



## RBF-PUM

Outline

Introduction

RBF-PUM

Theoretical results

Numerical results

RBF-QR

Convergence

Robustness

3-D results

Cost

Adaptivity

Summary

# Radial basis function partition of unity methods for PDEs

Elisabeth Larsson, Scientific Computing, Uppsala  
University

Credit goes to a number of RBF-PUM collaborators



Alfa Heryudono    Ali Safdari    Alison Ramage    Lina von Sydow    Victor Shcherbakov    Igor Tominec

Localized Kernel-Based Meshless Methods for Partial  
Differential Equations, ICERM, Aug 8, 2017



## RBF-PUM

### Outline

Introduction

RBF-PUM

Theoretical results

Numerical results

RBF-QR

Convergence

Robustness

3-D results

Cost

Adaptivity

Summary

# Outline

## Introduction

## RBF partition of unity methods for PDEs

## Theoretical results

## Numerical results

RBF-QR

Convergence

Robustness

3-D results

Cost

Adaptivity

## Summary



Outline

Introduction

RBF-PUM

Theoretical results

Numerical results

RBF-QR

Convergence

Robustness

3-D results

Cost

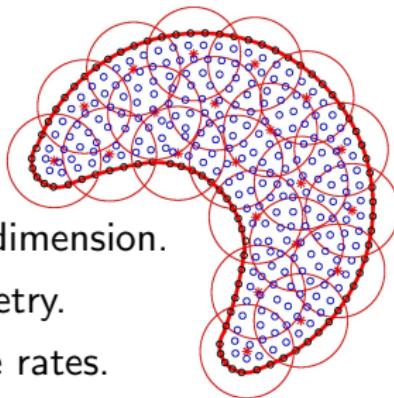
Adaptivity

Summary

# Motivation for RBF-PUM

## Global RBF approximation

- + Ease of implementation in any dimension.
- + Flexibility with respect to geometry.
- + Potentially spectral convergence rates.
- Computationally expensive for large problems.



## RBF-PUM

- ▶ Local RBF approximations on patches are blended into a global solution using a partition of unity.
- ▶ Provides spectral or high-order convergence.
- ▶ Solves the computational cost issues.
- ▶ Allows for local adaptivity.

*Wendland (2002), Fasshauer (2007), Cavoretto, De Rossi,  
Perracchione et al., Larsson, Heryudono et al.*



Outline

Introduction

RBF-PUM

Theoretical results

Numerical results

RBF-QR

Convergence

Robustness

3-D results

Cost

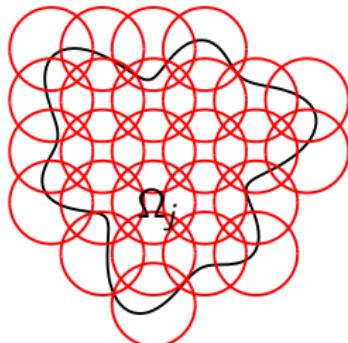
Adaptivity

Summary

# The RBF partition of unity method

## Global approximation

$$\tilde{u}(\underline{x}) = \sum_{j=1}^P w_j(\underline{x}) \tilde{u}_j(\underline{x})$$

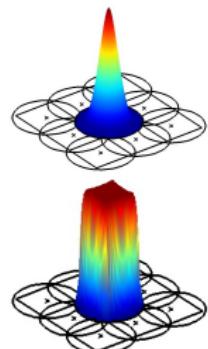


## PU weight functions

Generate weight functions from  
compactly supported  $C^2$  Wendland functions

$$\psi(\rho) = (4\rho + 1)(1 - \rho)_+^4$$

using Shepard's method  $w_i(\underline{x}) = \frac{\psi_i(\underline{x})}{\sum_{j=1}^M \psi_j(\underline{x})}$ .



## Cover

Each  $\underline{x} \in \Omega$  must be in the interior of at least one  $\Omega_j$ .  
Patches that do not contain unique points are pruned.



Outline

Introduction

RBF-PUM

Theoretical results

Numerical results

RBF-QR

Convergence

Robustness

3-D results

Cost

Adaptivity

Summary

# Differentiating RBF-PUM approximations

## Applying an operator globally

$$\Delta \tilde{u} = \sum_{i=1}^M \Delta w_i \tilde{u}_i + 2 \nabla w_i \cdot \nabla \tilde{u}_i + w_i \Delta \tilde{u}_i$$

## Local differentiation matrices

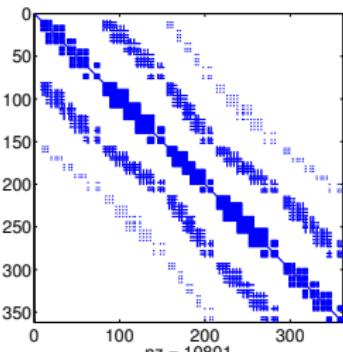
Let  $\underline{u}_i$  be the vector of nodal values in patch  $\Omega_i$ , then

$$\underline{u}_i = A \underline{\lambda}^i, \text{ where } A_{ij} = \phi_j(\underline{x}_i) \Rightarrow$$

$$\mathcal{L}\underline{u}_i = A^{\mathcal{L}} A^{-1} \underline{u}_i, \text{ where } A_{ij}^{\mathcal{L}} = \mathcal{L}\phi_j(\underline{x}_i).$$

