Anthony Gruber

Florida State University

Geometric Computing for Modeling and Approximation

Introduction

- Ph.D. Texas Tech University (2015-2019).
  - Advisors: Magdalena Toda, Hung Tran, Eugenio Aulisa.
  - Thesis: "Curvature Functionals and p-Willmore energy."
  - NSF Fellow at Oak Ridge National Lab (2018) in ML/DS.
- NTT Asst. Prof. at TTU satellite in San Jose, Costa Rica (2019-2020).
  - Served as Mathematics Program Director.
- Postdoc at Florida State University (2021-present).
  - Data-driven sci. comp. and reduced-order modeling.
  - Advisor: Max Gunzburger.

https://www.depts.ttu.edu/costarica/Jobs@TTUCR/index.php

https://www.lib.fsu.edu/dirac

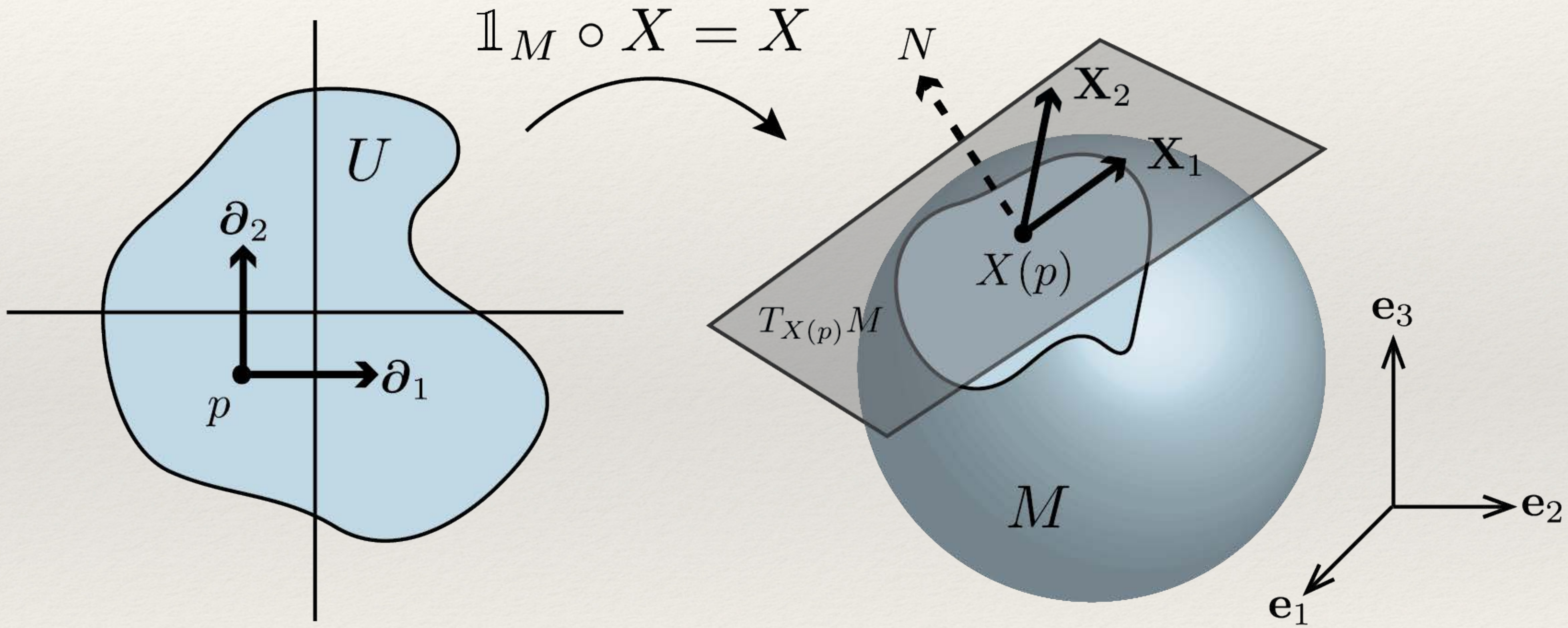
Overview

- *Where does modern scientific computing benefit from geometry-informed algorithms?*
- Examples:
  - High-dimensional function approximation.
    - Joint: M. Gunzburger, L. Ju, Z. Wang, Y. Teng, R. Bridges, M. Verma, C. Felder, G. Zhang.
  - Meshing for dynamical systems on general domains.
    - Joint: E. Aulisa.
  - **Funding:** NSF MSGI; NSF DMS 1912902, 1912705; DE SC0020418, SC0022254, SC0020270.

- Journal articles
  - A. Gruber. ``Planar Immersions with Prescribed Curl and Jacobian Determinant are Unique'', *Bull. Aust. Math. Soc.*, 1-6 (2021).
  - **A. Gruber, M. Gunzburger, L. Ju, Y. Teng, Z. Wang. ``Nonlinear Level Set Learning for Function Approximation on Sparse Data with Applications to Parametric Differential Equations'', *Numer. Math. Theor. Meth. Appl.*, (2021).**
  - A. Gruber, A. Pámpano, M. Toda. ``Regarding the Euler-Plateau Problem with Elastic Modulus'', *Ann. Mat. Pura Appl.*, (2021).
  - **A. Gruber, E. Aulisa. ``Computational p-Willmore Flow with Conformal Penalty'', *ACM Trans. Graph.* 39, 5, Article 161 (September 2020), 16 pages.**
