MPSpack tutorial

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Abstract

This tutorial shows how a variety of two-dimensional Laplace and Helmholtz boundary-value problems may be numerically solved simply and accurately with the MPSpack toolbox for MATLAB. We assume basic familiarity with MATLAB and with partial differential equations.

1 About this tutorial

This tutorial is designed for 'bottom-up' learning of the features of MPSpack, i.e. by progressing through simple examples. In that sense it complements the user manual which describes the theoretical framework in broad strokes and therefore could be considered 'top-down'. We will skip most of the mathematics behind the techniques, focusing on computing and plotting useful PDE solutions. We hope you will try each command as you read!

Throughout we will identify the plane \mathbb{R}^2 with the complex plane \mathbb{C} , by the usual map z=x+iy. In other words (2,3) and 2+3i represent the same point. We use teletype font to designate commands that may be typed at the MATLAB prompt. You may get help on any MPSpack command by typing help command. All the code examples in this document, including code to generate the figures, is found in the examples/ directory. The codes for Sections 2-7 are named tut_*.m according to the section names in tutorial.tex.

2 Solving Laplace's equation in a disc

We start by setting up a domain in \mathbb{R}^2 . Domains are built from segments which define their boundary. To make the unit disc domain, we first need a

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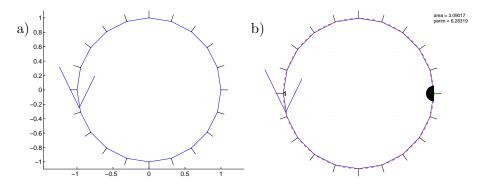


Figure 1: a) circular closed segment, b) unit disc domain. Both have a periodic trapezoidal quadrature rule with M=20 quadrature points

circle segment with center 0, radius 1, and angle range $[0, 2\pi)$, as follows,

The object s is indeed a circular segment, as we may check by typing s.plot, producing Fig. 1a. All segments have a natural *sense*, i.e. direction of travel: for this segment it is counter-clockwise, as shown by the downwards-pointing arrow symbol overlayed onto the segment at about 9 o'clock.¹ Notice also normal vectors (short 'hairs') pointing outwards at each boundary point; our definition is that normals on a segment always point to the *right* when traversing the sense of the segment.

We create the domain interior to this segment with

d = domain(s, +1)

where the second argument (here +1, the only other option being -1) specifies that the domain is to the 'standard' side of the segment, which we take to be such that the normals point away from the domain. That is, with +1 the domain lies to the left of the segment when traversed in its correct sense (with -1 the domain would lie to the right of the segment.) Typing $\mathtt{d.plot}$ produces² Fig. 1b. Note that perimeter and area are automatically labelled (these are only rough approximations intended for sanity checks).

Laplace's equation $\Delta u = 0$ is Helmholtz's equation with wavenumber zero, which we set for this domain with,

$$d.k = 0;$$

¹In fact, segments are parametrized internally as function z(t) of a real variable $t \in [0, 1]$, and the sense is the direction of increasing t. Segment s stores this function as s.Z.

²There are extra plotting options and features that are described in documentation such as help domain.plot. E.g. in this figure a grid of points interior to the domain has been included, achieved with opts.gridinside=0.05; d.plot(opts);

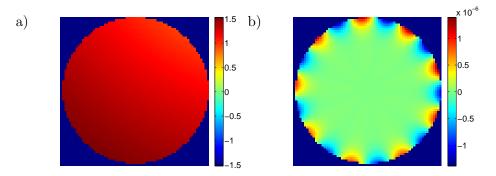


Figure 2: a) Numerical solution field u, b) pointwise error u-f, for Laplace's equation in the unit disc with M=20 quadrature points and 8th-order harmonic polynomials.

If the problem has many domains the wavenumber should be set globally using the method problem.setoverallwavenumber. Our philosophy is to approximate the solution in the domain by a linear combination of basis functions, each defined over the whole domain. We choose 8th-order harmonic polynomials $u(z) = \sum_{n=0}^{8} c_n \operatorname{Re} z^n + \sum_{n=1}^{8} c_{-n} \operatorname{Im} z^n$, where $\mathbf{c} := \{c_n\}_{n=-8}^8 \in \mathbb{R}^{17}$ is a coefficient vector, based at the origin 0, using the command

d.addregfbbasis(0, 8);

Let's specify Dirichlet boundary data $f(z) = \ln|z - 2 - 3i|$ for z on the segment³ by representing this as an anonymous function f and associating it with one side of the segment,

```
f = @(z) log(abs(z-2-3i));
s.setbc(-1, 'd', [], @(t) f(s.Z(t)));
```

Note that we needed to pass in a function not of location z, but of the segment parameter t; this was achieved by wrapping \mathbf{f} around the parametrization function $\mathbf{s}.\mathbf{Z}$. The first argument -1 expresses that the boundary condition is to be understood in the limit approaching from the side *opposite* the segment's normal direction, which is where the domain is located. The second argument 'd' specifies that the data is Dirichlet.

Finally we use the domain to make a boundary-value problem object p, p = bvp(d);

and may then solve (in the least-squares sense) a linear system for the coef-

³In other words, $f(x,y) = \ln \sqrt{(x-2)^2 + (y-3)^2}$ for points (x,y) on the boundary.

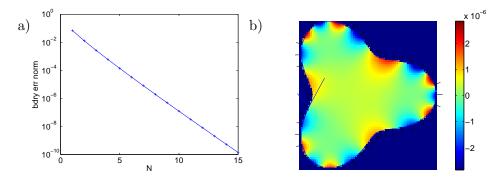


Figure 3: a) Convergence of boundary error L^2 norm for harmonic polynomials for Laplace equation in the unit disc, b) solution error for same boundary data f in a smooth star-shaped 'trefoil' domain (normals also shown).

ficients

p.solvecoeffs;

If it is needed, p.co now contains the coefficients vector c. To evaluate and plot the solution we simply use,

p.showsolution;

The software chose an appropriate grid covering the domain (points outside the domain are made transparent, but show up deep blue in this document), giving Fig. 2a.

3 Accuracy, convergence, and smooth domains

How accurate was our numerical solution u? One measure is the L^2 error on the boundary, and is estimated by

p.bcresidualnorm

which returns 2.09×10^{-6} . However, since the function f(z) is already harmonic in the domain, it is in fact the unique solution, and we may plot the pointwise error in u by passing in the analytic solution as an option,

opts.comparefunc = f; p.showsolution(opts); giving Fig. 2b. Note that the color scale is 10^{-8} .

