

MATH 590: Meshfree Methods

Chapter 43: RBF-PS Methods in MATLAB

Greg Fasshauer

Department of Applied Mathematics
Illinois Institute of Technology

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Outline

- 1 Computing the RBF-Differentiation Matrix in MATLAB
- 2 Use of the Contour-Padé Algorithm with the PS Approach
- 3 Computation of Higher-Order Derivatives
- 4 Solution of a 2D Helmholtz Equation
- 5 A 2D Laplace Equation with Piecewise Boundary Conditions
- 6 Summary



The coupling of RBF collocation and pseudospectral methods discussed in the previous chapter has provided a number of new insights.

- We can apply many standard pseudospectral procedures to RBF solvers.
- In particular, we now have “standard” procedures for solving time-dependent PDEs with RBFs.

In this chapter we illustrate how the RBF pseudospectral approach can be applied in a way very similar to standard polynomial pseudospectral methods.

Among our numerical illustrations are several examples taken from the book [Trefethen (2000)] (see Programs 17, 35 and 36 there).

We will also use the 1D transport equation from the previous chapter to compare the RBF and polynomial PS methods.



How to compute the discretized differential operators

In order to compute, for example, a **first-order differentiation matrix** we need to remember that — by the **chain rule** — the derivative of an RBF will be of the general form

$$\frac{\partial}{\partial \mathbf{x}} \varphi(\|\mathbf{x}\|) = \frac{\mathbf{x}}{r} \frac{d}{dr} \varphi(r).$$

We require both

- the **distances**, r ,
- and **differences in x** , where x is the first component of \mathbf{x} .

In our first MATLAB subroutine `DRBF.m` we compute these distance and difference matrices on lines 5 and 6.

The **differentiation matrix** is then given by (see lines 8–10)

$$D = A_x A^{-1}.$$

Note the use of the **matrix right division operator** `/` or `mrdivide` in MATLAB on line 10 used to solve the system $DA = A_x$ for D .



Program (DRBF.m)

```

1 function [D,x] = DRBF(N,rbf,dxrbf)
2 if N==0, D=0; x=1; return, end
3 x = cos(pi*(0:N)/N)'; x = flipud(x); % Chebyshev pts.
4 mine = .1; maxe = 10; % Shape parameter interval
5 r = DistanceMatrix(x,x);
6 dx = DifferenceMatrix(x,x);
7a ep=fminbnd(@ (ep) CostEpsilonDRBF(ep,r,dx,rbf,dxrbf), ...
7b                                     mine,maxe);
8 A = rbf(ep,r);
9 Ax = dxrbf(ep,r,dx);
10 D = Ax/A;

```

Remark

DRBF.m *is a little more complicated than it needs to be since we include an LOOCV-optimization of the RBF shape parameter.*

*Below we modify the basic routine CostEpsilon.m so that we optimize ε for the **matrix problem** $D = A_x A^{-1} \iff A^T D^T = (A_x)^T$.*

Program (CostEpsilonDRBF.m)

```

1 function ceps = CostEpsilonDRBF(ep,r,dx,rbf,dxrbf)
2 N = size(r,2);
3 A = rbf(ep,r);    % = A^T since A is symmetric
4 rhs = dxrbf(ep,r,dx)';    % A_x^T
5 invA = pinv(A);
6 EF = (invA*rhs)./repmat(diag(invA),1,N);
7 ceps = norm(EF(:));

```

Remark

*Note that CostEpsilonDRBF.m is very similar to CostEpsilon.m. Now, however, we compute a **right-hand side matrix** corresponding to the transpose of A_x .*

*Therefore, the **denominator** — which remains the same for all **right-hand sides** — needs to be **cloned** on line 6 via the `repmat` command.*

*The cost of ε is now the **Frobenius norm of the matrix** EF .*

We illustrate the use of the subroutine `DBRF.m` by solving a **1-D transport equation**.