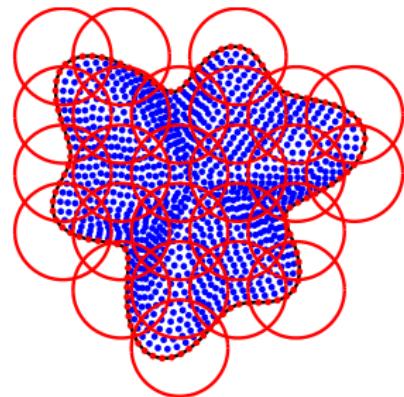
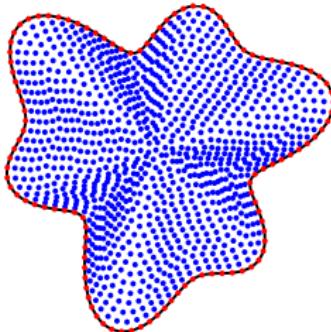
## The global differentiation matrix

Local contributions are added into the global matrix.





# An RBF-PUM collocation method

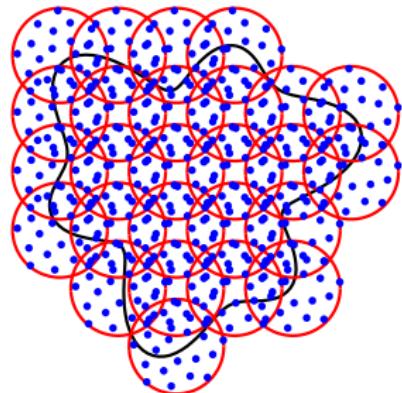


## Choices & Implications

- ▶ Nodes and evaluation points coincide.  
*Square matrix, iterative solver available (Heryudono, Larsson, Ramage, von Sydow 2015).*
- ▶ Global node set.  
*Solutions  $\tilde{u}_i(\underline{x}_k) = \tilde{u}_j(\underline{x}_k)$  for  $\underline{x}_k$  in overlap regions.*
- ▶ Patches are cut by the domain boundary.  
*Potentially strange shapes and lowered local order.*



# An RBF-PUM least squares method



## Choices & Implications

- ▶ Each patch has an identical node layout.  
*Computational cost for setup is drastically reduced.*
- ▶ Evaluation nodes are uniform.  
*Easy to generate both local and global high quality node sets.*
- ▶ Patches have nodes outside the domain.  
*Good for local order, but requires denser evaluation points.*



Outline

Introduction

RBF-PUM

Theoretical results

Numerical results

RBF-QR

Convergence

Robustness

3-D results

Cost

Adaptivity

Summary

# The RBF-PUM interpolation error

$$\mathcal{E}_\alpha = D^\alpha(I(u) - u) = \sum_{j=1}^M \sum_{|\beta| \leq |\alpha|} \binom{\alpha}{\beta} D^\beta w_j D^{\alpha-\beta}(I(u_j) - u_j)$$

## The weight functions

For  $C^k$  weight functions and  $|\alpha| \leq k$

$$\|D^\alpha w_j\|_{L_\infty(\Omega_j)} \leq \frac{C_\alpha}{H_j^{|\alpha|}}, \quad H_j = \text{diam}(\Omega_j).$$

## The local RBF interpolants (Gaussians)

Define the local fill distance  $h_j$  (Rieger, Zwicknagl 2010)

$$\|D^\alpha(I(u_j) - u_j)\|_{L_\infty(\tilde{\Omega}_j)} \leq c_{\alpha,j} h_j^{m_j - \frac{d}{2} - |\alpha|} \|u_j\|_{\mathcal{N}(\tilde{\Omega}_j)},$$

$$\|D^\alpha(I(u_j) - u_j)\|_{L_\infty(\tilde{\Omega}_j)} \leq e^{\gamma_{\alpha,j} \log(h_j)/\sqrt{h_j}} \|u_j\|_{\mathcal{N}(\tilde{\Omega}_j)}.$$



# RBF-PUM interpolation error estimates

Algebraic estimate for  $H_j/h_j = c$

$$\|\mathcal{E}_\alpha\|_{L_\infty(\Omega)} \leq K \max_{1 \leq j \leq M} C_j H_j^{m_j - \frac{d}{2} - |\alpha|} \|u\|_{\mathcal{N}(\tilde{\Omega}_j)}$$

$K$  — Maximum # of  $\Omega_j$  overlapping at one point

$m_j$  — Related to the local # of points

$\tilde{\Omega}_j$  —  $\Omega_j \cap \Omega$

Spectral estimate for fixed partitions

$$\|\mathcal{E}_\alpha\|_{L_\infty(\Omega)} \leq K \max_{1 \leq j \leq M} C e^{\gamma_j \log(h_j) / \sqrt{h_j}} \|u\|_{\mathcal{N}(\tilde{\Omega}_j)}$$

## Implications

- ▶ Bad patch reduces global order.
- ▶ Two refinement modes.
- ▶ Guidelines for adaptive refinement.



