Topics in Radial Basis Function methods for time-dependent PDEs

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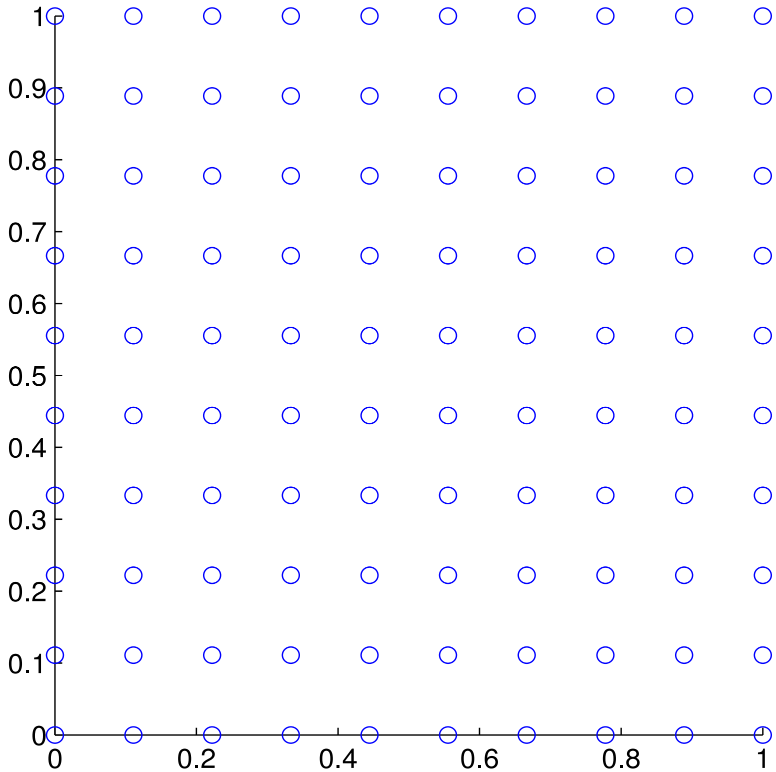
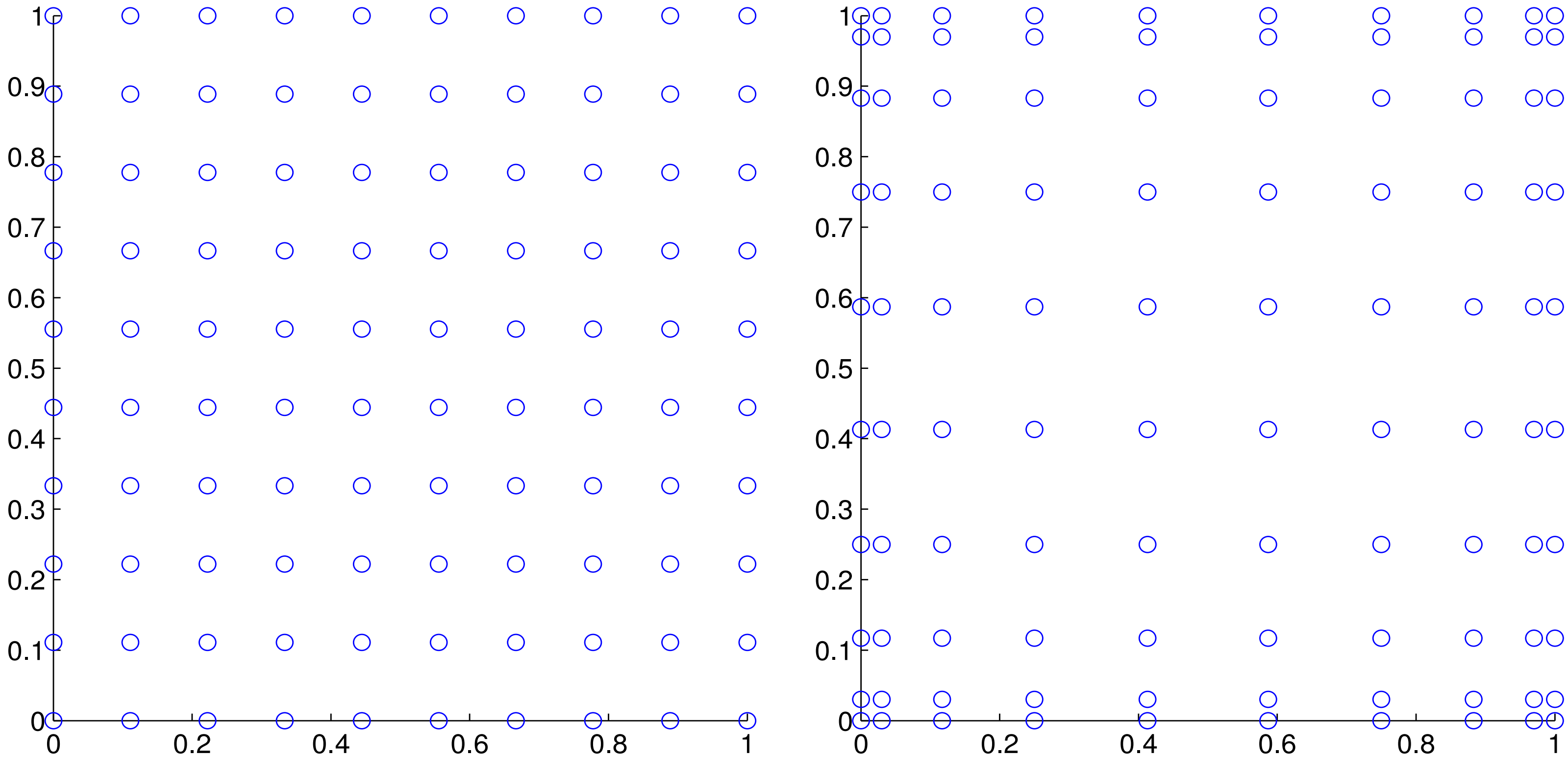
Talk Outline

- Symmetric and Asymmetric RBF Collocation Methods
- RBF methods for time-dependent PDEs
  - Eigenvalue Stability
  - Accuracy
  - Adaptive methods
  - Center Locations
- Approximating piecewise smooth functions
  - Digital Total Variation Filtering
- Future work and summary

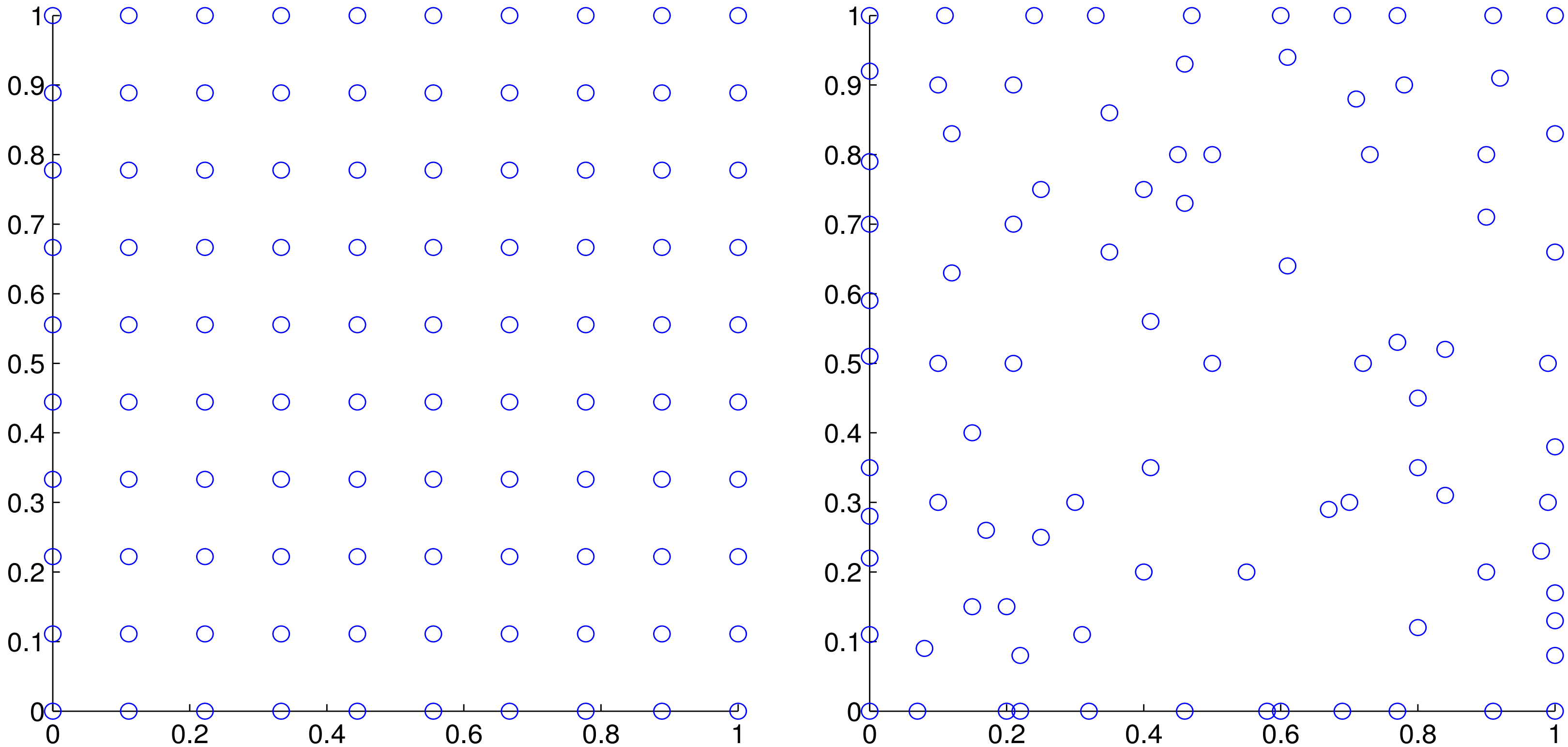
Scattered Approximations



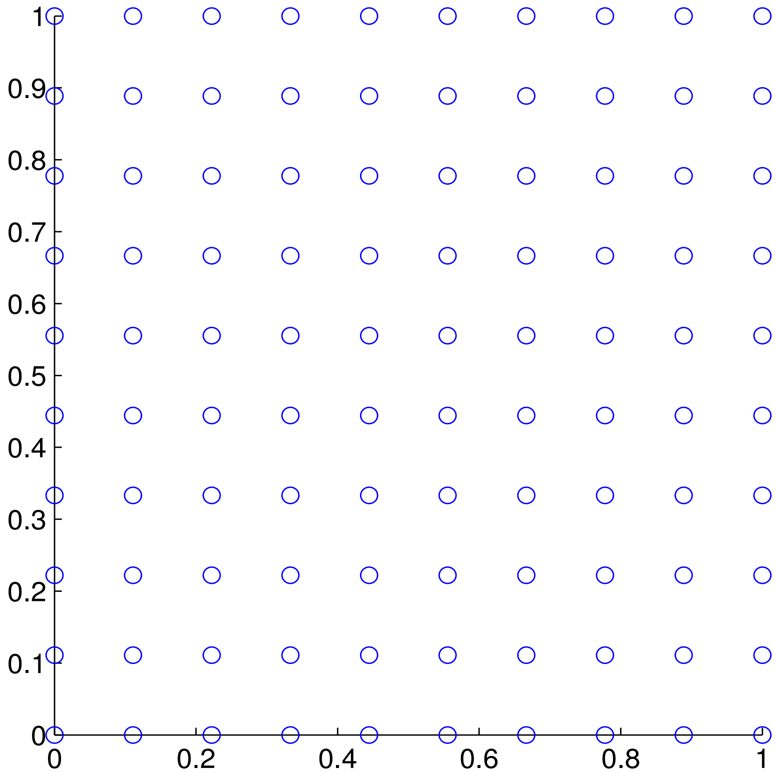
Scattered Approximations

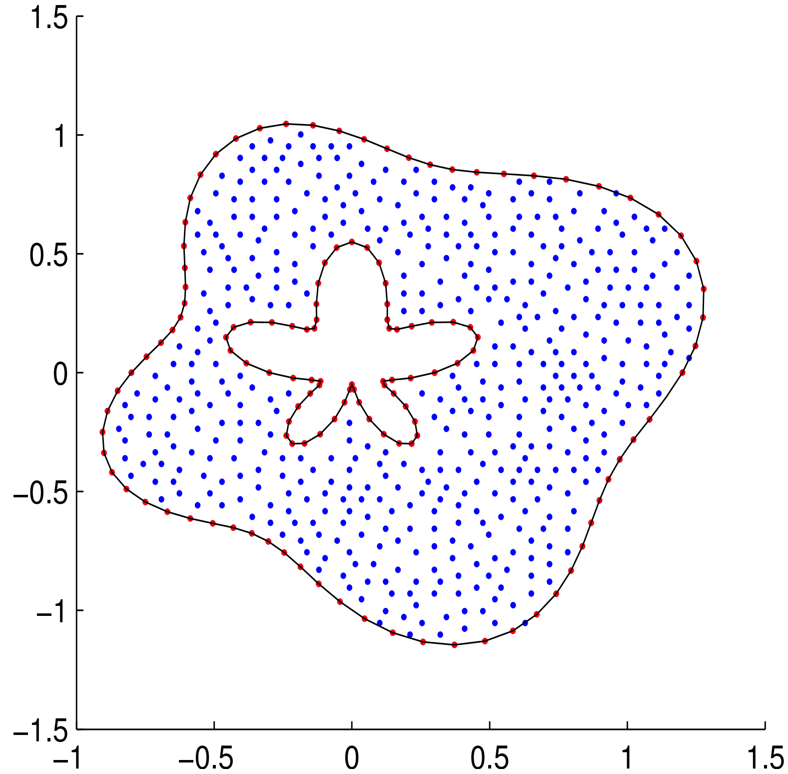


Scattered Approximations



Scattered Approximations





Definition - Radial Basis function

$$\phi(r = \|\mathbf{x}\|_2) : \mathbb{R}^d \rightarrow \mathbb{R}$$

- $\|\mathbf{x_1}\| = \|\mathbf{x_2}\| \Rightarrow \phi(\mathbf{x_1}) = \phi(\mathbf{x_2}), \quad \mathbf{x_1}, \mathbf{x_2} \in \mathbb{R}^d$
- approximation problems become insensitive to dimension
- use the same univariate function ϕ for all choices of d

