Radial Basis Function Methods: Developments and Applications to Planetary Scale Flows

Bengt Fornberg  
University of Colorado Boulder,  
Department of Applied Mathematics  
in collaboration with  
Natasha Flyer  
NCAR, IMAGe  
Institute for Mathematics Applied to the Geosciences
In context of RBFs for PDEs, \[ FD \Rightarrow PS \Rightarrow RBF \Rightarrow RBF-FD \]

Finite difference methods: Limits of increasing orders exist
Approximate derivatives by local difference formulas.

Examples of some explicit FD formulas on an equispaced grid:

\[
\frac{\partial u}{\partial x} = \begin{bmatrix} -\frac{1}{2} & 0 & \frac{1}{2} \end{bmatrix} \frac{u}{h} + O(h^2)
= \begin{bmatrix} \frac{1}{12} & -\frac{2}{3} & 0 & \frac{2}{3} & -\frac{1}{12} \end{bmatrix} \frac{u}{h} + O(h^4)
= \begin{bmatrix} -\frac{1}{60} & \frac{3}{20} & -\frac{3}{4} & 0 & \frac{3}{4} & -\frac{3}{20} & \frac{1}{60} \end{bmatrix} \frac{u}{h} + O(h^6)
\]

\[
\ldots -\frac{1}{3} & \frac{1}{2} & -1 & 0 & 1 & -\frac{1}{2} & \frac{1}{3} \ldots \frac{u}{h} \text{ PS limit}
\]

Very simple algorithm available for explicit or implicit FD formulas:
(Fornberg, 1998)

\[
\begin{array}{c}
\downarrow & \leftarrow s \rightarrow \downarrow & \leftarrow d \rightarrow \downarrow \\
\vdots - \cdot - \cdot - \cdot - \cdot - \cdot - \cdot - \cdot - \cdot \\
\uparrow & \leftarrow \ldots \rightarrow n \rightarrow \ldots \rightarrow \uparrow \\
\end{array}
\]

\[ t = \text{PadeApproximant}\left[x^s \left(\frac{\text{Log}[x]}{h}\right)^m,\{x,1,\{n,d\}\}\right]; \]

\[ \text{CoefficientList[\{Denominator[t],Numerator[t]\},x]} \]
Pseudospectral (PS) methods can be seen as limits of increasing order FD methods

**Periodic problem - Fourier-PS Method:**
Use equispaced grid: We get exactly the same derivative approximations at nodes if we:

i. Extend periodically, and then apply limiting FD method,
ii. Find interpolating trig polynomial by FFT, take its analytic derivative. \(O(N \log N)\) op. for \(N\) points

**Non-Periodic Problem - Chebyshev-PS Method:**
Runge Phenomenon  Does not arise if the nodes are suitably clustered near the boundaries.
Example:  \(f(x) = 1/(1+16x^2)\)

i. Create global FD formulas separately for each node point, \(O(N^2)\) operations for \(N\) points
ii. Get Chebyshev polynomial expansion (by FFT), take its analytic derivative; \(O(N \log N)\) operations.
How do PS methods work in more than 1-D?

2-D:

Can generalize to Tensor product type grids

BUT

NO set of basis functions can guarantee a nonsingular system in the case of scattered nodes

Scattered nodes

Interpolant \( s(x) = \sum_{k=0}^{N} c_k \Psi_k(x) \)

System that determines the expansion coefficients:

\[
\begin{bmatrix}
\Psi_0(x_0) & \Psi_1(x_0) & \cdots & \Psi_N(x_0) \\
\Psi_0(x_1) & \Psi_1(x_1) & \cdots & \Psi_N(x_1) \\
\vdots & \vdots & \ddots & \vdots \\
\Psi_0(x_N) & \Psi_1(x_N) & \cdots & \Psi_N(x_N)
\end{bmatrix}
\begin{bmatrix}
c_0 \\
c_1 \\
\vdots \\
c_N
\end{bmatrix}
= 
\begin{bmatrix}
f_0 \\
f_1 \\
\vdots \\
f_N
\end{bmatrix}
\]

Move two nodes so they exchange locations:

