

Some properties of RBF-FD differential operator approximations

Doctoral dissertation proposal

Author: Andrej Kolar-Požun

Mentor: Dr. Gregor Kosec

Jožef Stefan Institute
University of Ljubljana - Faculty of Mathematics and Physics

May 15, 2024

Numerical treatment of PDEs - Finite Difference Method

- Goal: Solve $\mathcal{L}u(x) = f(x), x \in \Omega$ (and boundary conditions)

Numerical treatment of PDEs - Finite Difference Method

- Goal: Solve $\mathcal{L}u(x) = f(x), x \in \Omega$ (and boundary conditions)
- Step 1 - discretise Ω to obtain a (regular) discretisation $\{x_i\}_i \subset \Omega$.

Numerical treatment of PDEs - Finite Difference Method

- Goal: Solve $\mathcal{L}u(x) = f(x), x \in \Omega$ (and boundary conditions)
- Step 1 - discretise Ω to obtain a (regular) discretisation $\{x_i\}_i \subset \Omega$.
- Step 2 - approximate the operator \mathcal{L} locally (i.e. 5-point, 9-point stencil,...).

Numerical treatment of PDEs - Finite Difference Method

- Goal: Solve $\mathcal{L}u(x) = f(x), x \in \Omega$ (and boundary conditions)
- Step 1 - discretise Ω to obtain a (regular) discretisation $\{x_i\}_i \subset \Omega$.
- Step 2 - approximate the operator \mathcal{L} locally (i.e. 5-point, 9-point stencil,...).
- Step 3 - Form a linear system by requiring the discretised PDE to hold at each x_i .

Numerical treatment of PDEs - Finite Difference Method

- Goal: Solve $\mathcal{L}u(x) = f(x), x \in \Omega$ (and boundary conditions)
- Step 1 - discretise Ω to obtain a (regular) discretisation $\{x_i\}_i \subset \Omega$.
- Step 2 - approximate the operator \mathcal{L} locally (i.e. 5-point, 9-point stencil,...).
- Step 3 - Form a linear system by requiring the discretised PDE to hold at each x_i .
- Step 4 - Invert the system to obtain the values $u(x_i)$.

RBF-FD - Radial Basis Function generated Finite Differences

- Strong-form meshless methods: $\{x_i\}_i \subset \Omega$ can be irregular.

RBF-FD - Radial Basis Function generated Finite Differences

- Strong-form meshless methods: $\{x_i\}_i \subset \Omega$ can be irregular.
- RBF-FD provides an approximation of the form
$$\mathcal{L}u(x_i) \approx \sum_{j \in S_i} w_j u(x_j).$$

RBF-FD - Radial Basis Function generated Finite Differences

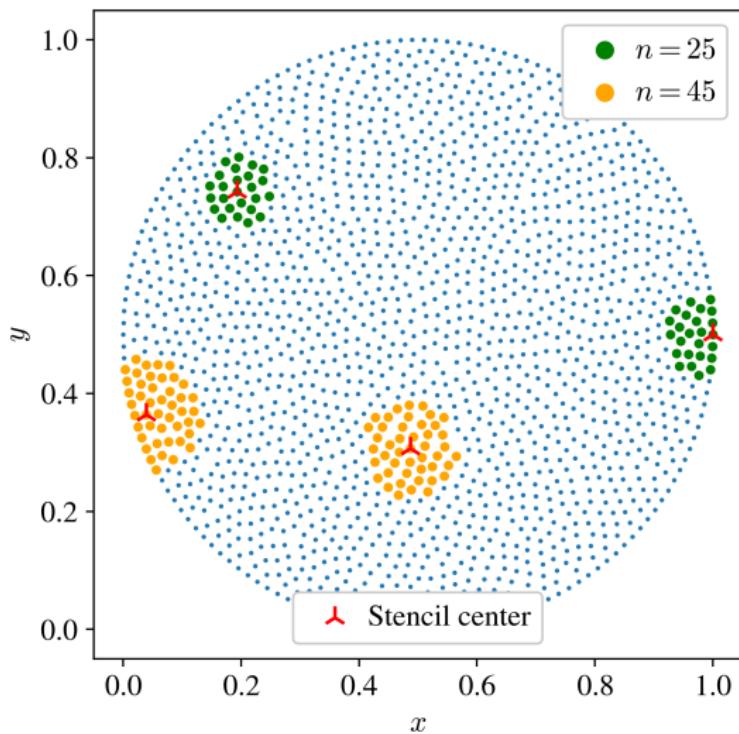
- Strong-form meshless methods: $\{x_i\}_i \subset \Omega$ can be irregular.
- RBF-FD provides an approximation of the form
$$\mathcal{L}u(x_i) \approx \sum_{j \in S_i} w_j u(x_j).$$

