zeta \)?

\[ \ times \] Projection using all degrees of freedom \( \zeta = \begin{bmatrix} \mathbf{Q} \\ \mathbf{U} \end{bmatrix} \) \rightarrow \text{Large offline computational cost} \]

\[ \times \] Projection using numerical traces \( \zeta = \begin{bmatrix} \mathbf{\hat{U}} \end{bmatrix} \) \rightarrow \text{Lose affine dependency} \]

\[ \checkmark \] Projection using \( \zeta = \begin{bmatrix} \mathbf{U} \\ \mathbf{\hat{U}} \end{bmatrix} \) \rightarrow \text{HDG natural norm, retain affine dependency} \]

\[ \mathbf{Q} = \mathbf{A}^{-1} \left( \mathbf{C} \mathbf{\hat{U}} - \mathbf{B} \mathbf{U} \right) \]

Eliminate \( \mathbf{Q} \) with first equation
**HDG formulation**

- **Approximation spaces**
  \[ W_h^p = \{ w \in L^2(D) : w|_K \in \mathcal{P}^p(K), \forall K \in \mathcal{T}_h \} \]
  \[ V_h^p = \{ v \in [L^2(D)]^d : v|_K \in [\mathcal{P}^p(K)]^d, \forall K \in \mathcal{T}_h \} \]
  \[ M_h^p = \{ \mu \in L^2(\mathcal{E}_h) : \mu|_F \in \mathcal{P}^p(F), \forall F \in \mathcal{E}_h \} \]

- **Define numerical traces**
  \[ \widehat{q}_h = q_h - \tau(u_h - \widehat{u}_h)n, \text{ on } \partial K \]

- **Find** \((q_h, u_h, \widehat{u}_h) \in V_h^p \times W_h^p \times M_h^p\) such that \(\forall (v, w, \mu) \in V_h^p \times W_h^p \times M_h^p\)
  \[
  (q_h, v)_{\mathcal{T}_h} + (u_h, \nabla \cdot v)_{\mathcal{T}_h} - \langle \widehat{u}_h, v \cdot n \rangle_{\partial \mathcal{T}_h} = 0, \\
  (\rho q_h, \nabla w)_{\mathcal{T}_h} - \langle \rho q_h \cdot n, w \rangle_{\partial \mathcal{T}_h} - (k^2 u_h, w)_{\mathcal{T}_h} + \langle \rho \tau (u_h - \widehat{u}_h), w \rangle_{\partial \mathcal{T}_h} = (f, w)_{\mathcal{T}_h} \\
  \langle \rho q_h \cdot n, \mu \rangle_{\partial \mathcal{T}_h} - \langle \rho \tau u_h, \mu \rangle_{\partial \mathcal{T}_h} + \langle \rho \tau \widehat{u}_h, \mu \rangle_{\partial \mathcal{T}_h} + \langle v \widehat{u}_h, \mu \rangle_{\partial D} = (g, w)_{\partial D}
  \]

\[
\begin{bmatrix}
A & B & -C \\
W & D & -E \\
N & -E^* & M
\end{bmatrix}
\begin{bmatrix}
Q \\
U \\
\widehat{U}
\end{bmatrix}
= 
\begin{bmatrix}
0 \\
F \\
G
\end{bmatrix}
\]

Solve for global dof \(TU = R\)

Recover local dof \(Q, U\)

Block-diagonal and invertible
Control variates \[ E[s] = E[s - s_{N_1}] + E[s_{N_1}] \]

MVR estimator \[ E_{M_0,M_1}[s] = E_{M_0}[s - s_{N_1}] + E_{M_1}[s_{N_1}] \]

\[ Z_0 = E[s - s_{N_1}] - E_{M_0}[s - s_{N_1}] \sim N\left(0; \frac{V[s - s_{N_1}]}{M_0}\right) \]

\[ Z_1 = E[s_{N_1}] - E_{M_1}[s_{N_1}] \sim N\left(0; \frac{V[s_{N_1}]}{M_1}\right) \]

\[ Z_0 + Z_1 = E[s] - E_{M_0,M_1}[s] \sim N\left(0; \frac{V[s - s_{N_1}]}{M_0} + \frac{V[s_{N_1}]}{M_1}\right) \]

Central limit theorem to establish confidence bounds

\[ \lim_{M_0 \to \infty} \lim_{M_1 \to \infty} \Pr \left( |E[s] - E_{M_0,M_1}[s]| \leq a \sigma_{MVR} \right) = \text{erf} \left( \frac{a}{\sqrt{2}} \right), \quad \forall a \geq 0 \]
Optimal weights (I)