Two rows become interchanged, determinant changes sign

\( \Rightarrow \) determinant is zero somewhere along the way.
RBF idea, In pictures:

1970  Invention of RBFs (for application in cartography)

Some other key dates:

1940  Unconditional non-singularity shown for many types of radial functions
1984  Unconditional non-singularity shown for multiquadrics \( \phi(r) = \sqrt{1 + (\epsilon r)^2} \)
1990  First application of RBFs to numerical solutions of PDEs
2002  Flat RBF limit exists: all 'classical' pseudospectral methods can be seen as RBF special cases
2004  First RBF algorithm that remains numerically stable in the flat basis function limit
2007  First application of RBFs to large-scale geophysical test problems
2009  A new physical phenomenon (a certain mantle convection instability) initially discovered in an RBF calculation
RBF idea, In formulas:

Given scattered data \((x_k, f_k), k = 1, 2, \ldots, N,\) in \(d\)-D, the RBF interpolant is

\[
s(x) = \sum_{k=1}^{N} \lambda_k \phi(||x - x_k||)
\]

The coefficients \(\lambda_k\) can be found by collocation:

\[
\begin{bmatrix}
\phi(||x_1 - x_1||) & \phi(||x_1 - x_2||) & \cdots & \phi(||x_1 - x_N||) \\
\phi(||x_2 - x_1||) & \phi(||x_2 - x_2||) & \cdots & \phi(||x_2 - x_N||) \\
\vdots & \vdots & \ddots & \vdots \\
\phi(||x_N - x_1||) & \phi(||x_N - x_2||) & \cdots & \phi(||x_N - x_N||)
\end{bmatrix}
\begin{bmatrix}
\lambda_1 \\
\vdots \\
\lambda_N
\end{bmatrix}
= \begin{bmatrix}
f_1 \\
\vdots \\
f_N
\end{bmatrix}
\]

**Two key theorems:**

- For most radial functions \(\phi(r)\), this system can never be singular
- The interpolation is spectrally accurate for smooth radial functions
Many types of RBFs are available:

### Piecewise smooth $\phi(r)$
- Cubics: $r^3$
- TP splines: $r^2 \log r$
- Compact support

### Infinitely smooth $\phi(r)$
- Multiquadric: $\sqrt{1 + (\varepsilon r)^2}$
- Gaussian: $e^{-(\varepsilon r)^2}$
- Inverse quadratic: $\frac{1}{1 + (\varepsilon r)^2}$

Interpolation guaranteed nonsingular for all commonly used radial functions.

- **Piecewise smooth RBFs:**
  - algebraic accuracy (cf. cubic splines)
  - often only mild Gibbs oscillations

- **Infinitely smooth RBFs:**
  - spectral accuracy (if no Runge phenomenon)
Numerical conditioning, and the flat RBF limit \((\varepsilon \to 0)\)

Classical basis functions are usually highly oscillatory.

RBFs are translates of one single function - here \(\phi(r) = e^{-(\varepsilon r)^2}\).

In case of 41 scattered nodes in 1-D:
\[
\text{cond}(A) = O(\varepsilon^{-80}), \quad \det(A) = O(\varepsilon^{1640}).
\]

2-D:
\[
\text{cond}(A) = O(\varepsilon^{-16}), \quad \det(A) = O(\varepsilon^{416}).
\]

Exact formulas available for any number of nodes in any number of dimensions (Fornberg and Zuev, 2007)

Extreme ill-conditioning typical as \(\varepsilon \to 0\).
Why are flat (or near-flat) RBFs interesting?

- Intriguing error trends as $\varepsilon \to 0$
  
  'Toy-problem' example: 41 node MQ interpolation of 
  $$f(x_1, x_2) = \frac{59}{67 + (x_1 + \frac{1}{7})^2 + (x_2 - \frac{1}{11})}$$

- RBF interpolant in 1-D reduces to Lagrange's interpolation polynomial
  (Driscoll and Fornberg, 2002)

- The $\varepsilon \to 0$ limit reduces to 'classical' PS methods if used on tensor type grids.

