Spectrally accurate Fourier methods in problems of wave propagation in inhomogeneous media

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Introduction

Problems of interest:

- Photonic crystals
- Optical fibers
- Volumetric scattering (radar and such ...)

Difficulties and accuracy requirements:

- Highly oscillatory fields
- Jumps of the field derivatives
- Wide range of field intensities
- Small band-gaps (photonic crystals)
- Convergence studies

Need fast, high-order accurate algorithms!

Promising numerical techniques

Fourier series and Fast Fourier transform (FFT)

- Fast ($\mathcal{O}(nlogn)$)
- High order convergence for smooth periodic functions

Tchebyshev polynomials

- Fast (can be implemented using FFT's)
- High order convergence for non periodic functions

Non-uniform Fast Fourier transforms

- ... for interpolation to/from non-Cartesian grids
- Asymptotically fast (can be implemented using FFT's)
- High order accuracy for smooth periodic functions

Problems of Interest I: Volumetric Acoustic Scattering

A wave $u^{inc}(x)$ with the wave number k propagates through inhomogeneous media with the density $\varepsilon(x) = 1 - m(x)$. The field $u(x) = u^{scat} + u^{inc})$ satisfies the equation

$$-\Delta u(x) + k^2 \varepsilon(x) u(x) = 0$$

or

$$-\Delta u^{scat} + k^2 u^{scat} = k^2 m(x)[u^{scat} + u^{inc}]$$

subject to the radiation boundary conditions

$$\lim_{r\to\infty} \sqrt{r}\left[\frac{\partial u^{scat}}{\partial r} - iku^{scat}(x)\right] = 0, \qquad r = |x|$$

Equivalently, $u(x)$ satisfies the Lippmann-Schwinger integral equation:

$$u^{scat} = -k^2 \left(m(x)(u^{scat} + u^{inc})\right) * \Phi$$

where $\Phi(x, y)$ is the free-space Green function

$$\Phi(x, y) = \frac{i}{4} H_0^{(1)}(k|x - y|)$$

Iterative Solution of the Scattering Problem

Solve for u^{scat} by iterating

$$\left(-\Delta + k^2\right) u^{(j)} = k^2 m(x)[u^{(j-1)} + u^{inc}]$$

or

$$u^{(j)} = -k^2 \left[m(x)(u^{(j-1)} + u^{inc})\right] * \Phi$$

Each iteration is equivalent to solving the Helmholtz equation

$$Hu^{(j)} = \left(-\Delta + k^2\right) u^{(j)} = f(x)$$

(Usually more advanced iterative techniques are used. However, they still require solution of the Helmholtz equation).

The Helmholtz equation is frequently solved by convolution with Φ, which can be computed fast using the Fast Fourier transform.

Problem: The Green's function $\Phi(x, y)$ has a logarithmic singularity when $x = y$. In order to achieve high-order accuracy one has to resort to sophisticated numerical techniques.

The simplest Helmholtz solver

1. Expand $f(x)$ in the Fourier series.
2. Find a periodic solution $u^*(x)$ to the Helmholtz equation

$$Hu^*(x) = f(x)$$

   by dividing the Fourier coefficients $C_{\mathbf{n}}$ by $k^2 + \mathbf{n}^2$.
3. Outside of support of $m(x)$ multiply $u^*(x)$ by C_0^∞ function $\eta(x)$ vanishing toward the boundaries of the computational domain.
4. Compute $g(x) = f(x) - Hu_1(x), \quad u_1(x) = \eta(x)u^*(x)$
5. Solve for $u_2(x)$ subject to the radiation boundary conditions

$$Hu_2(x) = g(x)$$

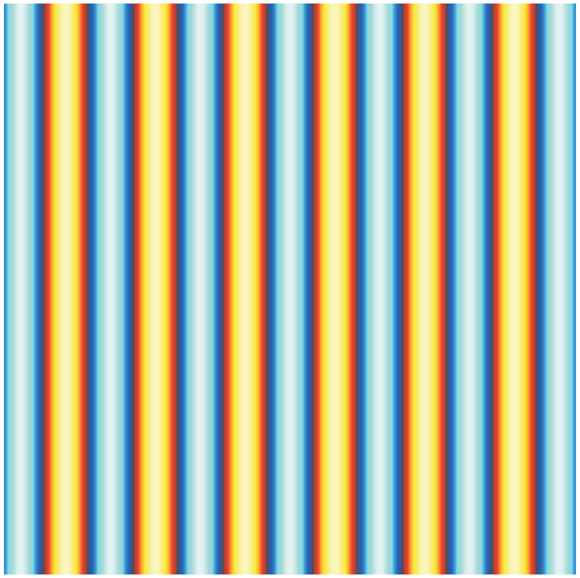
   by convolving the right hand side $g(x)$ with $\Phi(x, y)$.
6. Compute $u(x) = u_1(x) + u_2(x)$

   Since $F(x)$ is equal to zero within the support of $m(x)$ where the convolution needs to be computed, there is no problem with the singularity.

   The algorithm is spectrally accurate for smooth $\varepsilon(x)$!