  - A. Gruber, M. Toda, H. Tran. ``On the variation of curvature functionals in a space form with application to a generalized Willmore energy'', *Ann. Glob. Anal. Geom.* 56, 147–165 (2019).
- Conference papers
  - A. Gruber, E. Aulisa. ``Quaternionic remeshing during surface evolution'', *Proceedings of the 18th ICNAAM*, Rhodes, Greece, 2020, (in press).
  - A. Gruber, M. Toda, H. Tran. ``Willmore-stable minimal surfaces'', *Proceedings of the 18th ICNAAM*, Rhodes, Greece, 2020, (in press).
  - E. Aulisa, A. Gruber, M. Toda, H. Tran. ``New Developments on the p-Willmore Energy of Surfaces'', *Proceedings of 21st ICGIQ*, Sofia: Avangard Prima, 2020.
  - **R. Bridges, A. Gruber, C. Felder, M. Verma, C. Hoff. ``Active Manifolds: Reducing high dimensional functions to 1-D; A non-linear analogue to Active Subspaces''. *Proceedings of ICML*, 9-15 June 2019, Long Beach, California, USA. PMLR 97:764-772.**
- Submitted articles
  - Y. Teng, Z. Wang, L. Ju, A. Gruber, G. Zhang. "Learning Level Sets with Pseudo-Reversible Neural Networks for Dimension Reduction in Function Approximation." (under review).
  - **A. Gruber, M. Gunzburger, L. Ju, Z. Wang. ``A Comparison of Neural Network Architectures for Data-Driven Reduced-Order Modeling", (under review).**
  - **A. Gruber, E. Aulisa. ``Quasiconformal Mappings for Surface Mesh Optimization'', (under review).**
  - A. Gruber, A. Pámpano, M. Toda. ``On p-Willmore Disks with Boundary Energies'', (under review).
  - A. Gruber. ``Parallel Codazzi Tensors with Submanifold Applications'', (under review).
  - A. Gruber, M. Toda, H. Tran. ``Stationary Surfaces with Boundaries'', (under review).

What is a Riemannian geometry?