In the above, boundary integrals were approximated using the default of M=20 quadrature points, barely adequate given the oscillatory error function in Fig. 2b. M may be easily changed either by specifying a non-empty first argument in the **segment** constructor above, or for an existing segment

as follows,

s.requadrature(50); p.solvecoeffs; p.bcresidualnorm which now gives 1.98×10^{-6} , not much different than before. Notice that we did not have to redefine the domain d nor the BVP object p.

Exploring the convergence of the boundary error norm with the basis set order needs a simple loop over N,

```
for N=1:15
  p.updateN(N); p.solvecoeffs; r(N) = p.bcresidualnorm;
end
figure; semilogy(r, '+-'); xlabel('N'); ylabel('bdry err norm');
```

As the resulting Fig. 3a shows, the convergence is exponential.⁴ Notice we used updateN to change the basis set degree in a problem (in this simple case it is equivalent to d.bas{1}.N = N;)

Say we want to change the shape of segment s, to a smooth star-shaped 'trefoil' domain expressed as by radius $R(\theta) = 1 + 0.3\cos 3\theta$ as a function of angle $0 \le \theta < 2\pi$. This is achieved by passing a 1-by-2 cell array containing the function R and its derivative $R' = dR/d\theta$ to a variant of the segment constructor,

```
s = segment.radialfunc(50, \{@(q) 1 + 0.3*cos(3*q), @(q) -0.9*sin(3*q)\});
```

We again chose M = 50. The analytic formula for R' is needed to compute normal derivatives to high accuracy.

One might ask: has this change to s propagated to the existing domain object d and BVP object p, which both refer to it? In contrast to the case of quadrature point number M above, the answer is no: s is overwritten by a newly-constructed object, while d and p still contain handles pointing to the old s. Furthermore, the fact that the segment had domain d attached to its 'minus' or back side has been forgotten, as have the boundary conditions. (These segment properties are described in the MPSpack user manual.) We must therefore rerun the code from Sec. 2 to construct d and d are a fresh, before solving. The result, plotting the pointwise error as before, is shown by Fig. 3b for d and d and d and d and d solving d and d and d and d and d solving d and d and d and d solving d and d and d and d solving d and d and d solving d

⁴Asymptotically, error $\sim e^{-\alpha N}$. In fact the rate is $\alpha = \ln \sqrt{13}$, related to the conformal distance to the nearest singularity [2], which here is at 2+3i.

⁵Note that in theory it would be possible to change one by one each of the segment properties, t, w, speed, etc, to define the new segment without changing its identity, but this is cumbersome. Similarly, searching and changing all references to a segment in the properties of d and p is cumbersome. Neither has been implemented by us since problem setup time is very rapid.

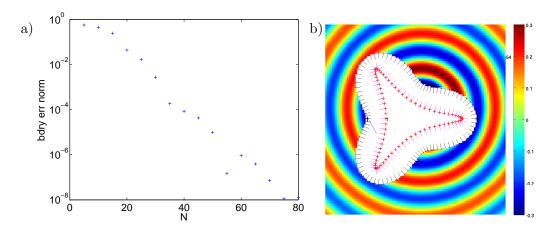


Figure 4: a) Convergence of exterior Helmholtz BVP with MFS basis, b) Domain boundary and MFS charge curve geometry, and (real part of) the solution field outside the domain.

The radialfunc constructor above is limited to radial functions with quadrature equidistant in angle. Instead you may create a segment from arbitrary smooth parametrizations z(t) for $t \in [0,1]$, as long as z'(t) is also given. For instance, a closed crescent-shaped analytic segment is produced (try it!) by,

```
a = 0.2; b = 0.8; w = @(t) \exp(2i*pi*t);

s = \text{segment}(100, \{@(t) w(t)-a./(w(t)+b), ...}

@(t) 2i*pi*w(t).*(1 + a./(w(t) + b).^2)\}, 'p');
```

Note that a convenient variable $w=e^{2\pi it}$ was used via nested anonymous functions. Heed also the new final argument 'p' which enforces periodic quadrature (the constructor doesn't try to guess your preferred rule). In order to get high-order (or spectral) convergence, it is recommended that you choose only smooth (or analytic) z. If periodic quadrature is used, this also applies to the 1-periodic extension of z to the real line. If $z(1) \neq z(0)$, the ends of the segment will not connect up, and the domain constructor above will report an error.

4 Helmholtz equation, exterior and multiply connected domains

Changing from the Laplace to Helmholtz equation is as simple as setting d.k to a positive value. We start a fresh example: an exterior Helmholtz BVP

with Neumann boundary data, and the Sommerfeld radiation condition [3]. This has a unique solution.

The simplest unbounded domain is \mathbb{R}^2 , which is created with

```
d = domain([], []);
```

One may check that its area d.area is ∞ . Exterior domains can be created by excluding from \mathbb{R}^2 a closed segment, for instance the trefoil segment introduced above,

```
tref = segment.radialfunc(100, \{0(q) 1 + 0.3*\cos(3*q), 0(q) -0.9*\sin(3*q)\});
d = domain([], [], tref, -1); % overwrites previous d
```

Note the choice -1 for the direction argument, which states that the domain lies on the 'nonstandard' side of the segment, i.e. to the right side as the segment is traversed in its natural sense, with the segment normals pointing *into* the exterior domain. As before, we set up Dirichlet boundary data corresponding to a known radiative solution (a point source lying in the segment interior),

```
d.k = 10; f = O(z) besselh(0,d.k * abs(z-0.3-0.2i)); tref.setbc(1, 'D', [], O(t) f(tref.Z(t)));
```

A convenient basis set for radiative solutions is a set of fundamental solutions ('MFS basis') with origins \mathbf{y}_j lying on a closed curve interior to the segment. The formula for the jth basis function at location $\mathbf{x} \in \mathbb{R}^2 \setminus \mathbf{y}_j$ is $\Phi(|\mathbf{x} - \mathbf{y}_j|)$, where the fundamental solution for the Helmholtz equation at wavenumber k is $\Phi(\mathbf{x}) = \frac{i}{4}H_0^{(1)}(k|\mathbf{x}|)$. We set this up and plot convergence of boundary error norm,

```
opts.tau = 0.06; d.addmfsbasis(tref, [], opts);
p = bvp(d);
for N=5:5:80,
   p.updateN(N); p.solvecoeffs; r(N) = p.bcresidualnorm;
end
figure; semilogy(r, '+-'); xlabel('N'); ylabel('bdry err norm');
```

This gives the convergence plot Fig. 4a, and executing d.plot; p.showbasesgeom; p.showsolution; gives Fig. 4b. Notice that the MFS charges lie some distance interior to the curve—this is controlled by the opts.tau parameter which makes use of the fact that the segment is specified as an analytic function and hence generates a new curve when the parameter t is displaced

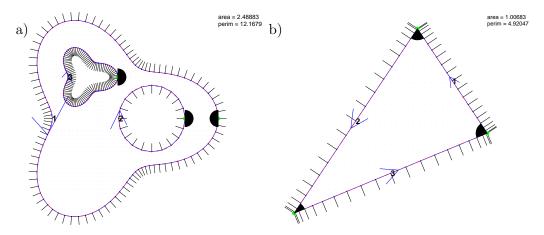


Figure 5: a) A multiply-connected domain. b) A polygonal domain.

by τ in the imaginary direction.⁶ Plotting pointwise error with opts.comparefunc = f; figure; p.showsolution(opts); shows that is it around 10^{-13} .

