High-accuracy computation of wave scattering and photonic crystal bands . . . and the software that makes it easy

COSI, September 14, 2009

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work with Leslie Greengard (Courant) and Timo Betcke (Reading)

Introduction

Light waves + structures = partial differential equation (PDE) problem

Device design requires accurate and robust numerical solvers

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- reliability: consider impact of LAPACK (e.g. via MATLAB)
- sensitivity analysis: assess response to small parameter changes

Seek: errors dying exponentially with number of degrees of freedom

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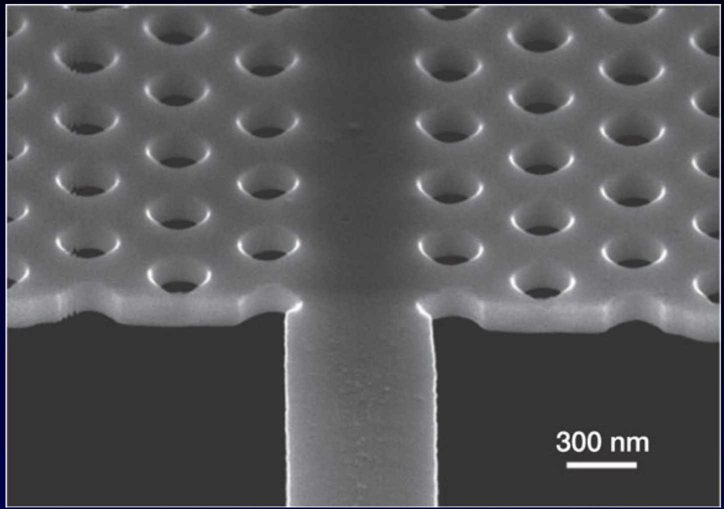
Outline

1.	photonic crystal band structure	eigenvalue problem
2.	scattering of waves from polygons	boundary value problem
3.	software	interface design problem

PART I: Photonic crystals



Si, $\lambda = 1.6\mu$m (Vlasov '05)

piecewise-const dielectric structures

period $\approx$ wavelength of light $\approx$ 1μm

control optical propagation in ways impossible in homogeneous media: dispersion relation, density of states

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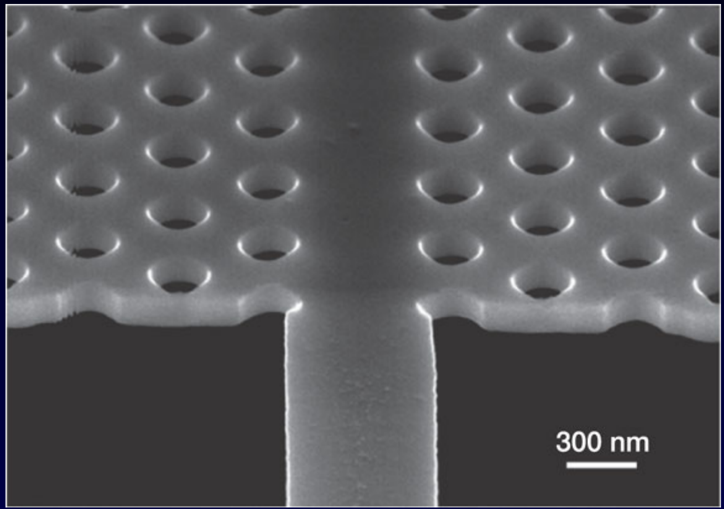

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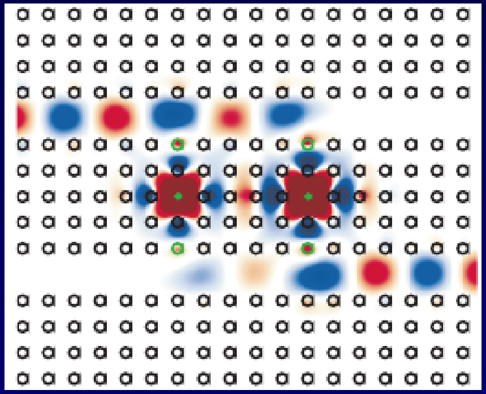
- bandgap freqs: all waves evanescent ('insulator')
- integrated devices: filters, couplers, optical computing, meta-materials ($n_{\text{eff}} < 0$), solar cells



channel-drop filter
(Johnson *et al.* '00)

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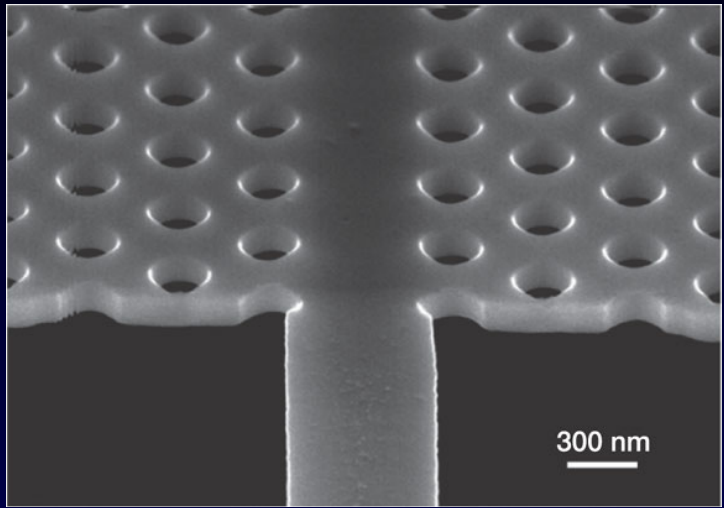

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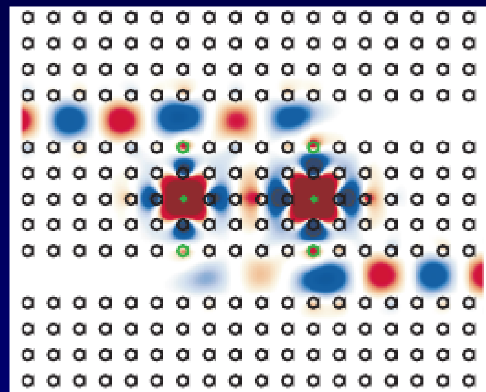

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Manufacturing costly $\Rightarrow$ numerical design/modeling/optimization key

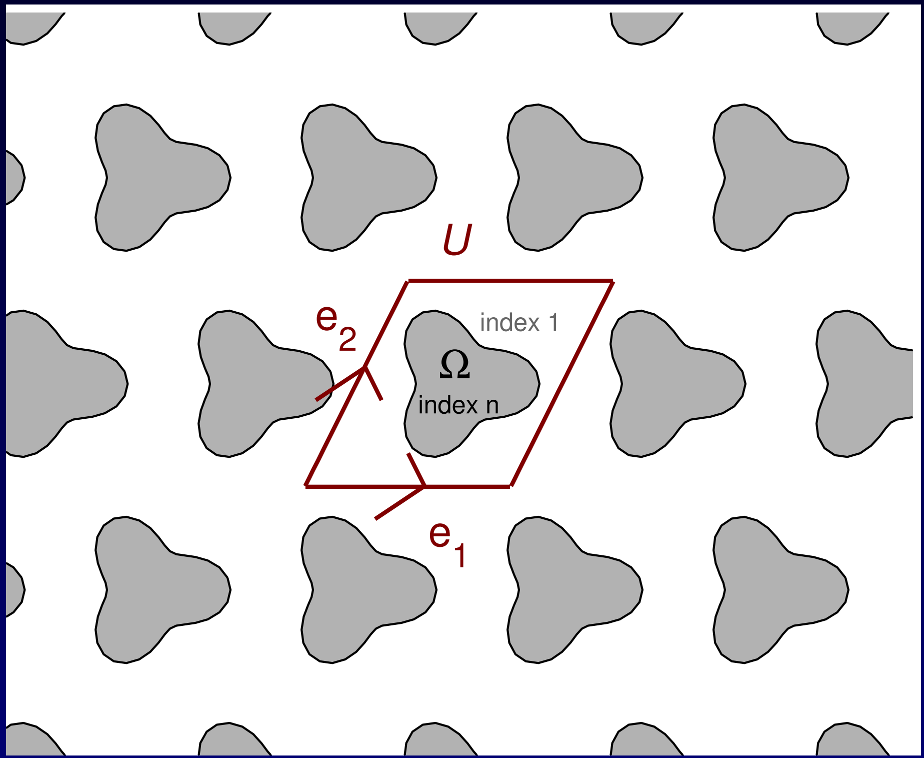
2D dielectric crystal

(z-invariant Maxwell, TM polarization)

unit cell U smooth inclusion $\Omega \Subset U$, refractive index n

lattice $\Lambda := \{m\mathbf{e}_1 + n\mathbf{e}_2 : n, m \in \mathbb{Z}\}$

dielectric inclusions $\Omega_\Lambda := \{\mathbf{x} : \mathbf{x} + \mathbf{d} \in \Omega \text{ for some } \mathbf{d} \in \Lambda\}$



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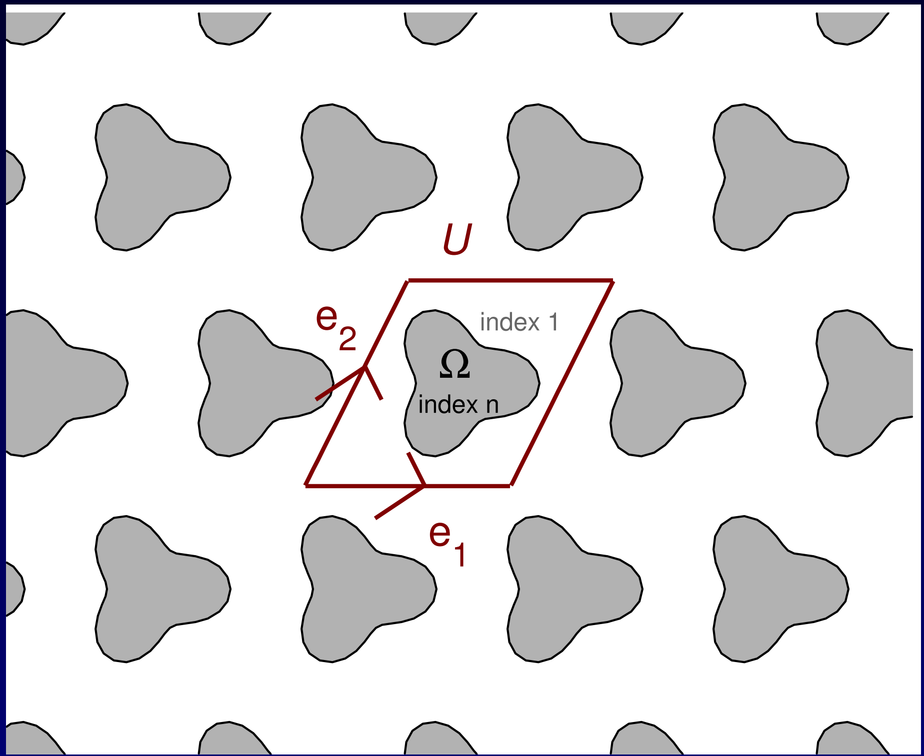

PDE (fixed frequency ω):

$$\begin{aligned}(\Delta + n^2\omega^2)u &= 0 \;\text{ in } \Omega_\Lambda\\ (\Delta + \omega^2)u &= 0 \;\text{ in } \mathbb{R}^2 \setminus \Omega_\Lambda\end{aligned}$$

material matching conditions:

$$\begin{aligned}u^+ - u^- &= 0 \;\text{ on } \partial\Omega_\Lambda\\ u_n^+ - u_n^- &= 0 \;\text{ on } \partial\Omega_\Lambda\end{aligned}$$

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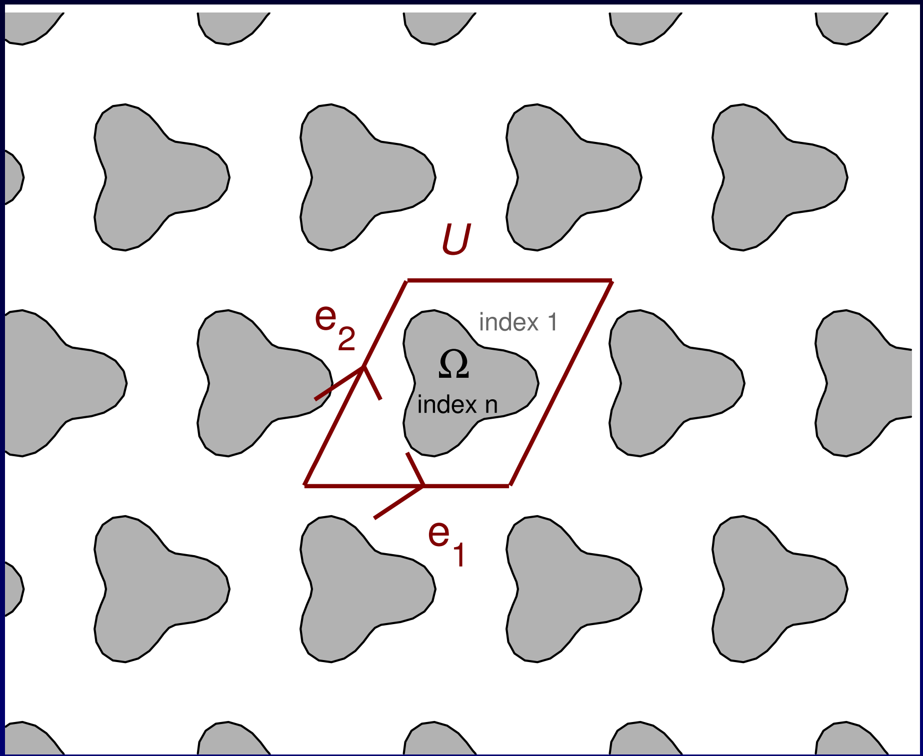

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Bloch 'theorem': solutions on $\mathbb{R}^2$ have the form (or are a sum of forms)

$u(\mathbf{x}) = e^{i\mathbf{k}\cdot\mathbf{x}}\tilde{u}(\mathbf{x})$, $\tilde{u}$ is periodic, $\mathbf{k} \in \mathbb{R}^2$ Bloch wavevector

(F. Bloch 1928 ... 3D version of Hill 1877, Floquet 1883, Lyapunov 1892)

