Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich

SAM

Simulation of Photonic Crystal Structures using Generalized FE in 2D

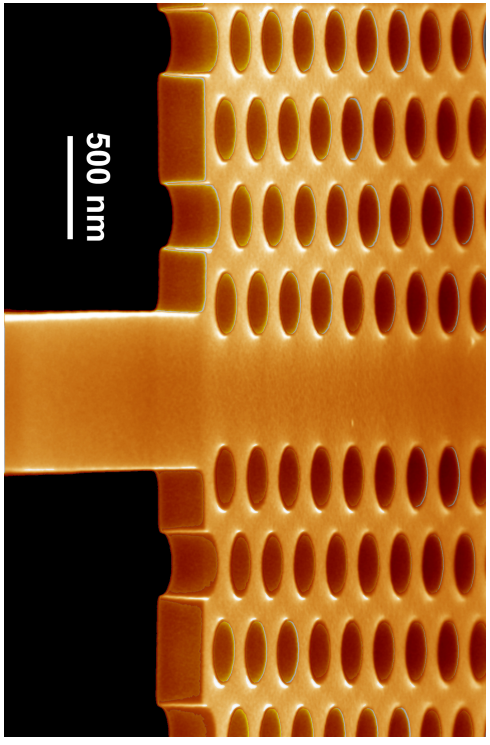
Holger Brandsmeier

ETH Zürich, Seminar for Applied Mathematics

Pro*Doc Workshop, Disentis 09

Overview of the method

- Simulation of Helmholtz type equations with locally periodic coefficients.
- **Application:** big networks of photonic crystal (PhC) structures.
- **Challenge:** avoid scale resolution. nDOFs scales as $O(n^2)$ with number of periods n.
- **g-FEM** approach with multiscale basis functions.
- **Micro basis**: problem adapted basis functions.
- **Macro basis**: polynomials.



[IBM Research]

Overview

Previous work

- Simulation of infinite PhCs:
  FDTD, MMP, FEM, ...
- Simulation of finite PhCs:
  - by FDTD [Lavrinenko et al., 2004],
  - by Wannier functions [Hermann et al., 2008],
  - by an expansion in a basis of Bloch modes from the infinite crystal [Jiang et al., 2005] and [Istrate et al., 2005].
- This work extends a multiscale FEM approach [Matache et al., 2000, Rüegg, 2002].
- Joint work with Kersten Schmidt and Christoph Schwab.

Governing Equations

- Scalar wave equations for e, h in $\mathbb{R}^2$

$$-\nabla\cdot\nabla e(\boldsymbol{x}) = \left(\frac{\omega}{c_0}\right)^2 \varepsilon(\boldsymbol{x})\, e(\boldsymbol{x}) \quad \text{(TM mode)},$$

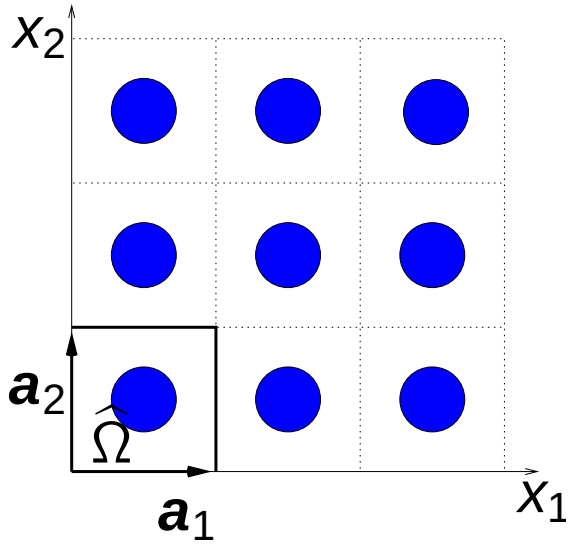
$$-\nabla\cdot\left(\varepsilon^{-1}(\boldsymbol{x})\nabla h(\boldsymbol{x})\right) = \left(\frac{\omega}{c_0}\right)^2 h(\boldsymbol{x}) \quad \text{(TE mode)}.$$

- TE/TM modes are of Helmholtz type

$$\nabla\cdot(a(\boldsymbol{x})\nabla u(\boldsymbol{x})) + b^2(\boldsymbol{x})u(\boldsymbol{x}) = 0.$$

Locally periodic material with *unit cell* $\widehat{\Omega}$

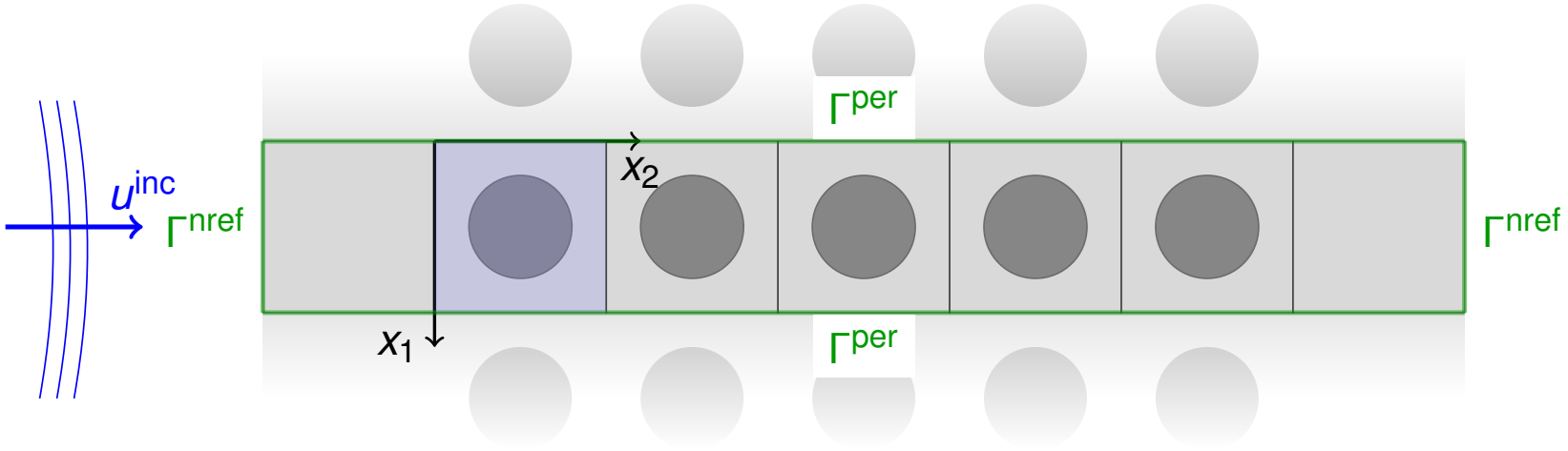
$$\varepsilon(\boldsymbol{x}+\boldsymbol{a_1}) = \varepsilon(\boldsymbol{x}) \quad \text{for all } \boldsymbol{x}, \boldsymbol{x}+\boldsymbol{a_1} \text{ in } \Omega^{\text{cr}},$$
$$\varepsilon(\boldsymbol{x}+\boldsymbol{a_2}) = \varepsilon(\boldsymbol{x}) \quad \text{for all } \boldsymbol{x}, \boldsymbol{x}+\boldsymbol{a_2} \text{ in } \Omega^{\text{cr}}.$$



Model problem – PhC barrier

crystal with $n_p = 5$ periods, incident plane wave $e^{i\boldsymbol{k}^{inc}\boldsymbol{x}}$,

$$\boldsymbol{k}^{inc} = (0, k)$$



find u in $H^1(\Omega)$

$$\nabla \cdot \left(a(\boldsymbol{x}) \nabla\, u(\boldsymbol{x})\right) + b^2(\boldsymbol{x}) u(\boldsymbol{x}) = 0 \qquad \text{for all } \boldsymbol{x} \text{ in } \Omega$$

$$u(\boldsymbol{x} + \boldsymbol{a_1}) = u(\boldsymbol{x}) \qquad \text{for all } \boldsymbol{x} \text{ on } \Gamma^{per}$$

$$\partial_{\boldsymbol{n}} u(\boldsymbol{x}) - i b_0 u(\boldsymbol{x}) = \partial_{\boldsymbol{n}} u^{inc}(\boldsymbol{x}) - i b_0 u^{inc}(\boldsymbol{x}) \qquad \text{for all } \boldsymbol{x} \text{ on } \Gamma^{nref}$$

Variational formulation

$$H^1_{\text{per}}(\Omega) := \left\{ u \in H^1(\Omega) : u(0, x_2) = u(\boldsymbol{a_1}, x_2) \quad \forall \boldsymbol{x} \in \Omega \right\}.$$

