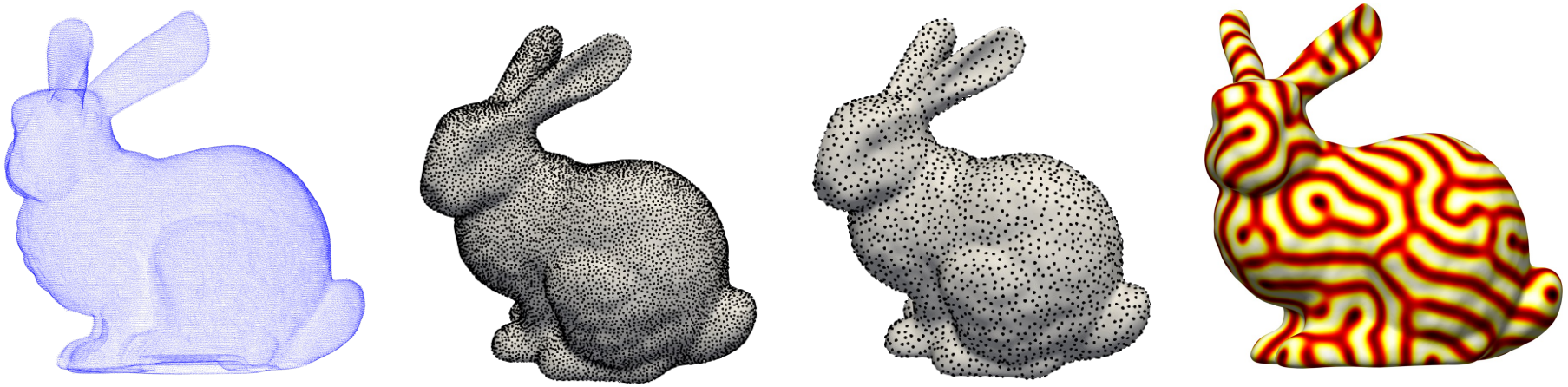
Computing on Point Cloud Surfaces:
PDEs, Multilevel Solvers, Quadrature, & Implicit Reconstruction



Grady B. Wright
Boise State University

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Collaborators

Varun Shankar
University of Utah

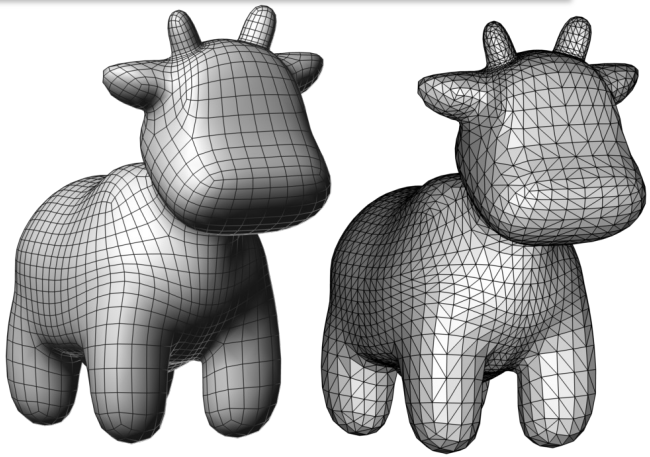
Andrew Jones
Sandia

Kathryn Drake
Apple

Meshes vs Point Cloud Surfaces

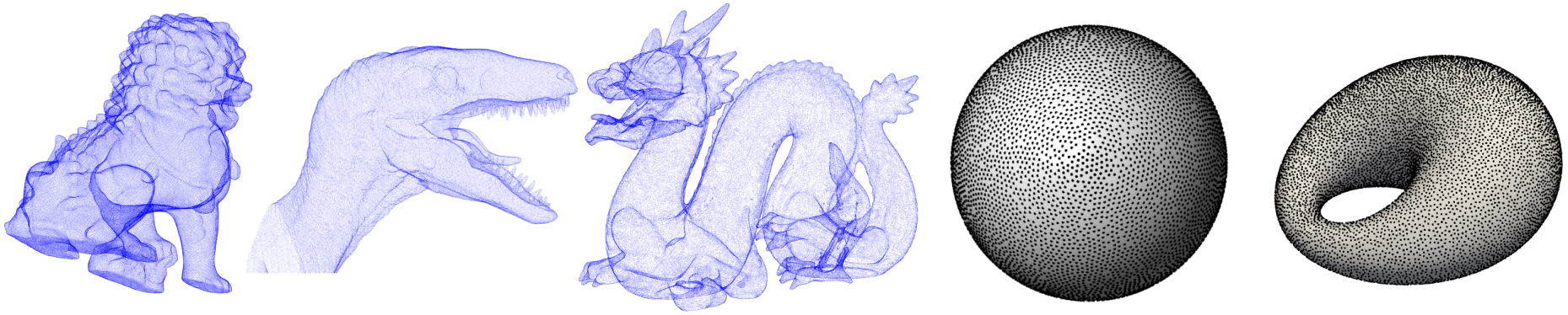
Mesh: a set of points that connects points into faces

(e.g., triangles or quads), forming a continuous surface.



- Great for computing when available:
  Surface finite elements (Dziuk & Elliot, 2013)
  Surface spectral elements (Fortunato 2024)

Point Cloud: a set of unstructured set of points without connectivity

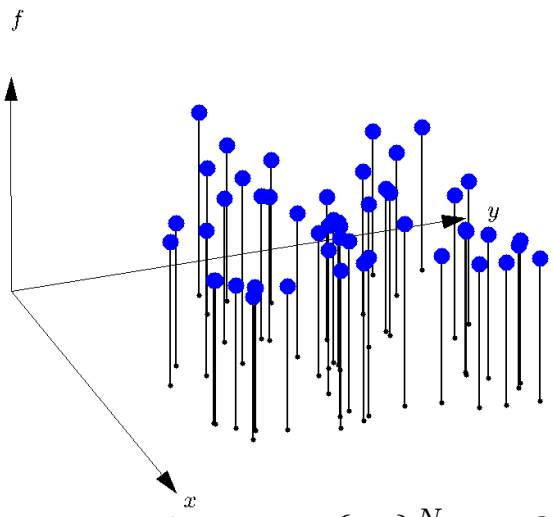


- More flexible representation for 3D geometry, especially for complex or data-defined shapes
- Easy to generate large point point sets
- No issues with mesh imprinting
- More difficult to develop high-order, scalable methods

Aim: Overview of a kernel-based framework for addressing these challenges

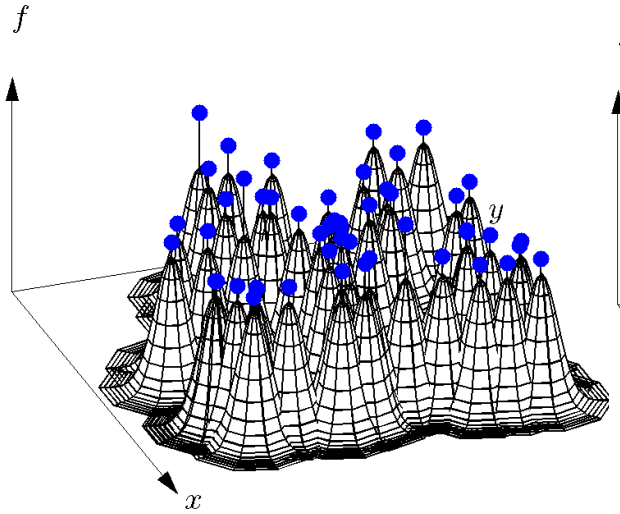
Kernel-based approximation

Interpolation with radial kernels: $\kappa(\mathbf{x}, \mathbf{y}) = \phi(\|\mathbf{x} - \mathbf{y}\|)$, $\mathbf{x}, \mathbf{y} \in \mathbb{R}^d$

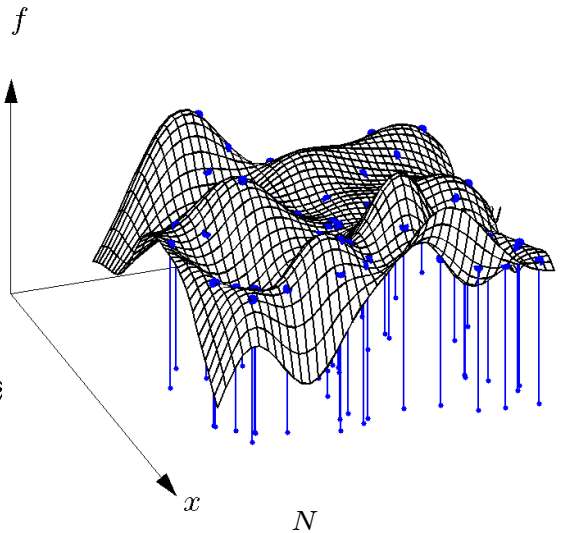


Nodes: $X = \{\mathbf{x}_j\}_{j=1}^N \subset \Omega$

Data: $\{f(\mathbf{x}_j)\}_{j=1}^N$



Collocation



$$s(\mathbf{x}) = \sum_{j=1}^{N} a_j \kappa(\mathbf{x}, \mathbf{x}_j),$$

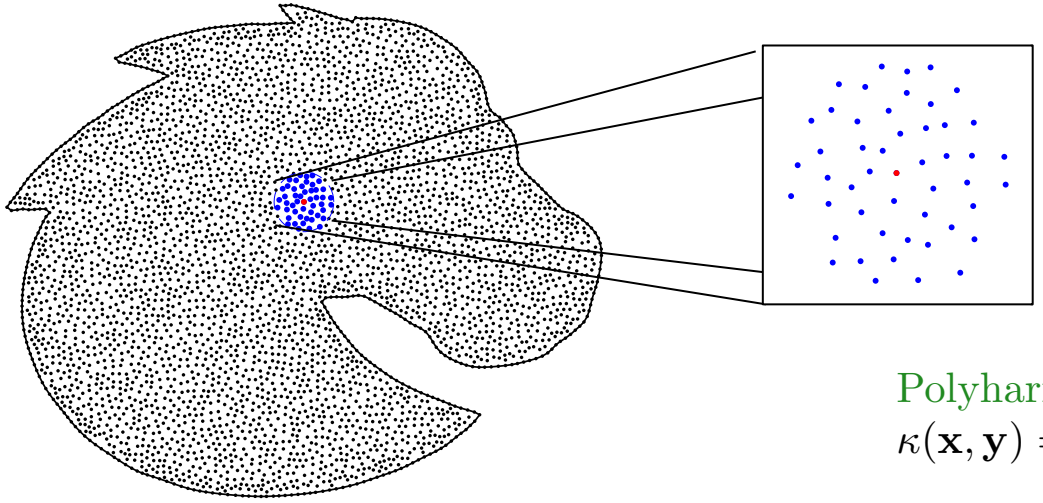
Linear system for expansion coefficients

$$\underbrace{\begin{bmatrix} \kappa(\mathbf{x}_1, \mathbf{x}_1) & \kappa(\mathbf{x}_1, \mathbf{x}_2) \cdots \kappa(\mathbf{x}_1, \mathbf{x}_N) \\ \kappa(\mathbf{x}_2, \mathbf{x}_1) & \kappa(\mathbf{x}_2, \mathbf{x}_2) \cdots \kappa(\mathbf{x}_2, \mathbf{x}_N) \\ \vdots & \vdots \quad \ddots \quad \vdots \\ \kappa(\mathbf{x}_N, \mathbf{x}_1) & \kappa(\mathbf{x}_N, \mathbf{x}_2) \cdots \kappa(\mathbf{x}_N, \mathbf{x}_N) \end{bmatrix}}_{K_{XX}} \underbrace{\begin{bmatrix} a_1 \\ a_2 \\ \vdots \\ a_N \end{bmatrix}}_{a_X} = \underbrace{\begin{bmatrix} f_1 \\ f_2 \\ \vdots \\ f_N \end{bmatrix}}_{f_X}$$

Similarities to Gaussian Processes and Kriging (Banff Workshop 26w5635, Fall 2026)

Localized approximation using polyharmonic spline kernels

Construct kernel approximations over local stencils of $X = \{\mathbf{x}_j\}_{j=1}^N \subset \Omega$



Stencil $X_i \subseteq X$ for center $\mathbf{x}_i$
with $n << N$ points

Polyharmonic spline (PHS) kernel:
$\kappa(\mathbf{x}, \mathbf{y}) = \|\mathbf{x} - \mathbf{y}\|^{2\ell+1}, \quad \ell \geq 0$

Augmented PHS kernel expansion with bivariate polynomials $\{p_k\}$ of degree ℓ

$$s(\mathbf{x}) = \sum_{j=1}^{n} a_j \kappa(\mathbf{x}, \mathbf{x}_j) + \sum_{k=1}^{L(\ell)} b_k p_k(\mathbf{x})$$

(Iske 2003; Bayona, Flyer, Fornberg, Barnett 2017)

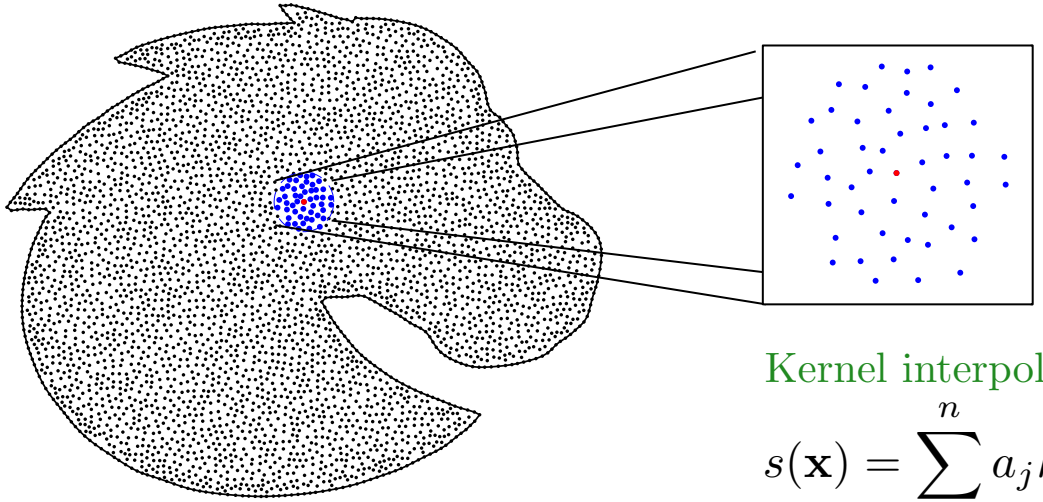
Enforce interpolation $s\big|_{X_i} = f\big|_{X_i}$, and moment conditions $\sum_{j=1}^{n} a_j p_k(\mathbf{x}_j) = 0$

$$\Longrightarrow \begin{bmatrix} K_{X_i X_i} & P \\ P^T & 0 \end{bmatrix} \begin{bmatrix} a_{X_i} \\ b_{X_i} \end{bmatrix} = \begin{bmatrix} f_{X_i} \\ 0 \end{bmatrix}$$

System is non-singular under mild restrictions on X_i (Duchon 1977)

Kernel-based Finite Difference (FD) Method

Construct kernel approximations over local stencils of $X = \{\mathbf{x}_j\}_{j=1}^N \subset \Omega$



Stencil $X_i \subseteq X$ for center $\mathbf{x}_i$
with $n << N$ points

Kernel interpolant:

$$s(\mathbf{x}) = \sum_{j=1}^{n} a_j \kappa(\mathbf{x}, \mathbf{x}_j) + \sum_{k=1}^{L(\ell)} b_k p_k(\mathbf{x})$$

Idea: Use $s(\mathbf{x})$ to produce local approximations to differential operators over X_i

$$\mathcal{L}u|_{\mathbf{x}_i} \approx c_1 u(\mathbf{x}_1) + c_2 u(\mathbf{x}_2) + \cdots c_n u(\mathbf{x}_n)$$

Generalization of finite difference (FD) method to scattered points and kernels

RBF-FD Method: Tolstykch & Shirobokov (2003), Shu, Ding, & Yeo (2003), W (2003), Fornberg & Flyer (2015), Flyer, Fornberg, Barnett (2017)

Kernel-based Finite Difference (FD) Method

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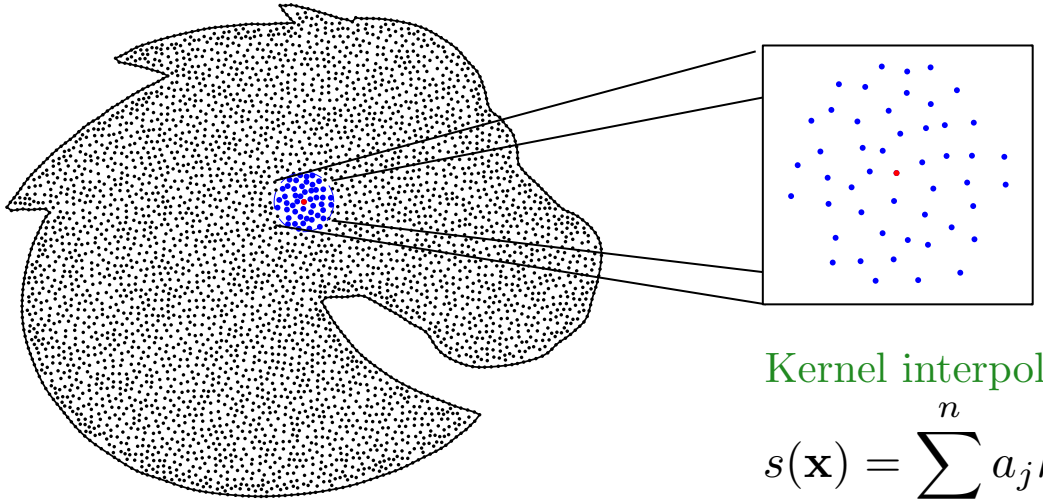

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Idea: Use $s(\mathbf{x})$ to produce local approximations to differential operators over X_i

$$\mathcal{L}u\big|_{\mathbf{x}_i} \approx c_1 u(\mathbf{x}_1) + c_2 u(\mathbf{x}_2) + \cdots c_n u(\mathbf{x}_n)$$

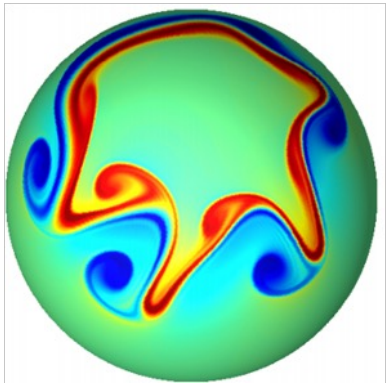
Solve a small system for the weights c_j