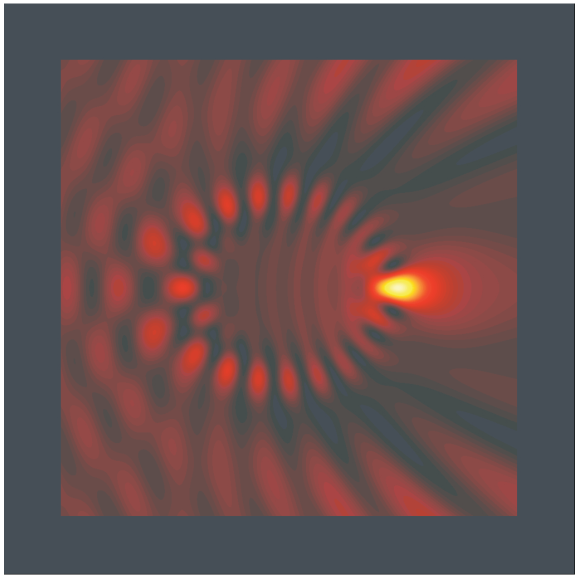
Scattering from a smooth inhomogeneity

Incoming wave



$\varepsilon(x)$

Total field (intensity)



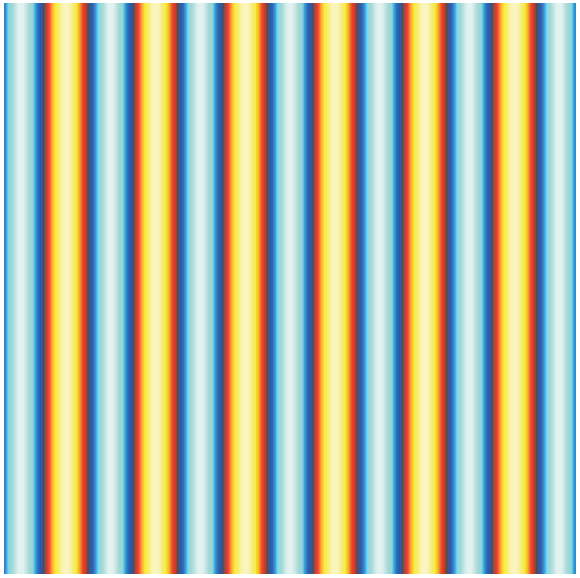
Convergence study:

Maximum error in the far field magnitude

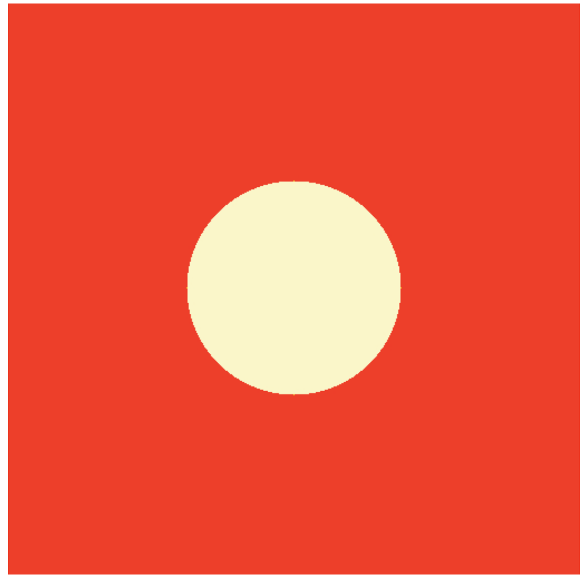
Grid size	Error
256×256	$2 \cdot 10^{-4}$
512×512	$5.7 \cdot 10^{-6}$
1024×1024	$1.2 \cdot 10^{-8}$

Scattering from a round lense

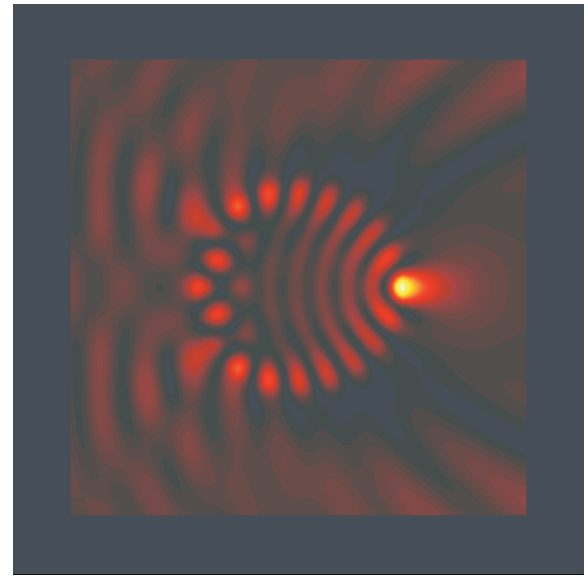
Incoming wave



$\varepsilon(x)$



Total field (intensity)