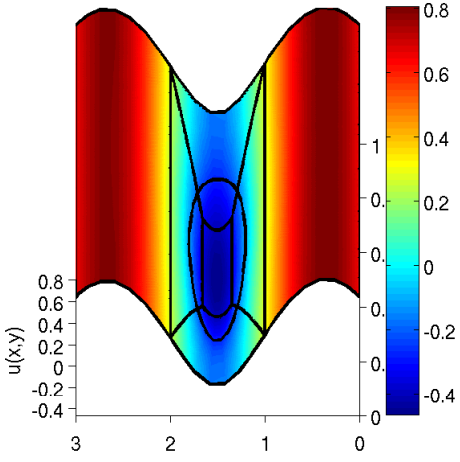
Find $u \in H^1_{\text{per}}(\Omega)$, such that

$$\Phi(u, v) = f(v) \qquad \text{for all } v \in H^1_{\text{per}}(\Omega),$$

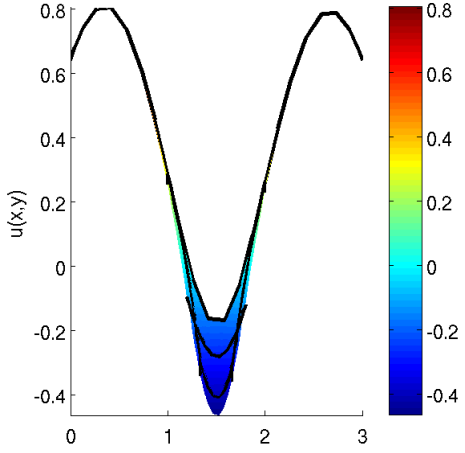
$$\Phi(u, v) := \int_\Omega a(\boldsymbol{x}) \nabla u(\boldsymbol{x}) \cdot \nabla \overline{v}(\boldsymbol{x}) \, \mathrm{d}\boldsymbol{x} - \int_\Omega b^2(\boldsymbol{x}) u(\boldsymbol{x}) \overline{v}(\boldsymbol{x}) \, \mathrm{d}\boldsymbol{x} + \mathrm{i} b_0 \int_{\Gamma^{\text{nref}}} u(\boldsymbol{x}) \overline{v}(\boldsymbol{x}) \, \mathrm{d}S$$

$$f(v) := - \int_{\Gamma^{\text{nref}}} a(\boldsymbol{x}) \, \partial_n u^{\text{inc}}(\boldsymbol{x}) \overline{v}(\boldsymbol{x}) \, \mathrm{d}S + \mathrm{i} b_0 \int_{\Gamma^{\text{nref}}} u^{\text{inc}}(\boldsymbol{x}) \overline{v}(\boldsymbol{x}) \, \mathrm{d}S$$

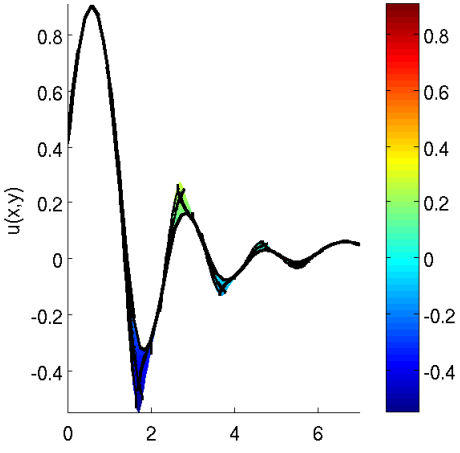
PhC barrier – example solutions (TM mode)



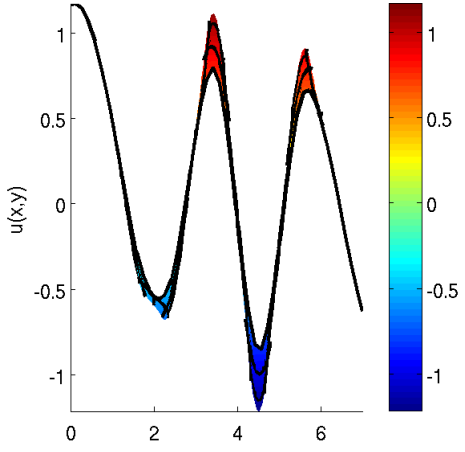
(top view, $n_\mathrm{p} = 1$)



(side view, $n_\mathrm{p} = 1$)



(bandgap frequency, $n_\mathrm{p} = 5$)



(propagating frequency, $n_\mathrm{p} = 5$)

Floquet Bloch transform

Floquet-Bloch transform $\mathscr{F} : H^s(\mathbb{R}^2) \to H^s(\widehat{\Omega} \times B)$

$$\widetilde{u}(\boldsymbol{k}, \boldsymbol{x}) = (\mathscr{F} u)(\boldsymbol{k}, \boldsymbol{x}) = \frac{1}{|B|} e^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x}} \sum_{\boldsymbol{m}\in\mathbb{Z}^2} u(\boldsymbol{x} - \boldsymbol{a_m})\, e^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{a_m}},$$

$$u(\boldsymbol{x}) = (\mathscr{F}^{-1}\widetilde{u})(\boldsymbol{x}) = \int_B e^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x}} \widetilde{u}(\boldsymbol{k}, \boldsymbol{x})\, \mathrm{d}\boldsymbol{k}.$$

- Brillouin zone $B = [-\pi/|\boldsymbol{a_1}|, \pi/|\boldsymbol{a_1}|] \times [-\pi/|\boldsymbol{a_2}|, \pi/|\boldsymbol{a_2}|]$.
- Functions $e^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x}}\widetilde{u}(\boldsymbol{k}, \boldsymbol{x})$ are called Bloch modes.
- Solution is a superposition of Bloch modes.
- each Bloch mode has to solve the Helmholtz equation
  e.g. for TM mode: Find $(\boldsymbol{k} \in \mathbb{C}^2, \omega \in \mathbb{R}, \widetilde{u}_{\boldsymbol{k}} \in H^1_{\mathrm{per}}(\widehat{\Omega})/\{0\})$

$$(\nabla + \mathrm{i}\boldsymbol{k})^T (\nabla + \mathrm{i}\boldsymbol{k})\, \widetilde{u}_{\boldsymbol{k}}(\boldsymbol{x}) + \left(\frac{\omega}{c_0}\right)^2 \varepsilon(\boldsymbol{x}) \widetilde{u}_{\boldsymbol{k}}(\boldsymbol{x}) = 0.$$

- **Assumption:** Bloch modes capture micro scale behavior in finite crystals.