A non-simply connected domain may be built by specifying excluded regions from a simply connected bounded domain. For example, to remove from an interior trefoil a circular 'hole',

```
tref.disconnect; % clears any domains from segment
c = segment([], [0.5 0.4 0 2*pi]); % new circular segment
d = domain(tref, 1, c, -1);
```

Note that segment tref had previously been 'linked' to the old domain d at the start of this section, hence the need to 'disconnect' it (or create a fresh segment) before building new domains from it. If the direction signs +1 and -1 are not correct as above, an error is reported (check this!) We may exclude two regions as follows, where the new region is a smaller copy of the trefoil.

 $^{^6}$ A general rule is that for good spectral convergence the MFS curve should be as far as possible from the solution domain boundary, while still 'shielding' this boundary from singularities in the analytic continuation of the solution field. The user will have to adjust this parameter, although it should not depend on k. See [1].

Typing d.plot gives Fig. 5a. Notice that the domain's boundary is the union of three segments. They are labeled 1, 2, and 3, showing the order in which segment handles are stored internally in the domain object d.seg. The convention for plotting domains is that the normals are those of the domain, rather than the normal intrinsic to each segment. The figure shows all normals pointing away from the domain, as it should. Similarly, the arrow directions are modified by the signs (1, -1, -1) that were passed in, so that, following the arrows the domain always lies to the *left*. (The black semicircles will be explained in the next section.)

More complicated domains similar to the above will be demonstrated later in Sec. 8.

5 Polygons, corners, and corner-adapted bases

So far each disconnected boundary piece of the domain has been a single segment connected to itself head-to-tail. More generally, a *list* of segments may be used to create these closed boundary pieces, as long as the last in the list connects back to the starting point of the first. For instance, a triangle is built by sending a list of three line segments to the domain command; such a list can simply be built from a list of vertices as follows,

```
s = segment.polyseglist([], [1 exp(3i*pi/8) exp(5i*pi/4)]);
tri = domain(s, 1);
```

Since s is a 1-by-3 array of (handles to) segments, the 2nd argument of the domain constructor is automatically vectorized to [1 1 1]. Each of the segments could have been made separately, e.g. the first by s(1) = segment([], [1 exp(3i*pi/8)]); etc. Fig. 5b shows tri.plot output for this domain.⁷

Let's discuss corners: their angles are indicated by the solid black 'fans' in the plot (before now these have had angle π , hence semicircles). A black fan at the junction of two segments indicates that a corner linkage was made (warnings will be given if any segment ends are left dangling), and shows the angle range pointing *into* the domain.

⁷Notice that periodic quadrature would now be inappropriate: in fact M=20 point Clenshaw-Curtis is used by default for open segments

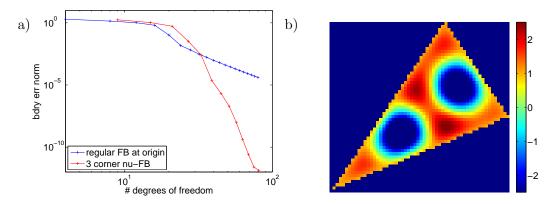


Figure 6: a) Comparing convergence of boundary error norm for Fourier Bessel vs corner-adapted fractional-order Fourier Bessel basis sets in a triangle with unity Dirichlet boundary data, for Helmholtz BVP with k=10, on log-log axes. b) The solution function.

Segment lists may also be sent to the excluded-region arguments of the domain constructor, for instance to create the domain exterior to the triangle,

```
exttri = domain([], [], s(end:-1:1), -1);
```

where it was important to reverse the order of the segment list so that they connect head-to-tail correctly. To create the domain exterior to two nearby triangles,

```
ss = s.translate(2);
exttwotri = domain([], [], {s(end:-1:1), ss(end:-1:1)}, {-1, -1});
```

We remind the reader that to create the above domains using the existing segment array s, each time a s.disconnect would be needed beforehand (this acts on all segments in the list).⁸ A universal rule is:

Each side of a segment may be associated with at most one domain

Say we want to solve an interior Helmholtz BVP on the original triangle of this section, and s and tri have been set up as with the first two commands of this section but with M=50 quadrature points. Say we want

⁸Also note that the domains previously linked to the segments, such as tri, would be left 'dangling' since s no longer is linked back to them. Attempts to use tri in a BVP would now be doomed unless the data s(:).dom were manually rewritten to point to the domain (see manual). When in doubt, disconnect segments then remake all domains.

constant boundary data 1. We may use a Fourier-Bessel basis set, solve, and plot error convergence with a simple code,

This produces the algebraic convergence shown in blue in Fig. 6a. Why is this so slow? The triangle has three *singular* corners (i.e. one whose angle is not π divided by an integer), and generically the exact solution to such a problem has a singularity at each such corner.⁹

We now show how corner-adapted basis sets achieve superior convergence and hence more efficiency. We clear the previous basis set from the domain then add fractional-order (i.e. 'wedge' expansion) Fourier-Bessel bases at each corner, of both cos and sin type.¹⁰ Repeating the convergence study and comparing against the previous data is easy,

```
tri.clearbases;
opts.rescale_rad = 2.0; tri.addcornerbases([], opts);
r = []; Ns = 1:13; for i=1:numel(Ns)
   p.updateN(Ns(i)); nn(i) = p.N; p.solvecoeffs; r(i) = p.bcresidualnorm;
end
hold on; loglog(nn, r, 'r+-'); % plot error vs total # dofs
```

The new convergence is shown in red in Fig. 6a, and is much faster; in fact it appears superalgebraic [2]. The solution field is Fig. 6b, and its large values shows that we are quite close to a Dirichlet resonance of the domain. The basis set geometry in the domain can be visualized by tri.showbasesgeom which shows wedges implied by the corner expansions.

⁹The power law for convergence is related to the corner angles and is discussed in [4].