- The RBF approach generalize PS methods in many ways:
  - Guaranteed nonsingular also for scattered nodes on irregular geometries
  - Allow spectral accuracy to be combined with mesh refinement
  - Best accuracy often obtained for non-zero $\varepsilon$.

Solving $A\vec{\lambda} = \vec{f}$ followed by evaluating 
$$s(x, \varepsilon) = \sum_{k=1}^{N} \lambda_k \phi(||x - x_k||)$$
is merely an unstable algorithm for a stable problem
Numerical computations for small values of $\varepsilon$ (near-flat RBFs)

It is possible to create algorithms that completely bypass ill-conditioning all the way into $\varepsilon \to 0$ limit, while using only standard precision arithmetic:

**Concept:** Find a computational path from $f$ to $s(x,\varepsilon)$ that does not go via the ill-conditioned expansion coefficients $\lambda$.

- **Contour-Padé algorithm**  
  First algorithm of its kind; established that the concept is possible  
  Based on contour integration in a complex $\varepsilon$-plane.  
  Limited to relatively small $N$-values

  First version  
  Improved algorithm RBF-RA  
  (Fornberg and Wright, 2004).

  Improved algorithm RBF-RA  
  (Fornberg and Wright, in progress).

- **RBF-QR method**  
  Initially developed for nodes scattered over the surface of a sphere  
  No limit on $N$; cost about five times that of RBF-Direct

  Original version (for nodes on sphere)  
  Versions for 1-D, 2-D, and 3-D  
  Codes for generating RBF-FD stencils  
  (Fornberg and Piret, 2007).  
  (Fornberg, Larsson, and Flyer, 2010).  
  (Larsson, Lehto, Heryudono, Fornberg, in progress).

Probably many more completely stable algorithms to come
The concept for the RBF-QR method

Recognize that the existence of an ill-conditioned basis does not imply that the spanned space is bad.

**Ex. 1:** 3-D space

**Ex. 2:** Polynomials of degree \( \leq 100 \)

\[
x^n, \ n = 0, 1, \ldots, 100
\]

**Ex. 3:** Space spanned by RBFs in their flat \( \varepsilon \to 0 \) limit

- The spanned space turns out to be excellent for computational work - just the basis that is bad.
- Is there any Good Basis in exactly the same space?
- RBF-QR finds such a basis through some analytical expansions, leading to numerical steps that all remain completely stable even in the flat basis function limit.
There is something strange about how FD and PS methods approximate \[ \frac{1}{\sqrt{2}} \left( \frac{\partial}{\partial x} + \frac{\partial}{\partial y} \right) \]

Where should \( \frac{\partial}{\partial x} \) pick up its data from?

Answer: \( \frac{x}{8} \, _0F_1 \left( 3, -\frac{1}{4} (x^2 + y^2) \right) \)

Turns out: RBFs on hexagonal or Halton (scattered) node types can be better conditioned and give higher accuracy than PS or RBFs on Cartesian lattices.
Interpolation on a sphere - RBF-Direct vs. RBF-QR
(Fornberg and Piret, 2007)

Test function: 1849 minimal energy nodes Errors as function of $\varepsilon$

\[ f(x) = e^{-7(x+\frac{1}{2})^2-8(y+\frac{1}{2})^2-9(z-\frac{1}{\sqrt{2}})^2} \]

RBF-Direct: \[ s(x) = \sum_{k=1}^{N} \lambda_k \phi(||x-x_k||) \] with the $\lambda_k$ from solving $A \lambda = f$; $\text{Cond}(A) = O(\varepsilon^{-84})$.

Lowering $\varepsilon$ by a factor of 100 increases $\text{cond}(A)$ a factor of $100^{84} = 10^{168}$. Maintaining >10 digits of accuracy by means of extended precision arithmetic requires the numerical precision to be raised from standard 16 digits to around 180 digits. Extended precision generally not a cost effective approach.

