Postdoc/ Graduate Student Introductions
Wednesday, January 31, 2024

John Carter, Rensselaer Polytechnic Institute
Casey Cavanaugh, Louisiana State University
Tristan Goodwill, University of Chicago
Sijing Liu, Brown University
Marissa Masden, ICERM
Henry von Wahl, Friedrich Schiller University Jena
Christopher Wang, Cornell University
Yukun Yue, University of Wisconsin, Madison

Introduction: John Carter

Rensselaer Polytechnic Institute

January 31, 2024

Background and Ph.D. Research

- **Ph.D. in Math:** Missouri University of Science and Technology (S&T), Spring 2023.
- **Research Focus:** Ensemble means for MHD equations, Scalar Auxiliary Variable approach for explicit discretization of nonlinear terms, error and stability analysis.
- **Results:** Significant time savings. Unconditional stability of schemes. Guaranteed positivity of scalar variables.

Post-Ph.D. Experience and Current Research

- **Postdoc at RPI:** Joined in 2023, working with Dr. Jeff Banks and Dr. Mark Shephard.
- **Current Focus:** Mesh adaptivity and development of standalone solvers for the multifluid plasma equations.
- **Involved Schemes:** Single-step Godunov scheme for fluids. 2nd and 4th order Maxwell solvers.
- **Applications:** Space weather simulations for planetary systems.

ICERM Expectations and Interests

- **Looking Forward To:** Potential research opportunities, engaging discussions, and interdisciplinary exploration.
- **Open to Discussions:** Let's connect and explore possible collaborations!

Introduction: Casey Cavanaugh

Postdoctoral Researcher

Louisiana State University

Center for Computation & Technology and Dept. of Mathematics

Supervisor: Susanne Brenner

PhD: Tufts University, 2022

Advisors: James Adler and Xiaozhe Hu

Thesis: *Structure-preserving discretizations for PDEs*

Research interests: finite element methods, finite difference methods, linear solvers, multigrid methods

CENTER FOR COMPUTATION & TECHNOLOGY

Thesis: Structure-preserving discretizations for PDEs

de Rham exact sequence

$$H(\text{grad}) \xrightarrow{\text{grad}} \boldsymbol{H}(\text{curl}) \xrightarrow{\text{curl}} \boldsymbol{H}(\text{div}) \xrightarrow{\text{div}} L^2$$

↙ ↘

discrete exterior calculus (DEC) | finite element exterior calculus (FEEC)

Idea: Draw connections to use FE theory for DEC scheme.

- **Maxwell's equations:** enforce $\text{div}\,\boldsymbol{B} = 0$

  Adler, C., Hu, Zikatanov, *A finite-element framework for a mimetic finite-difference discretization of Maxwell's equations*, SISC, 2021.

- **Convection-dominated diffusion equations:** stability

  Adler, C., Hu, Huang, Trask, *A stable mimetic finite-difference method for convection-dominated diffusion equations*. SISC, 2023.

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Current: FEM and multigrid for 3D quad-curl equation

Joint work with S. C. Brenner and L. -Y. Sung (LSU)

Find $\boldsymbol{u} \in \mathbb{E}$ such that for all $\boldsymbol{v} \in \mathbb{E}$,

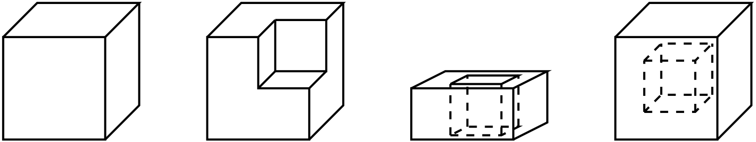
$$\langle \operatorname{curl} \operatorname{curl} \boldsymbol{u}, \operatorname{curl} \operatorname{curl} \boldsymbol{v} \rangle + \beta \langle \operatorname{curl} \boldsymbol{u}, \operatorname{curl} \boldsymbol{v} \rangle + \gamma \langle \boldsymbol{u}, \boldsymbol{v} \rangle = \langle \boldsymbol{f}, \boldsymbol{v} \rangle.$$

Hodge decomposition

A divergence-free vector field $\boldsymbol{u}$ has decomposition,

$$\boldsymbol{u} = \operatorname{curl} \varphi + \sum_{i=1}^{n} c_i \operatorname{grad} \lambda_i .$$

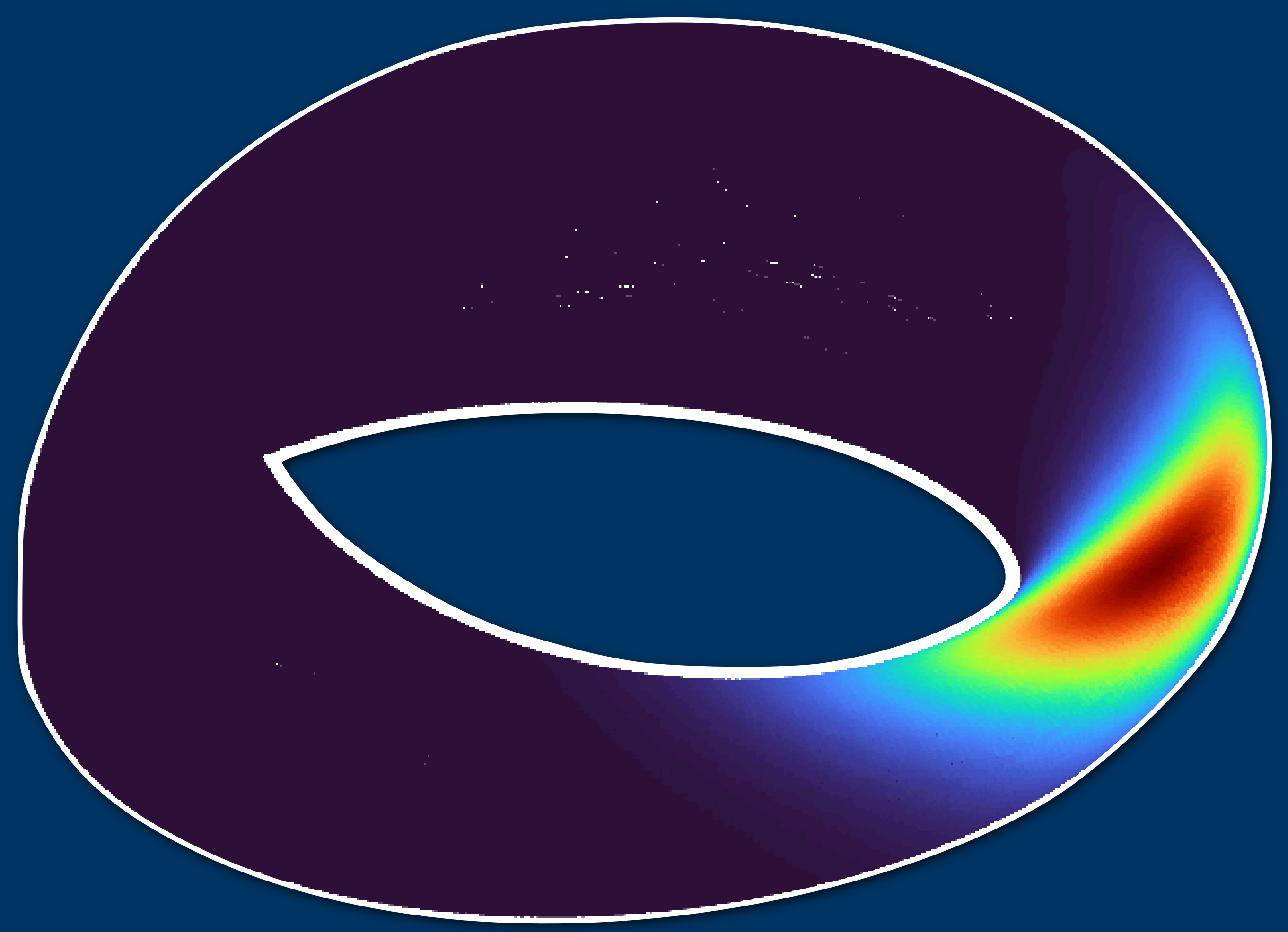
Idea: Reduce quad-curl to standard saddle point problems.

