

MATH 590: Meshfree Methods

Chapter 43: RBF-PS Methods in MATLAB

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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



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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.



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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

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

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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(:));
```



Program (CostEpsilonDRBF.m)

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6  EF = (invA*rhs)./repmat(diag(invA),1,N);
7  ceps = norm(EF(:));

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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)
```

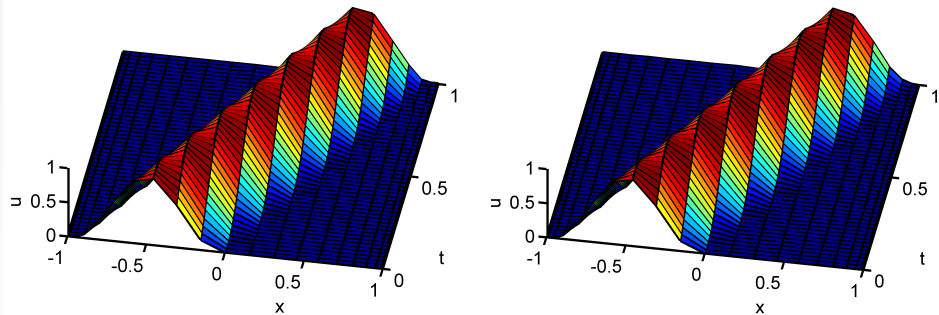


Figure: Time profiles of the solution to the transport equation for $0 \leq t \leq 1$ with initial profile $f(x) = \max(-64x^3(1+x)^3, 0)$ and unit wave speed based on **Gaussian RBFs** with $\varepsilon = 1.874049$ (left) and **Chebyshev PS** method (right). **Explicit Euler time-stepping** with $(\Delta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



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```
4  N=20; [D,x] = cheb(N); x = flipud(x); D = -D;
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where cheb.m is the subroutine provided on page 54 of [Trefethen (2000)] for spectral differentiation.



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



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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 $\mathbf{A}(\varepsilon)$.



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- 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

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



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- 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.



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- We will see that the non-limiting case (using `DRBF`) seems to work just as well.



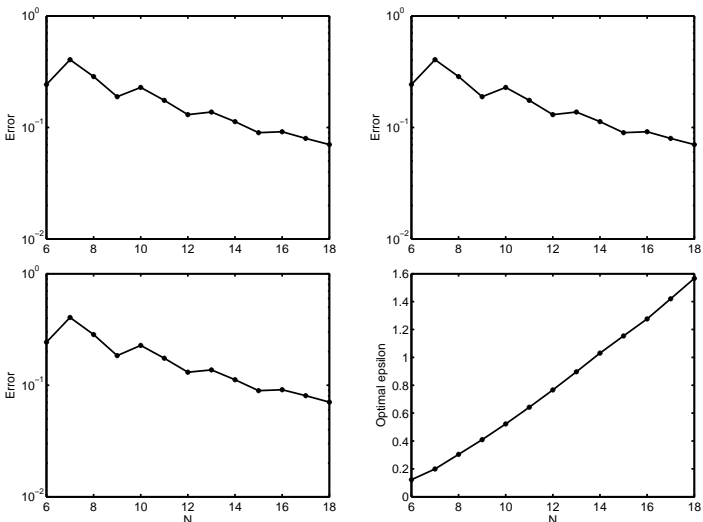


Figure: Errors at $t = 1$ for transport equation. Top: Gaussian RBF with $\epsilon = 0$ (left) and Chebyshev PS-solution (right). Bottom: Gaussian RBF with “optimal” ϵ (left) and corresponding ϵ -values (right). Variable spatial discretization N . Implicit Euler method with $\Delta t = 0.001$.



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- 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*.



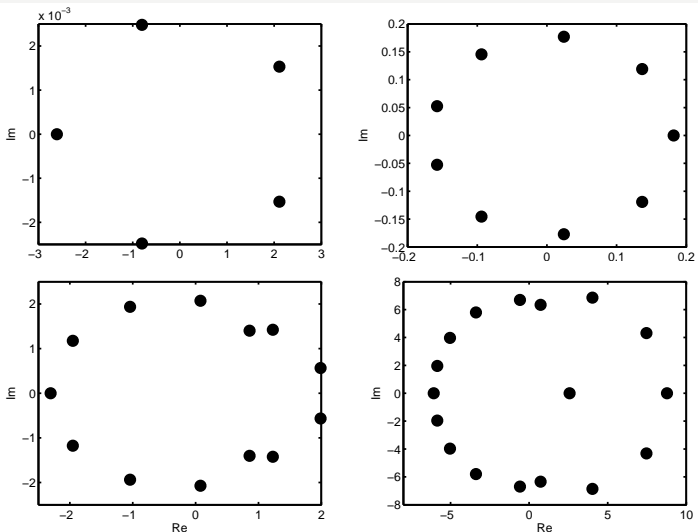


Figure: Spectra of differentiation matrices for **Gaussian RBF** with $\varepsilon = 0$ on Chebyshev collocation points obtained with the Contour-Padé algorithm and $N = 5, 9, 13, 17$.