¹⁰Sometimes an expansion is needed at some corners and not others. E.g. expansions at only the first two corners can be set up by passing in the options opts.cornermultipliers = [1 1 0];.

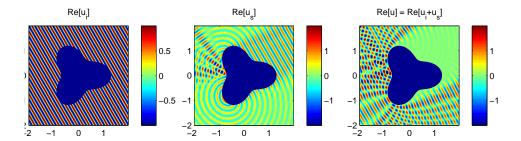


Figure 7: Sound-soft (homogeneous Dirichlet BC) scattering from a smooth trefoil at k = 30 using an MFS basis. Left: incident wave u_{inc} . Center: scattered wave u_s . Right: their sum, the total solution field u.

6 Scattering and transmission problems

Scattering of scalar waves (acoustic, or suitably-polarized Maxwell equations) involves finding a Helmholtz solution $u = u_{inc} + u_s$ with homogeneous boundary conditions on an obstacle, given an incident (often plane-wave) Helmholtz solution u_{inc} . The unknown u_s is then the solution to the radiative exterior BVP solved in Sec. 4 (see Sec. 8.3.1 for more detail), with inhomogeneous boundary data related to u_{inc} .

We designed a scattering class to implement this in a user-friendly fashion. Creating the analytic tref segment (with M=250) and its exterior domain d as in the start of Sec. 4, we set up and solve the sound-soft scattering problem as follows,

The quadrature approximation to the L^2 boundary error is 3×10^{-10} as given by p.bcresidualnorm; exponential convergence could be checked with a little loop as in Sec. 3. The incident wave, scattered wave, and solution are plotted¹¹ as in Fig. 7 by typing p.showthreefields. The solution took around 0.1 sec; the time for plotting is around 1 sec, but depends on the grid resolution requested. A good choice of the opts.tau distance parameter

¹¹We in fact tweaked the grid spacing and bounding-box options via o.dx=0.01; o.bb = 2*[-1 1 -1 1]; p.showthreefields(o);

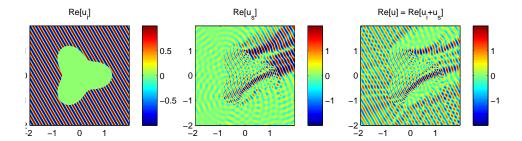


Figure 8: Transmission scattering from a smooth trefoil with refractive index (interior to exterior wavenumber ratio) 1.5 and exterior wavenumber k = 30, using MFS bases inside and out. Left: incident wave u_{inc} . Center: scattered wave u_s . Right: total solution field u.

must usually found by trial and error, examining the charge point locations and solution quality.

We may trivially switch to other physical boundary conditions by replacing the setbc command with either of the following,

```
s.setbc(1, 'N', []); % homogeneous Neumann: sound-hard s.setbc(1, 1i*k, 1); % homogeneous Robin: impedance
```

In the latter case a boundary condition $iku + u_n = 0$ is applied, which strongly absorbs incident waves.

A transmission problem involves coupled regions of different wavenumber, for instance wavenumber k in an exterior domain, and wavenumber nk in its complement, where n is the 'refractive index' of the interior. Reusing the above domain \mathbf{d} and its basis, we need a new interior domain \mathbf{d} and its MFS basis (with charge points this time outside the boundary curve),

The matching condition that u and u_n are continuous across the interface is appropriate for TM-polarized Maxwell (in two dimensions, i.e. z-invariant), for a dielectric problem, hence the setmatch arguments. Then, p.solvecoeffs; p.showthreefields; produces Fig. 8, which has error in

¹²Here we borrow notation from the optical application.

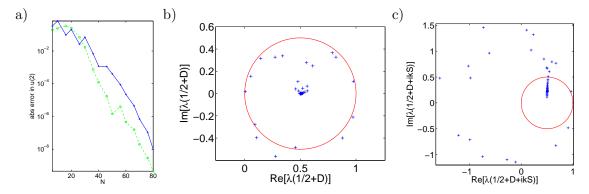


Figure 9: a) Pointwise convergence of exterior Helmholtz Dirichlet BVP with double-layer representation, at k=10 (solid: pure DLP, dotted, combined-field formulation). b) Spectrum of $(\frac{1}{2}I+D)$ in the complex plane (for M=80). We have superimposed a circle of radius 1/2 centered at 1/2, to which the eigenvalues appear to condense in the $k\to\infty$ limit—to prove this is an open problem! c) Spectrum of $(\frac{1}{2}I+D+ikS)$ relevant for combined-field formulation.

boundary matching (summing the L^2 errors in the jump in u and jump in u_n) of 10^{-6} given by p.bcresidualnorm. It can be verified that the convergence is exponential; MFS bases are an excellent choice for analytic boundaries.¹³

Notice that the scattering constructor takes two arguments (recall bvp took only one, the domain or list of domains in the problem). The first argument is the (list of) 'air' (as opposed to dielectric) domains, the second the 'non-air' domains. The former are interpreted as the domains which have the incident plane wave as their u_{inc} ; notice the non-air domain di has trivial u_{inc} in the left plot of Fig. 8, because this index $n \neq 1$ domain does not have the incident plane wave as a Helmholtz solution of the correct wavenumber nk. In the above, there was no freedom of choice of the air/non-air categorization, but in more complicated problems the exterior region may be divided into subdomains, some of which are passed in as air domains, others not; see Sec. 8.3. This enables dielectric-coated metals, dielectrics with interior holes, etc, to be solved; see Sec. 8.2.

¹³If condition number is not a problem [1]. For well-conditioned formulations, layer potentials are needed as described in the next section.

7 Layer potentials

Layer potentials are representations of Helmholtz solutions involving an integral over a boundary [3]. They are similar to the MFS representations discussed above, with the crucial advantage that a *second-kind* formulation is often possible, i.e. the operator involved is identity plus compact, and the resulting matrix problems are well-conditioned. It is easy to set up single-and double-layer potentials (SLP and DLP) living on a segment. Starting with the trefoil segment tref defined in Sec. 4, a DLP representation in its exterior is set up by,

The coefficients in p.co represent values of the double-layer density function at the quadrature points. In contrast to MFS bases, the segment's own quadrature points are always used. Therefore the number of degrees of freedom is the current value of numel(tref.x), and when you update N for a layerpot you actually change the quadrature point number of the underlying segment.