Bloch wave and eigenvalue problem

- Bloch eigenvalues: set of $(\omega, \mathbf{k})$ s.t. non-trivial Bloch waves u exist

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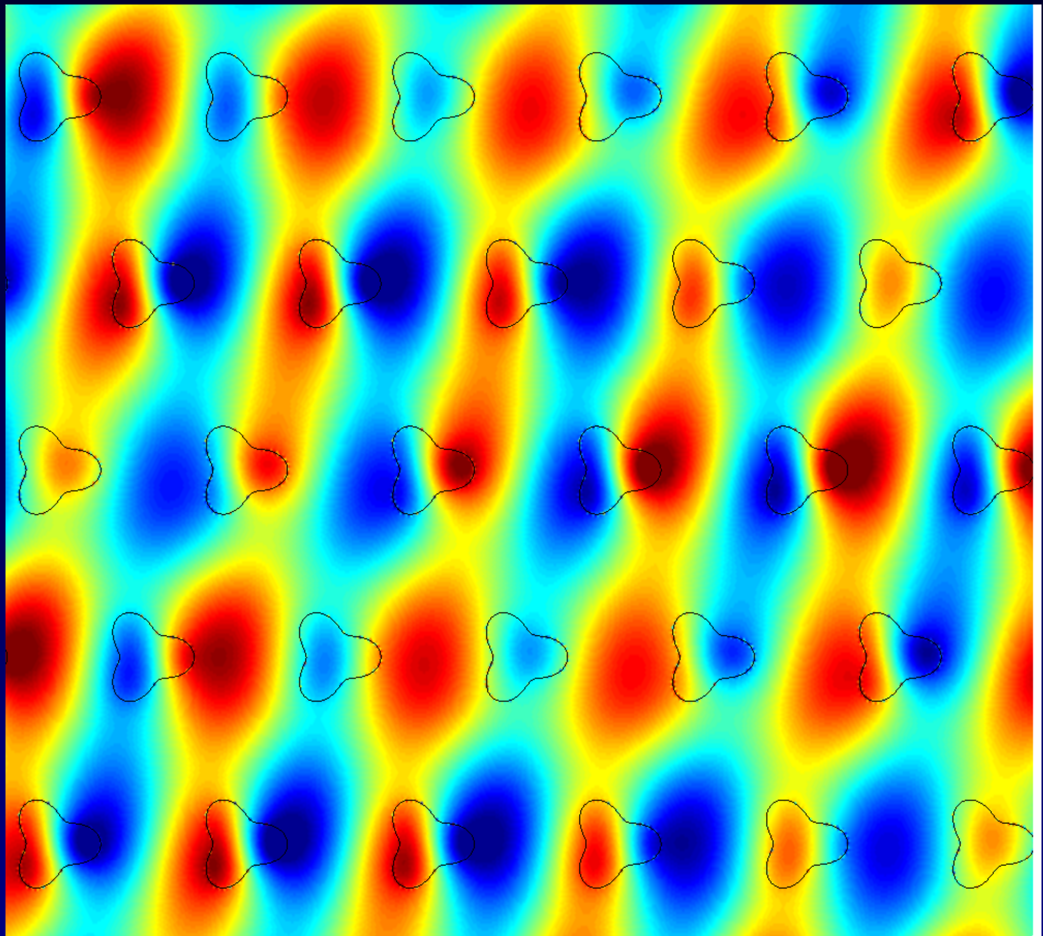
Example generalized eigenfunction u of Bloch wave form $e^{i\mathbf{k}\cdot\mathbf{x}}\tilde{u}(\mathbf{x})$:



Shown: $\mathrm{Re}[u]$ for

$\omega = 5, \quad \mathbf{k} = (-0.39, 2.08)$

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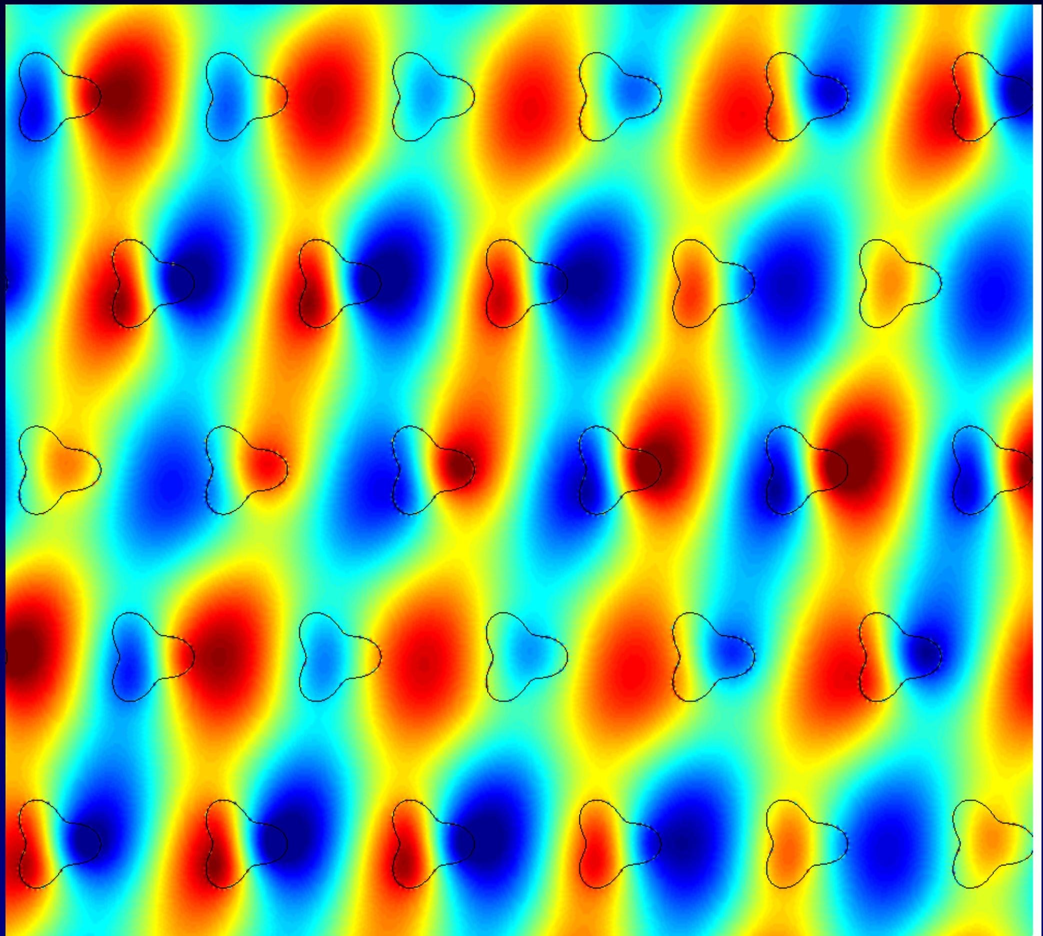

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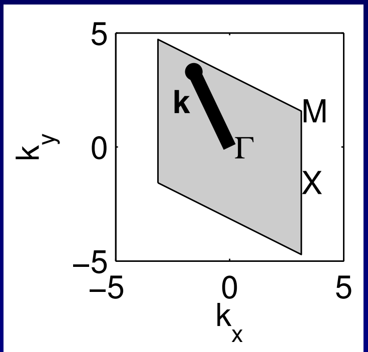
$\omega = 5, \quad \mathbf{k} = (-0.39, 2.08)$

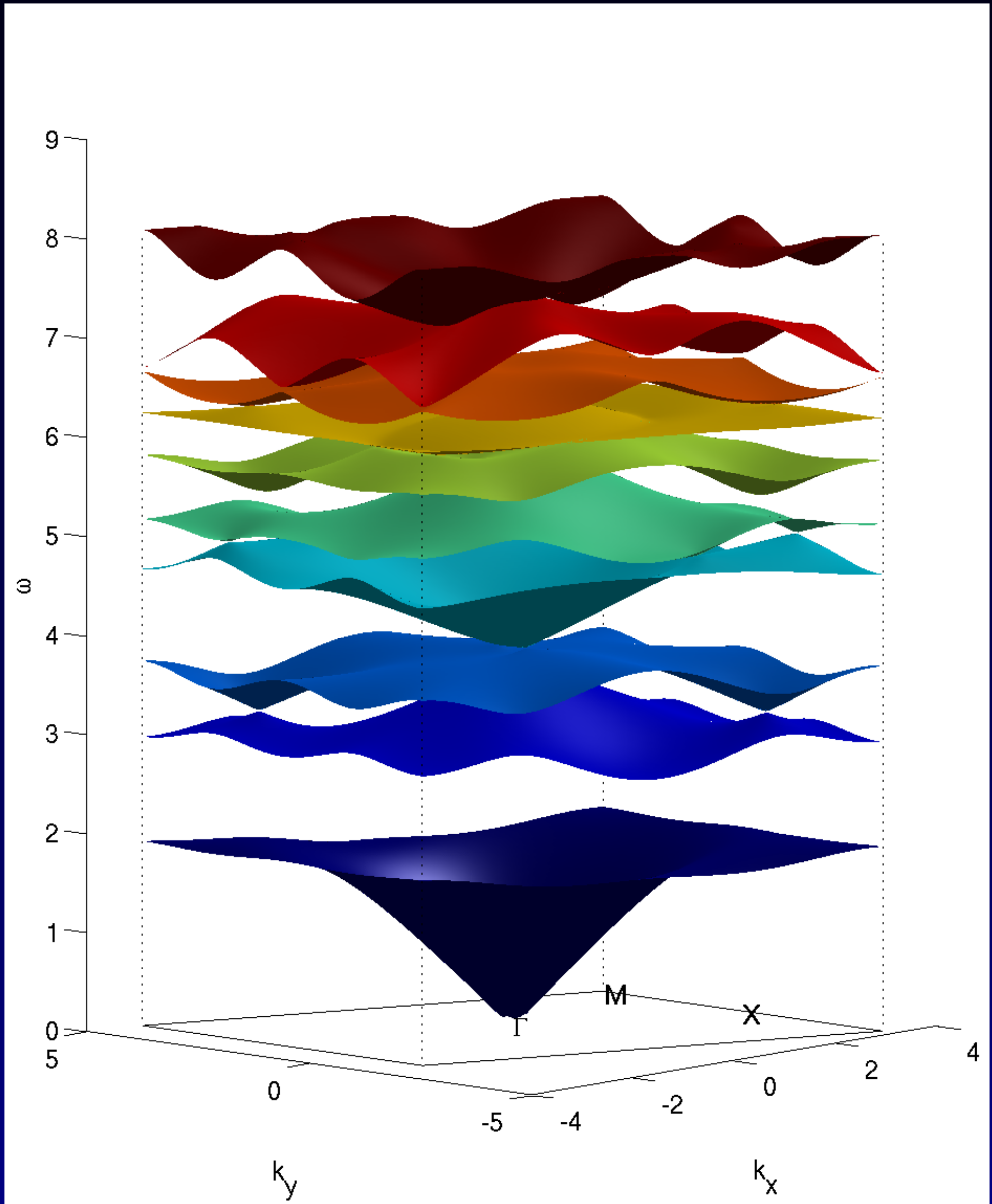
$\mathbf{k}$ equiv. to $\mathbf{k} + \mathbf{q}$, $\forall \mathbf{q} \in 2\pi\Lambda^*$

$\Lambda^* =$ dual (reciprocal) lattice

$\mathbf{k}$ lives on a torus, consider only $\mathbf{k}$ in *Brillouin zone* (BZ):



Band structure



For each wavevector $\mathbf{k} \in$ BZ,
$\exists$ discrete Bloch eigenvalues

$$\omega_1(\mathbf{k}) \leq \omega_2(\mathbf{k}) \leq \cdots \nearrow \infty$$

form ‘sheets’ above the BZ

note: conical at low freq ω

note: bandgap

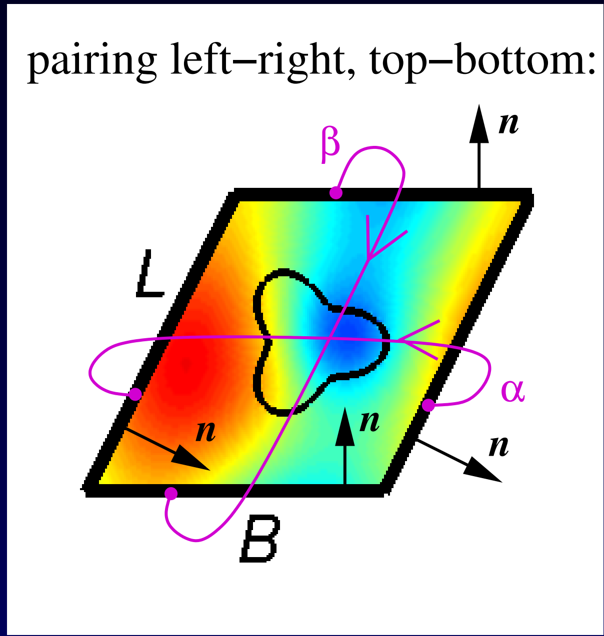
- is most important property of photonic crystal for applications

Recast problem on compact domain (torus)

- Bloch wave condition equiv. to quasi-periodic BCs on ∂U

Require vanishing unit cell discrepancy:

$$
\begin{aligned}
f &:= u|_L - \alpha^{-1} u|_{L+\mathbf{e}_1} = 0 \\
f' &:= u_n|_L - \alpha^{-1} u_n|_{L+\mathbf{e}_1} = 0 \\
g &:= u|_B - \beta^{-1} u|_{B+\mathbf{e}_2} = 0 \\
g' &:= u_n|_B - \beta^{-1} u_n|_{B+\mathbf{e}_2} = 0
\end{aligned}
$$



Bloch phase parameters $\alpha := e^{i\mathbf{k}\cdot\mathbf{e}_1}$, $\beta := e^{i\mathbf{k}\cdot\mathbf{e}_2}$, $|\alpha| = |\beta| = 1$

- Task: find Bloch eigenvalue triples (ω, k_x, k_y), i.e. (ω, α, β)