- "Smooth" manifold M equipped with "smooth" metric g.
- Metric g determines intrinsic behavior.
    - Laplacian, conformal structure
- Change in normal N determines extrinsic behavior.
    - Shape operator, mean curvature



Approximation of Functions

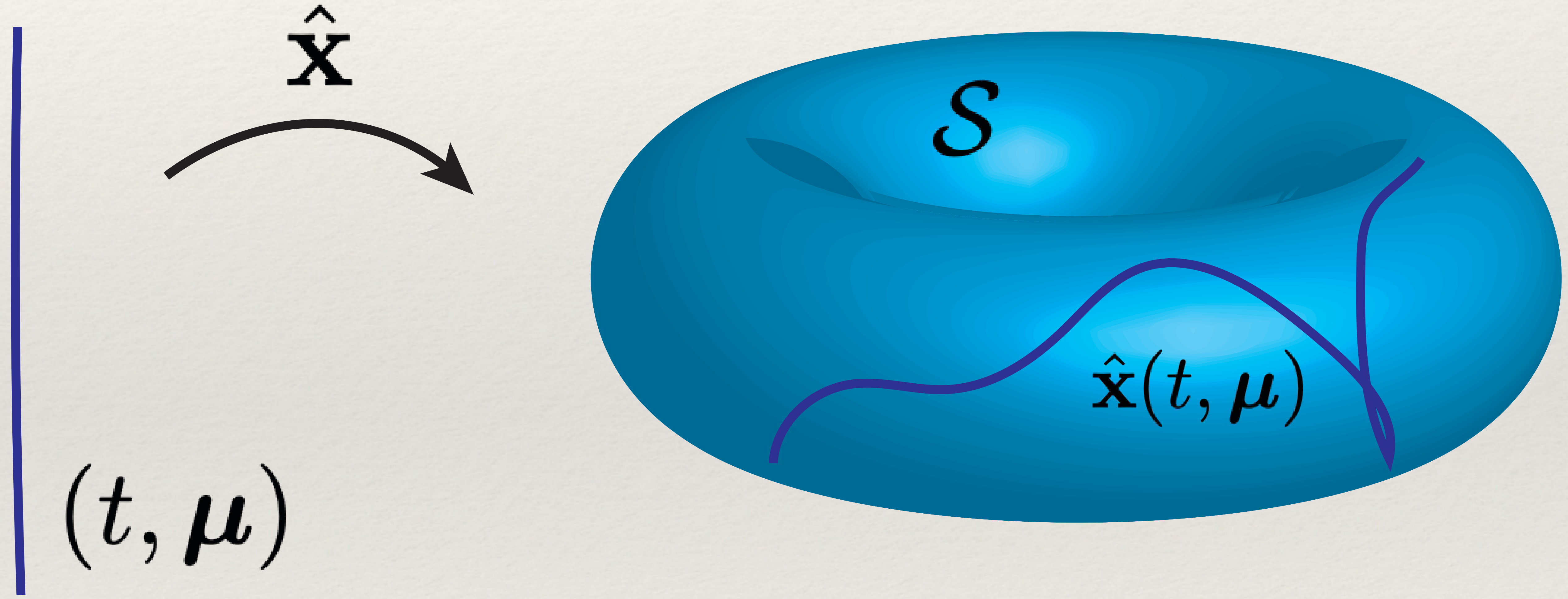
- Where does geometry meet sci. comp.?
- Real problems need measurements which are expensive (~10^{6+} DOFs).
  - DFT observables.
  - Disease metrics.
  - FEM/FVM consequences.
- Approximation benefits from *dimension reduction*.