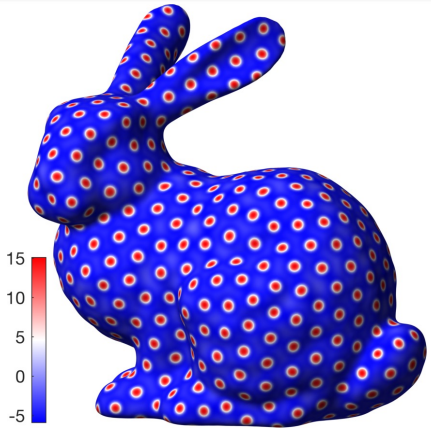
$$\Longrightarrow \begin{bmatrix} K_{X_i X_i} & P \\ P^T & 0 \end{bmatrix} \begin{bmatrix} c_{X_i} \\ \lambda \end{bmatrix} = \begin{bmatrix} \mathcal{L}\kappa(\mathbf{x}, \mathbf{x}_j)\big|_{\mathbf{x}_i} \\ \mathcal{L}p_k(\mathbf{x})\big|_{\mathbf{x}_i} \end{bmatrix}$$

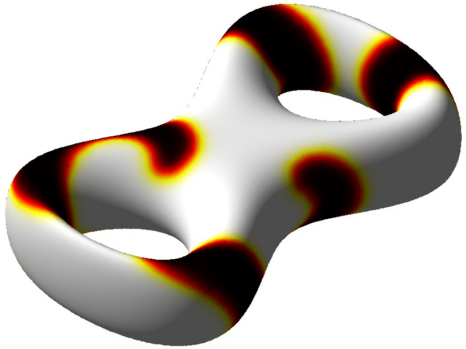
Polynomial degree ℓ controls the accuracy of the formulas (Davydov & Schaback 2019)

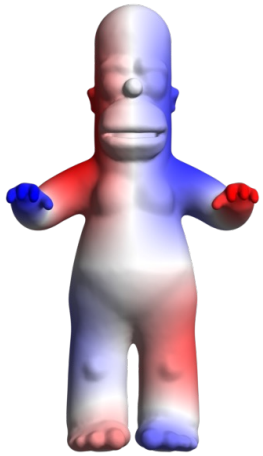
Solving Surface PDEs

Partial Differential Equations (PDEs) on Surfaces









Applications

Geophysics: numerical weather/climate prediction

Biology: advective/diffusive transport on a membrane, morphogenesis, pattern formation

Chemistry: waves in excitable media (cardiac arrhythmia, electrical signals in the brain)

Computer graphics: texture mapping, shape analysis, image processing

Prototypical PDE model:

$$(\mu\mathcal{I} - \Delta_{\mathcal{M}})u = f$$

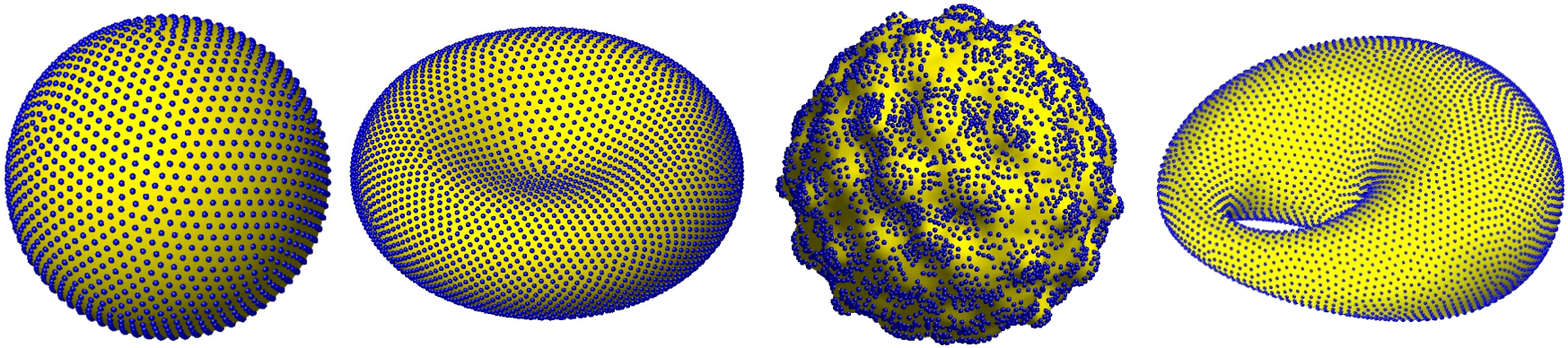
$$\begin{cases} \dfrac{\partial u}{\partial t} + \mathbf{w}\cdot\nabla_{\mathcal{M}}\, u = \delta_1 \Delta_{\mathcal{M}}\, u + f_1(t,u,v) \\ \dfrac{\partial v}{\partial t} + \mathbf{w}\cdot\nabla_{\mathcal{M}}\, v = \delta_2 \Delta_{\mathcal{M}}\, v + f_2(t,u,v) \end{cases}$$

$\mathcal{M}$ is a smooth embedded submanifold of co-dimension one in $\mathbb{R}^3$ with no boundary

$\Delta_{\mathcal{M}}$ is the Laplace-Beltrami operator

$\nabla_{\mathcal{M}}$ is the surface gradient

Kernel-based methods



Highlights:

- No mesh is required, just a point cloud
- Do not need additional points in the embedding space
- Can produce high orders of accuracy for smooth solutions

References

Global kernel methods and local finite difference methods

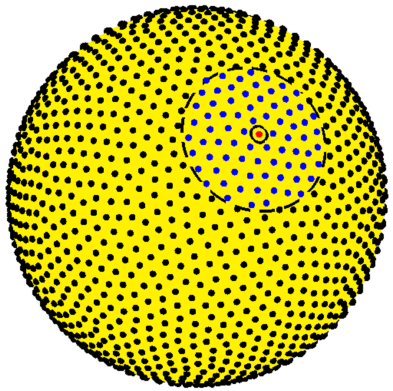
Piret (2012), Fuselier+W (2012, 2013), Shankar+W+Fogelson+Kriby (2014, 2015), Flyer+W+Fornberg (2015), Piret+Dunn (2016), Lehto+Shankar+W (2017), Shankar+Narayan+Kirby (2018), Shankar+W (2018), Petras+Ling+Ruuth (2018), Sokolov et. al. (2019), Petras et. al. (2019), Wendland+Künemund (2020), Shankar+W+Narayan (2020), Álvarez et. al. (2021), W+Jones+Shankar (2023), Jones et. al. (2023)

Generalized finite difference and moving least squares methods

Liang+Zhao (2013), Suchde+Kuhnert (2019), Trask+Kuberry (2020), Gross et. al. (2020), Hangelbroek+Rieger+W (2025)

Localized kernel-based methods for Laplace-Beltrami operator

Let $X_h = \{\mathbf{x}_i\}_{j=1}^{N_h} \subset \mathcal{M}$, where $\mathbf{x}_i = (x_i, y_i, z_i)$



- For each $\mathbf{x}_i \in X_h$, let σ_i^h be the index set for its n nearest neighbors in X_h

- $X_h^i = \{\mathbf{x}_j\}_{j \in \sigma_i^h}$ is the stencil for $\mathbf{x}_i$

- Find weights $\{c_{ij}\}_{j \in \sigma_i^h}$ such that for $u : \mathcal{M} \to \mathbb{R}$:

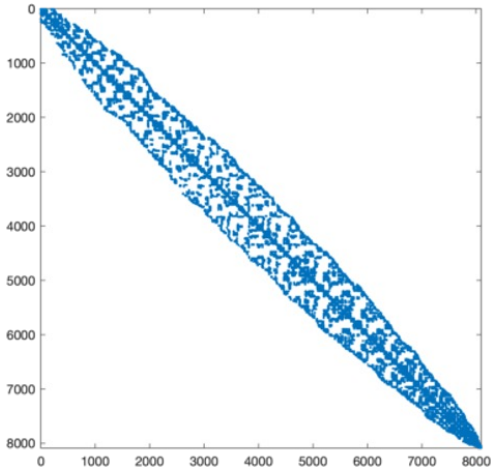
$$\Delta_{\mathcal{M}} u|_{\mathbf{x}_i} \approx \sum_{j \in \sigma_i^h} c_{ij} u(\mathbf{x}_j)$$

- Can assemble these weights into an N_h-by-N_h sparse differentiation matrix D_h to approximate $\mathcal{L}u = f$

  Let u^h, f^h contain samples of u and f at X_h

$$\mathcal{L}u = f \quad \longrightarrow \quad L_h u^h = f^h$$

$$L_h = \begin{cases} D_h & \text{if } \mathcal{L} = \Delta_{\mathcal{M}} \\ \mu I_h - D_h & \text{if } \mathcal{L} = \mu \mathcal{I} - \Delta_{\mathcal{M}} \end{cases}$$



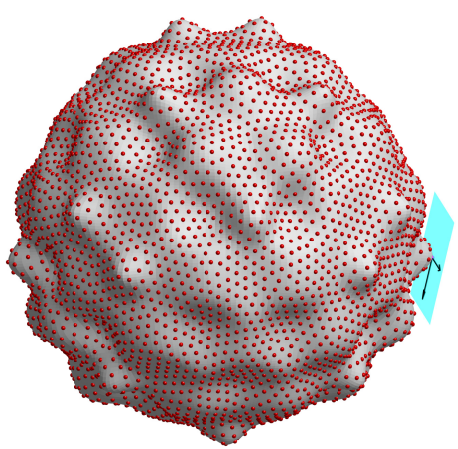
Tangent plane method for Laplace-Beltrami

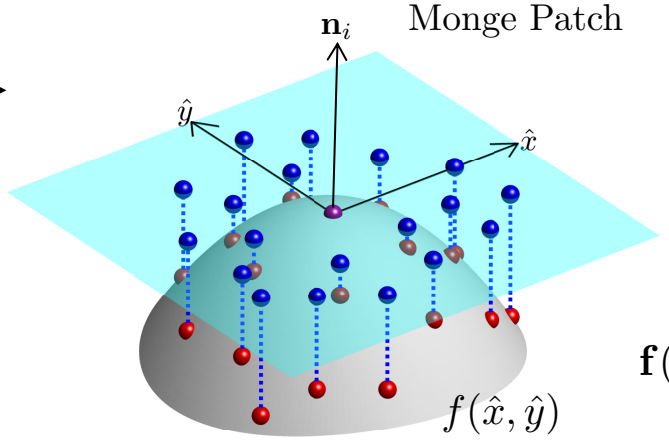
Tangent Plane method

Only requires point cloud $X_h \subset \mathcal{M}$ and normals $\{\mathbf{n}_j\}_{j=1}^{N_h}$

Demanet (2006), Shaw (2019), Suchde & Kuhnert (2020), Gunderman et. al. (2020), Jones et. al. (2023)

Idea: Consider local parameterization of the surface about each $\mathbf{x}_i$





Parameterization

$$\mathbf{f}(\hat{x},\hat{y}) = (\hat{x},\hat{y},f(\hat{x},\hat{y}))$$

Local metric tensor:

$$G = \begin{bmatrix} \partial_{\hat{x}}\mathbf{f}\cdot\partial_{\hat{x}}\mathbf{f} & \partial_{\hat{x}}\mathbf{f}\cdot\partial_{\hat{y}}\mathbf{f} \\ \partial_{\hat{y}}\mathbf{f}\cdot\partial_{\hat{x}}\mathbf{f} & \partial_{\hat{y}}\mathbf{f}\cdot\partial_{\hat{y}}\mathbf{f} \end{bmatrix} = \begin{bmatrix} 1+(\partial_{\hat{x}}f)^2 & (\partial_{\hat{x}}f)(\partial_{\hat{y}}f) \\ (\partial_{\hat{x}}f)(\partial_{\hat{y}}f) & 1+(\partial_{\hat{y}}f)^2 \end{bmatrix}, \qquad G^{-1} = \begin{bmatrix} g^{11} & g^{12} \\ g^{21} & g^{22} \end{bmatrix}, \qquad g = \det(G)$$

Laplace-Beltrami of u at $\mathbf{x}_i$

$$\Delta_{\mathcal{M}} u\big|_{\mathbf{x}_i} = \frac{1}{\sqrt{|g|}}\left(\partial_{\hat{x}}\left(\sqrt{|g|}g^{11}\partial_{\hat{x}}\right) + \partial_{\hat{x}}\left(\sqrt{|g|}g^{12}\partial_{\hat{y}}\right) + \partial_{\hat{y}}\left(\sqrt{|g|}g^{21}\partial_{\hat{x}}\right) + \partial_{\hat{y}}\left(\sqrt{|g|}g^{22}\partial_{\hat{y}}\right)\right)u\big|_{\hat{\mathbf{x}}_i}$$

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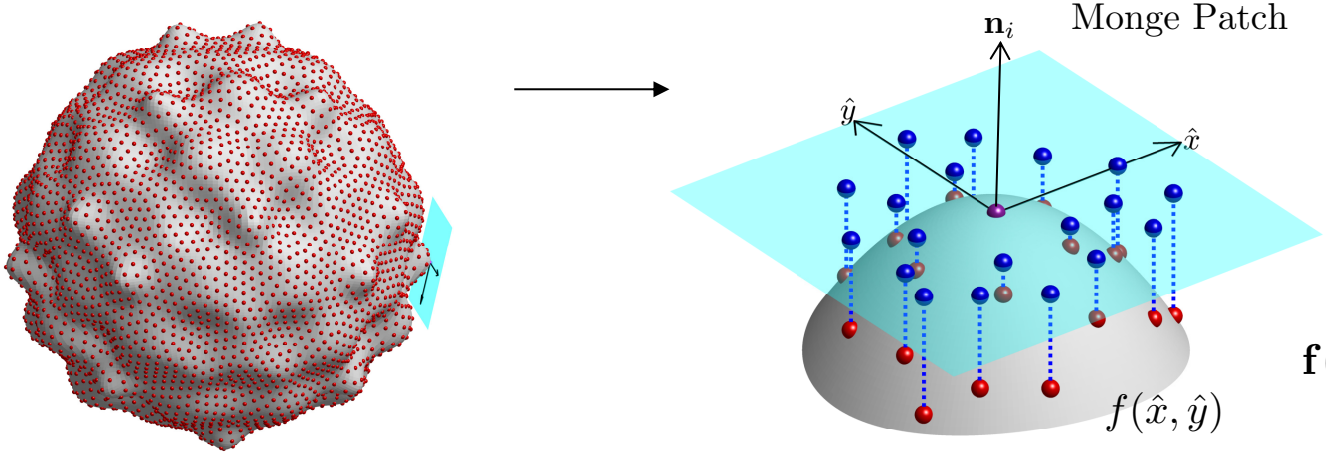

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Laplace-Beltrami of u at $\mathbf{x}_i$ simplifies

$$\Delta_{\mathcal{M}} u\big|_{\mathbf{x}_i} = \partial_{\hat{x}\hat{x}} u\big|_{\hat{\mathbf{x}}_i} + \partial_{\hat{y}\hat{y}} u\big|_{\hat{\mathbf{x}}_i} = \hat{\Delta} u\big|_{\hat{\mathbf{x}}_i}$$

Tangent plane method for Laplace-Beltrami

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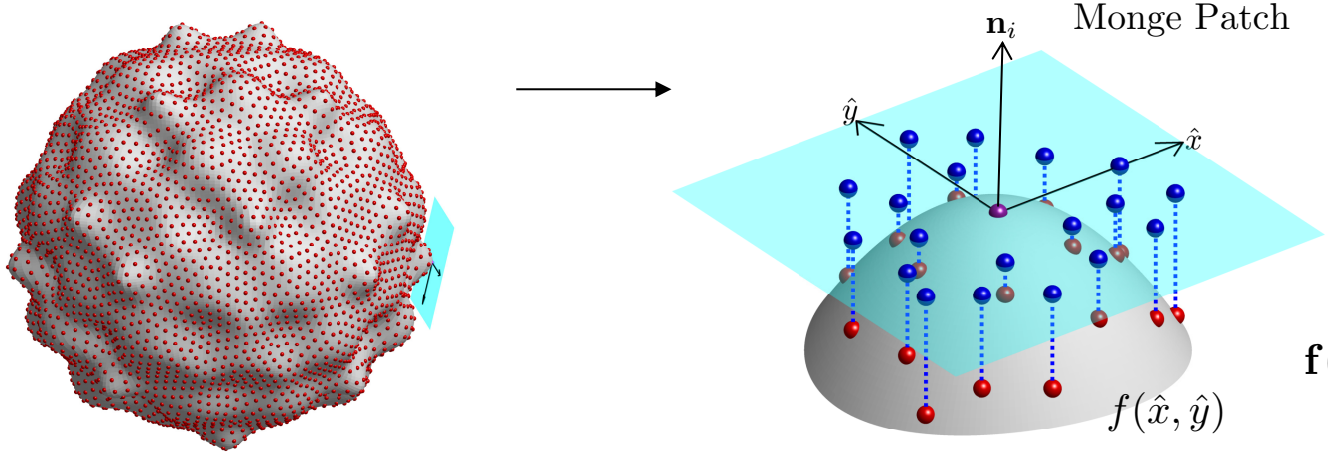


Parameterization

$$\mathbf{f}(\hat{x},\hat{y}) = (\hat{x},\hat{y},f(\hat{x},\hat{y}))$$

Consider PHS+Poly interpolant for the projected stencil X_h^i in the tangent plane

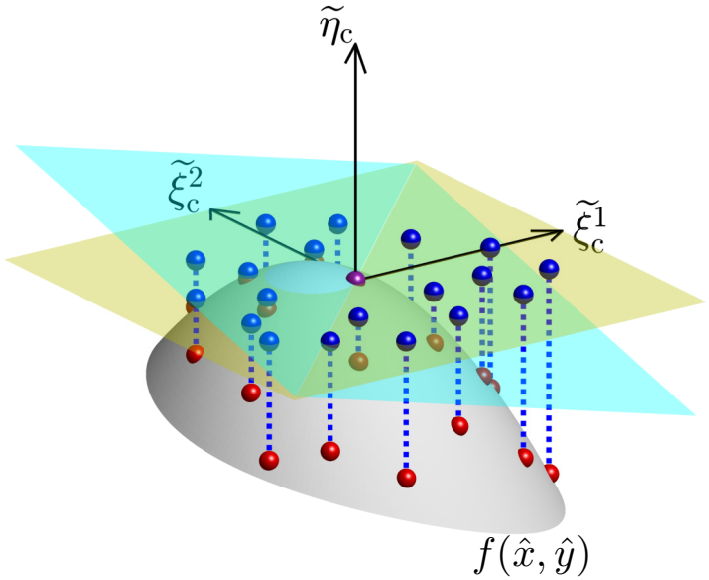
$$s(\hat{\mathbf{x}}) = \sum_{i=1}^{n} a_i \|\hat{\mathbf{x}} - \hat{\mathbf{x}}_i\|^{2\ell+1} + \sum_{k=1}^{L(\ell)} b_k p_k(\hat{\mathbf{x}})$$