Main numerical approaches

Time domain

a) time-stepping on finite-difference grid (FDTD) (*e.g.* Yee ’66)

low order (inaccurate); close freqs ⇒ large t needed, inefficent

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b) multiple-scattering, cylinder geometry only (McPhedran *et al.*)

c) Plane-wave method: all in Fourier space (Joannopoulos, Johnson, Sözüer)

discont. dielectric $\Rightarrow$ Gibbs phenom, slow $(1/N)$ convergence

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e) Integral equations: formulate problem *on* the discontinuity $\partial\Omega$

reduced dimensionality (small N), good scattering tools exist, Fast Multipole

rapid convergence: high accuracy with small effort

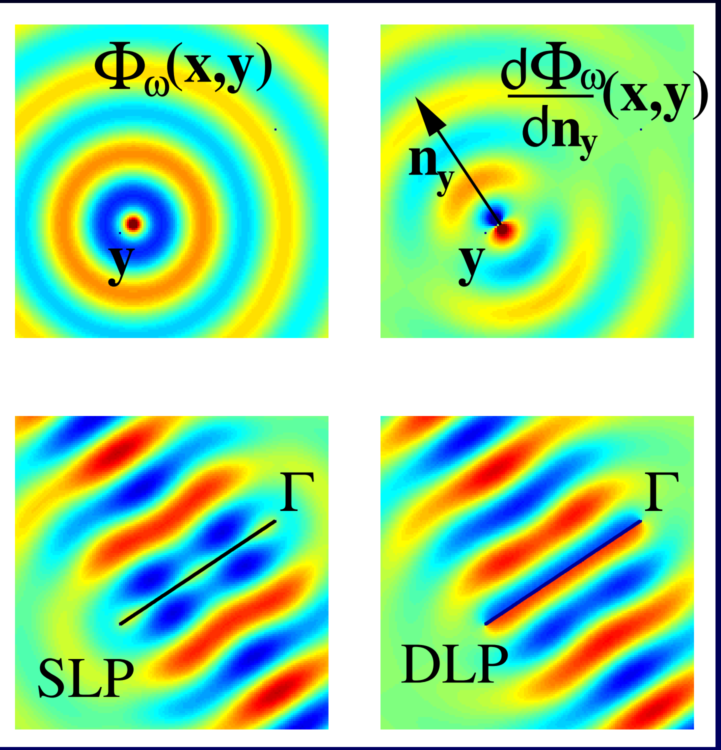
Integral equations (review)

'charge' (sources of waves) distributed along curve Γ w/ density func.

single-, double-layer potentials, $\mathbf{x} \in \mathbb{R}^2$:

$$u(\mathbf{x}) = \int_\Gamma \Phi_\omega(\mathbf{x},\mathbf{y})\sigma(\mathbf{y})ds_\mathbf{y} := (\mathcal{S}\sigma)(\mathbf{x})$$

$$v(\mathbf{x}) = \int_\Gamma \frac{\partial \Phi_\omega}{\partial n_\mathbf{y}}(\mathbf{x},\mathbf{y})\tau(\mathbf{y})ds_\mathbf{y} := (\mathcal{D}\tau)(\mathbf{x})$$



$$\Phi_\omega(\mathbf{x},\mathbf{y}) := \Phi_\omega(\mathbf{x}-\mathbf{y}) := \frac{i}{4}H_0^{(1)}(k|\mathbf{x}-\mathbf{y}|)$$

Helmholtz fundamental soln

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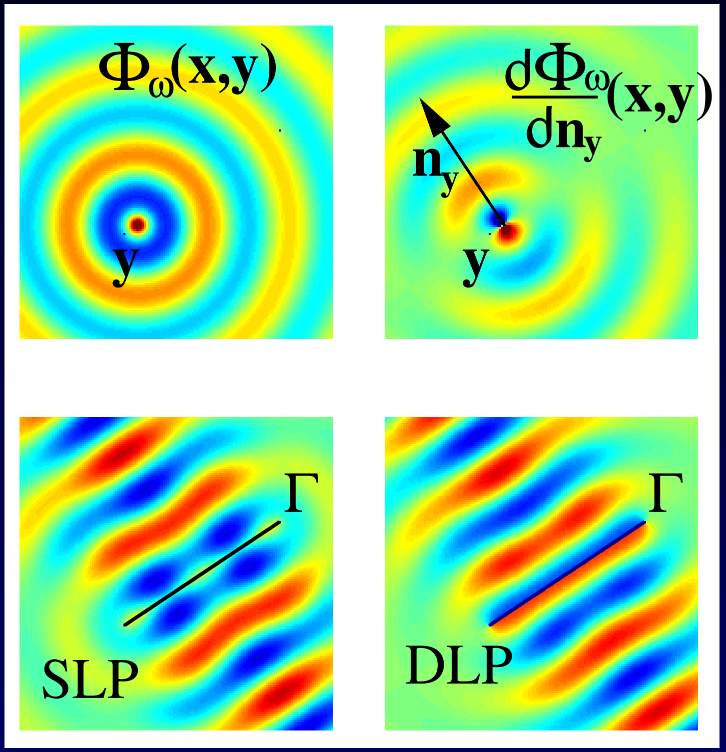

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Jump relations: limit as $\mathbf{x} \to \Gamma$ may depend on which side ($\pm$):

$$u^\pm = S\sigma$$
$$u_n^\pm = D^T\sigma \mp \tfrac{1}{2}\sigma$$
$$v^\pm = D\tau \pm \tfrac{1}{2}\tau$$
$$v_n^\pm = T\tau$$

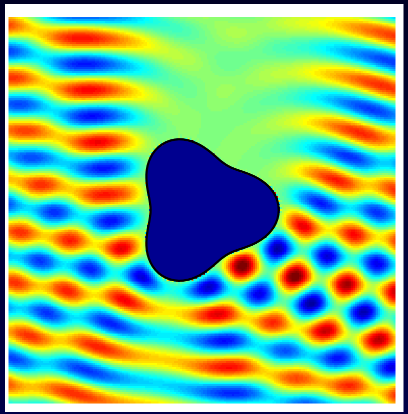
S, D are integral ops with above kernels

but defined on $C(\Gamma) \to C(\Gamma)$

T has kernel $\frac{\partial^2 \Phi_\omega}{\partial n_\mathbf{x} \partial n_\mathbf{y}}(\mathbf{x}, \mathbf{y})$

Integral equations for scattering (sketch)

e.g. sound-soft obstacle: represent $u = u^{\text{inc}} + \mathcal{D}\tau$ DLP on $\partial\Omega$



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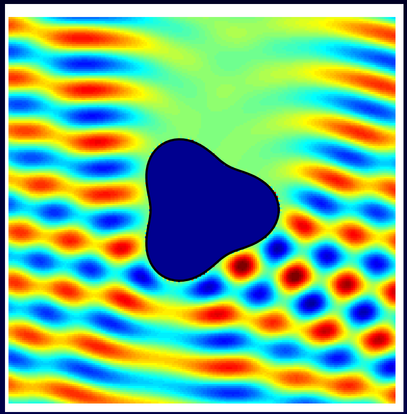

BC $\quad 0 = u^+ = u^{\text{inc}}|_{\partial\Omega} + (D + \frac{1}{2})\tau$ by JR3

integral eqn on $\partial\Omega$: $\quad (I + 2D)\tau = -2u^{\text{inc}}$

2nd-kind, D compact op so $(I + 2D)$ sing. vals. $\not\to 0$

Why important?

condition # small, iterative solvers (GMRES) fast

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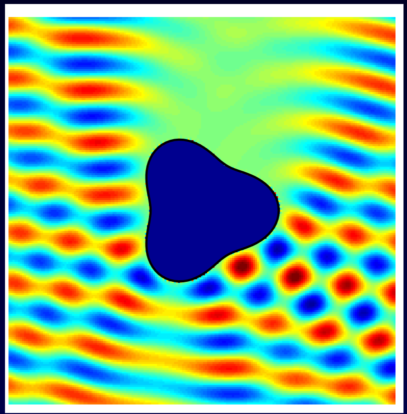

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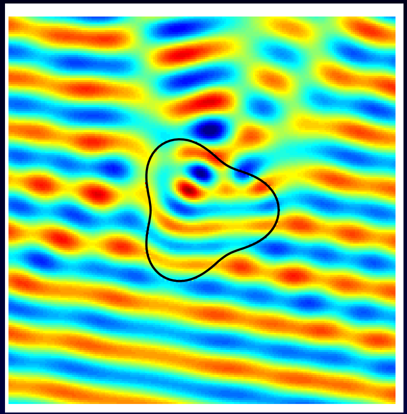
Quadrature: choose N nodes on $\partial\Omega$ to approximate integrals

Theorem: (Anselone, Kress) For analytic curve & incident wave, the 'Nyström method' has error $= O(e^{-cN})$

- called exponential or 'spectral' convergence
- e.g. for above: $N = 60$ enough for 10^{-6} error, $N = 100$ for 10^{-12}

Dielectric (transmission) scattering



Represent $u = u^{\text{inc}} + \mathcal{D}\tau + \mathcal{S}\sigma$ outside wavenumber ω

$u = \mathcal{D}_i\tau + \mathcal{S}_i\sigma$ inside wavenumber $n\omega$

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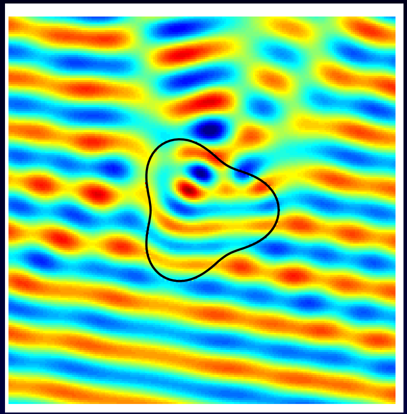

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$u = \mathcal{D}_i\tau + \mathcal{S}_i\sigma$ inside   wavenumber $n\omega$

mismatch on $\partial\Omega$: $h := u^+ - u^-$, $h' := u_n^+ - u_n^-$

BCs: mismatch $m := [h; h']$ vanishes, use JRs...

$$\begin{bmatrix} 0 \\ 0 \end{bmatrix} = \begin{bmatrix} u^{\text{inc}}|_{\partial\Omega} \\ u_n^{\text{inc}}|_{\partial\Omega} \end{bmatrix} + \left(\underbrace{\begin{bmatrix} I & 0 \\ 0 & I \end{bmatrix} + \begin{bmatrix} D - D_i & S_i - S \\ T - T_i & D_i^T - D^T \end{bmatrix}}_{A} \right) \underbrace{\begin{bmatrix} \tau \\ -\sigma \end{bmatrix}}_{\eta}$$

block 2nd-kind A maps densities to their effect on mismatch

- hypersingular part of T cancels, so $A = \text{Id} + \text{compact}$ (Rokhlin '83)
- kernel weakly singular, but still exist spectral quadratures   (Kress '91)

The standard way to periodize

replace kernel $\Phi_\omega(\mathbf{x})$ by $\Phi_{\omega,\mathrm{QP}}(\mathbf{x}) := \sum_{m,n\in\mathbb{Z}} \alpha^m \beta^n \Phi(\mathbf{x} - m\mathbf{e}_1 - n\mathbf{e}_2)$

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Theorem (*integral formulation of band structure*) :

$$\boxed{\text{If } A_{\mathrm{QP}} \text{ exists,} \quad \mathrm{Nul}\, A_{\mathrm{QP}} \neq \{0\} \quad \Leftrightarrow \quad (\omega, k_x, k_y) \text{ is eigenvalue}}$$

note: no u^{inc} since eigenvalue problem homogeneous

Not a robust method: A_{QP} does not exist for certain parameters (ω, k_x, k_y)

since there $\Phi_{\omega,\mathrm{QP}}(\mathbf{x}) \to \infty, \;\; \forall \mathbf{x}$

why… ?

Failure at spurious resonances

$\Phi_{\omega,\mathrm{QP}}(\mathbf{x})$ is Helmholtz Greens function in *empty* (index 1) torus

$$= \frac{1}{\mathrm{Vol}(U)} \sum_{\mathbf{q}\in 2\pi\Lambda^*} \frac{e^{i(\mathbf{k}+\mathbf{q})\cdot\mathbf{x}}}{\omega^2 - |\mathbf{k}+\mathbf{q}|^2}$$

spectral representation on torus

has simple pole wherever (ω, k_x, k_y) is eigenvalue of empty torus...

but physical field u well-behaved here: breakdown is non-physical!

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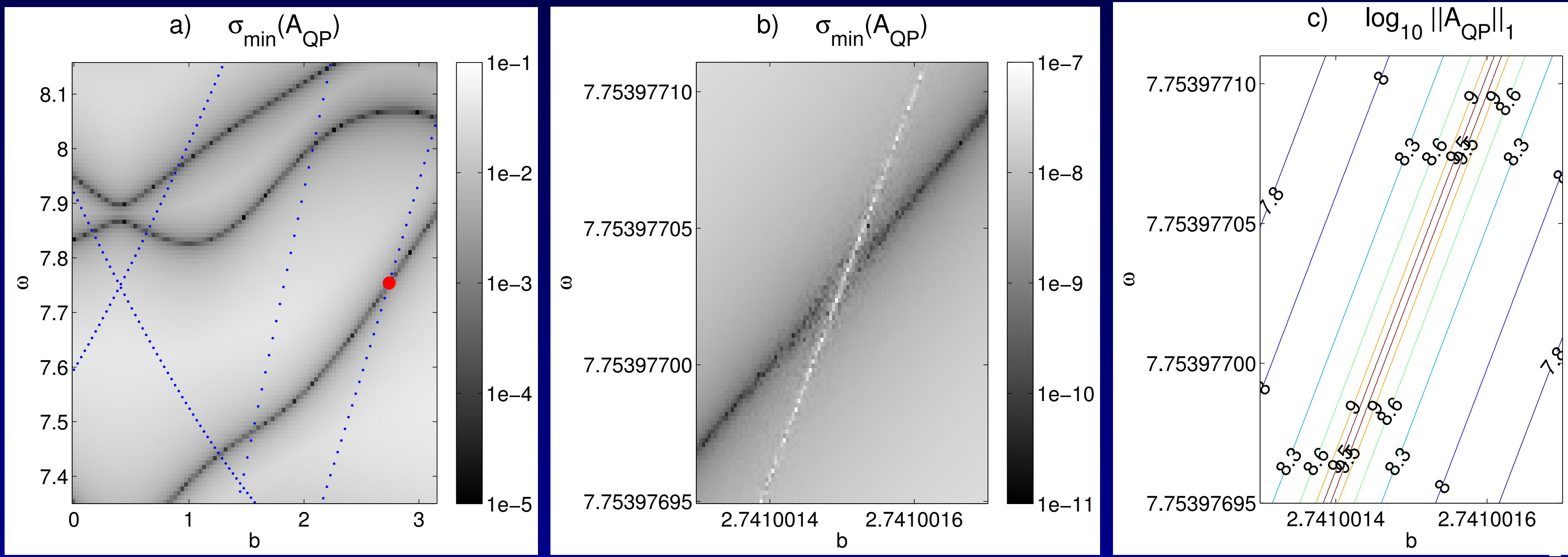

Our cure: robust way to periodize

represent $u = \mathcal{D}\tau + \mathcal{S}\sigma +$ (densities ξ on walls of U) outside

$\uparrow$ can enforce mismatch $m = 0$

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In block operator form $$\underbrace{\begin{bmatrix} A & B \\ C & Q \end{bmatrix}}_{M} \begin{bmatrix} \eta \\ \xi \end{bmatrix} = \begin{bmatrix} m \\ d \end{bmatrix}$$

- added extra degrees of freedom (a small #, indep. of complexity of Ω)

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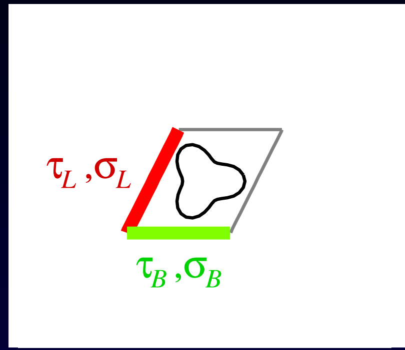
- added extra degrees of freedom (a small #, indep. of complexity of Ω)
- gain robustness: no matrix element blow-up at spurious resonances

Observe: $\boxed{\mathrm{Nul}\, M \neq \{0\} \quad \Leftrightarrow \quad (\omega, k_x, k_y) \text{ Bloch eigenvalue}}$

- idea of extra sources of waves not new (*e.g.* Hafner '02)
- what is new: $M = \mathrm{Id} + \text{compact}$ ideal for large-scale, iterative, FMM

How choose new densities on unit cell walls?

