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

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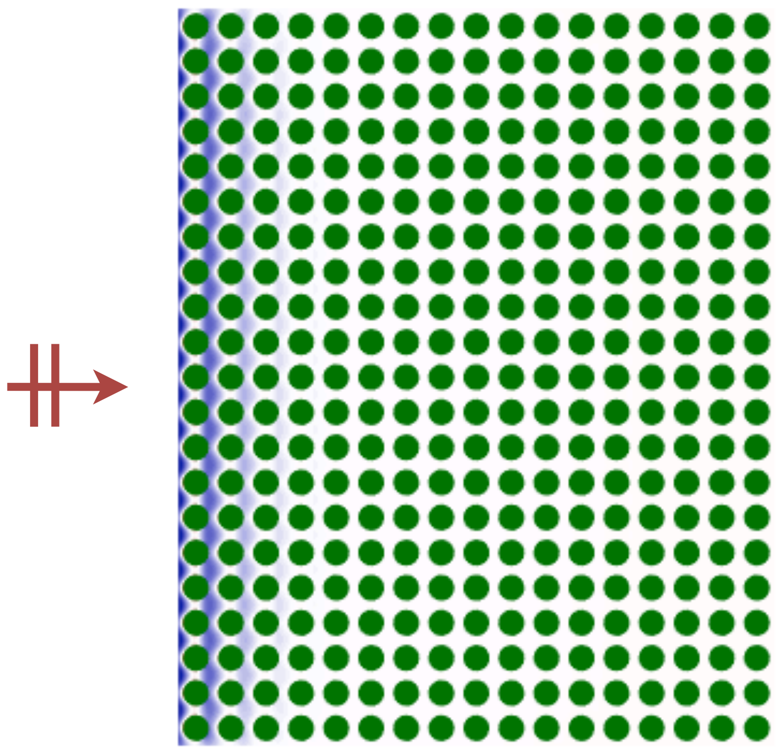
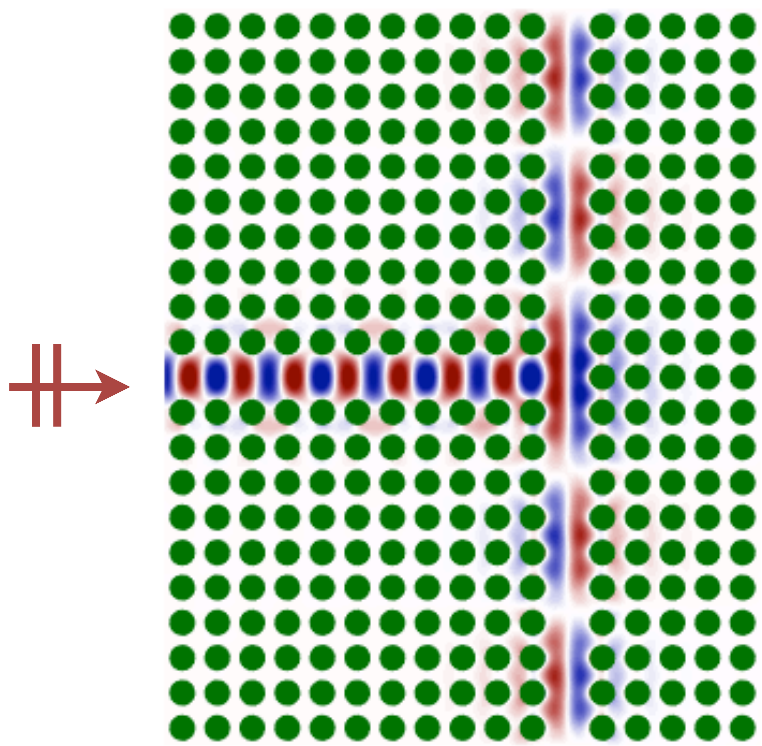
Motivation

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



photonic crystal

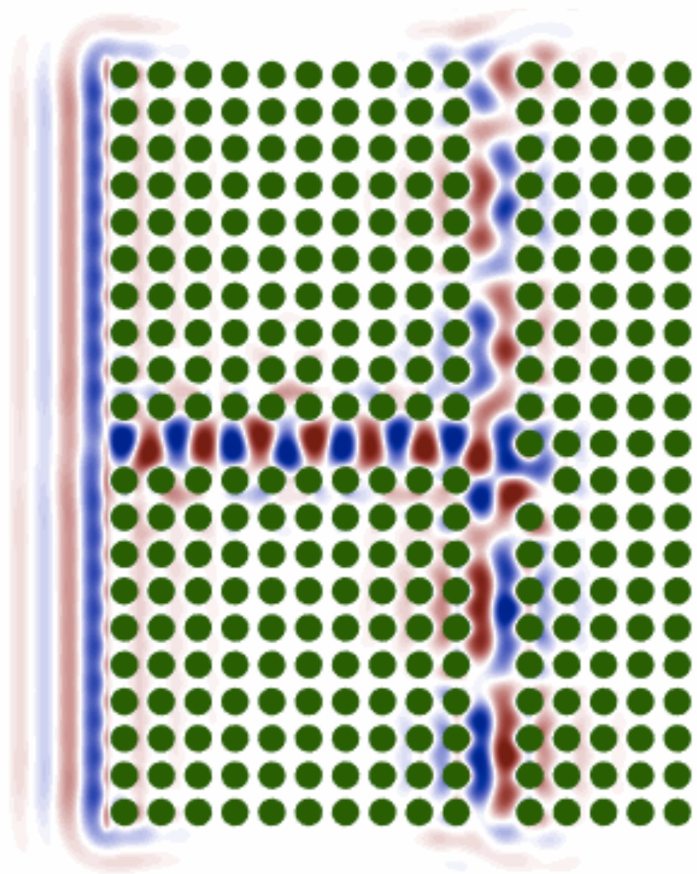


waveguide splitter

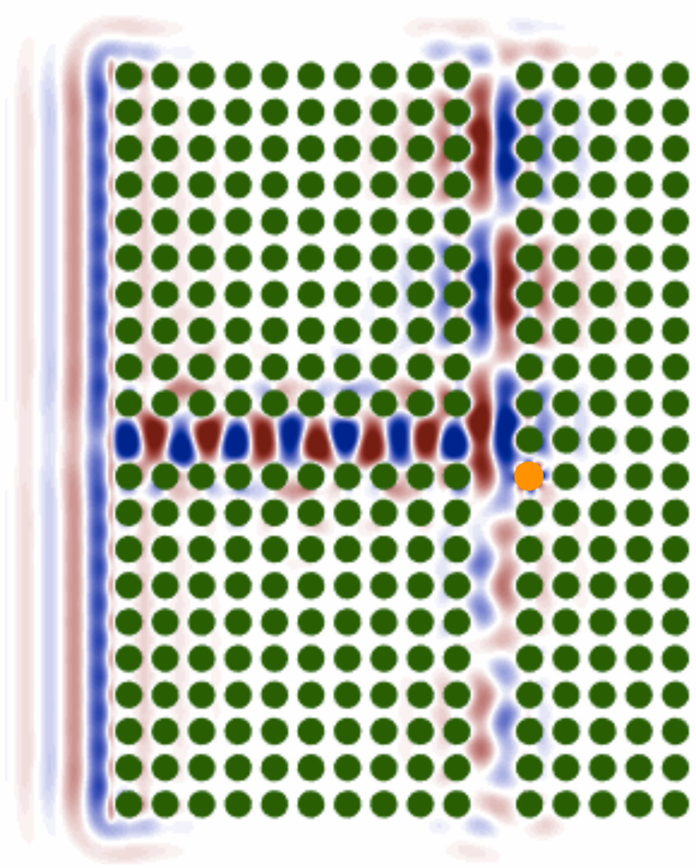
applications ⟶ waveguides, fibers, cavities...

Motivation: Photonic Bandgap

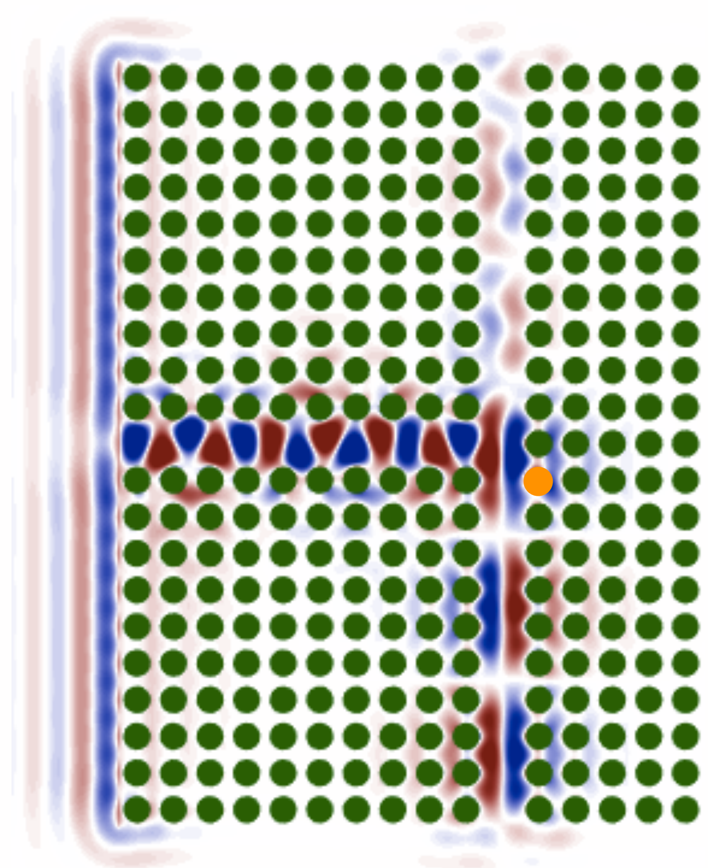
Highly **sensitive** to material properties and geometry **variations**



Remove rod



+15% permittivity



-3% radius

Accurate simulations are required

Problem statement

Consider the **Helmholtz** equation in 2d

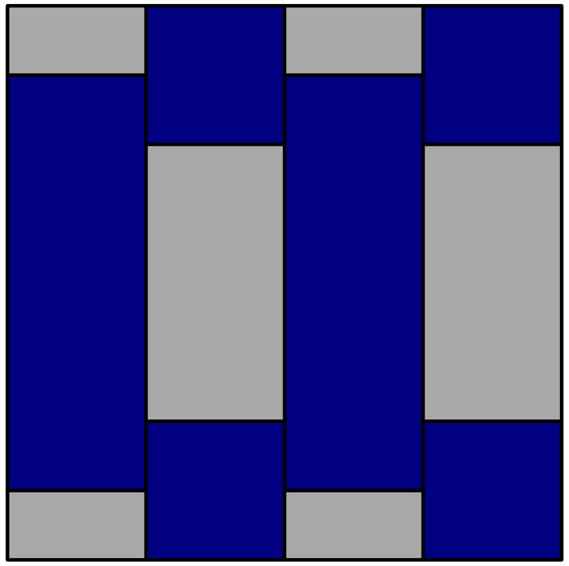
$$-\nabla \cdot (\rho(\mathbf{x}) \nabla u) - k^2(\mathbf{x}) u = f \qquad + \text{B.C.}$$

where $\rho(\mathbf{x})$, $k^2(\mathbf{x})$ represent material properties

- ✓ Time-harmonic solutions of scalar wave equation
- ✓ 2d Maxwell's equations for TE and TM polarizations ⟶ TE: $u = H_z$ TM: $u = E_z$

Wave propagation is considered for **structured** materials

Ω



Material 1 $\rho(\mathbf{x})$, $k^2(\mathbf{x})$

Material 2 $\rho(\mathbf{x})$, $k^2(\mathbf{x})$

piecewise constant

$$\Omega = \bigcup_{m=1}^{M} \Omega^m$$

Objectives

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

Simulate wave propagation in structured media

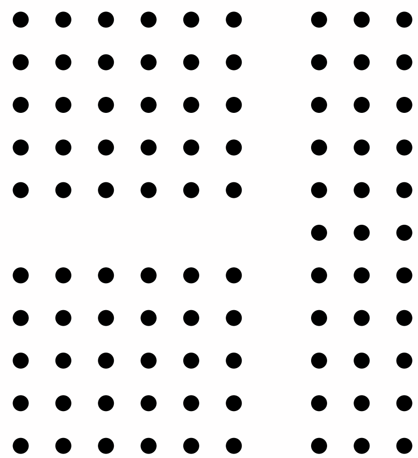
- Wave equation is **non-coercive,** need **high accuracy**
- Complex **geometries**, repeated **patterns**, mismatch in **length scales**

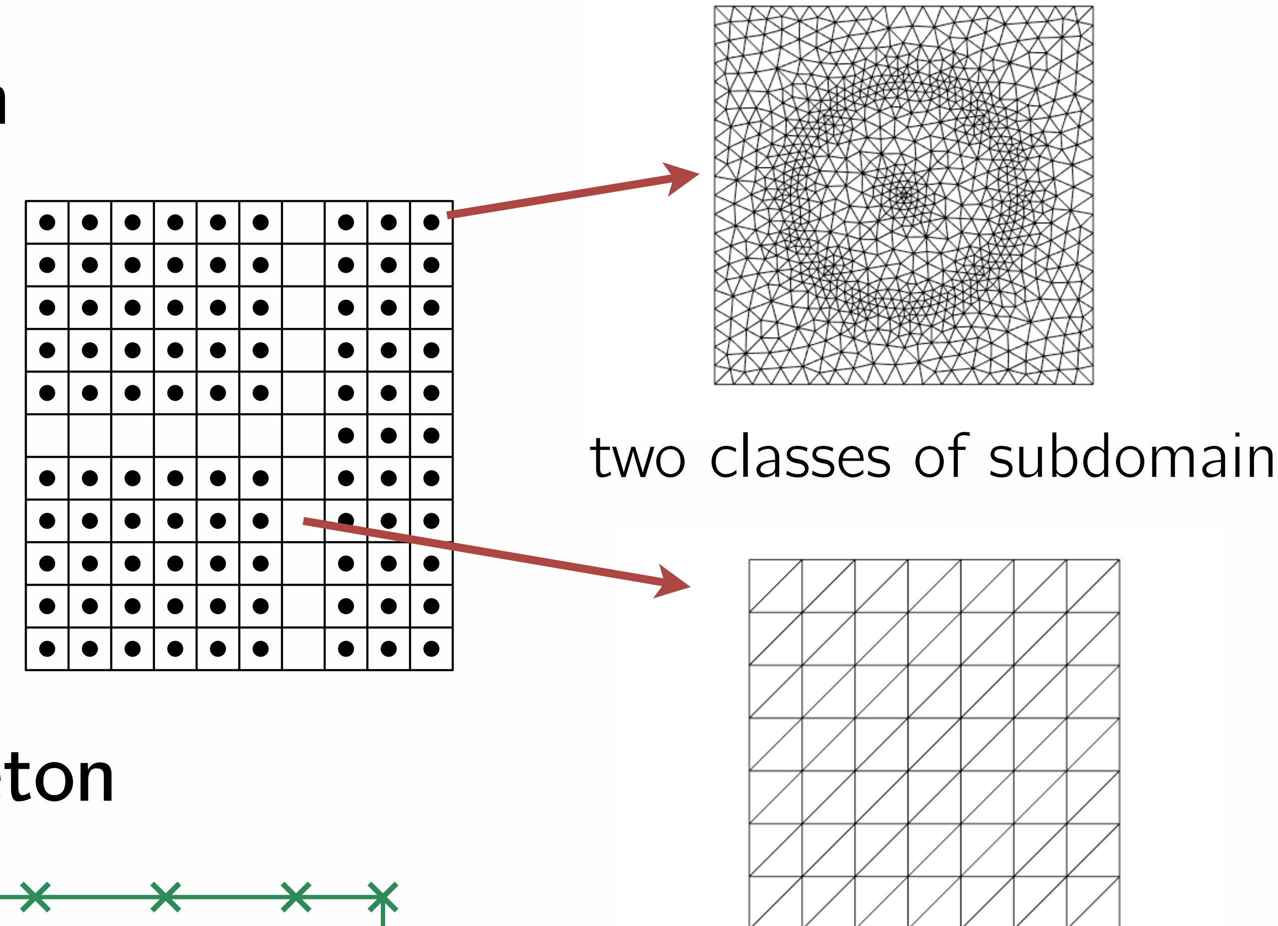
Stochastic simulation of wave propagation

- Framework to deal with **geometry** variations
- Models are expensive: develop **surrogates**, use **control variates**