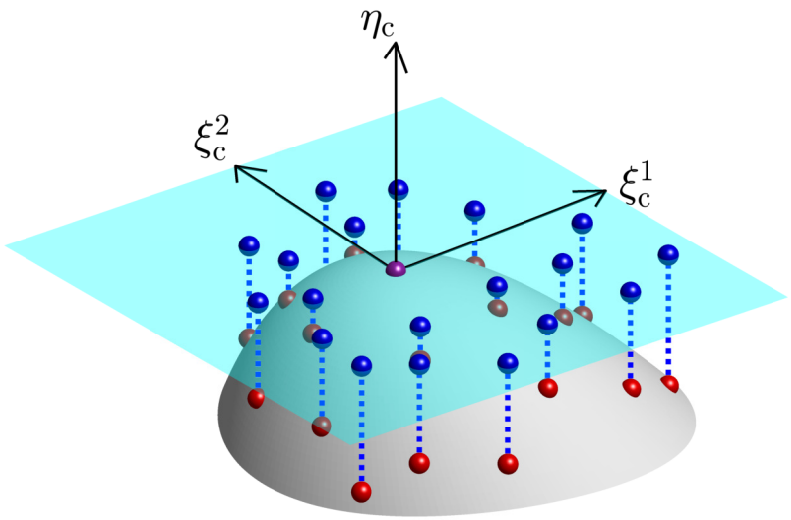
Use approximation $\Delta_{\mathcal{M}} u\big|_{\mathbf{x}_i} \approx \hat{\Delta} s\big|_{\hat{\mathbf{x}}_i}$ to find the stencil weights

Tangent plane method for Laplace-Beltrami

Approximating normals

Idea can also be used to approximate the normals $\{\mathbf{n}_j\}_{j=1}^{N_h}$ for $X_h \subset \mathcal{M}$





Start with a low-order approximation to the tangent plane about $\mathbf{x}_i$ using PCA (yellow plane)

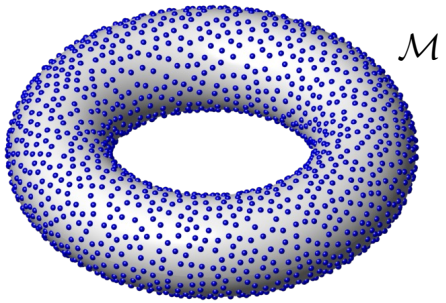
Fit local samples of f over the approximate tangent plane

$$s(\hat{\mathbf{x}}) = \sum_{i=1}^{n} a_i \|\hat{\mathbf{x}} - \hat{\mathbf{x}}_i\|^{2\ell+1} + \sum_{k=1}^{L(\ell)} b_k p_k(\hat{\mathbf{x}})$$

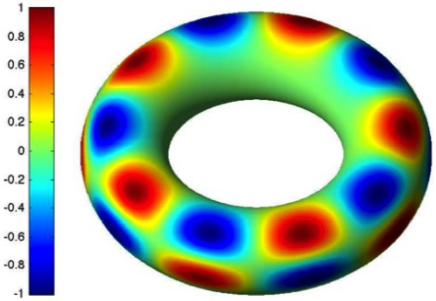
Use normal to this surface at $\mathbf{x}_i$ to improve the low-order approximation

Example: convergence of discrete surface Laplacian

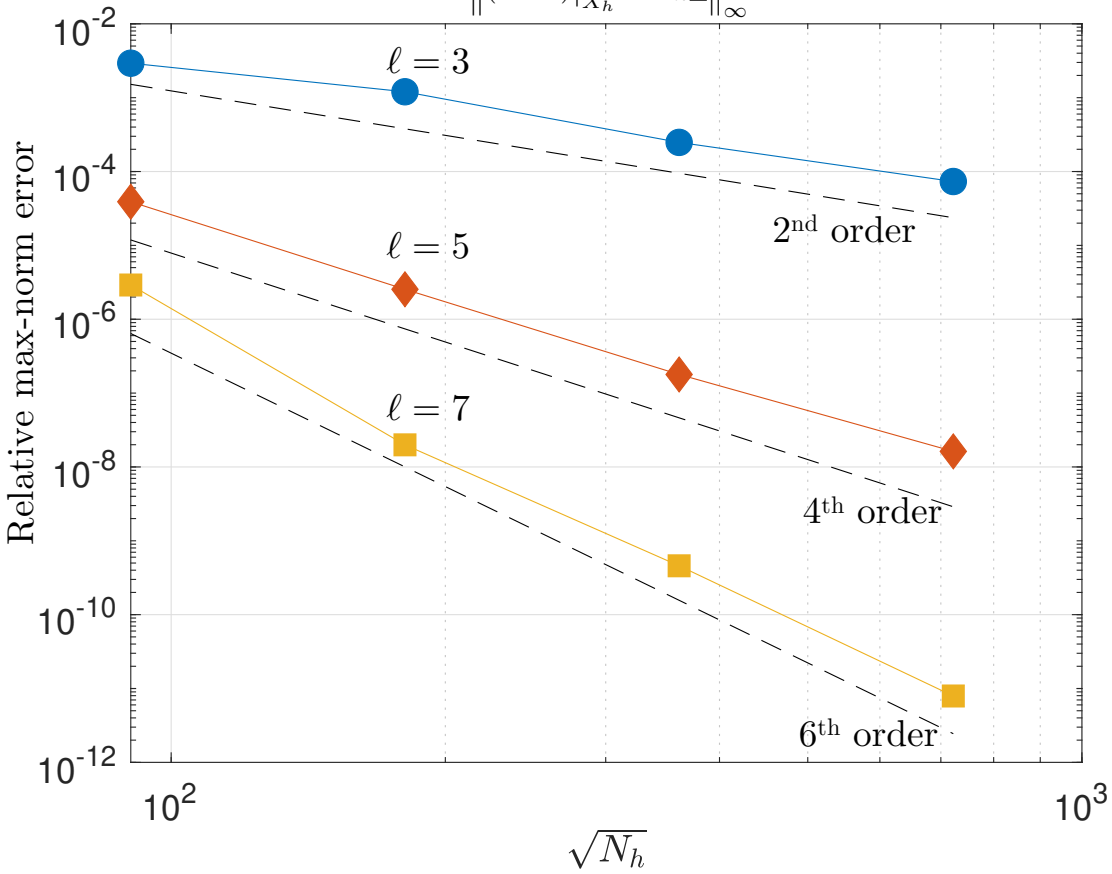
Problem: Approximate $\Delta_{\mathcal{M}} u$



Smooth target u



Error: $\left\| (\Delta_{\mathbb{M}} u)\big|_{X_h} - L_h \underline{u} \right\|_\infty$



Different poly. degrees ℓ in kernel approx.

Stencil size $n = \lceil (\ell+1)(\ell+2) \rceil$

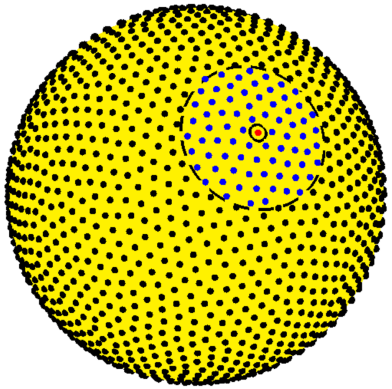
Point clouds with N_h unstructured nodes

$$h_{X_h} \sim 1/\sqrt{N_h}$$

Localized kernel methods for the Laplace-Beltrami

Let $X_h = \{\mathbf{x}_i\}_{j=1}^{N_h} \subset \mathcal{M}$, where $\mathbf{x}_i = (x_i, y_i, z_i)$

- For each $\mathbf{x}_i \in X_h$, let σ_i^h be the index set for its n nearest neighbors in X_h



- $X_h^i = \{\mathbf{x}_j\}_{j \in \sigma_i^h}$ is the stencil for $\mathbf{x}_i$
- Find weights $\{c_{ij}\}_{j \in \sigma_i^h}$ such that for $u : \mathcal{M} \to \mathbb{R}$:

$$\Delta_{\mathcal{M}} u|_{\mathbf{x}_i} \approx \sum_{j \in \sigma_i^h} c_{ij} u(\mathbf{x}_j)$$

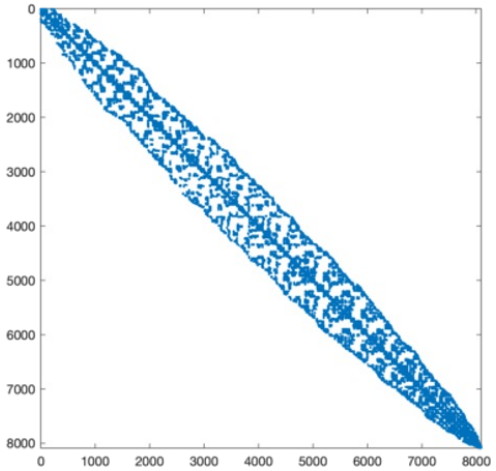
- Can assemble these weights into an N_h-by-N_h sparse differentiation matrix D_h to approximate $\mathcal{L}u = f$

Let u^h, f^h contain samples of u and f at X_h

$$\mathcal{L}u = f \quad \longrightarrow \quad L_h u^h = f^h$$

$$L_h = \begin{cases} D_h & \text{if } \mathcal{L} = \Delta_{\mathcal{M}} \\ \mu I_h - D_h & \text{if } \mathcal{L} = \mu \mathcal{I} - \Delta_{\mathcal{M}} \end{cases}$$

Large (sparse) non-symmetric linear systems

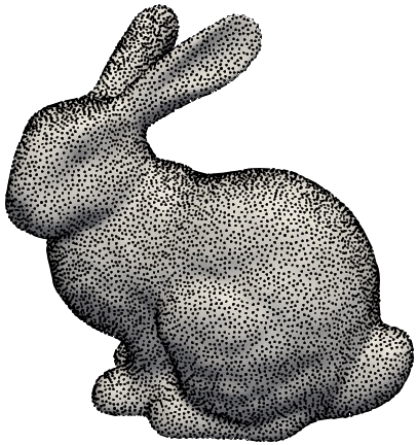


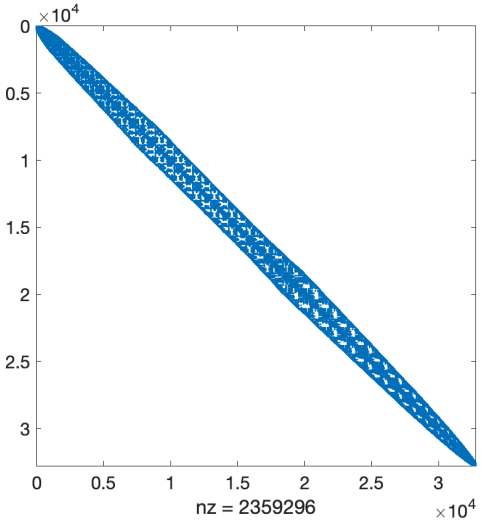
Geometric Multilevel Solver

Solving unstructured sparse linear systems

$$\mathcal{L}u = f \quad \longrightarrow \quad L_h u^h = f^h$$

$$L_h = \begin{cases} D_h & \text{if } \mathcal{L} = \Delta_{\mathcal{M}} \\ \mu I_h - D_h & \text{if } \mathcal{L} = \mu\mathcal{I} - \Delta_{\mathcal{M}} \end{cases}$$





Large (sparse) non-symmetric linear systems

Common general approaches:

- Direct sparse solver
- Preconditioned Krylov method
- Preconditioner:
  - Incomplete LU or Cholesky
  - Algebraic multigrid (AMG)

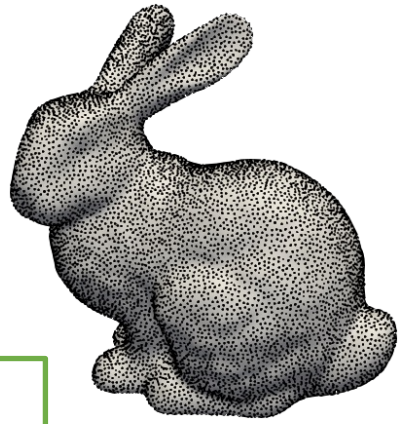
What about a general geometric multilevel solver/preconditioner?

W, Jones, Shankar (SISC 2023)
Meshfree geometric multilevel method for surface PDE on point clouds

Meshfree geometric multilevel (MGM) method: two-level cycle

Solve: $L_h u^h = f^h$

Level h nodes: X_h



1. Smooth initial guess:
   $\hat{u}^h \leftarrow \text{smooth}(\hat{u}^h, f^h, L_h)$

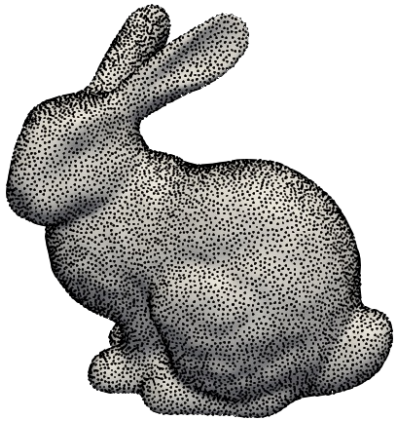
2. Compute residual:
   $r^h = f^h - L_h \hat{u}^h$

Defect correction:
- Solve for defect: $L_h e^h = r^h$
- Correct approximation: $\hat{u}^h \leftarrow \hat{u}^h + e^h$

MGM method: two-level cycle

Solve: $L_h u^h = f^h$

Level h nodes: X_h

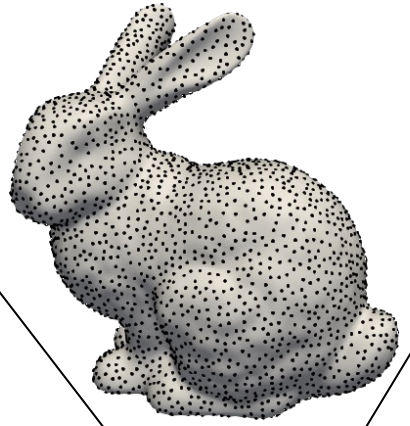


1. Smooth initial guess:
   $\hat{u}^h \leftarrow \text{smooth}(\hat{u}^h, f^h, L_h)$

2. Compute residual:
   $r^h = f^h - L_h \hat{u}^h$

3. Restrict residual:
   $r^H = I_h^H r^h$

Level H nodes: X_H



4. Solve for coarse level defect:
   $L_H e^H = r^H$

5. Interpolate defect:
   $e^h = I_H^h e^H$

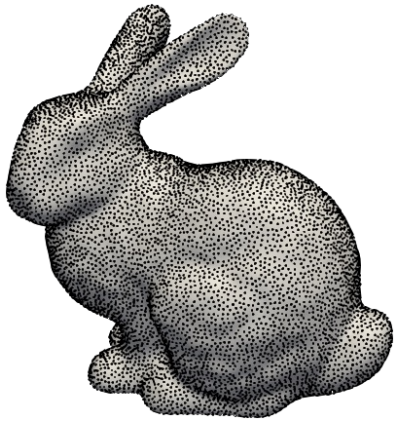
6. Correct approximation:
   $\hat{u}^h \leftarrow \hat{u}^h + e^h$

7. Smooth approximation:
   $\hat{u}^h \leftarrow \text{smooth}(\hat{u}^h, f^h, L_h)$

MGM method: two-level cycle

Solve: $L_h u^h = f^h$

Level h nodes: X_h



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   $\hat{u}^h \leftarrow \text{smooth}(\hat{u}^h, f^h, L_h)$

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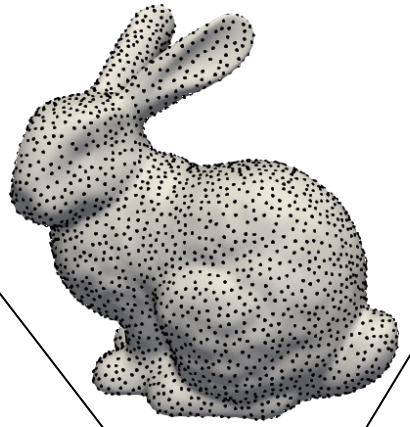
3. Restrict residual:
   $r^H = I_h^H r^h$

Level H nodes: X_H



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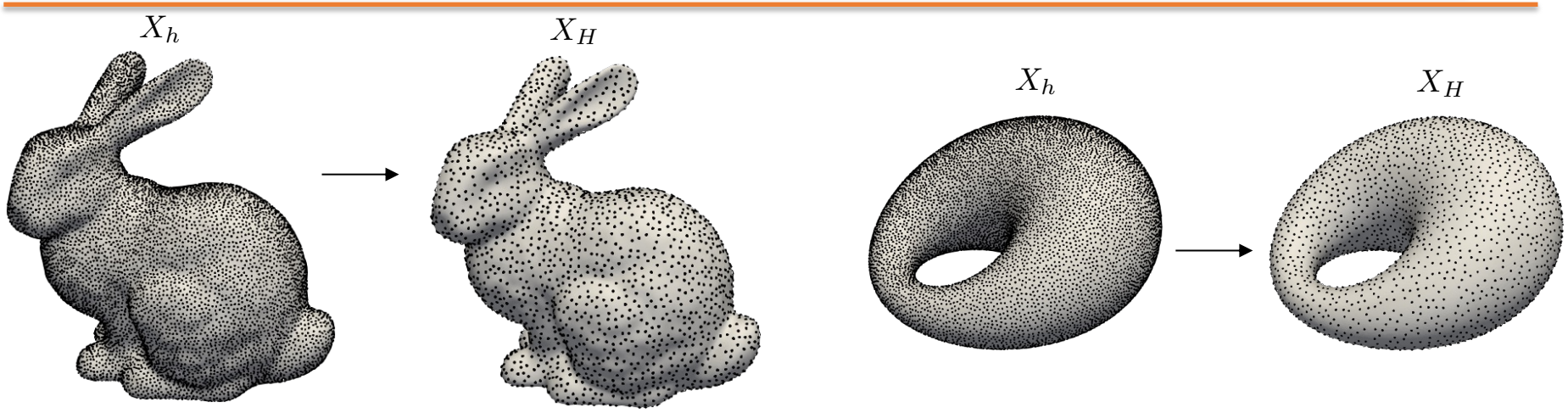
   $\hat{u}^h \leftarrow \hat{u}^h + e^h$

7. Smooth approximation:
   $\hat{u}^h \leftarrow \text{smooth}(\hat{u}^h, f^h, L_h)$

Node coarsening



Idea: Given a point cloud X_h with N_h samples, determine a subset X_H with N_H samples that has maximal Poisson disk (or separation) radius.