Radial Basis functions

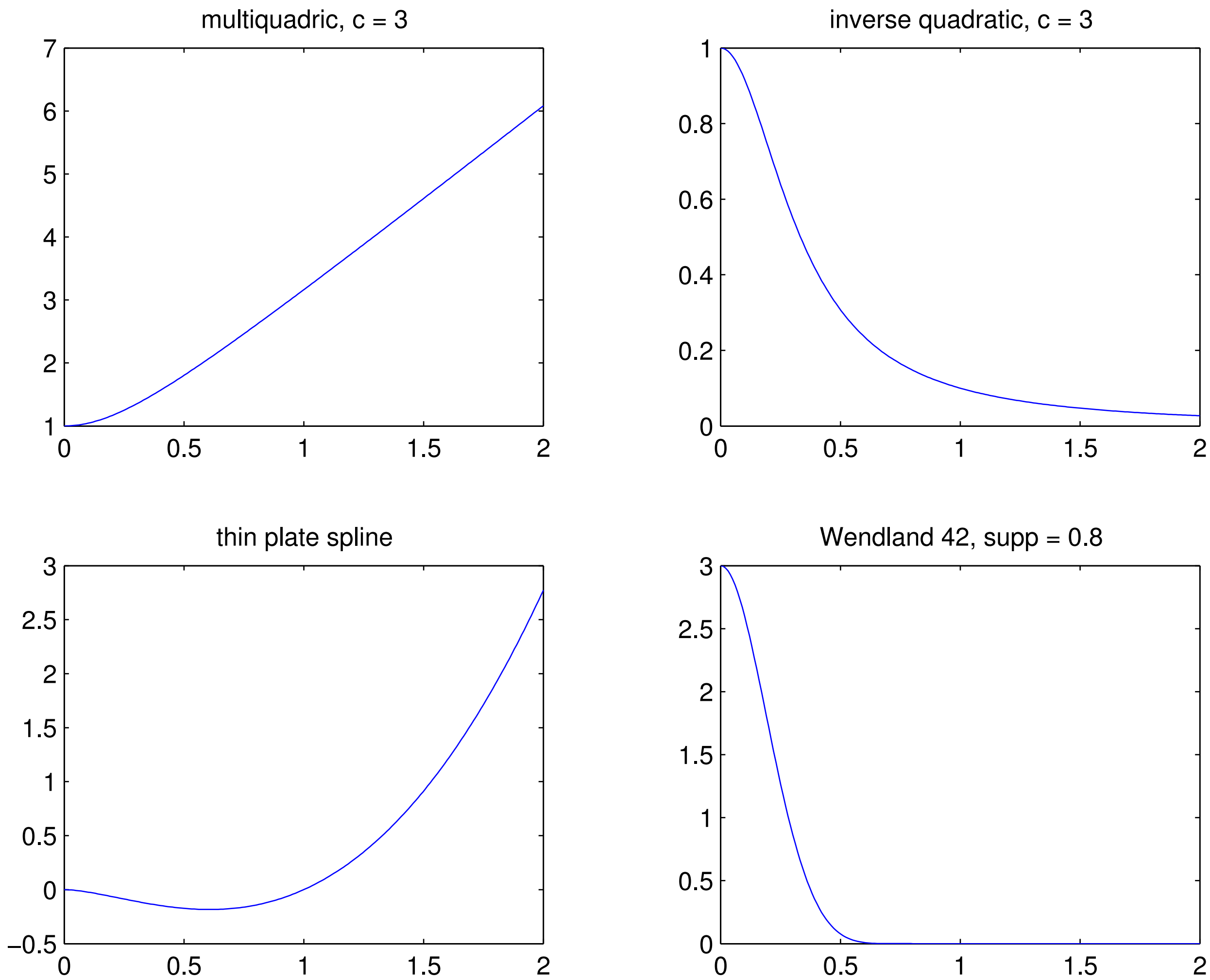
- **With shape parameter**
  - Multiquadric (MQ), $\phi(r,c) = \sqrt{1+c^2r^2}$
  - Inverse quadratic (IQ), $\phi(r,c) = 1/(1+c^2r^2)$
  - Gaussian (GS), $\phi(r,c) = e^{-(cr)^2}$

- **Without shape parameter**
  - Polyharmonic splines,

$$\phi(r) = \begin{cases} r^k & k \notin 2\mathbb{N} \\ r^{2k}\log r & k \in \mathbb{N}. \end{cases}$$

  - Wendland, $\phi(r) = (1-r)_+^{(l+2)} p(r)$ (compact support)

RBF graphs


multiquadric, c = 3
inverse quadratic, c = 3
thin plate spline
Wendland 42, supp = 0.8
7
6
5
4
3
2
1
1
0.8
0.6
0.4
0.2
0
3
2.5
2
1.5
1
0.5
0
–0.5
0
0.5
1
1.5
2

interpolation approximation orders

Fill distance

$$h = \sup_{y\in\Omega} \min_{0\le j\le N} \|\mathbf{y} - \mathbf{x}_j\|_2 \,.$$

Denotes the radius of the largest possible empty ball that can be placed among the data locations.

Convergence Results:

- polyharmonic splines, $\mathcal{O}\left(h^n\right)$
- multiquadric, $\mathcal{O}\left(e^{-K/h}\right)$, $K > 0$

good interpolation sites

Separation distance

$$q_\Xi = \frac{1}{2} \min_{i \neq j} \|\mathbf{x}_i - \mathbf{x}_j\|_2 \, .$$

The radius of the largest ball that can be placed around every point in Ξ such that no two balls overlap.

- for stability, q_Ξ can not be too small
- for convergence, h needs to be small
- obviously, not possible to minimize h and to maximize q_Ξ at the same time
- neither quantity depends on the RBF ϕ
- good points optimally balance h against q_Ξ by maximizing their **uniformity**

$$\rho_\Xi = \frac{q_\Xi}{h}$$

Shape parameter c

- "small" $c \Rightarrow$ better accuracy, worse conditioning of B.
- Uncertainty relation: The error and the condition number cannot both be kept small
- Interpolant equivalent to Lagrange interpolating polynomial as $c \to 0$ in 1d.
- $\nexists$ a formula to specify the optimal value of c.
- The optimal c is often unreachable with standard algorithms.

RBF Collocation Methods

- the **system matrix** H_m discretizes the differential operator L
- the **evaluation matrix** B_m consists of the functions serving as the basis of the approximation space.
- The methods derive their names from the fact that the **symmetric method** has a symmetric system matrix while the **asymmetric system** matrix is in general not symmetric.

Asymmetric Collocation

Assumes an approximant of the form

$$u(x) = \sum_{j=1}^{N} \lambda_j \phi(\|x - x_j\|_2), \quad x \in \mathbb{R}^d.$$

Discretizes L as

$$Lu(x_i) = \sum_{j=1}^{N} \lambda_j L\phi(\|x_i - x_j\|_2), \quad i = 1, \ldots, N_I,$$

Enforces boundary conditions

$$u(x_i) = \sum_{j=1}^{N} \lambda_j \phi(\|x_i - x_j\|_2), \quad i = N_I + 1, \ldots, N.$$

Asymmetric Differentiation matrix

$$D_a = H_a B_a^{-1} = \begin{bmatrix} L\phi \\ \phi \end{bmatrix} \begin{bmatrix} \phi \end{bmatrix}^{-1}$$

where the two blocks of H_a are generated as

$$\begin{aligned} (L\phi)_{i,j} &= L\phi(\|x_i - x_j\|_2), \qquad i = 1, \ldots, N_I \quad j = 1, \ldots, N \\ (\phi)_{i,j} &= \phi(\|x_i - x_j\|_2), \qquad i = N_I + 1, \ldots, N \quad j = 1, \ldots, N \end{aligned}$$

and B_a is defined by

$$(\phi)_{i,j} = \phi(\|x_i - x_j\|_2), \qquad i, j = 1, \ldots, N.$$

For all positive definite RBFs, as well as the conditionally positive definite MQ, the **evaluation matrix** B_a is known to be invertible. Thus we can always form D_a.

Symmetric Collocation

Assumes an approximant of the form

$$u(x) = \sum_{j=1}^{N-N_B} \lambda_j L^* \phi(\|x - x_j\|_2) + \sum_{N-N_B+1}^{N} \lambda_j \phi(\|x - x_j\|_2), \quad x \in \mathbb{R}^d.$$

Discretizes L as

$$Lu(x_i) = \sum_{j=1}^{N-N_B} \lambda_j L L^* \phi(\|x_i - x_j\|_2) + \sum_{N-N_B+1}^{N} \lambda_j L\phi(\|x_i - x_j\|_2), \quad x \in \mathbb{R}^d.$$

Enforces boundary conditions

$$u(x_i) = \sum_{j=1}^{N-N_B} \lambda_j L^* \phi(\|x_i - x_j\|_2) + \sum_{N-N_B+1}^{N} \lambda_j \phi(\|x_i - x_j\|_2), \quad i = N_I+1, \ldots, N.$$

Symmetric Differentiation matrix

$$D_s = H_s B_s^{-1} = \begin{bmatrix} LL^*\phi & L\phi \\ L^*\phi & \phi \end{bmatrix} \begin{bmatrix} L^*\phi & \phi \end{bmatrix}^{-1}$$

where the blocks of H_s are

$$\begin{aligned}
(LL^*\phi)_{i,j} &= LL^*\phi(\|x_i - x_j\|_2), \quad i = 1,\dots,N_I \quad j = 1,\dots,N_I \\
(L\phi)_{i,j} &= L\phi(\|x_i - x_j\|_2), \quad i = 1,\dots,N_I \quad j = N_I+1,\dots,N \\
(L^*\phi)_{i,j} &= L^*\phi(\|x_i - x_j\|_2), \quad i = N_I+1,\dots,N \quad j = 1,\dots,N_I \\
\phi_{i,j} &= \phi(\|x_i - x_j\|_2), \quad i = N_I+1,\dots,N \quad j = N_I+1,\dots,N
\end{aligned}$$

and the blocks of B_s are

$$\begin{aligned}
(L^*\phi)_{i,j} &= L^*\phi(\|x_i - x_j\|_2), \quad i = 1,\dots,N \quad j = 1,\dots,N_I \\
\phi_{i,j} &= \phi(\|x_i - x_j\|_2), \quad i = 1,\dots,N \quad j = N_I+1,\dots,N.
\end{aligned}$$

Kansa matrix

$$H_a = \begin{bmatrix} L\phi \\ \phi \end{bmatrix} = B_s^T = \begin{bmatrix} L^*\phi & \phi \end{bmatrix}^T = \begin{bmatrix} L\phi \\ \phi \end{bmatrix}$$

$Lu = f$

Asymmetric

$$\begin{aligned} D_a u &= f \\ u &= D_a^{-1} f \\ u &= B_a H_a^{-1} f \end{aligned}$$

Symmetric

$$\begin{aligned} D_s u &= f \\ u &= D_s^{-1} f \\ u &= B_s H_s^{-1} f \end{aligned}$$

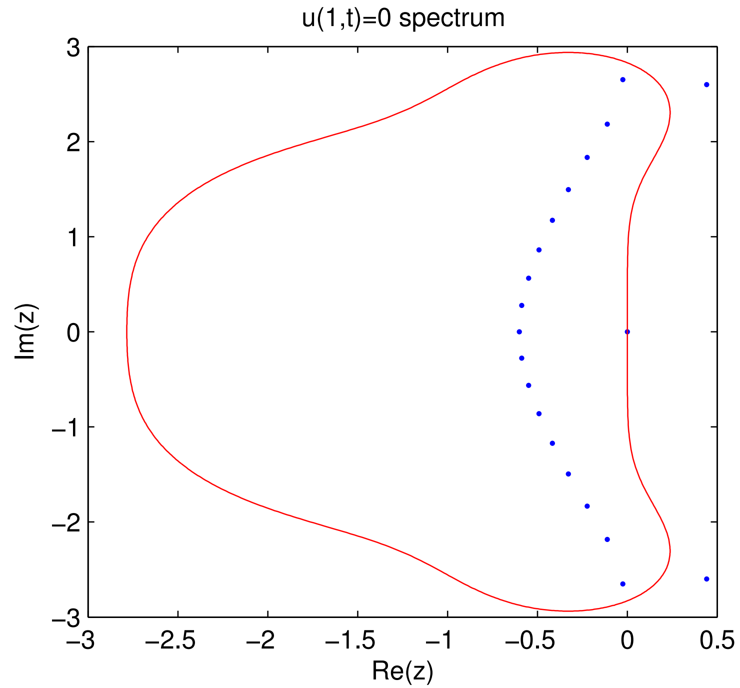
Time Dependent PDEs

Method of Lines

PDE is discretized in space with RBFs to get the semi-discrete system

$$\frac{\partial s}{\partial t} = F(s).$$

The system of ODEs advanced in time with any ODE method.



Some Examples

The one dimensional advection equation

$$\frac{\partial u}{\partial t} - \frac{\partial u}{\partial x} = 0$$

on the interval $\Omega = [-1, 1]$ with boundary condition $u(1, t) = 0$ and initial condition $u(x, t) = cos(\pi(x + t))$.