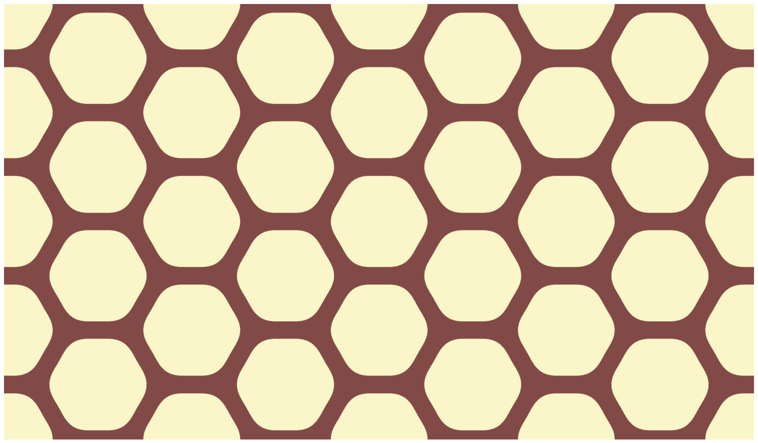
Convergence study:

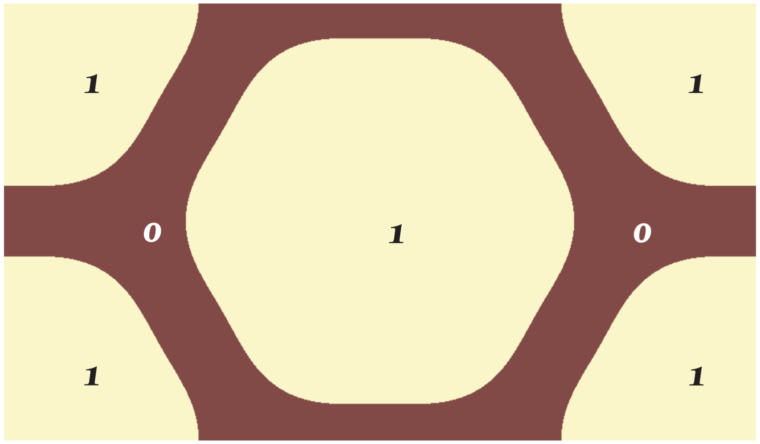
Maximum error in the far field magnitude

Grid size	Error
256×256	**0.17**
512×512	**0.057**
1024×1024	**0.019**

Problems of Interest II: Photonics

Periodic structures are obtained by infinite replication of the fundamental cell





Photonic gaps arise due to the sharp material interfaces

Photonics: Governing equations

Eigenvalue problem for the Poisson equation (TE polarization):

$$-\frac{1}{\varepsilon(x)}\Delta u(x) = \lambda u(x)$$

Eigenvalue problem for the divergence equation (TM polarization):

$$-\mathrm{div}\left(\frac{1}{\varepsilon(x)}\nabla u(x)\right) = \lambda u(x)$$

subject to quasi-periodic boundary conditions (Floquet-Bloch theory):

$$u(1, x_2) = u(0, x_2)e^{ik_1}, \quad u(x_1, 1) = u(x_1, 0)e^{ik_2}$$

The complete spectrum of the photonic crystal is obtained as the union of sets of eigenvalues of the both eigenvalue problems for all values of quasi-momenta

$$(k_1, k_2) \in [0, \pi] \times [0, \pi].$$

Problems of Interest III: Optical fibers

One of the simplest models:

$$-\Delta u(x) + k^2(1 - m(x))u(x) = \beta^2 u(x)$$

or

$$-\Delta u(x) + \left(k^2 - \beta^2\right) u(x) = k^2 m(x) u(x)$$

subject to the radiation boundary conditions.

Also an eigenvalue problem !!!

Methods for solving eigenvalue problems

Inverse power method: to find the smallest eigenvalue λ_0 of the problem

$$Au = \lambda u$$

iterate

$$u^{(k+1)} = A^{-1}u^{(k)}/||A^{-1}u^{(k)}||.$$

Then

$$u^{(k+1)} \longrightarrow u_0, \qquad ||A^{-1}u^{(k)}|| \longrightarrow \lambda_0$$

Krylov subspace methods are based on computing the sequence
$\{A^{-1}u^{(0)}, \left(A^{-1}\right)^2 u^{(0)}, \left(A^{-1}\right)^3 u^{(0)}, ...\}$.
They are very efficient in finding several lower eigenvalues.

Computation of $A^{-1}f$ is equivalent to the solution of the equation

$$Au = f$$

Our problems require solution of the Poisson, Helmholtz, or divergence equations with the radiation or periodic boundary conditions.

The main algorithm

The main building block is the solution of the following problem:

Find function $u(x)$ satisfying the Poisson equation on sub-domains:

$$-\frac{1}{\varepsilon_j}\Delta u_j(x) = f_j(x) \quad x \in \Omega_j$$

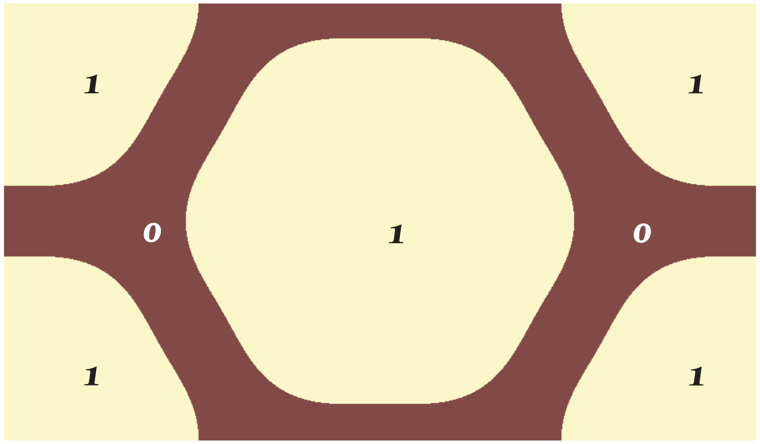
with prescribed jump conditions on the boundaries of material interfaces
and evaluate it at all nodes of computational grids.