Many algorithms developed in computer graphics to approximate the solution

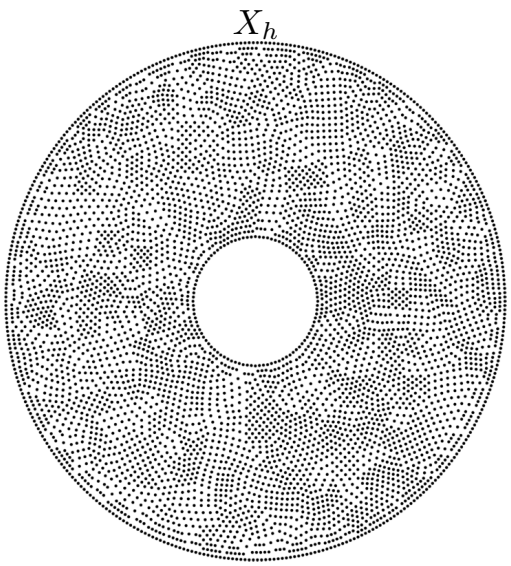
- Dart throwing – Cook (1986), Bridson (2007)
- Importance sampling - Ostromoukhov *et al.* (2004)
- Weighted Sample Elimination (WSE) – Yuksel (2015)

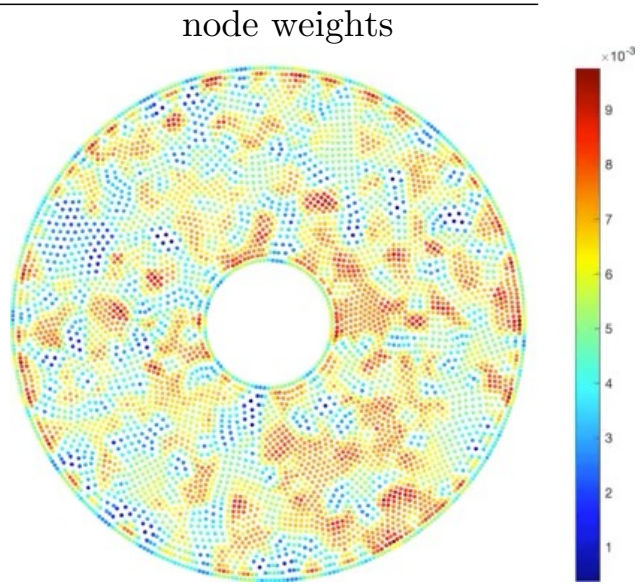
  Complexity: $\mathcal{O}(N_h - N_H) + \mathcal{O}(N_h \log N_h)$

We set $N_H = \lfloor N_h/4 \rfloor$, so that $H \approx 2h$

Node coarsening: Weighted Sample Elimination (WSE)

Input: X_h, N_h and N_H
Build a kd-tree for $\mathbf{X}_h$
for $i = N_h$ **do**
    Find all neighbors $\mathbf{x}_j$ contained in a ball of radius ρ centered at $\mathbf{x}_i$
    Assign weight w_{ij} for each $\mathbf{x}_j$ based on its distance to $\mathbf{x}_i$
    Compute weight $\overline{w}_i = \sum_j w_{ij}$
end for
Build a heap for X_h using weights $\overline{w}_i$
for $i = N_h - N_H$ **do**
    $\mathbf{x}_j \leftarrow$ pull sample from heap with highest priority
    for each sample $\mathbf{x}_i$ contained in a ball of radius ρ centered at $\mathbf{x}_j$ **do**
        Remove weight w_{ij} from $\overline{w}_i$: $\overline{w}_i \leftarrow \overline{w}_i - w_{ij}$
        Update the priority of $\mathbf{x}_i$ in the heap
    end for
end for





Meshfree interpolation/restriction operators

Interpolation operator: Stencil based approach

For each $\mathbf{x}_i \in X_h$, let σ_i^H be the index set for the m nearest neighbors in X_H to $\mathbf{x}_i$

Find weights $\{c_{ij}\}_{j \in \sigma_i^h}$ that interpolate $\{e_j^H\}_{j \in \sigma_i^H}$ to e_i^h:

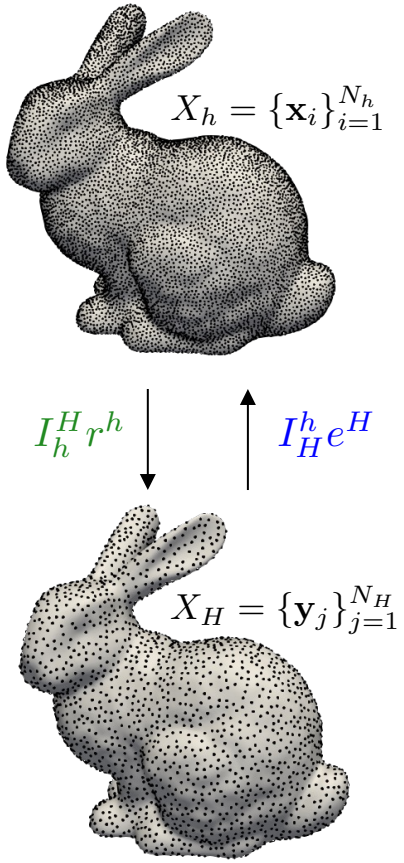
$$e_i^h = \sum_{j \in \sigma_H^i} c_{ij} e_j^H$$

Assemble these weights into an N_h-by-N_H sparse interpolation matrix I_H^h

We use a linear PHS interpolant to compute each set of weights $\{c_{i,j}\}_{j \in \sigma_H^i}$:

$$s_i(\mathbf{x}) = \sum_{j \in \sigma_H^i} a_{ij} \|\mathbf{x} - \mathbf{y}_j\| + b_i$$

Restriction operator: We use $I_h^H = (I_H^h)^T$



Coarse level operator

Two main ideas for constructing the coarse level operator

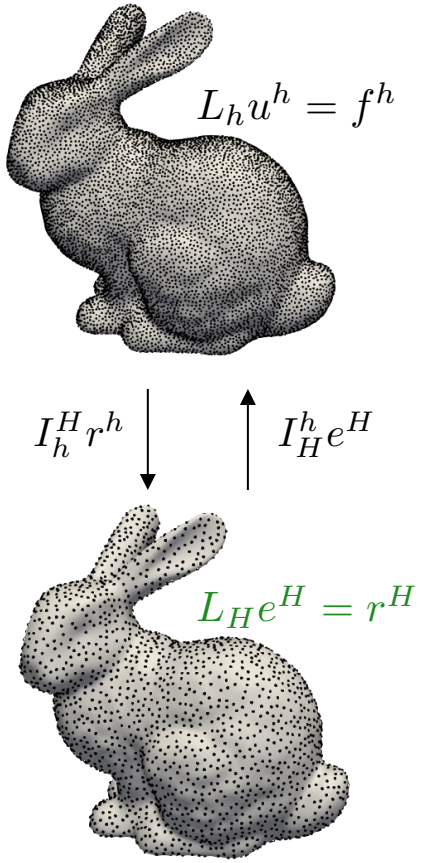
Direct discretization: Apply Kernel-FD method for $\Delta_{\mathcal{M}}$ on X_H

Galerkin projection: Use interpolation and restriction operators

$$L_H := I_h^H L_h I_H^h = (I_H^h)^T L_h I_H^h$$

We use this more general Galerkin approach

Leads to a variational principle for the coarse-level correction operator when L_h satisfies certain properties (Trottenberg et. al. 2000)



Other considerations

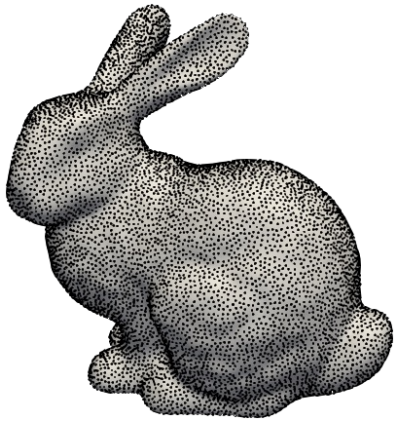
Smoother: Gauss-Seidel

Coarse level solver: Direct (sparse) solver

MGM method: two-level cycle

Solve: $L_h u^h = f^h$

Level h nodes: X_h

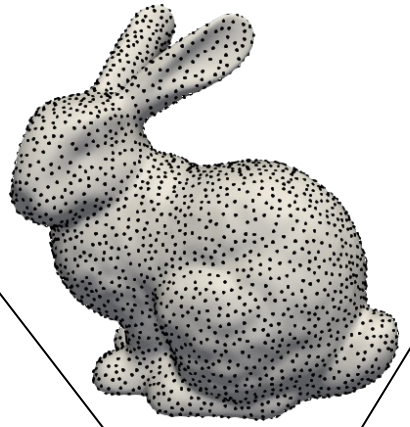


1. Smooth initial guess:
   $\hat{u}^h \leftarrow \text{smooth}(\hat{u}^h, f^h, L_h)$

2. Compute residual:
   $r^h = f^h - L_h \hat{u}^h$

3. Restrict residual:
   $r^H = I_h^H r^h$

Level H nodes: X_H



4. Solve for coarse level defect:
   $L_H e^H = r^H$

5. Interpolate defect:
   $e^h = I_H^h e^H$

6. Correct approximation:
   $\hat{u}^h \leftarrow \hat{u}^h + e^h$

7. Smooth approximation:
   $\hat{u}^h \leftarrow \text{smooth}(\hat{u}^h, f^h, L_h)$

Recursively apply two-level cycle

MGM: two-level cycle to multilevel

Algorithm MGM preprocessing phase

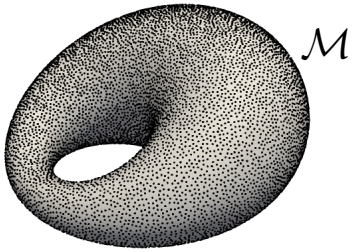
Input: Fine level nodes X_1 and operator L_1; min number of coarse level nodes $N_{\min}$
Compute number of levels: $p = \lfloor \log(N_1/N_{\min})/\log(4) \rfloor + 1$
for $j = 1 \dots p-1$ **do**
    Generate coarse point cloud X_{j+1} with $N_{j+1} = \lfloor N_1/4^j \rfloor$ points
    Generate interpolation operator I_{j+1}^j from X_{j+1} to X_j
    Set the restriction operator to $I_j^{j+1} = (I_{j+1}^j)^T$
    Generate Galerkin coarse level operator $L_{j+1} = I_{j+1}^j L_j I_j^{j+1}$
end for
Compute sparse LU decomposition of L_p

Algorithm MGM V(ν_1, ν_2)-cycle

Input: Right hand side f^1; Initial guess u^1; Number levels p; $\{L_j\}_{j=1}^{p-1}$; $\{I_{j+1}^j\}_{j=1}^{p-1}$;
    $\{I_j^{j+1}\}_{j=1}^{p-1}$; Sparse LU factorization of L_p;
Presmooth initial guess: $u^1 \leftarrow \text{presmooth}(L_1, u^1, f^1, \nu_1)$
Compute/restrict residual: $r^1 = I_1^2(f^1 - L_1 u^h)$
for $j = 2 \dots p-1$ **do**
    Presmooth defect: $e^j = \text{presmooth}(L_j, 0, r^j, \nu_1)$
    Compute/restrict residual: $r^{j+1} = I_j^{j+1}(r^j - L_j e^j)$
end for
Compute defect: Solve $L_p e^p = r^p$ using sparse LU decomposition of L_p
for $j = p-1, \dots, 2$ **do**
    Interpolate/correct defect: $e^j \leftarrow e^j + I_{j+1}^j e^{j+1}$
    Post smooth defect: $e^j \leftarrow \text{postsmooth}(L_j, e^j, r^j, \nu_2)$
end for
Interpolate defect/correct approximation: $u^1 \leftarrow u^1 + I_2^1 e^2$
Post smooth approximation: $u^1 \leftarrow \text{postsmooth}(L_1, u^1, f^1, \nu_2)$

Numerical results: convergence rates

Problem: $(\mathcal{I} - \Delta_{\mathcal{M}})u = f$



Different poly. degrees ℓ in kernel approx.

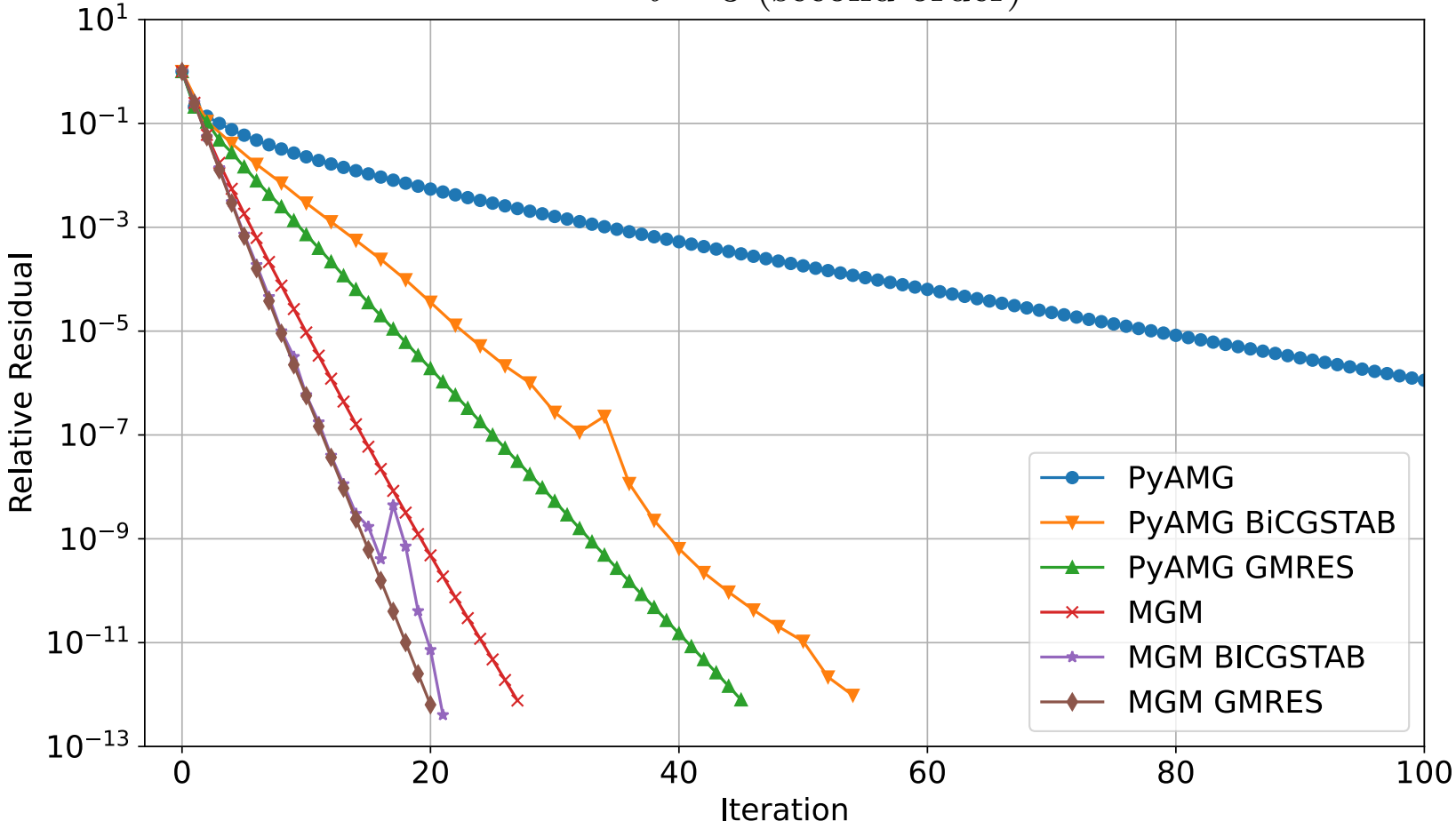
Stencil size $n = \lceil (\ell+1)(\ell+2) \rceil$

Point cloud with N_h=2,097,152 unstructured nodes

Use MGM as a solver or preconditioner

Compare with PyAMG (Olson & Schroder)

$\ell = 3$ (second order)



Numerical results: convergence rates

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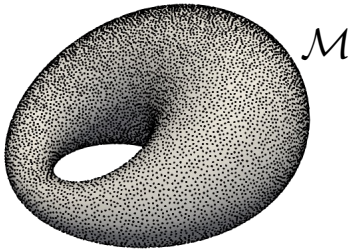