MultiScale continuous Galerkin (MSCG) method

Identify **repeated geometries** in domain



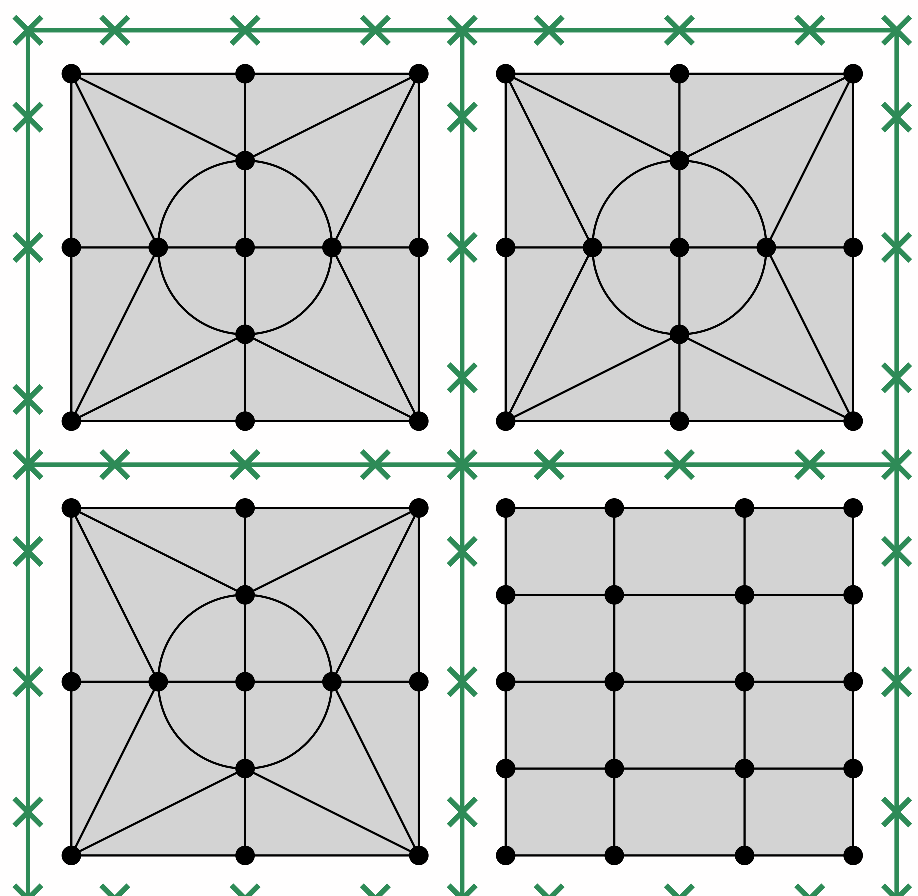


Discretize **subdomains** and **global skeleton**

Local problem

High-order CG discretization

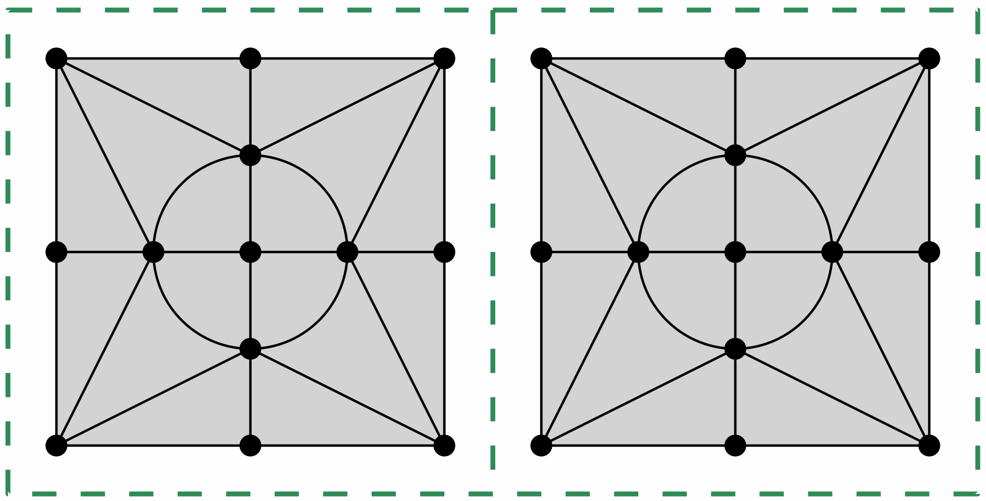
Capture small features

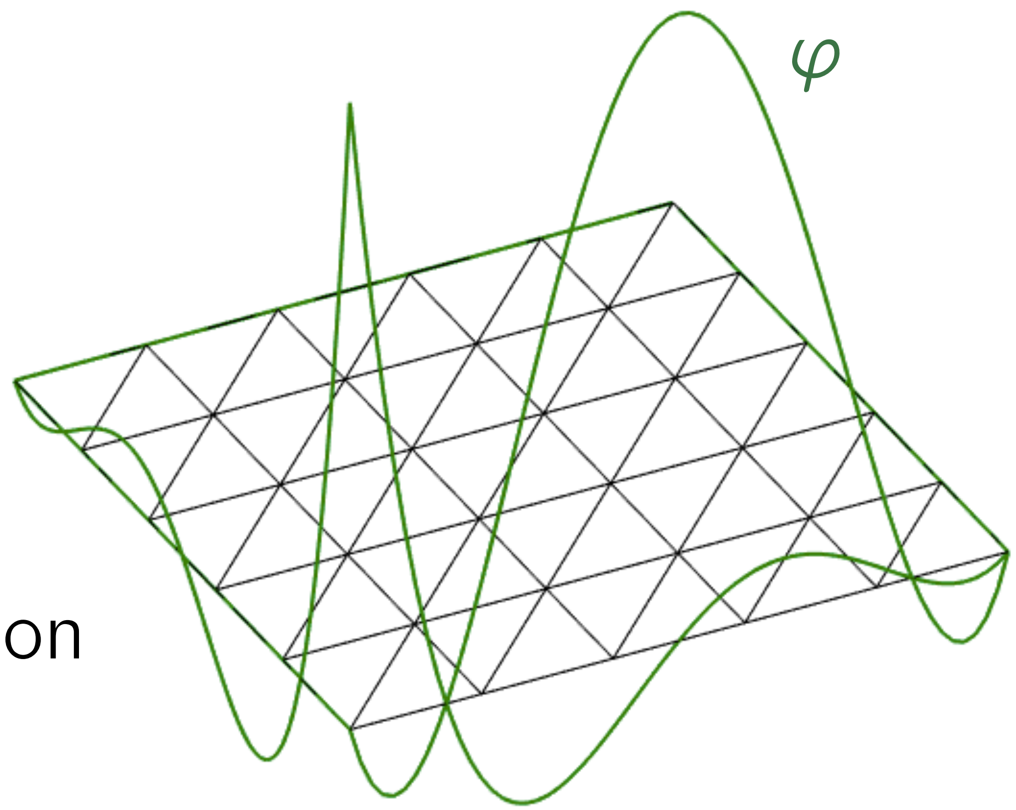


Global problem

Lagrange polynomial for solution on global faces

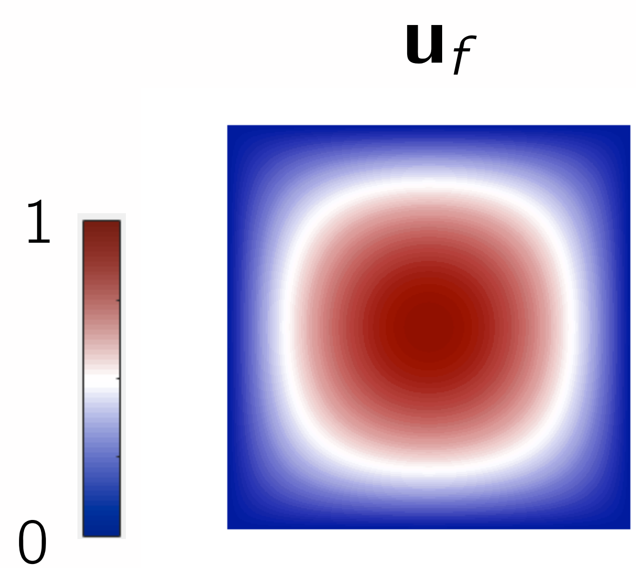
Capture frequencies on large scale

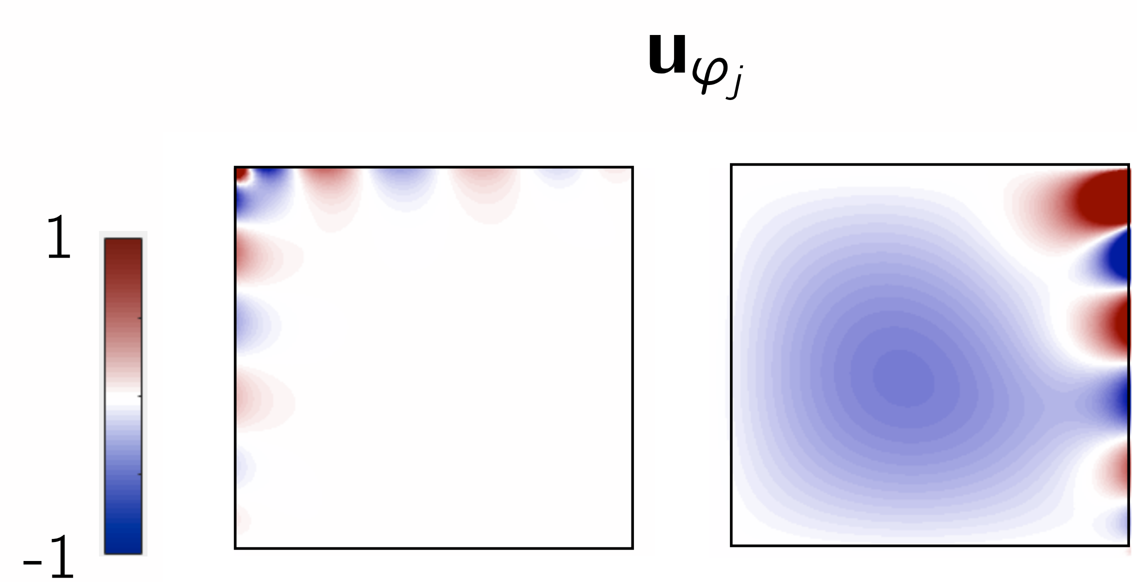




For every subdomain Ω^m, solve Helmholtz equation

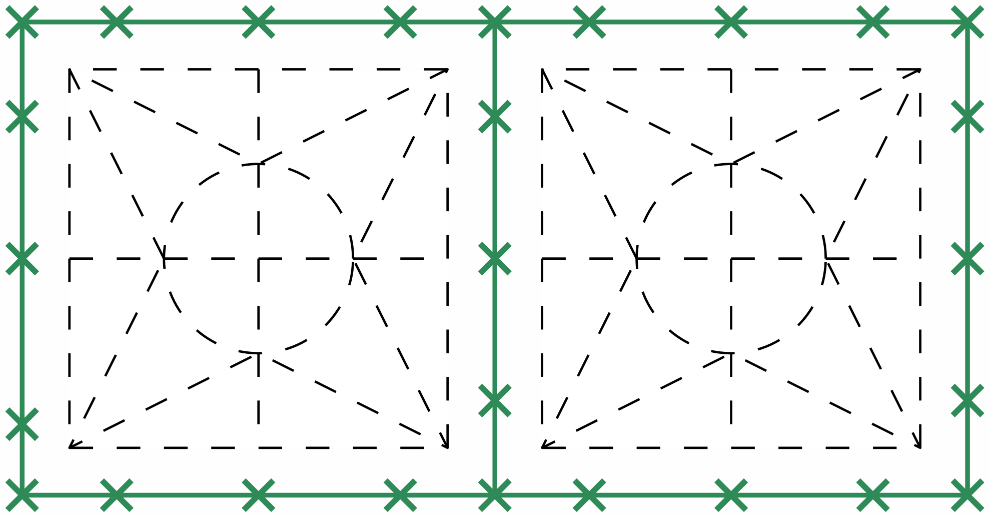
1. Source problem $\longrightarrow$ $\mathbb{A}\mathbf{u}_f = \mathbf{f}$
2. Inhomogeneous Dirichlet given by φ_j, $1 \leq j \leq J$ $\longrightarrow$ $\mathbb{A}\mathbf{u}_{\varphi_j} = \mathbf{d}_{\varphi_j}$





MultiScale CG - Global problem

On the subdomain level we apply **linearity** and **superposition**



$$\mathbf{u} = \mathbf{u}_f + \sum_{j=1}^{J} \lambda_j \mathbf{u}_{\varphi_j}$$

The contribution of each subdomain to the global problem is

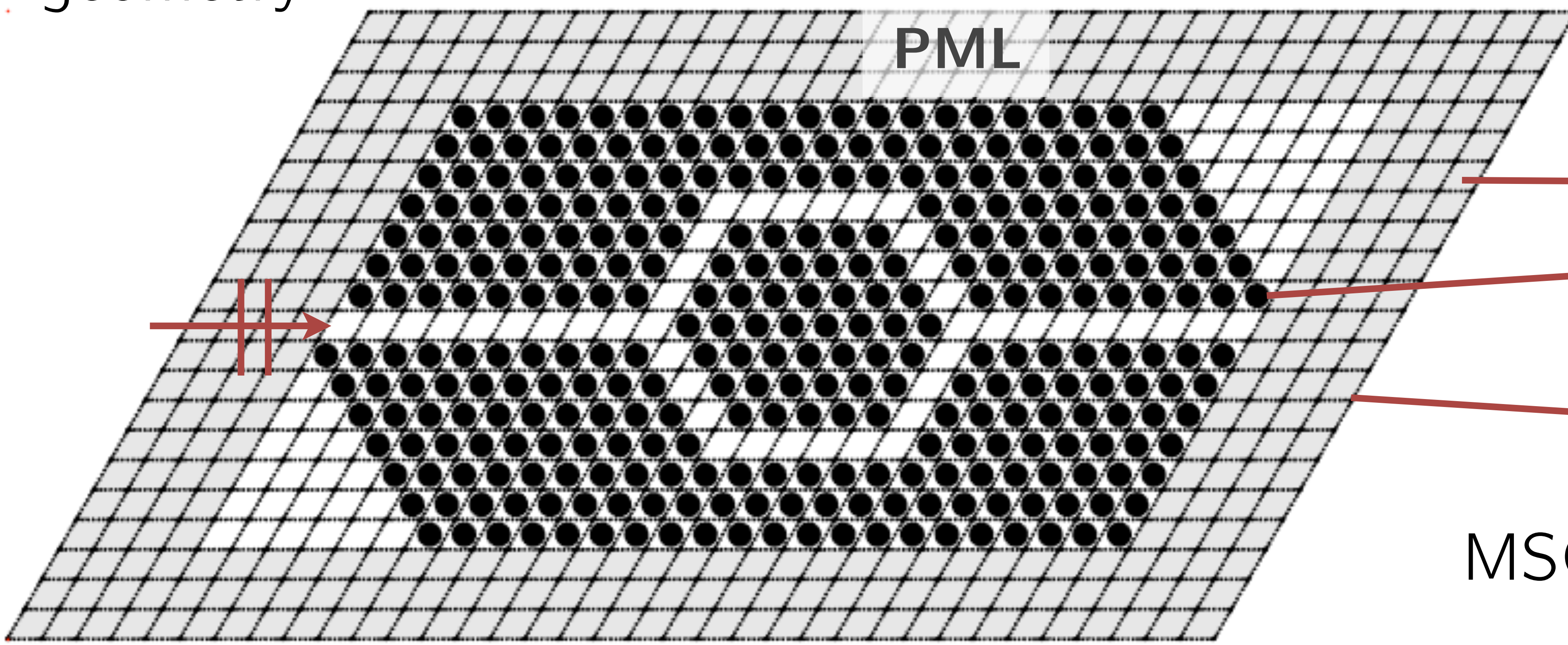
$$\mathbb{K}_{ij} = \mathbf{u}_{\varphi_i}^T \mathbb{A}\, \mathbf{u}_{\varphi_j}, \quad 1 \leq i, j \leq J$$