- to control 4 discrepancies (f, f', g, g')
  need 4 densities $\xi = [\tau_L; \sigma_L; \tau_B; \sigma_B]$



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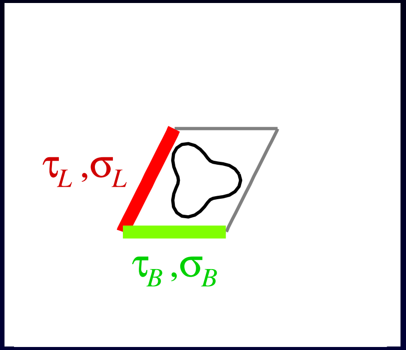


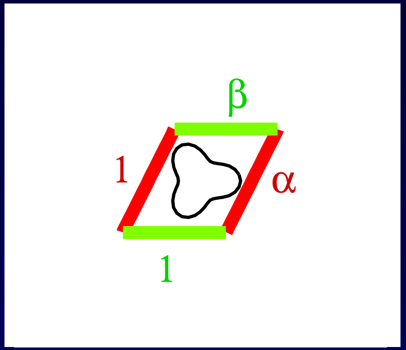
- add phased ghost copies on other 2 walls

  recall $f := u|_L - \alpha^{-1} u|_{L+\mathbf{e}_1}$

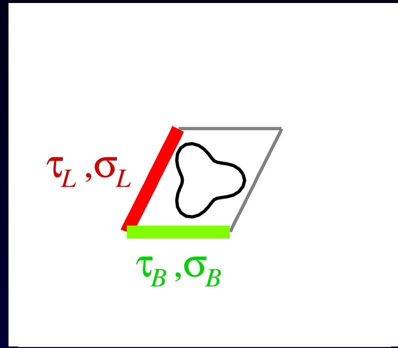
effect of σ_L on $u_n|_L$

effect of $\alpha\sigma_L$ on $\alpha^{-1} u_n|_{L+\mathbf{e}_1}$

} cancel apart from Id



How choose new densities on unit cell walls?

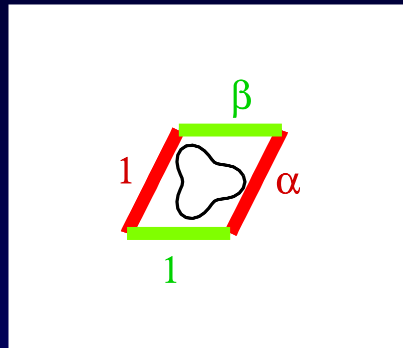


- to control 4 discrepancies (f, f', g, g')

  need 4 densities $\xi = [\tau_L; \sigma_L; \tau_B; \sigma_B]$

$Q = \frac{1}{2}\text{Id} + \text{(self-interactions)} + \text{(other interactions)}$

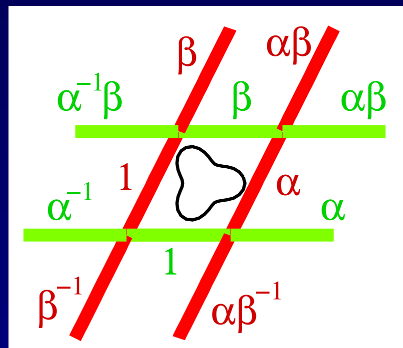
JRs $\quad \sigma_L \to u|_L \quad \sigma_L \to u|_B$



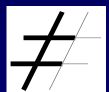
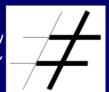
- add phased ghost copies on other 2 walls

  recall $f := u|_L - \alpha^{-1} u|_{L+\mathbf{e}_1}$

effect of σ_L on $u_n|_L$
effect of $\alpha\sigma_L$ on $\alpha^{-1} u_n|_{L+\mathbf{e}_1}$
} cancel apart from Id



- add more 'sticking-out' ghost images

effect of  on $u_n|_L$
effect of α  on $\alpha^{-1} u_n|_{L+\mathbf{e}_1}$
} cancel apart from Id

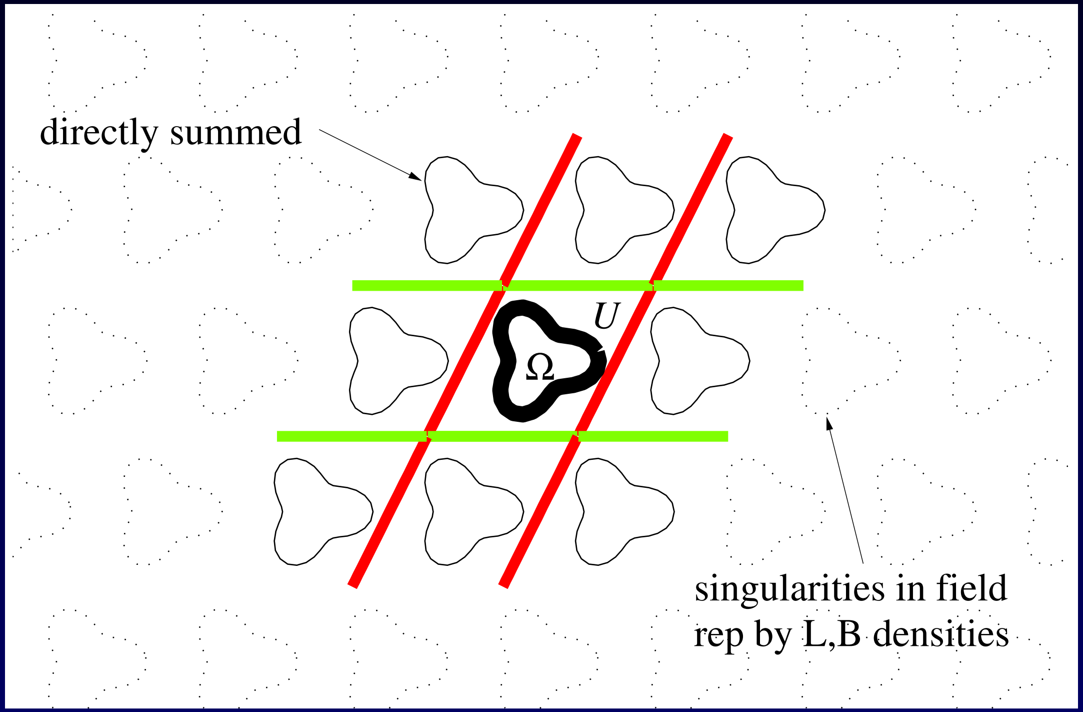
$\Rightarrow$ all corner interactions vanish!

- result: $\quad Q = I +$ (interactions of distance ≥ 1)

  $\Rightarrow$ low rank, rapid convergence: 20-pt Gauss quadr. on L, $B \Rightarrow 10^{-12}$ error

Full scheme

Finally we add 3x3 phased image copies of densities on $\partial\Omega$, giving:



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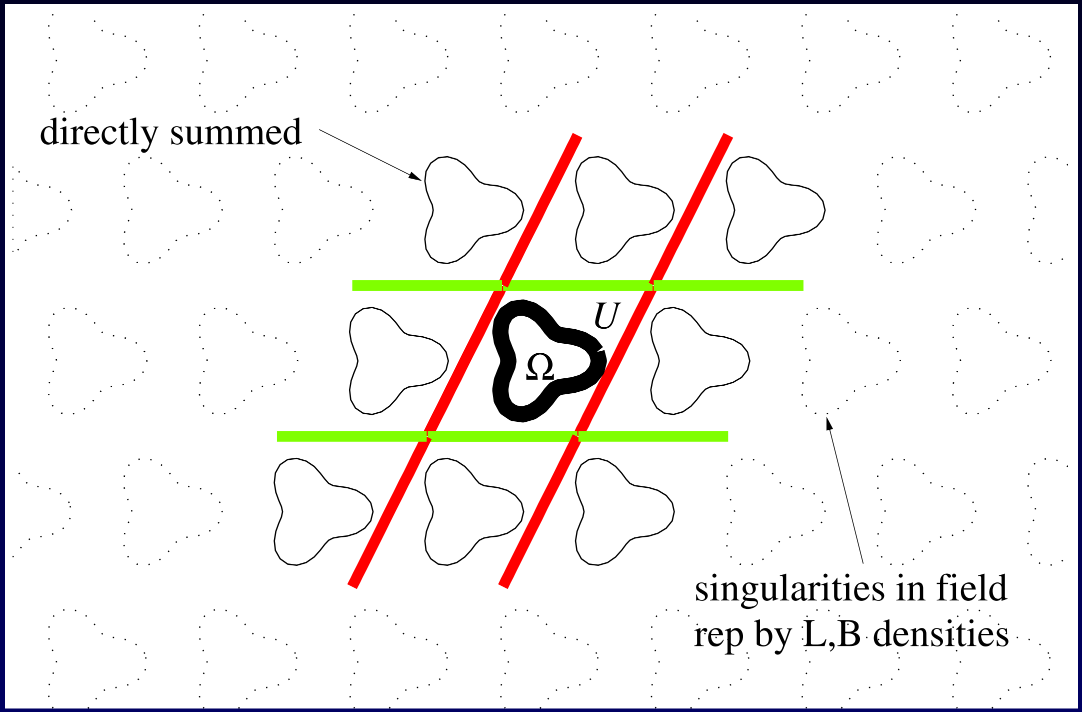

- Careful cancellations: B, C, Q have only interactions of distance ≥ 1
- This leads to rapid convergence rate, i.e. large c in error = $O(e^{-cN})$

Philosophy: sum neighboring image sources directly
so fields due to remainder of lattice have distant singularities

Results: small inclusion

band structure: simply plot log min sing. val. of M vs (ω, k_x, k_y) ...

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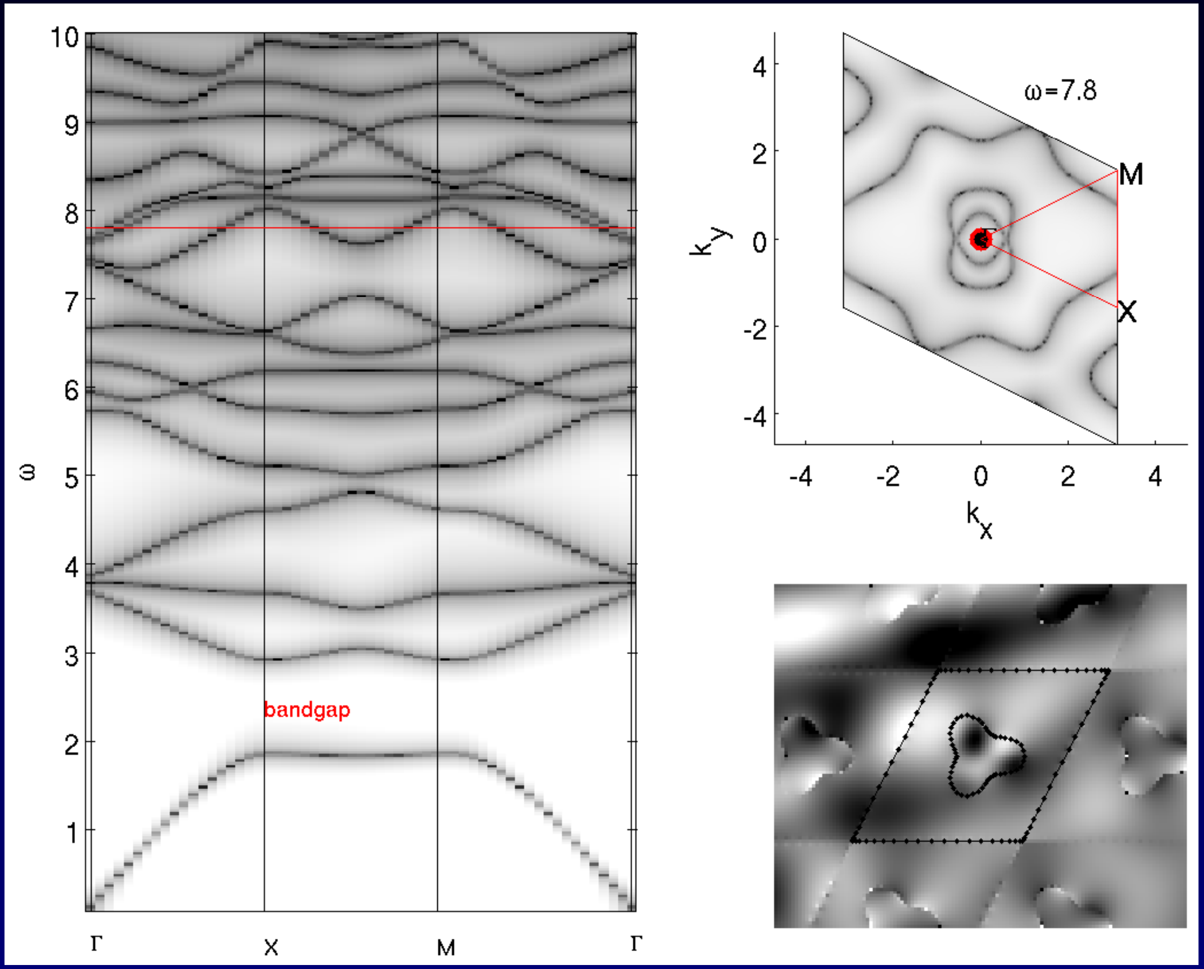