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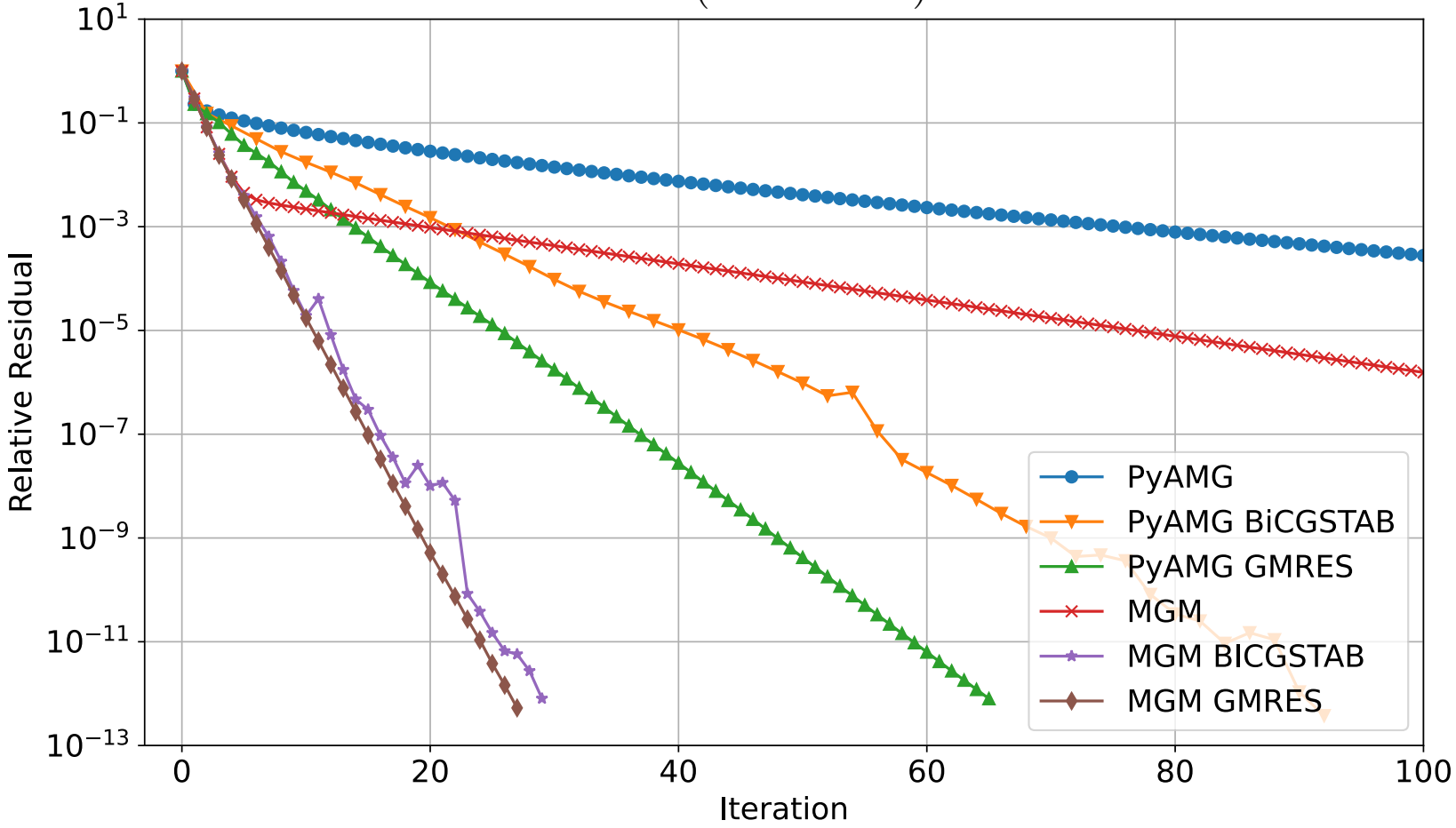
Stencil size $n = \lceil (\ell+1)(\ell+2) \rceil$

Point cloud with N_h=2,097,152 unstructured nodes

Use MGM as a solver or preconditioner

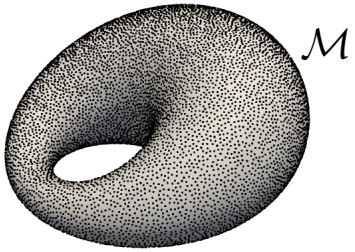
Compare with PyAMG (Olson & Schroder)

$\ell = 7$ (sixth order)



Numerical results: scaling

Problem: $(\mathcal{I} - \Delta_{\mathcal{M}})u = f$



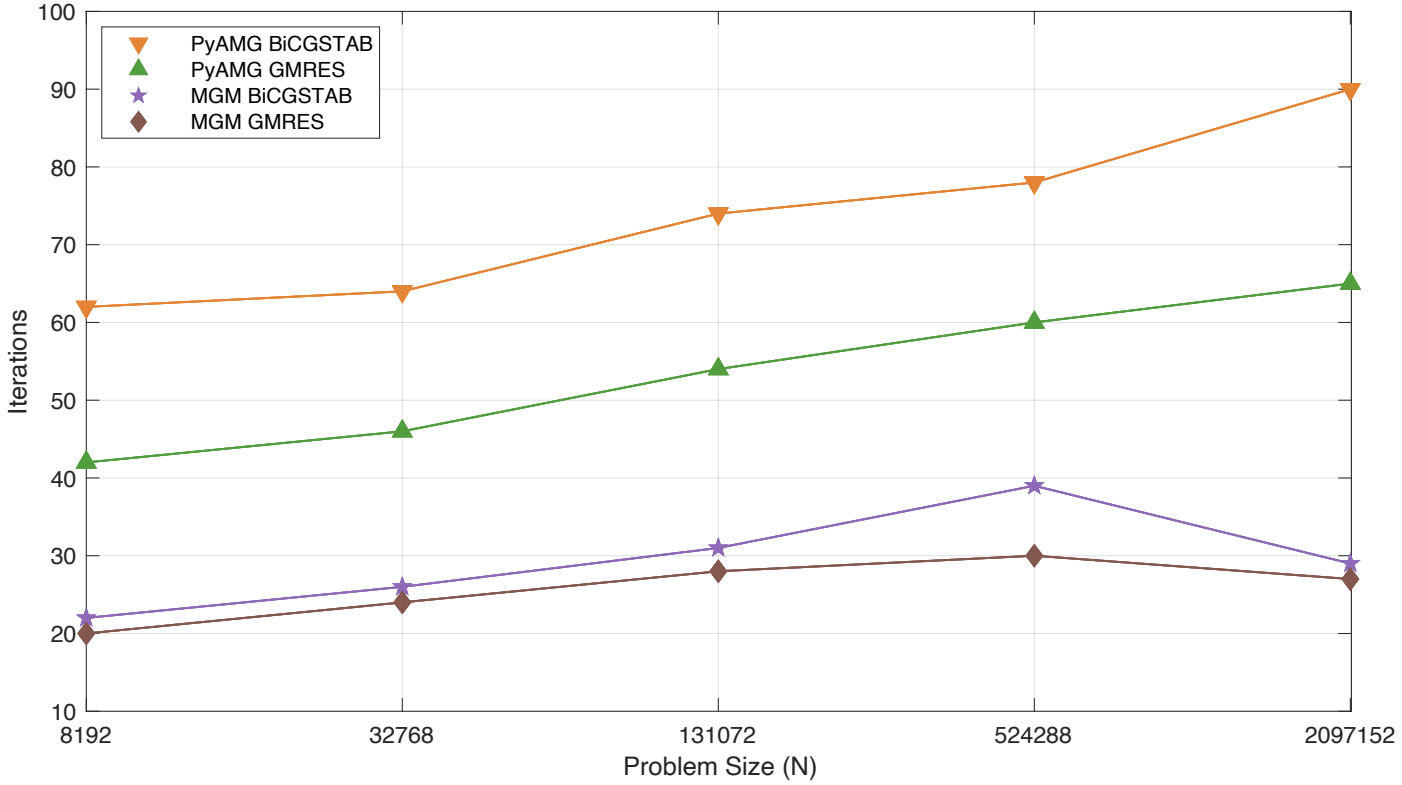
Different poly. degrees ℓ in kernel approx.

Stencil size $n = \lceil (\ell+1)(\ell+2) \rceil$

Use MGM as a solver or preconditioner

Compare with PyAMG (Olson & Schroder)

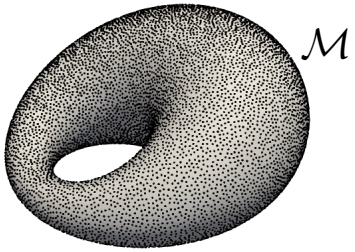
Scaling with N_h $(\ell = 7)$



Number of iterations to satisfy $\|f^h - L_h u^h\|_2 \leq 10^{-12} \|f^h\|_2$

Numerical results: timing

Problem: $(\mathcal{I} - \Delta_{\mathcal{M}})u = f$



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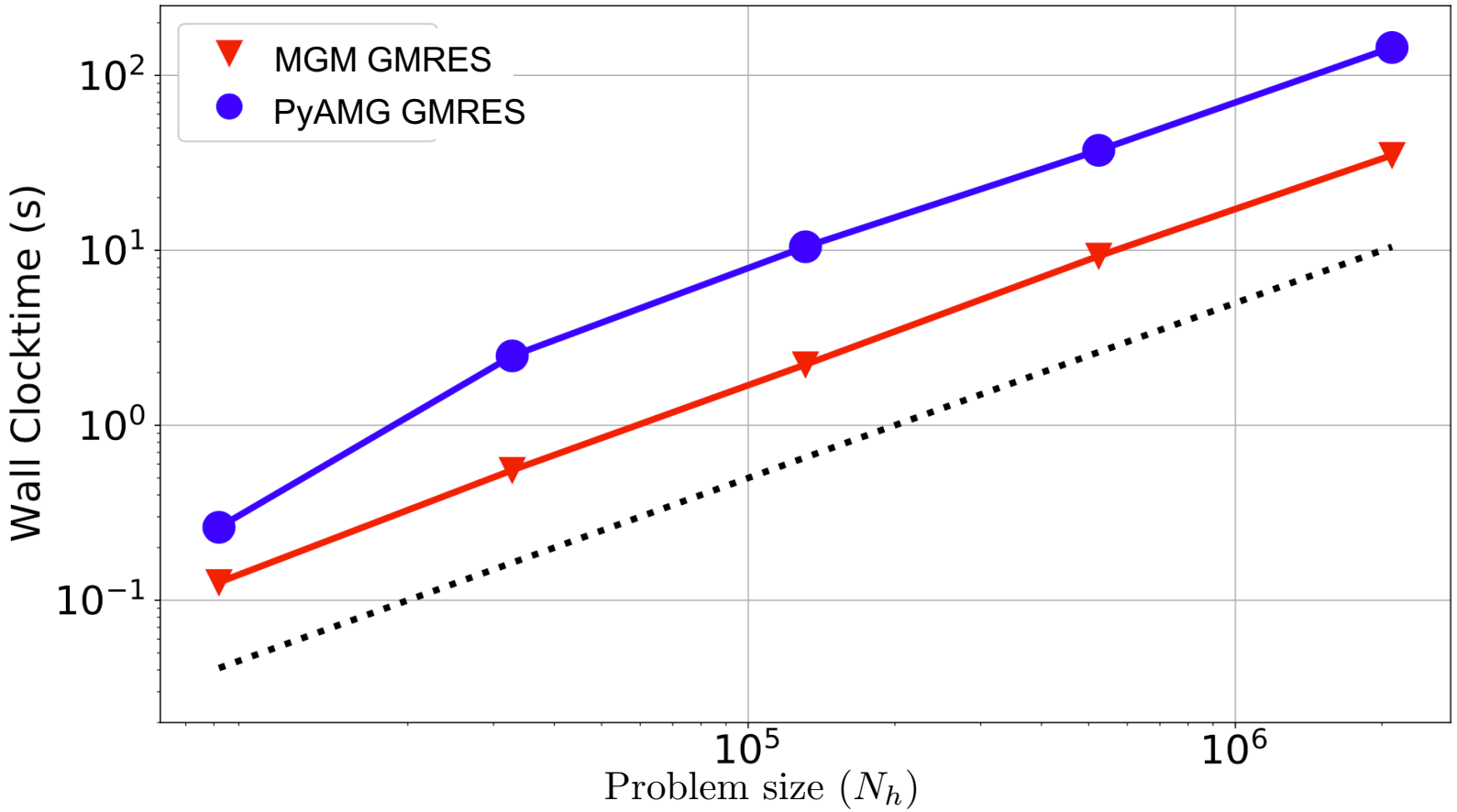
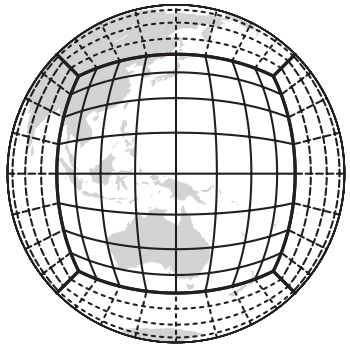


Also works well for mesh-based discretization!

Problem: $(\mathcal{I} - \Delta_{\mathcal{M}})u = f$



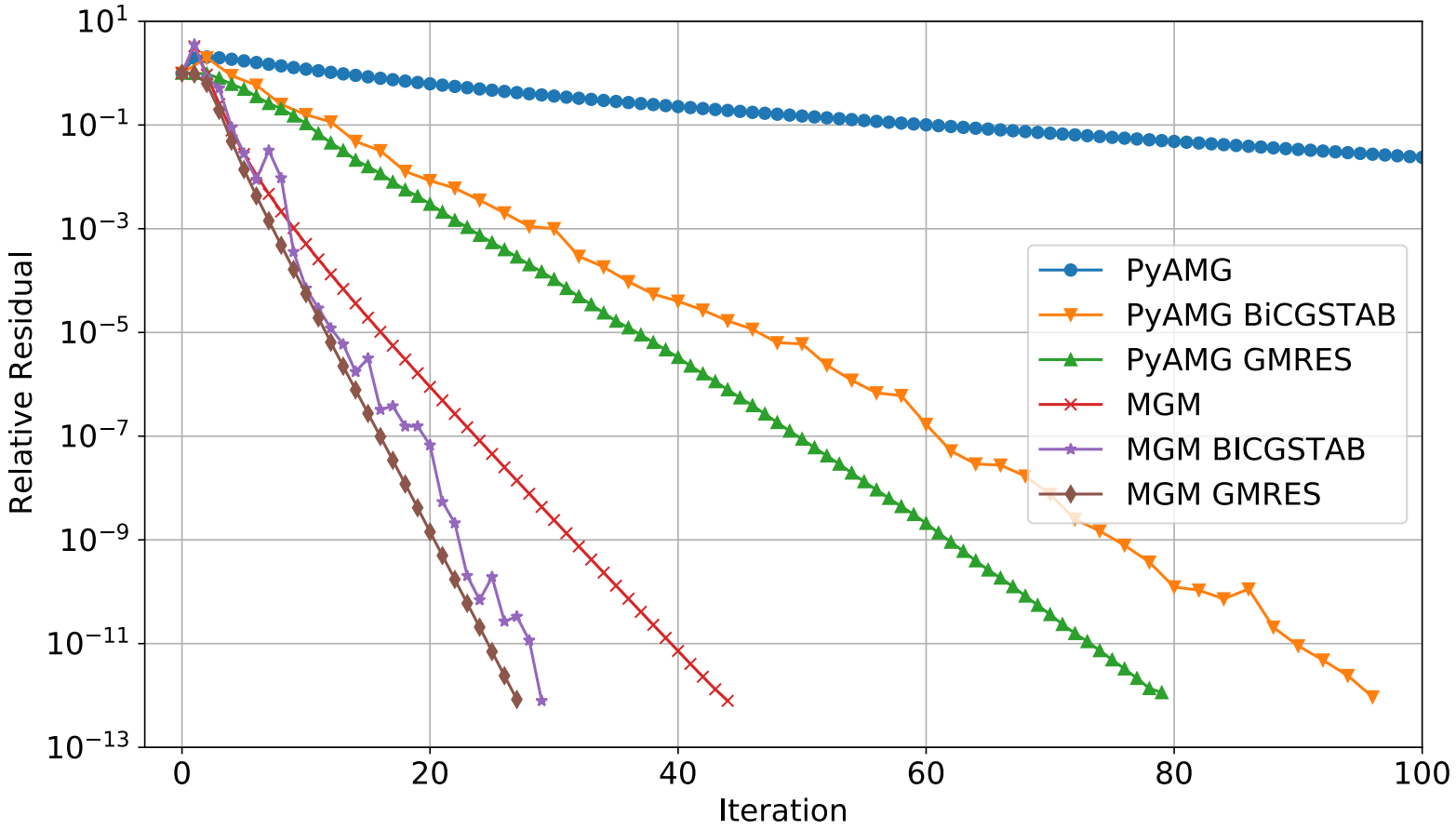
$\mathcal{M}$

Cubed sphere mesh with N_h=393216 (Grid: 64×64)

Discretization: Spectral elements with $p = 4$

Use MGM as a solver or preconditioner

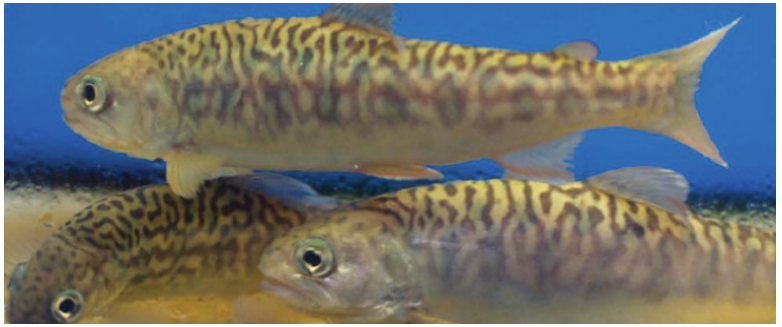
Compare with PyAMG (Olson & Schroder)



Application: Stationary Turing patterns

Pattern formation via non-linear reaction-diffusion systems; Turing (1952)

Possible mechanism for animal coat formation (and other morphogenesis phenomena)



Miyazawa, Okamoto, & Kondo (2010)

Example: Gierer–Meinhardt (1972)

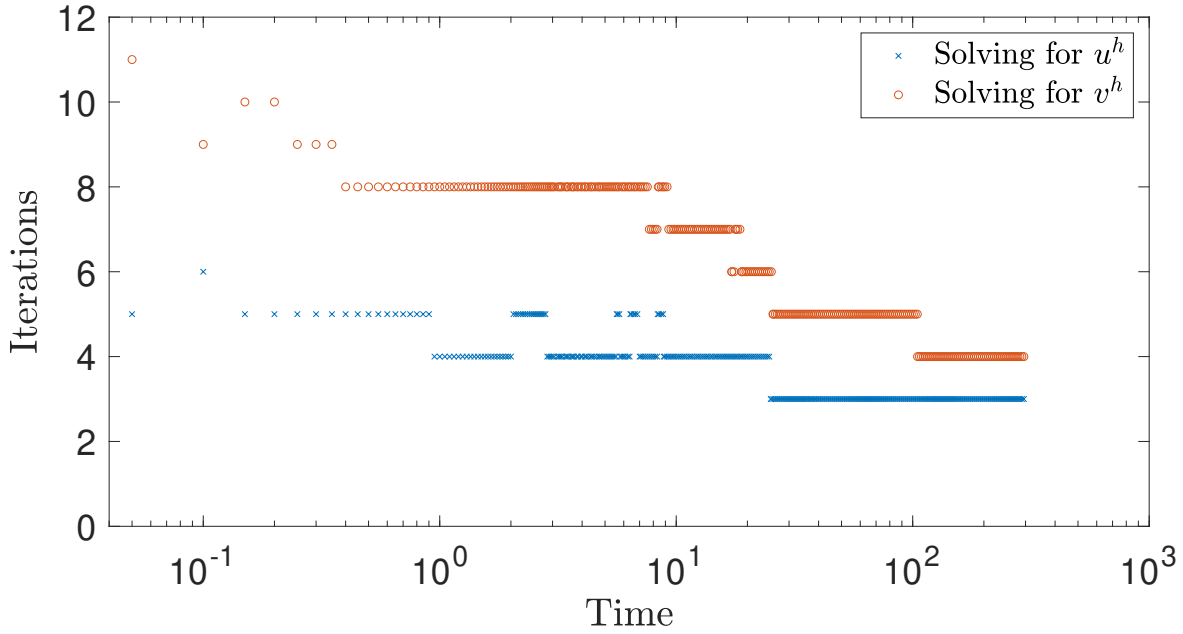
$$\frac{\partial u}{\partial t} = \delta_u \Delta_{\mathcal{M}} u + A - Bu + \left(\frac{u^2}{v(1 + Cu^2)} \right)$$

$$\frac{\partial v}{\partial t} = \delta_v \Delta_{\mathcal{M}} v + u^2 - v$$

Solution on bunny, $N_h = 291804$

Visualization of u at "steady-state"