$$\begin{pmatrix} A & P \\ P^T & 0 \end{pmatrix} \begin{pmatrix} w \\ \lambda \end{pmatrix} = \begin{pmatrix} \mathcal{L}(\phi) \\ \mathcal{L}(p) \end{pmatrix}$$

$$A = \begin{pmatrix} \phi(||x_1 - x_1||) & \dots & \phi(||x_1 - x_n||) \\ \vdots & \ddots & \vdots \\ \phi(||x_n - x_1||) & \dots & \phi(||x_n - x_n||) \end{pmatrix}$$

$$P = \begin{pmatrix} p_1(x_1) & \dots & p_M(x_1) \\ \vdots & \ddots & \vdots \\ p_1(x_n) & \dots & p_M(x_n) \end{pmatrix}$$

Example meshless discretisation



Some further properties of RBF-FD

- RBFs allow for interpolation on scattered data with provable invertibility guarantees.

Some further properties of RBF-FD

- RBFs allow for interpolation on scattered data with provable invertibility guarantees.
- RBF-FD approximation is obtained by applying \mathcal{L} to the interpolant.

Some further properties of RBF-FD

- RBFs allow for interpolation on scattered data with provable invertibility guarantees.
- RBF-FD approximation is obtained by applying \mathcal{L} to the interpolant.
- Polyharmonic Spline (PHS) RBF: $\phi(r) = r^3$ - no shape parameter, improved stability.

Some further properties of RBF-FD

- RBFs allow for interpolation on scattered data with provable invertibility guarantees.
- RBF-FD approximation is obtained by applying \mathcal{L} to the interpolant.
- Polyharmonic Spline (PHS) RBF: $\phi(r) = r^3$ - no shape parameter, improved stability.
- Monomial augmentation of order m - Polynomial reproduction up to order m .

Core topics

- Oscillatory behaviour of RBF-FD error under increasing stencil size.

Core topics

- Oscillatory behaviour of RBF-FD error under increasing stencil size.
- Superconvergent behaviour of the RBF-FD method.

Core topics

- Oscillatory behaviour of RBF-FD error under increasing stencil size.
- Superconvergent behaviour of the RBF-FD method.
- The "RBF FDM".

Core topics

- Oscillatory behaviour of RBF-FD error under increasing stencil size.
- Superconvergent behaviour of the RBF-FD method.
- The "RBF FDM".
- Smoothness of the RBF-FD approximation.

Typical research strategy

- Simple problem (circular domain, $\nabla^2 u(x, y) = f(x, y)$, Dirichlet BC)

Typical research strategy

- Simple problem (circular domain, $\nabla^2 u(x, y) = f(x, y)$, Dirichlet BC)
- Choose a function $u(x, y)$ and solve the corresponding PDE with RBF-FD

Typical research strategy

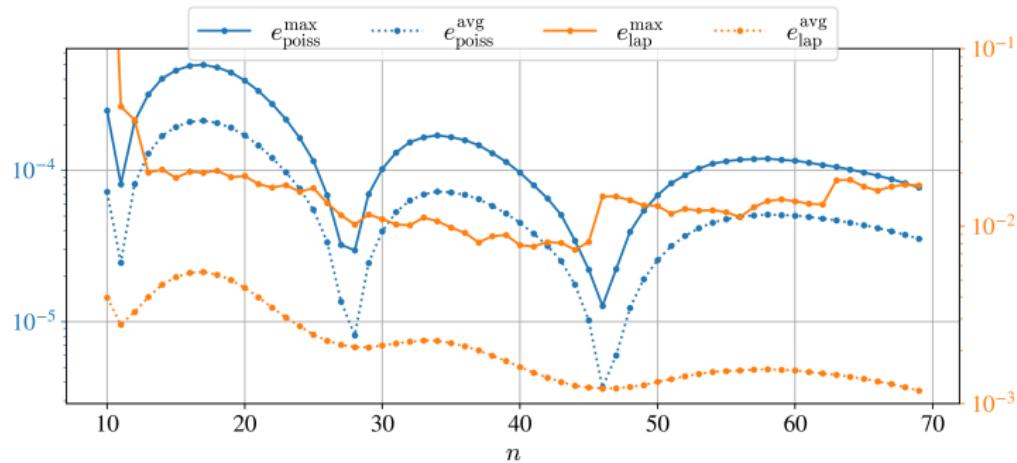
- Simple problem (circular domain, $\nabla^2 u(x, y) = f(x, y)$, Dirichlet BC)
- Choose a function $u(x, y)$ and solve the corresponding PDE with RBF-FD
- Study the error behaviour and the approximation properties.