Potential Copyright Issue

Image: https://mpas-dev.github.io/ocean/ocean.html

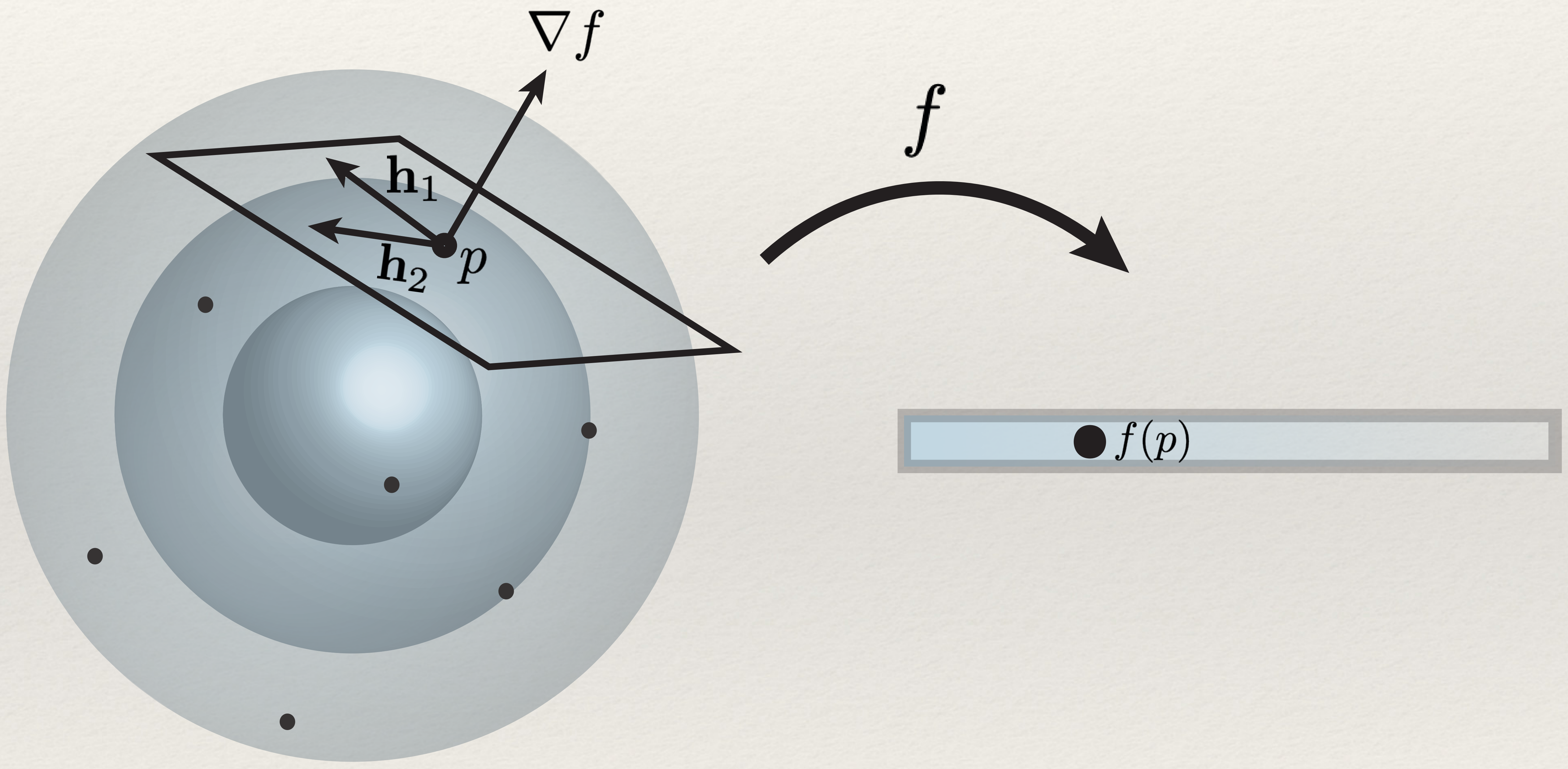
Two Broad Approaches

- **Intrinsic:** Data is *intrinsically* low-dimensional.
  - DR should exploit intrinsic features.
- Clustering, reduced basis, etc.
- DR according to local/global data properties.