RBF-QR:

With the new basis functions in exactly the same approximation space, $\text{cond}(A')$ remains $O(1)$. Cost increase over RBF-Direct about 6 times, no matter how small $\varepsilon$ is used.
Solving PDEs on a sphere

**Governing PDE:**

$$\frac{\partial u}{\partial t} + (\cos a - \tan \theta \sin \varphi \sin a) \frac{\partial u}{\partial \varphi} - \cos \varphi \sin a \frac{\partial u}{\partial \theta} = 0 \quad \Rightarrow$$

RBF collocation of PDE in spherical coordinates eliminates all coordinate-based singularities

**Spectrally accurate numerical methods:**

- **DF:** Double Fourier series
- **RBF:** Radial Basis Functions
- **SE:** Spectral Elements
  Implemented by means of *cubed sphere*
- **SPH:** Spherical Harmonics
  Collocation with orthogonal set of trig-like basis functions, which lead to entirely uniform resolution over surface of sphere
Snapshots of 4096 node RBF calculation after 12 days (1 full revolution) of a cosine bell

<table>
<thead>
<tr>
<th>Method</th>
<th>$l_2$ error</th>
<th>Number of node points/free parameters</th>
<th>Time step (RK4)</th>
<th>Code length (lines)</th>
<th>Local refinement feasible</th>
</tr>
</thead>
<tbody>
<tr>
<td>RBF Radial basis functions</td>
<td>0.006</td>
<td>4,096</td>
<td>1/2 hour</td>
<td>&lt; 40</td>
<td>yes</td>
</tr>
<tr>
<td>SPH Spherical harmonics</td>
<td>0.005</td>
<td>32,768</td>
<td>90 seconds</td>
<td>&gt; 500</td>
<td>no</td>
</tr>
<tr>
<td>DF Double Fourier</td>
<td>0.005</td>
<td>32,768</td>
<td>90 seconds</td>
<td>&gt; 100</td>
<td>no</td>
</tr>
<tr>
<td>SE Spectral elements</td>
<td>0.005</td>
<td>7,776</td>
<td>6 minutes</td>
<td>&gt; 1000</td>
<td>yes</td>
</tr>
</tbody>
</table>

(Fornberg and Piret, 2008): Time stepping thousands of full revolutions and using RBF-QR - still no significant error growth or trailing dispersive waves.
Moving Vortex Roll-Up on A Sphere: Local Node Refinement
(Flyer and Lehto, 2009)

Initial condition | Solution after 12 days

Linear convection with a vortex-like flow field

Numerical implementation

Minimal energy (ME) nodes

Refined nodes

IMQ RBFs: \( \phi(r) = \frac{1}{\sqrt{1 + \varepsilon^2 r^2}} \)

\( N = 3136 \) nodes
(1849 shown in figures to the right)

Method of lines (MOL) time stepping with standard Runge-Kutta, 4\(^{th}\) order
### Numerical RBF solution at 12 days

![Numerical RBF solution at 12 days](image1.png)

### Error at 12 days

$$ (10^{-4}) $$

![Error at 12 days](image2.png)

### Table of Methods, Resolution, Time step, and Error

<table>
<thead>
<tr>
<th>Method</th>
<th>Resolution</th>
<th>Time step</th>
<th>Error</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$N$ (total)</td>
<td>Typical angular</td>
<td>Minutes</td>
</tr>
<tr>
<td><strong>Without local refinement</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>RBF Radial basis functions</td>
<td>3,136</td>
<td>6.4 $^\circ$</td>
<td>60</td>
</tr>
<tr>
<td>FV Finite Volume (lat-long grid)</td>
<td>165,888</td>
<td>0.625 $^\circ$</td>
<td>10</td>
</tr>
<tr>
<td>FV Finite Volume (cubed sphere)</td>
<td>38,400</td>
<td>-</td>
<td>30</td>
</tr>
<tr>
<td>DG Discontinuous Galerkin</td>
<td>9,600</td>
<td>-</td>
<td>6</td>
</tr>
<tr>
<td><strong>With local refinement</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>RBF Radial basis functions</td>
<td>3,136</td>
<td>-</td>
<td>20</td>
</tr>
<tr>
<td>FV Finite Volume (3 levels. lat-long)</td>
<td>-</td>
<td>5 $^\circ$ - 0.625 $^\circ$</td>
<td>1-3</td>
</tr>
</tbody>
</table>
Forcing terms added to the shallow water equations to generate a flow that mimics a short wave trough embedded in a westerly jet.