Oscillatory behaviour of RBF-FD error under increasing stencil size

- $u(x, y) = \sin(\pi x) \sin(\pi y)$.

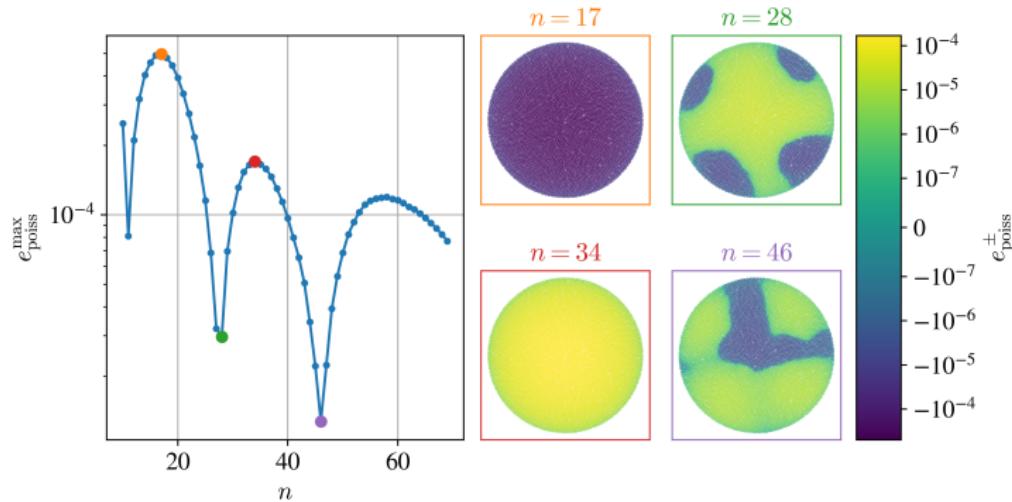
Oscillatory behaviour of RBF-FD error under increasing stencil size

- $u(x, y) = \sin(\pi x) \sin(\pi y)$.
- Fix monomial augmentation $m = 3$, $h = 0.01$, $\phi(r) = r^3$, increase the stencil size and observe that the solution error oscillates.



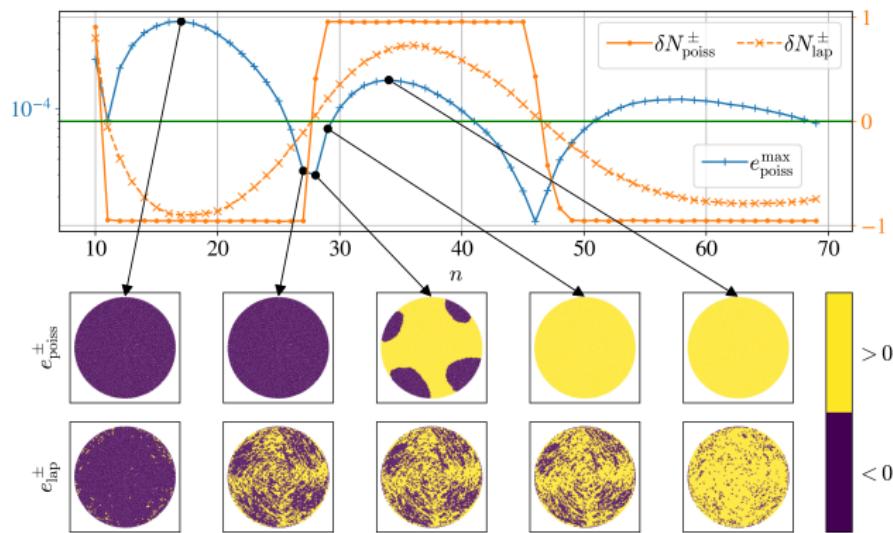
Oscillatory behaviour of RBF-FD error under increasing stencil size

- Oscillatory error can be connected to the pointwise error behaviour.