# Error estimate for PDE approximation

## The PDE estimate

$\|\tilde{u} - u\|_{L_\infty(\Omega)} \leq C_P \mathcal{E}_{\mathcal{L}} + C_P \|L_{\cdot, X} L_{Y, X}^+\|_\infty (C_M \delta_M + \mathcal{E}_{\mathcal{L}}),$   
where  $C_P$  is a well-posedness constant and  $C_M \delta_M$  is a small multiple of the machine precision.

## Implications

- ▶ Interpolation error  $\mathcal{E}_{\mathcal{L}}$  provides convergence rate.
- ▶ Norm of inverse/pseudoinverse can be large.
- ▶ Matrix norm better with oversampling.
- ▶ Finite precision accuracy limit involves matrix norm.

*Follows strategies from Schaback (2007) and Schaback (2016)*



Outline

Introduction

RBF-PUM

Theoretical results

Numerical results

RBF-QR

Convergence

Robustness

3-D results

Cost

Adaptivity

Summary

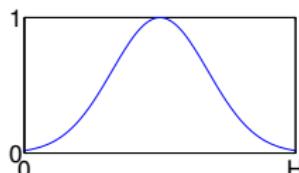
# Does RBF-PUM require stable methods?

In order to achieve convergence we have two options

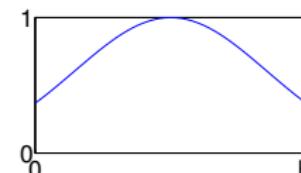
- ▶ Refine patches such that diameter  $H$  decreases.
- ▶ Increase node numbers such that  $N_j$  increases.
- ▶ In both cases, theory assumes  $\varepsilon$  fixed.

## The effect of patch refinement

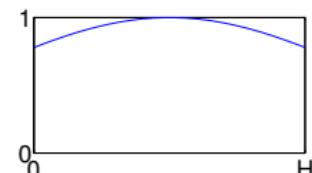
$$H = 1, \varepsilon = 4$$



$$H = 0.5, \varepsilon = 4$$



$$H = 0.25, \varepsilon = 4$$



The RBF-QR method: Stable as  $\varepsilon \rightarrow 0$  for  $N \gg 1$

Effectively a change to a stable basis.

Fornberg, Piret (2007), Fornberg, Larsson, Flyer (2011), Larsson, Lehto, Heryudono, Fornberg (2013)



# Effects on the local matrices

Local contribution to a global Laplacian

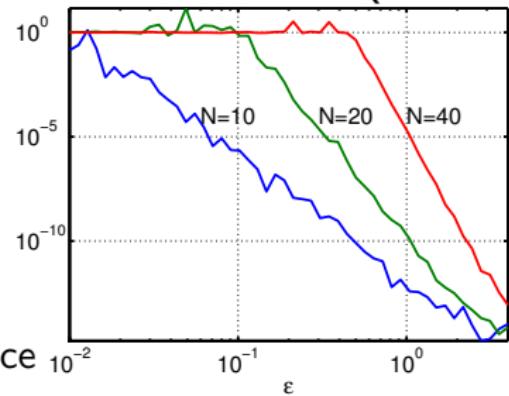
$$L_j = (W_j^\Delta A_j + 2W_j^\nabla \odot A_j^\nabla + W_j A_j^\Delta) A_j^{-1}.$$

Typically:  $A_j$  ill-conditioned,  $L_j$  better conditioned.

## RBF-QR for accuracy

- ▶ Stable for small RBF shape parameters  $\varepsilon$
- ▶ Change of basis  $\tilde{A} = A Q R_1^{-T} D_1^{-T}$
- ▶ Same result in theory  $\tilde{A}^{\mathcal{L}} \tilde{A}^{-1} = A^{\mathcal{L}} A^{-1}$
- ▶ More accurate in practice