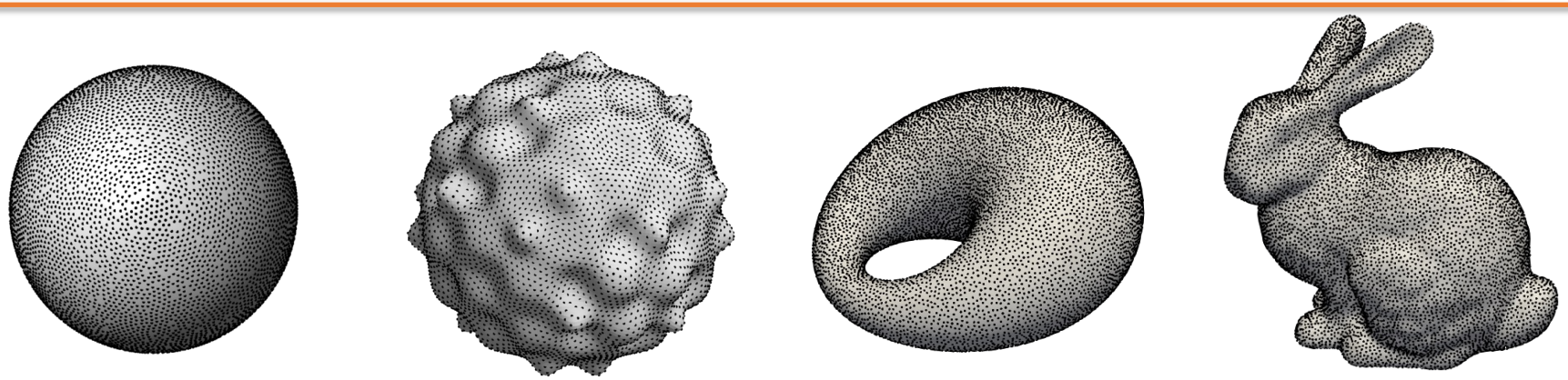
MGM GMRES Iterations, tol=10^{-8}



Quadrature

(cubature)

Quadrature (or cubature) for point clouds



$$I(f) := \int_{\mathcal{M}} f(\mathbf{x})\, dA \approx \sum_{j=1}^{N_h} w_j f(\mathbf{x}_j) =: I_{X_h}(f)$$

Nodes: $X_h = \{\mathbf{x}_j\} \subset \mathcal{M}$

Weights: $w^h = \{w_j\}$

Determine w^h so the error $E_{X_h}(f) = I(f) - I_{X_h}(f)$ is small for some space of functions and decreases rapidly to zero as $N_h \to \infty$

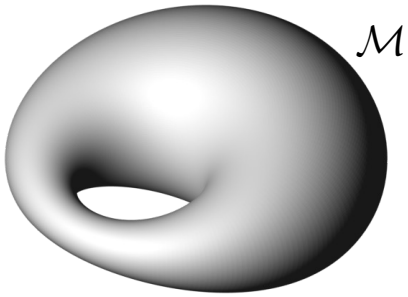
Dominant strategy for quadrature: Exactness

Pick a "good" vector space of functions $\mathcal{V}$ and enforce $E_{X_h}(f) = 0$ for all $f \in \mathcal{V}$

- What vector space of functions $\mathcal{V}$ should we use?
- How do we pick a bases for $\mathcal{V}$ and/or how do we integrate it over $\mathcal{M}$?

Introduce a new framework for quadrature that follows a different strategy

Motivation: Poisson problem on compact, connected manifold



Solve: $\Delta_{\mathcal{M}} u = g$

Issue: $\Delta_{\mathcal{M}}$ has a non-trivial null-space consisting of the constant function

Theorem (Fredholm alternative for surface Poisson problem)**.** *The solution of* $\Delta_{\mathcal{M}} u = g$*, with* $g \in L_2(\mathcal{M})$*, exists if and only if*

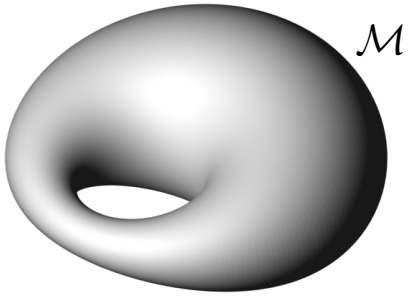
$$< g, w >= 0$$

for all w *in the nullspace of the adjoint of* $\Delta_{\mathcal{M}}$*.*

Poisson problem is self-adjoint and nullspace consists only of the constant function

$$\Longrightarrow \text{Solution exists if and only if } \int_{\mathcal{M}} g(\mathbf{x}) dA = 0$$

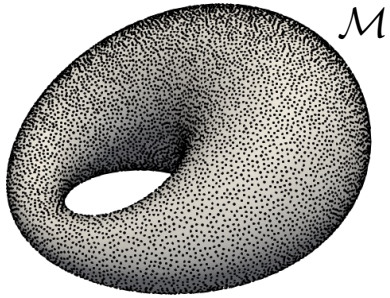
Motivation: Poisson problem on compact, connected manifold



New problem

Solve: $\Delta_{\mathcal{M}} u = g$ Constraint: $\dfrac{1}{|\mathcal{M}|}\displaystyle\int_{\mathcal{M}} u(\mathbf{x})\, dA = \mu$

Compatibility condition: $\int_{\mathcal{M}} g(\mathbf{x})\, dA = 0$



$X_h = \{\mathbf{x}_j\}_{j=1}^{N_h}$

Discretize

Solve: $L_h u^h = g^h$ Constraint: $\displaystyle\sum_{j=1}^{N_h} w_j u_j = (w^h)^T u^h = |\mathcal{M}|\mu$

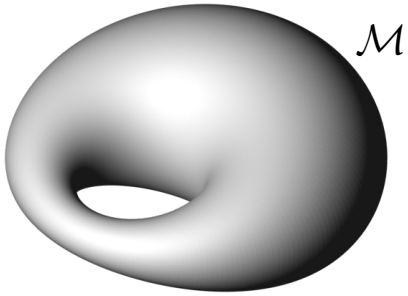
Compatibility condition: $(w^h)^T g^h = 0$

$$\Longrightarrow \begin{bmatrix} L_h & w^h \\ (w^h)^T & 0 \end{bmatrix} \begin{bmatrix} u^h \\ \lambda \end{bmatrix} = \begin{bmatrix} g^h \\ |\mathcal{M}|\mu \end{bmatrix}.$$

This problem has a unique solution provided $(w^h)^T e^h \neq 0$, where $e^h = [1\ 1\ \cdots\ 1]^T$

But, this solution satisfies $L_h u^h + \lambda w^h = g^h$, not the original problem $L_h u^h = g^h$ unless $\lambda = 0$

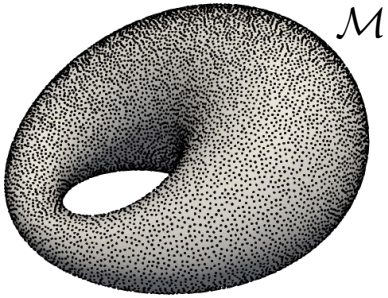
Motivation: Poisson problem on compact, connected manifold



New problem

Solve: $\Delta_{\mathcal{M}} u = g$ Constraint: $\dfrac{1}{|\mathcal{M}|}\displaystyle\int_{\mathcal{M}} u(\mathbf{x})\, dA = \mu$

Compatibility condition: $\int_{\mathcal{M}} g(\mathbf{x})\, dA = 0$



$X_h = \{\mathbf{x}_j\}_{j=1}^{N_h}$

Discretize

Solve: $L_h u^h = g^h$ Constraint: $\displaystyle\sum_{j=1}^{N_h} w_j u_j = (w^h)^T u^h = |\mathcal{M}|\mu$

Compatibility condition: $(w^h)^T g^h = 0$

$$\Longrightarrow \begin{bmatrix} L_h & w^h \\ (w^h)^T & 0 \end{bmatrix} \begin{bmatrix} u^h \\ \lambda \end{bmatrix} = \begin{bmatrix} g^h \\ |\mathcal{M}|\mu \end{bmatrix}.$$

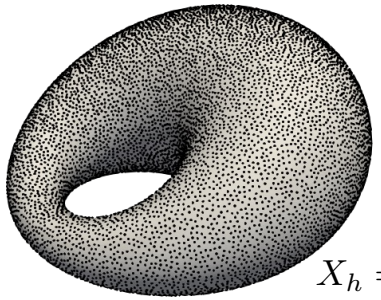
When does $\lambda = 0$?

$\lambda = 0$ if and only if $L_h^T w^h = 0$ and $(w^h)^T g^h = 0$

Fredholm alternative (1903) for linear systems

Main idea

Solve: $L_h u^h = g^h$



$X_h = \{\mathbf{x}_j\}_{j=1}^{N_h}$

Theorem (Fredholm alternative)**.**
A solution to $L_h u^h = g^h$ *exists if and only if* $(w^h)^T g^h = 0$ *for all* w^h *satisfying* $L_h^T w^h = 0$.

Suppose L_h only annihilates constant vectors so $\text{rank}(L_h) = N_h - 1$

The left null vector w^h of L_h will contain quadrature weights (after scaling), corresponding to the nodes X_h, for approximating the integral over $\mathcal{M}$

$$I(f) := \int_{\mathcal{M}} f(\mathbf{x})\, dA \approx \sum_{j=1}^{N_h} w_j f(\mathbf{x}_j) =: I_{X_h}(f)$$

We call $\{w^h, X_h\}$ a Fredholm alternative quadrature (FAQ) formula

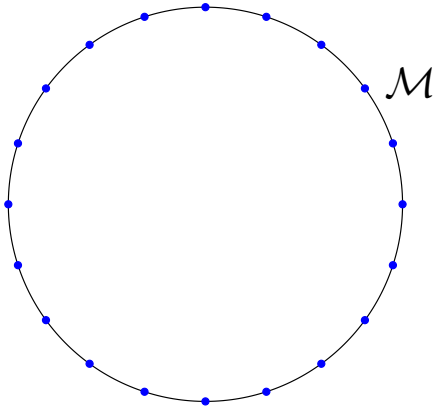
The quadrature formulas only depends on L_h and not on integrals of basis functions

Need to know or be able to approximate the surface area $|\mathcal{M}|$

What are FAQ formulas exact for?

Example: FAQ for the unit circle

Solve: $\Delta_{\mathcal{M}} u = g, \quad \mathcal{M} =$ unit disk



Discretize the domain using a grid of N equally spaced points $X_h = \{\mathbf{x}_j\}_{j=1}^N$, $\mathbf{x}_j = (\cos\theta_j, \sin\theta_j)$

$$u''(\theta) = g(\theta), \quad -\pi \le \theta \le \pi, \text{ periodic boundary conditions}$$

Use 2nd order finite differences

$$\underbrace{\frac{1}{h^2}\begin{bmatrix} -2 & 1 & & & & & 1 \\ 1 & -2 & 1 & & & & \\ & 1 & -2 & 1 & & & \\ & & \ddots & \ddots & \ddots & & \\ & & & \ddots & \ddots & \ddots & \\ & & & & 1 & -2 & 1 \\ 1 & & & & & 1 & -2 \end{bmatrix}}_{L_h} \underbrace{\begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ \vdots \\ \vdots \\ u_{N-1} \\ u_N \end{bmatrix}}_{u^h} = \underbrace{\begin{bmatrix} g_1 \\ g_2 \\ g_3 \\ \vdots \\ \vdots \\ g_{N-1} \\ g_N \end{bmatrix}}_{g^h}$$

What is the FAQ formula in this case?

Trapezoidal rule: $w^h = \frac{2\pi}{N}\begin{bmatrix} 1 & 1 & \cdots & 1 \end{bmatrix}^T$

What is this exact for?

Examples: FAQ for a 2D surface

Experiment:

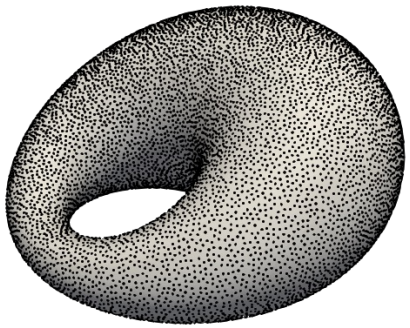
Scattered node set X_h with N_h points

Test convergence of the FAQ formulas as N increases

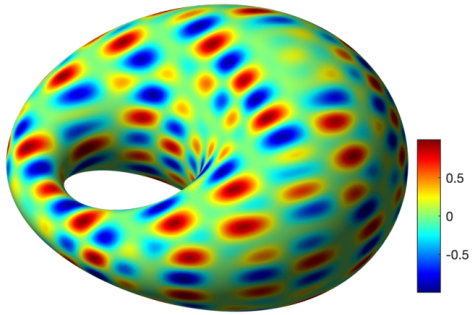
Different poly. degrees ℓ in kernel approx.

Stencil size $n = \lceil (\ell+1)(\ell+2) \rceil$

Example node set

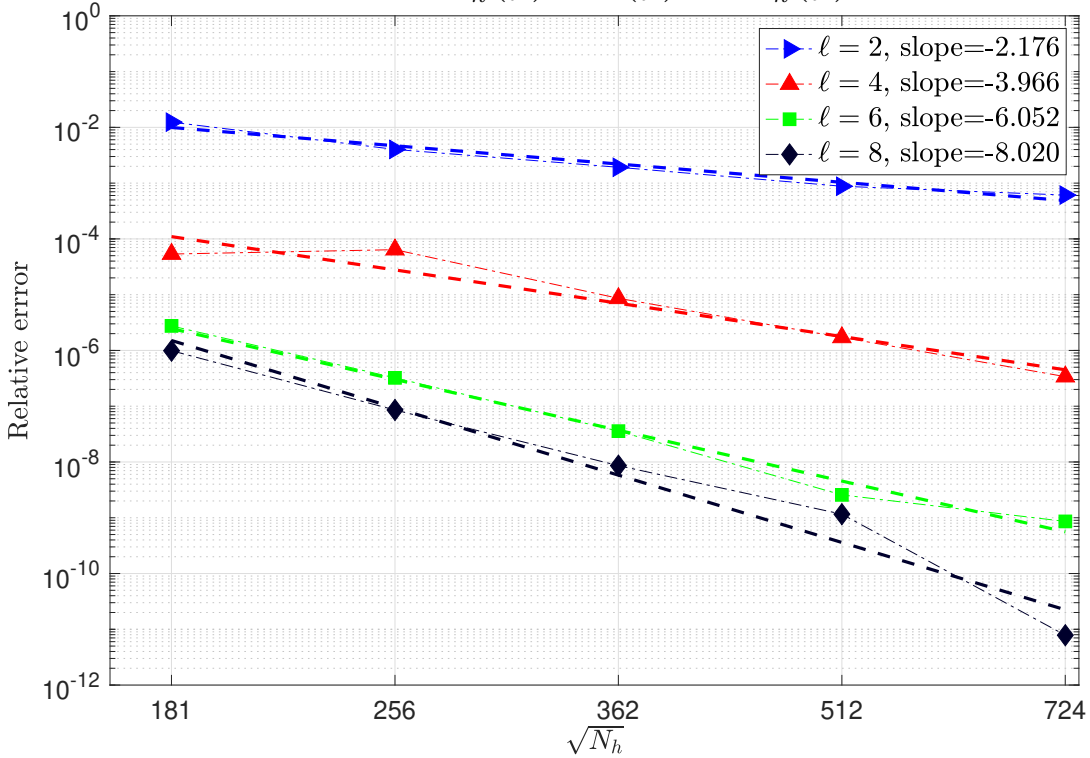


Target function f



$$\int_{\mathcal{M}} f(\mathbf{x})\, dA = 0.524555695704092\ldots$$

Error $E_{X_h}(f) = I(f) - I_{X_h}(f)$



Examples: FAQ for a 2D surface

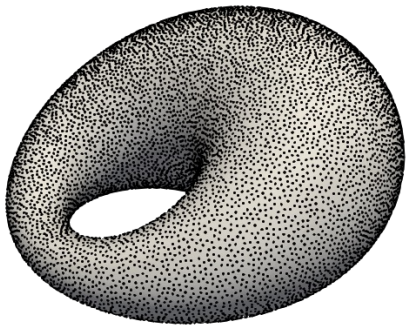
Experiment:

Scattered node set X_h with N_h points

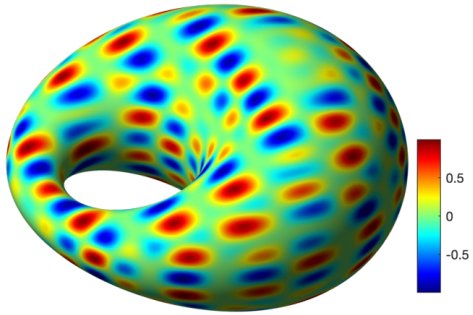
Test convergence of the FAQ formulas as N increases

Can obtain very high accuracy by using a global approximation of $\Delta_{\mathcal{M}}$ (Fuselier & W (2013))