$$\mathbf{F}_i = \mathbf{u}_{\varphi_i}^T \mathbf{f}, \quad 1 \leq i \leq J$$

Solve the global problem $\mathbb{K}\boldsymbol{\Lambda} = \mathbf{F}$

Simulation of waveguide bends

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



Subdomain dof

415 x 1K = 0.5M

320 x 17K = 5.4M

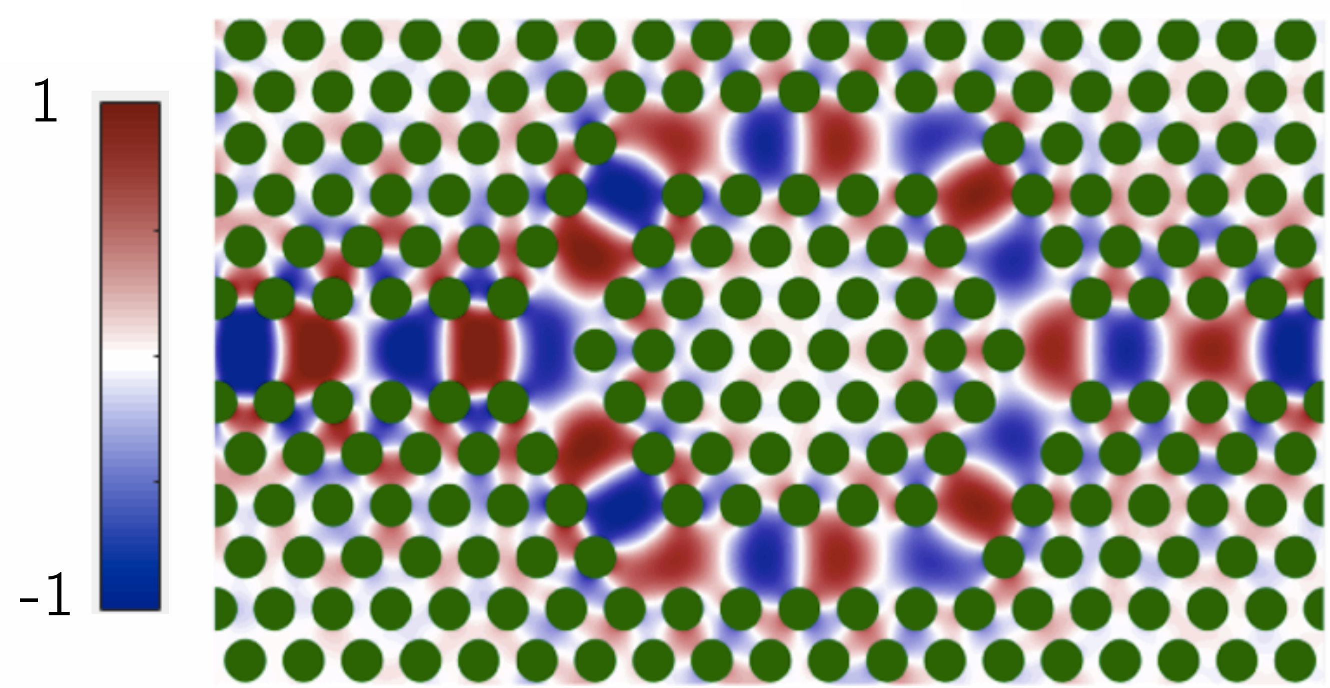
Skeleton dof 15K

MSCG solution in < 3s

Bandgap

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

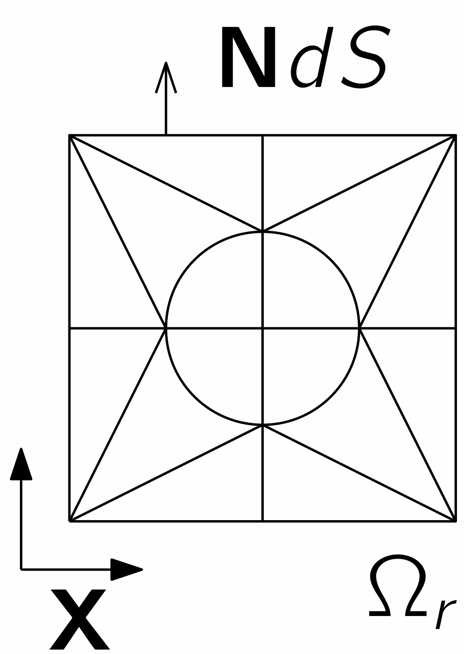
Results for $\dfrac{\omega\, a}{2\pi c} = 0.454$



Reference domain formulation

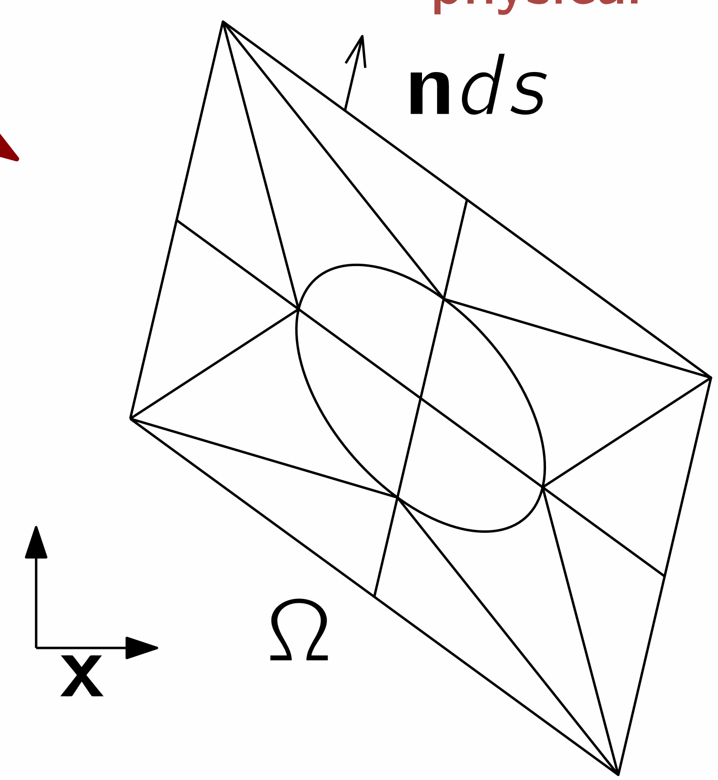
Reformulate governing equations [Persson *et.al.* 09] with deformation mapping parametrized by y

reference



$$\mathbf{x} = \mathcal{G}(\mathbf{X}, y)$$
$$\boldsymbol{G} = \nabla_r \mathcal{G}$$
$$g = \det \boldsymbol{G}$$

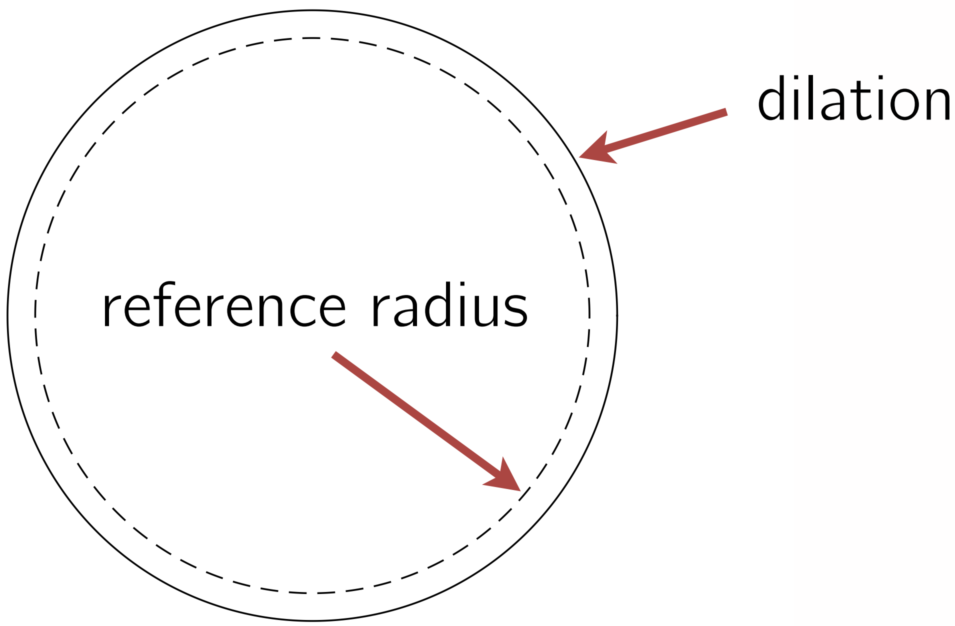
physical



$$-\nabla_r \cdot (\rho(\mathbf{X}) g \boldsymbol{G}^{-1} \boldsymbol{G}^{-T} \nabla_r u) - k^2(\mathbf{X}) u\, g = f\, g$$

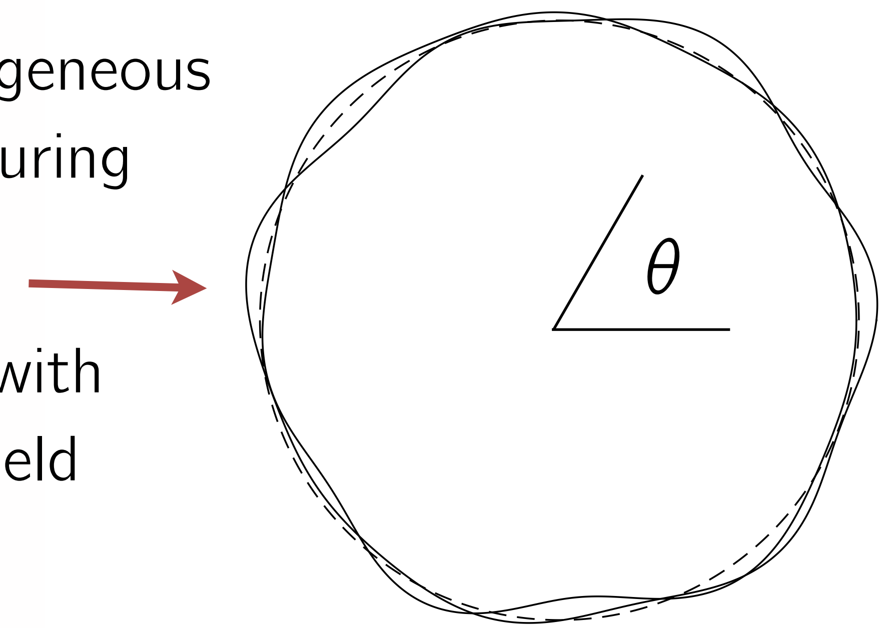
$$-\nabla \cdot (\rho(\mathbf{x}) \nabla u) - k^2(\mathbf{x}) u = f$$

Analyze response of a structured medium under geometry variations



nonhomogeneous
manufacturing
errors

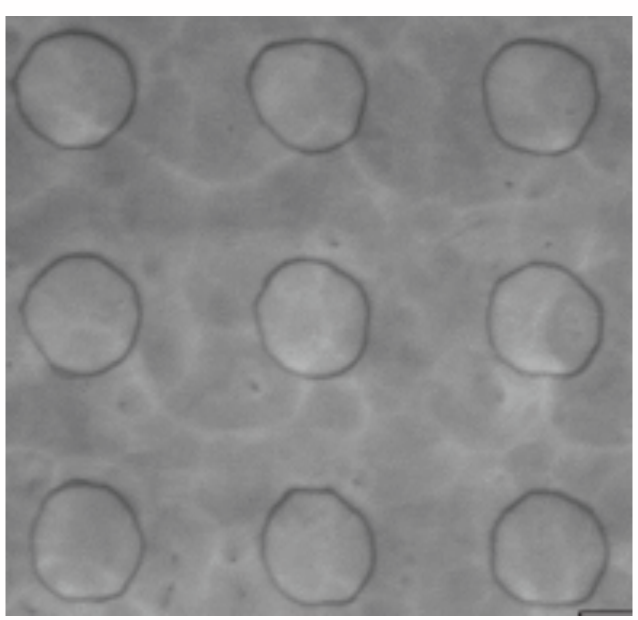
modeled with
random field



variance and
correlation length

uniform r.v.

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



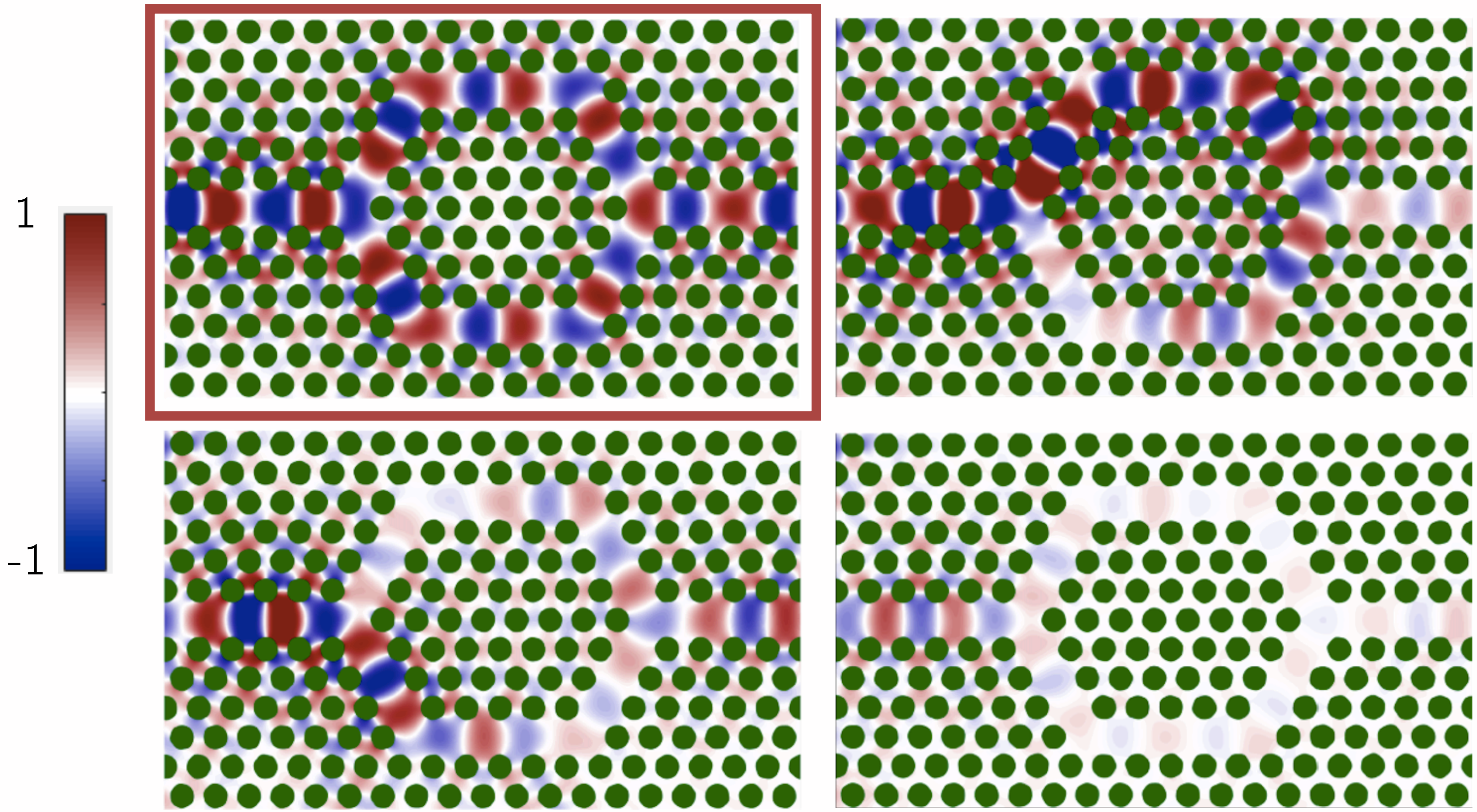
Nanogaps of Al_2O_3 on gold substrate

[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

$\longrightarrow$ **no** longer capitalize **repetition** of subdomains



Reduced basis for MSCG (1/2)

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]