We may repeat the exterior BVP convergence of Sec. 4 using the DLP,

```
f = @(z) besselh(0, d.k * abs(z-0.3-0.2i));  % known exterior field
tref.setbc(1, 'D', [], @(t) f(tref.Z(t)));  % its Dirichlet data
p = bvp(d);
Ns = 5:5:80; for i=1:numel(Ns)
   p.updateN(Ns(i)); p.solvecoeffs; N(i) = p.N;
   e(i) = f(2) - p.pointsolution(pointset(2));  % error at a point in d
end
figure; semilogy(N, abs(e), '+-'); xlabel('N'); ylabel('error in u(2)');
```

The result is the solid line in Fig. 9a. The condition number of the problem is O(1), viz. cond(p.A) gives 69, as opposed to the ill-conditioned value 1.8×10^7 for MFS in Sec. 4. Note that errors can no longer be estimated by p.bcresidualnorm since it always around machine precision, 10^{-16} .

What actually happened above? Quite a lot! The BVP class needed to know how to evaluate the DLP on its own source segment, which requires two new ingredients:

- 1. the jump relation that states that $u^+ = (\frac{1}{2}I + D)\tau$ where τ is the density function and D the integral operator on the boundary with the double-layer kernel, and,
- 2. a good quadrature scheme to evaluate $D\tau$ at the quadrature points themselves is needed; by default for periodic quadrature¹⁴ the Martensen-Kussmaul scheme recommended by Kress is used [3], and this requires z''(t), hence the need for R'' in radialfunc.

The above scheme is called the Nyström method [3]. How did MPSpack know to evaluate u^+ rather than u^- ? Only the + side of the segment is connected to the evaluation domain. Note that our choice of normalization is that the matrix $\mathbf{p}.\mathbf{A}$ maps density values to field values multiplied by the square-root of quadrature weights. To recover the unweighted matrix and check its eigenvalues, which approximate well eigenvalues of $(\frac{1}{2}I+D)$, we use

figure; plot(eig(diag(1./p.sqrtwei)*p.A), '+'); axis equal giving Fig. 9b.

This plot shows an eigenvalue alarmingly close to zero. Why? It is well-known that $\frac{1}{2}I + D$ goes singular when k^2 is a Dirichlet eigenvalue of the interior domain [3]. This leads to blow-up of the condition number, hence non-robustness. A cure due to Brakhage, Werner, Leis and Panich [3] is to use a combined-field representation of DLP plus ik times SLP, which is done by replacing the above basis setup by

d.addlayerpot(tref, [1i*d.k 1]);

Delightfully, the spectrum of $\frac{1}{2}I+D+ikS$ avoids zero like the plague (Fig. 9c) and now cond(p.A) is reduced to 5.

In a future edition we will discuss sound-hard scattering, direct formulations, and how to solve transmission problems with layer potentials. For now, the latter is implemented in test/testdielscatrokh.m. Please get in touch with the authors if you have any questions or suggestions!

8 More elaborate examples

In this section we describe in detail some more complicated worked examples and give the corresponding code. All examples can also be found in the examples subdirectory of MPSpack.

¹⁴MPSpack also implements Kapur-Rokhlin schemes of order 2, 4, and 10, which for non-FMM-accelerated problems sich as this are inferior to Kress'. For non-periodic open segments, no special quadratures are currently implemented.

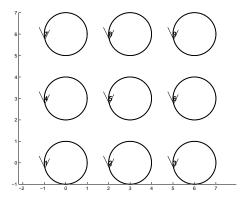


Figure 10: An array of 9 scatterers.

Scattering from an array of discs

In this section we describe how to solve the problem of scattering from an array of circular scatterers in MPSpack using a basis of fundamental solutions.

Problem description and solution approach

Let Ω be the union of disks D_j with radius r whose midpoints have the coordinates $(an_1^{(j)},an_2^{(j)}) \in \mathbb{R}^2$, where $n_1^{(j)},n_2^{(j)} \in \mathbb{N}$ and a>0 is the distance between two neighboring midpoints. An example for 9 scatterers is shown in Figure 10. The PDE is the following.

$$\Delta u + k^2 u = 0 \quad \text{in } \mathbb{R}^2 \backslash \Omega \tag{1}$$

$$u = 0 \text{ on } \partial\Omega$$
 (2)

$$u = 0 \text{ on } \partial\Omega$$

$$\frac{\partial u_s}{\partial r} - iku_s = o(r^{-1/2}),$$
(2)

Here, $u = u_{inc} + u_s$ is the total field, u_{inc} is the incident wave, u_s is the scattered field, and r is the radial coordinate. The Sommerfeld radiation condition (6) is to be understood to hold uniformly in all directions.

We solve the problem using fundamental solutions approximations in each disk, where the charge points lie on circles with radius $r_{mfs} < r$.

Implementation in MPSpack

Initialization of the problem parameters We have the following problem parameters.

```
N1=3; N2=3; % Number of scatterers in each direction r=1; % Radii of circles a=3; % Distance of midpoints of neighboring circles in each dimension k=10; % Wavenumber M=300; % Number of points on each circle N=150; % Number of MFS basis fct. in each circle Rmfs=0.8*r; % Radius of fundamental solutions inside circles
```

Setup of the geometry The geometry is setup using a simple for loop.

```
y0=0;
s=segment.empty(N1*N2,0);
for i=1:N1,
    x0=0;
    for j=1:N2
        seg=segment(M,[x0+1i*y0 r 0 2*pi],'p');
        seg.setbc(1,'D',[]);
        s((i-1)*N2+j)=seg;
        x0=x0+a;
    end
    y0=y0+a;
end
```

In the inner for loop circular segments are created whose handle is the variable seg. We directly assign the homogeneous Dirichlet boundary conditions using the command

```
seg.setbc(1,'D',[]);
```

The segments are then stored in the array **s**. Storing the circular segments in an array makes plotting easy. Figure 10 is simply created with the commands

```
o.normals=0;
plot(s,1,o);
```

Once all segments are created we define the domain by

```
d=domain([],[],num2cell(s),num2cell(-1*ones(N1*N2,1)));
```

This command might look complicated at first because of the use of num2cell. We need to convert the array ${\tt s}$ into a cell structure so that the domain constructor recognizes that each element of s is a closed shape in itself. Otherwise, the constructor would try to combine the elements of ${\tt s}$ into one connected shape, which is not possible.

Basis functions We want to use a basis of fundamental solutions in each of the circular scatterers. This is achieved with the following for loop.

```
x0=0; y0=0; opts.fast=1;
for i=1:N1,
    x0=0;
    for j=1:N2
        Z=@(w) rmfs*exp(2i*pi*w)+x0+1i*y0;
        Zp=@(w) rmfs*2i*pi*w.*exp(2i*pi*w);
        d.addmfsbasis({Z,Zp},N,opts);
        x0=x0+a;
    end
    y0=y0+a;
end
```

The function handle Z defines the fundamental solutions curve and Zp its derivative. We have to shift the curves according to the midpoints of the circles.