0.1 sec per eval

30 sec per const-ω slice

spectral convergence

- errors 10^{-9} for 40 pts on $\partial\Omega$, 20 on each wall (total $N = 160$)
- nonlinear EVP: spectral Chebychev rootfinder (Boyd '02) on det M

PART II: Scattering of waves from polygons

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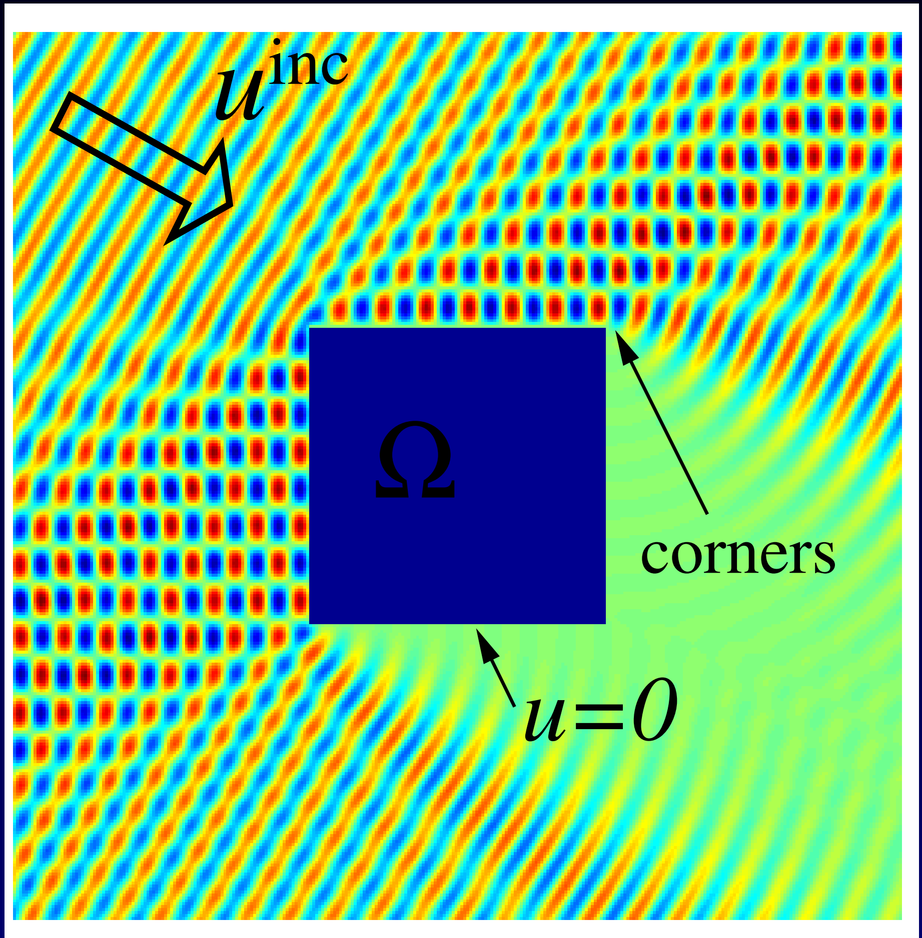


total field $\quad u = u^{\text{inc}} + u_s$

e.g. E_z, Maxwell TM, $\partial\Omega =$PEC

Solve for scattered field u_s:

$$\begin{aligned} (\Delta + \omega^2) u_s &= 0 && \text{in } \mathbb{R}^2 \backslash \overline{\Omega} \\ u_s &= -u^{\text{inc}} && \text{on } \partial\Omega \\ \frac{\partial u_s}{\partial r} - i\omega u_s &= o(r^{-1/2}) && r \to \infty \end{aligned}$$

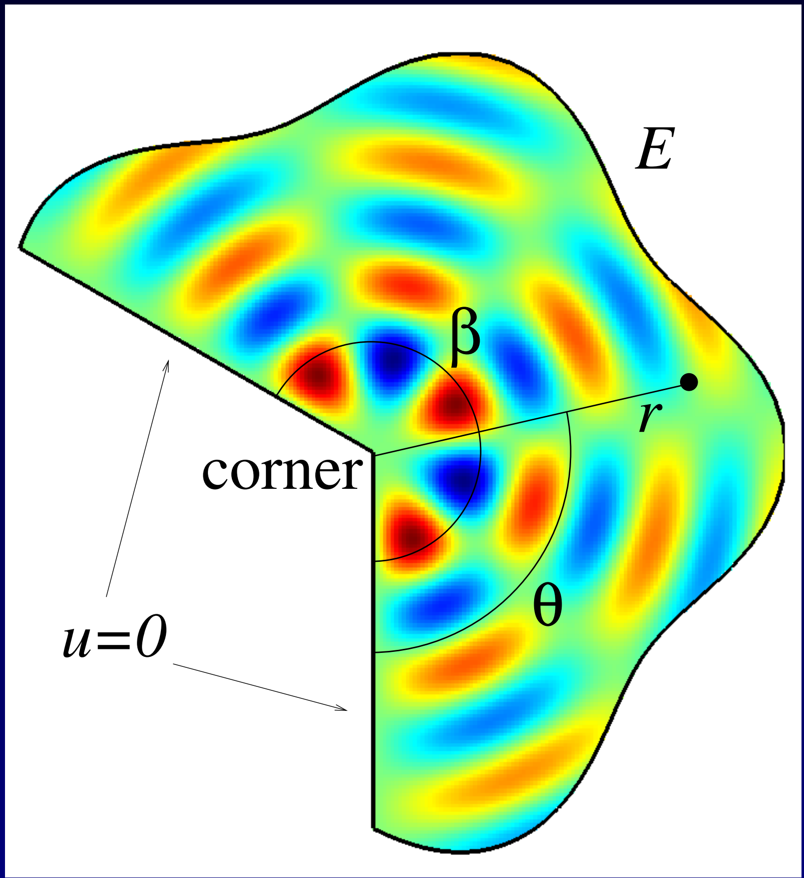
plane wave: $u^{\text{inc}}(\mathbf{x}) = e^{i\omega\hat{n}\cdot\mathbf{x}}$

- Apps: acoustics, radar, imaging, photonics, ...

Helmholtz equation in a wedge

Solution u at corner with angle $\beta \neq \frac{\pi}{\text{integer}}$ has singularity

- finite-difference, FEM, integral equations usually slow to converge



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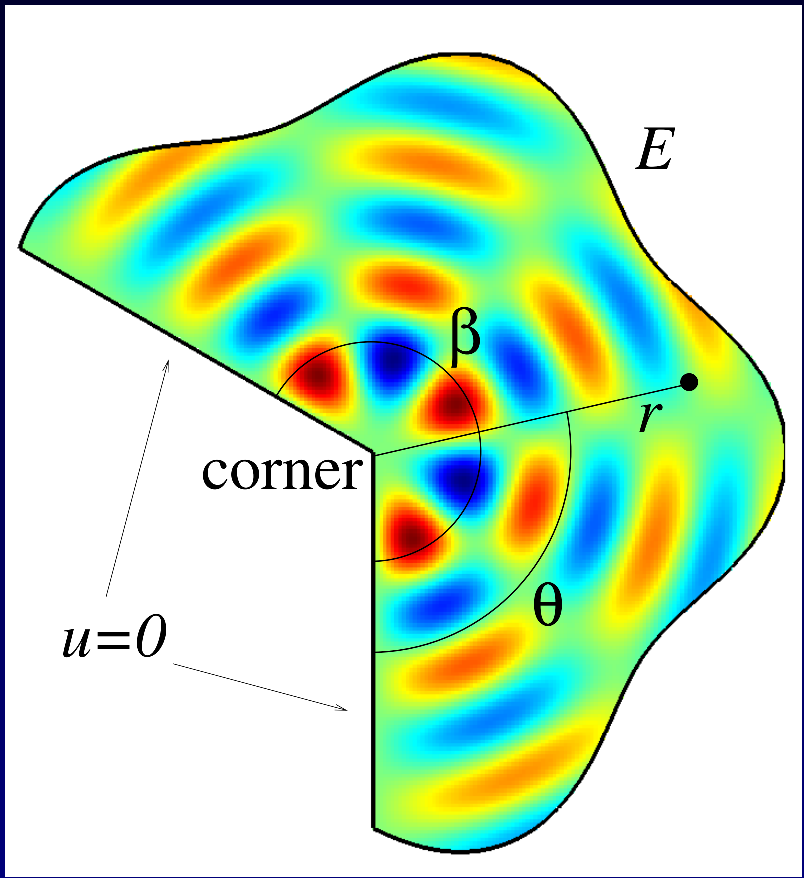


Separable basis functions:

$$u \approx v = \sum_{n=1}^{N} c_n J_{n\pi\theta/\beta}(\omega r) \sin(n\pi\theta/\beta)$$

each term solves Helmholtz

Theorem (Vekua, Betcke): *there exist coefficients* $\mathbf{c} \in \mathbb{R}^N$ *and* $\rho > 1$ *such that*

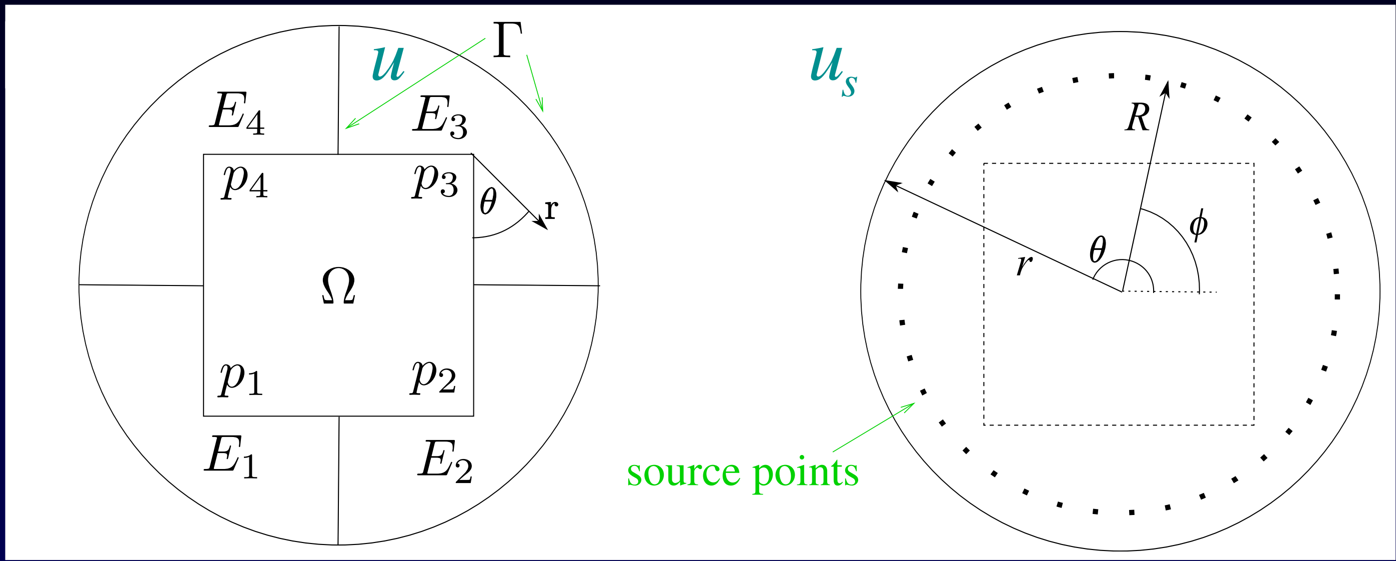
$$\max_{\mathbf{x}\in E} |v(\mathbf{x}) - u(\mathbf{x})| = O(\rho^{-N}), \quad N \to \infty$$

Exponential convergence (efficient representation)

- best (largest) rate ρ is known (need: conformal maps & other corners)

Representation & boundary matching

Divide space into artificial domains with new boundaries Γ:



- non-polynomial FEM: huge elements, PDE solutions as basis funcs
- outside circle: $u_s \approx$ sum of effective sources (radiative)

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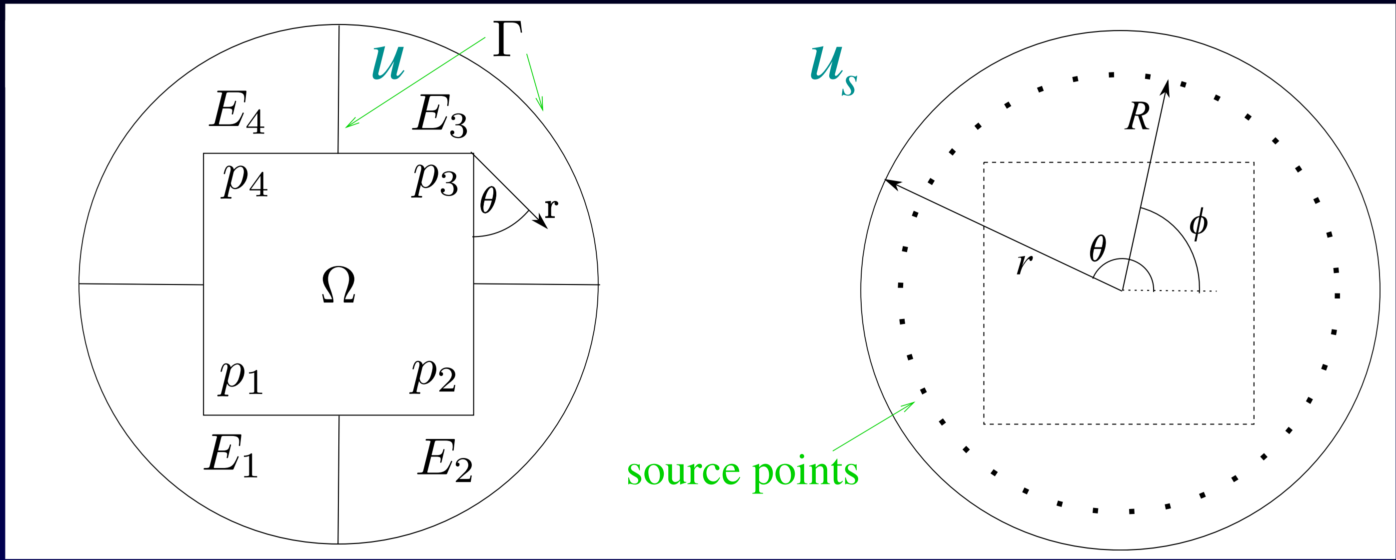