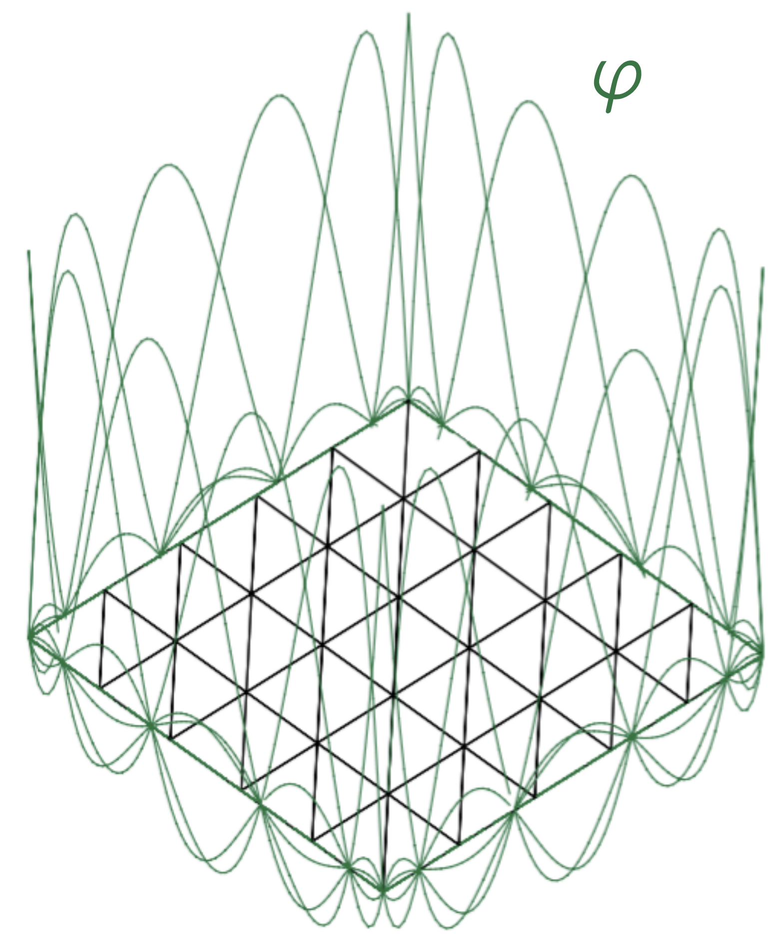
✓ Empirical interpolation [Barrault *et al.* 04] for parameter dependent mapping $\mathcal{G}(y)$

$$\mathbb{A}(y)\mathbf{u}_{\varphi_j} = \mathbf{d}_{\varphi_j}(y)$$

$$\downarrow$$

$$\sum_{q=1}^{Q} \sigma_q(y)\mathbb{A}_q\mathbf{u}_{\varphi_j} = \sum_{q=1}^{Q} \sigma_q(y)\mathbf{d}_{q,\varphi_j}$$

Reduced basis for MSCG (2/2)



- For each Dirichlet BC φ_j, compute snapshots sampling y
- **Single** RB Z compressing snapshots for all Dirichlet BC $\varphi_j, 1 \leq j \leq J$

$$\mathbf{u}^N_{\varphi_j} = \boldsymbol{Z}\mathbf{c}_j$$

- Linear system with **multiple** RHS

$$\sum_{q=1}^{Q} \sigma_q(y) \boldsymbol{Z}^\dagger \mathbb{A}_q \boldsymbol{Z}\mathbf{c}_j = \sum_{q=1}^{Q} \sigma_q(y) \boldsymbol{Z}^\dagger \mathbf{d}_{q,\varphi_j}$$

- RB approximation to local contribution to stiffness matrix

$$\mathbb{K}^N_{ij} = \sum_{q=1}^{Q} \sigma_q(y) \mathbf{c}_i^\dagger \boldsymbol{Z}^\dagger \mathbb{A}_q \boldsymbol{Z}\mathbf{c}_j, \quad 1 \leq i,j \leq J$$

Model and variance reduction method

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

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

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

Variance reduction (statistical correlation) + **Model reduction (cheaper output evaluation)**

Estimate of expectation

Choose $N_1 < N_2 < \ldots < N_L$ and define L-MVR estimator

$$\overset{\text{output evaluation complexity}}{\longrightarrow}$$

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

$$\underset{\#\text{ samples } M_\ell}{\longleftarrow}$$

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

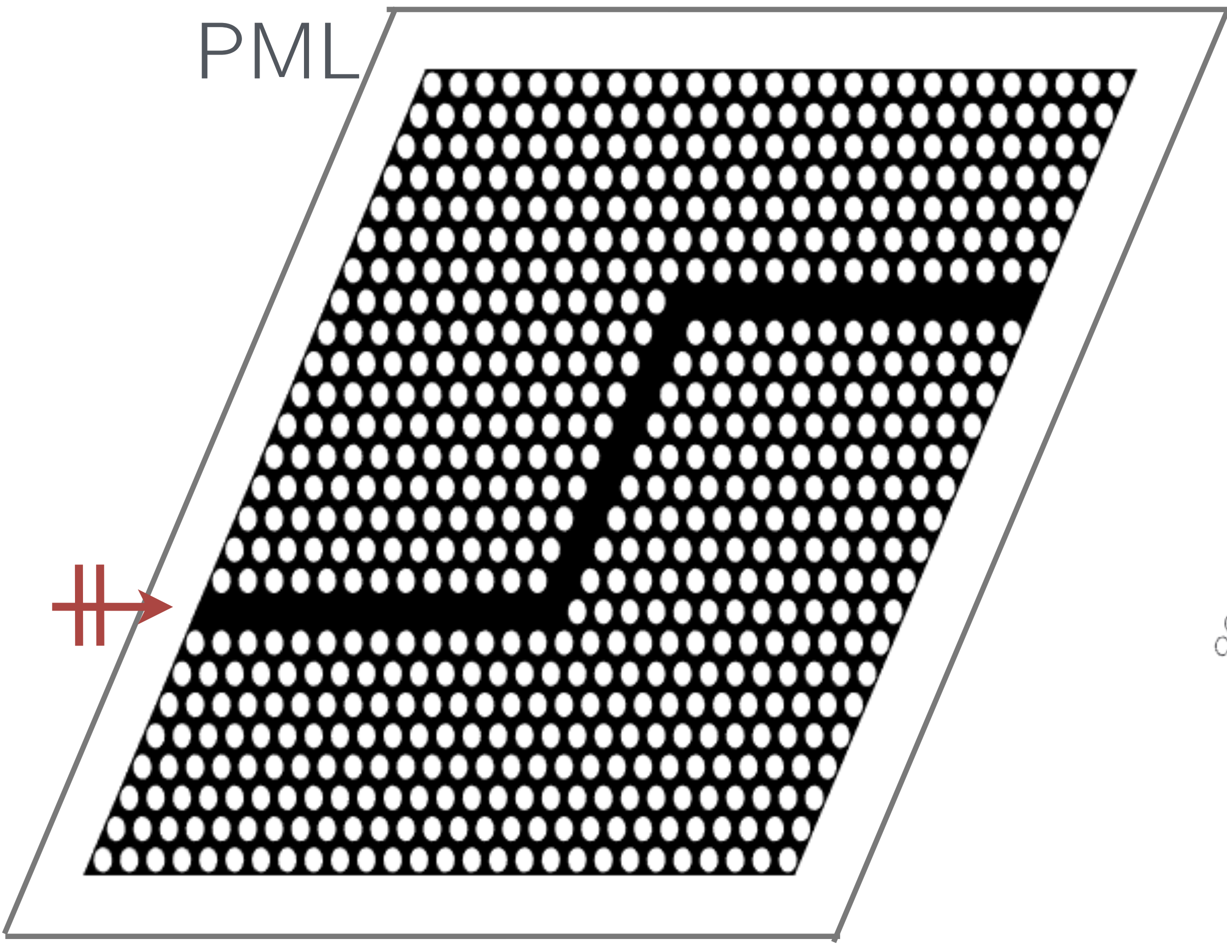
$$\lim_{M_0\to\infty} \ldots \lim_{M_L\to\infty} \Pr\left(\left|E[s] - E_{M_0,\ldots,M_L}[s]\right| \le \Delta_E\right) = \operatorname{erf}\left(\frac{a}{\sqrt{2}}\right), \quad \forall a \ge 0$$

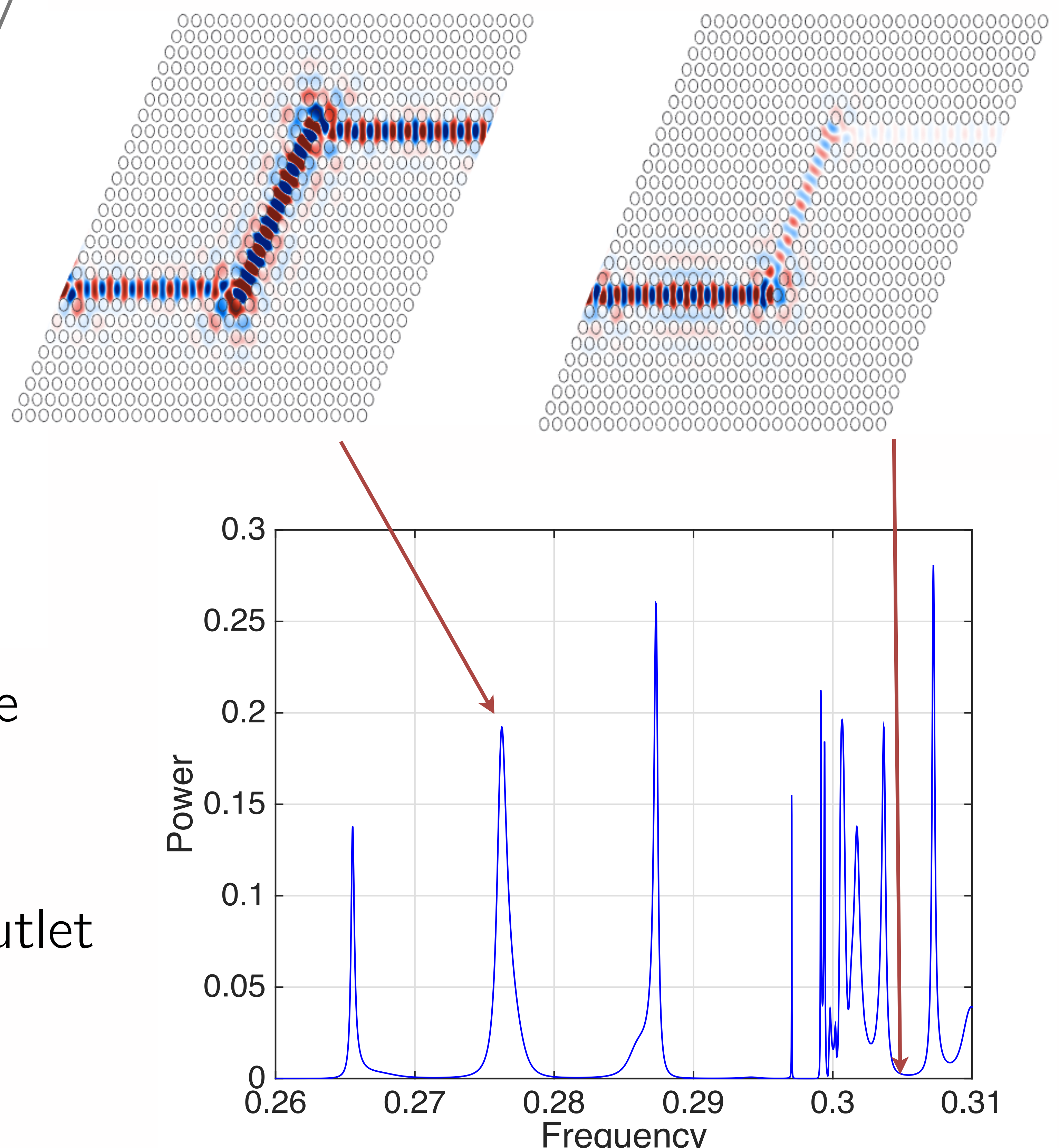
obtain ***a posteriori*** sampling error estimates

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

Similar estimators for the **variance**

Robust design of photonic slab

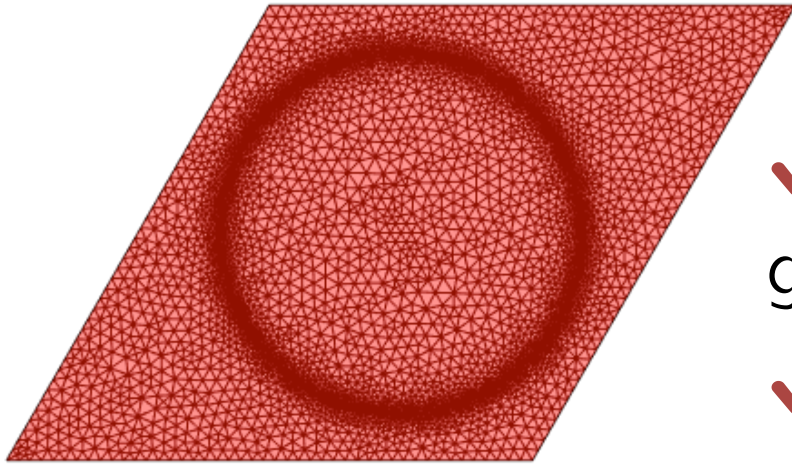




- ✓ Silicon slab on triangular lattice with air holes
- ✓ TE polarization, solve for H_z
- ✓ Output s is optical power at outlet

Computational domain and subproblem selection

Subdomain #1 (optimization)