Consider

$$\begin{aligned}u_t(x, t) + cu_x(x, t) &= 0, & x > -1, t > 0, \\u(-1, t) &= 0, \\u(x, 0) &= f(x),\end{aligned}$$

with the **well-known solution**

$$u(x, t) = f(x - ct).$$



Program (TransportDRBF.m)

```
1  rbf = @(e,r) exp(-(e*r).^2);          % Gaussian RBF
2  dxrbf = @(e,r,dx) -2*dx*e.^2.*exp(-(e*r).^2);
3  f = @(x) max(64*(-x).^3.*(1+x).^3,0);
4  N = 20; [D,x] = DRBF(N,rbf,dxrbf);
5  dt = 0.001; t = 0; c = 1; v = f(x);
6  tmax = 1; tplot = .02; plotgap = round(tplot/dt);
7  dt = tplot/plotgap; nplots = round(tmax/tplot);
8  data = [v'; zeros(nplots,N+1)]; tdata = t;
9  for i = 1:nplots
10     for n = 1:plotgap
11         t = t+dt;
12         vv = v(end-1);
13         v = v - dt*c*(D*v);          % explicit Euler
14         v(1) = 0; v(end) = vv;
15     end
16     data(i+1,:) = v'; tdata = [tdata; t];
17 end
18 surf(x,tdata,data), view(10,70), colormap('default');
19 axis([-1 1 0 tmax 0 1]), ylabel t, zlabel u, grid off
20 xx = linspace(-1,1,101); vone = f(xx-c);
21 w = interp1(x,v,xx);
22 maxErr = norm(w-vone,inf)
```

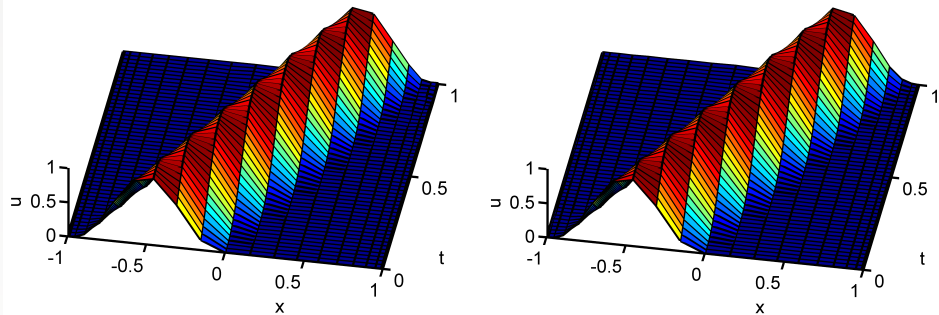



Figure: Time profiles of the solution to the transport equation for $0 \leq t \leq 1$ with initial profile $f(x) = \max(-64x^3(1+x)^3, 0)$ and unit wave speed based on **Gaussian RBFs** with $\varepsilon = 1.874049$ (left) and **Chebyshev PS** method (right). **Explicit Euler time-stepping** with $(\Delta t = 0.001)$, and 21 Chebyshev points.

The maximum error for the Gaussian solution at time $t = 1$ is 0.0416 while for the PS solution we get 0.0418.



Remark

- We could use almost the identical code to solve this problem with a Chebyshev pseudospectral method as discussed in [Trefethen (2000)].
- The only difference in the PS-code is the replacement of line 4 in `TransportDRBF.m` by

```
4  N=20; [D,x] = cheb(N); x = flipud(x); D = -D;
```

where `cheb.m` is the subroutine provided on page 54 of [Trefethen (2000)] for spectral differentiation.
- Note that Trefethen's `cheb` is based on a “right-to-left” orientation of the collocation points, and therefore we need to “correct” the points and matrix `D`.



We now explain how the Contour-Padé algorithm of [Fornberg and Wright (2004)] can be used to compute RBF differentiation matrices.

In its original form the Contour-Padé algorithm allows us to stably evaluate RBF interpolants based on infinitely smooth RBFs for extreme choices of the shape parameter ε (in particular $\varepsilon \rightarrow 0$).

The Contour-Padé algorithm uses FFTs and Padé approximations to evaluate the function

$$\hat{u}(\mathbf{x}, \varepsilon) = \mathbf{b}^T(\mathbf{x}, \varepsilon)(\mathbf{A}(\varepsilon))^{-1} \mathbf{f} \quad (1)$$

with $\mathbf{b}(\mathbf{x}, \varepsilon)_j = \varphi_\varepsilon(\|\mathbf{x} - \mathbf{x}_j\|)$ at some evaluation point \mathbf{x} and $\mathbf{A}(\varepsilon)_{i,j} = \varphi_\varepsilon(\|\mathbf{x}_i - \mathbf{x}_j\|)$.