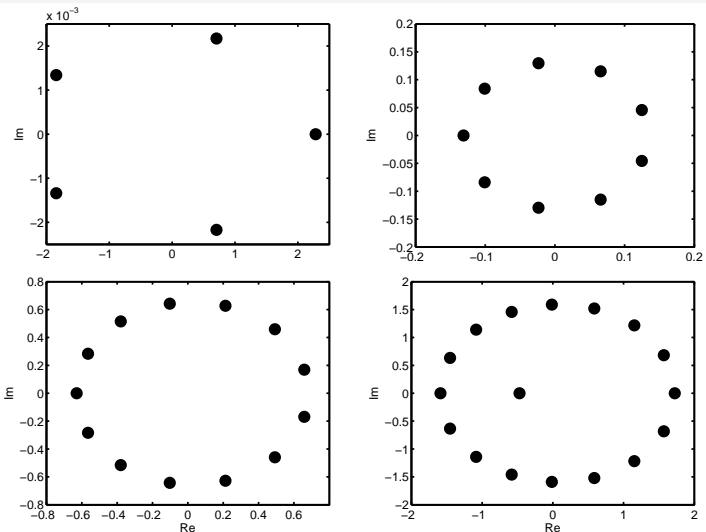


Figure: Spectra of differentiation matrices for Chebyshev pseudospectral method on Chebyshev collocation points with $N = 5, 9, 13, 17$.



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- 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* .



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

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



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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`.



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- *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**.



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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**

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



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**.

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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**.



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**.

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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.

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- In fact, this is the *main difference between the RBF-PS approach and the collocation approach* of Chapters 38–40.

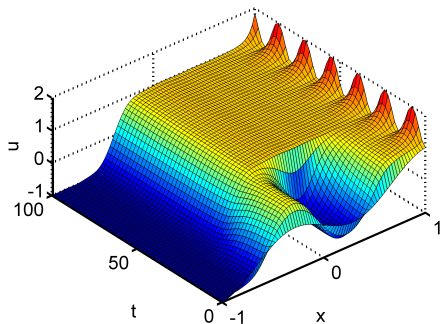
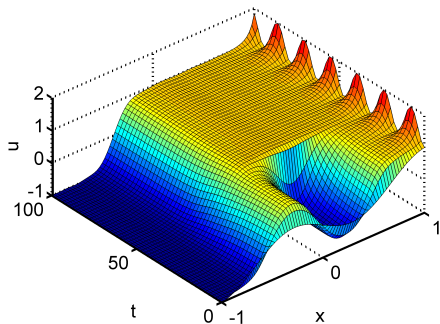


Figure: Solution of the Allen-Cahn equation using the **Chebyshev PS-method** (left) and an **RBF-PS method with cubic Matérn functions**

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



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- 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”.



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- 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 $\epsilon > 0$.*



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- 1 Computing the RBF-Differentiation Matrix in MATLAB
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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**

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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).



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- 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,
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- 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))

```

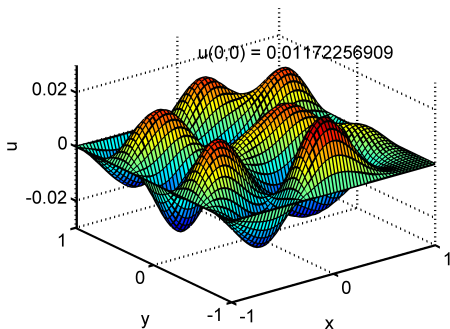
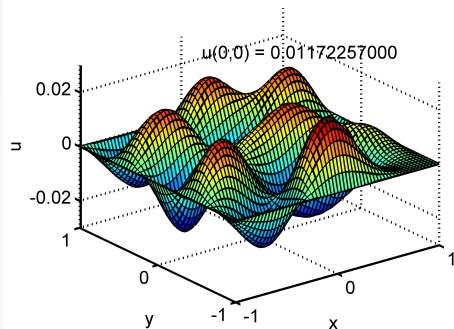


Figure: Solution of the 2D Helmholtz equation with $N = 24$ using the **Chebyshev pseudospectral method** (left) and **Gaussians** with $\varepsilon = 2.549845$ (right).



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- 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.

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- 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);
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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;