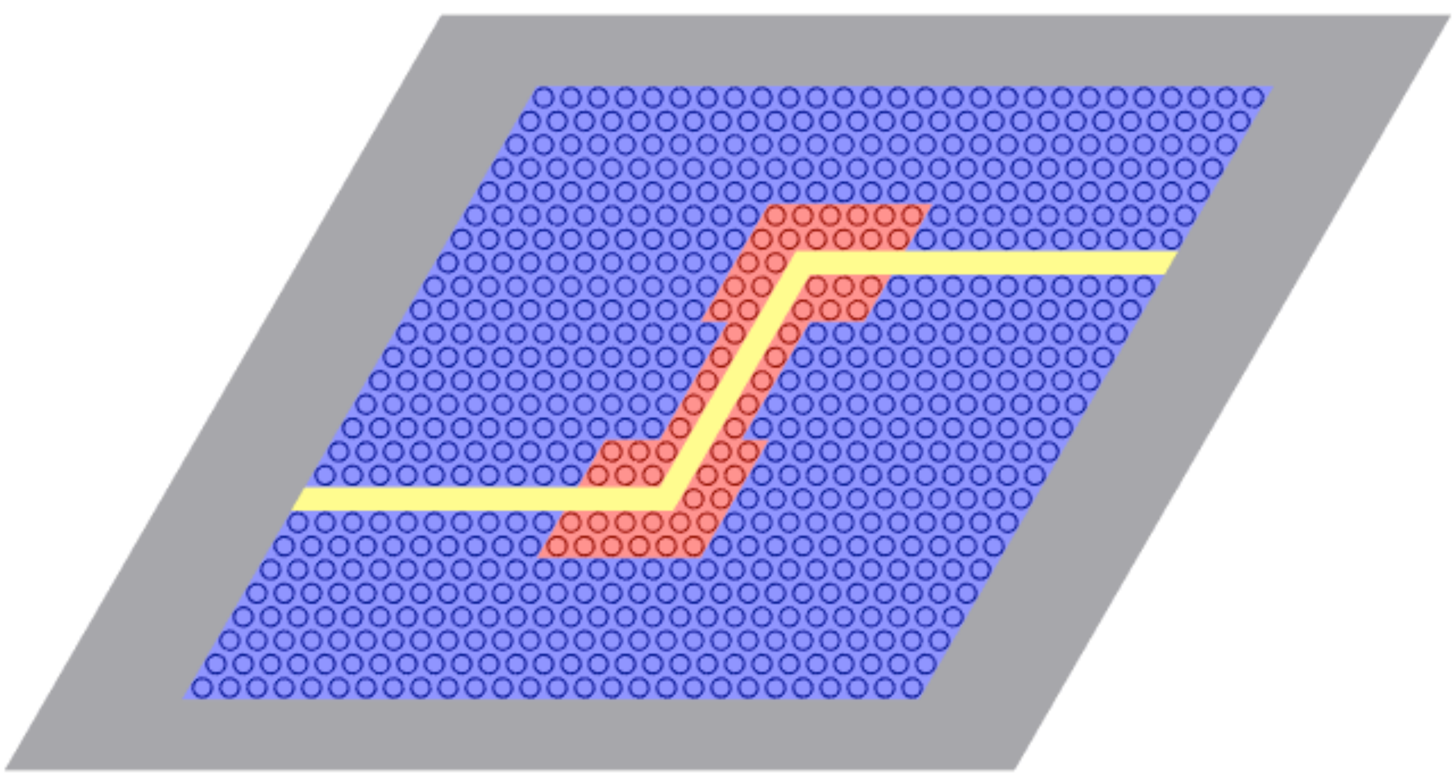


18K dof

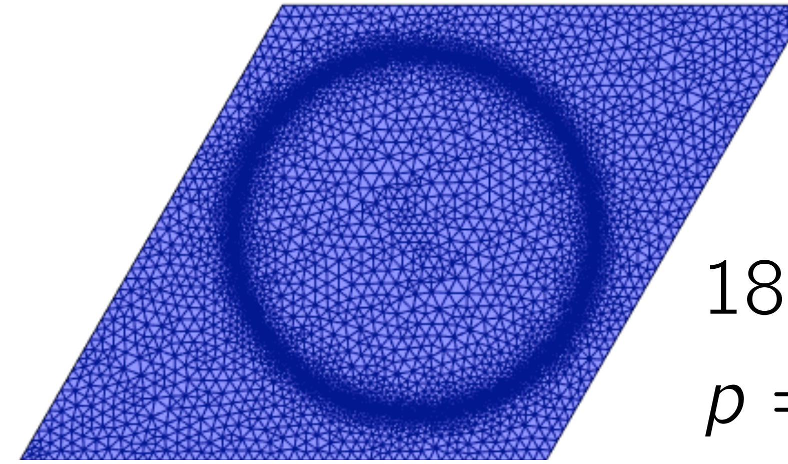
$p = 2$

✓ Develop RB for geometry and frequency

✓ Lagrange polynomial of order 10



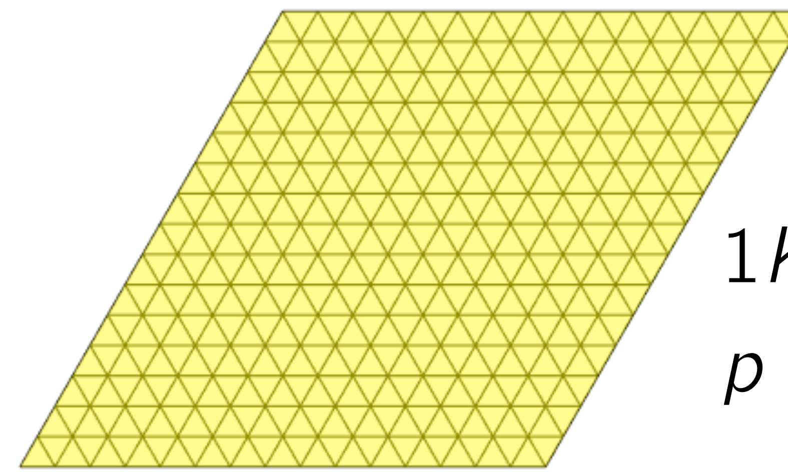
Subdomain #2



18K dof

$p = 2$

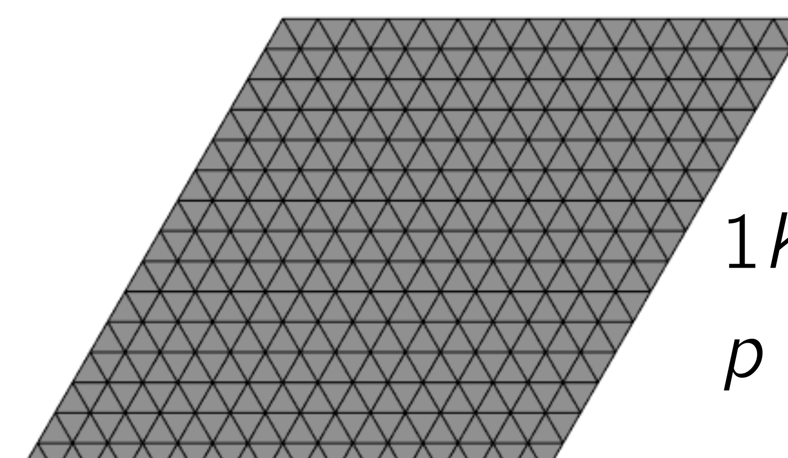
Subdomain #3



1K dof

$p = 2$

Subdomain #4



1K dof

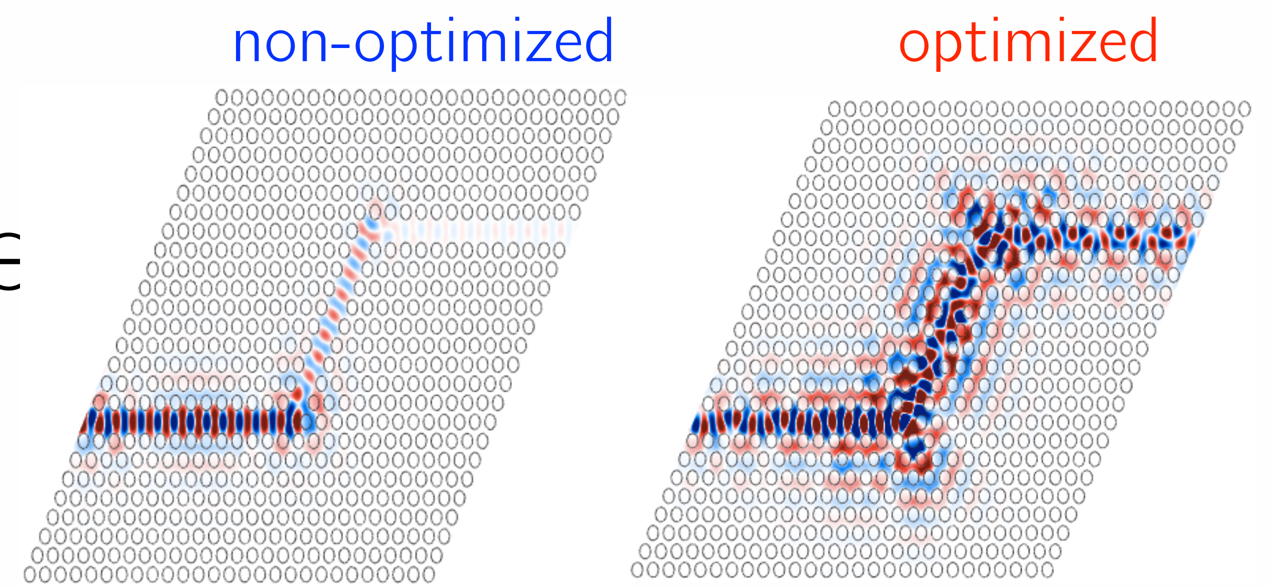
$p = 2$

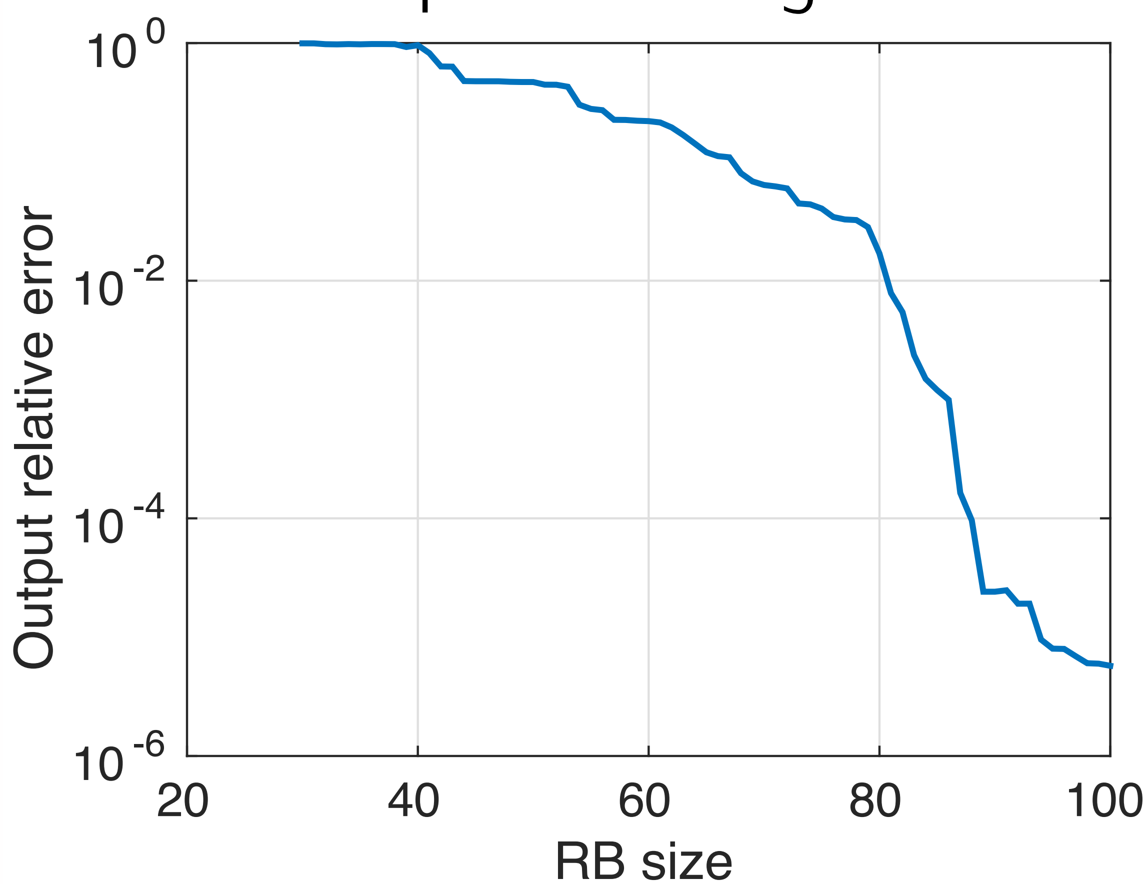
Shape optimization at discrete frequencies

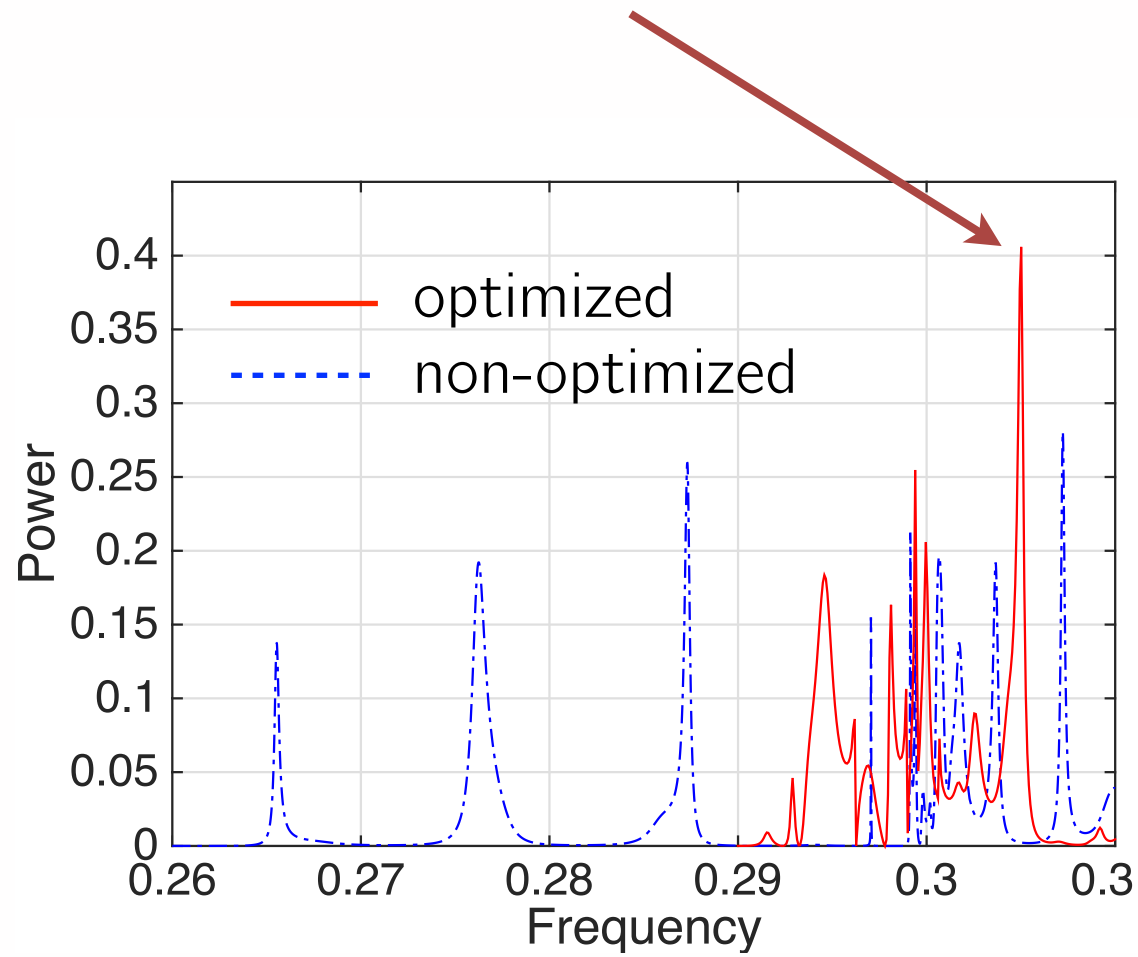
✓ Optimize radius of holes to maximize transmission [NLOPT-Johnson 10]

$$\max_{\theta} s \quad \text{where} \quad r_i = r_0(1+\theta_i),\ \theta_i \in \epsilon$$

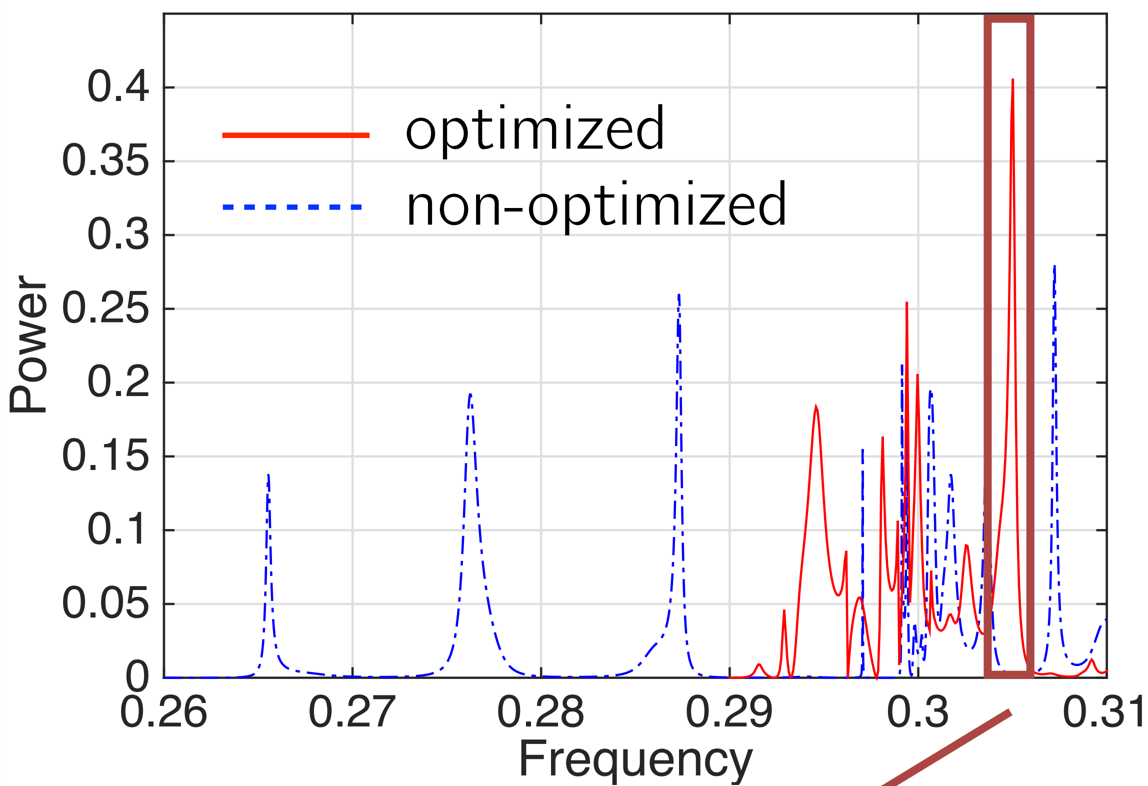
✓ Replace CG for RB on optimization subdomains: speedup ~ 150