- If we evaluate \hat{u} at all of the collocation points \mathbf{x}_i , $i = 1, \dots, N$, for some fixed value of ε , then $\mathbf{b}^T(\mathbf{x}, \varepsilon)$ turns into the matrix $\mathbf{A}(\varepsilon)$.
- In the case of interpolation this is pointless.
- If the Contour-Padé algorithm is adapted to replace the vector $\mathbf{b}^T(\mathbf{x}, \varepsilon)$ (corresponding to evaluation at a single point \mathbf{x}) with the matrix $\mathbf{A}_{\mathcal{L}}$ based on the differential operator (corresponding to evaluation at all collocation points), then

$$\mathbf{A}_{\mathcal{L}}(\varepsilon)(\mathbf{A}(\varepsilon))^{-1} \mathbf{u}$$

computes the values of the (spatial) derivative of \mathbf{u} on the collocation points \mathbf{x}_i .

- Boundary conditions can be incorporated later as in the standard PS approach (see, e.g., [Trefethen (2000)] or Chapter 42).



- This means that we can add another subroutine to compute the differentiation matrix on line 4 of `TransportDRBF.m` via the Contour-Padé algorithm.
- We compare
 - a solution based on the Contour-Padé algorithm for Gaussian RBFs in the limiting case $\varepsilon \rightarrow 0$
 - to the two methods described earlier (based on `DRBF` and `cheb`).
- All methods use an implicit Euler method with time step $\Delta t = 0.001$ for the time discretization.
- For an implicit time-stepping method both the Contour-Padé approach and the `DRBF` approach require an inversion of the differentiation matrix.
- Recall that our theoretical discussion suggested that this is justified as long as we're in the limiting case $\varepsilon \rightarrow 0$ and one space dimension.
- We will see that the non-limiting case (using `DRBF`) seems to work just as well.



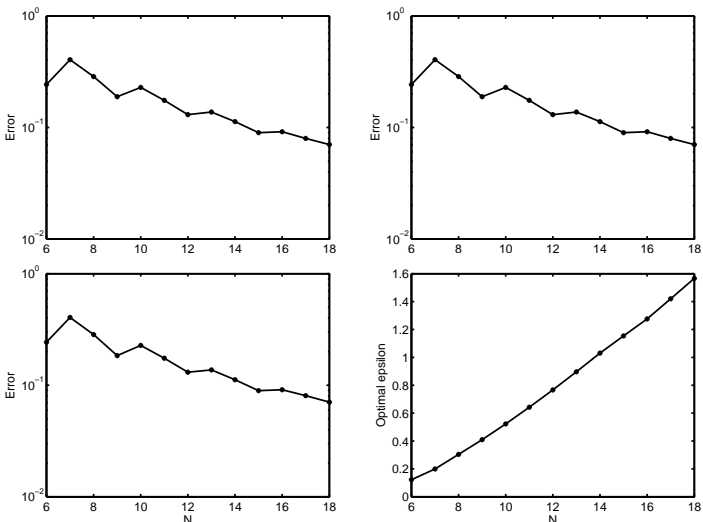


Figure: Errors at $t = 1$ for transport equation. Top: Gaussian RBF with $\varepsilon = 0$ (left) and Chebyshev PS-solution (right). Bottom: Gaussian RBF with “optimal” ε (left) and corresponding ε -values (right). Variable spatial discretization N . Implicit Euler method with $\Delta t = 0.001$.



Remark

- The “*optimal*” ε ranges *almost linearly* increasing from 0.122661 at $N = 6$ to 1.566594 at $N = 18$.
- We can see that the *errors for all three methods are virtually identical*.
- Unfortunately, in this *experiment we are limited to this small range of N* since for $N \geq 19$ the Contour-Padé solution becomes *unreliable*.
- The remarkable agreement of all three solutions for these small values of N seems to indicate that the *errors in the solution are mostly due to the time-stepping method used*.