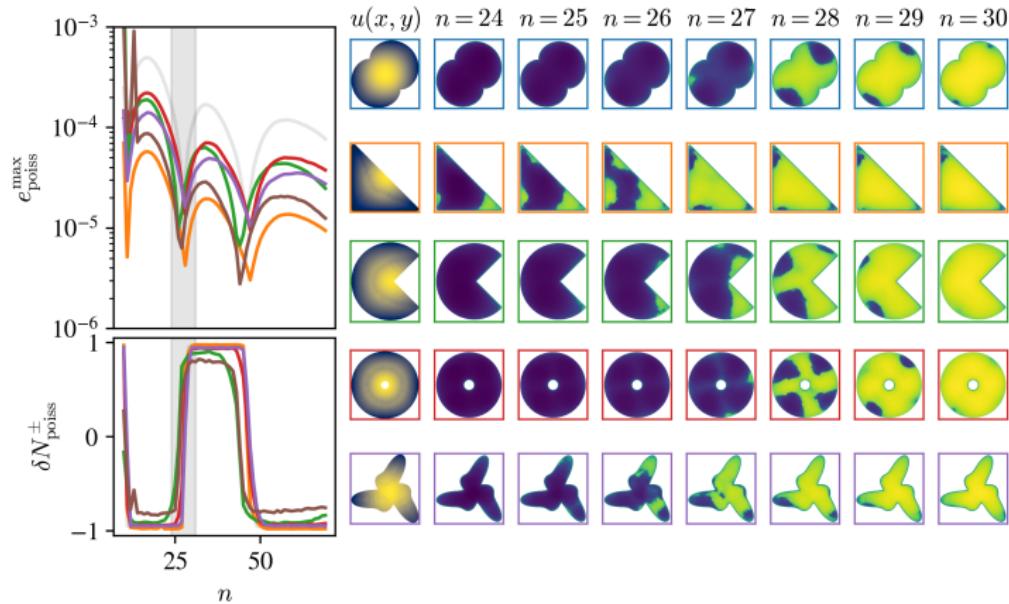
Oscillatory behaviour of RBF-FD error under increasing stencil size

- Quantity $\delta N_{\text{poiss}}^{\pm}$ ("mean sign of pointwise error") - minima indicator?



Oscillatory behaviour of RBF-FD error under increasing stencil size

- The behaviour is robust under various different changes of the problem setup and method parameters.

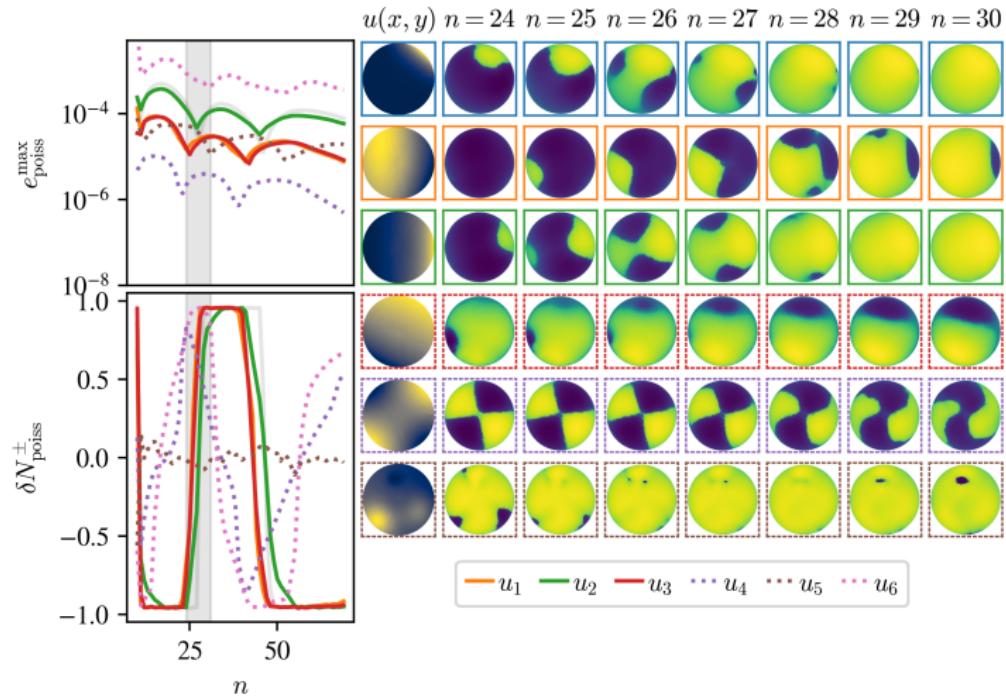


Oscillatory behaviour of RBF-FD error under increasing stencil size

- ... But there are exceptions.