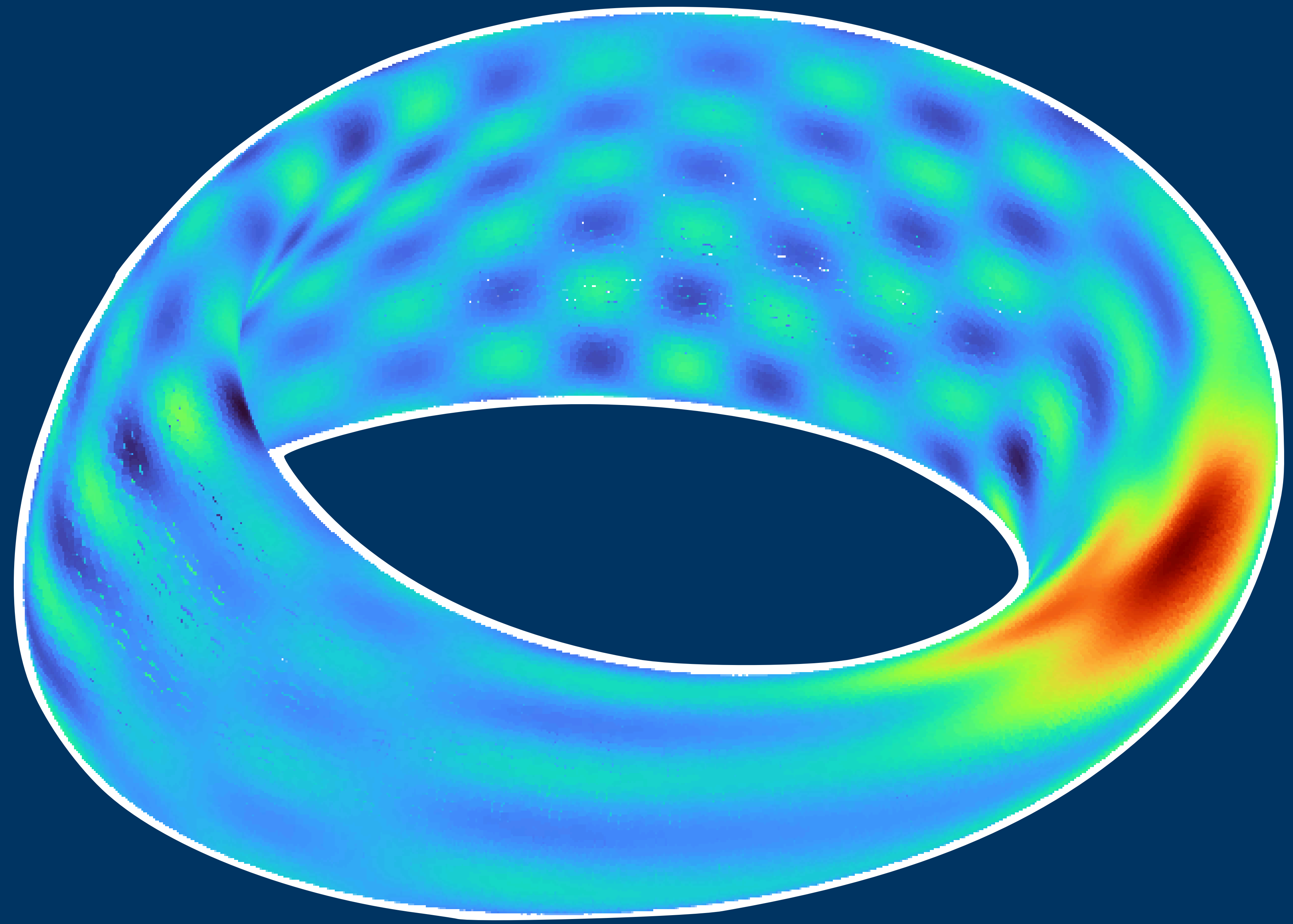


LSU CENTER FOR COMPUTATION & TECHNOLOGY

Tristan Goodwill

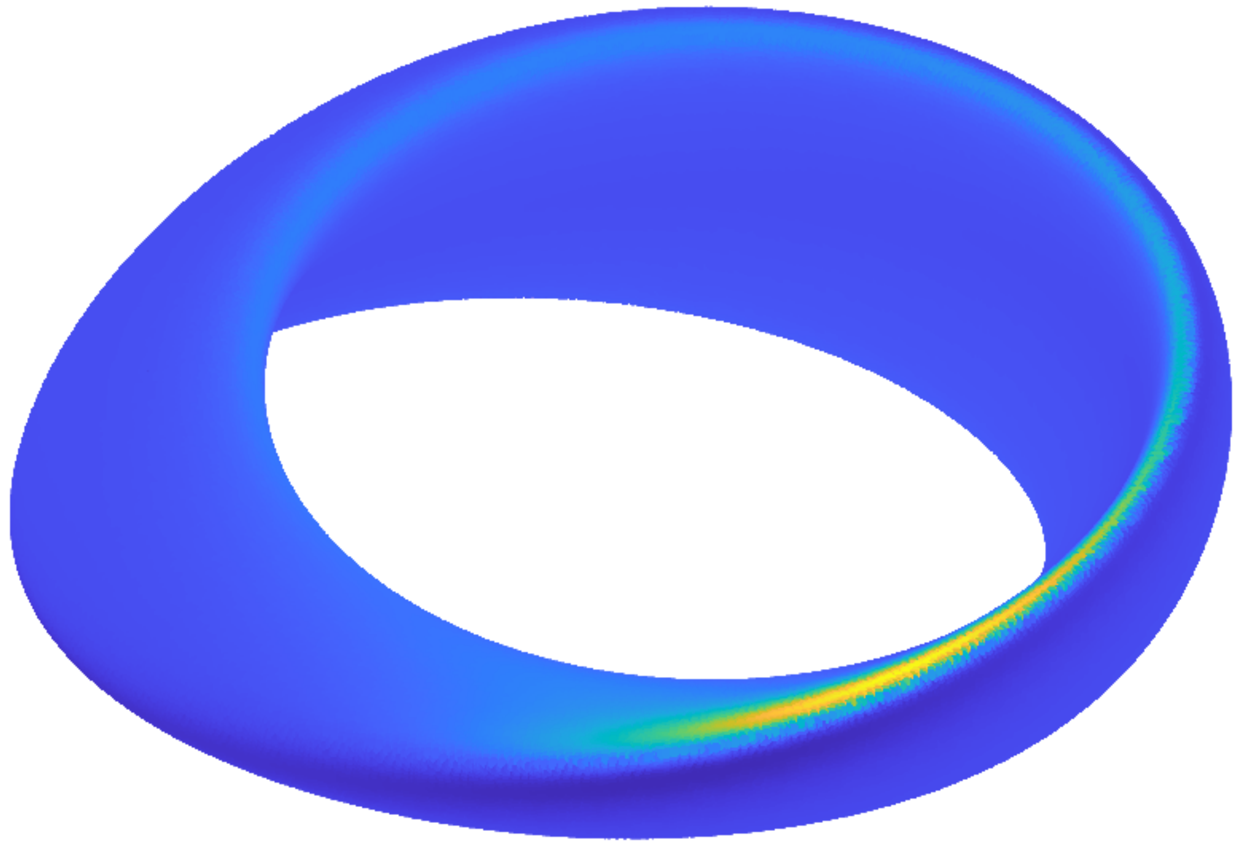
William H. Kruskal Instructor
University of Chicago