Example #1 Find a smooth solution of the Poisson equation.

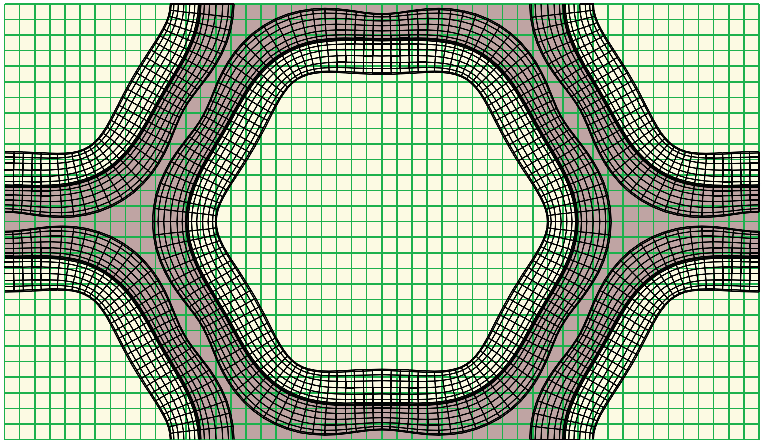
Example #2 Evaluate double- or -single layer potential

First step: Solving around interfaces

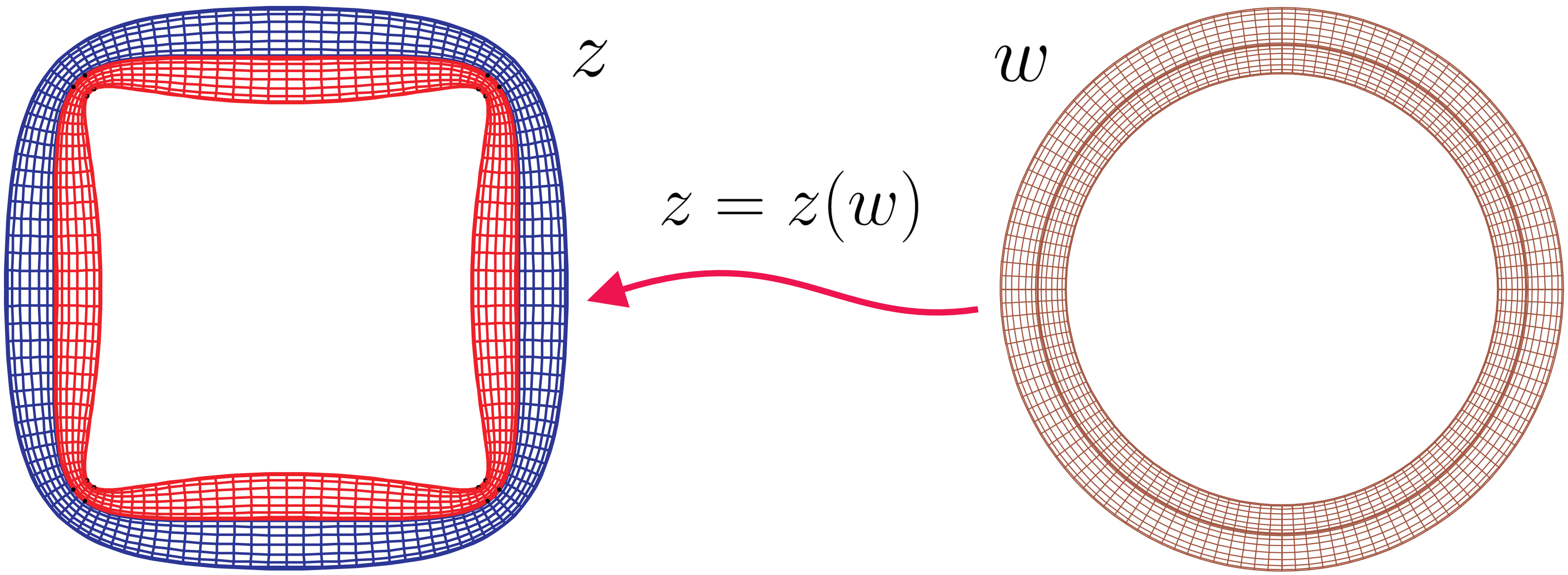
Fundamental cell



Introduce conforming grids overlapping with the Cartesian grid



Reduction to an annular domain



Equation

$$\Delta u(z) = f(z)$$

under conformal change of variable

$$v(w) = u(z(w)), \quad z = z(w),$$

transforms to

$$\Delta v(w) = |z'(w)|^2 \Delta_z u = f(w)|z'(w)|^2$$

Solving Poisson equation in the annuli

$$\Delta v(r,\theta) = f(r,\theta)$$

Expand in Fourier series in θ:

$$v(r,\theta) = \sum v_k(r)e^{ik\theta}, \qquad f(r,\theta) = \sum f_k(r)e^{ik\theta}$$