**Initial Velocity Field**  
**Initial geopotential height field**  
(equivalent to pressure field)
Comparison with numerical implementations reported in the literature

**Total physical run time 5 days (wave trough traveled one revolution)**

<table>
<thead>
<tr>
<th>Method</th>
<th>(N)</th>
<th>Time step</th>
<th>Relative (L_2) error</th>
</tr>
</thead>
<tbody>
<tr>
<td>RBF</td>
<td>784</td>
<td>40 minutes</td>
<td>(4.8 \cdot 10^{-1})</td>
</tr>
<tr>
<td></td>
<td>1,849</td>
<td>24 minutes</td>
<td>(3.5 \cdot 10^{-1})</td>
</tr>
<tr>
<td></td>
<td>3,136</td>
<td>15 minutes</td>
<td>(8.8 \cdot 10^{-6})</td>
</tr>
<tr>
<td></td>
<td>4,096</td>
<td>8 minutes</td>
<td>(2.5 \cdot 10^{-7})</td>
</tr>
<tr>
<td></td>
<td>5,041</td>
<td>6 minutes</td>
<td>(1.0 \cdot 10^{-8})</td>
</tr>
<tr>
<td>Double Fourier</td>
<td>2,048</td>
<td>6 minutes</td>
<td>(3.9 \cdot 10^{-1})</td>
</tr>
<tr>
<td></td>
<td>8,192</td>
<td>3 minutes</td>
<td>(8.2 \cdot 10^{-4})</td>
</tr>
<tr>
<td></td>
<td>32,768</td>
<td>90 seconds</td>
<td>(4.0 \cdot 10^{-4})</td>
</tr>
<tr>
<td>Spherical Harmonic</td>
<td>8,192 (1,849)</td>
<td>3 minutes</td>
<td>(2.0 \cdot 10^{-3})</td>
</tr>
<tr>
<td>Spectral Element</td>
<td>6,144</td>
<td>90 seconds</td>
<td>(6.5 \cdot 10^{-3})</td>
</tr>
<tr>
<td></td>
<td>24,576</td>
<td>45 seconds</td>
<td>(4.0 \cdot 10^{-5})</td>
</tr>
</tbody>
</table>

**Computational times for the RBF method, in Matlab on 2.66 GHz PC**

<table>
<thead>
<tr>
<th>(N)</th>
<th>Runtime per time step (s)</th>
<th>Total Runtime</th>
</tr>
</thead>
<tbody>
<tr>
<td>784</td>
<td>0.03</td>
<td>5 seconds</td>
</tr>
<tr>
<td>1,849</td>
<td>0.11</td>
<td>33 seconds</td>
</tr>
<tr>
<td>3,136</td>
<td>0.25</td>
<td>2 minutes</td>
</tr>
<tr>
<td>4,096</td>
<td>0.41</td>
<td>6 minutes</td>
</tr>
<tr>
<td>5,041</td>
<td>0.60</td>
<td>24 minutes</td>
</tr>
</tbody>
</table>
Thermal Convection in a 3-D Spherical Shell
(Flyer and Wright, 2009)

Equations:  
(Ra = Rayleigh number; related to ratio of heat convection to heat conduction)

\[
\begin{align*}
\nabla \cdot \mathbf{u} &= 0 \\
\Delta \mathbf{u} - \nabla p + Ra \mathbf{e}_r &= 0 \\
\frac{\partial T}{\partial t} + \mathbf{u} \cdot \nabla T &= \Delta T
\end{align*}
\]

Node Layout for hybrid RBF-Chebyshev discretization:
Ra = 7,000 test case

Initial condition \( Y_4^0 + \frac{5}{7} Y_4^4 \)

\( N = 1849 \) nodes on each spherical shell
\( M = 31 \) shells, Perturbation temperature shown
Blue - down flow, Yellow - up flow, Red - core