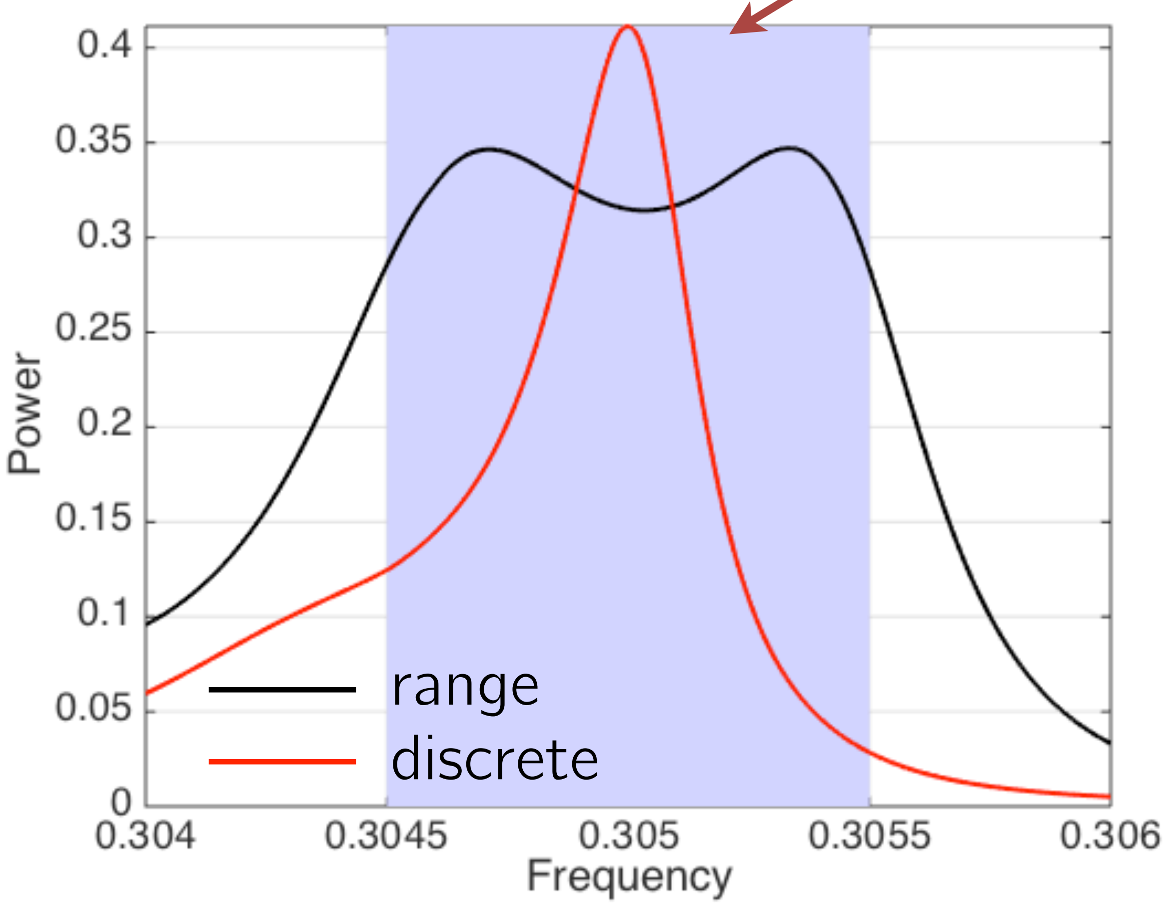






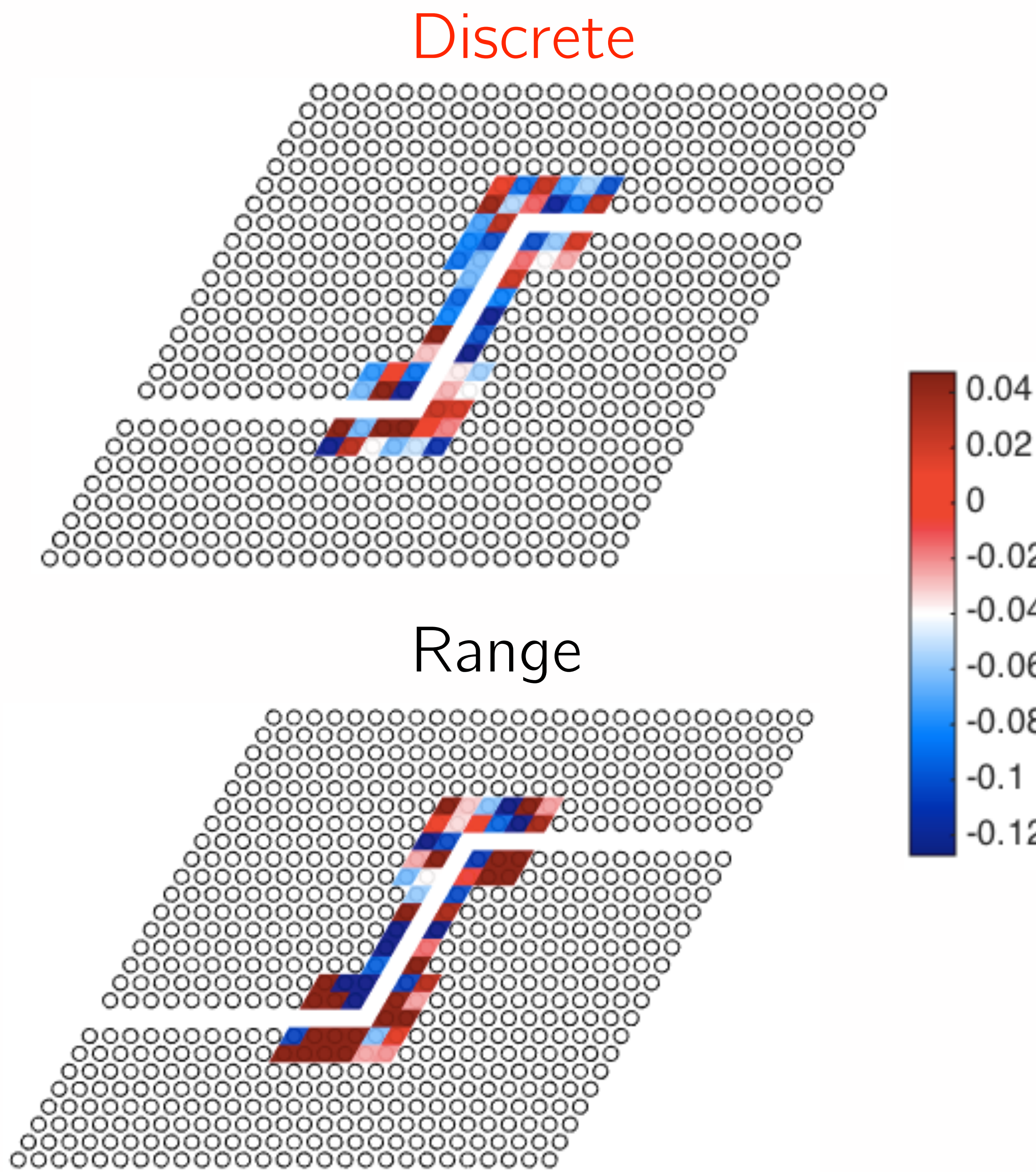
Shape optimization for range of frequencies





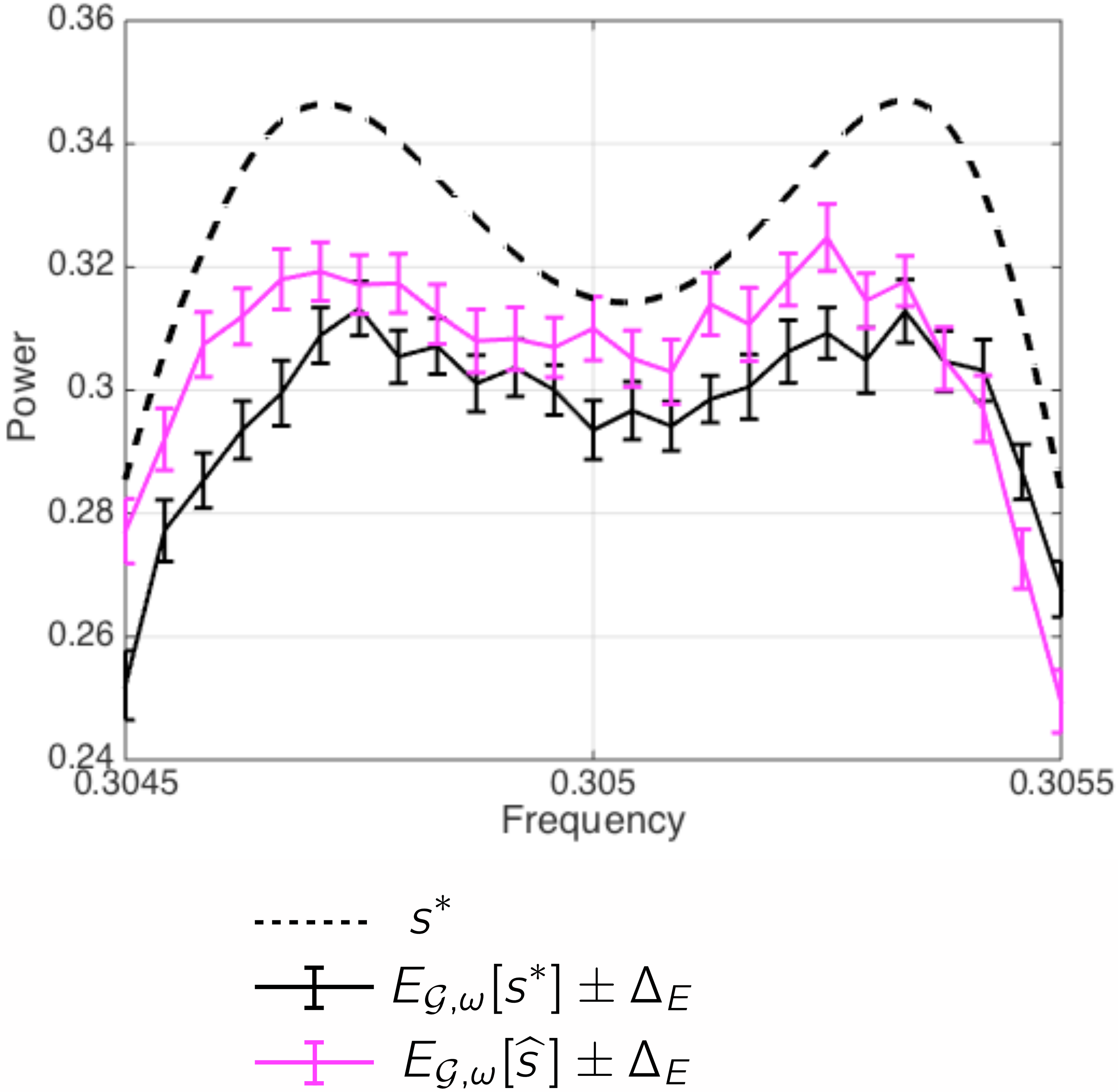
Objective function

$$s^* = \max_{\theta} E_\omega[s] - \gamma\sqrt{V_\omega[s]}$$



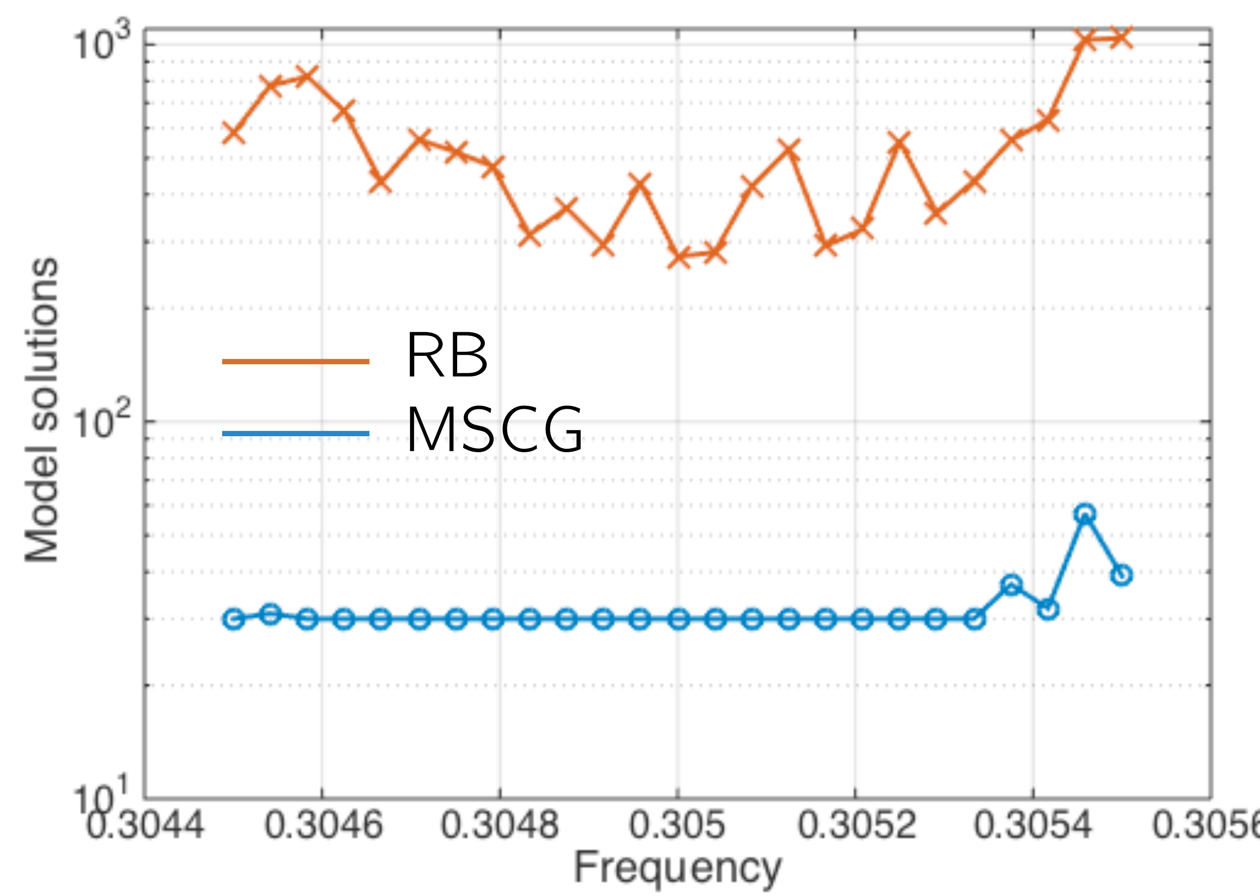
Robust shape optimization for range of frequencies

$\widehat{s} = \max_{\theta} E_{\mathcal{G},\omega}[s] - \gamma\sqrt{V_{\mathcal{G},\omega}[s]}$ $\longrightarrow$ 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

- Multiscale CG method
- Deformable domains
- Helmholtz

- RB for MSCG
- Multilevel variance reduction

Advanced wave propagation simulation

Stochastic simulation

Robust design of structured materials

- Waveguides, splitters
- Nanogaps

Thanks for your attention

Questions?

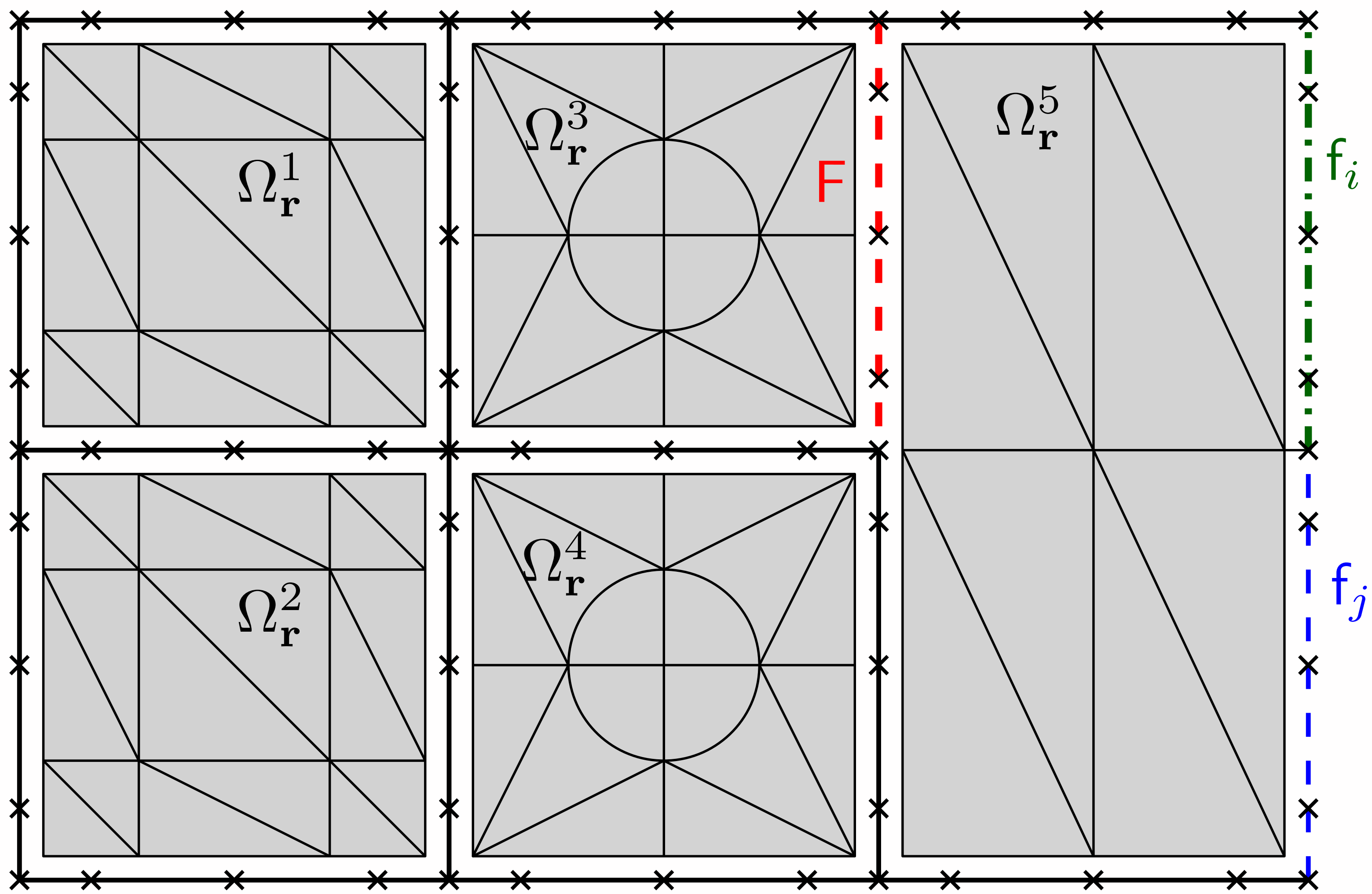
MultiScale CG - Spaces

$$W_h = \{w \in L^2(\Omega) : w \in \mathcal{C}^0(\Omega^m),\ w|_T \in \mathcal{P}^{p^m}(T), \forall T \in \mathcal{T}_h^m,\ 1 \le m \le M\},$$