Solving the problem We now have everything together to setup a problem instance. This is easily done with the scattering class and the following three commands.

```
pr=scattering(d,[]);
pr.setoverallwavenumber(k);
pr.setincidentwave(-pi/3);
```

The solution and timing results are then obtained by

On a standard Core 2 Duo Laptop this takes just under 40 seconds with a boundary error of about $2\cdot 10^{-13}$. We can plot the solution using the following commands.

```
o.bb=[-a N2*a -a N1*a];
o.dx=0.05;
o.sepfigs=1;
pr.showthreefields(o);
```

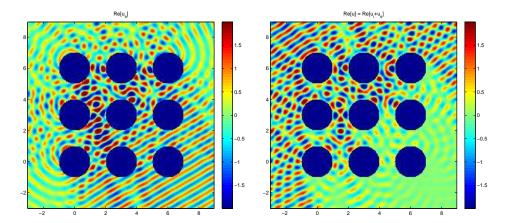


Figure 11: The scattered (left) and the full field (right) for the problem of scattering from an array of circles.

The command pr.showthreefields(o) plots the incoming wave, scattered field and full field using the parameters given in o. We have specified o.sepfigs=1. This creates three separate figures for the three different fields instead of plotting everything into one figure.

The scattered and the full field are shown in Figure 11. Note that plotting can take a long time since the array of scatterers spans many wavelenghts for which we need a sufficiently high resolution. The solution is not symmetric with respect to the diagonal since the incident angle for the incoming wave is $-\frac{\pi}{3}$, destroying the symmetry given by the configuration of scatterers.

8.2 Transmission scattering with 'metal' and air holes

Here we demonstrate how the fundamental solutions introduced in Sec. 4 can be used to solve efficiently the scattering of TE (transverse-electric) polarized z-invariant plane-wave (2D Maxwell equations) from a smooth dielectric body with various inclusions. We will be somewhat brief in this example.

The mathematical set up is identical to the previous example, except that there is a bounded dielectric region which has refractive index n=1.5 and hence a Helmholtz solution with larger wavenumber than in the surrounding vacuum (or 'air'). The field u represents H_z , the out-of-plane magnetic field. The solution in the dielectric must match that in the air at their common boundary, as we describe shortly. We also have a homogeneous boundary

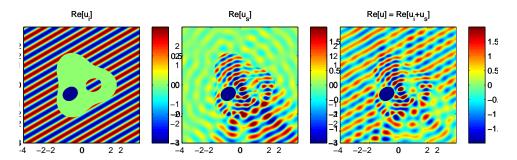


Figure 12: Transmission scattering (TE-polarized) from dielectric with two inclusions: an air hole (to the right side) and a 'metallic' PMC inclusion (to the left side). Multiple MFS basis curves are used. Left: incident wave u_{inc} . Center: scattered wave u_s . Right: their sum, the total solution field u.

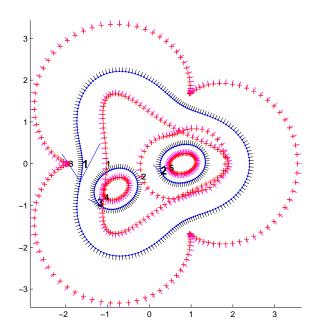


Figure 13: MFS curves (red) and boundary curves (blue) used for transmission scattering from dielectric with two inclusions.

condition on a 'metallic' inclusion inside the dielectric; see Fig. 12.

First we set up some curves, formed by scaling, translating and rotating standard 'radius-1' segments 's' and 'c', and build the three domains from them,

```
s = segment.smoothstar(200, 0.2, 3);
                                               % weak trefoil shape
c = segment.smoothstar(70, 0.1, 2);
                                               % squashed circle
sd = s.scale(2);
                                               % outer bdry of dielectric
sa = translate(rotate(sm, .3), .8);
                                               % air inclusion bdry
sm = c.scale(0.5); sm.rotate(pi/5); sm.translate(-.8-.6i); % 'metal' bdry
de = domain([], [], sd, -1);
                                               % exterior air domain
da = domain(sa, 1);
                                               % air inclusion domain
d = domain(sd, 1, \{sm sa\}, \{-1 -1\});
                                               % dielectric w/ 2 holes
d.setrefractiveindex(1.5);
                                               % choose dielectric index
```

Assuming relative permeability of unity, the relative permittivity of the dielectric is $\epsilon = n^2$. The TE boundary condition is that u is continuous across a dielectric interface (segments sd and sa), while for the normal derivatives $\epsilon^{-1}\partial u/\partial n$ is continuous. We set this up, and a Dirichlet BC on the other inclusion, with,

The domains are then collected into a scattering problem as follows (note that by including da in the first argument list, it is set up as an 'air' domain thus receives a nonzero u_{inc} plane-wave field, although results are similar if de is the only air domain),

MFS bases are very convenient for such analytic boundaries, and we use the analytic continuation of the boundary parametrization to generate MFS curves either inside or outside the actual segment curves (tau>0 is inside, and tau<0 outside, for CCW segments). Fig. 13 shows the five MFS curves and the three segments. The reason the dielectric needs three MFS curves is that (analogous with Runge's Theorem in complex approximation), singularities

¹⁵See [5]. See segment.dielectriccoeffs for where this is set up in MPSpack.

are needed in *each* disconnected component of the domain's complement. The distances tau in the following should be chosen as large as possible while still keeping the coefficient norm norm(pr.co) not too large (i.e. 10⁴ or less).

```
de.addmfsbasis(sd, 120,struct('tau',0.05));  % exterior domain
da.addmfsbasis(sa, 60, struct('tau',-0.1));  % inside air pocket
d.addmfsbasis(sd, 150,struct('tau',-0.05));  % 1st of 3 curves for diel...
d.addmfsbasis(sm, 60, struct('tau',0.1));  % ...2nd curve in 'metal' hole
d.addmfsbasis(sa, 60, struct('tau',0.1));  % ...3rd curve in air hole
```

Note that the basis set degrees were optimized roughly for this k value, giving only 450 total degrees of freedom for a problem around 8 wavelengths in size. Solving for the coefficients of the solution takes 0.67 sec,

```
pr.solvecoeffs; pr.bcresidualnorm
```

The L^2 boundary error is less than 10^{-7} . We then plot the incident, scattered, and total field as usual with pr.showthreefields; giving Fig. 12. Evaluating the solution on a 400×400 grid takes 11 sec.