Relative error in  $A_j^\Delta A_j^{-1}$   
without RBF-QR





UPPSALA  
UNIVERSITET

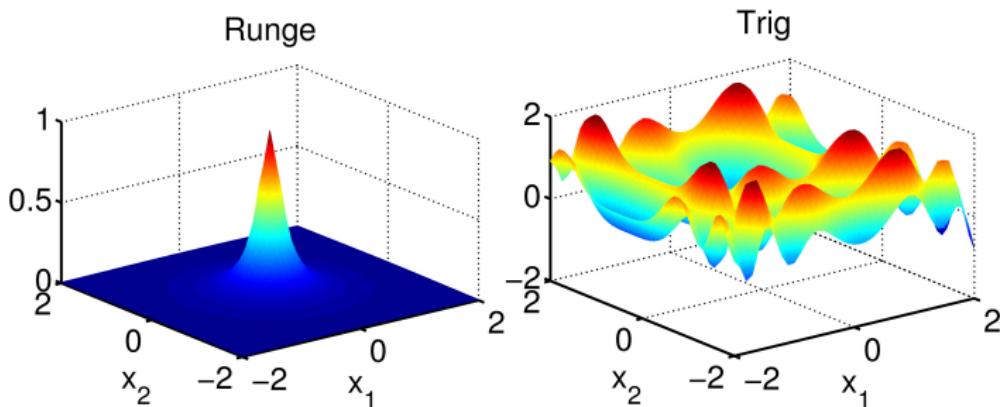
## RBF-PUM

Outline  
Introduction  
RBF-PUM  
Theoretical results  
Numerical results  
RBF-QR  
**Convergence**  
**Robustness**  
**3-D results**  
**Cost**  
**Adaptivity**  
Summary

# Poisson test problems in 2-D

Domain  $\Omega = [-2, 2]^2$ .

Uniform nodes in the collocation case.



$$u_R(x, y) = \frac{1}{25x^2+25y^2+1}$$

$$u_T(x, y) = \sin(2(x-0.1)^2) \cos((x-0.3)^2) + \sin^2((y-0.5)^2)$$



Outline

Introduction

RBF-PUM

Theoretical results

Numerical results

RBF-QR

Convergence

Robustness

3-D results

Cost

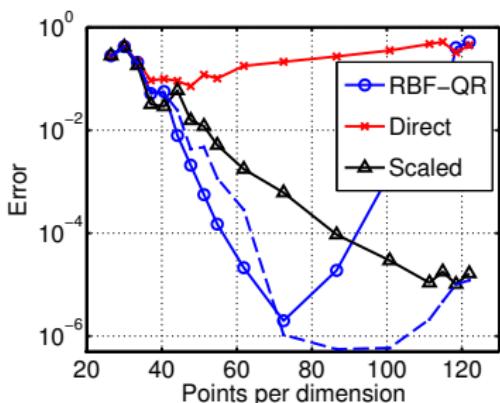
Adaptivity

Summary

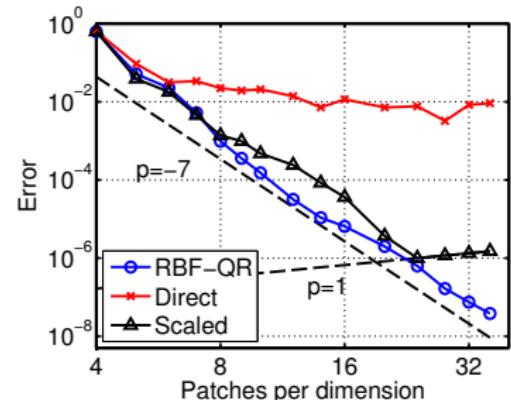
# Error results with and without RBF–QR

- ▶ Least squares RBF-PUM
- ▶ Fixed shape  $\varepsilon = 0.5$  or scaled such that  $\varepsilon h = c$
- ▶ Left:  $5 \times 5$  patches    Right: 55 points per patch

Spectral mode



Algebraic mode



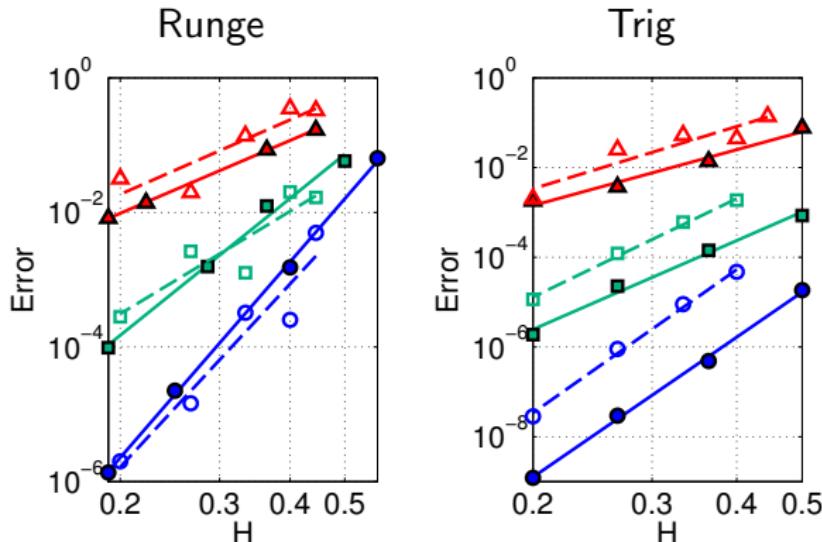
- ▶ With RBF–QR better results for  $H/h$  large.
- ▶ Scaled approach good until saturation.



## RBF-PUM

Outline  
Introduction  
RBF-PUM  
Theoretical results  
Numerical results  
**RBF-QR**  
Convergence  
Robustness  
3-D results  
Cost  
Adaptivity  
Summary

# Convergence as a function of patch size



Collocation (dashed lines) and Least Squares (solid lines).