Laplacian in polar coordinates reduces to Bessel's eqation:

$$\left[\frac{\partial}{\partial}\left(r\frac{\partial}{\partial r}\right) - \frac{k^2}{r}\right] v_k(r) = r f_k(r)$$

Integrate twice:

$$v_n(r) - \int\limits_a^r \frac{1}{r'}\left[\int\limits_a^{r'} \frac{k^2}{r''} v_k(r'')dr''\right] dr' = \int\limits_a^r \left[\frac{1}{r'}\int\limits_a^{r'} r'' f_k(r'')dr''\right] dr'$$

Volterra style equation, well-posed problem, ideally suited for iterative solution

Solving the problem in the whole domain

1. Find a solution $u_1^*(x)$ in thin subdomains around interfaces, so that

$$\Delta u_1^*(x) = f(x) \quad \text{within the subdomains}$$

2. Glue solutions across interfaces by adding harmonic $w(x)$

$$u_1^{**}(x) = u_1^*(x) + w(x)$$

3. Multiply by a C_0^∞ function $\eta(x)$

$$u_1(x) = \eta(x) u_1^{**}(x),$$

so that

$$\Delta u_1(x) = f(x) \quad \text{around interfaces}$$

4. Solve for $u_2(x)$ subject to (quasi)periodic BC

$$\Delta u_2(x) = f(x) - \Delta u_1(x)$$

5. And the solution is ....

$$u(x) = u_1(x) + u_2(x)$$

since

$$\Delta(u_2(x) + u_1(x)) = [f(x) - \Delta u_1(x)] + \Delta u_1(x) = f(x)$$

Divergence equation, piece-wise constant case

In order to find solution $v(x)$ of the divergence equation, solve

$$-\Delta v_0(x) = \varepsilon(x)g(x)$$

The difference $h(x) = v(x) - v_0(x)$ is a harmonic function on subdomains. It can be represented by the single-layer potential

$$h(x) = \int_\Gamma \varphi(x'(s))G(x'(s), x)ds.$$

Jumps of the potential:

$$\begin{aligned} &\lim_{\delta\to 0} \frac{\partial}{\partial n} h(x+\delta n) = -\frac{1}{2}\varphi(x) + \int_\Gamma \varphi(x'(s)) \frac{\partial}{\partial n} G(x'(s), x)ds, \\ &\lim_{\delta\to 0} \frac{\partial}{\partial n} h(x-\delta n) = \frac{1}{2}\varphi(x) + \int_\Gamma \varphi(x'(s)) \frac{\partial}{\partial n} G(x'(s), x)ds, \qquad x \in \Gamma. \end{aligned}$$

To find $\varphi(x)$ solve

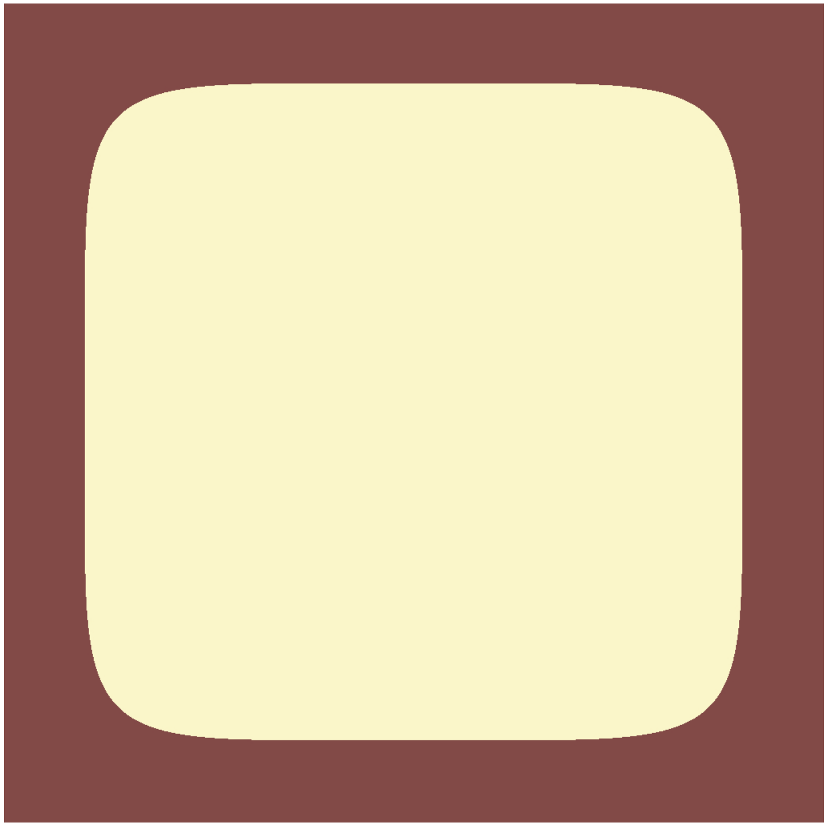
$$-\frac{1}{2}\left(\frac{1}{\varepsilon(x+0n)} + \frac{1}{\varepsilon(x-0n)}\right)\varphi(x) + \left(\frac{1}{\varepsilon(x+0n)} - \frac{1}{\varepsilon(x-0n)}\right)\int_\Gamma ...ds = F(x)$$