✓ Precompute MSCG-RB outputs \( s, s_{N_{\ell}}, 1 \leq N_{\ell} \leq N_{\text{max}} \) for \( M \) samples

✓ Approximate \( V_{M_{\ell}}[s_{N_{\ell}} - s_{N_{\ell}+1}] \) (a posteriori) with \( V_M[s_{N_{\ell}} - s_{N_{\ell}+1}] \) (a priori)

✓ Surrogate online cost can be expressed as

\[
\hat{C}_{L-MVR} = \sum_{\ell=0}^{L} \frac{\hat{C}^\ell}{w_{\ell}} = \frac{a^2}{\Delta_E^2} \left[ (t_s + t_{N_1}) \frac{V_M[s - s_{N_1}]}{w_0} + t_{N_L} \frac{V_M[s_{N_L}]}{w_L} ight.
\]

\[
+ \sum_{\ell=1}^{L-1} \left( t_{N_{\ell}} + t_{N_{\ell+1}} \right) \frac{V_M[s_{N_{\ell}} - s_{N_{\ell+1}}]}{w_\ell} \right]
\]
Optimal weights (II)

✓ Fix level sizes \((\overline{N}_1, \ldots, \overline{N}_L)\) \(\rightarrow\) optimize over weights

\[
(w_0^*, w_1^* \ldots, w_L^*) = \arg \min \, \hat{C}_{L-MVR}(\overline{N}_1, \ldots, \overline{N}_L)
\]

\[
\text{s.t. } \sum_{\ell=0}^{L} w_{\ell} = 1, \quad w_{\ell} \geq 0
\]

✓ Optimal weights have closed formula

\[
w_{\ell}^* = \frac{\sqrt{\hat{C}_\ell / \hat{C}^0}}{\sum_{\ell'=0}^{L} \sqrt{\hat{C}_{\ell'}/\hat{C}^0}}, \quad \ell = 0, \ldots, L.
\]

✓ Exhaustive search \(\rightarrow\) select \((L,N,w)\) with lowest \(\hat{C}_{L-EIMVR}\)
Empirical interpolation applied to MVR

Choose \( N_1 > N_2 > \ldots > N_L \) and define \( L \)-EIMVR estimator

\[
E_{M_0, \ldots, \hat{M}_L} [s] = E_{M_0} [s - s_{N_1}] + \sum_{\ell=1}^{L-1} E_{M_{\ell}} [s_{N_{\ell}} - s_{N_{\ell+1}}] + E_{M_L} [s_{N_L} - \hat{s}_{N_L}] + E_{\hat{M}_L} [\hat{s}_{N_L}]
\]

For i.i.d. samples between levels, we apply the central limit theorem

\[
\lim_{M_0 \to \infty} \ldots \lim_{\hat{M}_L \to \infty} \Pr \left( |E[s] - E_{M_0, \ldots, \hat{M}_L} [s]| \leq \Delta_{\hat{E}} \right) = \text{erf} \left( \frac{a}{\sqrt{2}} \right), \quad \forall a \geq 0
\]

and obtain the \textit{a posteriori} error bound

\[
\Delta_{\hat{E}} = a \sqrt{\frac{V_{M_0} [s - s_{N_1}]}{M_0} + \sum_{\ell=1}^{L-1} \frac{V_{M_{\ell}} [s_{N_{\ell}} - s_{N_{\ell+1}}]}{M_{\ell}} + \frac{V_{M_L} [s_{N_L} - \hat{s}_{N_L}]}{M_L} + \frac{V_{\hat{M}_L} [\hat{s}_{N_L}]}{\hat{M}_L}}
\]
Empirical interpolation applied to MVR

Estimator for variance

Define \( \zeta = \left( s - E_{M_0, M_1, \hat{M}_1}[s] \right)^2 \), \( \zeta_N = \left( s_N - E_{M_0, M_1, \hat{M}_1}[s] \right)^2 \)

\( \hat{\zeta}_N = \left( \hat{s}_N - E_{M_0, M_1, \hat{M}_1}[s] \right)^2 \)

and reuse multilevel expression

\[
V_{M_0, M_1, \hat{M}_1}[s] = E_{M_0}[\zeta - \zeta_N] + E_{M_1}[\zeta_N - \hat{\zeta}_N] + E_{\hat{M}_1}[\hat{\zeta}_N]
\]