- ▶ Points per patch  $n = 28, 55, 91$ .
- ▶ Theoretical rates  $p = 4, 7, 10$ .
- ▶ Numerical rates  $p \approx 3.9, 6.9, 9.8$ .

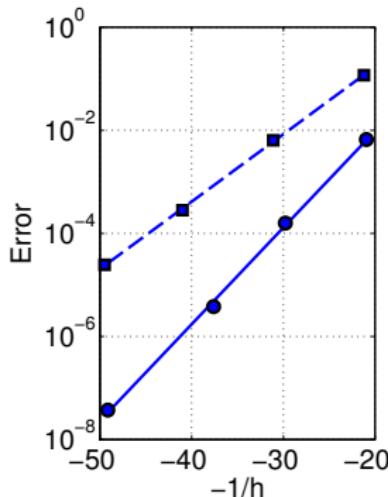


## RBF-PUM

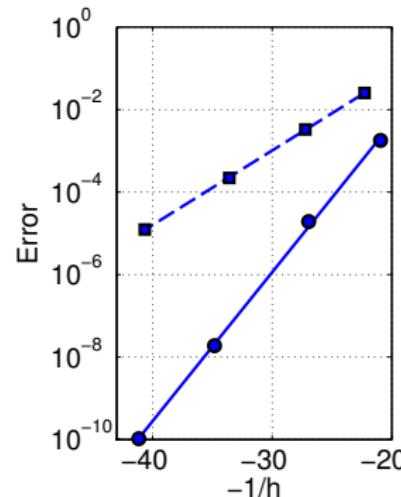
- Outline
- Introduction
- RBF-PUM
- Theoretical results
- Numerical results
  - RBF-QR
  - Convergence
  - Robustness
  - 3-D results
  - Cost
  - Adaptivity
- Summary

# Spectral convergence for fixed patches

Runge



Trig



Collocation (dashed lines) and Least Squares (solid lines).

LS-RBF-PU is significantly more accurate due to the constant number of nodes per patch.



Outline

Introduction

RBF-PUM

Theoretical results

Numerical results

RBF-QR

Convergence

Robustness

3-D results

Cost

Adaptivity

Summary

# Robustness and large scale problems

## The global error estimate

$$\|\tilde{u} - u\|_{L_\infty(\Omega)} \leq C_P \mathcal{E}_{\mathcal{L}} + C_P \|L_{\cdot, X} L_{Y, X}^+\|_\infty (C_M \delta_M + \mathcal{E}_{\mathcal{L}})$$

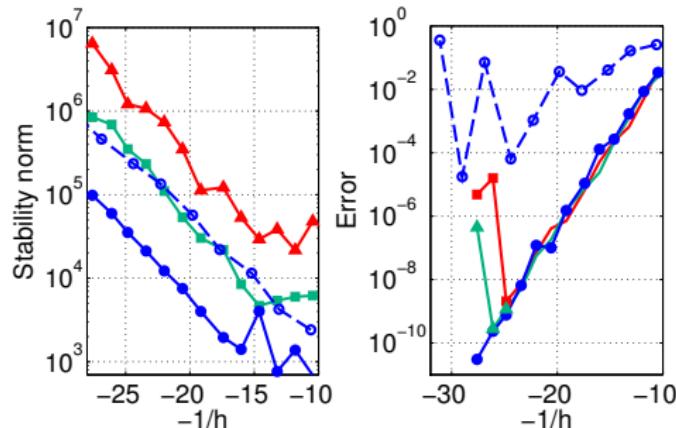
The dark horse is the 'stability matrix norm'

- ▶ The stability norm is related to conditioning.
- ▶ In the collocation case,  $\|L_{X, X}^{-1}\|$  grows with  $N$ .
- ▶ How does it behave with least squares?



# The stability matrix norm: fill distance

- ▶ Fixed patch size with  $10 \times 10$  patches.
- ▶ Oversampling  $M/N = 1.1, 1.2, 1.5$



Collocation (dashed) and Least Squares (solid)

- ▶ Stability norm grows exponentially as  $h$  decreases.
- ▶ Oversampling reduces the norm.
- ▶ Collocation is less robust.



Outline

Introduction

RBF-PUM

Theoretical results

Numerical results

RBF-QR

Convergence

Robustness

3-D results

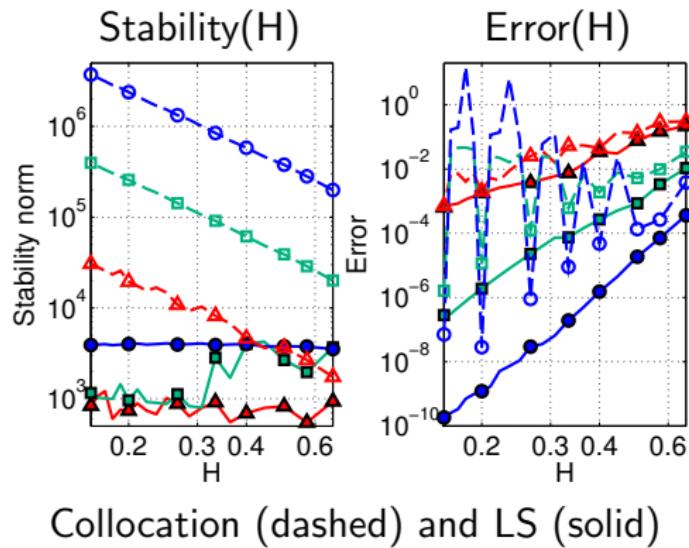
Cost

Adaptivity

Summary

# Stability norm: Patch size

- ▶ Fixed number of points per patch  $n = 28, 55, 91$
- ▶ Results as a function of patch diameter  $H$