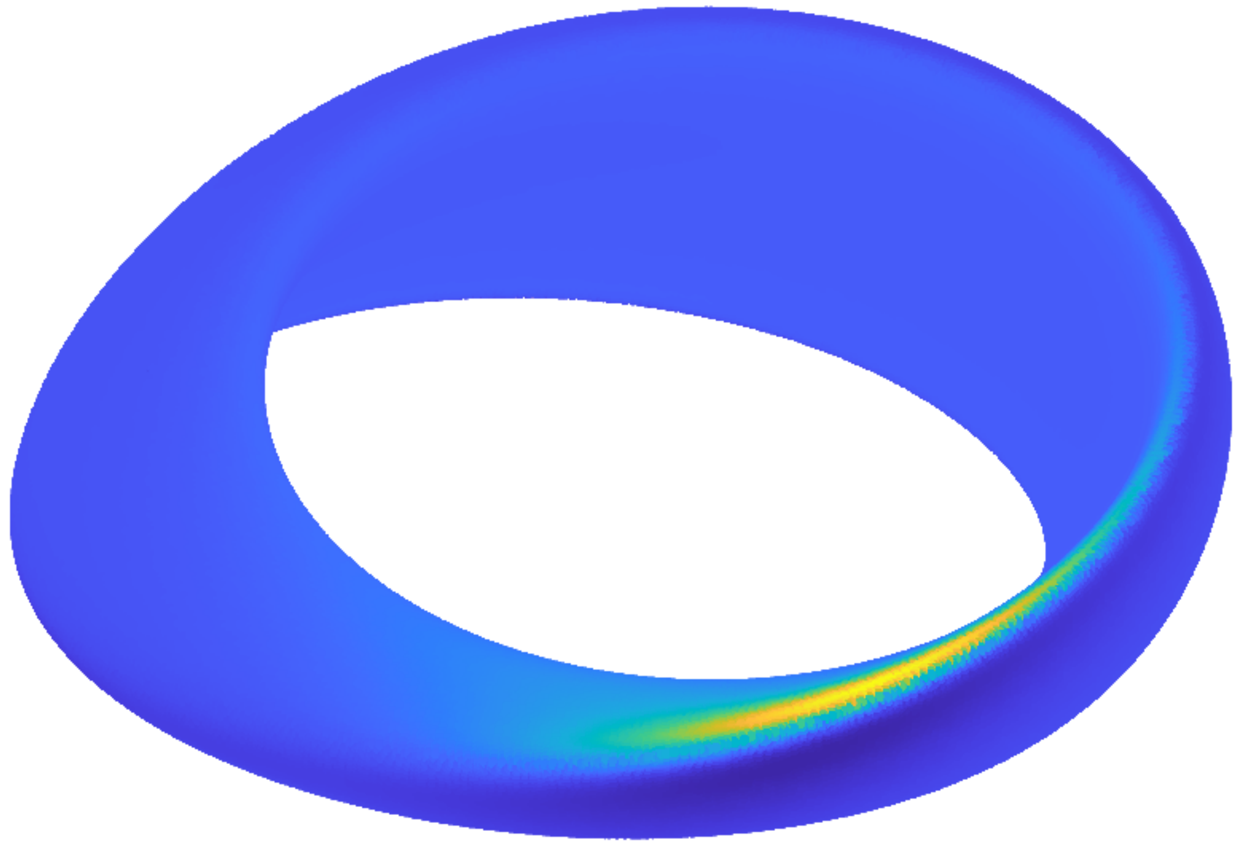


- High order methods for PDEs
- Particularly fast and accurate integral equation methods
- Fast hierarchical linear algebra (FMM, etc…)
- PDEs on surfaces
- PDEs with discontinuous coefficients

Laplace-Beltrami equation



f



σ

We want to solve

$$\Delta_\Gamma u = f \text{ on } \Gamma$$

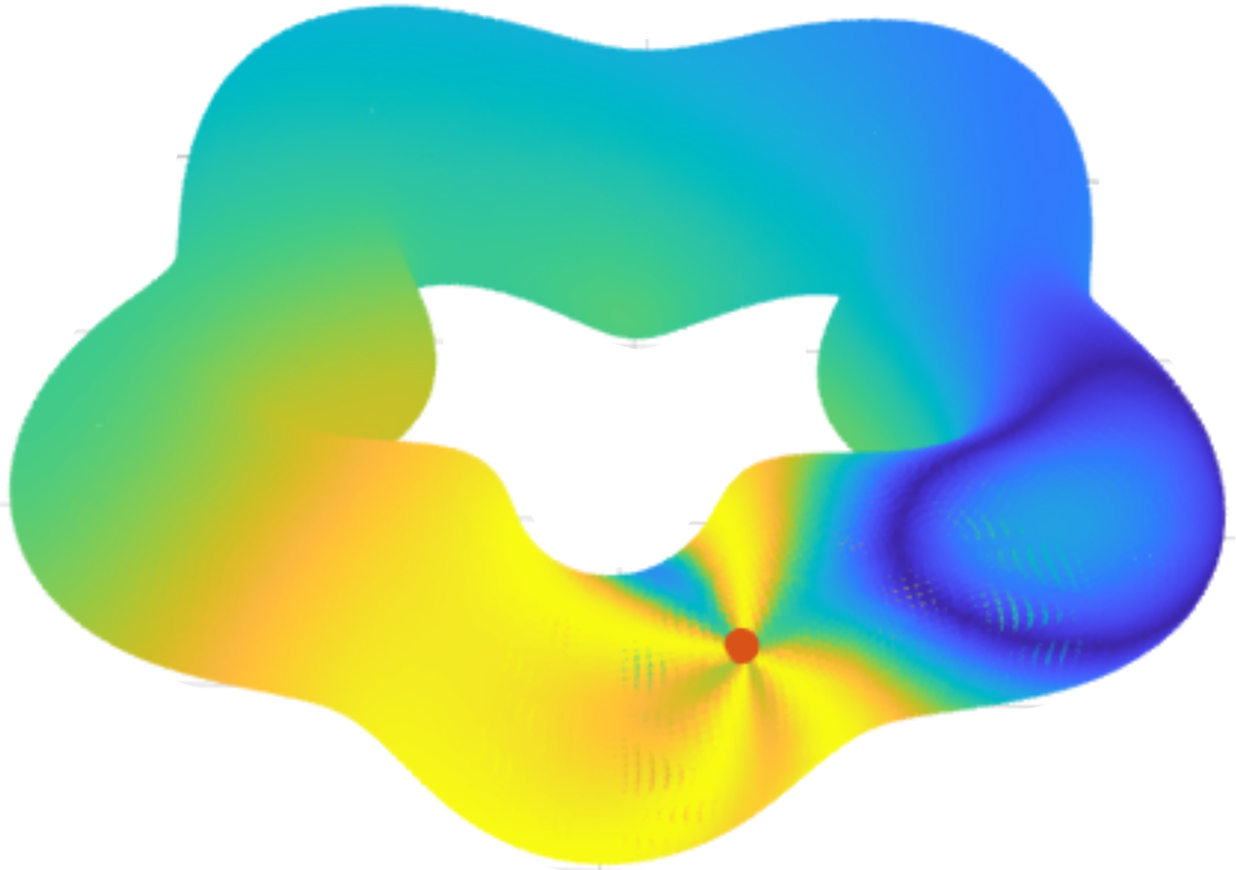
The 2D Green's function $K(\boldsymbol{x}, \boldsymbol{x}') = \log \|\boldsymbol{x} - \boldsymbol{x}'\|$ satisfies

$$\Delta_\Gamma K(\boldsymbol{x}, \boldsymbol{x}') = \delta(\boldsymbol{x} - \boldsymbol{x}') + R(\boldsymbol{x}, \boldsymbol{x}').$$