where

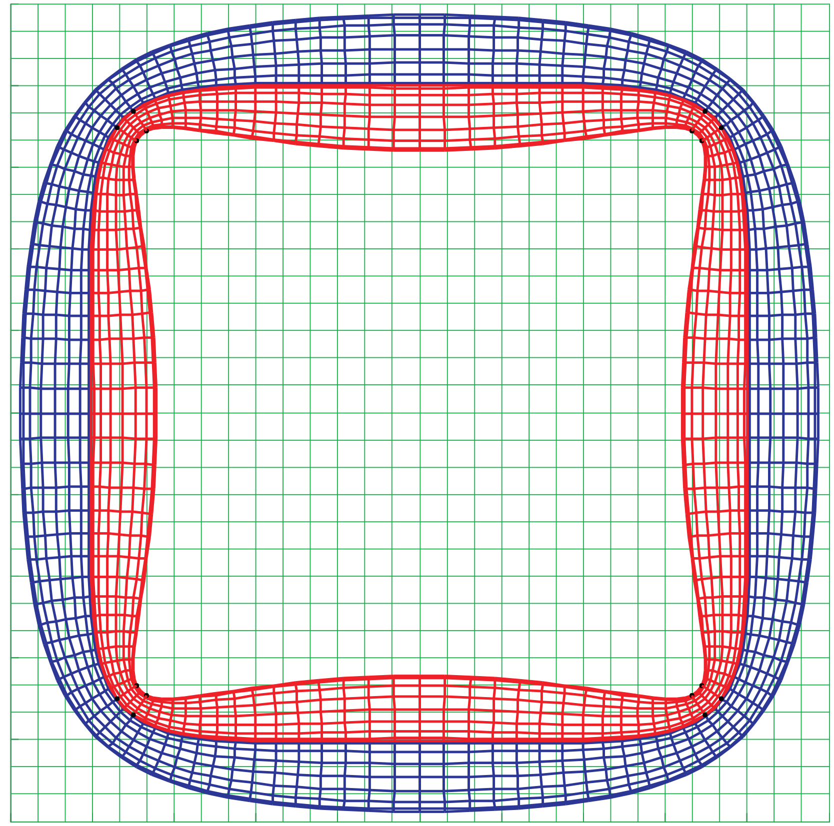
$$F(x) = -\lim_{\delta\to 0}\left(\frac{1}{\varepsilon(x+\delta n)}\frac{\partial}{\partial n}v_0(x+\delta n) - \frac{1}{\varepsilon(x-\delta n)}\frac{\partial}{\partial n}v_0(x-\delta n)\right) \qquad x \in \Gamma,$$

Accuracy checks and convergence studies

An almost-square structure, $\varepsilon(x) = \varepsilon_0$

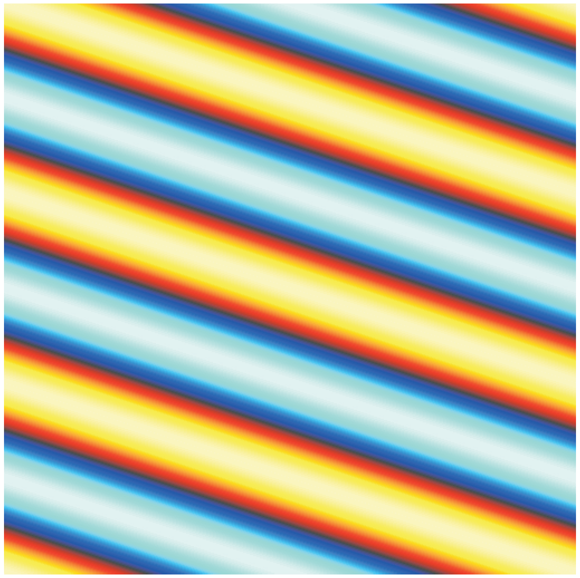


(a)

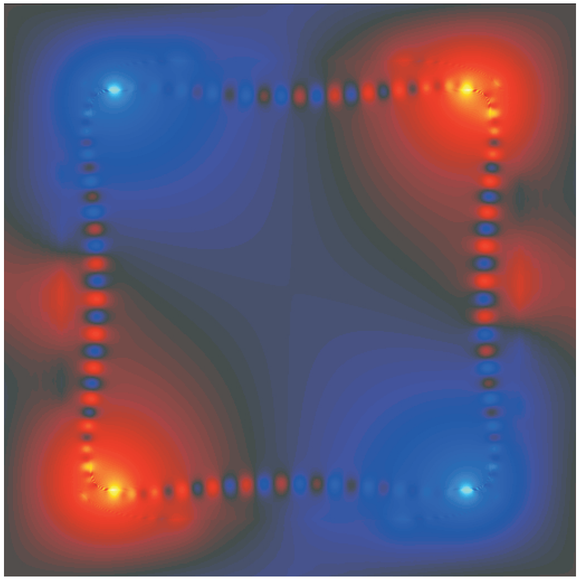


(b)