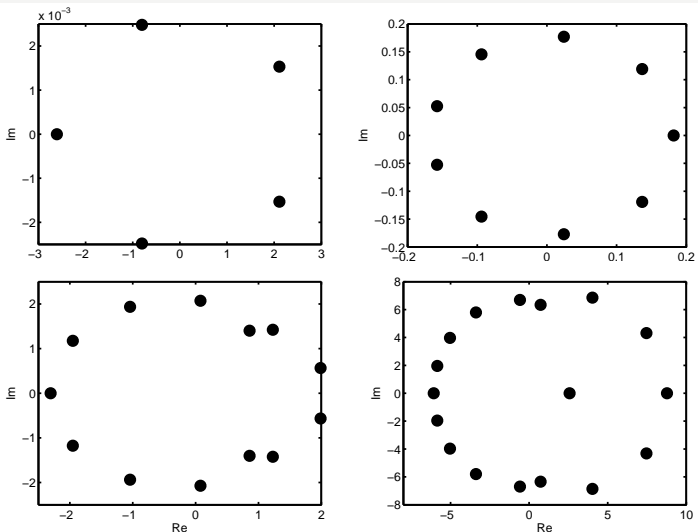


Figure: Spectra of differentiation matrices for **Gaussian RBF** with $\varepsilon = 0$ on Chebyshev collocation points obtained with the Contour-Padé algorithm and $N = 5, 9, 13, 17$.



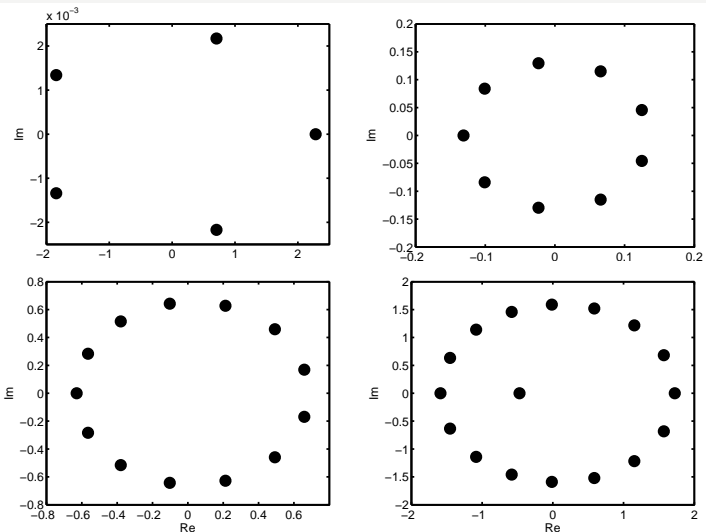


Figure: Spectra of differentiation matrices for Chebyshev pseudospectral method on Chebyshev collocation points with $N = 5, 9, 13, 17$.



Remark

- The *plots* for the Gaussian and Chebyshev methods *show some similarities*, but also *some differences*.
- The general *distribution of the eigenvalues* for the two methods is *quite similar*.
- The *spectra* for the Contour-Padé algorithm with Gaussian RBFs seem to be more or less *a slightly stretched reflection about the imaginary axis* of the spectra of the Chebyshev pseudospectral method.
- The *differences increase as N increases*.
- This is not surprising since the *Contour-Padé algorithm is known to be unreliable for larger values of N* .



For polynomial differentiation matrices higher-order derivatives can be computed by repeatedly applying the first-order differentiation matrix, i.e.,

$$D^{(k)} = D^k,$$

where D is the standard first-order differentiation matrix and $D^{(k)}$ is the matrix corresponding to the k -th (univariate) derivative.

Unfortunately, this **does not carry over to the general RBF case** (just as it does not hold for periodic Fourier spectral differentiation matrices, either).

We therefore **need to provide separate MATLAB code for higher-order differentiation matrices**.