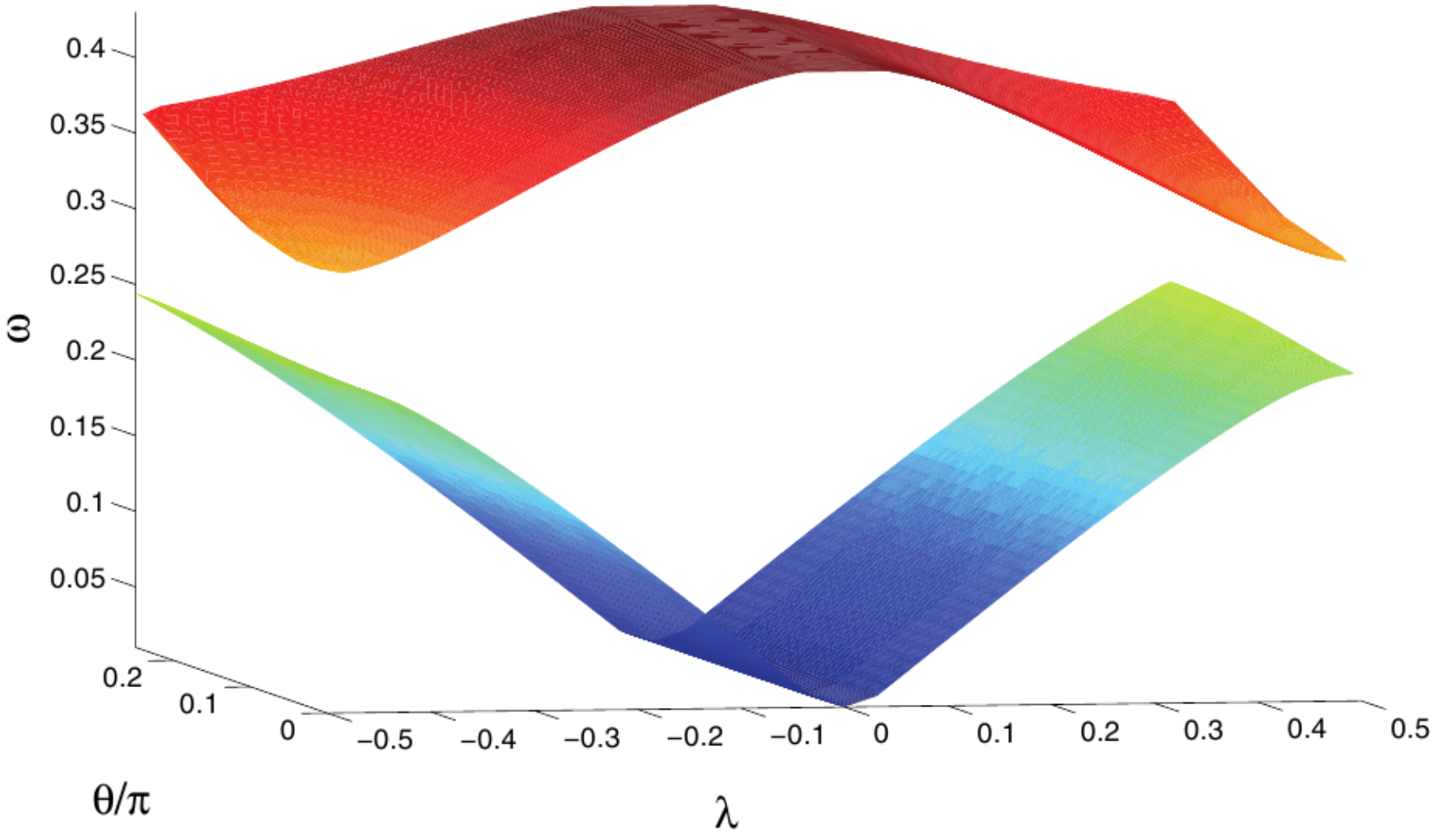
Unit cell problem

- **(from last slide)** for TM mode: Find $(\boldsymbol{k} \in \mathbb{C}^2, \omega \in \mathbb{R}, \widetilde{u} \in H^1_{\text{per}}(\widehat{\Omega}))$

$$(\nabla + \mathrm{i}\boldsymbol{k})^T (\nabla + \mathrm{i}\boldsymbol{k})\ \widetilde{u}_{\boldsymbol{k}}(\boldsymbol{x}) + \left(\frac{\omega}{c_0}\right)^2 \varepsilon(\boldsymbol{x}) \widetilde{u}_{\boldsymbol{k}}(\boldsymbol{x}) = 0.$$

- Linear (generalized) Eigenvalue problem: specify $\boldsymbol{k} \in \mathbb{C}^2$ or $\boldsymbol{k} \in \mathbb{R}^2$, search for $(\omega \in \mathbb{R}, \widetilde{u}_{\boldsymbol{k}} \in H^1_{\text{per}}(\widehat{\Omega})/\{0\})$.
- Quadratic Eigenvalue problem: specify $\omega \in \mathbb{R}$, use representation $\boldsymbol{k} = \lambda\big(\sin(\theta), \cos(\theta)\big)$, sample θ, search for $(\lambda \in \mathbb{R}, \widetilde{u}_{\boldsymbol{k}} \in H^1_{\text{per}}(\widehat{\Omega})/\{0\})$.
- Both formulations are important.
- Solving using Standard FEM (p-FEM).

Infinite Photonic Crystals – bandstructure 2D

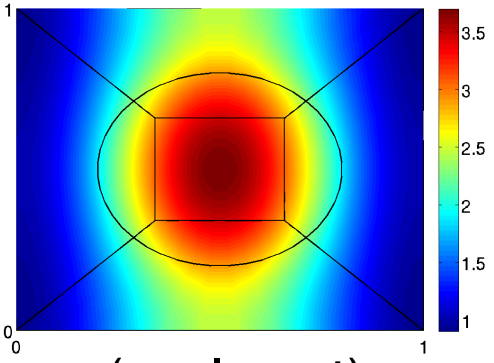


[Engström and Richter, 2009]

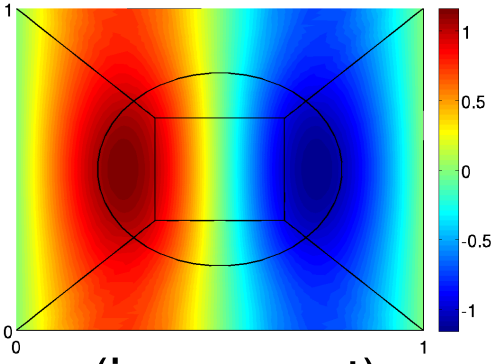
Infinite Photonic Crystals – bandstructure

TM, $\omega a/2\pi = 0.21$

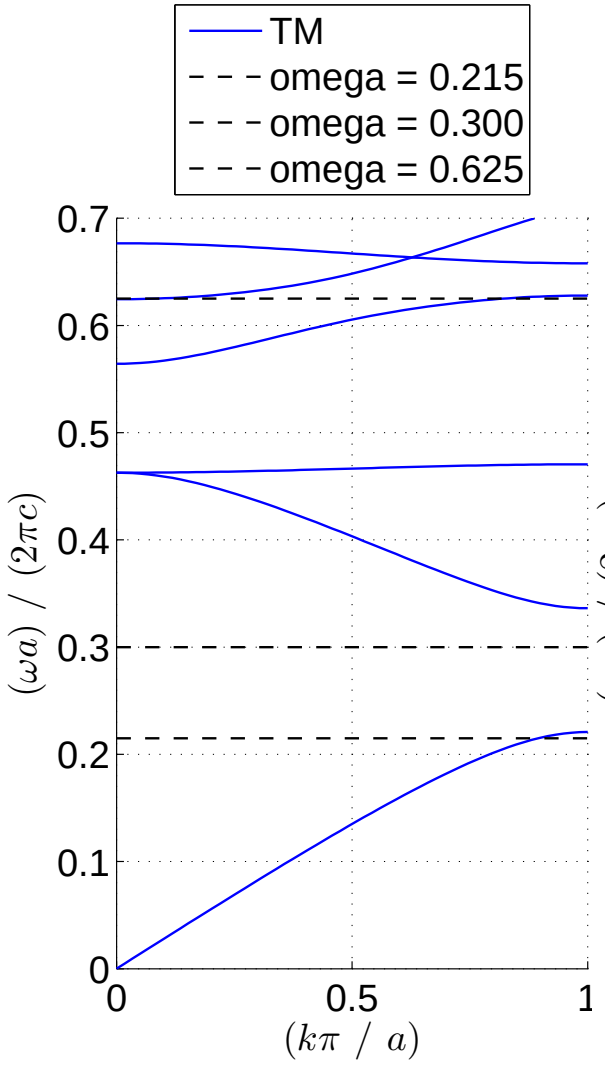
$k/a = 2.81$

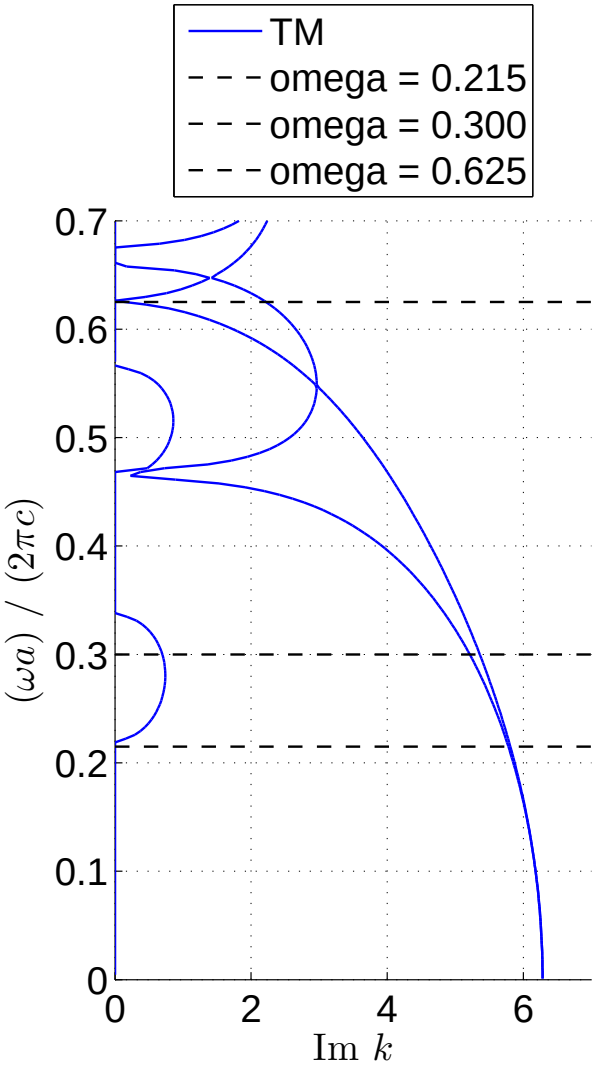


(real part)