+ error bounds

Estimator for gradient

\[
E_{M_0, M_1, \hat{M}_1}[\nabla s] = E_{M_0}[\nabla s - \nabla s_N] + E_{M_1}[\nabla s_N - \nabla \hat{s}_N] + E_{\hat{M}_1}[\nabla \hat{s}_N]
\]

+ error bounds

Extension to arbitrary number of levels is straightforward
Error and cost equation

For a prescribed tolerance $\Delta$

$$\Delta^2 = a^2 \frac{V_{M_0} [s - s_{N_1}]}{M_0} = w_0 \Delta^2$$

$$+ \sum_{\ell=1}^{L-1} a^2 \frac{V_{M_\ell} [s_{N_\ell} - s_{N_{\ell+1}}]}{M_\ell} = w_\ell \Delta^2$$

$$+ a^2 \frac{V_{M_L} [s_{N_L} - \hat{s}_{N_L}]}{M_L} = w_L \Delta^2$$

Level 0

Level $\ell$

Level $L$

Level $\hat{L}$

Termination condition MC

Cost of $L$-MVR estimator

$$C_{L-EIMVR} = (t_s + t_{N_1}) M_0 + t_{N_L} M_L + \sum_{\ell=1}^{L-1} (t_{N_\ell} + t_{N_{\ell+1}}) M_\ell$$

alternatively...

$$C_{L-EIMVR} = \frac{a^2}{\varepsilon_{tol}^2} \left[ (t_s + t_{N_1}) \frac{V_{M_0} [s - s_{N_1}]}{w_0} + t_{N_L} \frac{V_{M_L} [s_{N_L} - \hat{s}_{N_L}]}{w_L} ight.$$  

$$+ \sum_{\ell=1}^{L-1} (t_{N_\ell} + t_{N_{\ell+1}}) \frac{V_{M_\ell} [s_{N_\ell} - s_{N_{\ell+1}}]}{w_\ell} \left] 

\right.$$
✓ Fix $N_L$ and precompute EI output at $M_L + \hat{M}_L$ samples

✓ Precompute HDG-RB outputs $s, s_{N_L}, N_L \leq N_L \leq N_{\text{max}}$ for $M$ samples

✓ Approximate $V_{M_L}[s_{N_L} - s_{N_{L+1}}]$ (a posteriori) with $V_M[s_{N_L} - s_{N_{L+1}}]$ (a priori)

✓ Surrogate online cost can be expressed as

$$\hat{C}_{L-EIMVR} = \sum_{\ell=0}^{L} \frac{\hat{C}^\ell}{W^\ell} = \frac{a^2}{\Delta^2} \left[ (t_s + t_{N_1}) \frac{V_M[s - s_{N_1}]}{W_0} + t_{N_L} \frac{V_M[s_{N_L} - \hat{s}_{N_L}]}{W_L} \right.$$

$$+ \sum_{\ell=1}^{L-1} (t_{N_{\ell}} + t_{N_{\ell+1}}) \frac{V_M[s_{N_{\ell}} - s_{N_{\ell+1}}]}{W_\ell} \left. \right]$$
Optimal weights (II)

✓ Compute weight for EI level $\widehat{w}_L = \frac{a^2}{\Delta^2} \frac{V_{\widehat{M}_L}[\widehat{s}_{N_L}]}{\widehat{M}_L}$

✓ Fix level sizes $(\overline{N}_1, \ldots, \overline{N}_L)$ → optimize over weights

$$(w_0^*, w_1^* \ldots, w_L^*) = \arg\min \widehat{C}_{L-EIMVR}(\overline{N}_1, \ldots, \overline{N}_L)$$

s.t. $\sum_{\ell=0}^{L} w_\ell = 1 - \widehat{w}_L$, $w_\ell \geq 0$

✓ Optimal weights have closed formula

$$w_\ell^* = \frac{\sqrt{\widehat{C}_\ell / \widehat{C}_0}}{\sum_{\ell'=0}^{L} \sqrt{\widehat{C}_{\ell'}/\widehat{C}_0}}, \quad \ell = 0, \ldots, L.$$  

✓ Exhaustive search → select $(L, N, w)$ with lowest $\widehat{C}_{L-EIMVR}$
Stochastic simulation: 1d numerical verification

\[-\nabla \cdot (\rho \nabla u) = f \quad x \in \Omega\]

\[\rho \nabla u = 0 \quad x = 1\]

\[\rho = \sum_{q=1}^{10} y_q 1_{\Omega_q}\]

\[u = 0 \quad x = 0\]

Compare MC with MVR given by

\[E_{M/10,M}[s] = E_{M/10}[s - s_5] + E_M[s_5]\]