Program (D2RBF.m)

```

1 function [D2,x] = D2RBF(N,rbf,d2rbf)
2 if N==0, D2=0; x=1; return, end
3 x = cos(pi*(0:N)/N)'; % Chebyshev points
4 mine = .1; maxe = 10; % Shape parameter interval
5 r = DistanceMatrix(x,x);
6a ep=fminbnd(@(ep) CostEpsilonD2RBF(ep,r,rbf,d2rbf),...
6b                                     mine,maxe);
7 A = rbf(ep,r);
8 AD2 = d2rbf(ep,r);
9 D2 = AD2/A;

```

The only new thing that is needed for D2RBFs is the **appropriate formula for the derivative of the RBF** passed to D2RBF via the parameter `d2rbf`.



Remark

- *We do not list `CostEpsilonD2RBF`.*
- *It differs from `CostEpsilonDRBF` only in the definition of the right-hand side matrix which now becomes*

$$4 \quad \text{rhs} = \text{d2rbf}(\text{ep}, \text{r})';$$
- *Also, the number and type of parameters that are passed to the functions are different since the first-order derivative requires differences of collocation points and the second-order derivative does not.*



We illustrate the use of the subroutine `D2RBF.m` with a modification of Program 35 in [Trefethen (2000)] which is concerned with the solution of the **nonlinear reaction-diffusion (or Allen-Cahn) equation**.

Consider

$$u_t = \mu u_{xx} + u - u^3, \quad x \in (-1, 1), \quad t \geq 0,$$

with **parameter** μ , **initial condition**

$$u(x, 0) = 0.53x + 0.47 \sin\left(-\frac{3}{2}\pi x\right), \quad x \in [-1, 1],$$

and **non-homogeneous (time-dependent) boundary conditions**

$$\begin{aligned} u(-1, t) &= -1 \\ u(1, t) &= \sin^2(t/5). \end{aligned}$$

The **solution has three steady states** ($u = -1, 0, 1$) with the two **nonzero states being stable**.

The **transition between these states is governed by the parameter** μ . Below we use $\mu = 0.01$, and the **unstable state should vanish around** $t = 30$.

Program (Modification of Program 35 of [Trefethen (2000)])

```

1  rbf = @(e,r) exp(-e*r).*(15+15*e*r+6*(e*r).^2+(e*r).^3);
2  d2rbf = @(e,r) e^2*((e*r).^3-3*e*r-3).*exp(-e*r);
3  N = 20; [D2,x] = D2RBF(N,rbf,d2rbf);
   % Here is the rest of Trefethen's code.
4  mu = 0.01; dt = min([.01,50*N^(-4)/mu]);
5  t = 0; v = .53*x + .47*sin(-1.5*pi*x);
6  tmax = 100; tplot = 2; nplots = round(tmax/tplot);
7  plotgap = round(tplot/dt); dt = tplot/plotgap;
8  xx = -1:.025:1; vv = polyval(polyfit(x,v,N),xx);
9  plotdata = [vv; zeros(nplots,length(xx))]; tdata = t;
10 for i = 1:nplots
11     for n = 1:plotgap
12         t = t+dt; v = v + dt*(mu*D2*v + v - v.^3); % Euler
13         v(1) = 1 + sin(t/5)^2; v(end) = -1; % BC
14     end
15     vv = polyval(polyfit(x,v,N),xx);
16     plotdata(i+1,:) = vv; tdata = [tdata; t];
17 end
18 surf(xx,tdata,plotdata), grid on
19 axis([-1 1 0 tmax -1 2]), view(-40,55)
20 colormap('default'); xlabel x, ylabel t, zlabel u

```

Remark

- Note *how easily the nonlinearity is dealt with* by incorporating it into the time-stepping method on line 12.
- The original program in [Trefethen (2000)] is obtained by deleting lines 1–2 and replacing line 3 by a call to `cheb.m` followed by the statement $D2 = D^2$.
- In our RBF-PS implementation the *majority of the matrix computations are required only once outside the time-stepping procedure* when computing the derivative matrix.
- *Inside the time-stepping loop* (on line 12) we require *only matrix-vector multiplication*.
- We point out that this approach is *much more efficient than computation of RBF expansion coefficients at every time step* (as suggested, e.g., in [Hon and Mao (1999)]).
- In fact, this is the *main difference between the RBF-PS approach and the collocation approach* of Chapters 38–40.