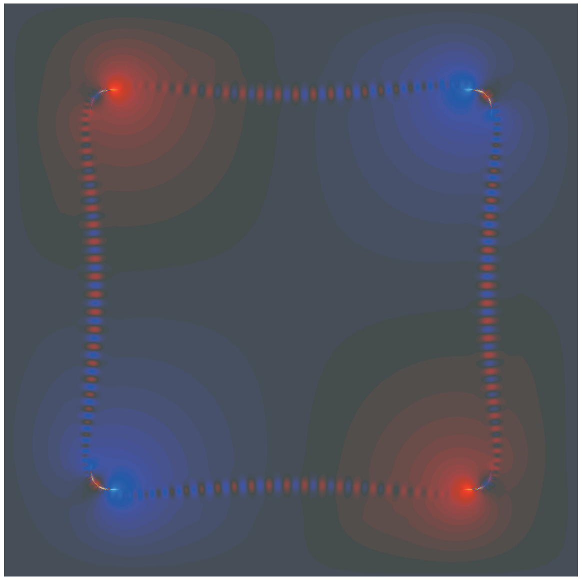
Solving Poisson equation, $\varepsilon(x) = \varepsilon_0$



Right-hand side
=
Exact solution



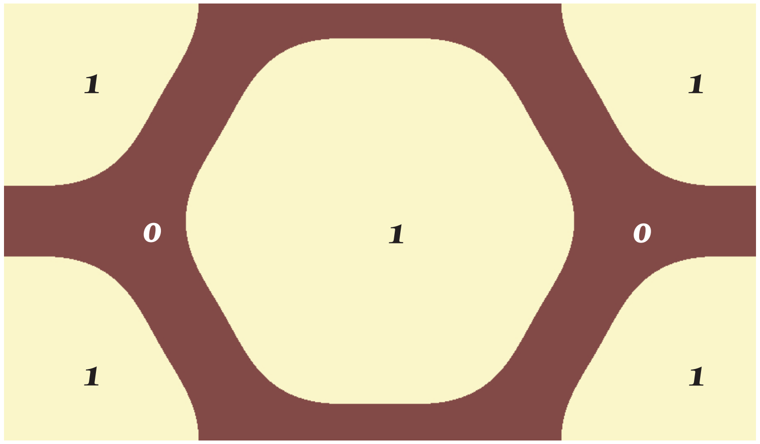
Error in solution
on 512×512 grid
Error $< 4.7 \cdot 10^{-5}$



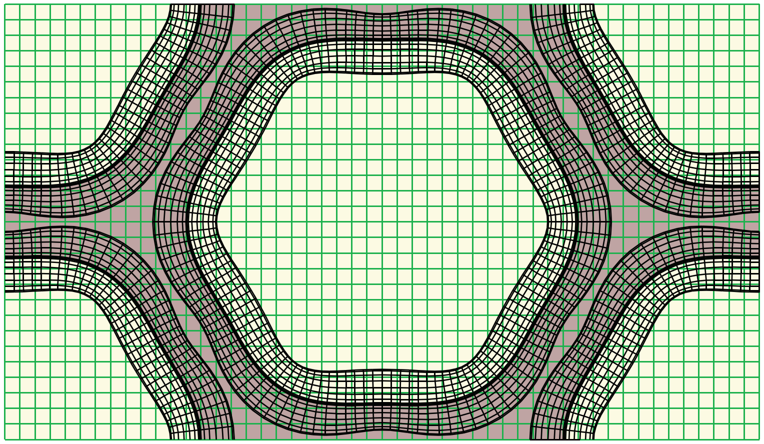
Error in solution
on 1024×1024 grid
Error $< 6.4 \cdot 10^{-10}$

Hexagonal structure

Fundamental cell



Grids



Eigenvalue problem for Poisson eq-n; convergence study

When $\varepsilon_0 = \varepsilon_1 = \pi^2$, the exact eigenvalues are integers $l^2 + 3m^2$. Pink highlights incorrect digits.

Eig #	Grid 256×448	Grid 360×648	Grid 512×896	Exact
1	0.0000000000000	0.0000000000000	0.0000000000000	0.0
2	0.9999999980087	0.9999999999813	0.9999999999998	1.0
3	1.0000000011731	1.0000000000011	0.9999999999998	1.0
4	2.9999999933818	3.0000000000414	2.9999999999957	3.0
5	3.0000000032706	3.0000000001951	3.0000000000001	3.0
6	3.9999999855360	3.9999999999274	3.9999999999891	4.0
7	3.9999999918374	3.9999999999974	3.9999999999979	4.0
8	4.0000000003077	4.0000000000054	3.9999999999982	4.0
9	4.0000000012973	4.0000000000167	3.9999999999983	4.0
10	4.0000000014669	4.0000000000699	3.9999999999999	4.0
11	4.0000000038250	4.0000000006347	4.0000000000001	4.0
12	6.9999999976126	6.9999999995311	6.9999999999973	7.0
13	7.0000000015684	6.9999999999895	6.9999999999984	7.0
14	7.0000000043222	6.9999999999953	7.0000000000023	7.0
15	7.0000000188245	7.0000000000194	7.0000000000055	7.0
16	8.9999999878827	8.9999999999085	8.9999999999921	9.0
17	8.9999999897990	9.0000000006835	8.9999999999980	9.0
18	11.9999999663406	11.9999999997943	11.9999999999852	12.0
19	11.9999999725875	11.9999999999910	11.9999999999857	12.0
20	11.9999999901527	11.9999999999936	11.9999999999892	12.0
21	12.0000000028481	11.9999999999986	11.9999999999989	12.0
22	12.0000000122244	12.0000000002511	11.9999999999998	12.0
23	12.0000000122387	12.0000000009899	12.0000000000009	12.0
24	12.9999999810157	12.9999999999757	12.9999999999786	13.0
25	12.9999999884013	13.0000000000019	12.9999999999858	13.0