Label	$u(x, y)$
u_1	$x^4 y^5$
u_2	$1 + \sin(4x) + \cos(3x) + \sin(2y)$
u_3	$\exp(x^2)$
u_4	$\text{arsinh}(x + 2y)$
u_5	$\cos(\pi x) \cos(\pi y)$
u_6	$\text{franke}(x, y)$

Oscillatory behaviour of RBF-FD error under increasing stencil size



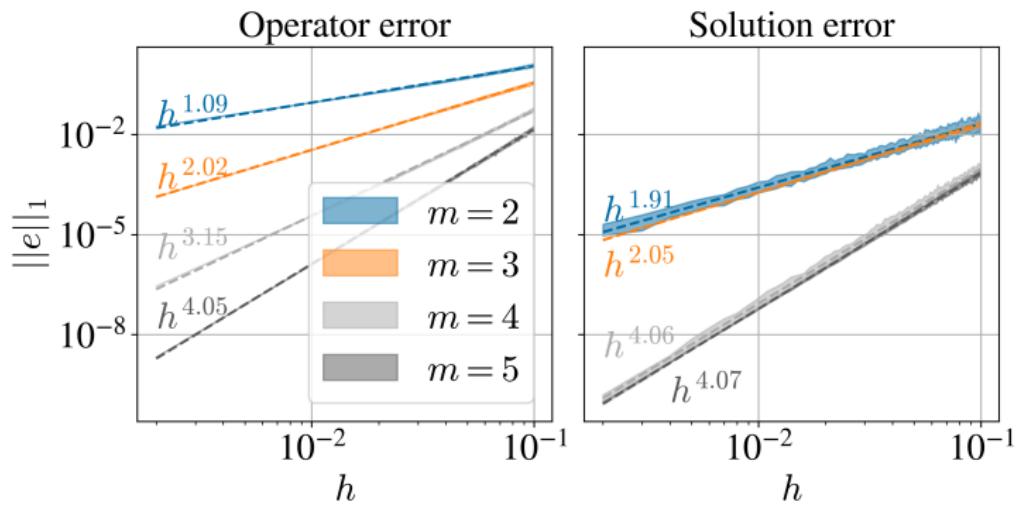
Superconvergence of the RBF-FD method

- Solve the Poisson equation with

$$u(x, y) = 1 + \sin(4x) + \cos(3x) + \sin(2y).$$

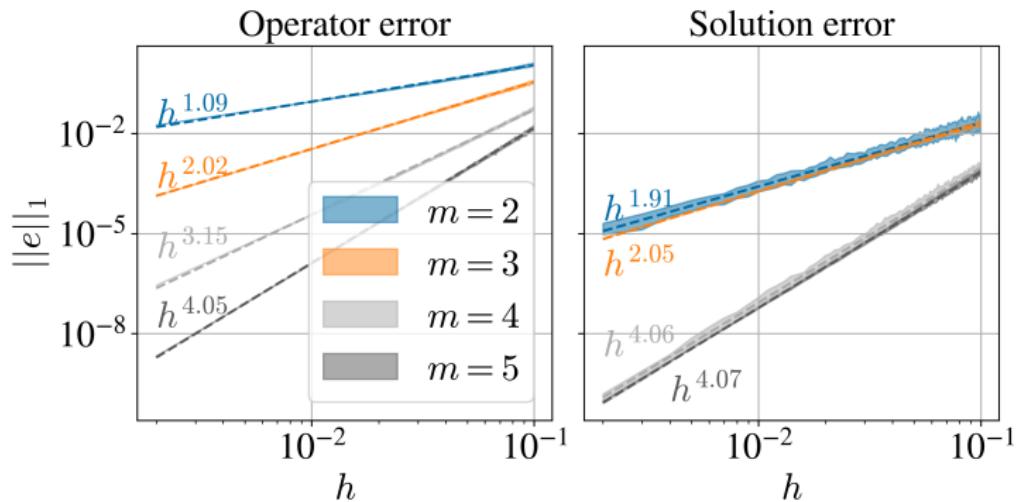
Superconvergence of the RBF-FD method

- Solve the Poisson equation with $u(x, y) = 1 + \sin(4x) + \cos(3x) + \sin(2y)$.
- Calculate the error dependence on h (over different discretisations)



Superconvergence of the RBF-FD method

- Solve the Poisson equation with $u(x, y) = 1 + \sin(4x) + \cos(3x) + \sin(2y)$.
- Calculate the error dependence on h (over different discretisations)
- Operator approximation order matches theory - h^{m-1} (h^{m+1-k}).
- Solution order is h^{m-1} or h^m



Superconvergence of the RBF-FD method

- The solution error can be obtained as a solution to $Ae_{\text{sol}} = e_{\text{op}}$.