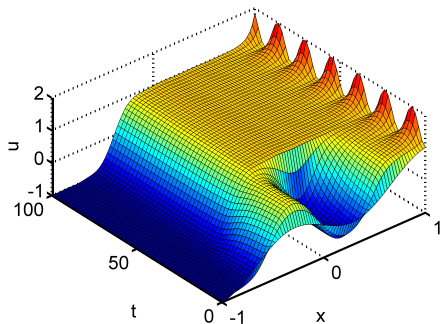
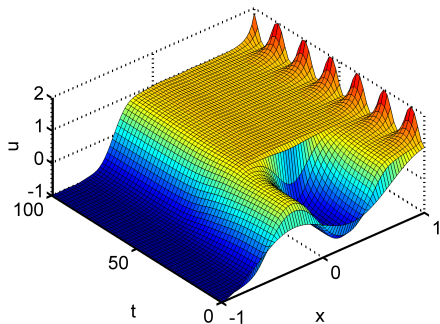


Figure: Solution of the Allen-Cahn equation using the **Chebyshev PS-method** (left) and an **RBF-PS method with cubic Matérn functions**

$\varphi(r) = (15 + 15\epsilon r + 6(\epsilon r)^2 + (\epsilon r)^3)e^{-\epsilon r}$ with “optimal” shape parameter $\epsilon = 0.350952$ (right) with $N = 20$.



Remark

- We can see that the solution based on *Chebyshev polynomials* appears to be slightly more accurate since the transition occurs at a slightly later and correct time (i.e., at $t \approx 30$) and is also a little “sharper”.
- The *differentiation matrix RBF* is obtained directly with `D2RBF.m` (i.e., *without the Contour-Padé algorithm* – since that method is not reliable for 21 points).
- The plots show that *reasonable solutions can also be obtained via this direct (and much simpler) RBF approach*.
- *True spectral accuracy will no longer be given if $\epsilon > 0$.*



Consider the **2D Helmholtz equation** (see Program 17 in [Trefethen (2000)])

$$u_{xx} + u_{yy} + k^2 u = f(x, y), \quad x, y \in (-1, 1)^2,$$

with **boundary condition**

$$u = 0$$

and **exact solution**

$$f(x, y) = \exp \left(-10 \left[(y - 1)^2 + \left(x - \frac{1}{2}\right)^2 \right] \right).$$



Remark

- To solve this type of (elliptic) problem we *need to assume invertibility of the differentiation matrix* (even though this may be theoretically questionable).
- We compare
 - a *non-symmetric RBF pseudospectral method*
 - with a *Chebyshev pseudospectral method*.
- We attempt to solve the problem with radial basis functions in *two different ways*.



Approach 1:

We apply the same **tensor-product technique** as in [Trefethen (2000)] **using the `kron` function** to express the discretized Laplacian on a tensor-product grid of $(N + 1) \times (N + 1)$ points as

$$L = I \otimes D2 + D2 \otimes I, \quad (2)$$

where

D2: is the (univariate) second-order differentiation matrix,

I: is an identity matrix of size $(N + 1) \times (N + 1)$, and

\otimes : denotes the **Kronecker tensor-product**.

- For polynomial PS methods we have $D2 = D^2$.
- For RBFs $D^2 \neq D^{(2)}$, and we **generate D2 with `D2RBF`**.
- However, **as long as we use tensor-product collocation points and the RBF is separable** (such as a Gaussian or a polynomial), **we can still use the Kronecker tensor-product construction (2)**.

Program (Modification of Program 17 of [Trefethen (2000)])

```

1  rbf = @(e,r) exp(-(e*r).^2);
2  d2rbf = @(e,r) 2*e^2*(2*(e*r).^2-1).*exp(-(e*r).^2);
3  N = 24; [D2,x] = D2RBF(N,rbf,d2rbf); y = x;
4  [xx,yy] = meshgrid(x,y); xx = xx(:); yy = yy(:);
5  I = eye(N+1);
6  k = 9;
7  L = kron(I,D2) + kron(D2,I) + k^2*eye((N+1)^2);
8  b = find(abs(xx)==1 | abs(yy)==1); % boundary pts
9  L(b,:) = zeros(4*N,(N+1)^2); L(b,b) = eye(4*N);
10 f = exp(-10*((yy-1).^2+(xx-.5).^2));
11 f(b) = zeros(4*N,1);
12 u = L\f;
13 uu = reshape(u,N+1,N+1);
14 [xx,yy] = meshgrid(x,y);
15 [xxx,yyy] = meshgrid(-1:.0333:1,-1:.0333:1);
16 uuu = interp2(xx,yy,uu,xxx,yyy,'cubic');
17 figure, clf, surf(xxx,yyy,uuu),
18 xlabel x, ylabel y, zlabel u
19 text(.2,1,.022,sprintf('u(0,0)=%13.11f',uu(N/2+1,N/2+1))