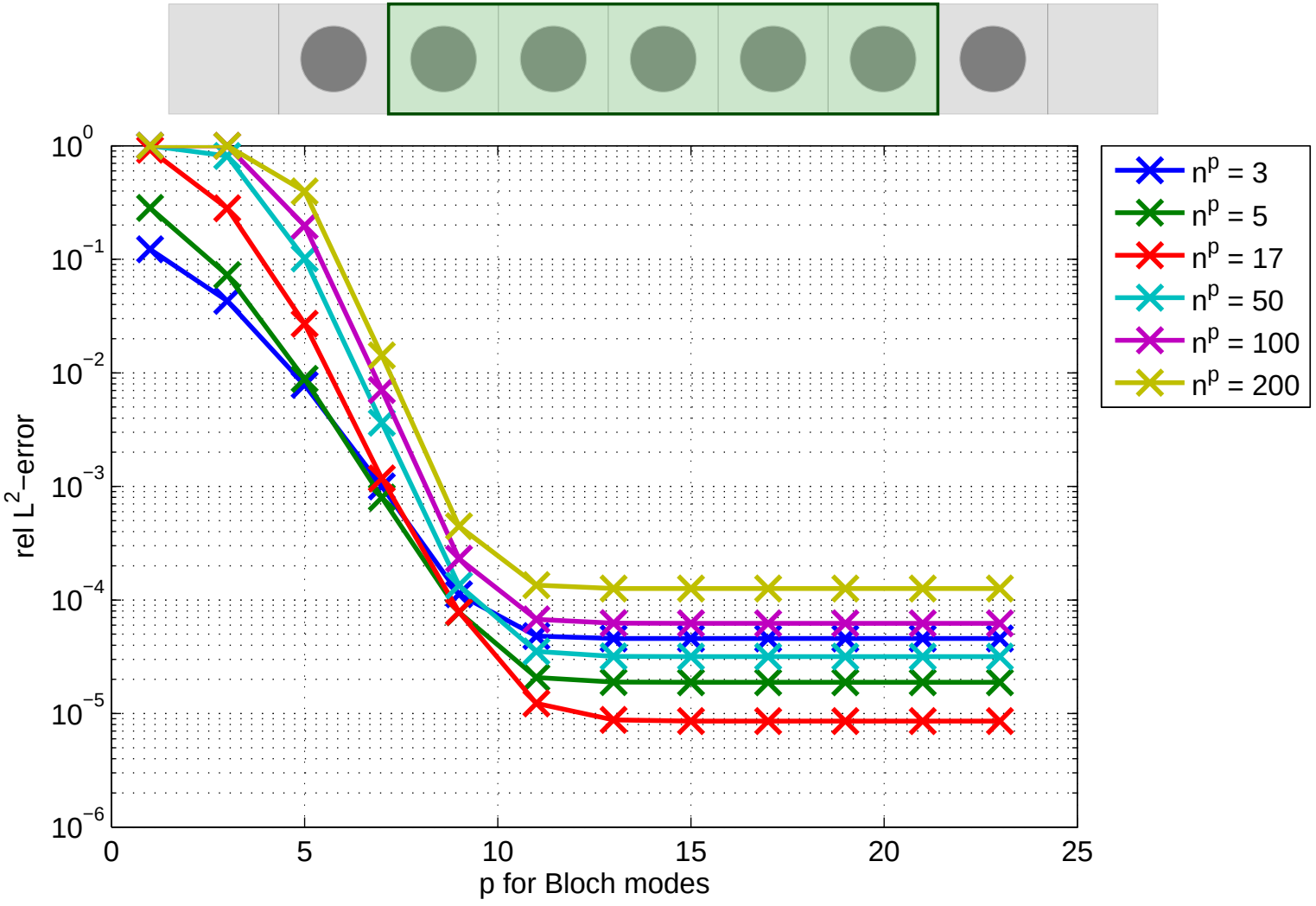


(imag part)