Comparisons against main previous results from the literature

<table>
<thead>
<tr>
<th>Method</th>
<th>No of nodes</th>
<th>( \text{Nu}_{\text{outer}} )</th>
<th>(&lt; V_{\text{RMS}} &gt;)</th>
<th>( T )</th>
</tr>
</thead>
<tbody>
<tr>
<td>FE</td>
<td>393,216</td>
<td>3.6254</td>
<td>31.09</td>
<td>0.2176</td>
</tr>
<tr>
<td>FD</td>
<td>12,582,912</td>
<td>3.4945</td>
<td>32.6308</td>
<td>0.21597</td>
</tr>
<tr>
<td>FV</td>
<td>663,552</td>
<td>3.5983</td>
<td>31.0226</td>
<td>0.21594</td>
</tr>
<tr>
<td>SH-FD</td>
<td>552,960</td>
<td>3.6096</td>
<td>31.0821</td>
<td>0.21578</td>
</tr>
<tr>
<td>RBF-CH</td>
<td>57,319</td>
<td>3.6096</td>
<td>31.0823</td>
<td>0.21578</td>
</tr>
</tbody>
</table>
Example of computed solution for Ra = 500,000

Isosurfaces of perturbed temperature:

(Single frame from a movie)

Calculation on PC system;

At somewhat lower Ra numbers, a similar RBF calculation revealed an unexpected physical instability, afterwards confirmed on the Japanese Earth Simulator.
IDEA 1: Consider local \(n\)-node FD stencils centered at each of the domain's \(N\) nodes. Find the weights NOT by requiring exact result for increasing order (multivariate) polynomials, but instead for RBFs centered at each of the \(n\) nodes within the stencil.

1849 ME nodes  
Eigenvalues for *convective flow over a sphere* \((N = 3600, n = 17, \varepsilon = 2.5)\)

IDEA 2: Over the same stencil size, apply also a RBF-FD 'hyperviscosity' operator (such as approximating \(\Delta^{10}\)). Spurious EVs in right half plane can then be shifted to left half plane with insignificant disturbance to the physically relevant ones.

COSTS:  
Global RBFs:  \(O(N^3)\) initially, \(O(N^2)\) per time step.  
RBF-FD: \(O(N)\) initially, and per time step.
Revisit two previous test problems with RBF-FD approximations

**Convective flow**

- Solutions
- Errors

- 1 revolution
- 10 revolutions
- 1,000 revolutions

**Vortex roll-up**

- Solutions
- Errors

- $t = 3$
- $t = 6$
- $t = 9$

$N = 25,600$, $n = 74$

$N = 25,600$, $n = 50$
Cost effectiveness of RBF-FD vs. global RBFs

Vortex rollup test case at $t = 3$; costs for different end accuracies.

Run time

Memory requirement
Modeling geophysical flows with RBF-FD methods

Some things currently on the radar:

1) 3-D RBF-FD formulas, implemented on scattered nodes.

2) Dynamically adaptive node refinement.

3) Study the interaction of RBF-FD stencils with boundaries.

4) Implement RBF-FD codes on parallel architectures, for example on GPUs (Graphical Processing Units).
Conclusions

Established:
- RBFs can be seen as a generalization of PS methods to arbitrarily shaped domains.
- RBFs combine spectral accuracy with flexible opportunities for local node refinement.
- RBFs can offer excellent accuracy also over very long integration times.
- The near-flat basis function regime ($\epsilon$ small) is of particular interest, and stable numerical algorithms for it have been developed.
- For certain classes of convective flow problems, RBF-based solutions can be more accurate and cost-effective than any previous numerical method.

Some current research issues:
- Develop further the RBF-FD approach.
- Compare both global RBFs and RBF-FD implementations against previous methods in more major applications.
- Explore further the combination of spectral accuracy with local node refinement.
- Try to find still more options for RBF algorithms that bypass all numerical instability issues.
- Develop effective implementations of RBF-FD methods, first on GPUs, and later on massively parallel (peta-scale) computer hardware.

References:
- Flyer, N. and Fornberg, B., Radial basis functions: Developments and applications to planetary scale flows, *Computers and Fluids*, in press.