```

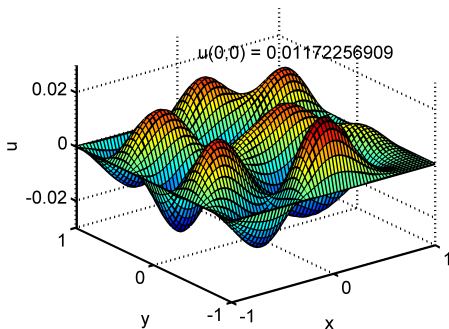
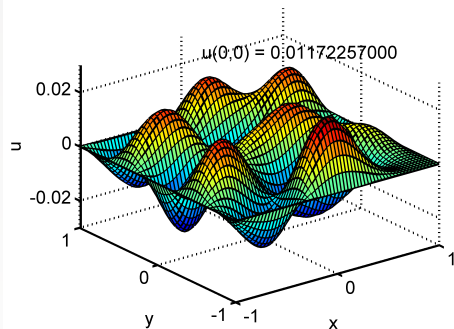


Figure: Solution of the 2D Helmholtz equation with $N = 24$ using the **Chebyshev pseudospectral method** (left) and **Gaussians** with $\varepsilon = 2.549845$ (right).



Approach 2:

- This approach allows the use of non-tensor product collocation grids.
- We use a direct implementation of the Laplacian of the RBFs.
- The only advantage of doing this on a tensor-product grid is that now all RBFs can be used.
- This approach takes considerably longer to execute since the differentiation matrix is now computed with matrices of size 625×625 instead of the 25×25 univariate differentiation matrix D2 used before.
- Moreover, the results are likely to be less accurate since the larger matrices are more prone to ill-conditioning.
- However, the advantage of this approach is that it frees us of the limitation of polynomial PS methods to tensor-product collocation grids.

Program (Modification II of Program 17 of [Trefethen (2000)])

```

1  rbf=@(e,r) max(1-e*r,0).^8.*(32*(e*r).^3+25*(e*r).^2+8*
2a Lrbf = @(e,r) 44*e^2*max(1-e*r,0).^6.*...
2b          (88*(e*r).^3+3*(e*r).^2-6*e*r-1);
3  N = 24; [L,x,y] = LRBF(N,rbf,Lrbf);
4  [xx,yy] = meshgrid(x,y);
5  xx = xx(:); yy = yy(:);
6  k = 9;
7  L = L + k^2*eye((N+1)^2);
8  b = find(abs(xx)==1 | abs(yy)==1); % boundary pts
9  L(b,:) = zeros(4*N,(N+1)^2); L(b,b) = eye(4*N);
10 f = exp(-10*((yy-1).^2+(xx-.5).^2));
11 f(b) = zeros(4*N,1);
12 u = L\f;
13 uu = reshape(u,N+1,N+1);
14 [xx,yy] = meshgrid(x,y);
15 [xxx,yyy] = meshgrid(-1:.0333:1,-1:.0333:1);
16 uuu = interp2(xx,yy,uu,xxx,yyy,'cubic');
17 figure, clf, surf(xxx,yyy,uuu),
18 xlabel x, ylabel y, zlabel u
19 text(.2,1,.022,sprintf('u(0,0)=%13.11f',uu(N/2+1,N/2+1))