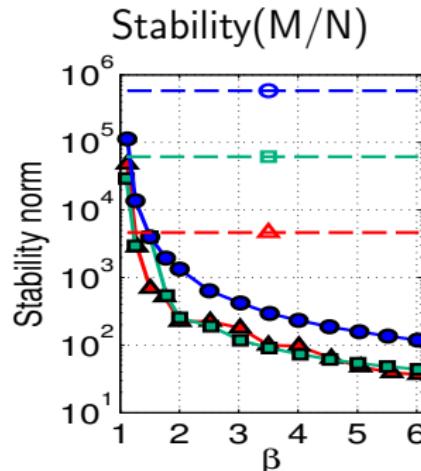


- ▶ The norm does not grow for LS-RBF-PUM (!)



## Stability norm: Oversampling

- ▶ Fixed number of local points  $n = 55$ .
- ▶ Patches:  $5 \times 5, 10 \times 10, 15 \times 15$



Collocation (dashed) and LS (solid)

- ▶ Oversampling provides stability (at a cost).
- ▶ For robustness in  $h$ ,  $M/N$  needs to grow with  $N$ .



UPPSALA  
UNIVERSITET

## RBF-PUM

Outline

Introduction

RBF-PUM

Theoretical results

Numerical results

RBF-QR

Convergence

Robustness

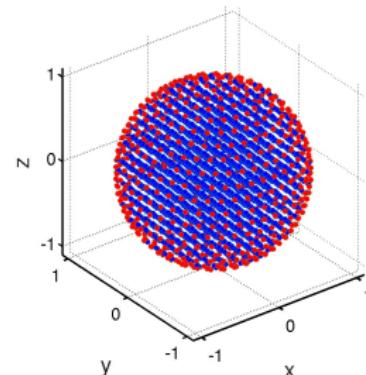
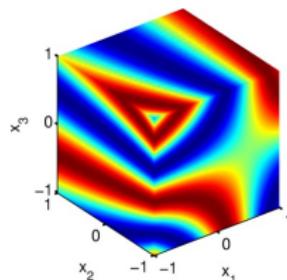
3-D results

Cost

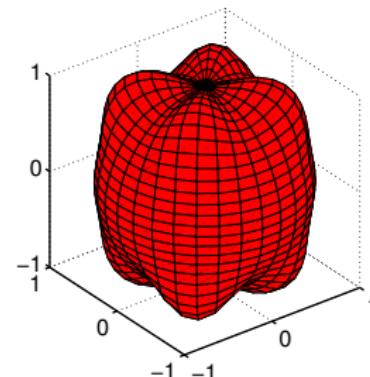
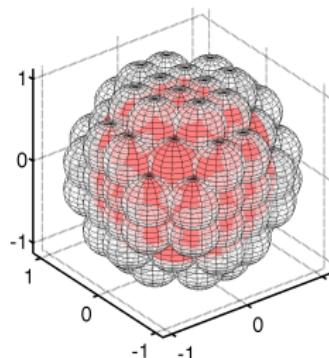
Adaptivity

Summary

# Poisson test problems in 3-D



$$u(\underline{x}) = \sin \left( \frac{\pi(x_1 - 0.5)x_3}{\log(x_2 + 3)} \right)$$