- $L = \frac{\partial}{\partial x}$
- $L^* = -\frac{\partial}{\partial x}$
- $LL^* = -\frac{\partial^2}{\partial x^2}$

Center Locations, $N = 100$

1. equidistant
2. Chebyshev pseudospectral (CPS) grid

$$x_i = -\cos(i\pi/N), \quad i = 0, 1, \ldots, N$$

3. mapped CPS grid

$$x_i = \frac{\arcsin\left[-\gamma\cos(i\pi/N)\right]}{\arcsin\gamma}, \quad i = 0, 1, \ldots, N \text{ and } 0 < \gamma < 1,$$

4. a “RBF grid” consisting of 86 equidistant interior centers and 7 mapped CPS centers near each boundary.
5. Random center locations generated by the following Matlab script:

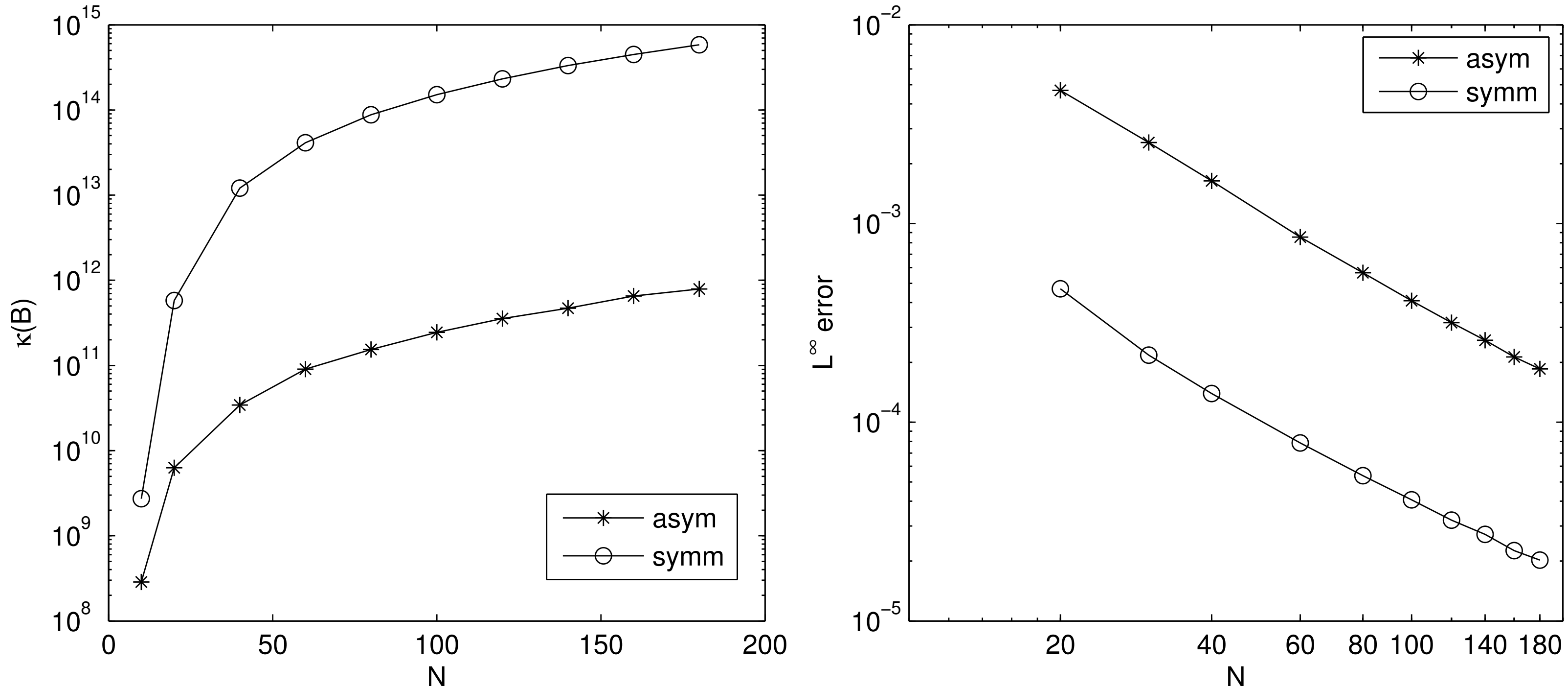
```
x = rand(100,1);  x = sort(x);
x(1) = 0;   x(end) = 1;
x = 2*x - 1;   % [0,1] -> [-1,1].
```

Condition Number Bounds on B

RBF	$\max(\kappa_s)$	$\max(\kappa_a)^\star$
MQ	1e14	1e10
IQ	1e13	1e9
IMQ	1e13	1e9
GA	1e11	1e7

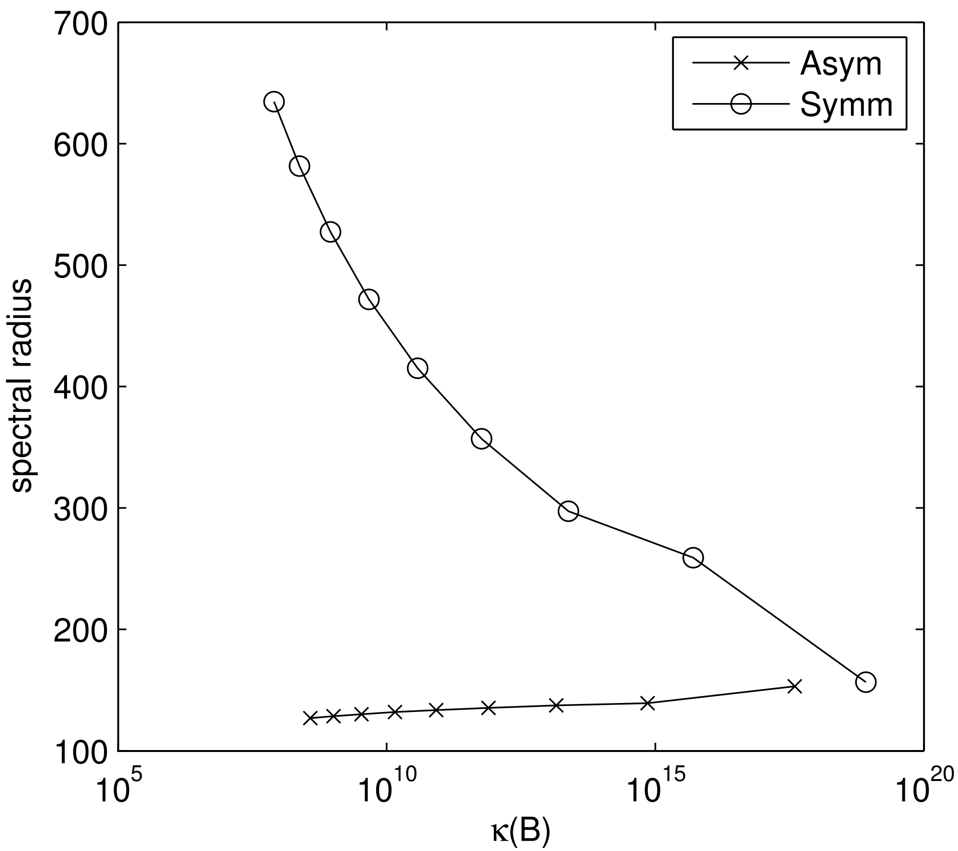
Stable condition number bounds for the symmetric and asymmetric methods for five $N = 100$ center distributions (* For randomly located centers, the asymmetric method does not have a stable spectrum for any condition number.)

Accuracy on Uniform Centers



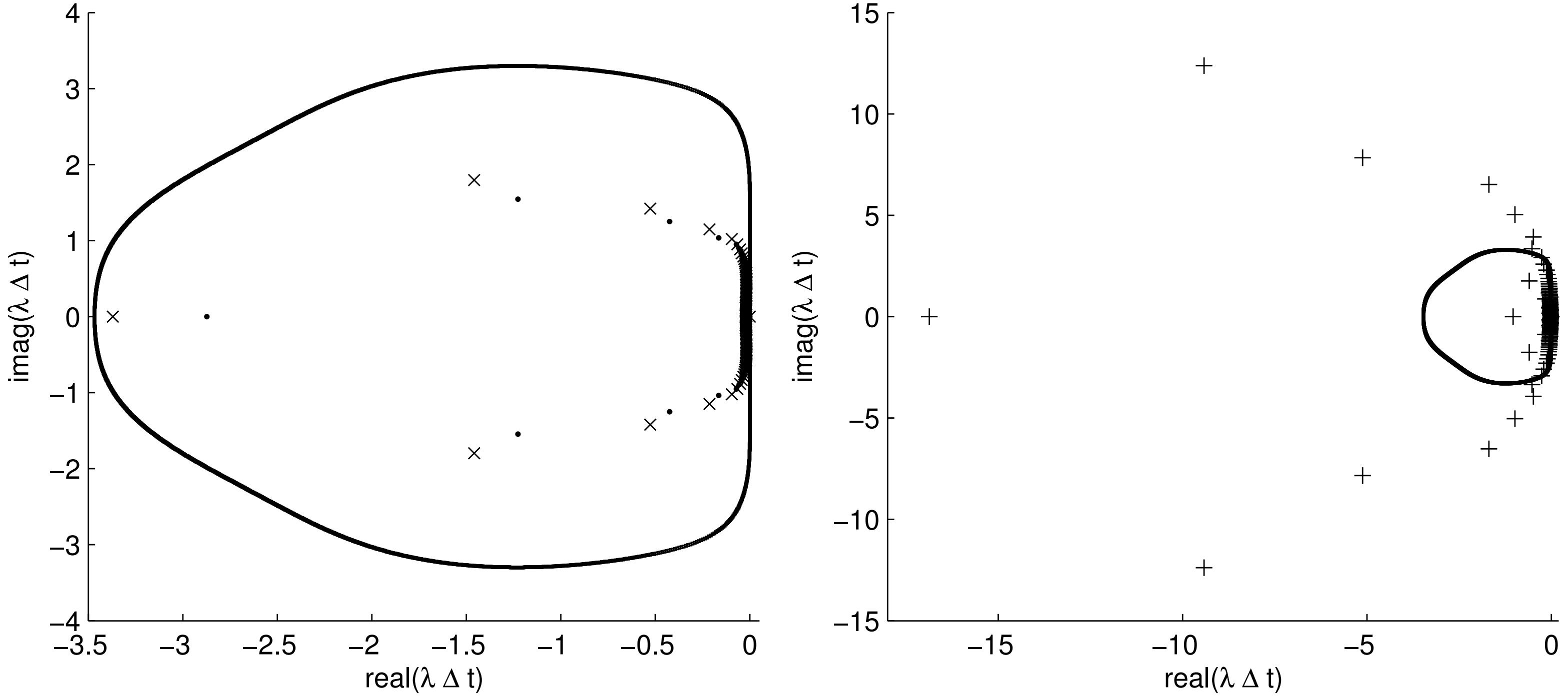
Left: Upper bound of the stable condition number range of the MQ B_a and B_s with increasing N equidistant center distributions. Right: Maximum error from equidistant center MQ approximation at $t = 5$ for increasing N.

Spectral Radius of D



Spectral radius of D versus $\kappa(B)$ for a first order PDE.

Larger c, smaller $\kappa(B)$



Stability region of LDDRK46 and spectra of the MQ D_s scaled by $\Delta t = 0.005$. Left: $c = 11$ and $\kappa(B_s) = 3.7e13$ (.), $c = 13$ and $\kappa(B_s) = 2.3e12$ (x). Right: $c = 100$ and $\kappa(B_s) = 2.7e6$ (+).

$N_B = 0$

$$\frac{\partial u}{\partial t} + x\frac{\partial u}{\partial x} = 0$$

on the interval $[-1, 1]$. The initial condition is taken from the exact solution $u(x,t) = e^{-400(xe^{-t})^2}$. The differentiation matrix for this example is $D =$ diag$(-x)D_m$.

- B_s is singular
- $\kappa(B_a) \leq 5e15$ produces stable DM on all center locations except random

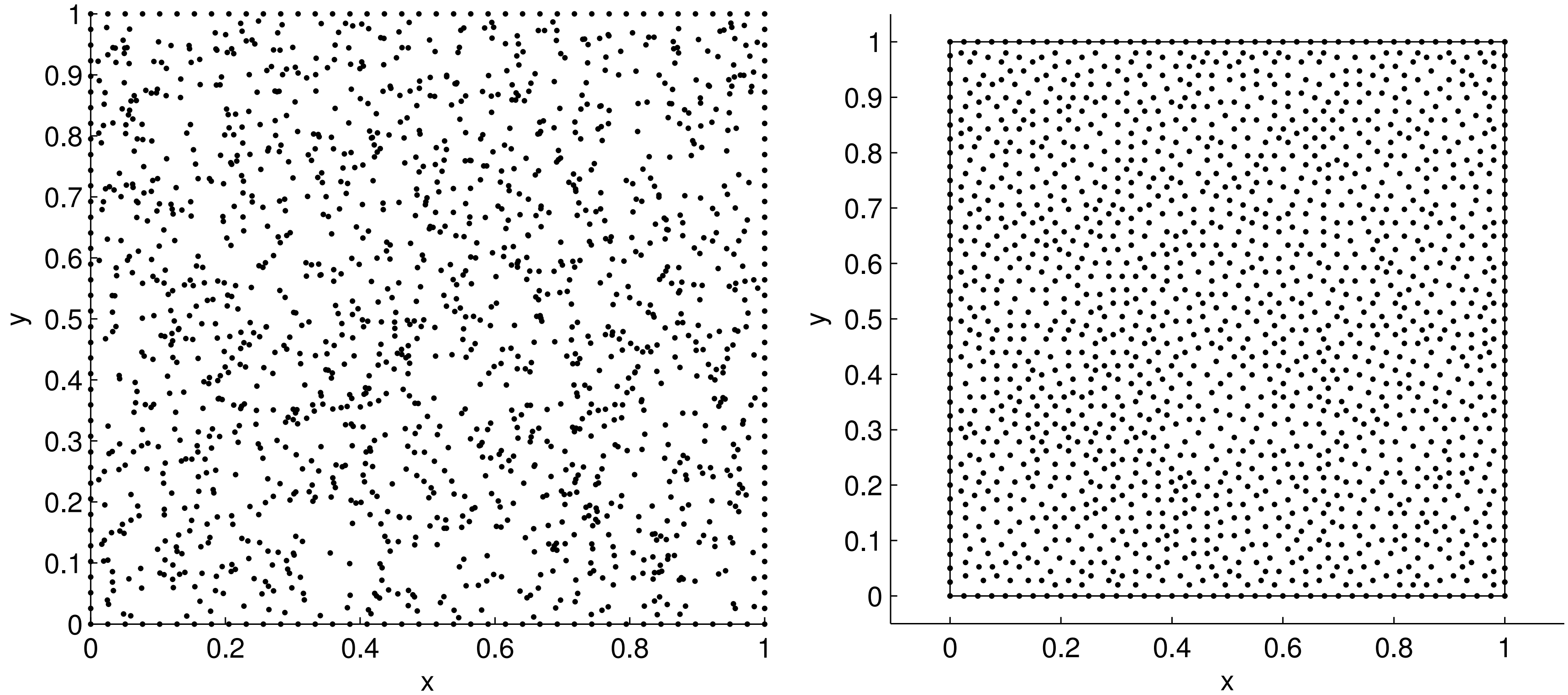
2d

$$\frac{\partial u}{\partial t} - \mu_x \frac{\partial u}{\partial x} - \mu_y \frac{\partial u}{\partial y} = 0$$

on the unit square $[0,1] \times [0,1]$ with $\mu_x = \mu_y = 1$. Dirichlet boundary conditions, $u(1,y,t) = 0$ and $u(x,1,t) = 0$, initial condition $u(x,y,0) = e^{-100[(x-0.7)^2+(y-0.7)^2]}$