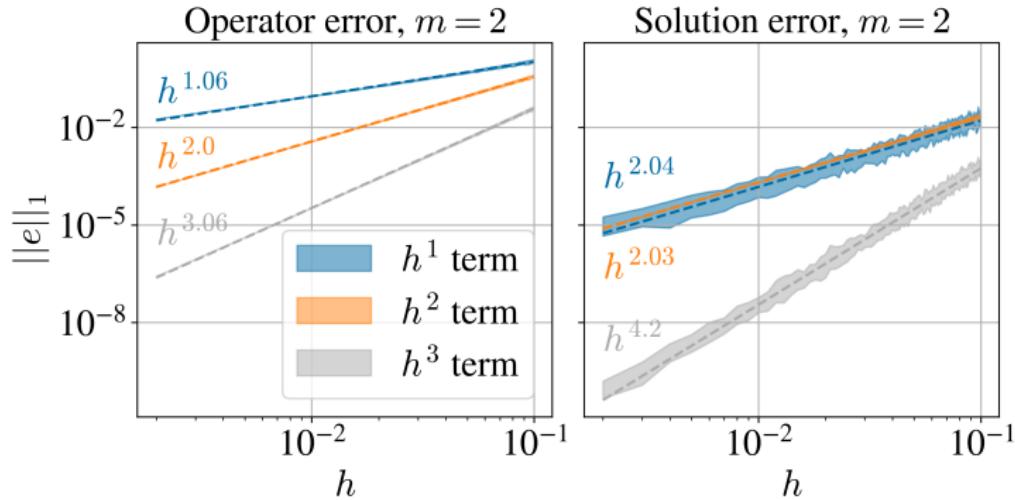
Superconvergence of the RBF-FD method

- The solution error can be obtained as a solution to $Ae_{\text{sol}} = e_{\text{op}}$.
- The form of e_{op} is actually known¹:
- $\nabla^2 \hat{u}(x_i, y_i) - \nabla^2 u(x_i, y_i) = \sum_{k=s+1}^{\infty} L_k[u(x_i, y_i)](\mathbf{p}_k^T \cdot \mathbf{w})$.

¹Bayona V., An insight into RBF-FD approximations augmented with monomials,
2019

Superconvergence of the RBF-FD method

- The solution error can be obtained as a solution to $Ae_{\text{sol}} = e_{\text{op}}$.
- The form of e_{op} is actually known¹:
- $\nabla^2 \hat{u}(x_i, y_i) - \nabla^2 u(x_i, y_i) = \sum_{k=s+1}^{\infty} L_k[u(x_i, y_i)](\mathbf{p}_k^T \cdot \mathbf{w})$.
- Study the error behaviour term by term in powers of h .



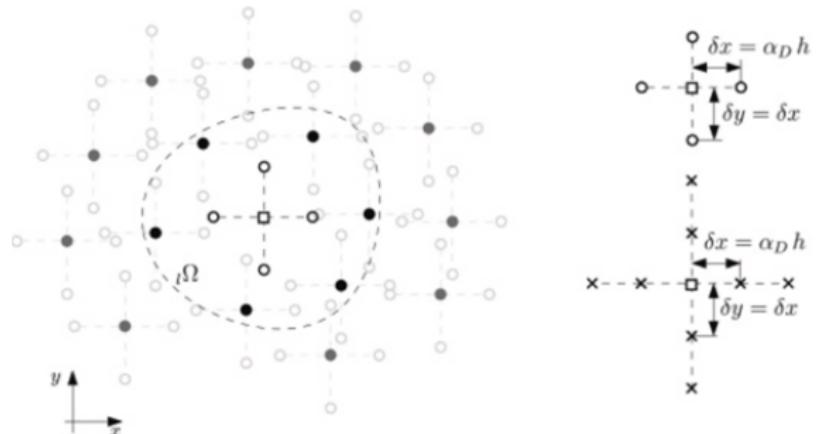
¹Bayona V., An insight into RBF-FD approximations augmented with monomials, 2019

RBF FDM

- "Radial Basis Function Finite Difference Method".

RBF FDM

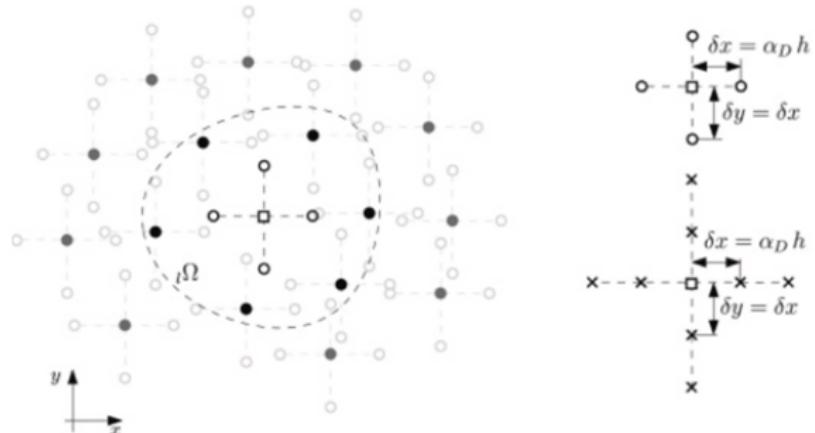
- "Radial Basis Function Finite Difference Method".
- Employing RBF interpolants, interpolate scattered nodes to a "virtual" FDM stencil and apply FDM formulas.
- Already successfully applied to physical problems²