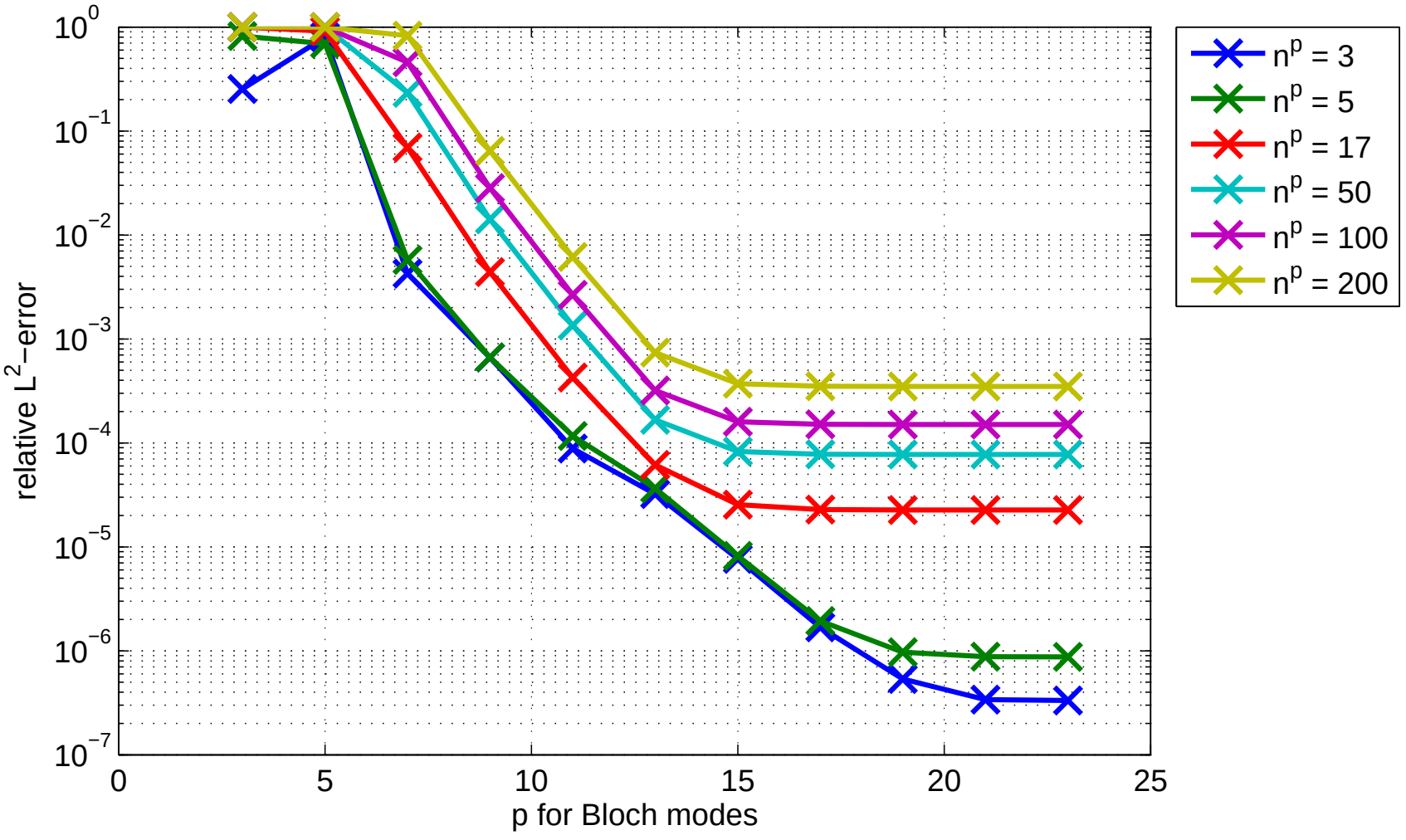


L^2-projection with 2 Bloch modes $\hat{\omega} = 0.215$



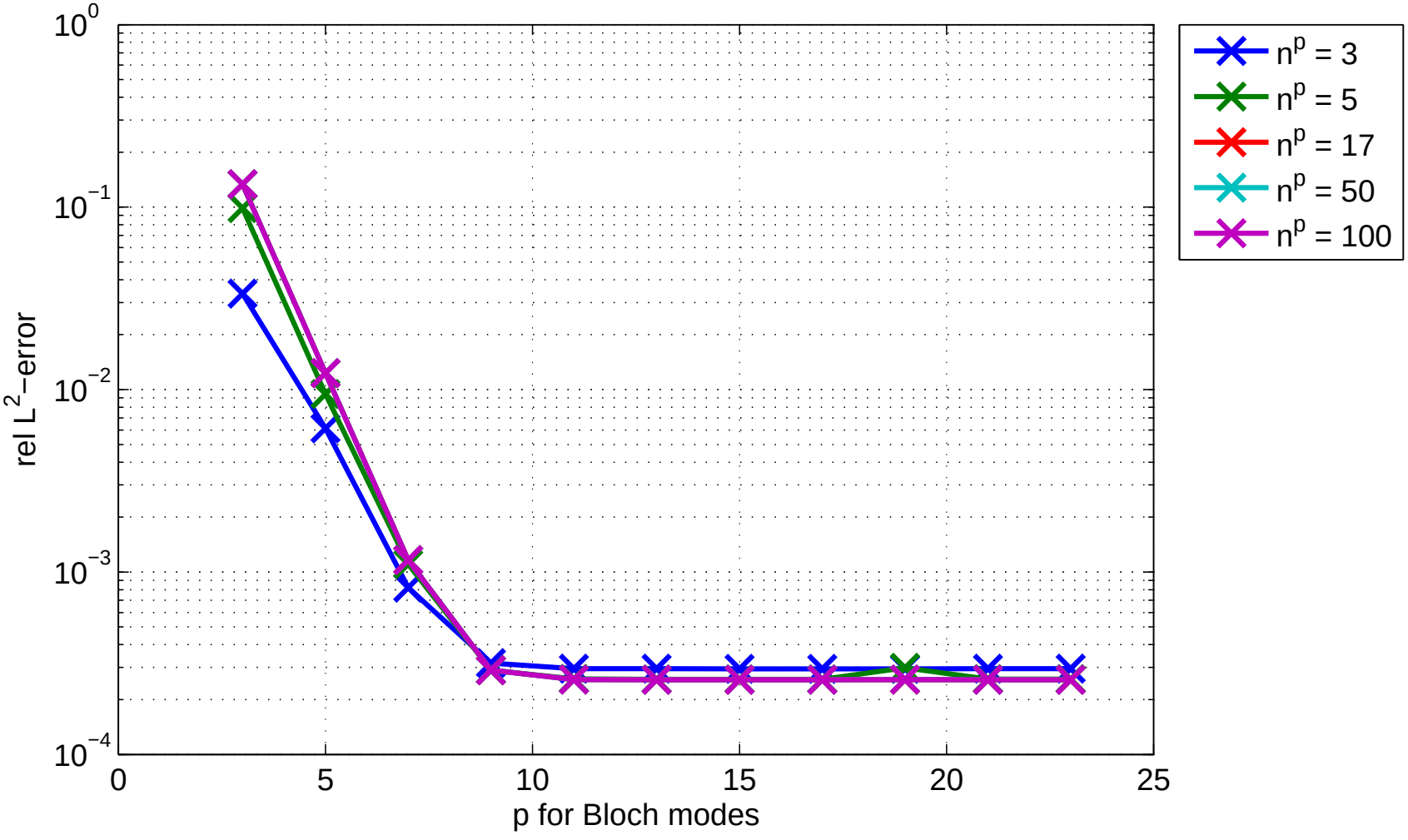
(number of g-FEM DOFs: 2!)

L^2-projection with 4 Bloch modes $\hat{\omega} = 0.615$



(number of g-FEM DOFs: 4!)

L^2-projection with 2 Bloch modes $\hat{\omega} = 0.300$



(number of g-FEM DOFs: 2!)

Approximation with Bloch modes – summary

- Approximation quality nearly independent of n_p.
- Relative L^2-errors less than 10^{-3} are reached.
- Problems close to the boundary, especially for bandgap frequencies.
- Best approximation results of solutions computed with Standard FEM.

$\Rightarrow$ Focus on FEM.

$\Rightarrow$ Relevant error norm relative H^1-error, approximately factor 10 bigger than L^2-error.

Multiscale FEM – idea

- FEM discretisation $V_N^{\text{gfem}} \subset H^1_{\text{per}}(\Omega)$

  find $u_N \in V_N^{\text{gfem}}$: $\quad \Phi(u_N, v_N) = f(v_N) \quad$ for all $v_N \in V_N^{\text{gfem}}(\Omega)$,

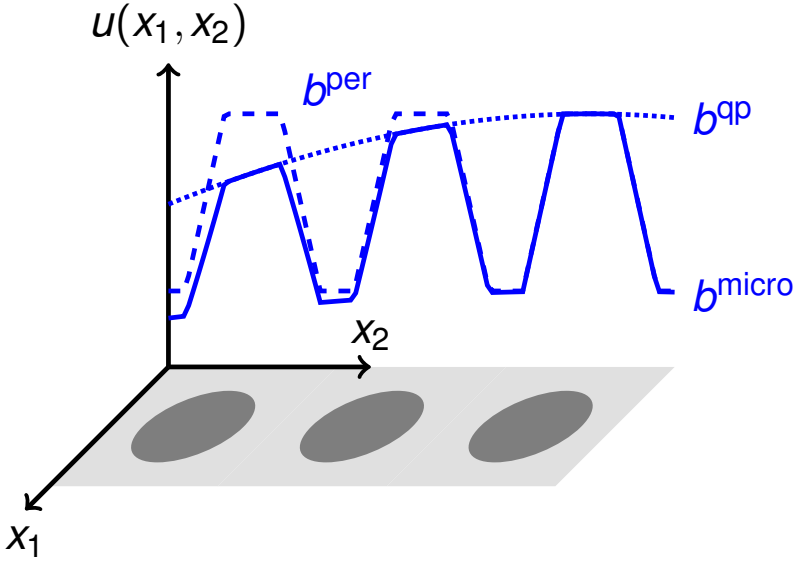
  $$\text{where} \quad u_N(\boldsymbol{x}) = \sum_{i=1}^{N} \alpha_i b_i^{\text{gfem}}(\boldsymbol{x}).$$

- Special multiscale basis functions

  $$b_{i,j}^{\text{gfem}}(\boldsymbol{x}) = b_i^{\text{macro}}(\boldsymbol{x})\, b_j^{\text{micro}}(\boldsymbol{x}) = b_i^{\text{macro}}(\boldsymbol{x})\, e^{\mathrm{i}\boldsymbol{k}_j \cdot \boldsymbol{x}}\, b_j^{\text{per}}(\boldsymbol{x})$$

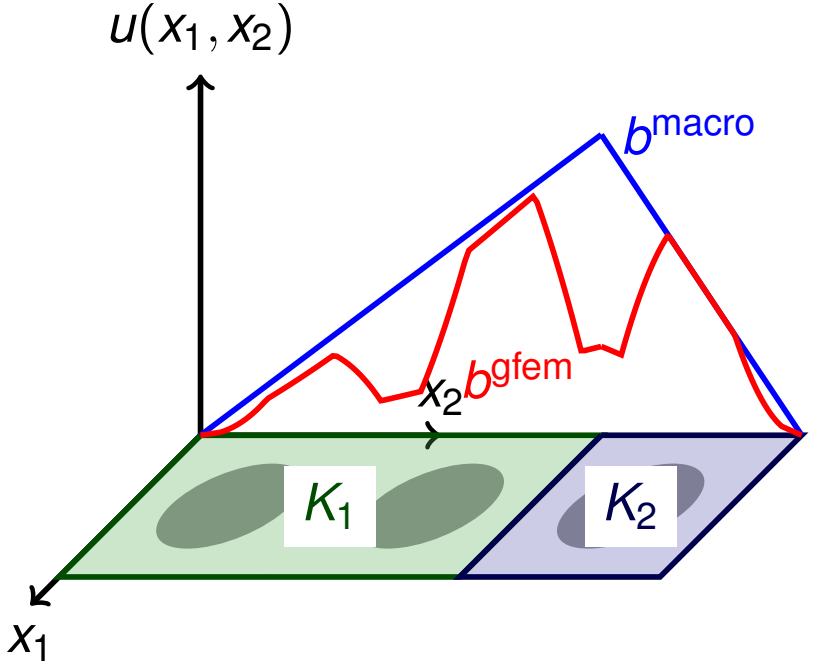
- macro polynomial basis b^{macro}
- Bloch modes as micro oscillations b^{micro}

g-FEM basis functions



micro basis function:

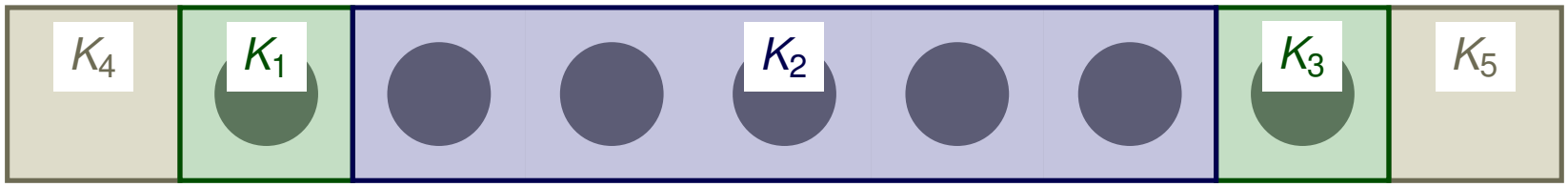
$$b^{\text{micro}}(\boldsymbol{x}) = e^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x}} b^{\text{per}}(\boldsymbol{x})$$



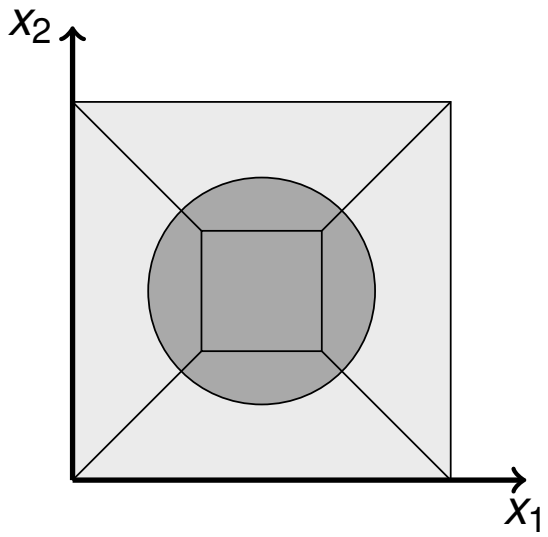
g-FEM basis function:

$$b^{\text{gfem}}(\boldsymbol{x}) = b^{\text{micro}} b^{\text{macro}}$$

g-FEM interface



Macro Mesh $\mathscr{M}^{\text{macro}}$



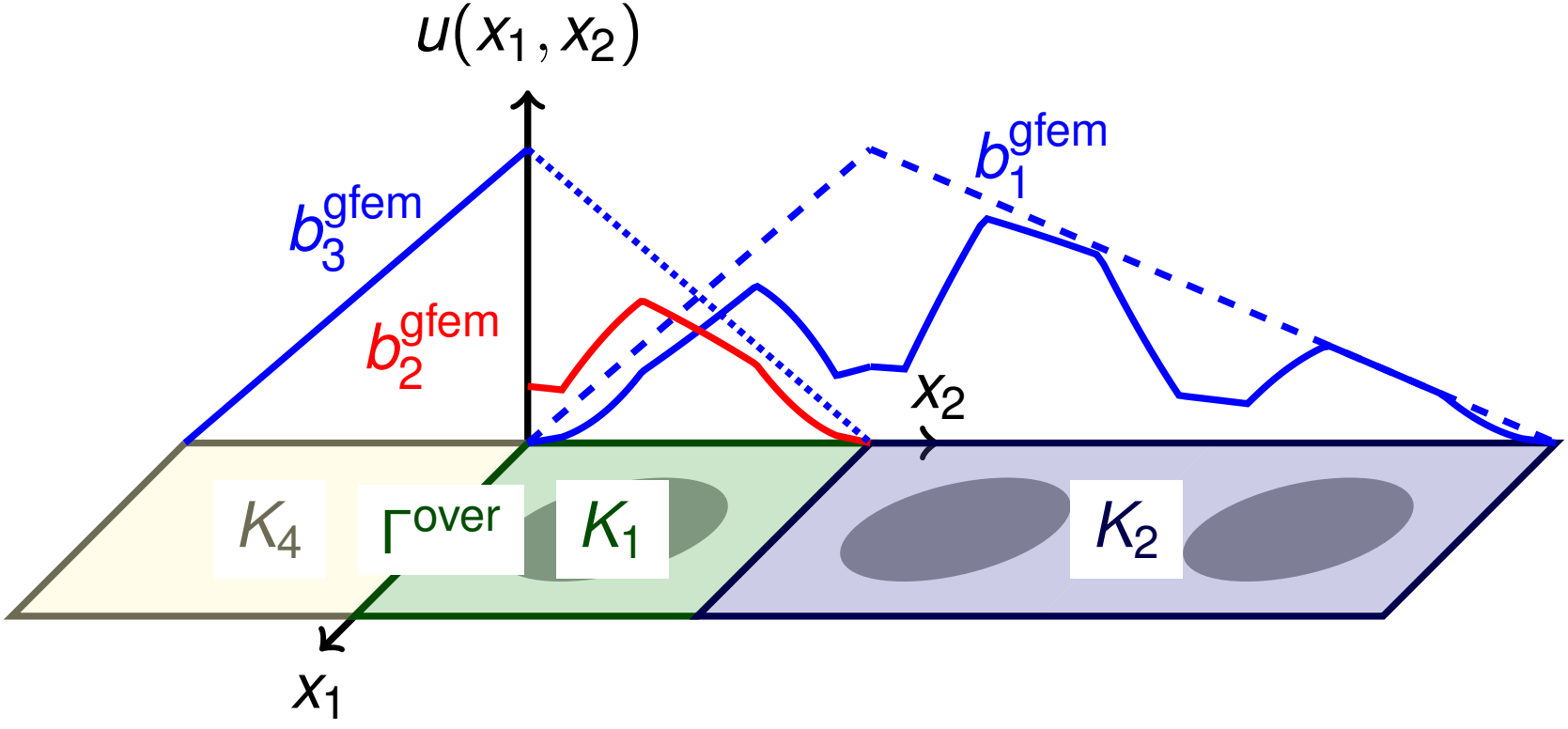
Micro Mesh $\mathscr{M}^{\text{micro}}$

- g-FEM in crystal cells K_1, K_2, K_3
- standard FEM in air cells K_4, K_5
- special handling K_1, K_3 (global continuity)

parameters:

- pol. deg. p in air cells
- p^{macro} in g-FEM cells
- set of Bloch modes $e^{i\boldsymbol{k}_j \cdot \boldsymbol{x}}\, b_j^{\text{per}}(\boldsymbol{x})$
- pol. deg. p^{bloch}

Global C^0-continuity



- drop b_2^{gfem}, it can not be matched on Γ^{over}
- add special micro function $b^{\text{micro}}(\boldsymbol{x}) \equiv 1$ to match b_3^{gfem} in K_1.

Computation of matrix entries

$$\mathrm{b}(u,v) := \int_{K^{\text{macro}}} f(\boldsymbol{x}) u(\boldsymbol{x}) \overline{v}(\boldsymbol{x}) \,\mathrm{d}\boldsymbol{x}$$