- $L = \mu_x \frac{\partial}{\partial x} + \mu_y \frac{\partial}{\partial y}$
- $L^* = -\mu_x \frac{\partial}{\partial x} - \mu_y \frac{\partial}{\partial y}$
- $LL^* = -\mu_x^2 \frac{\partial}{\partial x} - \mu_x \mu_y \frac{\partial^2}{\partial x \partial y} - \mu_y^2 \frac{\partial}{\partial y}$

2d center locations



Left: 1600 randomly located centers. Right: $N = 1600$ near optimal center locations for example

Near optimal centers

- S. De Marchi, R. Schaback, and H. Wendland. Near-optimal data- independent point locations for radial basis function interpolation. Advances in Computational Mathematics, pages 1-14, 2004.
- center sets have small fill distances
- large separation distances
- add new centers to fill the largest hole in the existing center set

Condition Number Bounds

	symmetric		asymmetric	
centers	$\kappa(B_s)$ bound	$er_{t=.4}$	$\kappa(B_a)$ bound	$er_{t=.4}$
uniform	$1e14$	2.4e-4	$1e14$	3.7e-5
optimal	$1e14$	8.6e-5	$1e12$	4.2e-5
random	$1e14$	7.4e-4	$-$	4.7e-2

Stable condition number bounds for the symmetric and asymmetric methods for five $N = 1600$ center distributions (* For randomly located centers, the asymmetric method does not have a stable spectrum for any condition number.)

$N_B = 0$

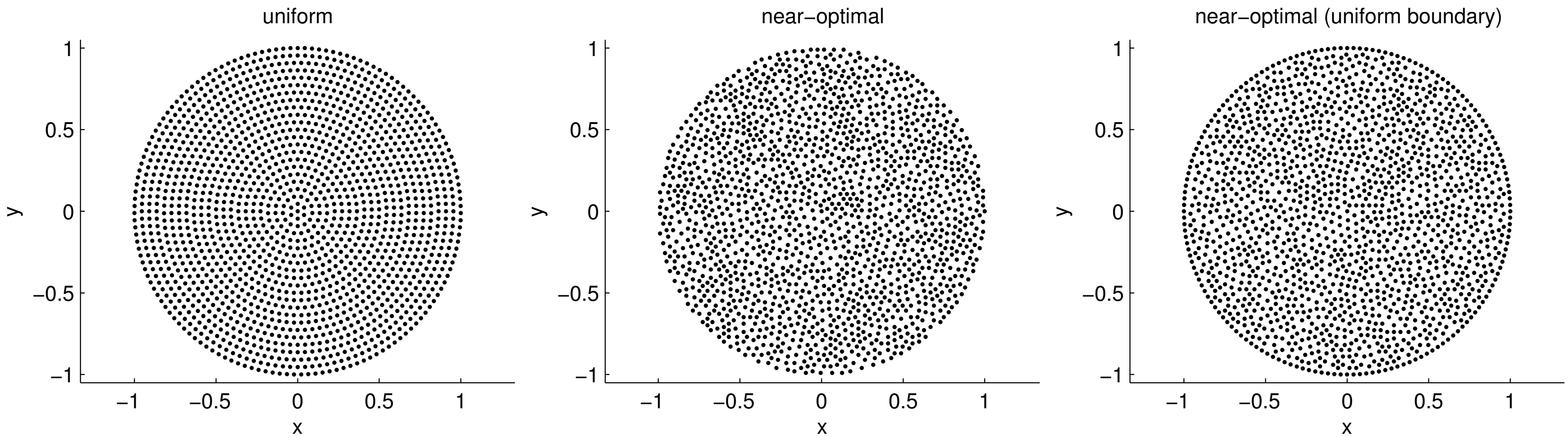
$$\frac{\partial u}{\partial t} - 2y\frac{\partial u}{\partial x} + 2x\frac{\partial u}{\partial y} = 0.$$

on the unit circle centered at the origin with initial condition

$$u(x,y) = e^{-200((x-0.3)^2+(y-0.3)^2)}.$$

$$\mathsf{D}_a = \text{ diag } (-2\mathsf{y})\ \mathsf{DX}_a + \text{ diag } (2\mathsf{x})\ \mathsf{DY}_a$$

center locations

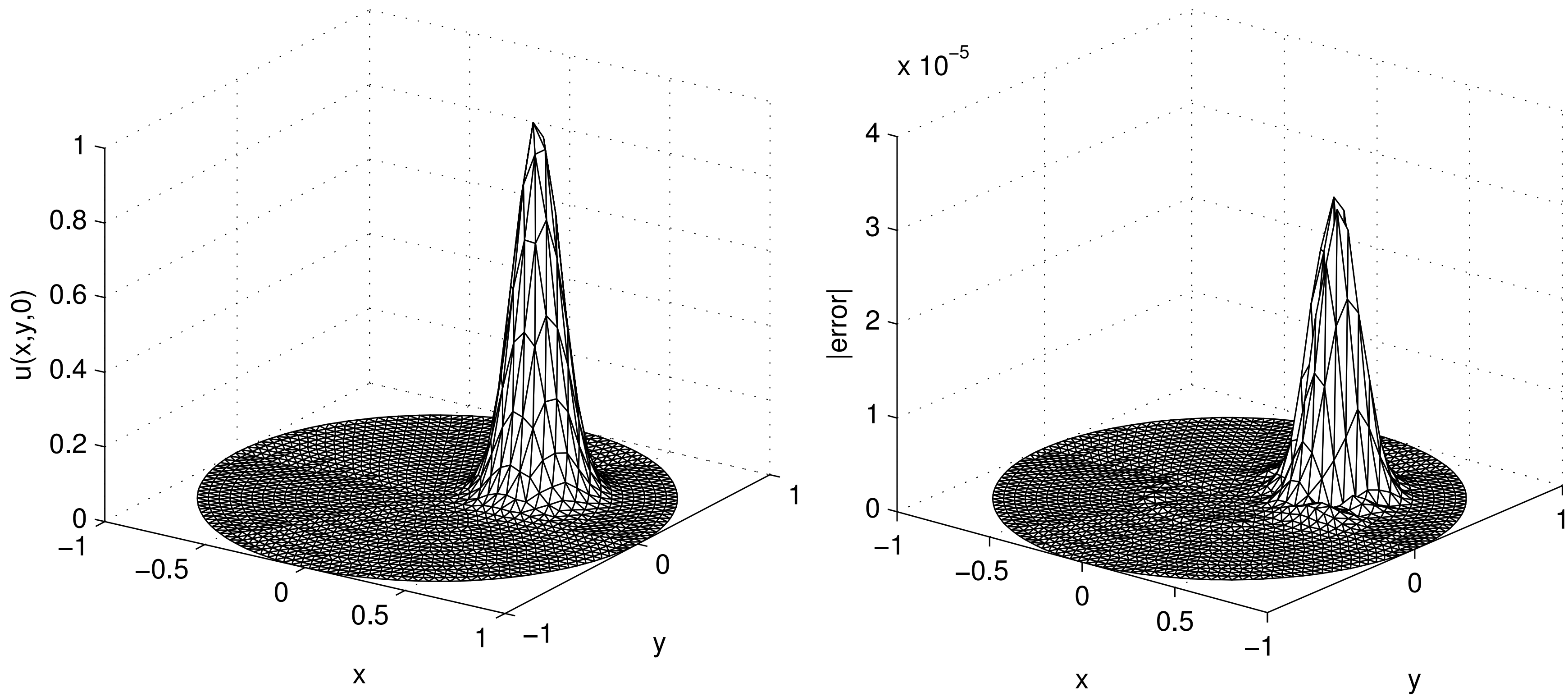


Left: uniformly distributed. Middle: near-optimal. Right: near-optimal with uniform boundary.

Accuracy

center distribution	$er_{t=\pi}$	$er_{t=5\pi}$	$er_{t=10\pi}$
uniform	3.1e-6	1.6e-5	3.1e-5
near-optimal (n-o)	2.3e-5	1.3e-4	2.4e-4
n-o w/uniform boundary	8.9e-6	4.6e-5	8.8e-5

solution and error



Exact solution and error after 10 rotations.

A second order operator

$$\frac{\partial^2 E}{\partial t^2} = \frac{\partial^2 E}{\partial x^2} + \frac{\partial^2 E}{\partial y^2}$$

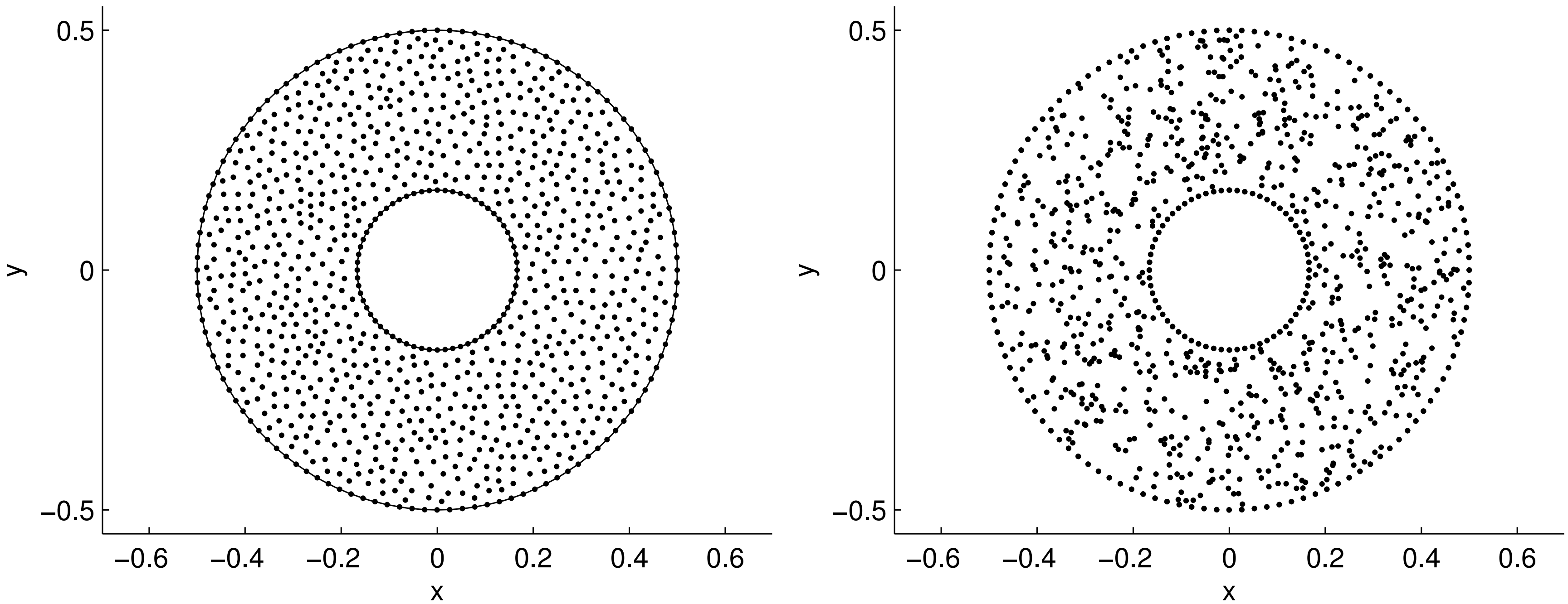
The initial conditions are taken from the exact solution

$$E(r, \theta, t) = \cos\left(\omega t + \theta\right)\left[J_1(\omega r) + \alpha Y_1(\omega r)\right]$$

$\theta = \arctan(y/x)$, J and Y are Bessel functions,
$\alpha = 1.76368380110927$, $\omega = 9.813695999428405$

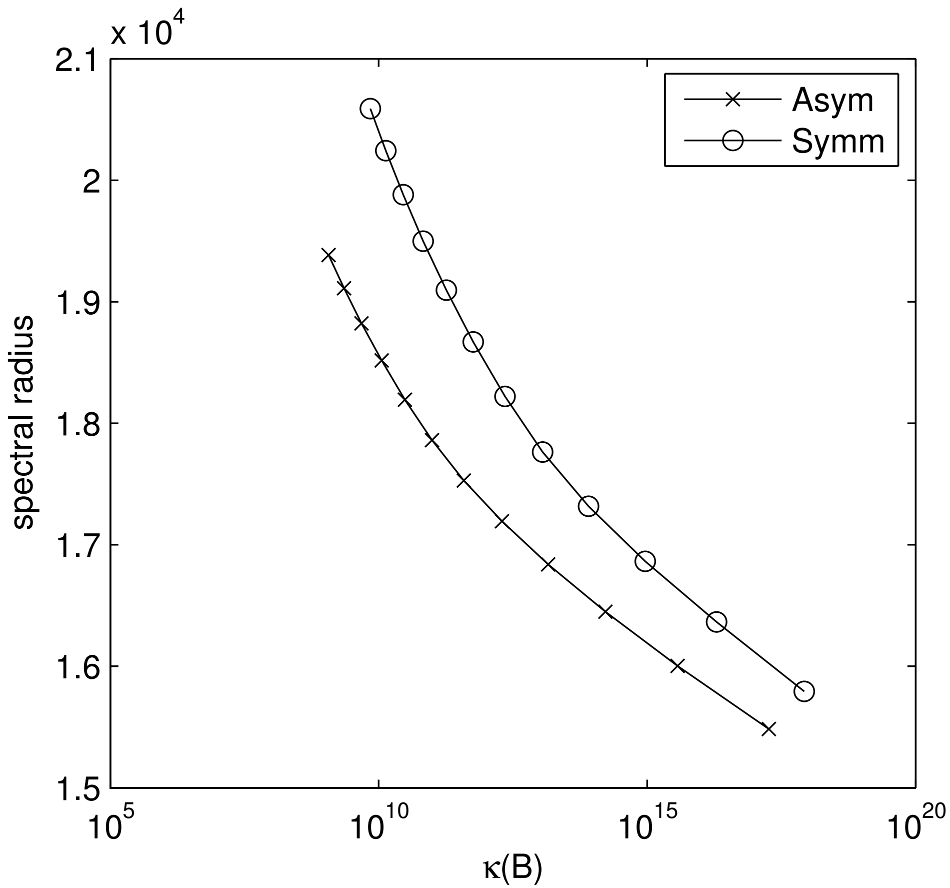
- $L = L^* = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}$
- $LL^* = \frac{\partial^4}{\partial x^4} + 2\frac{\partial^4}{\partial x^2 \partial y^2} + \frac{\partial^4}{\partial y^4}$