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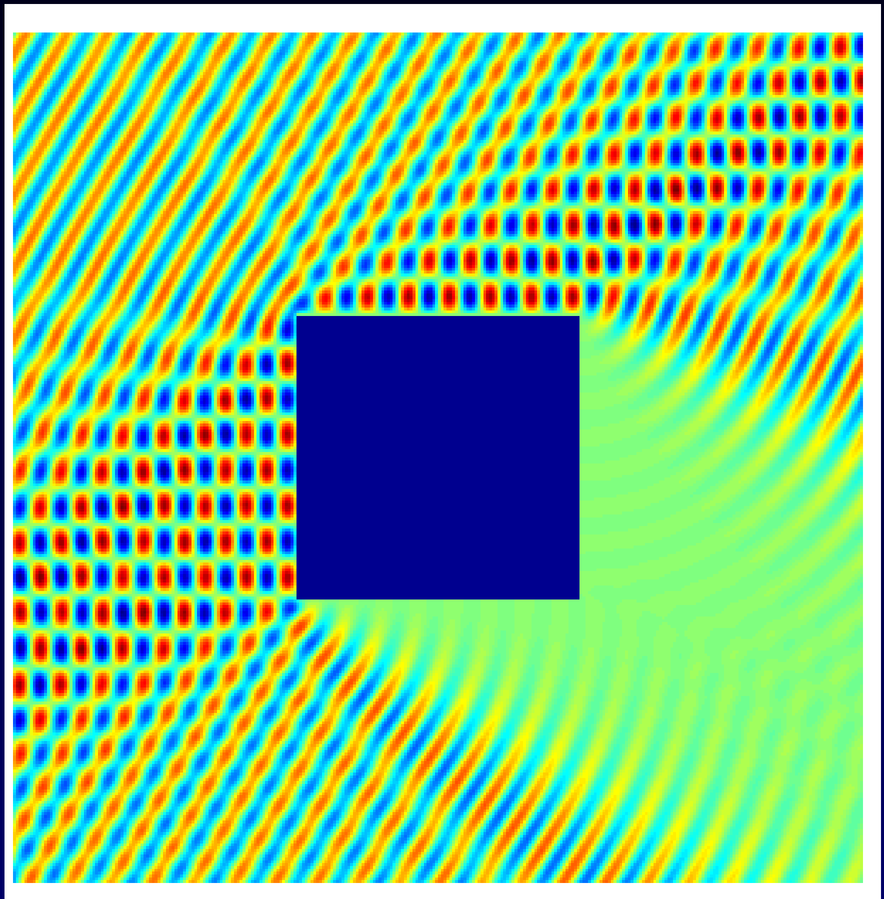
Matching L^2 error: $\quad t(v) = \left(\int_\Gamma |v^+ - v^-|^2 + |v_n^+ - v_n^-|^2 ds\right)^{1/2}$

Want $\min_{\boldsymbol{c}} t$: Gauss quadrature for $\int_\Gamma$ gives least-squares system,

$$\hat{c} = \arg\min_{\boldsymbol{c}} \|A\boldsymbol{c} - \boldsymbol{b}\|_2$$

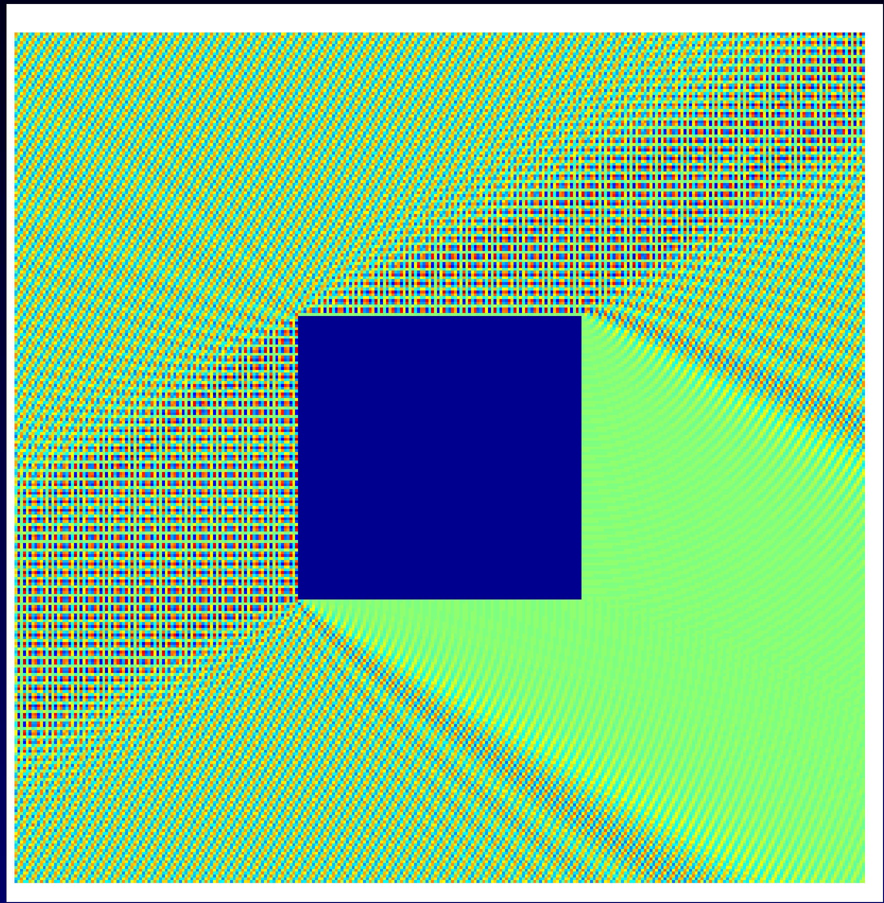
efficient basis: A is small (order $\sim 10^3$), dense

Results: square



8 wavelengths (λ) per side $\quad N = 549$

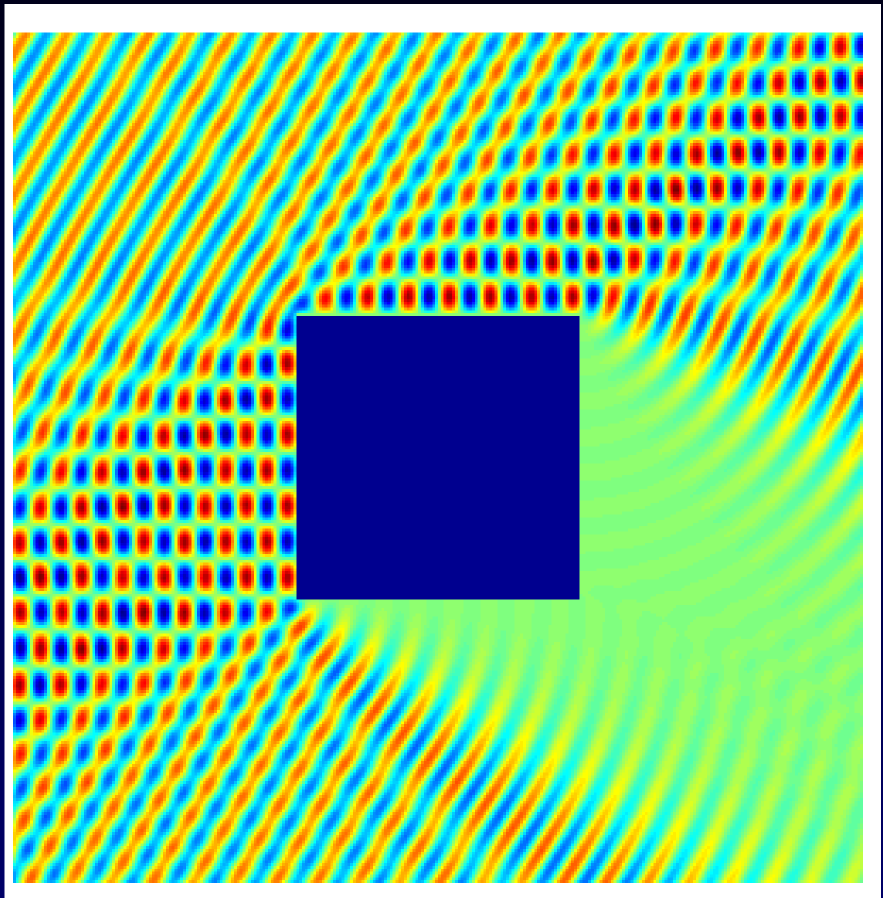
error $t = 8 \times 10^{-11}$ $\quad$ 13 sec on laptop



32 λ $\quad N = 1464$ $\quad t = 2 \times 10^{-9}$

100 sec

Results: square



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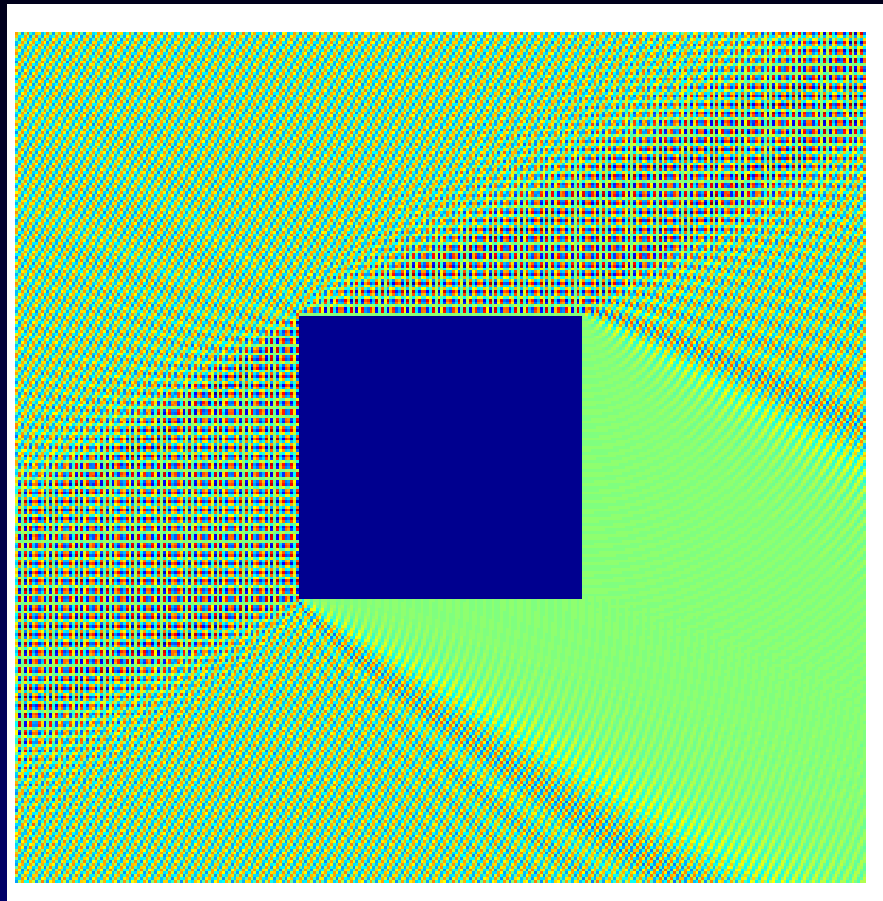
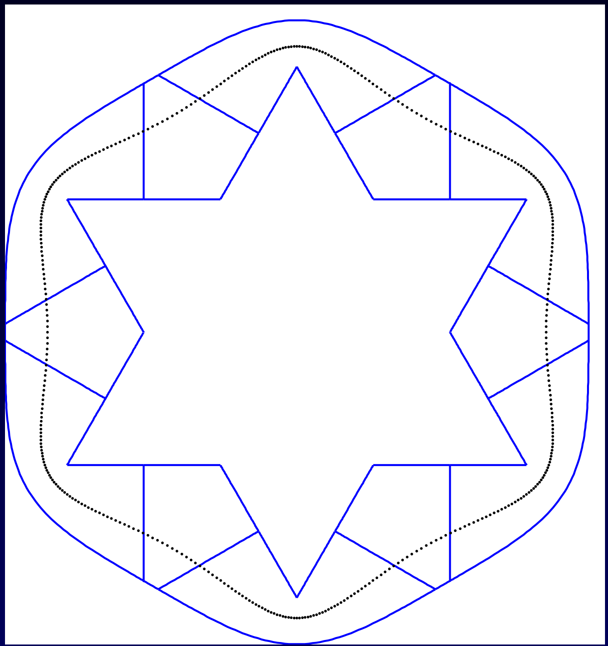