8.2.1 Convergence study

Once a good set of MFS basis sizes has been chosen, as above, they may all be changed at once conveniently with the nmultiplier option. We could have redone the basis sets as follows,

```
d.clearbases; de.clearbases; da.clearbases;
de.addmfsbasis(sd, [], struct('tau',0.05, 'nmultiplier', 120/450));
da.addmfsbasis(sa, [], struct('tau',-0.1, 'nmultiplier', 60/450));
d.addmfsbasis(sd, [], struct('tau',-0.05, 'nmultiplier', 150/450));
d.addmfsbasis(sm, [], struct('tau',0.1, 'nmultiplier', 60/450));
d.addmfsbasis(sa, [], struct('tau',0.1, 'nmultiplier', 60/450));
```

The mutipliers were set up to be the fraction of the total degrees of freedom that they were before, but now they can be scaled with a single command, viz, pr.updateN(450) sets up the original basis sizes, as may be checked with diff([pr.basnoff pr.N]) which gives the numbers of degrees of freedom in each problem basis set. We put this in a convergence loop,

```
Ns=300:50:600; for i=1:numel(Ns)
  pr.updateN(Ns(i)); pr.solvecoeffs; u0 = pr.pointsolution(pointset(0));
  fprintf('N=%d, co-norm=%g, bc-norm=%g, |u(0)|=%.16g\n', Ns(i), ...
```

norm(pr.co), pr.bcresidualnorm, abs(u0));

end

We actually doubled the number of quadrature points on the original segments to perform this high-accuracy study, giving 680 quadrature points in total. The output shows very rapid convergence,

```
N=300, co-norm=2125.38, bc-norm=0.000363003, |u(0)|=3.045222448551815
N=350, co-norm=1968.37, bc-norm=1.26165e-05, |u(0)|=3.045222451567895
N=400, co-norm=1844.05, bc-norm=4.21908e-07, |u(0)|=3.045222451435764
N=450, co-norm=1746.25, bc-norm=9.77848e-08, |u(0)|=3.045222451435782
N=500, co-norm=1651.79, bc-norm=3.96167e-09, |u(0)|=3.045222451436035
N=550, co-norm=1581.87, bc-norm=1.1487e-09, |u(0)|=3.045222451436006
N=600, co-norm=1521.16, bc-norm=1.44025e-10, |u(0)|=3.045222451436037
```

This suggests that, at least for u at the origin, we had 12 correct digits in the solution with the total N=450 used above, and probably achieved 14 digits with N = 600, computed in just a couple of seconds.

8.3 Acoustic scattering from the unit square

This example introduces a new feature: the use of decomposition of a region of constant wavenumber into computational subdomains connected by fictitious boundaries. The code is in examples/tut_square.m

Problem description and solution approach

In this example we solve the problem of time-harmonic acoustic sound-soft scattering from the unit square $\Omega = (-0.5, 0.5)^2$. The full PDE has the following form.

$$\Delta u + k^2 u = 0 \quad \text{in } \mathbb{R}^2 \backslash \Omega \tag{4}$$

$$u = 0 \text{ on } \partial\Omega \tag{5}$$

$$\Delta u + k^2 u = 0 \text{ in } \mathbb{R}^2 \backslash \Omega$$

$$u = 0 \text{ on } \partial \Omega$$

$$\frac{\partial u_s}{\partial r} - iku_s = o(r^{-1/2}),$$
(4)
(5)

Here, $u = u_{inc} + u_s$ is the total field, u_{inc} is the incident wave, u_s is the scattered field, and r is the radial coordinate. The Sommerfeld radiation condition (6) is to be understood to hold uniformly in all directions.

To achieve high accuracy we cannot simply use fundamental solutions to approximate the scattered field. The problem is the singularities of the solution u at the corners. If these are not represented in the basis our

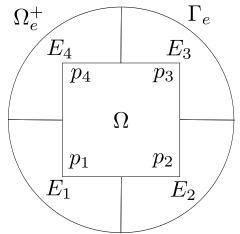


Figure 14: Geometry of the problem

approximation error will decay very slowly as the number of basis functions increases. To solve this problem we use the domain decompositon shown in Figure 14. The idea is that each of the elements E_i only contains one corner p_i of the square. We can then match the corner behavior in each domain by using fractional order Bessel functions. Since furthermore, u=0 on $\partial\Omega$ it will be sufficient to use Fourier-Bessel sine functions that automatically satisfy the zero boundary conditions on the sides of the square. Hence, the total field u is approximated in each element E_i using an approximation of the form

$$u(r,\theta) \approx \sum_{j=1}^{N_i} c_j^{(i)} J_{\frac{2}{3}j}(kr) \sin(\frac{2j}{3}\theta).$$

The polar coordinate system in each element E_i is rotated in such a way that the basis functions are zero on the sides adjacent to the corner at p_i .

In the infinite domain Ω_e^+ we use a basis of fundamental solutions to represent the scattered field u_s . Hence, for $\mathbf{x} \in \Omega^+$ we have

$$u_s(\mathbf{x}) \approx \sum_{j=1}^{N_e} \frac{i}{4} c_j^{(e)} H_0^{(1)}(|\mathbf{x} - \mathbf{y}_j|),$$

where $\mathbf{y}_j = r_{mfs}e^{i\phi_j}$ and $\phi_j = \frac{2\pi j}{N_e}$. Note that we approximate with the fundamental solutions the scattered field u_s while in the finite subdomains E_i we approximate the total field u. The compatibility conditions between approximations u^i und u^j in two neighboring elements E_i and E_j with common

boundary Γ_{ij} are given by

$$u^{(i)}(\mathbf{x}) \approx u^{(j)}(\mathbf{x}), \quad \frac{\partial u}{\partial n_i} u^{(i)}(\mathbf{x}) \approx \frac{\partial u}{\partial n_i} u^{(j)}(\mathbf{x}),$$

where $\mathbf{x} \in \Gamma_{ij}$ and $\frac{\partial}{\partial \nu_i}$ is the outward normal derivative at the boundary of E_i . On the interface Γ_{ie} between an element E_i and the exterior domain Ω_e^+ we have the compatibility conditions

$$u^{(i)}(\mathbf{x}) \approx u_{inc}(\mathbf{x}) + u_s^{(e)}(\mathbf{x}), \quad \frac{\partial}{\partial n_i} u^{(i)}(\mathbf{x}) \approx \frac{\partial}{\partial n_i} (u_s^{(e)} + u_{inc})(\mathbf{x}),$$

where $u_s^{(i)}$ is the fundamental solutions approximation to the scattered field in Ω_e^+ . We have to add the incident field to the approximate scattered field since we are matching with the total field in the elements E_i . An approximate solution to the whole problem is now computed by minimizing the L^2 error of the compatibility conditions on all interfaces.