Centers



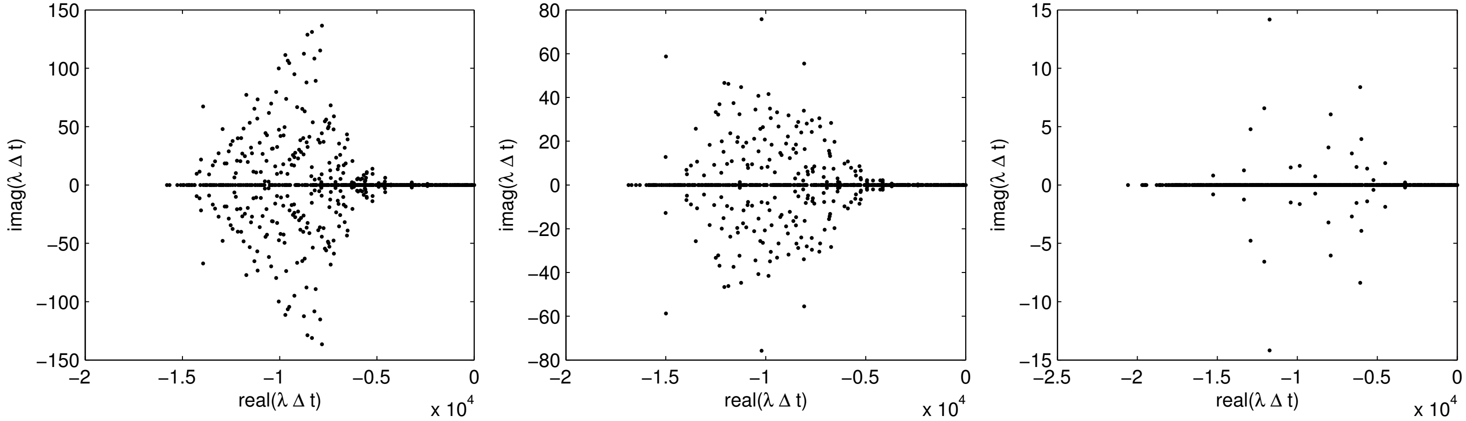
Left: Domain and $N = 1000$ near optimal centers. Right: Randomly located centers.

Spectral Radius of D

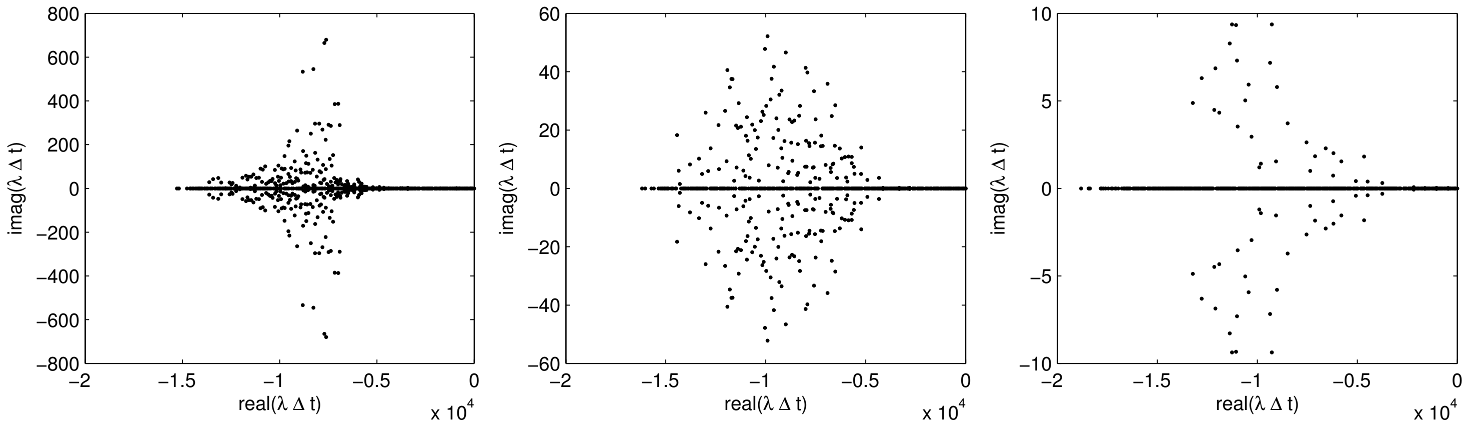


Spectral radius of D versus $\kappa(B)$ for a second order PDE.

Eigenvalues of D



From left to right: $\kappa(B_s)$ =1e18, $\kappa(B_s)$ =1e15, $\kappa(B_s)$ =1e10



From left to right: $\kappa(B_a)$ =1e18, $\kappa(B_a)$ =1e15, $\kappa(B_a)$ =1e10

Accuracy, $\kappa(B) \approx$ 1e15

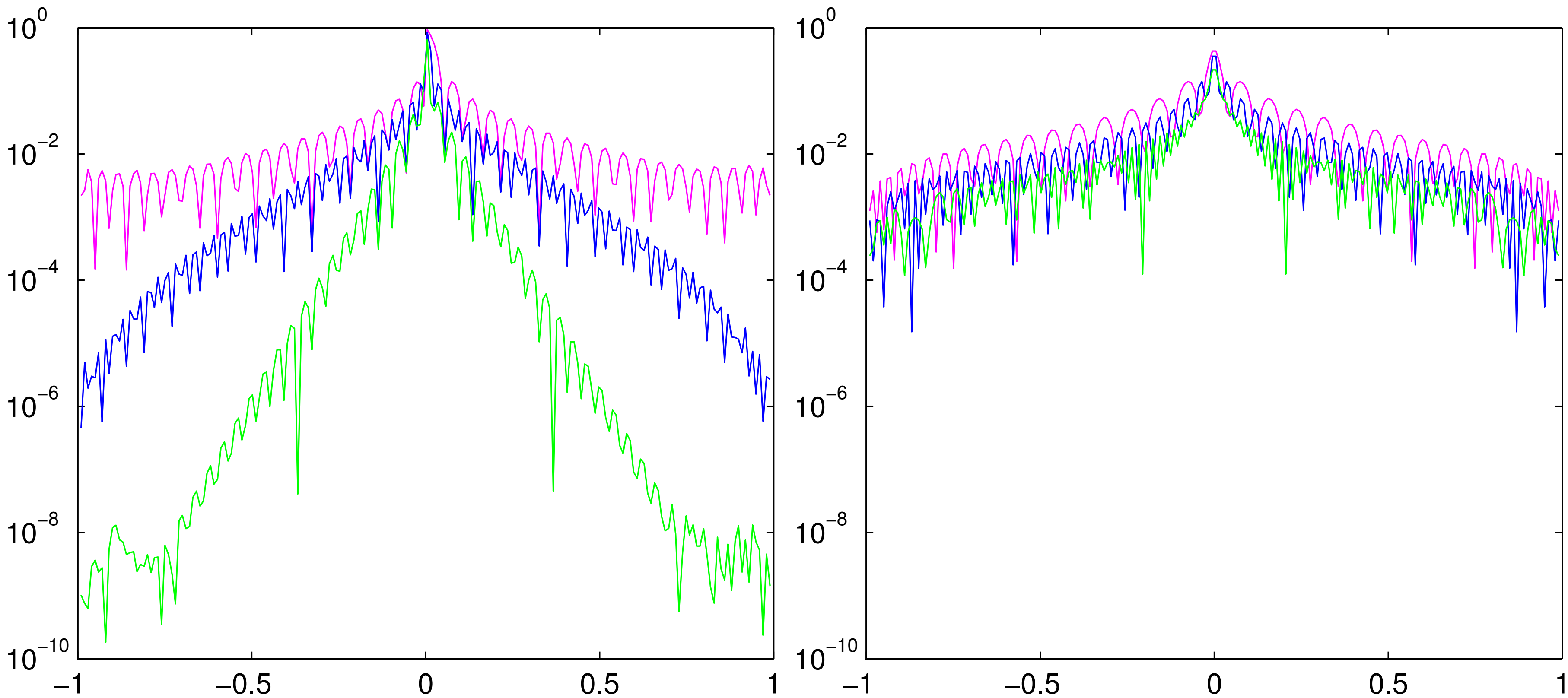
	t = 1	t = 10
Symm	6.8 e-3	6.1 e-2
Asym	6.1 e-3	4.7 e-2

Asym vs. Symm summary

- Symmetric method for first-order IBVPs
- Asymmetric method when BCs not applied - limited to structured grid
- Second-order operators do not have the stability issues that first-order operators do

Approximating Discontinuous Functions

RBF vs. Pseudospectral Gibbs



From top to bottom, $N = 39, 79, 159$. Left: MQ RBF. Right: Chebyshev.

DTV Postprocessing

Digital Total Variation filtering as postprocessing for Radial Basis Function Approximation Methods, Computers and Mathematics with Applications, 2006.

Digital TV Filtering - overview

- Originated in Image Processing
- Built-in Edge Detection
- Simple and Computationally Efficient
- A potential Black-Box algorithm
- Applicable to other approximations, for example see *Digital Total Variation filtering as postprocessing for Chebyshev Pseudospectral Methods for Conservation Laws*, Numerical Algorithms, vol. 41, p. 17-33, 2006.

Digital TV Filtering - notation

- Let $[\Omega, G]$ be a finite set Ω of points and a dictionary of edges G.
- vertices are denoted by $\alpha, \beta, \cdots$.
- $\alpha \sim \beta$ indicates that α and β are linked by an edge
- All the neighbors of α are denoted by

$$N_\alpha = \{\beta \in \Omega \,|\, \beta \sim \alpha\}$$

- u^0, Gibbs contaminated data on Ω that is an approximation to exact data u

Digital TV Filtering

- Postprocess by by solving the unconstrained minimization problem, minimize the fitted TV energy

$$E_\lambda^{TV}(u) = \sum_{\alpha \in \Omega} \|\nabla_g u_\alpha\|_a + \frac{\lambda}{2} \|u - u^0\|_\Omega^2$$

- The *regularized location variation* is

$$\|\nabla_g u_\alpha\|_a = \left[\sum_{\beta \in N_\alpha} (u_\beta - u_\alpha)^2 + a^2 \right]^{1/2}$$

DTV - parameters

the parameter λ is *fitting parameter* corresponding to a Lagrange multiplier in the variational problem that has been digitized

The *regularization parameter* a is a small constant to avoid a zero local variation

Digital TV Filtering

- Leads to a system of nonlinear equations which has a unique solution that depends on λ and u^0.
- Solved by a linearized Jacobi iteration as

$$
\begin{aligned}
u_\alpha^{[n+1]} &= \frac{\lambda}{\lambda + \sum_{\beta \in N_\alpha} w_{\alpha\beta}(u^{[n]})} u_\alpha^0 \\
&+ \sum_{\beta \in N_\alpha} \frac{w_{\alpha\beta}(u^{[n]})}{\lambda + \sum_{\beta \in N_\alpha} w_{\alpha\beta}(u^{[n]})} u_\beta^{[n]}
\end{aligned}
$$

where

$$
w_{\alpha\beta}(u) = \frac{1}{\|\nabla_g u_\alpha\|_a} + \frac{1}{\|\nabla_g u_\beta\|_a}
$$

DTV: specifying λ

- Typically, a wide range of λ results in an accurate postprocessing
- Currently, no way to specify an optimal λ
- Strong oscillations - small λ
- Weak oscillations - large λ

DTV: maximum principle

The DTV filter is a lowpass filter

It satisfies the *maximum principle*

$$\min_{\beta} u_{\beta}^{0} \leq u_{\alpha}^{[n]} \leq \max_{\beta} u_{\beta}^{0}$$