Poisson equation; convergence study

$$\varepsilon_0 = 10, \quad \varepsilon_1 = 1$$

The accuracy is estimated by comparison with the last column.

Eig #	Grid 256×448	Grid 360×648	Grid 512×896	Grid 720×1296
1	0.0000000000000	0.0000000000000	0.0000000000000	0.0000000000000
2	1.8627946671758	1.8627946701743	1.8627946702077	1.8627946702090
3	2.6448743873941	2.6448743855294	2.6448743854103	2.6448743854153
4	5.3319077431592	5.3319077419544	5.3319077419620	5.3319077419626
5	6.5923933810198	6.5923933763970	6.5923933763512	6.5923933763492
6	6.9651096538640	6.9651096794944	6.9651096794805	6.9651096795023
7	6.9651096833625	6.9651096812038	6.9651096795080	6.9651096795149
8	8.5093161533517	8.5093161273396	8.5093161279372	8.5093161279301
9	11.6581467835013	11.6581467039362	11.6581467039542	11.6581467039584
10	14.7168652095953	14.7168652727793	14.7168652729969	14.7168652730249
11	14.7168653051258	14.7168652734616	14.7168652730229	14.7168652730319
12	15.0007420113235	15.0007423207952	15.0007422987149	15.0007422981166
13	15.6247295235227	15.6247294783675	15.6247294783469	15.6247294783366
14	17.2913522447176	17.2913522269694	17.2913522234990	17.2913522235487
15	20.4524226803744	20.4524226945979	20.4524226946617	20.4524226946761
16	23.8215095663657	23.8215073077432	23.8215073056977	23.8215073057745
17	23.8784037737822	23.8784035788934	23.8784035773945	23.8784035774149
18	24.2961079262918	24.2961068953961	24.2961069628187	24.2961069646527
19	26.3074340464543	26.3074338363974	26.3074338377855	26.3074338377806
20	26.3074341020334	26.3074338375519	26.3074338377913	26.3074338377832
21	26.4806307232110	26.4806320949416	26.4806320956537	26.4806320957007
22	26.4806346818460	26.4806320986140	26.4806320957384	26.4806320957903
23	30.7991239547820	30.7991245850027	30.7991245853872	30.7991245854037
24	31.6258862976232	31.6258847207720	31.6258847208370	31.6258847208477
25	33.1285628299182	33.1285603901680	33.1285603873808	33.1285603874728

Divergence eq-n; convergence study

$$\varepsilon_0 = 10, \quad \varepsilon_1 = 1$$

In the table below the accuracy of computed eigenvalues is estimated by comparison with the last, most accurate column. The incorrect decimal places are highlighted by pink background.

Eig #	Grid 256 × 448	Grid 360 × 648	Grid 512 × 896	Grid 720 × 1296
1	0.0000000000000	0.0000000000000	0.0000000000000	0.0000000000000
2	2.1731174774192	2.1731187717163	2.1731187554192	2.1731187558991
3	6.8731048645056	6.8731057488855	6.8731058162982	6.8731058252217
4	12.3530050269053	12.3530148593262	12.3530147946306	12.3530147911515
5	12.4494677485520	12.4494684161349	12.4494684096257	12.4494684153581
6	12.9024679473623	12.9024693423057	12.9024693592060	12.9024693609620
7	15.1401173590018	15.1401364387912	15.1401370610179	15.1401370875472
8	15.1401301295557	15.1401370381847	15.1401370904606	15.1401370878992
9	17.3007546432239	17.3007538200413	17.3007537726319	17.3007537722860
10	17.7283401544538	17.7283382016667	17.7283383112427	17.7283383120929
11	17.7283513595176	17.7283388323950	17.7283383140630	17.7283383125987
12	19.6158901501799	19.6158909798907	19.6158910436875	19.6158910468127
13	23.7382433148613	23.7382388591566	23.7382384636753	23.7382384672381
14	25.6831858514213	25.6831865558878	25.6831868284518	25.6831868265801
15	27.2531989891292	27.2532150213182	27.2532149359520	27.2532149390233
16	29.3567730277499	29.3567789168132	29.3567789643385	29.3567789669999
17	30.0286018522408	30.0286040246721	30.0286039871221	30.0286039910703
18	30.8795095625380	30.8795125145484	30.8795125222064	30.8795125231751
19	30.8795106371952	30.8795125171392	30.8795125234805	30.8795125235263
20	32.2590029578916	32.2589921087838	32.2589918118383	32.2589918147145
21	37.0770671964050	37.0770662275087	37.0770661914075	37.0770661849947