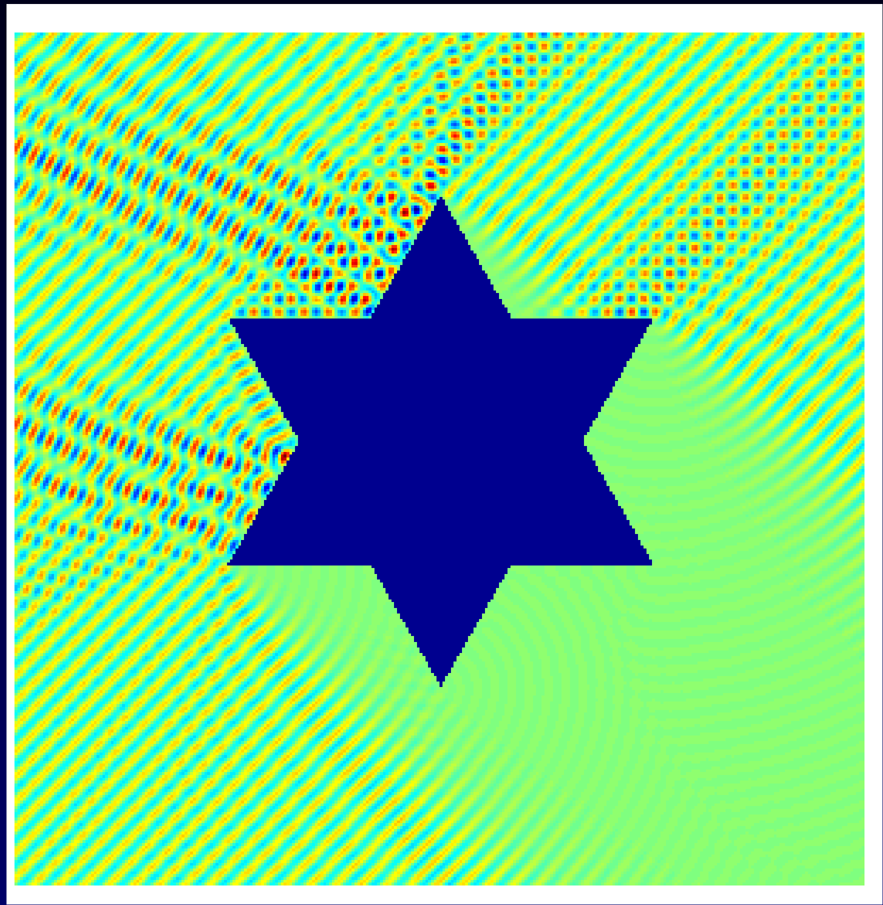
$32\ \lambda$ $N = 1464$ $t = 2 \times 10^{-9}$
100 sec

- $N = O(\omega)$ at high freq: total cost $O(\omega^3)$, but prefactor small
- low-to-medium freqs fast; then loses to $O(1)$ (Chandler-Wilde, Graham)

Results: snowflake

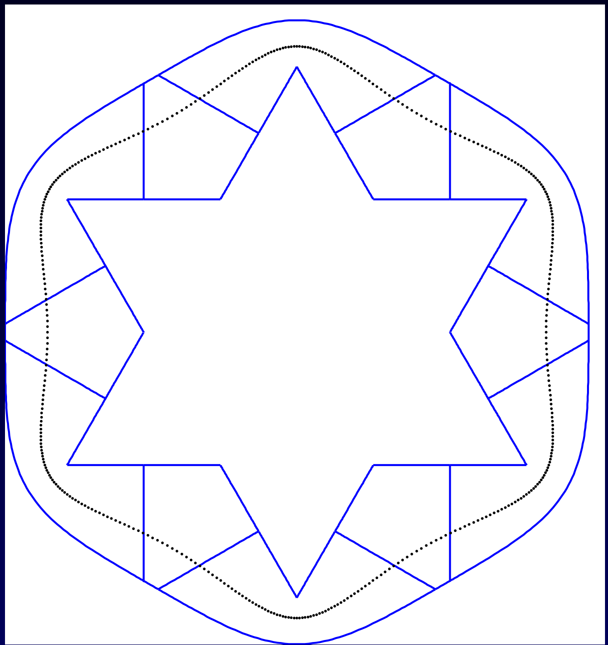


non-circular artificial curve, charges 'shield' the corners



24 λ $\quad N = 1800 \quad t = 2 \times 10^{-11} \quad$ 43 sec

Results: snowflake



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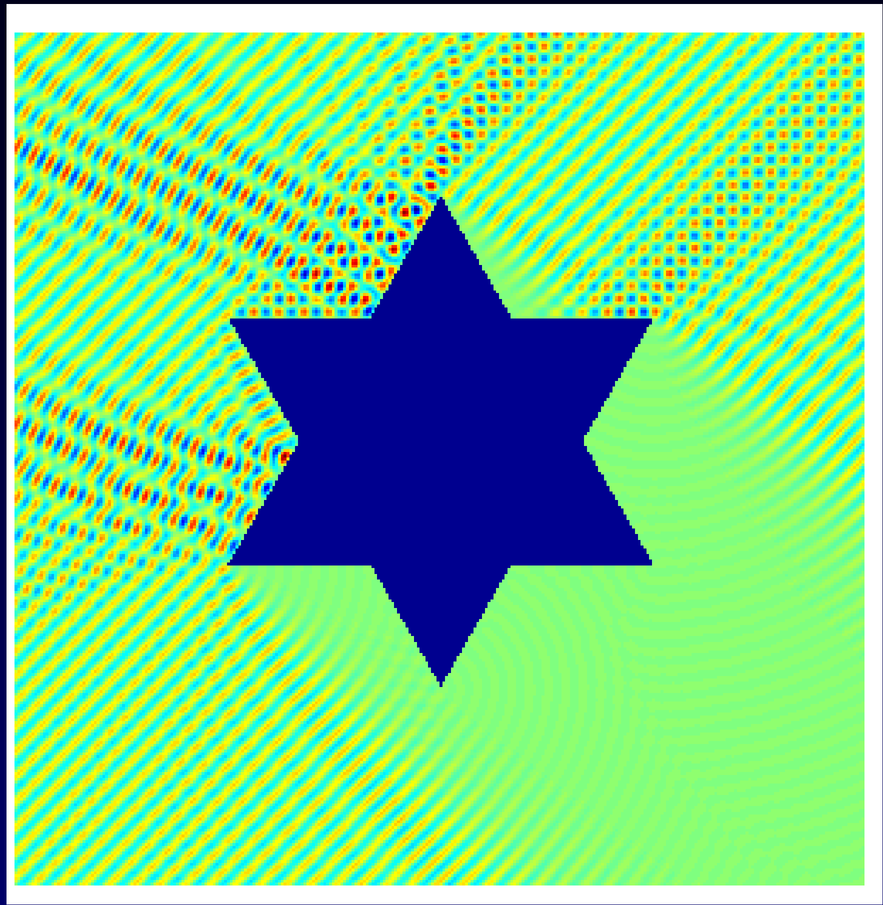
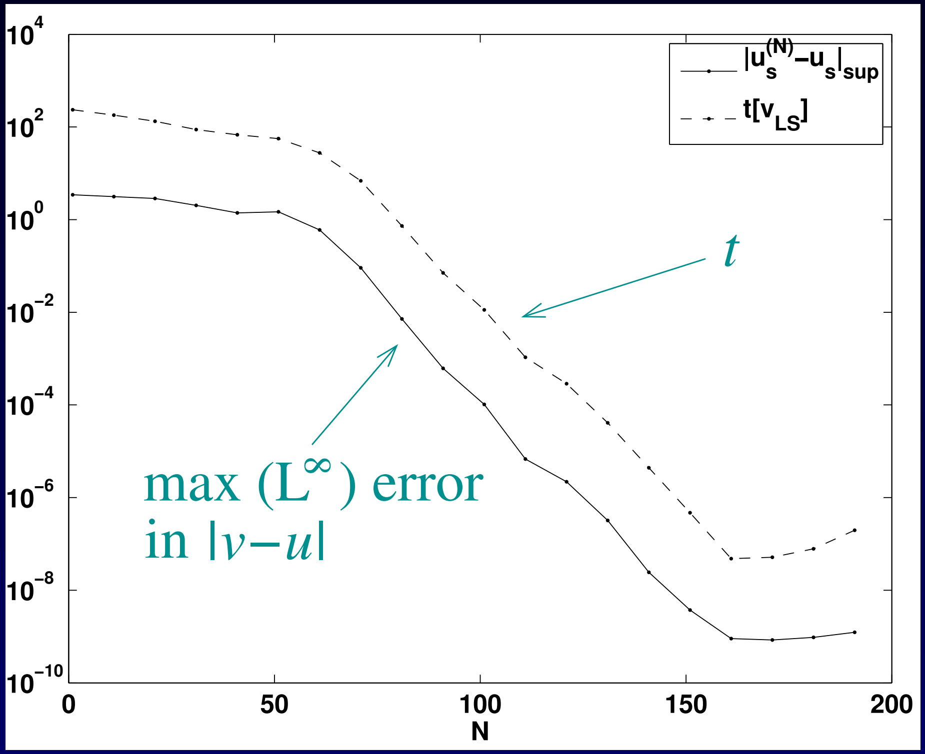


24 λ $N = 1800$ $t = 2 \times 10^{-11}$ 43 sec

- dense QR: a new right-hand side takes only 0.1 sec (unlike iterative)
- Apps: radar scattering cross section (RCS), multiple u^{inc} angles

Convergence & stability

Theorem: *boundary L^2 error $t = O(\rho^{-N})$ for computable rate $\rho > 1$*



Also observe $\max\limits_{\mathbb{R}^2 \setminus \Omega} |u - v| \leq C_\Omega t$

here $C_\Omega \approx 10^{-2}$

- we would like to prove this!

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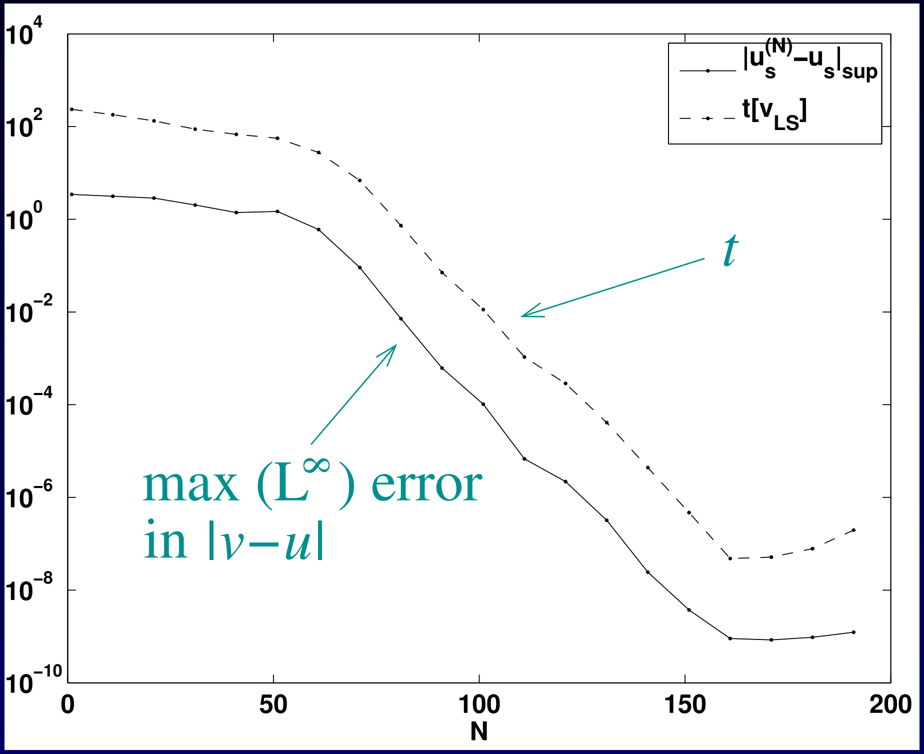

Also observe $\max_{\mathbb{R}^2\setminus\Omega} |u - v| \le C_\Omega t$

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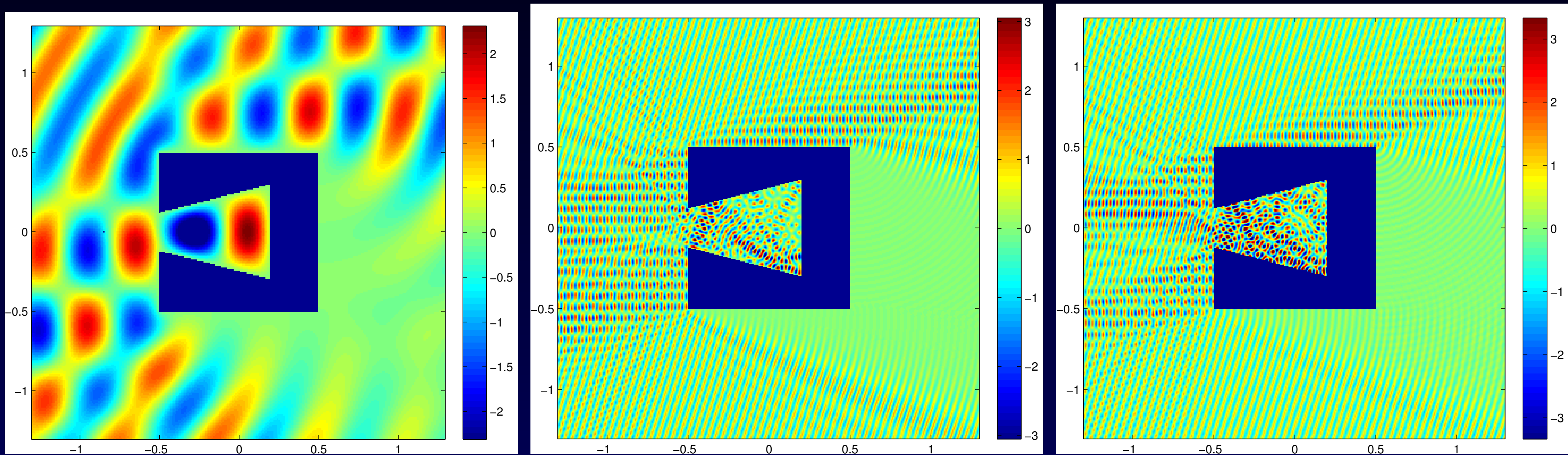
- we would like to prove this!

- A is ill-conditioned, but least-squares solvers backwards stable

$\Rightarrow$ accuracy can approach machine precision if $|\mathbf{c}| = O(1)$

goal: *keep coeff norm $|\mathbf{c}|$ small, e.g. by careful choice of charge curve*

Results: resonant cavity



Dirichlet $u = 0$ Neumann $u_n = 0$

$24\ \lambda$ $N = 1933$ $t = 10^{-7}$ 35 sec

- Neumann hard to handle with integral equations (hypersingular T)
- here simply switch sin to cos in corner expansions
- but, no series expansion known for dielectric corners, …

PART III: Software (teaser)

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`MPSpack`: object-oriented 2D PDE toolbox in MATLAB (B-Betcke '09)

- implements above methods & more: Helmholtz, Laplace, scattering
- intuitive interface: curves, domains, basis sets, problems, are objects

E.g.