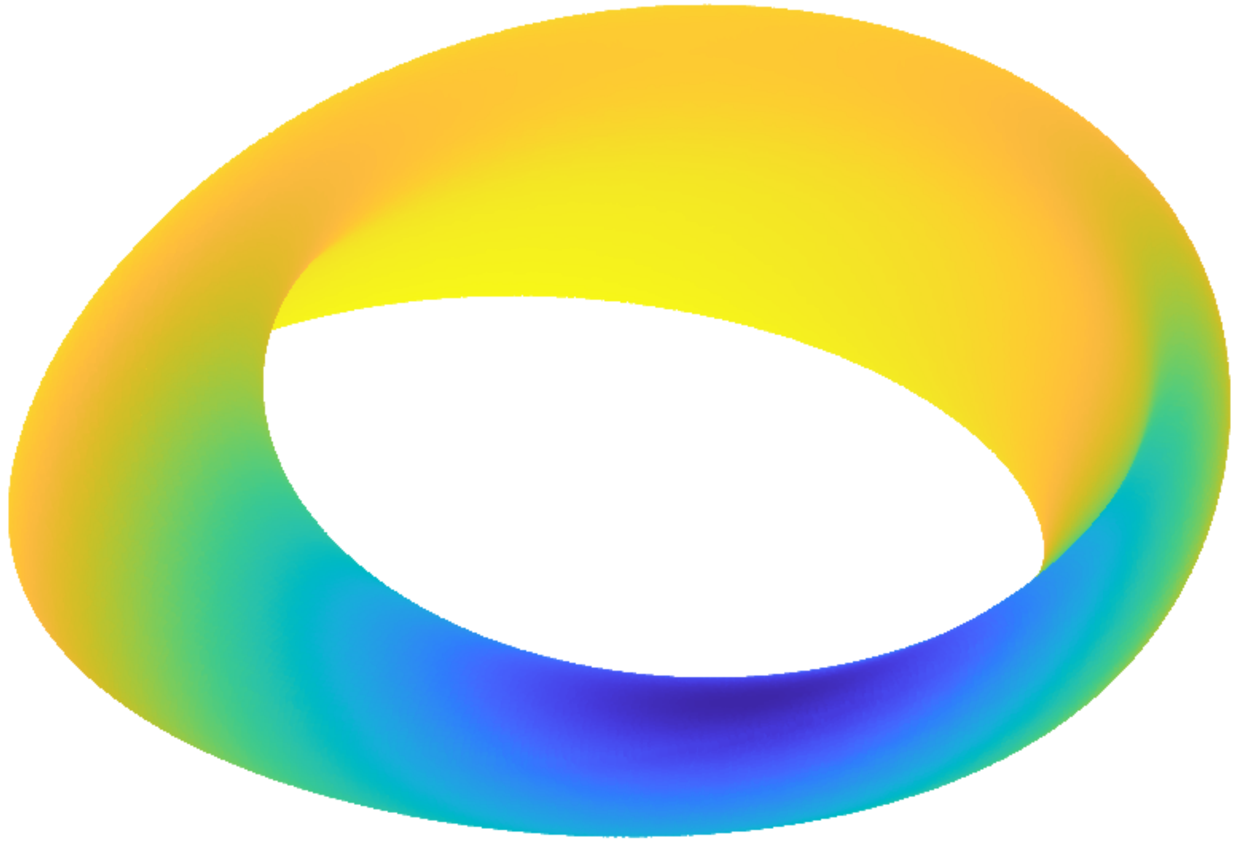
Thus if $u(\mathbf{x}) = \int_\Gamma K(\mathbf{x}, \mathbf{x}')\sigma(\mathbf{x}')da(\mathbf{x}')$,

then σ must solve

$$\sigma(\mathbf{x}) + \int_\Gamma R(\mathbf{x}, \mathbf{x}')\sigma(\mathbf{x}')da(\mathbf{x}') = f(\mathbf{x}).$$