8.3.2 Implementation in MPSpack

Although the setup of the problem seems quite complicated we will see that it is very simple to set it up in MPSpack. Indeed, the most part of the code will be devoted to creating the mesh structure from Figure 14.

Initialization of the problem parameters We need to define the following problem parameters.

Setup of the geometry We now need to define the geometry. Fortunately, MPSpack gives some support for the construction of the geometry.

The list of segments is defined by the following three commands.

```
s = segment.polyseglist(M, [1i*r 1i*a a+1i*a a r]);
s=[s(1:3) segment(2*M, [0 r 0 pi/2])];
s = [s rotate(s, pi/2) rotate(s, pi) rotate(s, 3*pi/2)];
```

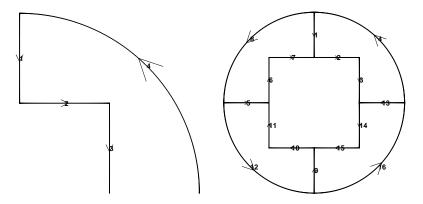


Figure 15: The segments in the right plot are created by rotating the segments shown in the left plot.

The first command defines all the straight lines that form part of the boundary of E_3 . For this we use polyseglist. The command polyseglist constructs a closed polygon. We then delete the last two segments of the array s and add instead the circular line segment. This results in the segments shown in the left plot of Figure 15. We now rotate this element three times to obtain the segments shown in the right plot of Figure 15.

For later it is important to have a separate list of all segments not belonging to the square and all segments belonging to the outer circle.

```
sdecomp=s([1 4 5 8 9 12 13 16]); % All artificial boundaries
extlist=s([4 8 12 16]); % Segments forming the outer circle
```

We now define the domains. By taking the rotational symmetry into account we can do this in a simple for loop.

```
d=domain.empty(4,0); for j=1:4, d(j)=domain(s(1+mod(4*(j-1)+[0 1 2 12 3],16)),[1 1 1 -1 1]); end ext = domain([], [],extlist(end:-1:1), -1);
```

The for loop looks slightly complicated. But all it does is pick out the right indices for the elements forming a domain and creating it together with the right sense of direction. At the end we have an array d containing the four fine domains E_i . The exterior domain ext is created by traversing extlist in reverse order with reversed sense -1. This is necessary since we now have the boundary of an exterior domain, which has a reversed sense of direction.

Boundary conditions and basis functions Setting up the compatibility conditions between the elements is trivial. It is done by the command

```
sdecomp.setmatch([k -k],[1 -1]);
```

The matching conditions for the function values are scaled by the wavenumber k to balance the different scaling between the L^2 error in the function and the L^2 error in the derivative.¹⁶

We can now add the basis functions to the domains. The fractional Bessel functions are added to the interior domains by the following command.

```
nuopts=struct('type','s','cornermultipliers',[0 0 1 0 0],'rescale_rad',1);
for j=1:4, d(j).addcornerbases(N,nuopts); end
```

The options structure nuoopts specifies that we only want Fourier-Bessel sine functions at the third corner of each domain. This is the corner belonging to the square. The option 'rescale_rad' specifies that the basis functions are rescaled to balance out the bad scaling of Bessel functions. The method addcornerbases automatically finds out the right fractional orders, offsets and suitable branch vectors.

The exterior fundamental solutions are added with the following command.

```
Z=@(t) rmfs*exp(2i*pi*t); Zp=@(t) 2i*pi*rmfs*exp(2i*pi*t);
opts=struct('eta','k','fast',1,'nmultiplier',2);
ext.addmfsbasis({Z, Zp},N,opts);
```

Note that now nmultiplier is set to 2. It turns out to be effective for this problem to use twice as many fundamental solutions as there are Fourier-Bessel sine functions in each domain.

Solving the problem We now have everything together to setup the problem class and solve the scattering problem. The following commands setup the scattering problem and define an incident plane wave.

```
pr=scattering(ext,d);
pr.setoverallwavenumber(k);
pr.setincidentwave(-pi/4);
```

¹⁶Consider the one dimensional plane wave e^{ikx} . The derivative is ike^{ikx} . Hence, in general it makes sense to scale the L^2 error of function values by k to give it the same dimension as the L^2 error of the derivative.

There is one small specialty here. In the first line we have defined ext to be an air-domain and the array d to be a non-air domain. This tells MPSpack to add the incident field to the exterior basis functions in assembling the least-squares problem. In the finite domains this is not necessary since there we approximate directly the full field.

The following commands now solve the problem and plot the solution u.

The incident field ui is automatically evaluated only in air-domains. If we want to evaluate it in all domains we have to set o.all=1. But here the default behavior is fine for us. The sum ui+u is now the total field in all domains (remember that u approximates the total field in the interior domains and the scattered field in the exterior domain). The scattering class also provides a routine showthreefields to plot the incident wave, scattered field and total field. However, the routine assumes that the computed solution is the scattered field, which is not correct for the way we have set up this problem. The resolution if the plot can easily be increased by decreasing the variable o.dx, which influences the distance of two grid points.

The output of the example problem is shown in Figure 16. The L^2 boundary error of the solution is approximately $1.5 \cdot 10^{-10}$. On a standard laptop with Intel Core 2 Duo processor the solution vector is computed in around 11 seconds. The plot takes slightly longer.

A wonderful feature of this approach is that we can trivially switch to a sound-hard scattering problem, that is instead of requiring u=0 on $\partial\Omega$ we require $\frac{\partial}{\partial n}u=0$ on $\partial\Omega$. All we have to do is switch to Fourier-Bessel cosine functions. These automatically satisfy the required condition for the

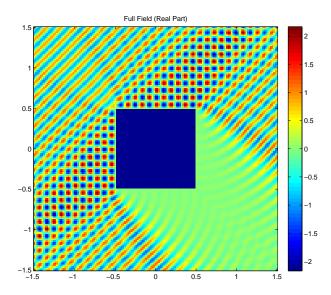


Figure 16: The solution of the scattering problem on the unit square with sound-soft boundary conditions.

normal derivative. The solution to this problem is shown in Figure 17. The accuracy and solution time are comparable to the sound-soft scattering case.

References

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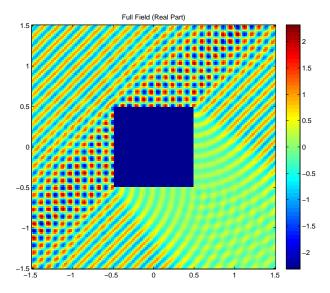


Figure 17: The solution of the scattering problem on the unit square with sound-hard boundary conditions.