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

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

$$V_h = \{v \in \mathcal{C}^0(\mathcal{F}_\mathrm{f}) : v|_\mathrm{f} \in \mathcal{P}^{p^\mathrm{f}}(\mathrm{f}), \forall \mathrm{f} \in \mathcal{F}_\mathrm{f}\}$$



$$\mathcal{F}_\mathrm{f} = \{\mathrm{f}_i,\ 1 \le i \le \sum_{\ell=1}^{L} N^\ell\}$$

MultiScale CG - Formulation

Introduce auxiliary variable $\mathbf{q}_h$ approximating the flux, with $[\![\mathbf{q}_h \cdot \mathbf{n}]\!]$ the normal component

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

$$
\begin{aligned}
(\mathbf{q}_h, \nabla w)_\Omega - (k^2 u_h, w)_\Omega - \sum_{m=1}^{M} \langle \mathbf{q}_h \cdot \mathbf{n}, w \rangle_{\partial\Omega^m} &= (f, w)_\Omega \\
u_h &= \mathrm{P}^{W_h^m}(\lambda_h), \qquad \text{on } \mathcal{F}_\mathrm{f} \\
\langle [\![\mathbf{q}_h \cdot \mathbf{n}]\!], v \rangle_{\mathcal{F}_\mathrm{f}} &= \langle g_N, v \rangle
\end{aligned}
$$

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

MultiScale CG - Formulation

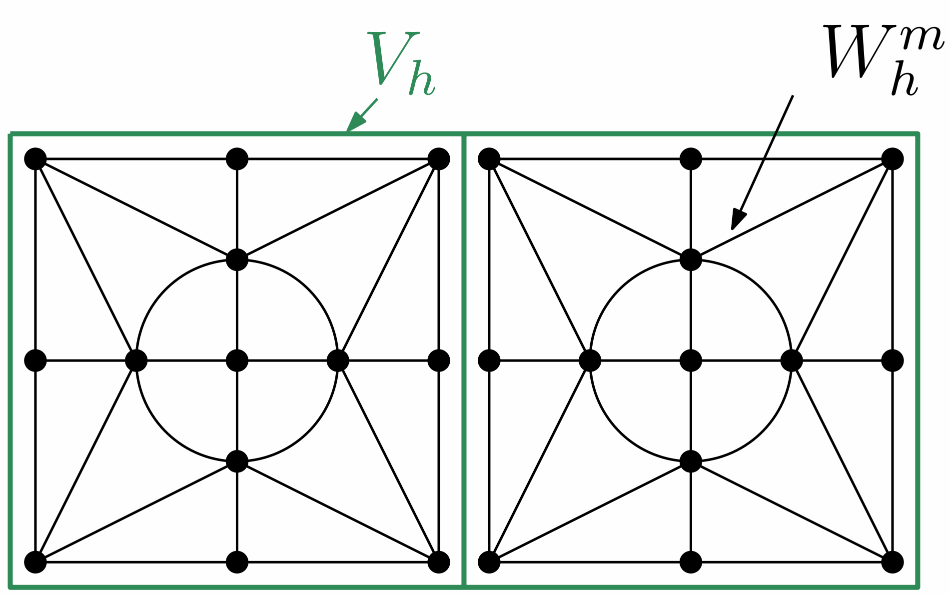
Seek $(u_h^f|_{\Omega^m}, u_h^\eta|_{\Omega^m}) \in W_h^m(0) \times W_h^m(\eta)$

$$(\rho \mathrm{G} \nabla_{\mathrm{X}} u_h^f, \nabla_{\mathrm{X}} w)_{\Omega^m} - (k^2 u_h^f, w\, g)_{\Omega^m} = (f, w\, g)_{\Omega^m}, \quad \forall w \in W_h^m(0),$$

$$(\rho \mathrm{G} \nabla_{\mathrm{X}} u_h^\eta, \nabla_{\mathrm{X}} w)_{\Omega^m} - (k^2 u_h^\eta, w\, g)_{\Omega^m} = 0, \quad \forall w \in W_h^m(0)$$

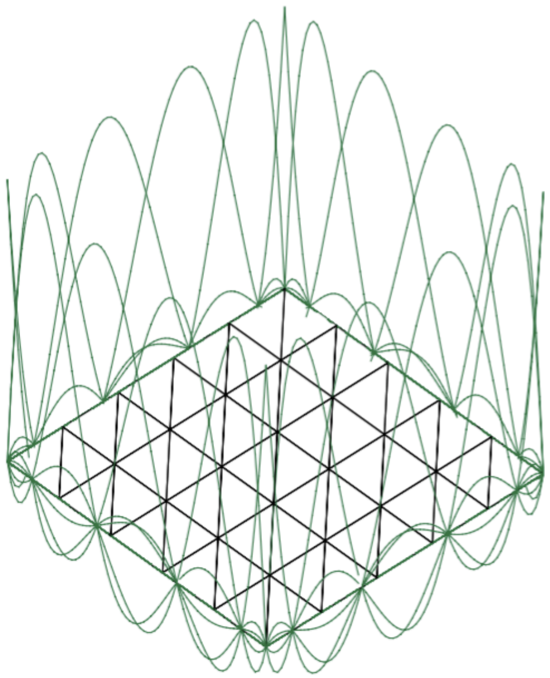
Applying **linearity** and **superposition** we have $u_h = u_h^f + u_h^{\lambda_h}$
and the Lagrange multipliers $\lambda_h \in V_h(u_D)$ satisfy

$$(\rho \mathrm{G} \nabla_{\mathrm{X}} u_h^{\lambda_h}, \nabla_{\mathrm{X}} u_h^\mu)_\Omega - (k^2 u_h^{\lambda_h}, u_h^\mu\, g)_\Omega = (f, u_h^\mu\, g)_\Omega + \langle g_N, \mu \rangle_{\Omega_N}, \quad \forall \mu \in V_h(0)$$



MultiScale CG - Implementation

For each subdomain
$$\mathbb{A}^m \mathbf{u}_f^m = \mathbf{f}^m$$
$$\mathbb{A}^m \mathbf{u}_{\varphi_i}^m = \mathbb{A}_{\varphi_i}^m$$
for BC $\varphi = \{\varphi_i\}_{i=1}^{\mathrm{N}_m}$



Assemble the elementary global matrices

$$\mathbb{K}_{ij}^m = \left(\mathbf{u}_{\varphi_i}^m\right)^T \mathbb{A}^m \mathbf{u}_{\varphi_j}^m, \qquad 1 \le i, j \le \mathrm{N}_m$$
$$\mathbb{F}_i^m = \left(\mathbf{u}_{\varphi_i}^m\right)^T \mathbf{f}^m + \mathbf{g}_i^m, \qquad 1 \le i \le \mathrm{N}_m$$

Solve the global problem $\mathbb{K}\boldsymbol{\Lambda} = \mathbb{F}$ where $\boldsymbol{\lambda}_h = \sum_{i=1}^{\mathrm{N}} \Lambda_i \varphi_i$

Recover the solution at each subdomain

$$\mathbf{u}^m = \mathbf{u}_f^m + \sum_{i=1}^{\mathrm{N}_m} \Lambda_i \mathbf{u}_{\varphi_i}^m$$

Weak formulation for the Dirichlet problem

$$(\rho \mathrm{G} \nabla_X u_h^\eta, \nabla_X w)_{\Omega^m} - (k^2 u_h^\eta, w\, g)_{\Omega^m} = 0, \quad \forall w \in W_h^m(0)$$

Approximate geometry quantities using DEIM

$$\sum_{q=1}^{Q} \sigma_q(y)(\phi_q^{\mathrm{G}}\, \rho \nabla_X u_h^\eta, \nabla_X w)_{\Omega^m} - \sum_{q=1}^{Q'} \sigma'_q(y)(k^2\, u_h^\eta, w\, \phi_q^g)_{\Omega^m} = 0, \quad \forall w \in W_h^m(0)$$

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

$$\sum_{q=1}^{Q} \sigma_q(y)(\phi_q^{\mathrm{G}}\, \rho \nabla_X u_N^{\varphi_i}, \nabla_X w)_{\Omega^m} - \sum_{q=1}^{Q'} \sigma'_q(y)(k^2 u_N^{\varphi_i}, w\, \phi_q^g)_{\Omega^m} = 0, \quad \forall w \in W_N^m(0)$$

Approximate the elementary global matrix

$$\mathbb{K}_{ij}^m \approx \sum_{q=1}^{Q} \sigma_q(y)(\phi_q^{\mathrm{G}} \rho \nabla_X u_N^{\varphi_j}, \nabla_X u_N^{\varphi_i})_{\Omega^m} - \sum_{q=1}^{Q'} \sigma'_q(y)(k^2 u_N^{\varphi_j}, u_N^{\varphi_i}\, \phi_q^g)_{\Omega^m}$$

MultiScale CG - Reduced basis implementation

Empirical interpolation of mapping

$$\sum_{q=1}^{Q} \sigma_q(y) \mathbb{A}_q^m \mathbf{u}_{\varphi_i}^m = \boldsymbol{\varphi}_i$$

POD basis with all possible Dirichlet BC $\quad \Phi = \{\zeta_1, \dots, \zeta_N\} \longrightarrow \quad \mathbf{u}_{\varphi_i}^m = \Phi \mathbf{c}_i$

Galerkin projection to compute coefficients

$$\sum_{q=1}^{Q} \sigma_q(y) \Phi^T \mathbb{A}_q^m \Phi \mathbf{c}_i = \Phi^T \boldsymbol{\varphi}_i$$

Approximate global elementary matrix

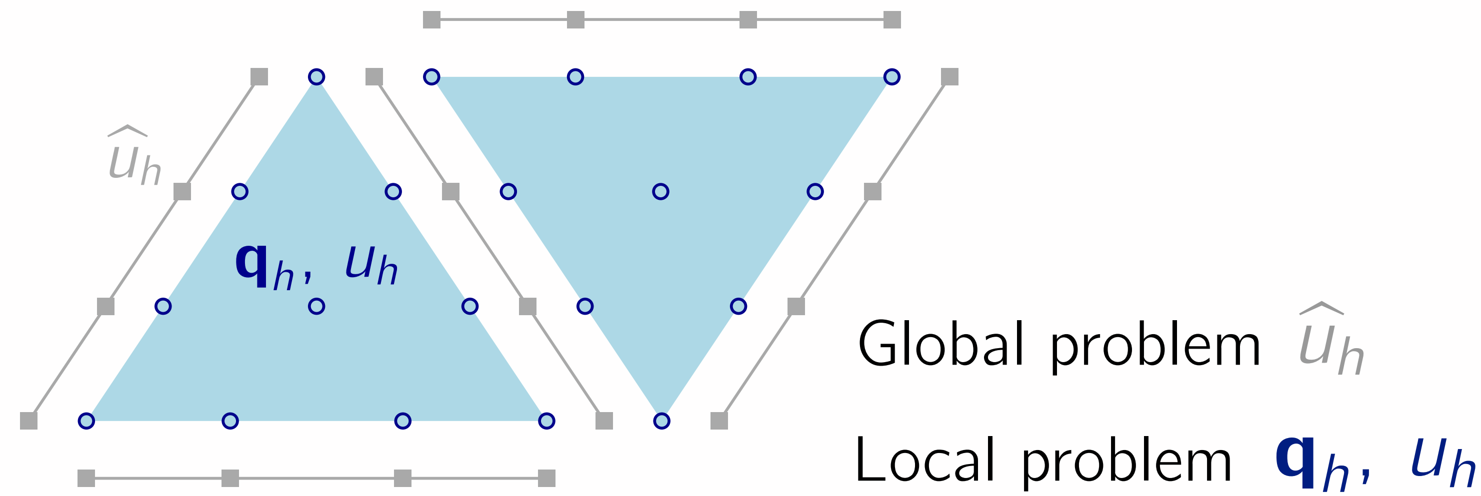
$$\mathbb{K}_{ij}^m \approx \sum_{q=1}^{Q} \sigma_q(y) \mathbf{c}_i^T \Phi^T \mathbb{A}_q^m \Phi \mathbf{c}_j, \qquad 1 \leq i, j \leq \mathrm{N}_m$$

$$\mathbb{F}_i^m \approx \mathbf{c}_i^T \Phi^T \mathbf{f}^m + \mathbf{g}_i^m, \qquad 1 \leq i \leq \mathrm{N}_m$$

Contribution #2: Reduced basis for HDG

Reduced basis for hybridizable discontinuous Galerkin method

$$
\begin{aligned}
\mathbf{q} - \nabla u &= 0 && \mathbf{x} \in \Omega \\
-\nabla \cdot (\rho\,\mathbf{q}) + k^2 u &= f && \mathbf{x} \in \Omega \\
\rho\,\mathbf{q} \cdot \mathbf{n} + \nu u &= g && \mathbf{x} \in \partial\Omega
\end{aligned}
$$



In [158] we propose a new weak formulation

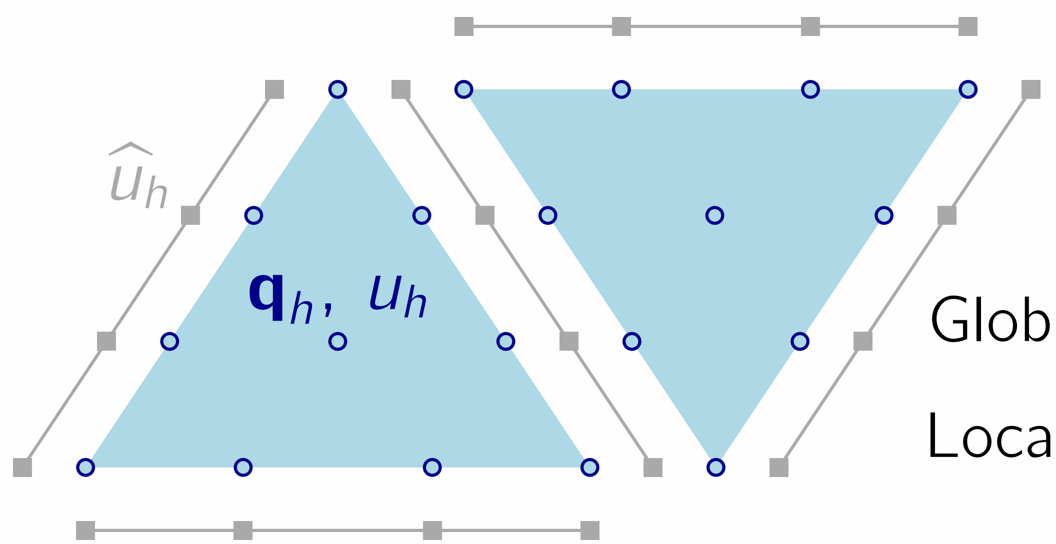
- ✓ Approximate only $u_h,\ \widehat{u}_h$ by setting $\mathbf{q}_h(u_h,\ \widehat{u}_h)$ $\longrightarrow$ RB projection
- ✓ Retain affine parametric dependence of $\rho,\ k^2,\ \nu$
- ✓ Solve a system with global variables $\widehat{u}_h$ only

Wave Propagation - HDG formulation

Hybridizable Discontinuous Galerkin (HDG) method

Helmholtz equation

$$\begin{aligned} \mathbf{q} - \nabla u &= 0 && \mathbf{x} \in \Omega \\ -\nabla \cdot (\rho\, \mathbf{q}) + k^2 u &= f && \mathbf{x} \in \Omega \\ \rho\, \mathbf{q} \cdot \mathbf{n} + \nu u &= g && \mathbf{x} \in \partial\Omega \end{aligned}$$



Global problem $\widehat{u}_h$

Local problem $\mathbf{q}_h,\ u_h$

Why HDG?