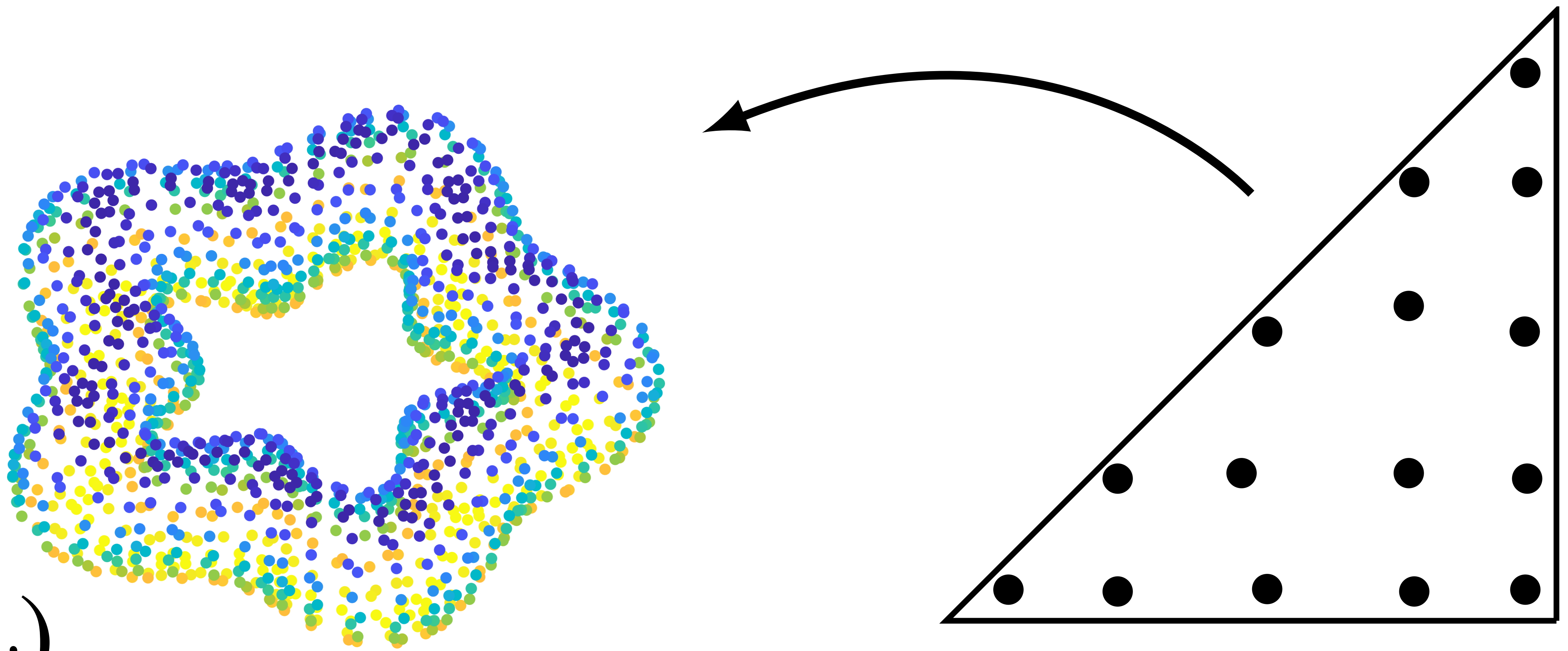
$R(\mathbf{x}, \cdot\,)$



u

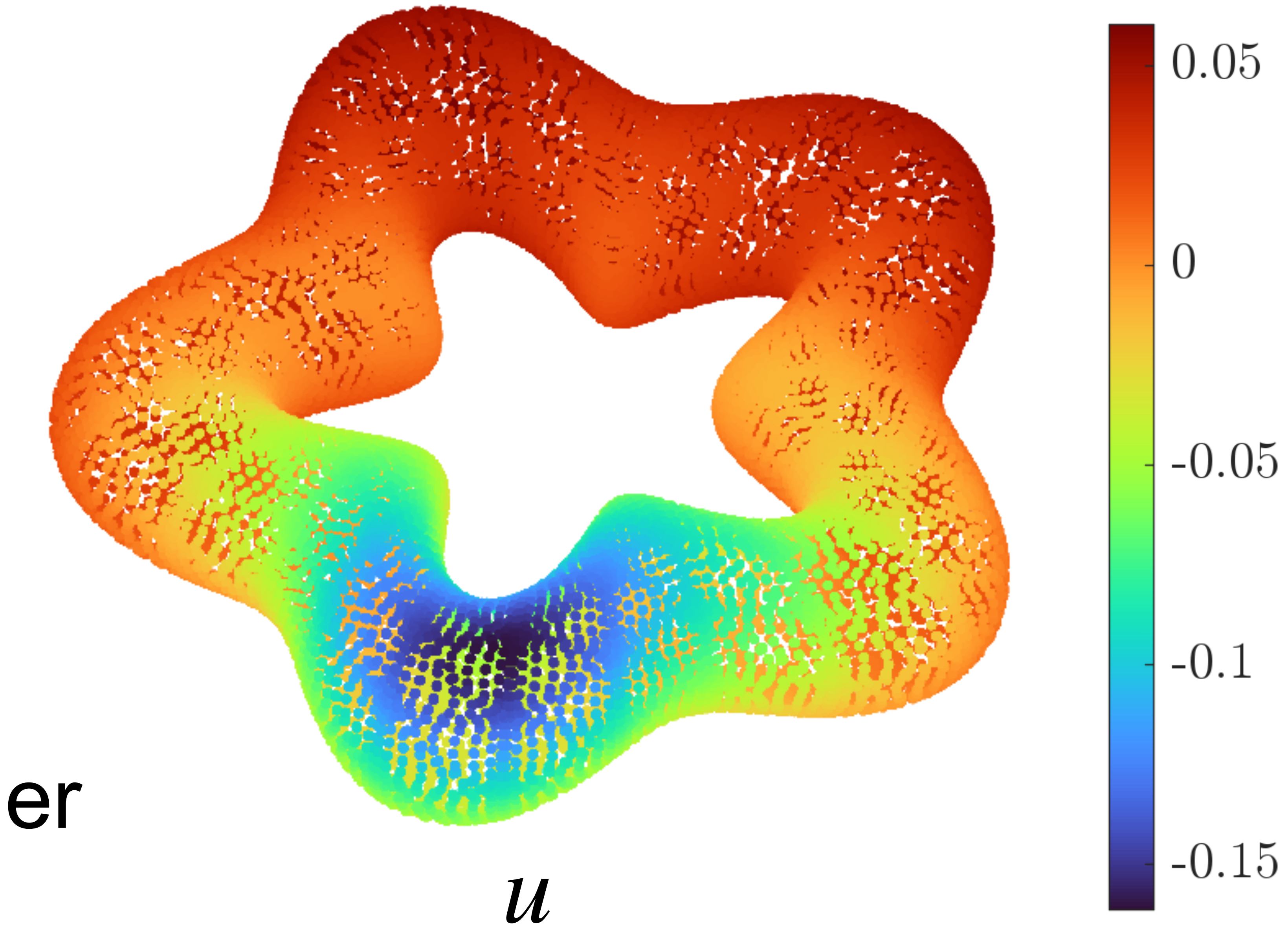
Discretized system

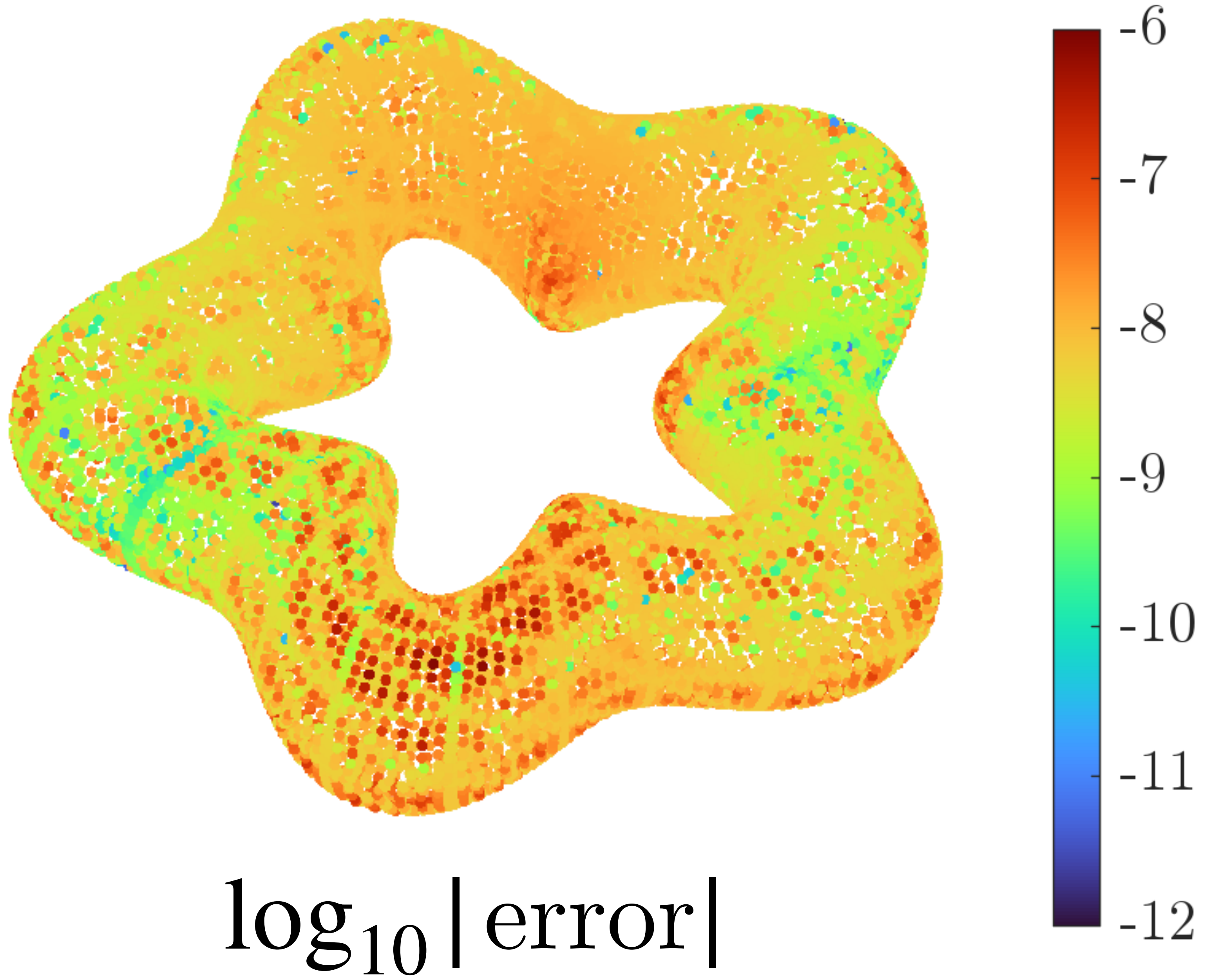
Discretize the integrals and enforce at nodes



$$\sigma_i + \sum_{j=1}^{N} R(\mathbf{x}_i, \mathbf{x}_j)\ \sigma_j \sqrt{(\det g)(\mathbf{x}_j)}\ w_{i,j} = f(\mathbf{x}_i)$$

Use recursive skeletonization to build an $O(N)$ direct solver.