```



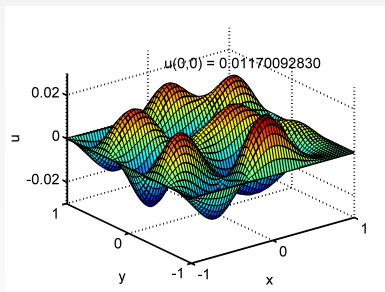


Figure: Solution of the 2D Helmholtz equation using a **direct implementation of the Laplacian** based on $\varphi_{3,3}(r) = (1 - \varepsilon r)_+^8 (32(\varepsilon r)^3 + 25(\varepsilon r)^2 + 8\varepsilon r + 1)$ with $\varepsilon = 0.129444$ on 625 tensor-product Chebyshev points.



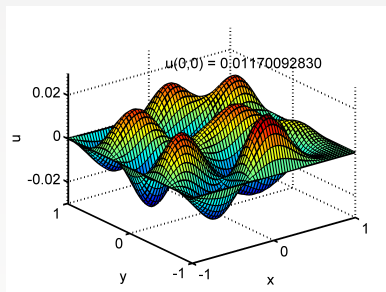


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Remark

- We use *compactly supported Wendland functions* in “*global mode*”.

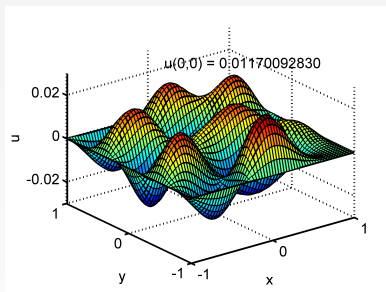


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- This *explains the definition of the basic function* in the MATLAB code as needed for `DistanceMatrix.m` in `LRBF.m`.

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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**

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



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



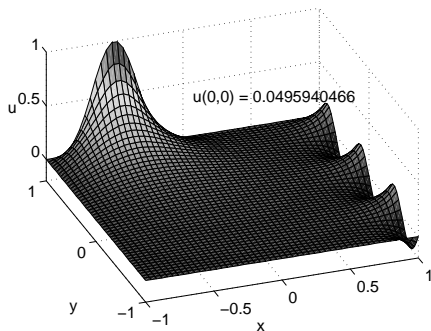
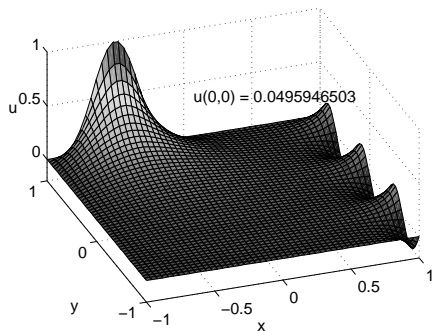


Figure: Solution of the 2D Laplace equation using a **Chebyshev PS** approach (left) and **Gaussian RBFs** (right) with $\varepsilon = 2.549845$ on 625 tensor-product Chebyshev collocation points.



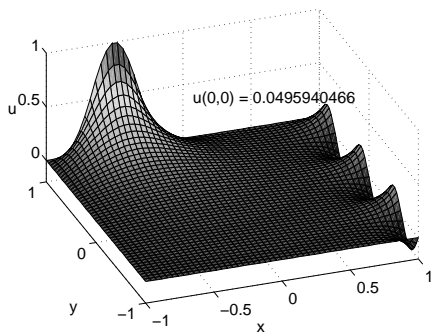
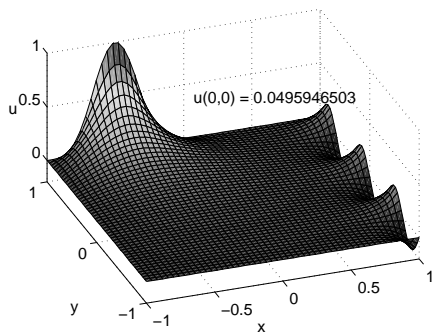


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The differentiation matrix for the RBF-PS approach is computed using the `D2RBF` and `kron` construction.



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- *Eigenvalue stability* of RBF-PS methods have been reported in [Platte and Driscoll (2006)].




References I

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