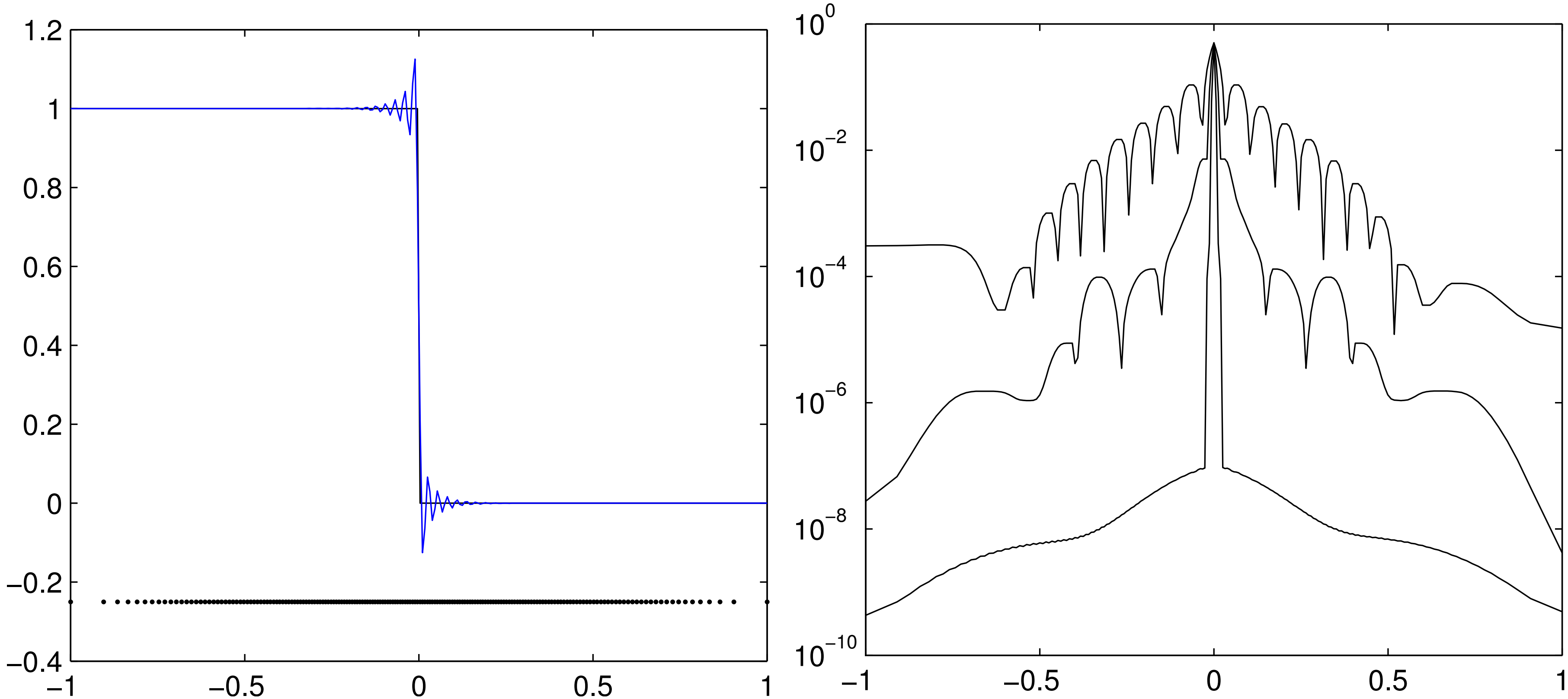
at each node α

DTV: built-in edge detection

A jump in the data will be indicated by the weights $w_{\alpha\beta}$ being small compared to λ and leads to a large portion of the original data being retained

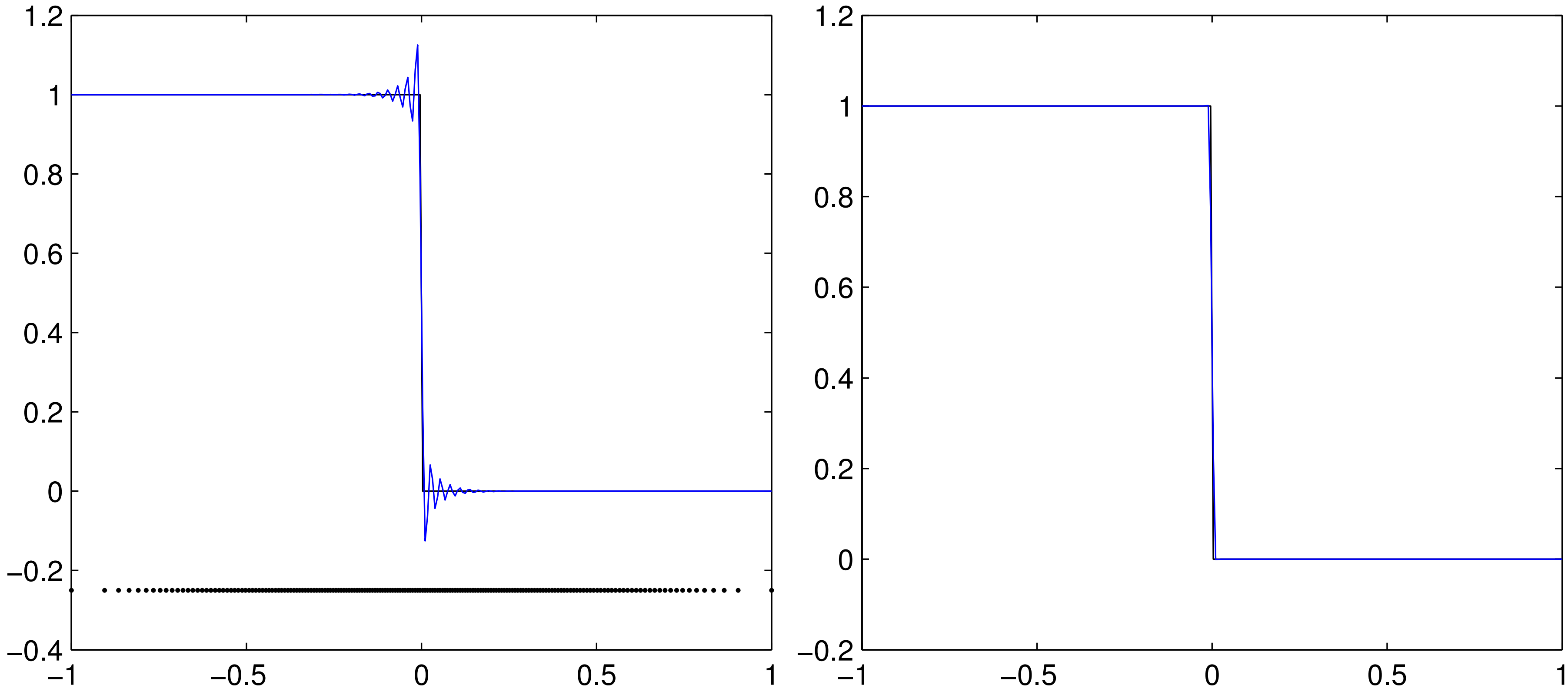
In smooth regions, the weights are large compared to λ which leads to the oscillations in the data being smoothed.

RBF DTV example



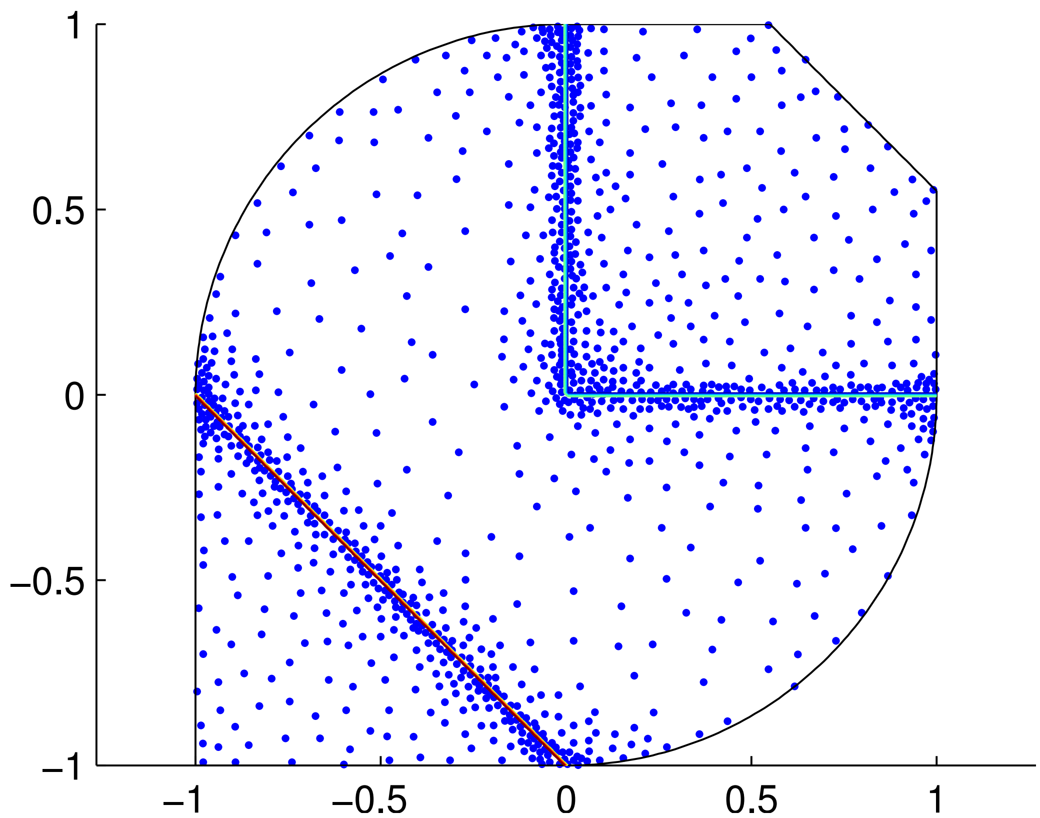
Left: $N = 79$ MQ RBF, Right: DTV postprocessed convergence $N = 39, 79, 159$.

RBF DTV example



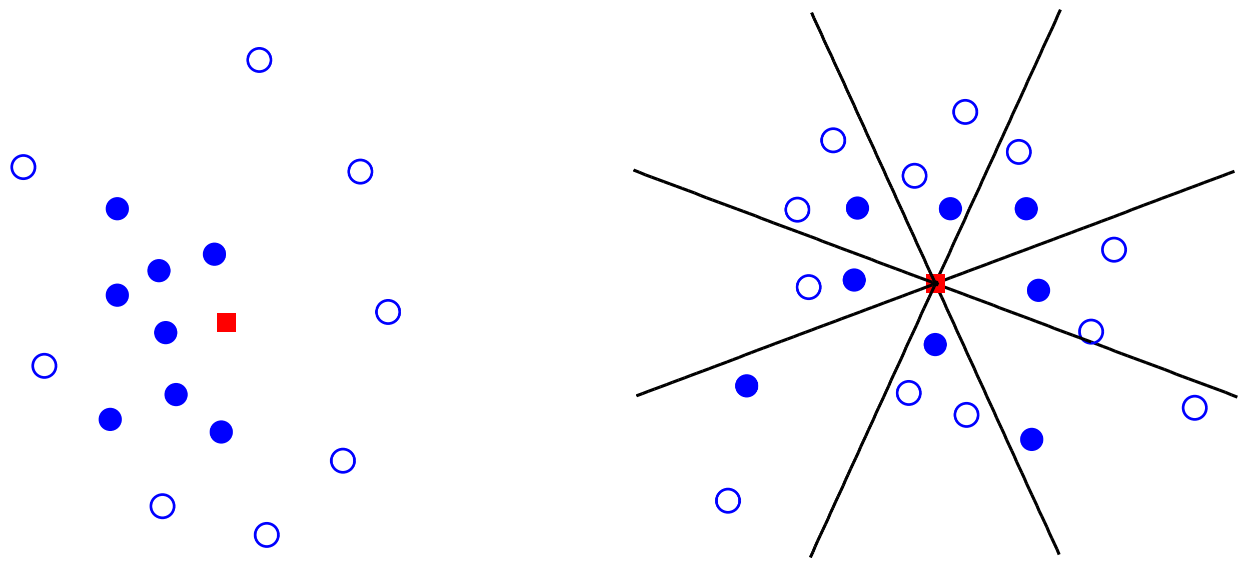
Left: $N = 79$ MQ RBF, Right: DTV postprocessed $N = 79$.

2d Complex Domain - Scattered Data

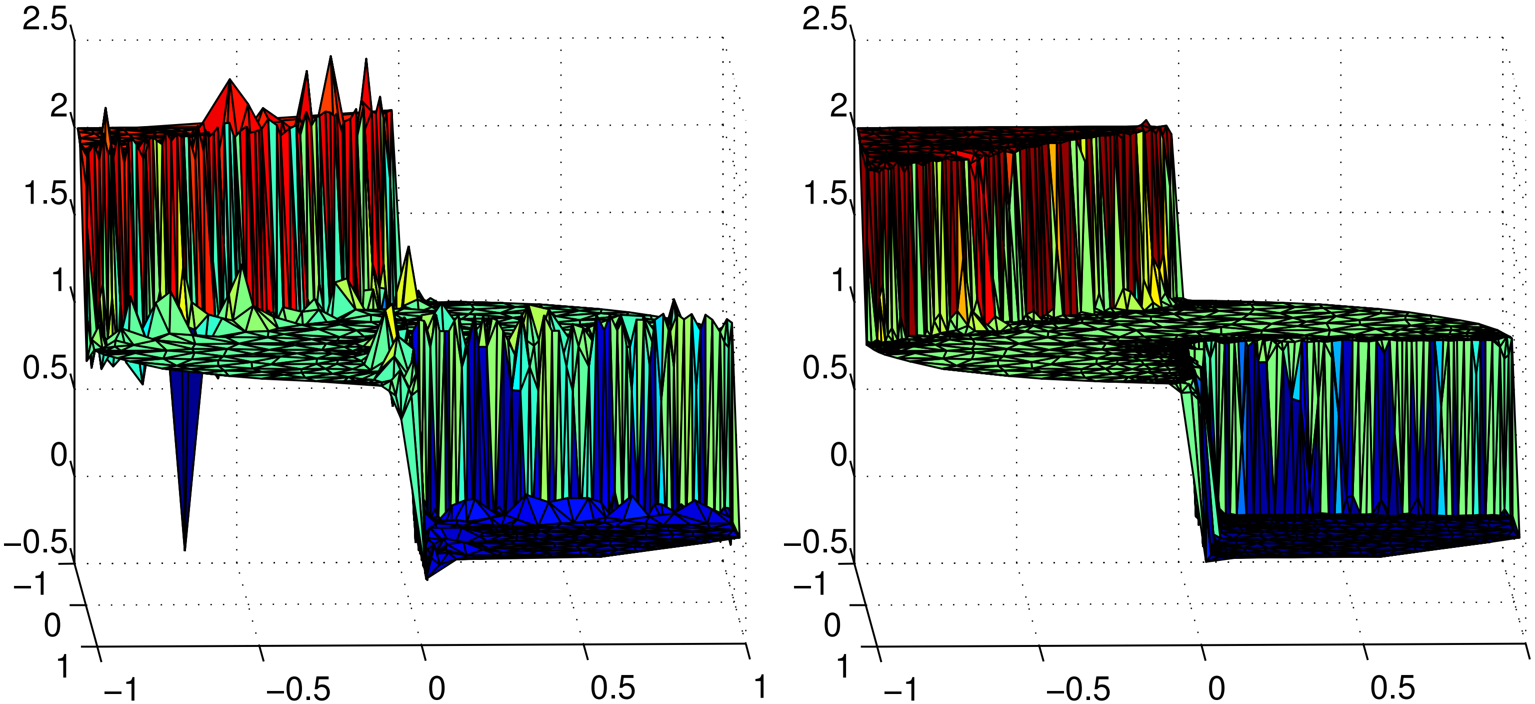


$N = 1126$ scattered points on a complexly shaped domain.