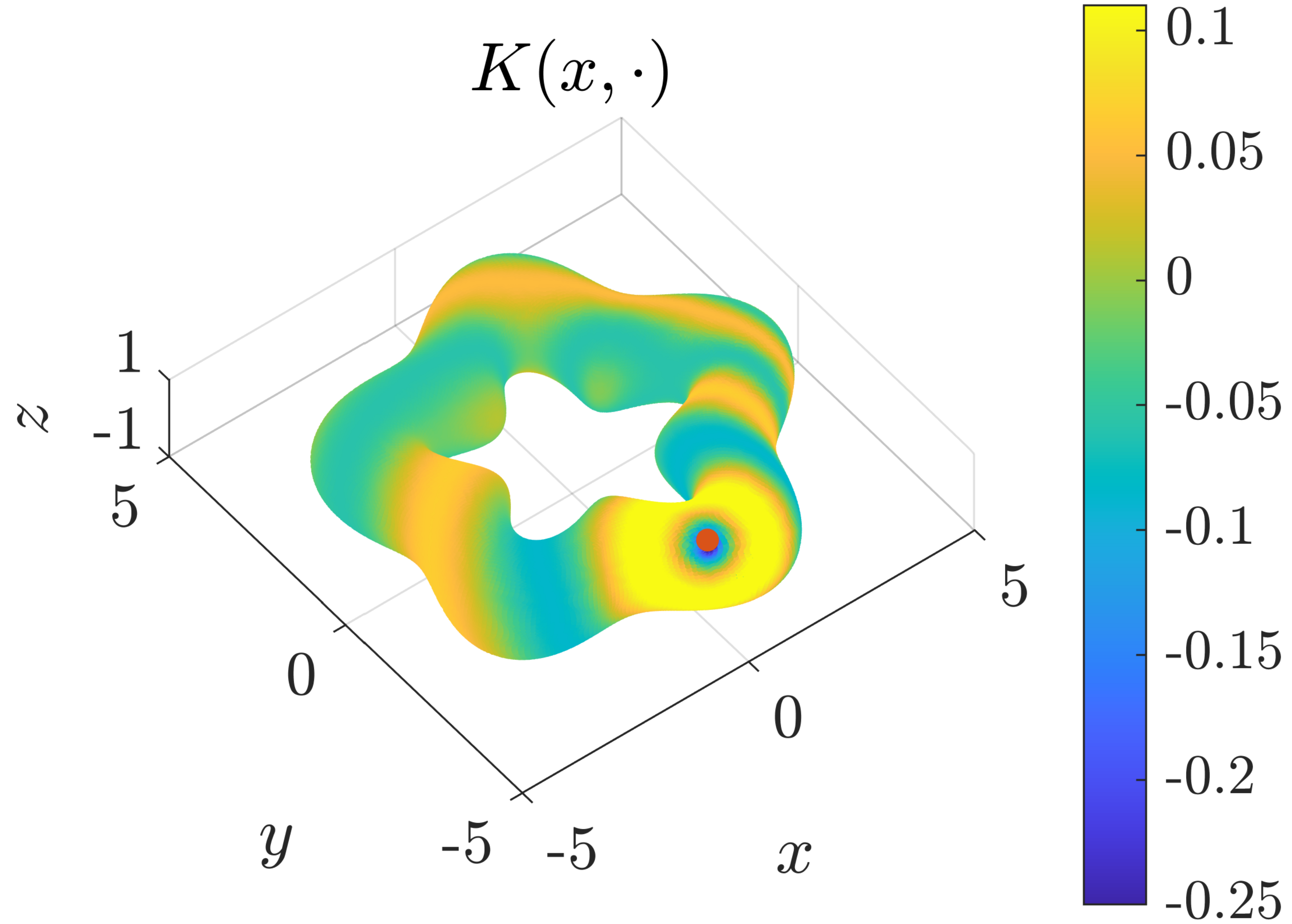


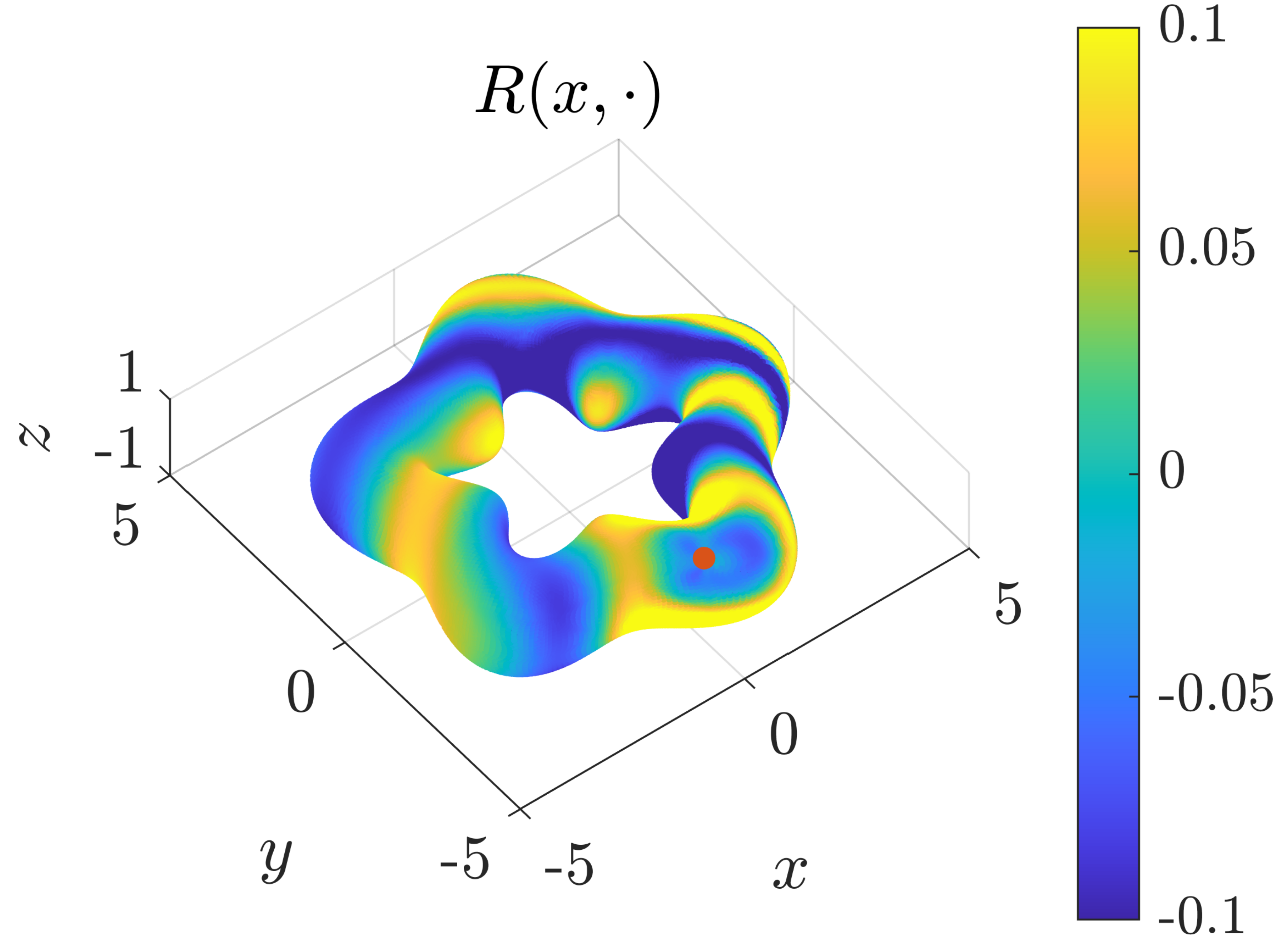


384 8th order patches

Other elliptic equations

General form $\nabla_\Gamma \cdot a(\mathbf{x})\,\nabla_\Gamma u + \mathbf{b}(\mathbf{x}) \cdot \nabla_\Gamma u + c(\mathbf{x})u = f$