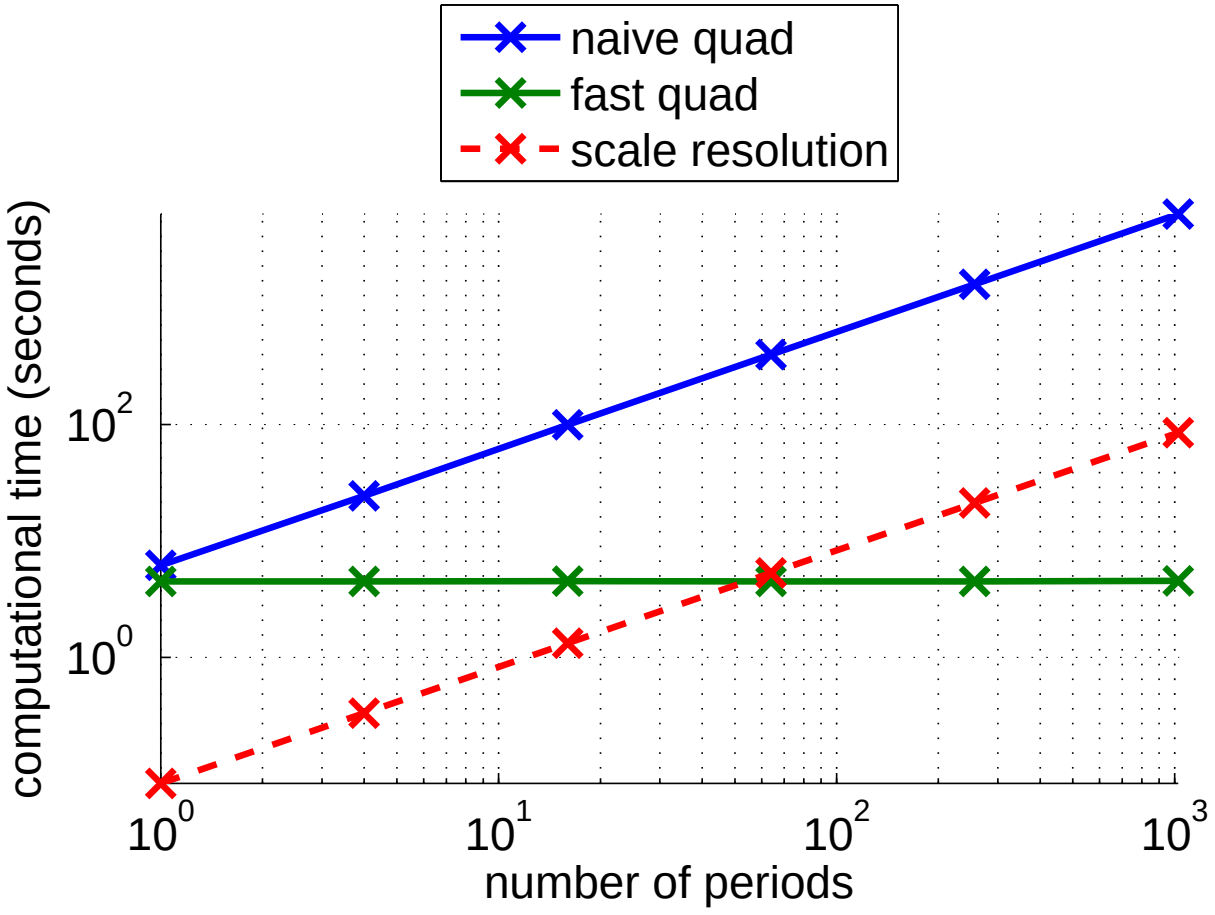
$$\mathrm{a}(u,v) := \int_{K^{\text{macro}}} f(\boldsymbol{x}) \nabla u(\boldsymbol{x}) \cdot \nabla \overline{v(\boldsymbol{x})} \,\mathrm{d}\boldsymbol{x}$$

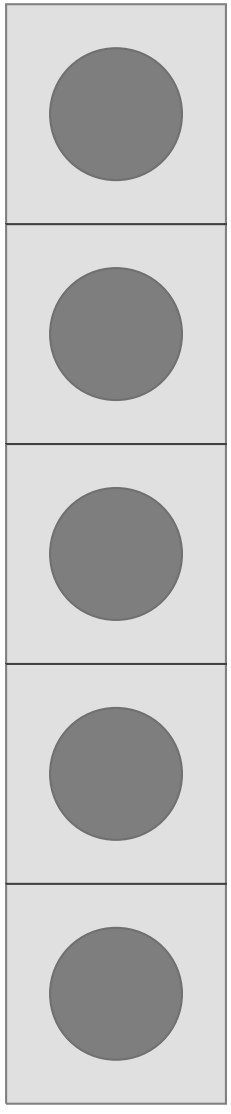
- test with g-FEM basis functions

$$b_{i,j}^{\text{gfem}}(\boldsymbol{x}) = b_i^{\text{macro}}(\boldsymbol{x})\, e^{\mathrm{i}\boldsymbol{k}_j \cdot \boldsymbol{x}}\, b_j^{\text{per}}(\boldsymbol{x})$$

- Use quadrature from micro cells K^{micro}.
- Integrate over macro cells K^{macro}.

Fast quadrature – assembly times





crystal $n_p \times 1$ periods

- g-FEM: $p^{\text{macro}} = 4$, 3 micro oscillations
- scale res: $p = 8$

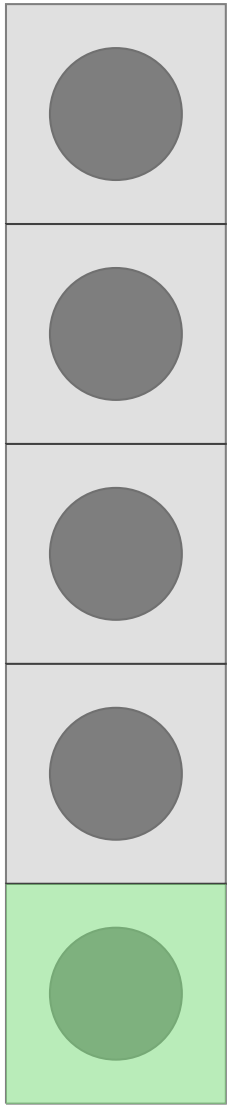
Fast quadrature – idea

Example: mass bilinear form

$$\mathrm{b}(b_i^{\mathrm{gfem}}, b_j^{\mathrm{gfem}}) = \int_{K^{\mathrm{macro}}} f(\boldsymbol{x})\, b^{\mathrm{macro}}(\boldsymbol{x})\, b^{\mathrm{macro}}(\boldsymbol{x}) \left(b^{\mathrm{per}}(\boldsymbol{x})\, e^{\mathrm{i}\boldsymbol{k}_i\cdot\boldsymbol{x}}\right)\left(\overline{b^{\mathrm{per}}}(\boldsymbol{x})\, e^{-\mathrm{i}\overline{\boldsymbol{k}_j}\cdot\boldsymbol{x}}\right) \mathrm{d}\boldsymbol{x}$$

$$= \sum_{l=0}^{n_{\mathrm{p}}-1} e^{\mathrm{i}(\boldsymbol{k}_i-\overline{\boldsymbol{k}_j})\cdot l\boldsymbol{a}_2} \int_{\widehat{\Omega}} f(\hat{\boldsymbol{x}})\, b^{\mathrm{macro}}(\hat{\boldsymbol{x}}+l\boldsymbol{a}_2)\, b^{\mathrm{macro}}(\hat{\boldsymbol{x}}+l\boldsymbol{a}_2) \left(b^{\mathrm{per}}(\hat{\boldsymbol{x}})\, e^{\mathrm{i}\boldsymbol{k}_i\cdot\hat{\boldsymbol{x}}}\right)\left(\overline{b^{\mathrm{per}}}(\boldsymbol{x})\, e^{-\mathrm{i}\overline{\boldsymbol{k}_j}\cdot\hat{\boldsymbol{x}}}\right) \mathrm{d}\hat{\boldsymbol{x}}.$$

goal: factor out integration on $\widehat{\Omega}$.