²Vuga G., Mavrič B. and Šarler B., An improved local radial basis function method for solving small-strain elasto-plasticity, 2024

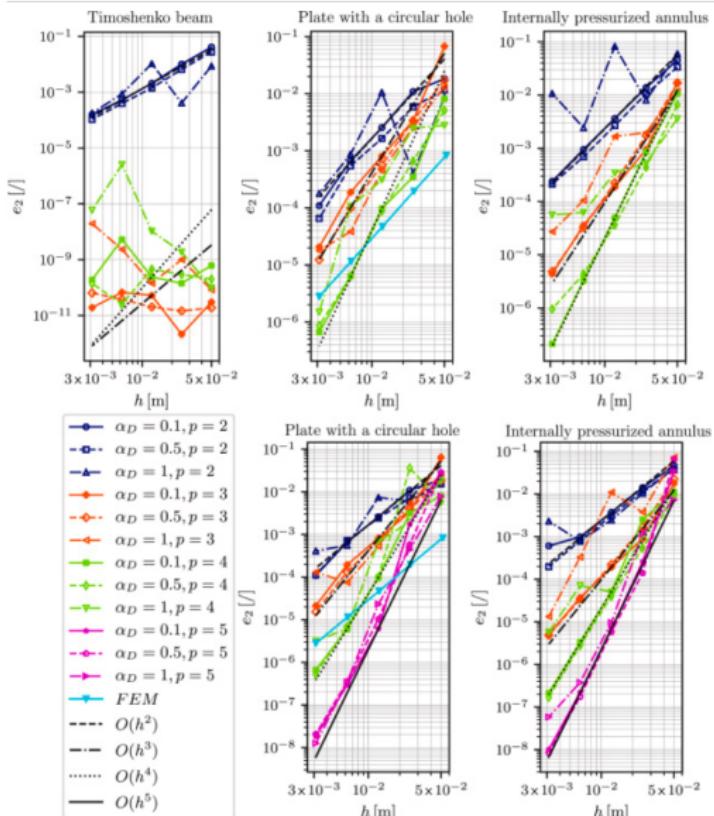
RBF FDM

- "Radial Basis Function Finite Difference Method".
- Employing RBF interpolants, interpolate scattered nodes to a "virtual" FDM stencil and apply FDM formulas.
- Already successfully applied to physical problems²
- New parameters - shape and spacing of the "virtual" FDM stencil.



²Vuga G., Mavrič B. and Šarler B., An improved local radial basis function method for solving small-strain elasto-plasticity, 2024

RBF-FDM applications



RBF FDM motivation

- Greater stability under decreasing h .

RBF FDM motivation

- Greater stability under decreasing h .
- Potentially better suited for problems with discontinuity.

RBF FDM motivation

- Greater stability under decreasing h .
- Potentially better suited for problems with discontinuity.
- Sometimes a grid may also be desired, i.e. Yee's algorithm.

Smoothness of the approximation

- The usual error estimates assume the solution in question is sufficiently smooth.

Smoothness of the approximation

- The usual error estimates assume the solution in question is sufficiently smooth.
- In a numerical setting, a similar notion is well-resolvedness of a function.

Smoothness of the approximation

- The usual error estimates assume the solution in question is sufficiently smooth.
- In a numerical setting, a similar notion is well-resolvedness of a function.
- Taylor series remainder - $\propto f^{(p+1)}(\xi)h^{p+1}$

Smoothness of the approximation

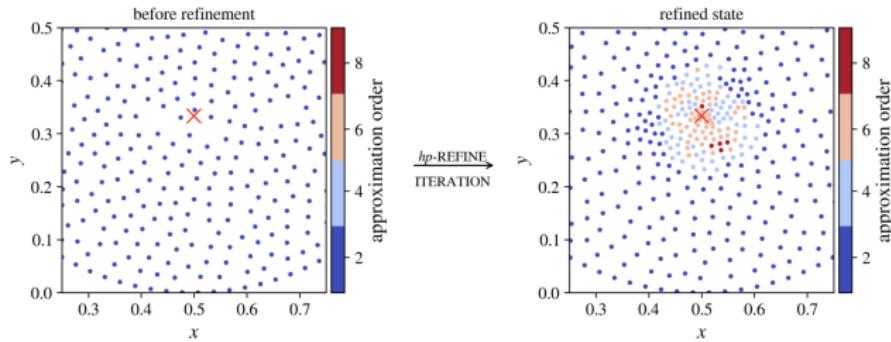
- The usual error estimates assume the solution in question is sufficiently smooth.
- In a numerical setting, a similar notion is well-resolvedness of a function.
- Taylor series remainder - $\propto f^{(p+1)}(\xi)h^{p+1}$
- For a badly resolved function, increasing the method order is undesirable!