## RBF-PUM

Outline

Introduction

RBF-PUM

Theoretical results

Numerical results

**RBF-QR**

**Convergence**

**Robustness**

**3-D results**

**Cost**

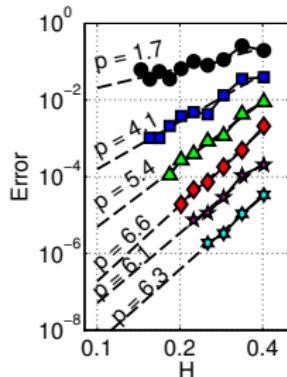
**Adaptivity**

Summary

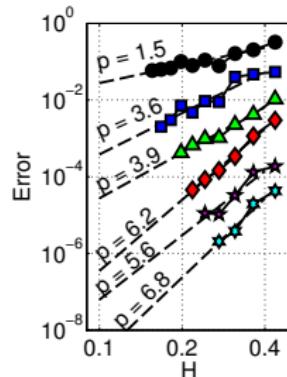
# Convergence in 3-D

- ▶  $n = 20, 35, 56, 84, 120, 165$  points per patch

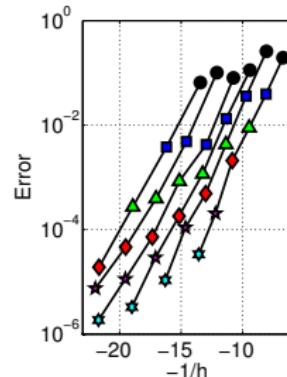
Sphere



Pepper



Spectral



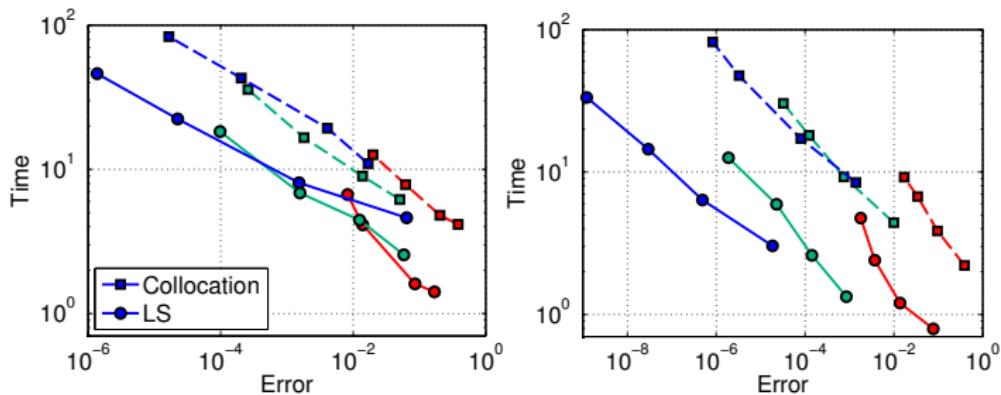
- ▶ Convergence order is a bit better than expected.
- ▶ Refinement modes work as expected.



## RBF-PUM

Outline  
Introduction  
RBF-PUM  
Theoretical results  
Numerical results  
**RBF-QR**  
**Convergence**  
**Robustness**  
**3-D results**  
**Cost**  
**Adaptivity**  
Summary

# Computational time comparison in 2-D



- ▶ Experiments with fixed  $n = 28, 55, 91$ .
- ▶ For a fixed problem size, RBF-PU-LS involves more work, but yields a smaller error.
- ▶ Overall, the LS approach is the winner.
- ▶ Strategy: Points per patch adjusted to tolerance.



Outline

Introduction

RBF-PUM

Theoretical results

Numerical results

**RBF-QR**

Convergence

Robustness

3-D results

Cost

Adaptivity

Summary

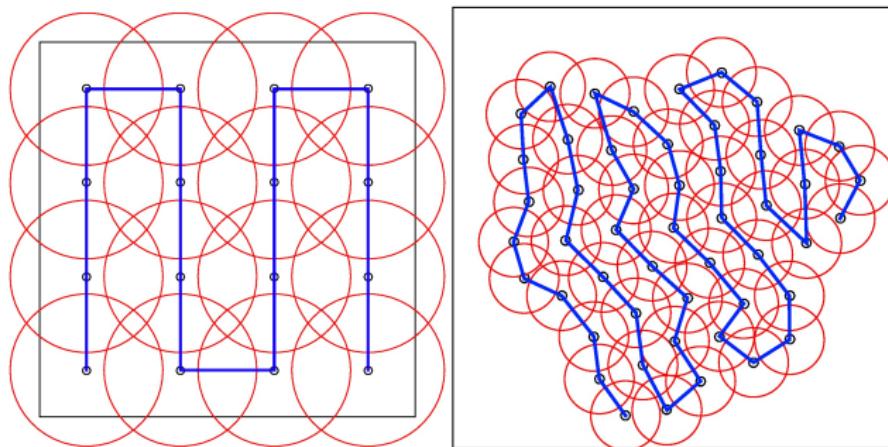
## Solution using iterative methods

So far implemented for the collocation approach. First step: Re-ordering of the unknowns to improve structure.