Example node set

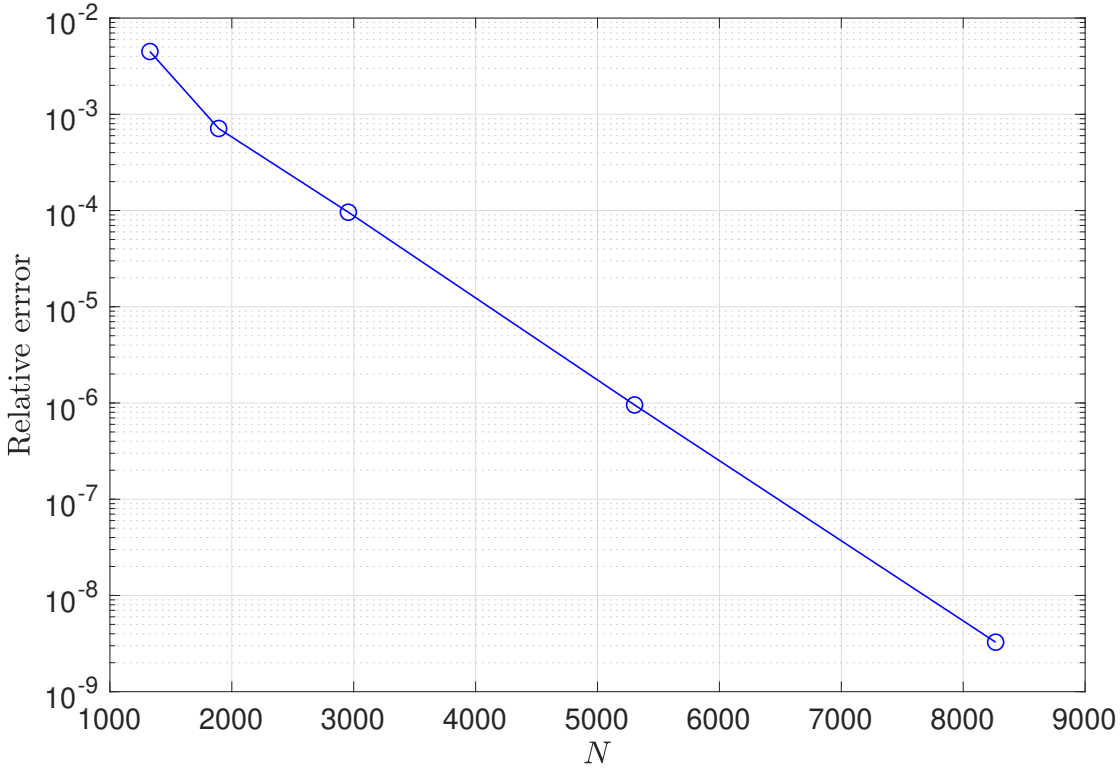


Target function f

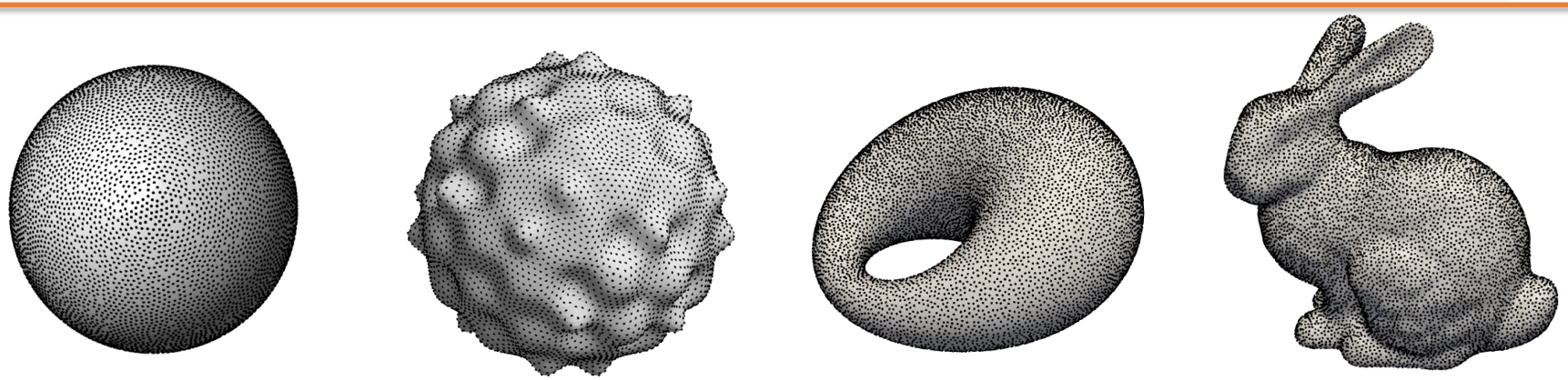


$$\int_{\mathcal{M}} f(\mathbf{x})\, dA = 0.524555695704092\ldots$$

Error $E_{X_h}(f) = I(f) - I_{X_h}(f)$



How to compute the FAQ weights



L_h is some N-by-N matrix representing a consistent discrete approximation to $\Delta_{\mathcal{M}}$ over some set of N nodes $X_h = \{\mathbf{x}_j\}_{j=1}^N \subset \mathcal{M}$.

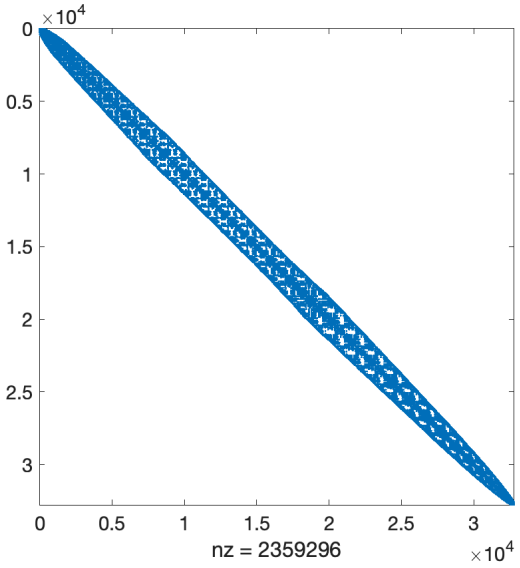
Determine FAQ weights by finding w^h that satisfies

$$L_h^T u^h = 0, \text{ subject to } \sum_{j=1}^{N} w_j = |\mathcal{M}|$$

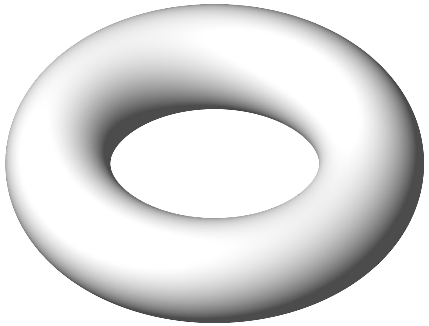
$$\implies \text{Solve } \begin{bmatrix} L_h^T & 1_h \\ 1_h^T & 0 \end{bmatrix} \begin{bmatrix} w^h \\ \lambda \end{bmatrix} = \begin{bmatrix} 0 \\ |\mathcal{M}| \end{bmatrix}$$

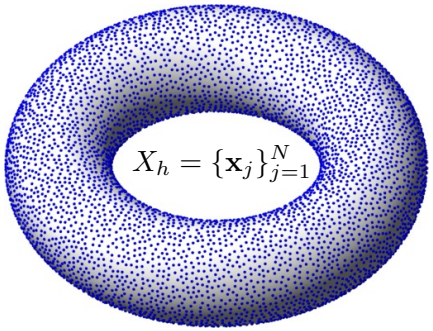
MGM can be used to solve this system efficiently

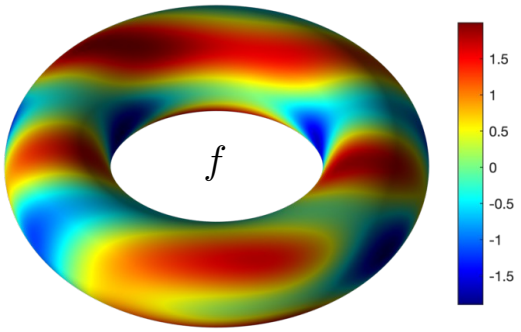
Pattern of non-zero entries of L_h



FAQ Summary







Continuous problem on Ω

$\Delta_{\mathcal{M}} u = g$

$\longrightarrow$

Discrete problem on X_h

$L_h u^h = g^h$

Solve: $L_h^T w^h = 0$, $\sum_j w_j = |\mathcal{M}|$

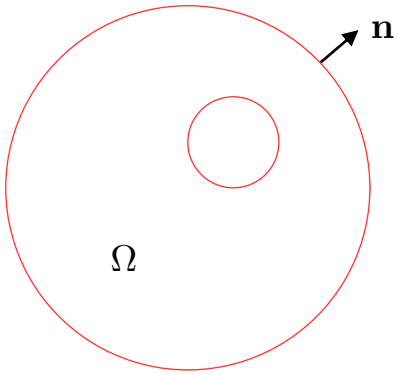
$\Longrightarrow$

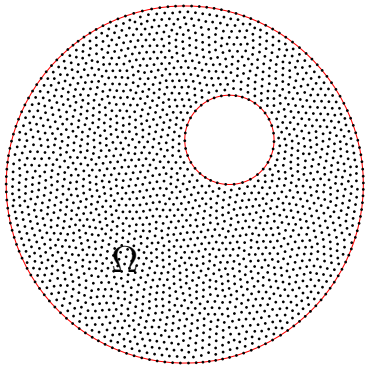
FAQ formula:

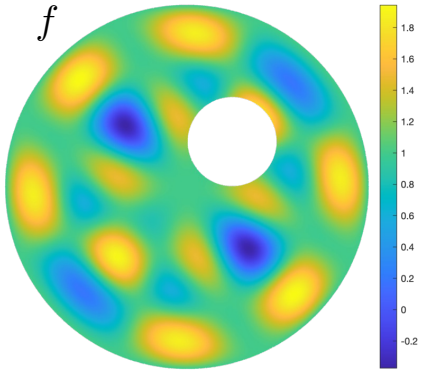
$\int_{\mathcal{M}} f(\mathbf{x}) dA \approx \sum_j w_j f(\mathbf{x}_j)$

Relative err: 6.17×10^{-7}

Can be extended to Euclidean domains via the Neumann-Poisson problem







Continuous problem on Ω

$\Delta u = g$ in Ω

$\mathbf{n} \cdot \nabla u = 0$ on $\partial\Omega$

$\longrightarrow$

Discrete problem on $X_h = \{\mathbf{x}_j\}_{j=1}^N$

$L_h u^h = g^h$

Solve: $L_h^T w^h = 0$, $\sum_j w_j = |\Omega|$

$\Longrightarrow$

Quadrature formula:

$\int_{\Omega} f(\mathbf{x}) d\mathbf{x} \approx \sum_j w_j f(\mathbf{x}_j)$

Relative err: 2.277×10^{-6}

Implicit Surface Reconstruction

Motivation

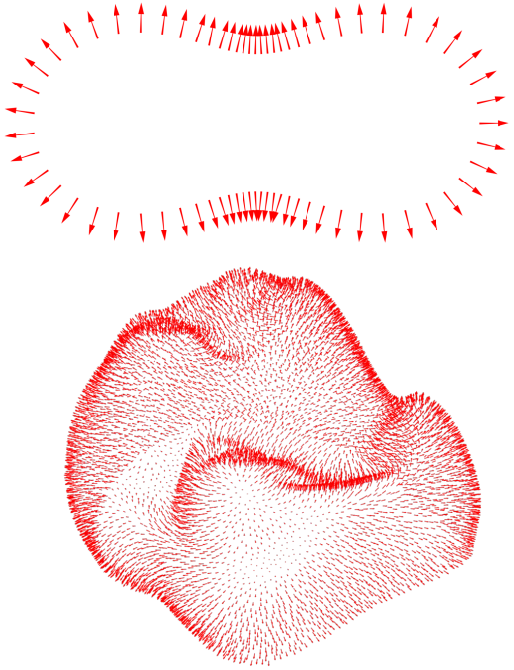
Reconstructing a surface from an (oriented) point cloud has many applications

computer graphics, computer-aided design, medical imaging, manufacturing, remote sensing

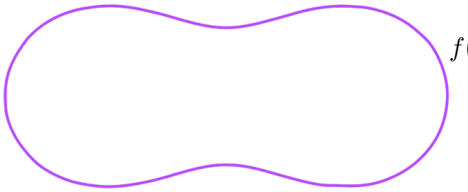
Common approach: implicit surface (zero-level set) methods

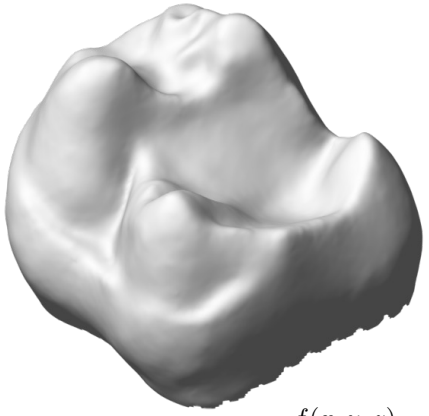
Problem: Given an oriented point cloud $\{(\mathbf{x}_j, \mathbf{n}_j)\}_{j=1}^N$, find a function f such that the level-set $S = \{\mathbf{x} \in \mathbb{R}^d \big| f(\mathbf{x}) = 0\}$ fits the point cloud. S is called the zero-level implicit surface.

Oriented point cloud



Implicit surface





Curl-free Partition of Unity (CFPU) method (Drake, Fuselier, & W, 2022)

Overview of CFPU method

Uses the following fundamental result from vector calculus

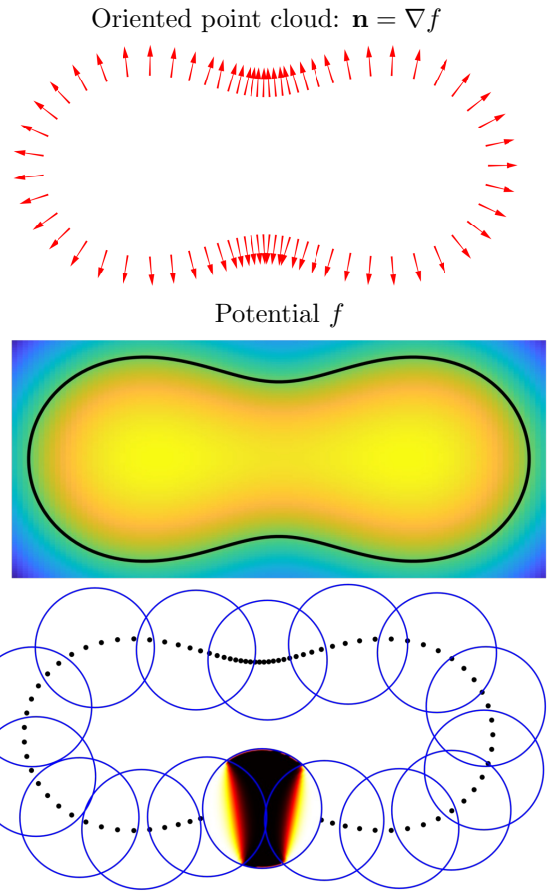
Proposition 1 *A vector field* $\mathbf{n}$ *is curl-free in* $\mathbb{R}^d$ *if and only if locally there exists a scalar potential* $f : \mathbb{R}^d \longrightarrow \mathbb{R}$ *such that* $\mathbf{n} = \nabla f$*. Furthermore,* f *is unique up to a constant.*

Overview of our approach:

- Fit a curl-free Kernel interpolant to the normal vectors

$$\mathbf{s}(\mathbf{x}) = \sum_{j=1}^{N} \Phi(\mathbf{x}, \mathbf{x}_j)\mathbf{c}_j = \sum_{j=1}^{N} \left[\nabla\nabla^T \phi\left(\|\mathbf{x} - \mathbf{x}_j\|\right)\right] \mathbf{c}_j$$

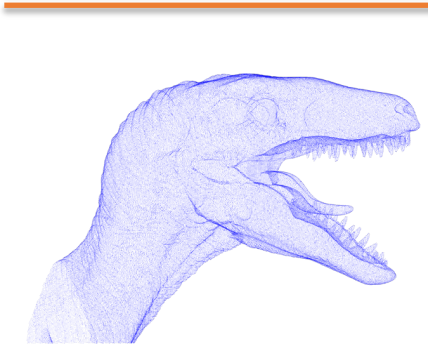
- Extract a scalar potential $\tilde{f}$ for the interpolant
- Shift the potential to be zero at the point cloud
- Include regularization if the data is noisy
- Combine the above in a partition of unity (PU) framework
- Use isosurface extractor to obtain the zero-level set



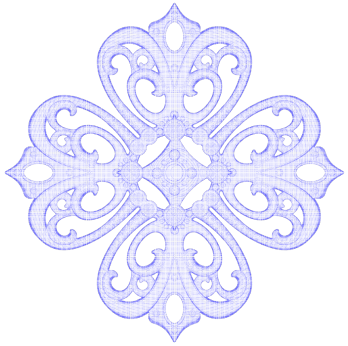
Relationship to previous work

Narrow band: Carr et. al. (1997, 2001), Turk & O'Brien (1999), Morse et. al. (2001), Fasshauer (2007)
Indicator function: Kazhdan et. al. (2006, 2013, 2019), Calakli & Taubin (2011),
Hermite: Walder et. al. (2006), Süßmuth et. al. (2010), Macêdo et. al. (2011), Liu et. al. (2016),

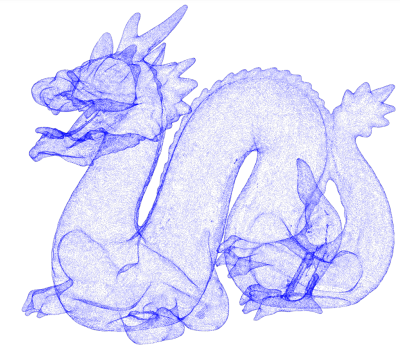
Computational performance



Raptor



Filigree



Dragon

Buddha

Armadillo

Surface	N	M	Grid size	Time in seconds			
				Number of cores			
				1	2	4	8
Raptor	135740	10337	384×143×258	18.2 (16.5)	6.67 (8.84)	4.14 (7.22)	3.35 (5.69)
Filigree	514300	35130	383×63×384	30.4 (7.70)	10.9 (4.10)	6.63 (3.39)	4.99 (3.13)
Dragon	434856	14400	384×175×272	42.73 (11.83)	17.24 (6.46)	10.7 (5.46)	9.20 (4.82)
Buddha	583079	42861	161×162×384	37.34 (7.71)	14.0 (4.20)	8.32 (3.43)	5.99 (3.02)
Armadillo	172974	14349	323×294×384	9.42 (10.0)	3.62 (5.54)	2.25 (4.85)	1.61 (4.55)