```

Program (LRBF.m)

```

1 function [L,x,y] = LRBF(N,rbf,Lrbf)
2 if N==0, L=0; x=1; return, end
3 x = cos(pi*(0:N)/N)'; % Chebyshev points
4 y = x; [xx,yy] = meshgrid(x,y);
   % Stretch 2D grids to 1D vectors and put in one array
5 points = [xx(:) yy(:)];
6 mine = .1; maxe = 10; % Shape parameter interval
7 r = DistanceMatrix(points,points);
8a ep = fminbnd(@(ep) CostEpsilonLRBF(ep,r,rbf,Lrbf), ...
8b                                     mine,maxe);
9 fprintf('Using epsilon = %f\n', ep)
10 A = rbf(ep,r);
11 AL = Lrbf(ep,r);
12 L = AL/A;

```



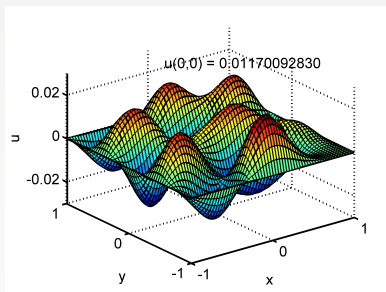


Figure: Solution of the 2D Helmholtz equation using a **direct implementation of the Laplacian** based on $\varphi_{3,3}(r) = (1 - \varepsilon r)_+^8 (32(\varepsilon r)^3 + 25(\varepsilon r)^2 + 8\varepsilon r + 1)$ with $\varepsilon = 0.129444$ on 625 tensor-product Chebyshev points.

Remark

- We use *compactly supported Wendland functions* in “*global mode*”.
- This *explains the definition of the basic function* in the MATLAB code as needed for `DistanceMatrix.m` in `LRBF.m`.

Consider the **2D Laplace equation** (see Program 36 of [Trefethen (2000)] and earlier examples)

$$u_{xx} + u_{yy} = 0, \quad x, y \in (-1, 1)^2,$$

with **boundary conditions**

$$u(x, y) = \begin{cases} \sin^4(\pi x), & y = 1 \text{ and } -1 < x < 0, \\ \frac{1}{5} \sin(3\pi y), & x = 1, \\ 0, & \text{otherwise.} \end{cases}$$

Remark

We don't list the code since it is too similar to previous examples and the original code in [Trefethen (2000)].



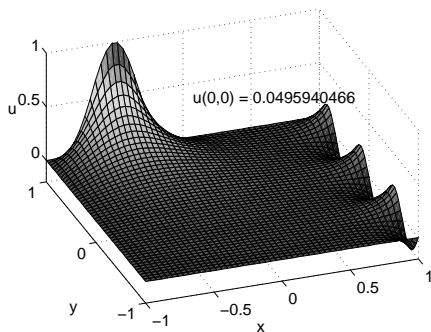
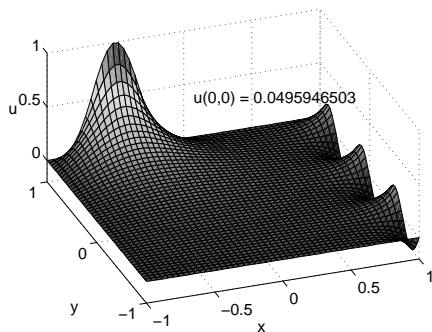


Figure: Solution of the 2D Laplace equation using a **Chebyshev PS** approach (left) and **Gaussian RBFs** (right) with $\varepsilon = 2.549845$ on 625 tensor-product Chebyshev collocation points.

The differentiation matrix for the RBF-PS approach is computed using the `D2RBF` and `kron` construction.








Remark

- While there is *no advantage in going to arbitrarily spaced irregular collocation points for any of the problems presented here*, there is *nothing that prevents us from doing so for the RBF-PS approach*.
- A potential *advantage of the RBF-PS approach* over the standard polynomial methods is the fact that we are *not limited to using tensor product grids* for higher-dimensional spatial discretizations.
- More *applications* of the RBF-PS method can be found in [Ferreira and Fasshauer (2006), Ferreira and Fasshauer (2007)].
- Future *challenges* include
 - dealing with *larger problems in an efficient and stable way*, and
 - coming up with *preconditioning and FFT-type algorithms*.
- *Eigenvalue stability* of RBF-PS methods have been reported in [Platte and Driscoll (2006)].



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