**Patches:** Preceded and followed by a neighbour.

**Nodes  $x_k$ :** Define home patch  $\Omega_j$  such that  $w_j \geq w_i(x_k)$ .

**Within patch:** Sub-order according to node memberships.



*Heryudono, Larsson, Ramage, and von Sydow (2015)*



UPPSALA  
UNIVERSITET

RBF-PUM

Outline

Introduction

RBF-PUM

Theoretical results

Numerical results

RBF-QR

Convergence

Robustness

3-D results

Cost

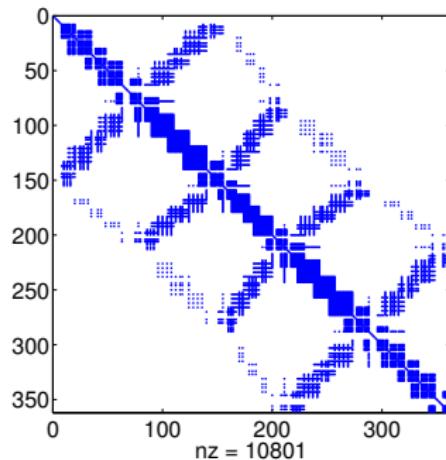
Adaptivity

Summary

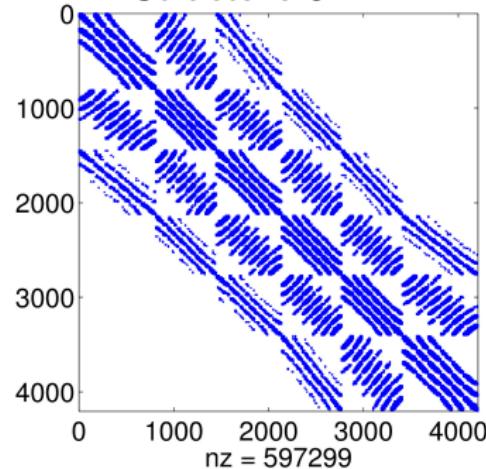
# Matrix structures with snake order

- ▶ The patch order fills in gaps in the band.
- ▶ The node order minimizes the central band width.
- ▶ Chosen preconditioner, ILU(0) of central band.

Structure 2-D



Structure 3-D





## RBF-PUM

Outline  
Introduction  
RBF-PUM  
Theoretical results  
Numerical results  
**RBF-QR**  
**Convergence**  
**Robustness**  
**3-D results**  
**Cost**  
**Adaptivity**  
Summary

## Results for the iterative method contd.

## Results in 2-D with Halton nodes

$N$	# it no prec	# it ILU(0)	Time gain
436	189	72	3.1
583	209	91	2.4
681	231	112	2.7
884	262	125	2.3
1 090	295	135	3.0

## Results in 3-D with Halton nodes

$N$	# it no prec	# it ILU(0)	Time gain
4 206	100	47	1.1
9 534	166	69	1.5
18 101	224	85	2.5
99 568	454	174	4.6
231 284	755	417	2.9

*Memory gain not to be forgotten.*



Outline

Introduction

RBF-PUM

Theoretical results

Numerical results

RBF-QR

Convergence

Robustness

3-D results

Cost

Adaptivity

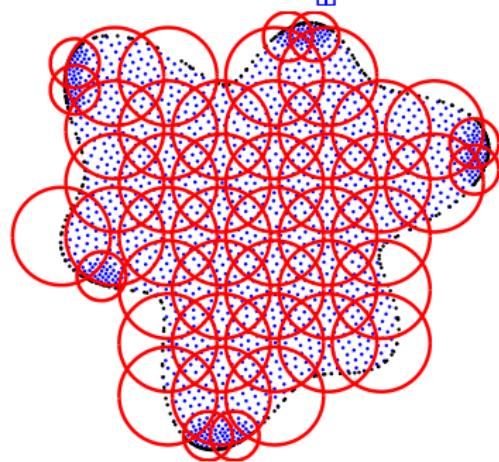
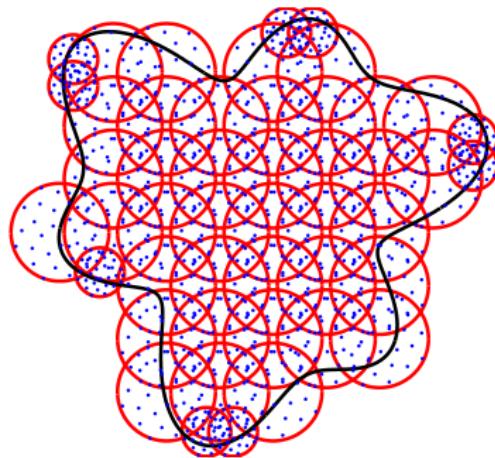
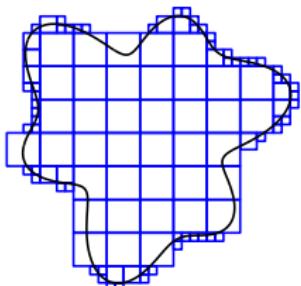
Summary

# Current project: Adaptivity

*With Alfa Heryudono, Danilo Stocchino and Stefano De Marchi*

- ▶ Box structure helps book keeping.
- ▶ Overlaps complicate things.
- ▶ Evaluation points placed using node placing algorithm.

*Fornberg & Flyer (2015)*





Outline

Introduction

RBF-PUM

Theoretical results

Numerical results

RBF-QR

Convergence

Robustness

3-D results

Cost

Adaptivity

Summary

# Summary

## Results

- ▶ RBF-PUM is a flexible tool for solving PDEs.
- ▶ By using template patches, LS RBF-PUM becomes computationally efficient.
- ▶ LS RBF-PUM is numerically stable for large scale problems.

## Things to do

- ▶ Change patch type to reduce unnecessary overlap.
- ▶ Adaptive algorithms based on LS RBF-PUM.
- ▶ Time-stability for LS RBF-PUM.  
*For collocation and hyperbolic PDEs on the sphere,  
see poster by Igor Tominec et al.*