Smoothness of the approximation

- The usual error estimates assume the solution in question is sufficiently smooth.
- In a numerical setting, a similar notion is well-resolvedness of a function.
- Taylor series remainder - $\propto f^{(p+1)}(\xi)h^{p+1}$
- For a badly resolved function, increasing the method order is undesirable!
- Main question - when should the order be increased?

Smoothness of the approximation - Application and Motivation

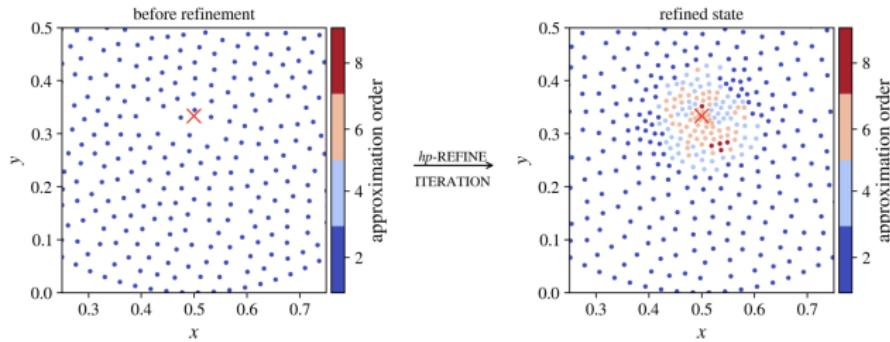
- hp refinement - iterative spatial modification of nodal density (h -) and method order (p)³.



³ Jančič M. and Kosec G., Strong form mesh-free hp-adaptive solution of linear elasticity problem, 2023

Smoothness of the approximation - Application and Motivation

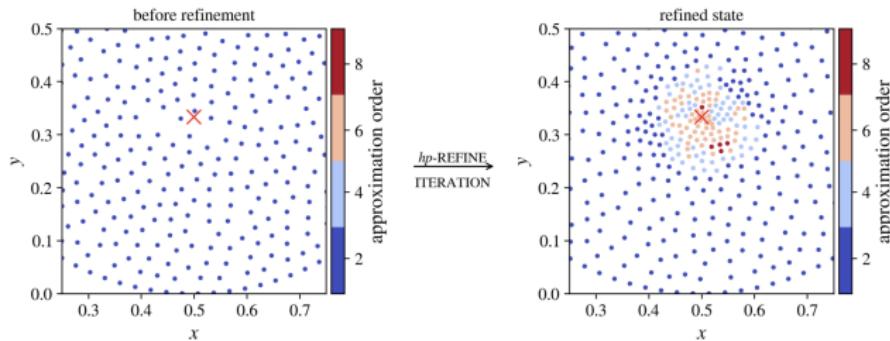
- hp refinement - iterative spatial modification of nodal density (h -) and method order (p)³.
- h-refining should be preferred in the areas, where the solution is less smooth - smoothness indicator?



³ Jančič M. and Kosec G., Strong form mesh-free hp-adaptive solution of linear elasticity problem, 2023

Smoothness of the approximation - Application and Motivation

- hp refinement - iterative spatial modification of nodal density (h -) and method order (p -)³.
- h-refining should be preferred in the areas, where the solution is less smooth - smoothness indicator?
- Connection with RBFs.



³ Jančič M. and Kosec G., Strong form mesh-free hp-adaptive solution of linear elasticity problem, 2023

Summary

- Our work aims to further the understanding of PHS RBF-FD approximations.

Summary

- Our work aims to further the understanding of PHS RBF-FD approximations.
- We aim to analyse the two observed behaviours - oscillating error and order elevation.

Summary

- Our work aims to further the understanding of PHS RBF-FD approximations.
- We aim to analyse the two observed behaviours - oscillating error and order elevation.
- We plan to systematically research the RBF FDM.

Summary

- Our work aims to further the understanding of PHS RBF-FD approximations.
- We aim to analyse the two observed behaviours - oscillating error and order elevation.
- We plan to systematically research the RBF FDM.
- We wish to incorporate solution smoothness information in the solution procedure.