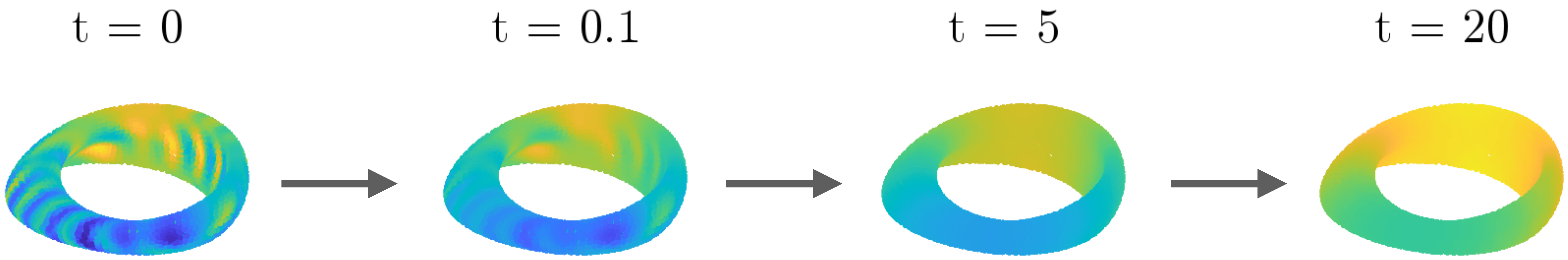




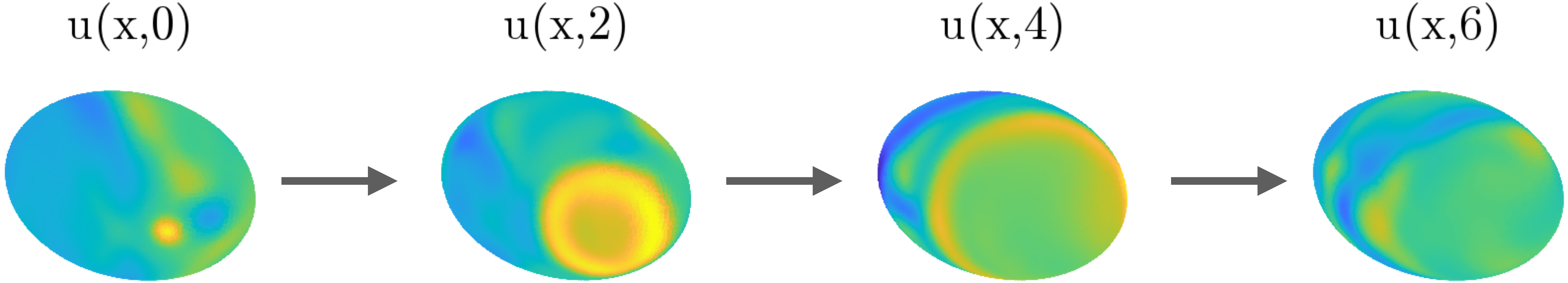
$$K(\mathbf{x},\mathbf{x}') = \frac{i}{4a(\mathbf{x}')} H_0^{(1)}\left(\sqrt{\frac{c(\mathbf{x}')}{a(\mathbf{x}')}}\,\|\,\mathbf{x}-\mathbf{x}'\,\|\right)$$

Time dependent problems

Solve $\partial_t u = \Delta_\Gamma u$ with Crank-Nicolson



Solve $\partial_t^2 u + \gamma \partial_t u = \Delta_\Gamma u + f(\mathbf{x}) g(t)$ in frequency space



ICERM Introduction

Sijing Liu

ICERM

Brown University

January 31, 2024

Background

- Louisiana State University, PhD, 2020.
- University of Connecticut, Assistant Research Professor, 2020-2023.
- ICERM, Institute Postdoc, 2023-2024.
  - Numerical PDEs: Analysis, Algorithms, and Data Challenges, Spring 2024.
- Research Interests:
  - (Stabilized) Finite Element Methods, Discontinuous Galerkin Methods.
  - Multigrid Methods.
  - PDE-constrained Optimizations, Optimal Control Problems.
  - Fluid-structure Interaction.

Elliptic Optimal Control Problems

We consider a region $\Omega \subset \mathbb{R}^2$ or $\mathbb{R}^3$ to be heated or cooled.

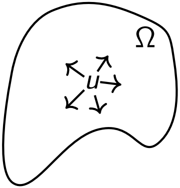


Figure: Distributed Control

The linear-quadratic elliptic optimal control problem is to find

$$\min_{(y,u)} \left[\frac{1}{2} \|y - y_d\|^2_{L^2(\Omega)} + \frac{\beta}{2} \|u\|^2_{L^2(\Omega)} \right],$$

subject to

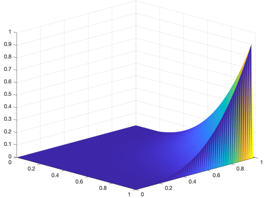
$$\begin{aligned} -\Delta y &= u \quad \text{in} \quad \Omega, \\ y &= 0 \quad \text{on} \quad \partial\Omega. \end{aligned}$$

Convection-dominated Problems

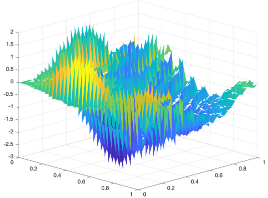
We consider

$$-\varepsilon \Delta u + \zeta \cdot \nabla u + \gamma u = f \quad in \quad \Omega,$$
$$u = g \quad on \quad \partial\Omega,$$

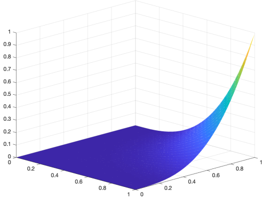
where $\varepsilon \ll \|\zeta\|_\infty$.



Exact Solution



No Stabilization



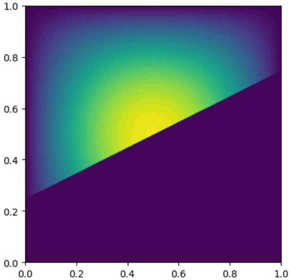
Upwind DG

Stabilization methods:

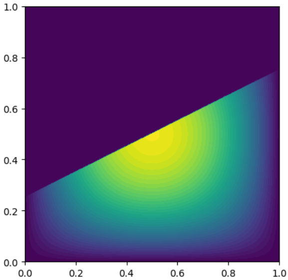
- SUPG, Local Projection, EAFE, DG, DWDG, etc.

Fluid-Structure Interaction

Fluid-Structure Interaction (FSI) is the multiphysics interaction of a fluid flow with a solid structure.



"Solid Problem"



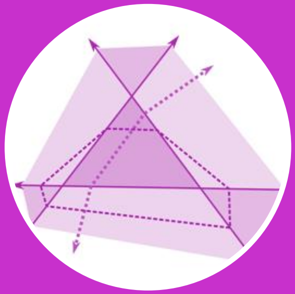
"Fluid Problem"

Marissa Masden

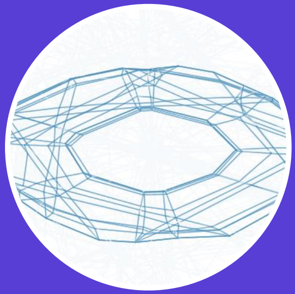
- B.S. Math and Chemistry 2015
  Walla Walla University
- High school math teacher
- Ph.D. Mathematics, 2023
  University of Oregon
- Postdoctoral Fellow, 2023-2024
  ICERM

https://mmasden.github.io

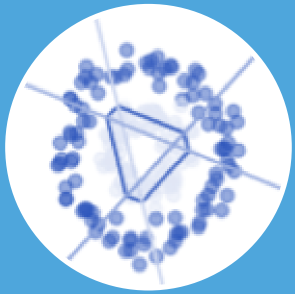
Research Interests



(Combinatorial, algebraic) approaches to topology of neural network functions

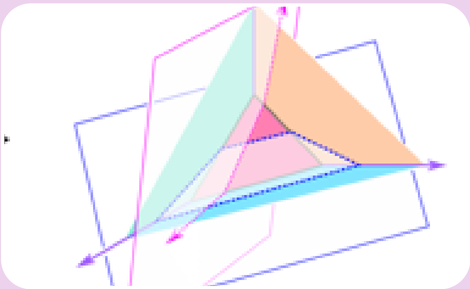


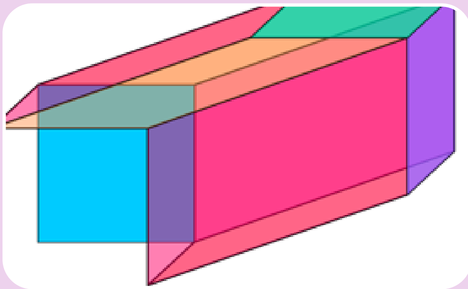
Relationships between shape of training data and shape of neural networks