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s=segment.radialfunc(100,{@(q)1+.3*cos(3*q),@(q)-.9*sin(3*q)})
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piecewise analytic curves

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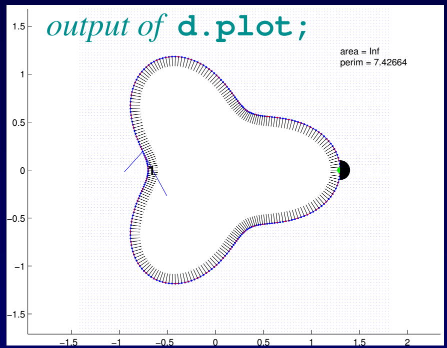


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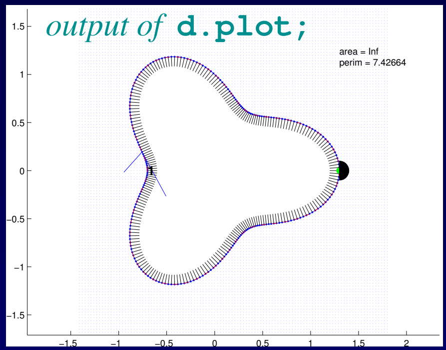


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d.setbc(1, 'N', []);
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Neumann BCs on exterior

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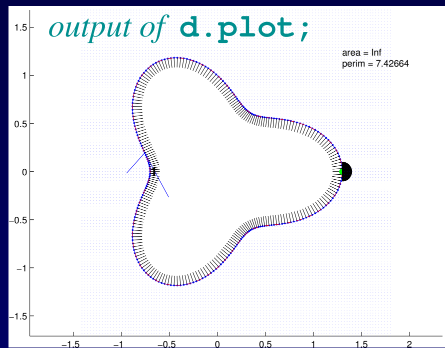


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choose basis set for solution

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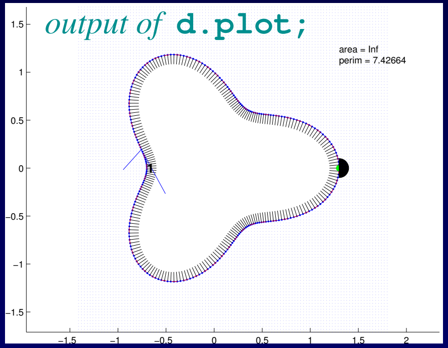

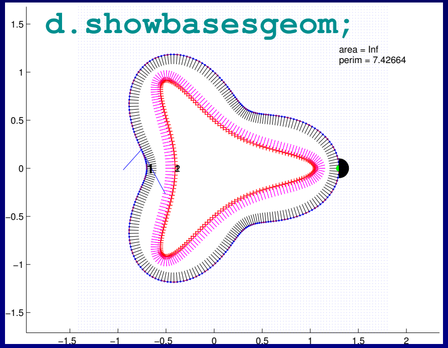


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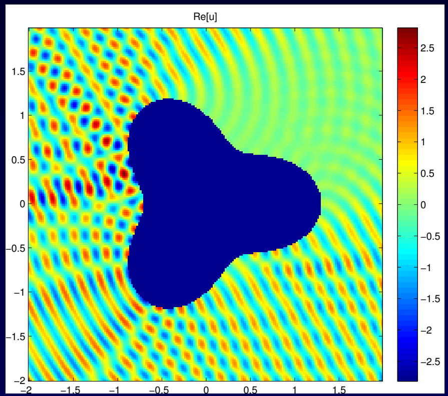
p.showfullfield(struct('bb',[-2 2 -2 2]));
```



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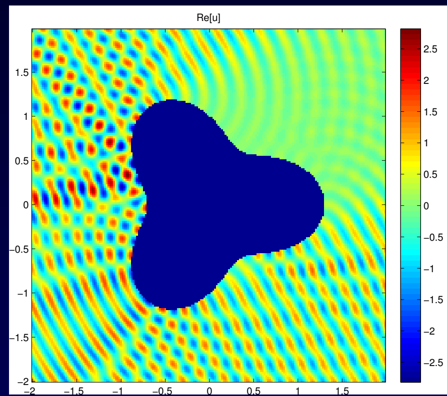

- was easy case: 8 lines (could have done in 80 lines of MATLAB)
- multiple (sub)domains: basis, quadrature, bookkeeping hidden
  - e.g. square scattering still only 20 lines of code
- human-readable, rapid to code, sensible defaults (you can change)

To do: automatic meshing, GUI, Dirichlet eigenvalue problem...

Dirichlet eigenvalue prob:

$$(\Delta + \omega_j^2) u_j = 0, \quad u_j|_{\partial\Omega} = 0$$

Scaling method:

- fastest by factor 10^3

(star-shaped domains)

(Vergini ’94, B ’00)

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- High-freq. asymptotic study of Ω with chaotic ray dynamics (B '06)

shown: mode numbers $j = 1, 10, 10^2, 10^3, 10^4, 10^5$

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Notices

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Volume 55, Number 1

Quantum chaos (see page 41)

Conclusions

Theme: spectral representations $\rightarrow$ fast and accurate wave modeling

- photonic crystals: periodize robustly, 2nd kind integral equations
- scattering: corner-adapted expansions, great for low-to-medium freqs
- `MPSpack` software makes 2D problems simple to set up and solve

Future:

Use wall densities to periodize scattering problems
Extend to 3D (easy-ish for photonic crystals, hard for corners)

code:
http://code.google.com/p/mpspack

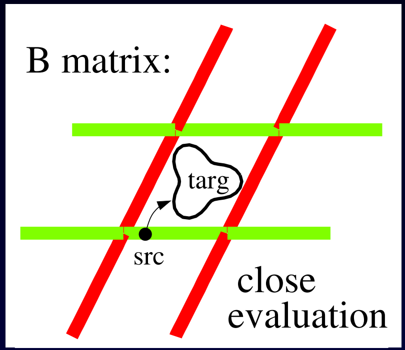
funding: NSF DMS-0507614
DMS-0811005

Preprints, talks, movies:
http://math.dartmouth.edu/~ahb

made with: Linux, LaTeX, `Prosper`

EXTRA SLIDES

Large inclusion passing through unit cell



As dist$(\Omega, \partial U) \to 0$ standard quadrature v. poor

- fix via adaptive quadrature of Lagrange interpolant?
- faster: project wall densities onto J-expansion using Graf addition thm (needs $N{=}35$ per wall)

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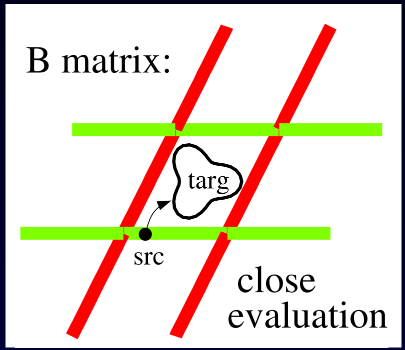

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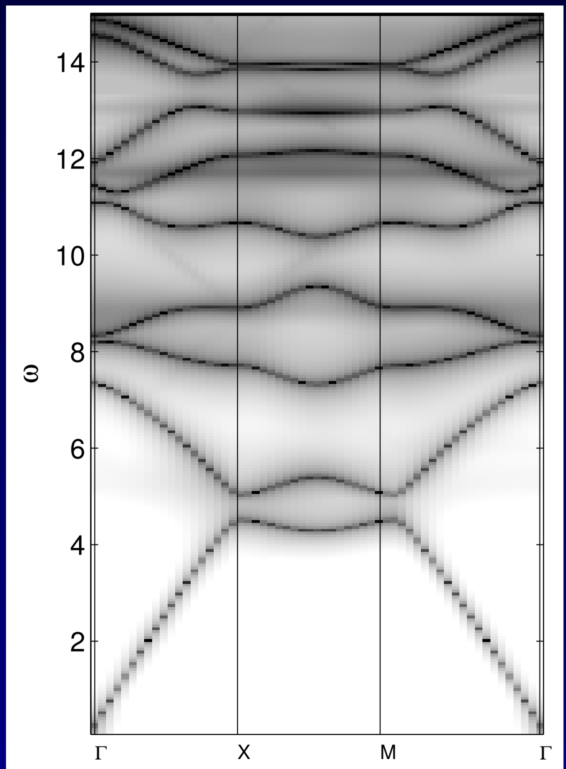
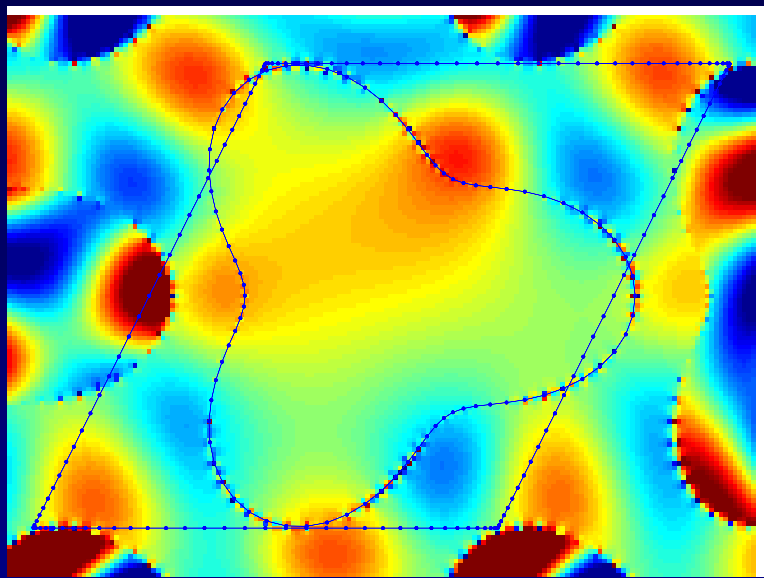


Amazingly (due to far singularities), J-exp analytically continues the field to outside U:



$\omega = 4.47$

$\mathbf{k} \approx (0.17, 2.11)$

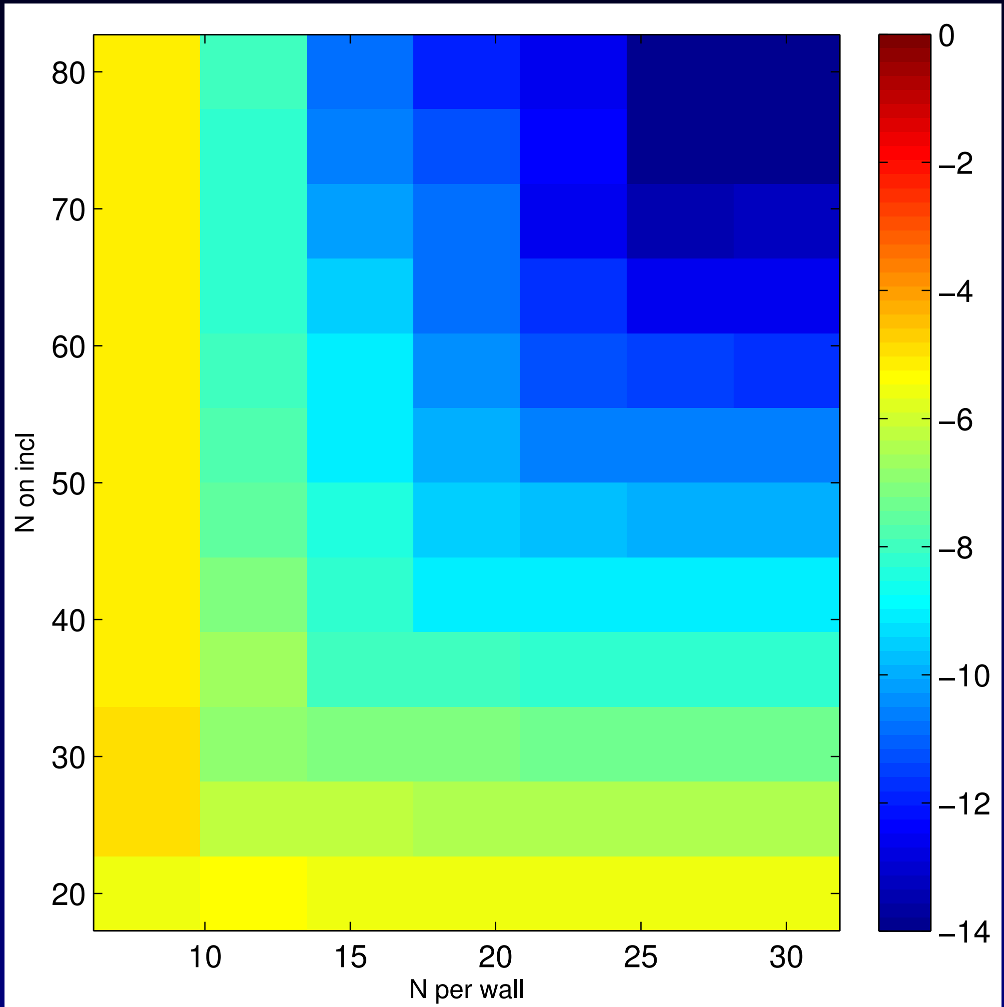
$n{=}1$ inside

$n{=}3.3$ outside

movie

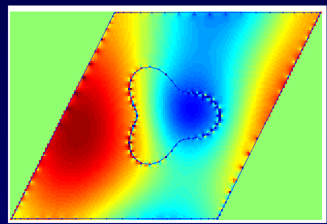
Error convergence

$\log_{10}$ min sing. val M for known Bloch eigenvalue (should be zero):



Note: is eigenvalue error up to $O(1)$ const

$\omega = 5, \mathbf{k} = (-0.39\cdots, 2.08\cdots)$

mode: 

- spectral (exponential) convergence: error $\sim e^{-cN}$

Avoiding the root search

Holding ω constant, can rapidly explore the slice (ω, α, β):

operator (hence matrix) M is of the form $\sum_{m,n=-2}^{1} \alpha^m \beta^n M_{mn}$

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- pre-store coeffs M_{nm} for quick filling of M at any (α, β)
- fix ω, β so get a cubic (polynomial) eigenvalue problem in α
  – only eigenvalues with $|\alpha| = 1$ are traveling Bloch waves
  – can be turned into $3N$-by-$3N$ dense generalized EVP (slow)
  – could use iterative methods since only couple eigvals wanted
  – similar linearizations known (Yuan '08, Dossou '06)

Hope: find an approximate linearization in ω, as in scaling method ?