2d Neighborhoods N_α



2d RBF DTV example



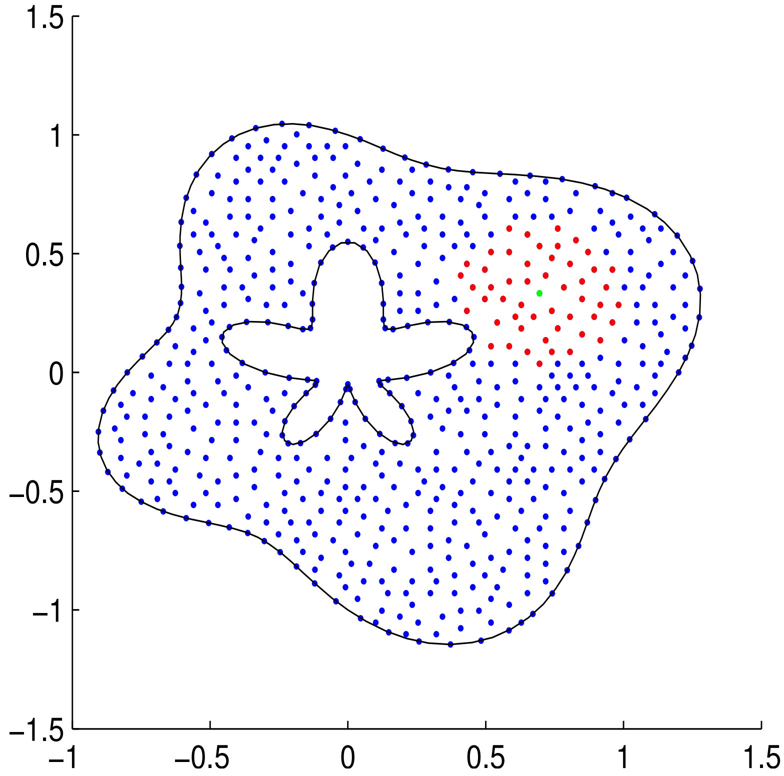
Summary

- Symmetric and Asymmetric RBF Collocation Methods
- RBF methods for time-dependent PDEs
  - Eigenvalue Stability
  - Accuracy
  - Center Locations
- Approximating piecewise smooth functions
  - Digital Total Variation Filtering

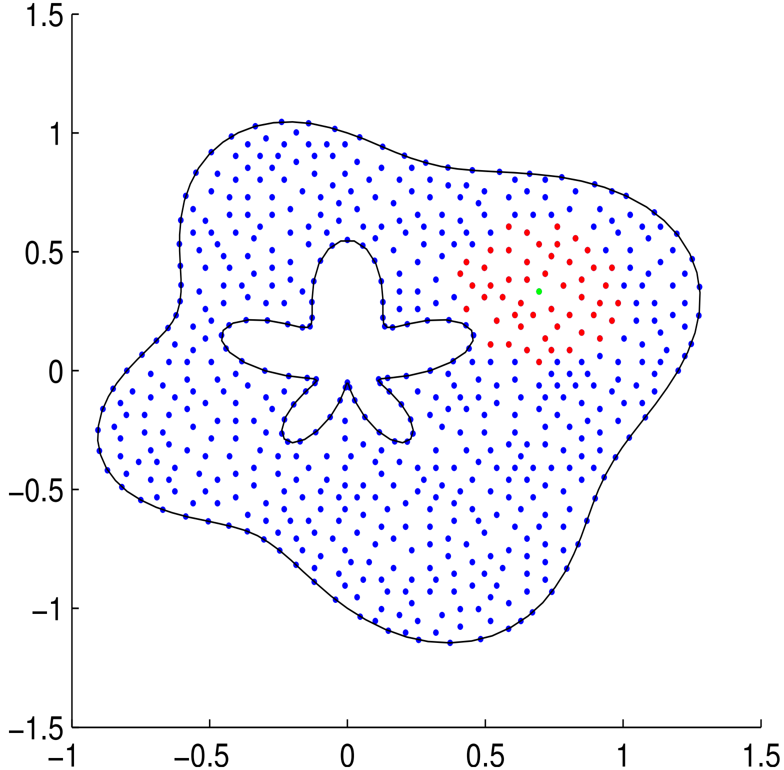
Future Work

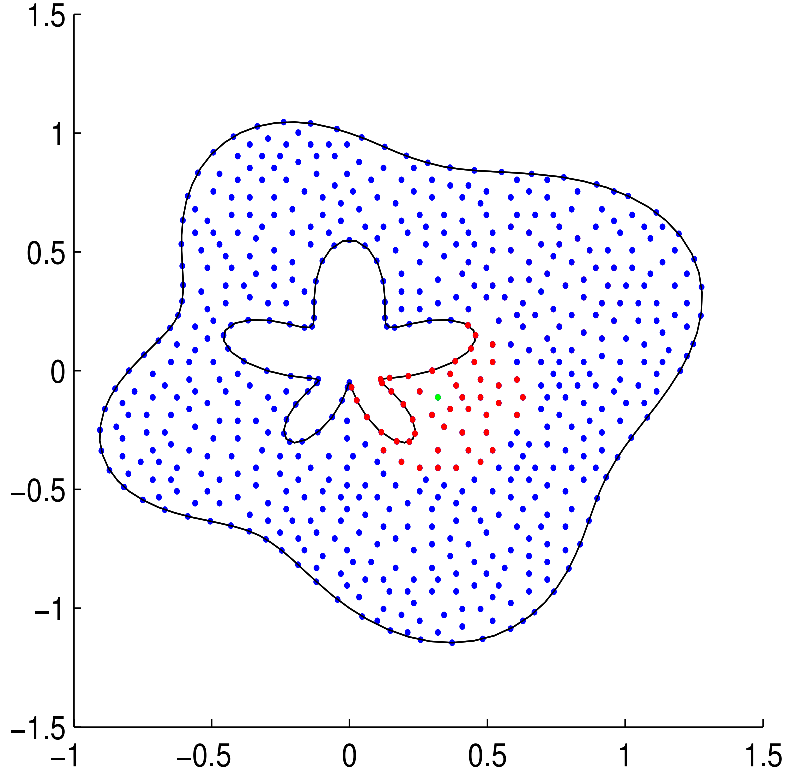
- Enforcing Boundary Conditions
- RBF finite difference mode
- Adaptive methods in 2d
- RBF Collocation methods for Conservation Laws

RBF FD mode 2d

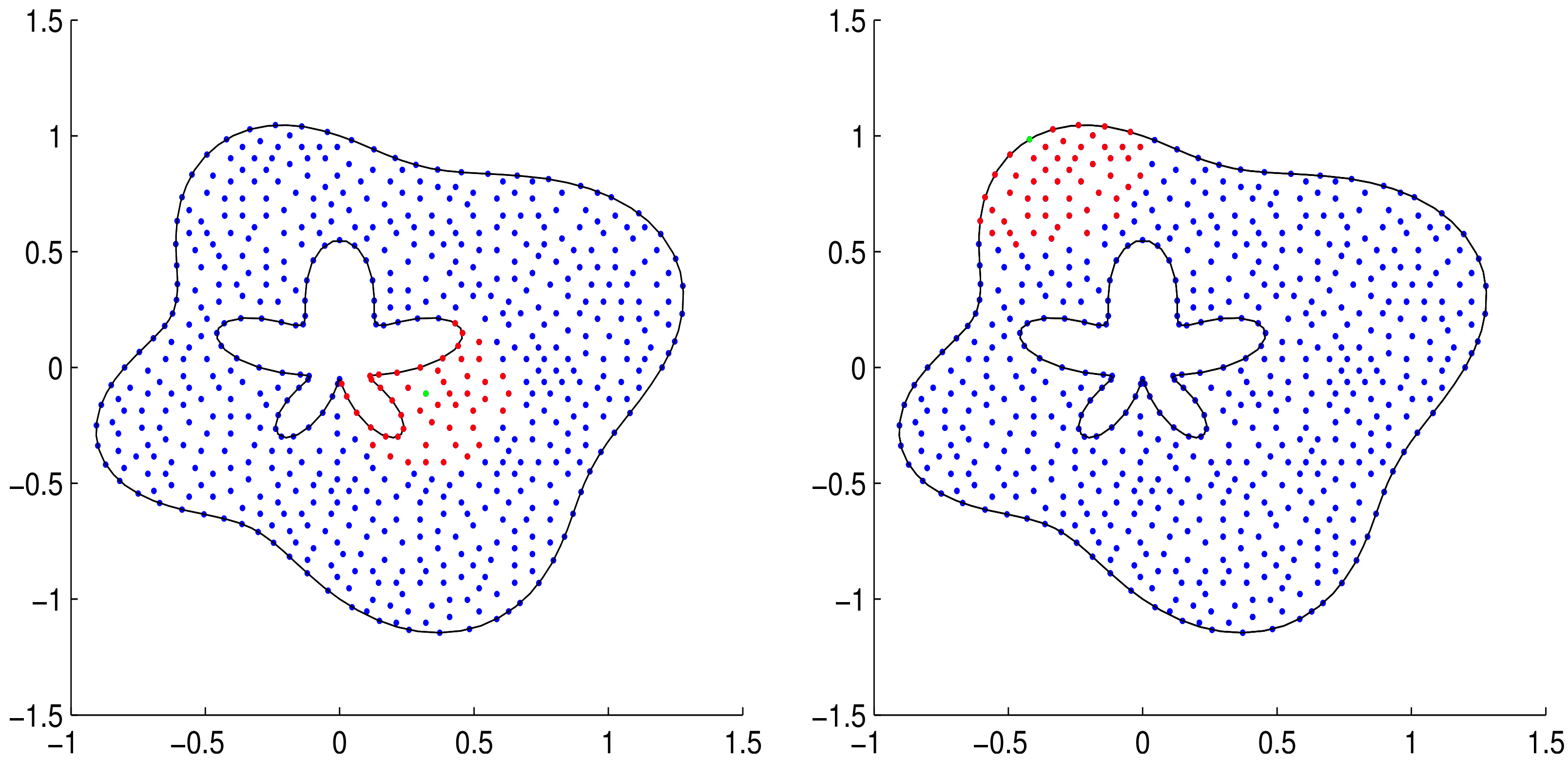


RBF FD mode 2d





RBF FD mode 2d



Adaptive methods in 2d

1. no existing applications in literature
2. RBF finite difference mode
3. stencil size and form
4. adaptive algorithm
5. eigenvalue stability

Adaptive Methods

Applied Numerical Mathematics

Adaptive radial basis function methods for time dependent partial differential equations, Applied Numerical Mathematics, 54 (2005), p. 79 - 94.

1d Adaptive Algorithm

Equidistribution of Arclength

1. Compute the length of the polygon through the points (x_j^n, s_j^n).
2. Find the points p_j^n on the polygon that divides it into N equal segments.
3. The new centers x_j^{n+1} are found by projecting the points p_j^n onto the x-axis.
4. Use RBFs to interpolate s_j^n to the new grid as s_j^{n+1}.

1d Adaptive Algorithm parameters

1. η causes the adaptation to be performed every η time steps
2. β controls the relative size of the largest and smallest grid spacings by ensuring that

$$\max_i \Delta x_i \leq \sqrt{1+\beta} \min_i \Delta x_i$$

where $\Delta x_i = x_i - x_{i-1}$.

The **uniformity** of the grid specified by the method is

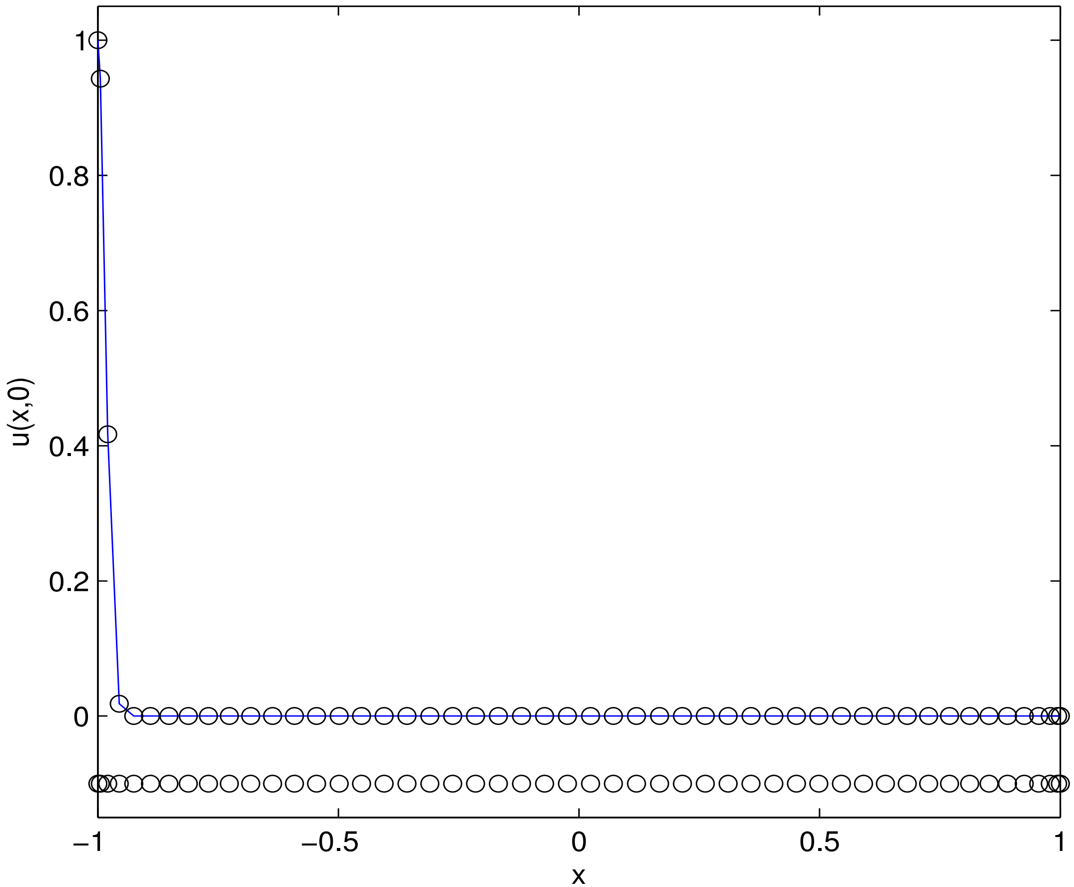
$$\rho_\Xi = \frac{q_\Xi}{h} = \frac{\min_i \Delta x_i}{\max_i \Delta x_i} = \frac{1}{\sqrt{1+\beta}}.$$