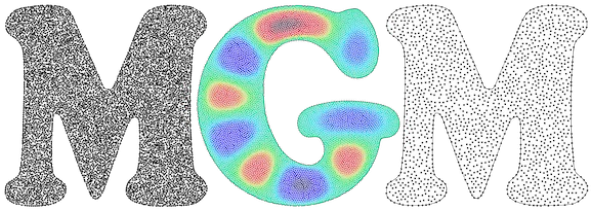
fit time & eval. time

Concluding remarks

Surface PDEs

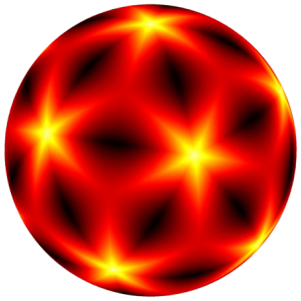
- Incorporation of advection using semi-Lagrangian method
- Anisotropic diffusion
- PDEs on moving surfaces
- KernelDMSuite (https://github.com/gradywright/kerneldmsuite)

Meshfree geometric multilevel (MGM) method



- Generalize to other discretization methods, both meshfree and mesh-restrained
- Euclidean domains
- Going beyond Poisson equation
- Parallelization
- MGM (https://github.com/gradywright/mgm)

Fredholm Alternative Quadrature (FAQ)

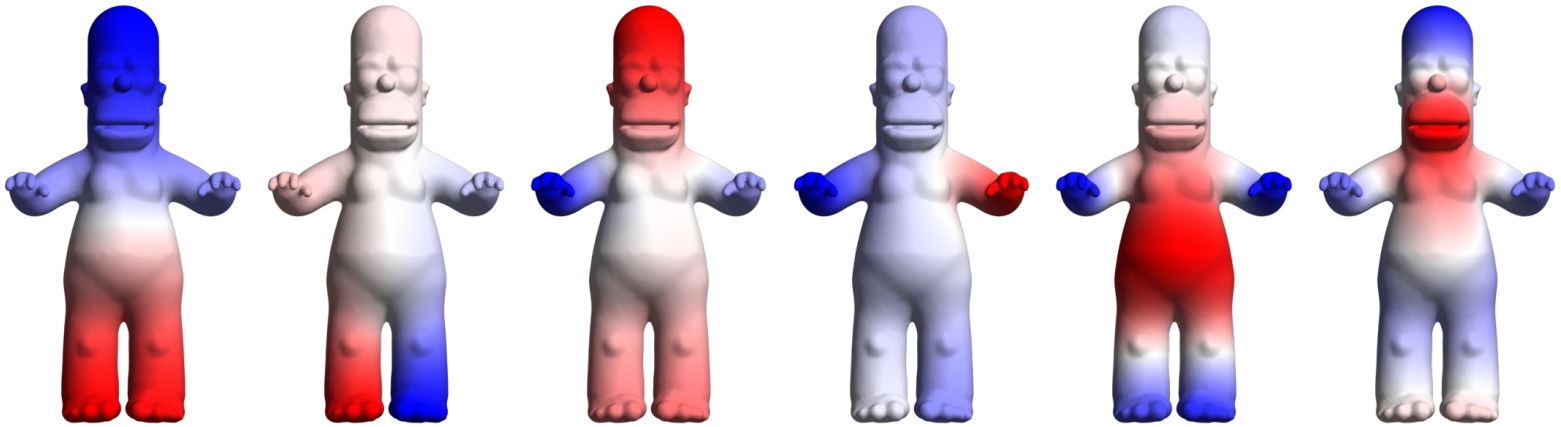


- Positive weight quadrature
- Error estimates
- Domain decomposition
- Non-smooth integrands

Implicit surface reconstruction

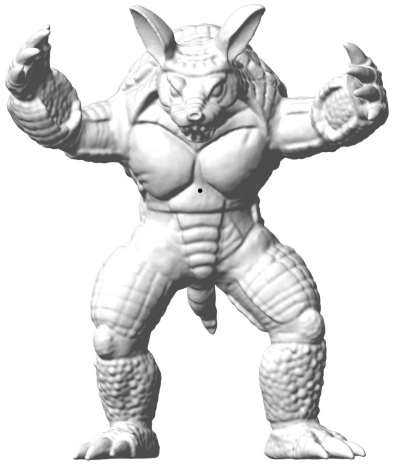
- Curl-free Partition-of-Unity Method (https://github.com/gradywright/cfpu)

Questions?



Application: Geodesic distance

Problem: Compute the geodesic distance from a single point on a surface $\mathcal{M}$



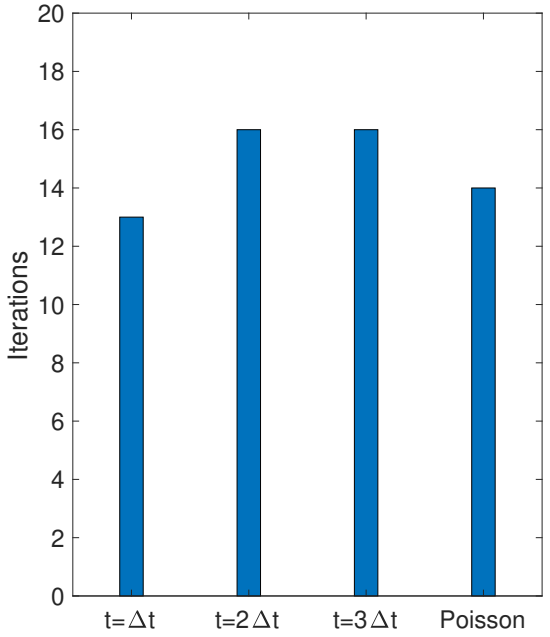
Heat flow method: Crane, Weischedel, Wardetzky (2013)

1. Solve $u_t = \Delta_{\mathcal{M}} u$, with $u_0 = \delta(\mathbf{x}^*)$, for $0 < t \leq m\Delta t$
2. Compute the vector field $\boldsymbol{\eta} = -\nabla_{\mathcal{M}} u / |\nabla_{\mathcal{M}} u|$
3. Solve the Poisson problem $\Delta_{\mathcal{M}} \phi = \nabla_{\mathcal{M}} \cdot \boldsymbol{\eta}$

$\Longrightarrow$ Potential ϕ approximates the geodesic distance from $\mathbf{x}^*$ on $\mathcal{M}$

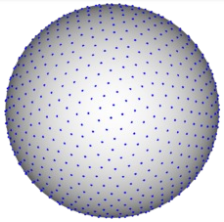
Solution on armadillo, $N_h = 872773$

MGM GMRES Iterations, tol=10^{-8}



Numerical results: accuracy vs. iteration

Problem: $\Delta_{\mathcal{M}} u = f$

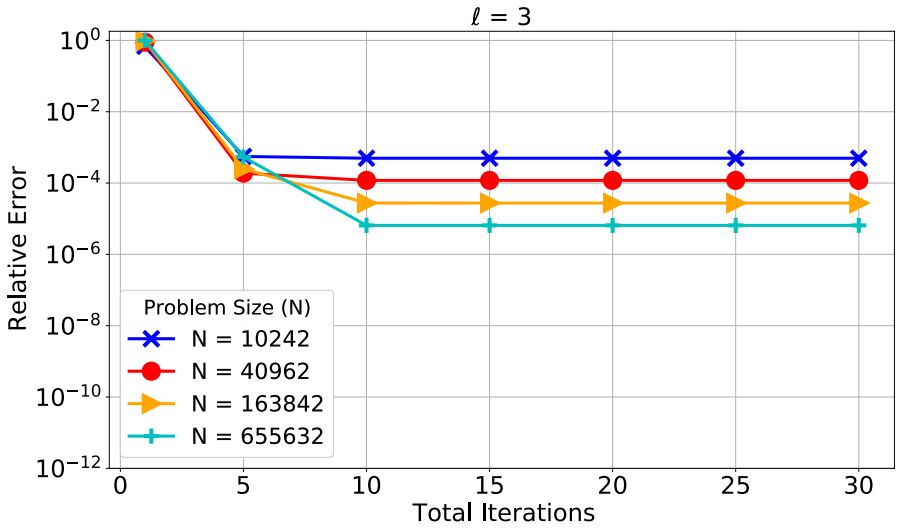


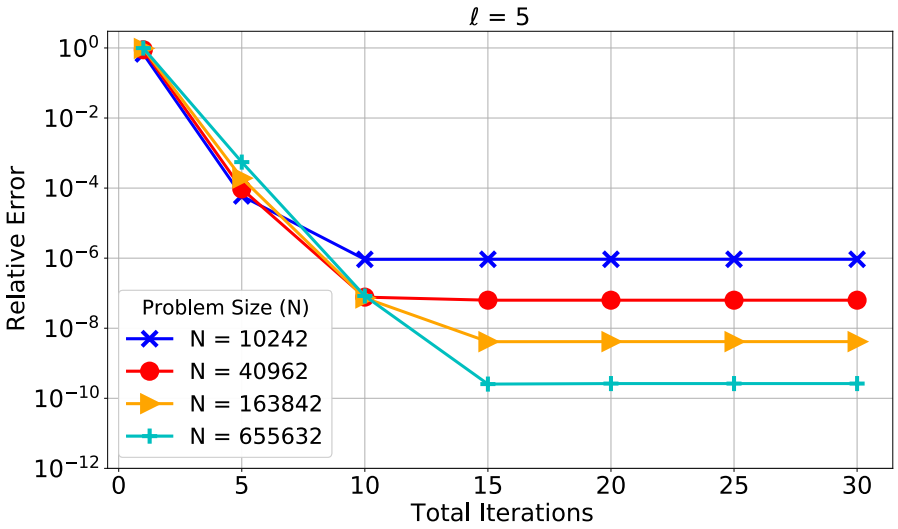
$\mathcal{M}$

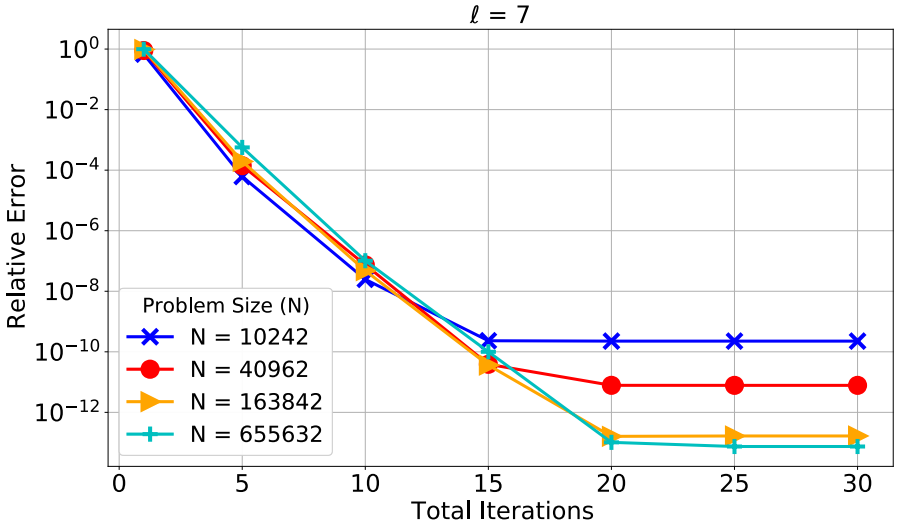
Test different poly. degrees ℓ in RBF-FD

RBF-FD stencil size $n = \lceil (\ell+1)(\ell+2) \rceil$

Exact solution is Y_5^4 spherical harmonic

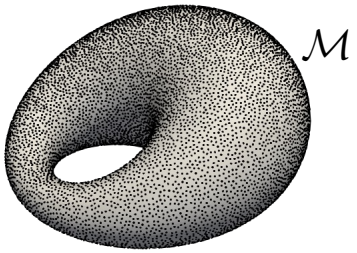




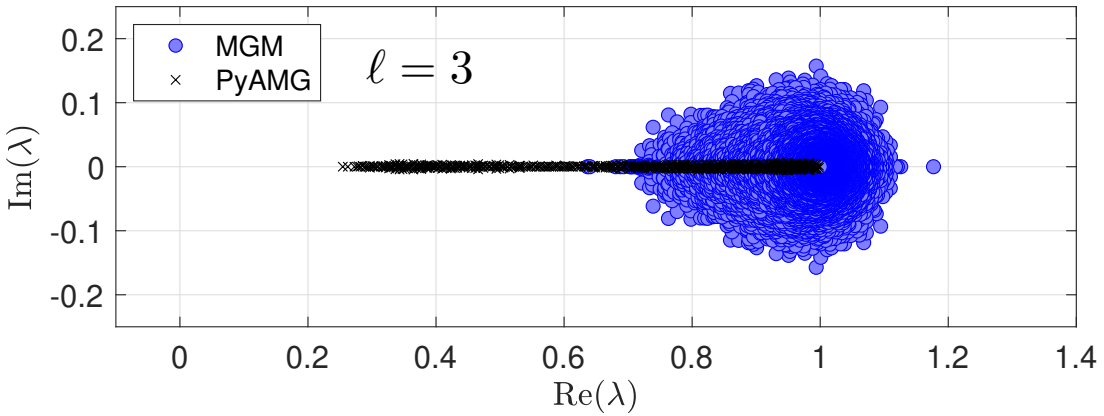


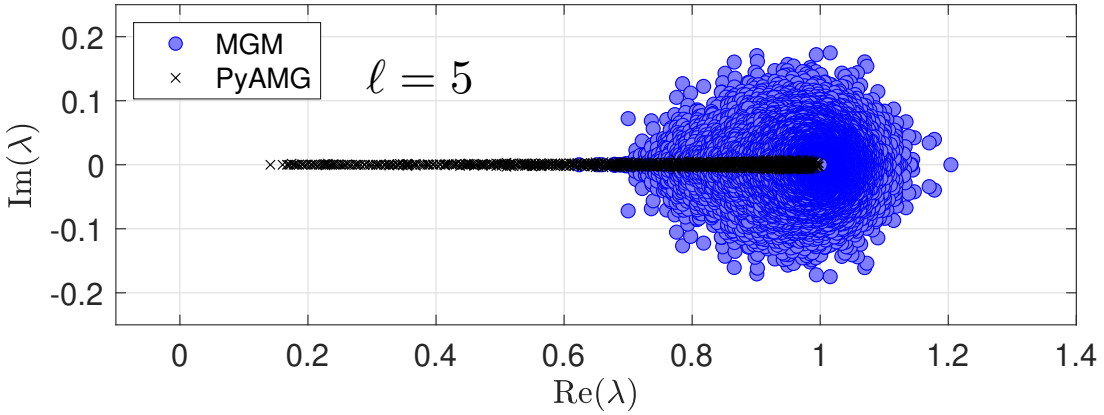
Numerical results: spectrum analysis

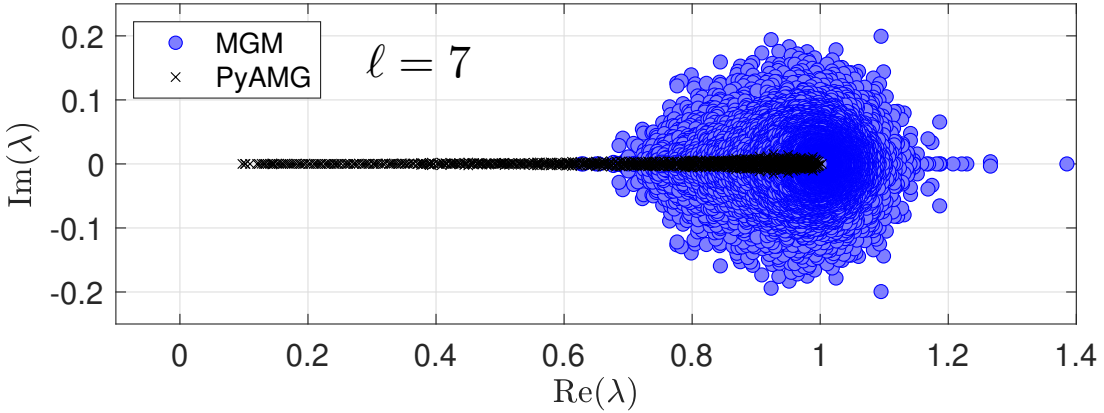
Problem: $(\mathcal{I} - \Delta_{\mathcal{M}})u = f$



Eigenvalues of the preconditioned matrix $L_h M_h$







Modifications required for surface Poisson problem

Suppose $\mathcal{L} = \Delta_{\mathcal{M}}$, so we want to solve

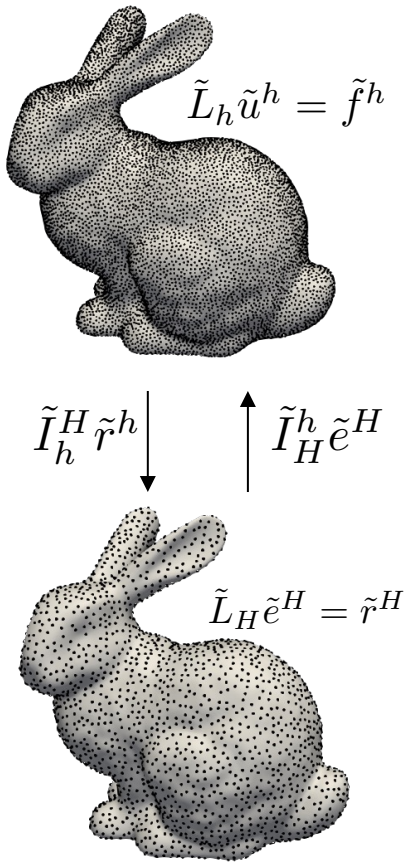
$$\Delta_{\mathcal{M}} u = f$$

Provided f satisfies the compatibility condition $\int_{\mathcal{M}} f dA = 0$, the solution is unique up to a constant

$L_h u^h = f^h$ is singular since L_h annihilates constants

Need to add another condition:

$$\frac{1}{N_h} \sum_{j=1}^{N_h} u_j = 0 \quad \longrightarrow \quad \underbrace{\begin{bmatrix} L_h & b_h^T \\ b_h & 0 \end{bmatrix}}_{\tilde{L}_h} \underbrace{\begin{bmatrix} u^h \\ \lambda^h \end{bmatrix}}_{\tilde{u}^h} = \underbrace{\begin{bmatrix} f^h \\ 0 \end{bmatrix}}_{\tilde{f}^h}$$



Requires modifications to the transfer and coarse level operators (Adams 2004)

$$\tilde{L}_H = \underbrace{\begin{bmatrix} I_h^H & 0 \\ 0 & 1 \end{bmatrix}}_{\tilde{I}_h^H} \underbrace{\begin{bmatrix} L_h & b_h^T \\ b_h & 0 \end{bmatrix}}_{\tilde{L}_h} \underbrace{\begin{bmatrix} I_H^h & 0 \\ 0 & 1 \end{bmatrix}}_{\tilde{I}_H^h} = \begin{bmatrix} I_h^H L_h I_H^h & I_h^H b_h^T \\ b_h I_H^h & 0 \end{bmatrix}$$