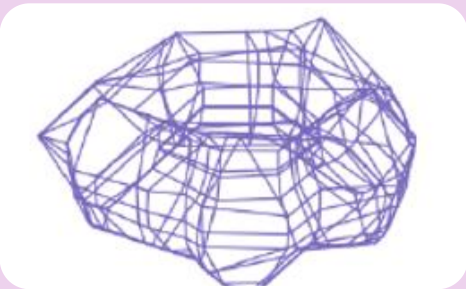


Geometry and topology in scientific data, machine learning

Obtaining topological properties of the true decision boundary of a neural network





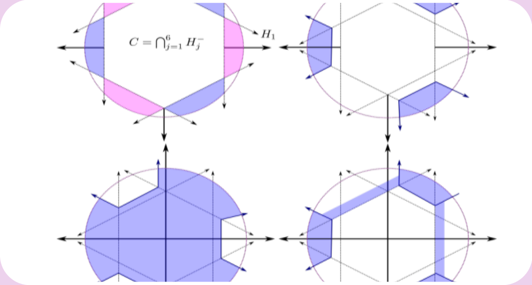


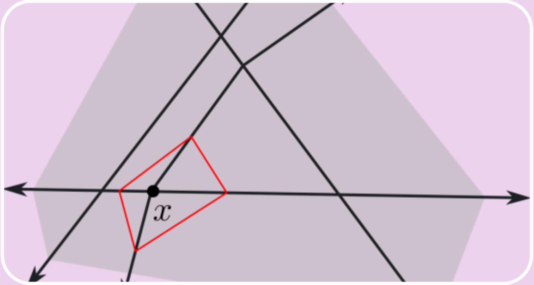
Establish conditions when face poset is determined by combinatorial information. (Differential Topology)

Understand algebraic properties and establish its duality to a cubical complex. (Oriented Matroid Theory)

Tracking Betti numbers of ReLU networks during training. (Algebraic Topology)

Obtaining topological properties of the true decision boundary of a neural network





Extend PL Morse theory concepts to non-compact, non-general position ReLU functions (With Grigsby, Lindesy)

Current: Using face poset knowledge to develop algorithms for PL and Discrete Morse theory on ReLU networks (With R. Brooks)

Local and global topological complexity measures of ReLU neural network functions: E.Grigsby, K. Lindsey & M. Masden (2022)

Other Projects (Near Future):

- Probability distributions of geometric properties (e.g. discrete curvature of substructures) under random initialization assumptions
- Developing theory describing combinatorial changes on paths in parameter space.
- Expanding tools about ReLU networks to other architectures (non-fully-connected, convolutional)
- Using tools from this work to computationally analyze dynamical systems

Thank you!

Personal Introduction

ICERM Semester Program “Numerical PDEs: Analysis, Algorithms, and Data Challenges”

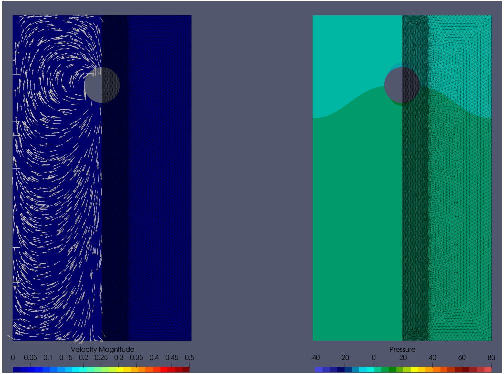
Henry von Wahl

Institute for Mathematics, Friedrich-Schiller-University Jena, Ernst-Abbe-Platz 2, Jena, Germany

30th January 2024

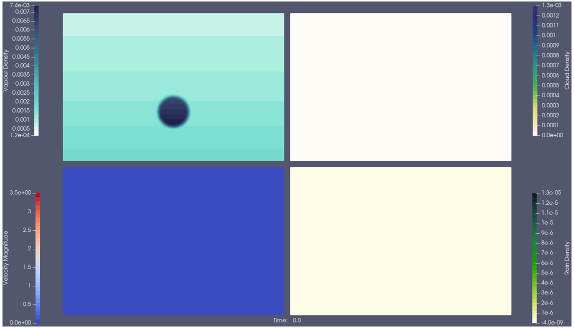
Unfitted Finite Element Methods

- Unfitted Finite Elements
  - Geometry representation implicit through level sets.
  - Stability through ghost-penalties.
  - Error estimates including higher-order geometry approximation.
- Moving domain problems.
  - Time-stepping with fixed background mesh.
  - Application: Fluid-structure interaction.
    - Artificial neural network to predict forces governing rigid-body motion.
- Structure preserving discretisations $\longrightarrow H(div)$-conforming.
- Trefftz methods $\longrightarrow$ Reduced basis to gain efficiency.
- `ngsxfem`: Add-on package to `NGSolve` for unfitted FEM.



Video: Unfitted FEM simulation of an experiment with a ball falling in a fluid.

- Discontinuous Galerkin for moist air
  - Hyperbolic balance law with multiple densities.
  - Mass exchange between densities contain algebraic constraints.
  - Highly-parallelisable scheme to use HPC.
- Crack-propagation
  - Phase-field approach to simulate pressurised crack.
  - Geometry reconstruction to couple with FSI with ALE discretisation.



Video: Stabilised DG discretisation for a rising thermal in an under-saturated atmosphere leading to rain.

Christopher Wang

- My name is Christopher Wang (I go by Chris)
- 2nd year PhD
- Cornell University
- Adviser: Alex Townsend

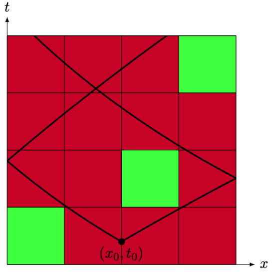
Research Interests: Operator Learning

- data-driven algorithms for learning solution operators of PDEs

$$\{(u_j, f_j)\}_{j=1}^{N}, \qquad \mathcal{L}u_j = f_j$$

$$u_j(x) = \int_\Omega K(x,y) f_j(y) \mathrm{d}y$$

- learning characteristics of hyperbolic PDEs



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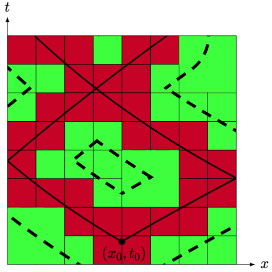

(b)

Research Interests: Complexity & RandNLA

- operator learning for nonlinear PDEs
- curvature flows
- Solvability Complexity Index (SCI) hierarchy
  - classify complexity of computational problems, like computing the spectrum of a differential operator
- randomized numerical linear algebra (RandNLA), e.g., rSVD

Other Interests

- hiking, skiing, rock climbing, swimming
- singing, piano

Introduction

Yukun Yue

University of Wisconsin-Madison

January 29, 2024

Introduction

- I received my Ph.D. in Mathematics from Carnegie Mellon University in 2023, under the guidance of Prof. Franziska Weber and Prof. Noel Walkington.
- Following my graduation, I joined the University of Wisconsin-Madison as a Van Vleck Visiting Assistant Professor in Fall 2023, collaborating with Prof. Qin Li.

Research Interest

Classical Numerical Analysis

- Studying convergence and stability analysis of different numerical schemes.
- Constructing more efficient numerical schemes to solve PDE-related problems.
- Both computational and theoretical performance are emphasized.

PDE-Constrained Optimization

- Focus on finding optimal control in a PDE system.
- Applying data-related method to solve inverse problem

Current Research Problems

Gradient-Flow Related Physics Problems

- Liquid crystals
- Phase-field problems.
- Application of Invariant Energy Quadratization (IEQ), Scalar Auxiliary Variable (SAV) and Convex-Splitting method

Analysis of HDG Method

- Application onto various problems
- Focus on stability analysis.

Plasma-Related Problems

- Control of plasma instability based on Vlasov equation.
- Simulation of plasma behavior.