Fast quadrature – idea

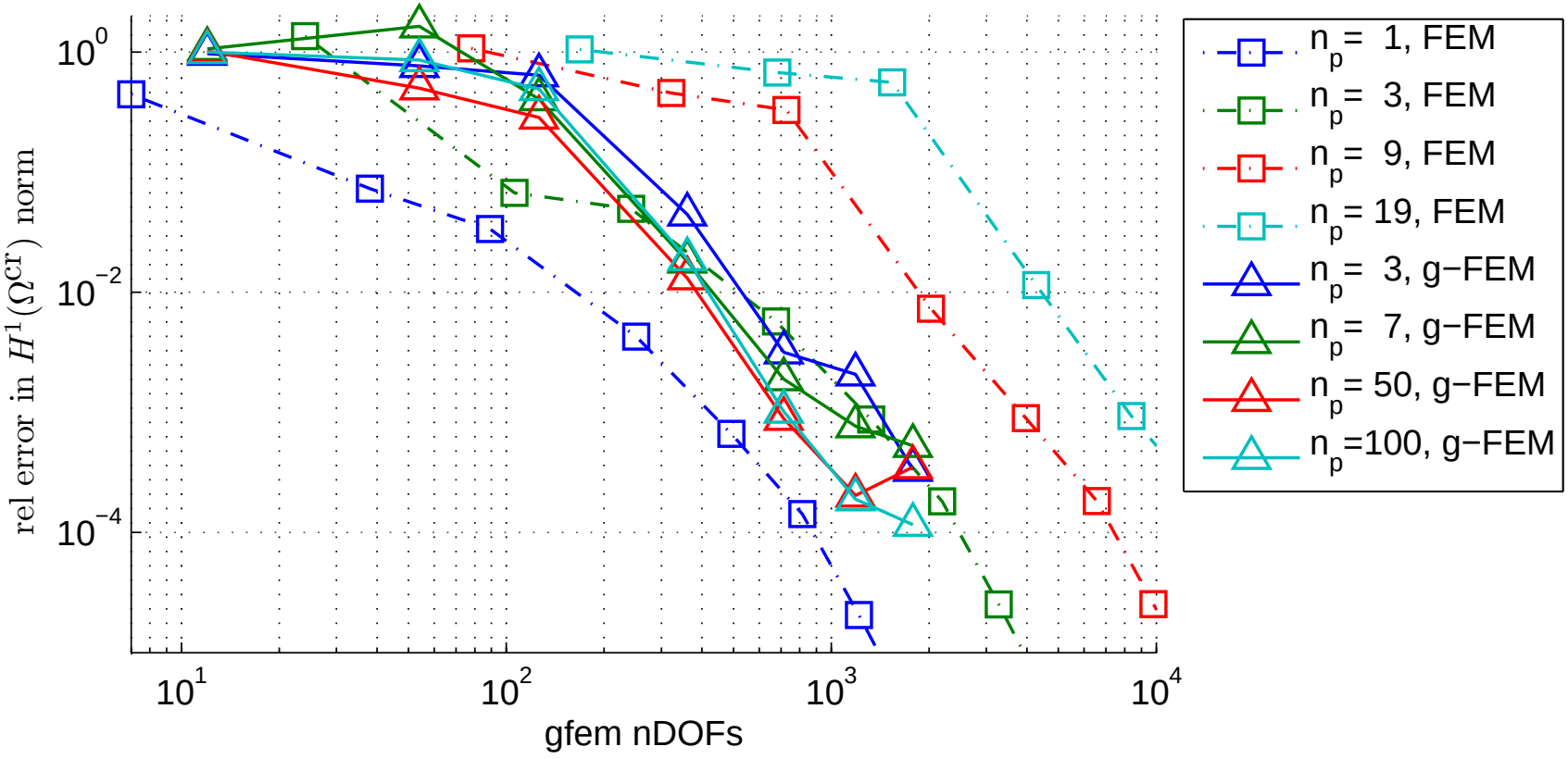
$$\sum_{l=0}^{n_\mathrm{p}-1} e^{\mathrm{i}(\boldsymbol{k}_i-\overline{\boldsymbol{k}_j})\cdot l\boldsymbol{a}_2} \int_{\widehat{\Omega}} f(\hat{\boldsymbol{x}})\, b^{\mathrm{macro}}(\hat{\boldsymbol{x}}+l\boldsymbol{a}_2)\, b^{\mathrm{macro}}(\hat{\boldsymbol{x}}+l\boldsymbol{a}_2) \left(b^{\mathrm{per}}(\hat{\boldsymbol{x}})\, e^{\mathrm{i}\boldsymbol{k}_i\cdot\hat{\boldsymbol{x}}}\right)\left(\overline{b^{\mathrm{per}}}(\boldsymbol{x})\, e^{-\mathrm{i}\overline{\boldsymbol{k}_j}\cdot\hat{\boldsymbol{x}}}\right) \mathrm{d}\hat{\boldsymbol{x}}.$$

- monomial expansion $b^{\mathrm{macro}}(\boldsymbol{x}) = \sum_{\nu\in[0,p]^2} \alpha_\nu \boldsymbol{x}^\nu$
- tensor product structure
- binomial theorem $(x+l)^\nu = \sum_{k=0}^{\nu} \binom{\nu}{k} x^{\nu-k} l^k$
- integral $\int_{\widehat{\Omega}}$ independent of l $\Rightarrow$ precompute
- remaining sum $\sum_{l=0}^{n_\mathrm{p}-1} a^l l^k$

$$= \begin{cases} \text{Bernoulli polynomials} & a = 1, \\ \text{Geometric sum} & k = 0, \\ \text{derivative of Geometric sum} & \text{otherwise.} \end{cases}$$

- in each case, evaluation time independent of n_p.

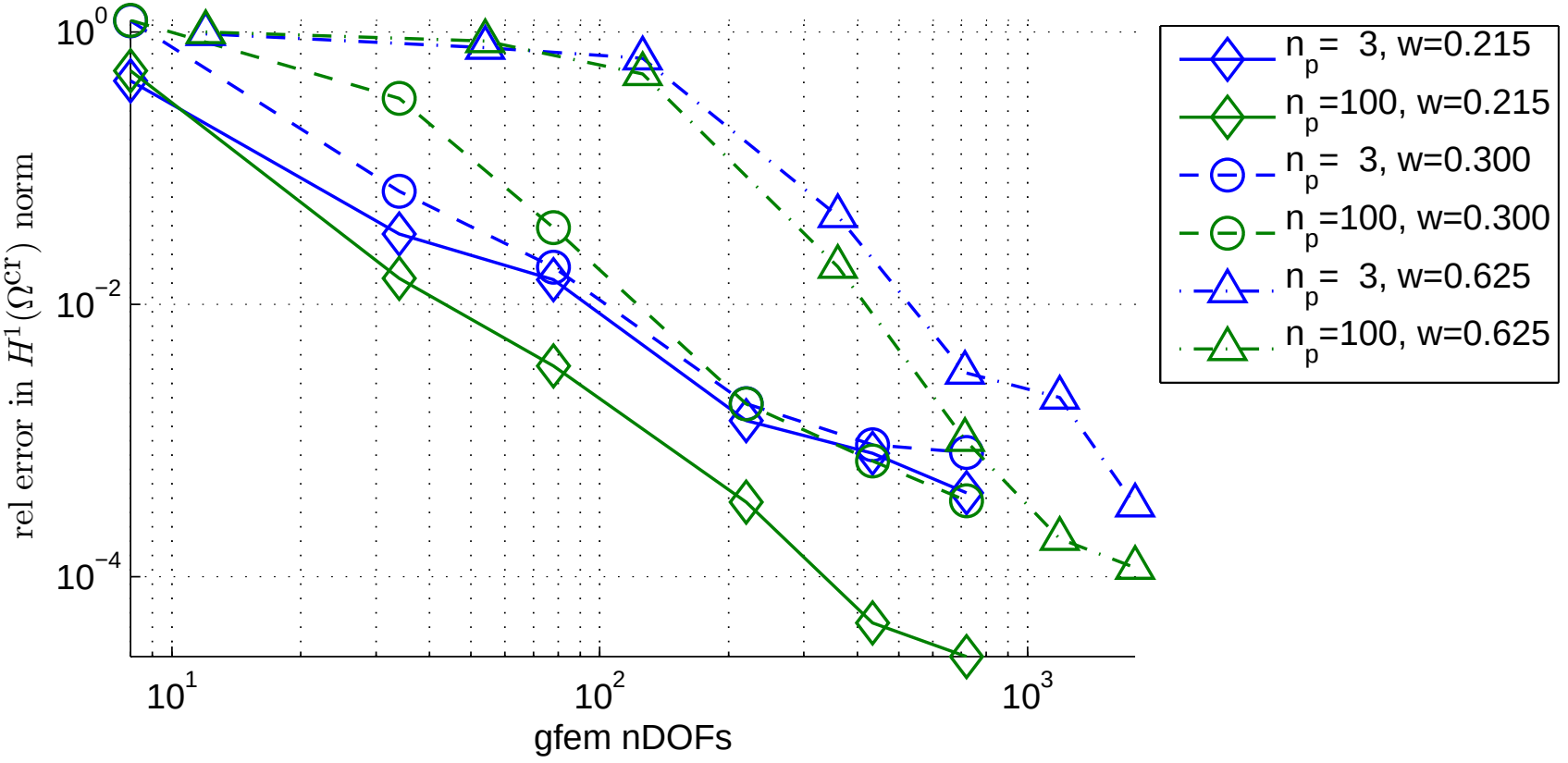
Comparison to standard FEM



error independent of n_p

($\hat{\omega} = 0.625$, 4 Bloch modes)

Convergence for different frequencies



- $\hat{\omega} = 0.625$, 4 Bloch modes
- $\hat{\omega} = 0.215$, 2 Bloch modes
- $\hat{\omega} = 0.300$, 2 Bloch modes, positive decay direction

Conclusion and outlook

- Effective method for finite crystals.
- nDOFs independent of n_p.
- Computational time independent of n_p.
- Problem: high condition numbers (10^{20}).
- Works for propergating and bandgap frequencies,
- Works for non-perpendicular incident fields,

* finite 2D crystal and PhC waveguide,
* robust convergence analysis,
* 1D, 3D simulations,
* large crystal simulation and comparison to measurements.

Thank you for your attention.

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IBM Watson Research Cent.

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IBM's Thomas J. Watson Research Center.

Silicon photonic crystal waveguide connected to photonic wire waveguide.

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