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

HDG solution

block diagonal

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

- Solve for global DOF $\mathbb{T}\widehat{\mathbb{U}} = \mathbb{R}$ (Schur complement)
- Recover local DOF $\mathbb{Q}$, $\mathbb{U}$ element-wise

Projection for RB with HDG

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

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

Which DOF should we use to parametrize snapshot ζ ?

✗ Projection using all degrees of freedom $\zeta = \begin{bmatrix} \mathbb{Q} \\ \mathbb{U} \\ \widehat{\mathbb{U}} \end{bmatrix} \longrightarrow$ Large offline computational cost

✗ Projection using numerical traces $\zeta = \begin{bmatrix} \widehat{\mathbb{U}} \end{bmatrix} \longrightarrow$ Lose affine dependency

$$\mathbb{T}\widehat{\mathbb{U}} = \mathbb{R}$$

$$\mathbb{T} = \mathbb{M} + [\mathbb{N} \quad -\mathbb{E}^*] \begin{bmatrix} \mathbb{A} & \mathbb{B} \\ \mathbb{W} & \mathbb{D} \end{bmatrix}^{-1} \begin{bmatrix} \mathbb{C} \\ \mathbb{E} \end{bmatrix} \qquad \mathbb{R} = \mathbb{G} - [\mathbb{N} \quad -\mathbb{E}^*] \begin{bmatrix} \mathbb{A} & \mathbb{B} \\ \mathbb{W} & \mathbb{D} \end{bmatrix}^{-1} \begin{bmatrix} 0 \\ \mathbb{F} \end{bmatrix}$$

✓ Projection using $\zeta = \begin{bmatrix} \mathbb{U} \\ \widehat{\mathbb{U}} \end{bmatrix} \longrightarrow$ **HDG natural norm, retain affine dependency**

$$\mathbb{Q} = \mathbb{A}^{-1}\left(\mathbb{C}\widehat{\mathbb{U}} - \mathbb{B}\mathbb{U}\right) \longrightarrow \begin{bmatrix} \mathbb{D} - \mathbb{W}\mathbb{A}^{-1}\mathbb{B} & \mathbb{W}\mathbb{A}^{-1}\mathbb{C} - \mathbb{E} \\ -\mathbb{E}^* - \mathbb{N}\mathbb{A}^{-1}\mathbb{B} & \mathbb{M} + \mathbb{N}\mathbb{A}^{-1}\mathbb{C} \end{bmatrix} \begin{bmatrix} \mathbb{U} \\ \widehat{\mathbb{U}} \end{bmatrix} = \begin{bmatrix} \mathbb{F} \\ \mathbb{G} \end{bmatrix}$$

Eliminate $\mathbb{Q}$ with first equation

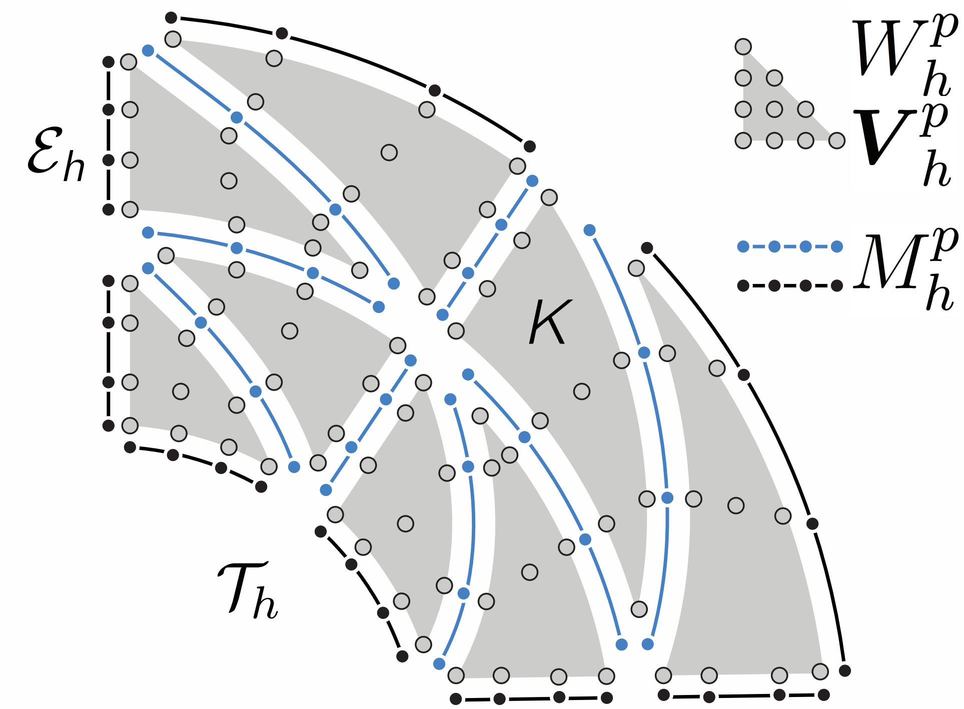
HDG formulation

- Approximation spaces

$$W_h^p = \{w \in L^2(D) : w|_K \in \mathcal{P}^p(K), \forall K \in \mathcal{T}_h\}$$

$$\boldsymbol{V}_h^p = \{\boldsymbol{v} \in [L^2(D)]^d : \boldsymbol{v}|_K \in [\mathcal{P}^p(K)]^d, \forall K \in \mathcal{T}_h\}$$

$$M_h^p = \{\mu \in L^2(\mathcal{E}_h) : \mu|_F \in \mathcal{P}^p(F), \forall F \in \mathcal{E}_h\}$$



- Define numerical traces

$$\widehat{\boldsymbol{q}}_h = \boldsymbol{q}_h - \tau(u_h - \widehat{u}_h)\boldsymbol{n}, \ \text{on } \partial K$$

- Find $(\boldsymbol{q}_h, u_h, \widehat{u}_h) \in \boldsymbol{V}_h^p \times W_h^p \times M_h^p$ such that $\forall(\boldsymbol{v}, w, \mu) \in \boldsymbol{V}_h^p \times W_h^p \times M_h^p$

$$(\boldsymbol{q}_h, \boldsymbol{v})_{\mathcal{T}_h} + (u_h, \nabla \cdot \boldsymbol{v})_{\mathcal{T}_h} - \langle \widehat{u}_h, \boldsymbol{v} \cdot \boldsymbol{n} \rangle_{\partial \mathcal{T}_h} = 0,$$

$$(\rho \boldsymbol{q}_h, \nabla w)_{\mathcal{T}_h} - \langle \rho \boldsymbol{q}_h \cdot \boldsymbol{n}, w \rangle_{\partial \mathcal{T}_h} - (k^2 u_h, w)_{\mathcal{T}_h} + \langle \rho\tau(u_h - \widehat{u}_h), w \rangle_{\partial \mathcal{T}_h} = (f, w)_{\mathcal{T}_h}$$

$$\langle \rho \boldsymbol{q}_h \cdot \boldsymbol{n}, \mu \rangle_{\partial \mathcal{T}_h} - \langle \rho \tau u_h, \mu \rangle_{\partial \mathcal{T}_h} + \langle \rho \tau \widehat{u}_h, \mu \rangle_{\partial \mathcal{T}_h} + \langle \nu\, \widehat{u}_h, \mu \rangle_{\partial \mathcal{D}} = (g, w)_{\partial \mathcal{D}}$$

$\rightarrow$ Local

$\rightarrow$ Global

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

Solve for global dof $\mathbb{T}\widehat{\mathbb{U}} = \mathbb{R}$

Recover local dof $\mathbb{Q}$, $\mathbb{U}$

$\begin{bmatrix} \mathbb{A} & \mathbb{B} \\ \mathbb{W} & \mathbb{D} \end{bmatrix}$ Block-diagonal and invertible

A posteriori error estimate for expectation

Control variates $\longrightarrow$ $E[s] = E[s - s_{N_1}] + E[s_{N_1}]$

MVR estimator $\longrightarrow$ $E_{M_0,M_1}[s] = E_{M_0}[s - \underbrace{s_{N_1}] + E_{M_1}[s_{N_1}}_{\text{i.i.d samples}}]$

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

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

$$Z_0 + Z_1 = E[s] - E_{M_0,M_1}[s] \sim N\left(0\,;\, \underbrace{\frac{V[s - s_{N_1}]}{M_0} + \frac{V[s_{N_1}]}{M_1}}_{\sigma^2_{MVR}}\right)$$

Central limit theorem to establish confidence bounds

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

Optimal weights (I)

- ✓ Precompute MSCG-RB outputs $s, s_{N_\ell},\ 1 \le N_\ell \le N_{\max}$ 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

$$\widehat{C}_{L\text{-}MVR} = \sum_{\ell=0}^{L} \frac{\widehat{C}^\ell}{w_\ell} = \frac{a^2}{\Delta_E^2}\Bigg[(t_s + t_{N_1})\frac{V_M[s - s_{N_1}]}{w_0} + t_{N_L}\frac{V_M[s_{N_L}]}{w_L} + \sum_{\ell=1}^{L-1}(t_{N_\ell} + t_{N_{\ell+1}})\frac{V_M[s_{N_\ell} - s_{N_{\ell+1}}]}{w_\ell}\Bigg]$$

Optimal weights (II)

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

$$(w_0^*, w_1^* \ldots, w_L^*) = \arg\min\ \widehat{C}_{L-MVR}(\overline{N}_1, \ldots, \overline{N}_L)$$
$$\text{s.t.} \quad \sum_{\ell=0}^{L} w_\ell = 1, \quad w_\ell \geq 0$$

✓ Optimal weights have closed formula

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

✓ Exhaustive search $\longrightarrow$ select $(\boldsymbol{L}, \boldsymbol{N}, \boldsymbol{w})$ with lowest $\widehat{C}_{L\text{-}EIMVR}$

Empirical interpolation applied to MVR

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

$$\xrightarrow{\#\text{ samples } M_\ell}$$

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

$$\xleftarrow{\text{output evaluation complexity}}$$

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

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

and obtain the *a posteriori* error bound

$$\Delta_{\widehat{E}} = a\sqrt{\frac{V_{M_0}[s - s_{N_1}]}{M_0} + \sum_{\ell=1}^{L-1} \frac{V_{M_\ell}[s_{N_\ell} - s_{N_{\ell+1}}]}{M_\ell} + \frac{V_{M_L}[s_{N_L} - \widehat{s}_{N_L}]}{M_L} + \frac{V_{\widehat{M}_L}[\widehat{s}_{N_L}]}{\widehat{M}_L}}$$

Empirical interpolation applied to MVR

Estimator for variance

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

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

and reuse multilevel expression

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

+ error bounds

Estimator for gradient

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

+ error bounds

Extension to arbitrary number of levels is straightforward

Error and cost equation

For a prescribed tolerance Δ

$$\Delta^2 = \underbrace{a^2 \frac{V_{M_0}[s - s_{N_1}]}{M_0}}_{\text{Level } 0,\ = w_0 \Delta^2} + \sum_{\ell=1}^{L-1} \underbrace{a^2 \frac{V_{M_\ell}[s_{N_\ell} - s_{N_{\ell+1}}]}{M_\ell}}_{\text{Level } \ell,\ = w_\ell \Delta^2} + \underbrace{a^2 \frac{V_{M_L}[s_{N_L} - \widehat{s}_{N_L}]}{M_L}}_{\text{Level } L,\ = w_L \Delta^2} + \underbrace{a^2 \frac{V_{\widehat{M}_L}[\widehat{s}_{N_L}]}{\widehat{M}_L}}_{\text{Level } \widehat{L},\ = \widehat{w}_L \Delta^2}$$

Termination condition MC

Cost of L-MVR estimator

$$C_{L\text{-}EIMVR} = (t_s + t_{N_1})\, M_0 + t_{N_L} M_L + \sum_{\ell=1}^{L-1} \left(t_{N_\ell} + t_{N_{\ell+1}}\right) M_\ell \quad \text{alternatively...}$$

$$C_{L\text{-}EIMVR} = \frac{a^2}{\epsilon_{\text{tol}}^2} \Bigg[(t_s + t_{N_1}) \frac{V_{M_0}[s - s_{N_1}]}{w_0} + t_{N_L} \frac{V_{M_L}[s_{N_L} - \widehat{s}_{N_L}]}{w_L} + \sum_{\ell=1}^{L-1} \left(t_{N_\ell} + t_{N_{\ell+1}}\right) \frac{V_{M_\ell}[s_{N_\ell} - s_{N_{\ell+1}}]}{w_\ell} \Bigg]$$

Optimal weights (I)

- Fix N_L and precompute EI output at $M_L + \widehat{M}_L$ samples
- Precompute HDG-RB outputs $s, s_{N_\ell},\ N_L \leq N_\ell \leq N_{\max}$ 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

$$\widehat{C}_{L\text{-}EIMVR} = \sum_{\ell=0}^{L} \frac{\widehat{C}^\ell}{w_\ell} = \frac{a^2}{\Delta^2}\left[(t_s + t_{N_1})\frac{V_M[s - s_{N_1}]}{w_0} + t_{N_L}\frac{V_M[s_{N_L} - \widehat{s}_{N_L}]}{w_L} + \sum_{\ell=1}^{L-1}(t_{N_\ell} + t_{N_{\ell+1}})\frac{V_M[s_{N_\ell} - s_{N_{\ell+1}}]}{w_\ell}\right]$$

Optimal weights (II)

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

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

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

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

✓ Optimal weights have closed formula

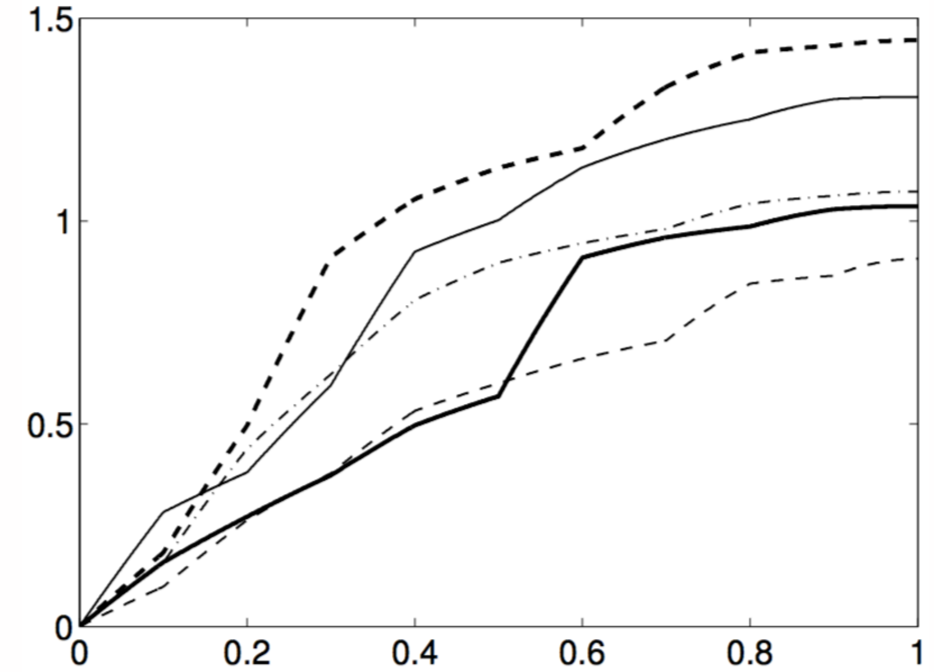
$$w_\ell^* = \frac{\sqrt{\widehat{C}^\ell / \widehat{C}^0}}{\sum_{\ell'=0}^{L} \sqrt{\widehat{C}^{\ell'} / \widehat{C}^0}}, \qquad \ell = 0, \ldots, L.$$

✓ Exhaustive search $\longrightarrow$ select (***L*,*N*,*w***) with lowest $\widehat{C}_{L\text{-}EIMVR}$

Stochastic simulation: 1d numerical verification

$$-\nabla\cdot(\rho\nabla u) = f \quad x\in\Omega$$
$$\rho\nabla u = 0 \quad x = 1$$
$$u = 0 \quad x = 0$$

$$\rho = \sum_{q=1}^{10} y_q \mathbf{1}_{\Omega_q}$$



Compare MC with MVR given by

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