Adaptive Grids

- Advection equation

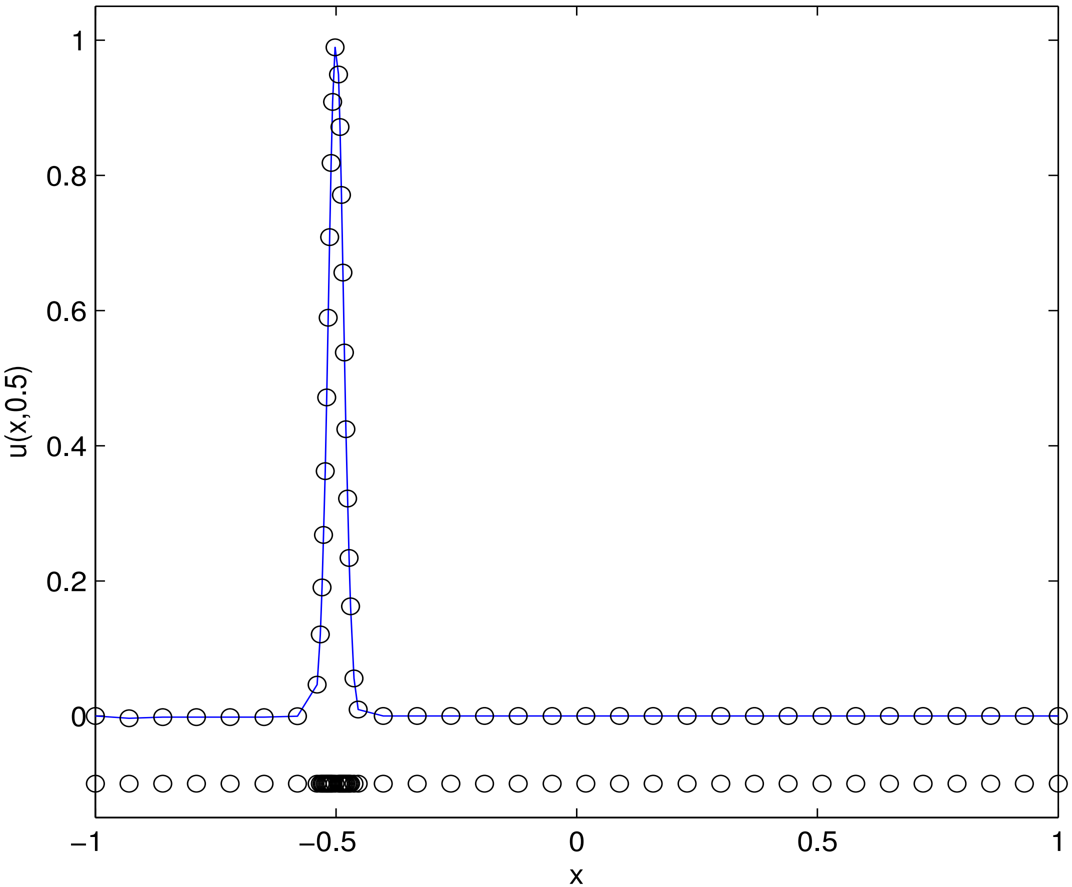
$$\begin{aligned} \frac{\partial u}{\partial t} + \frac{\partial u}{\partial x} &= 0 \\ u(x,0) &= e^{-2000(x+1)^2} \\ u(-1,t) &= e^{-2000(x+1-t)^2} \end{aligned}$$

Adaptive Grids



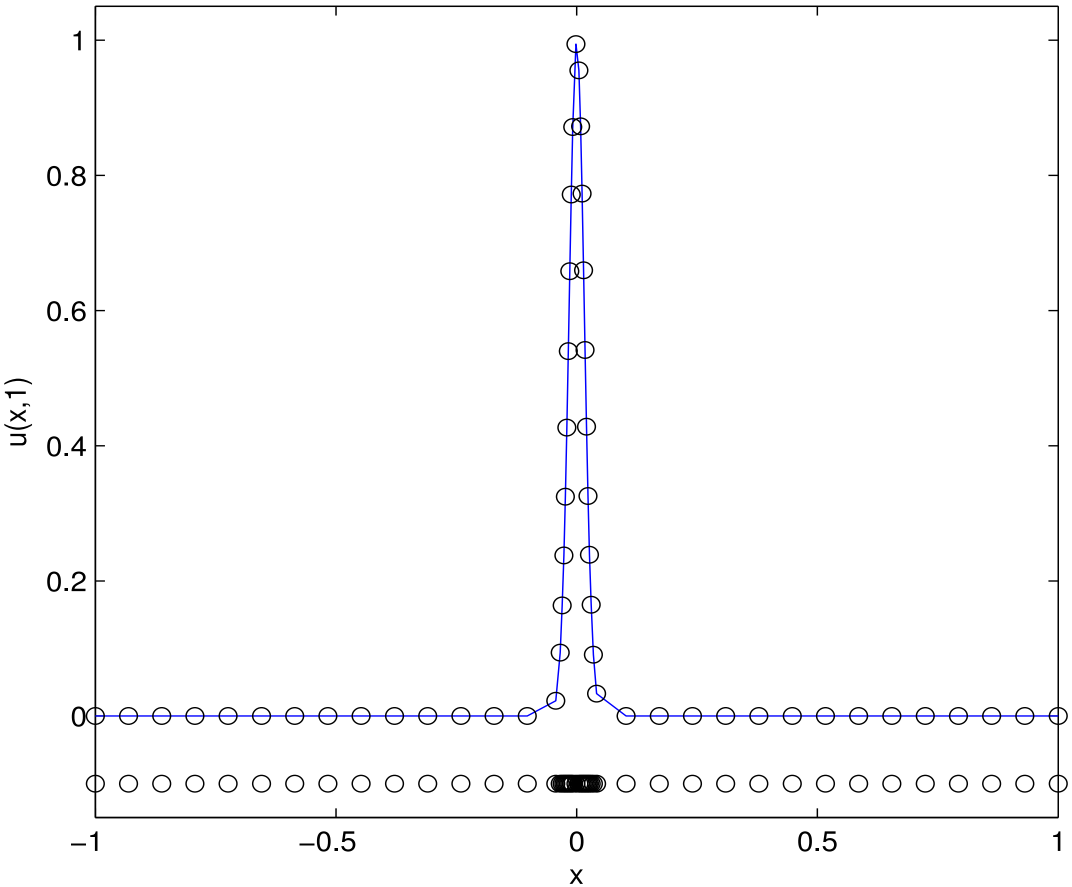
$N = 49$, Wendland W42 with $supp = 0.07$

Adaptive Grids



$N = 49$, Wendland W42 with $supp = 0.07$

Adaptive Grids



$N = 49$, Wendland W42 with $supp = 0.07$

Burger's Equation

$$\frac{\partial u}{\partial t} + \frac{\partial}{\partial x}\left(\frac{u^2}{2}\right) = \nu \frac{\partial^2 u}{\partial x^2}$$

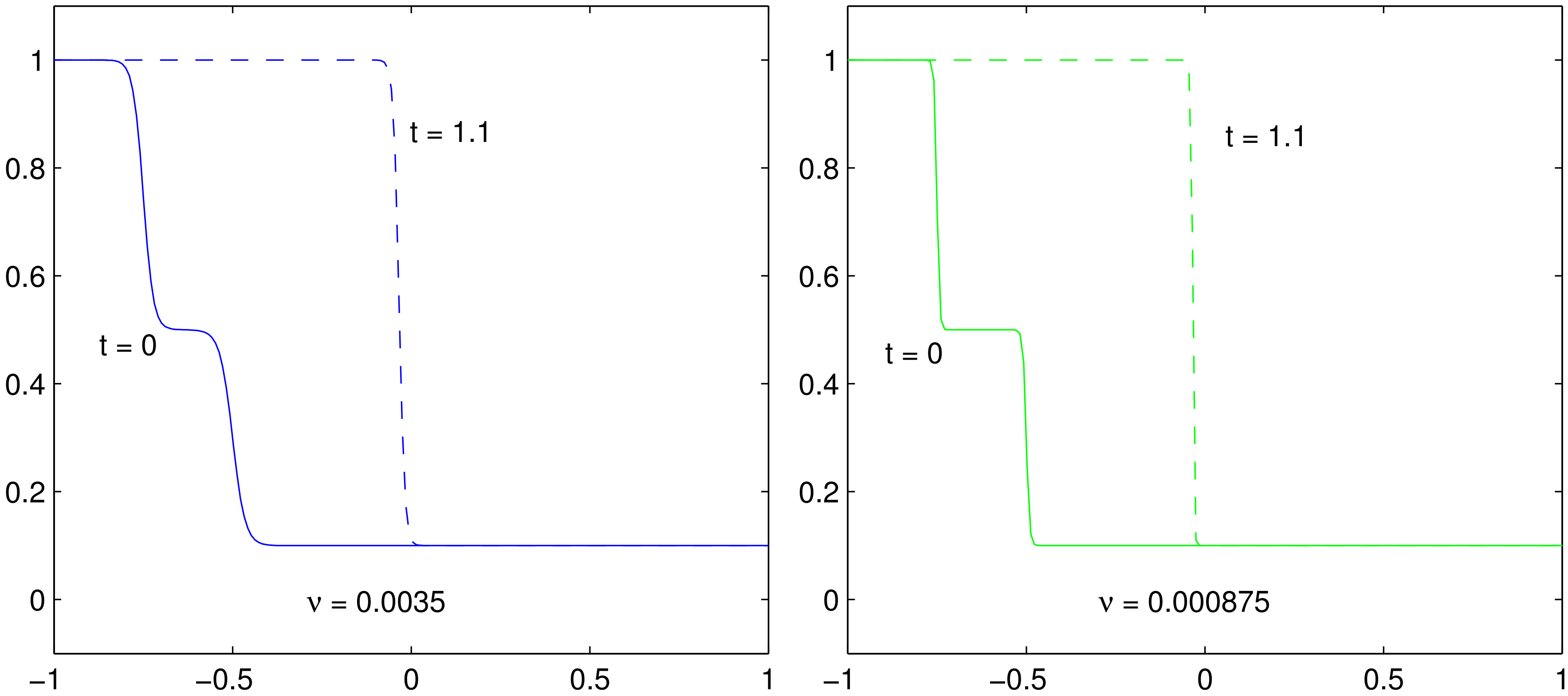
on $\Omega = [-1, 1]$.

The exact solution is

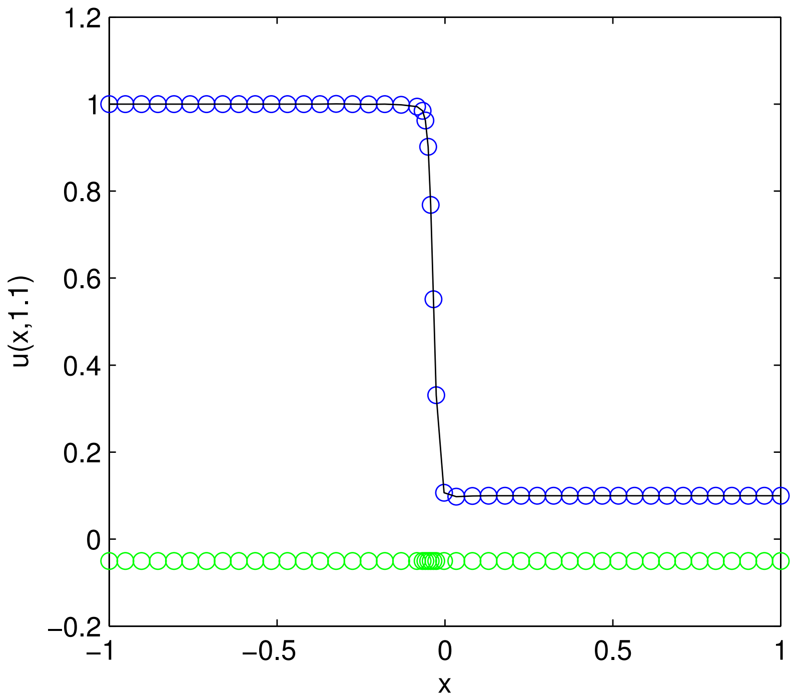
$$u(x,t) = \frac{0.1e^a + 0.5e^b + e^c}{e^a + e^b + e^c}.$$

where $a = -(x + 0.5 + 4.95t)/(20\nu)$, $b = -(x + 0.5 + 0.75t)/(4\nu)$, and $c = -(x + 0.625)/(2\nu)$.

Burger's Solution



Burger's Adaptive Solution



Exact solution of Burgers' equation (solid) at $t = 1.1$. Open circles represent the center locations at time $t = 1.1$ using the MQ RBF and $N = 47$.

Conservation Laws

1. stability
2. viscosity methods

A Brief Advertisement

Matlab Postprocessing Toolbox (MPT), version 2.0

- edge detection
- spectral filtering
- rational reconstruction
- Gegenbauer reprojection
- Freud reprojection
- Digital Total Variation (DTV) filtering

The development of the MPT is partially supported by NSF grant DMS-0609747.