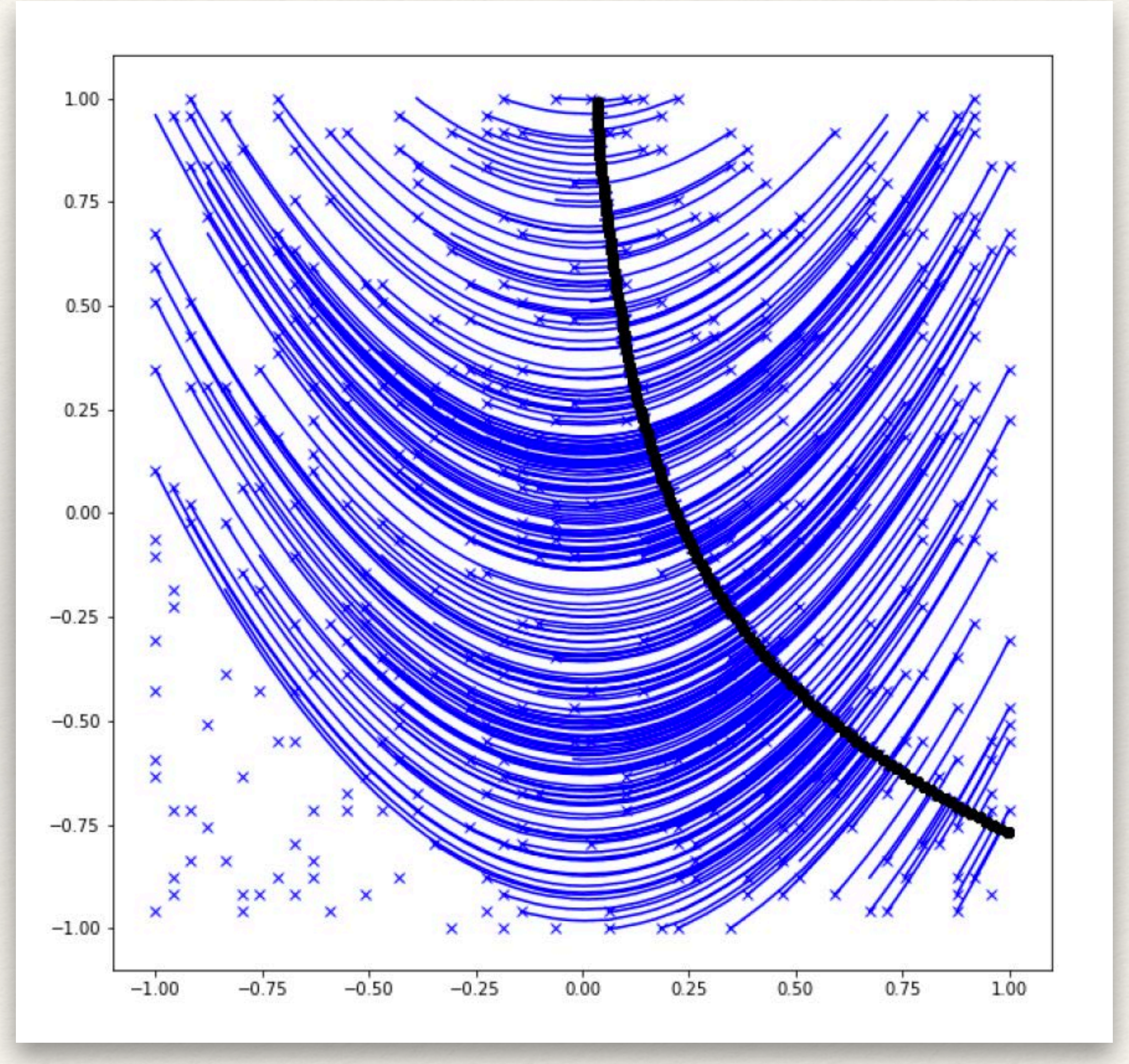
Two Broad Approaches

- **Extrinsic:** Low-dim structure is *induced* by external mapping.
  - Structure on data imposed by objective.
- Ridge regression
- Active subspaces/manifolds
- Nonlinear level set learning



Active Manifolds

- Solve $\dot{\mathbf{x}} = \dfrac{\nabla f(\mathbf{x})}{|\nabla f(\mathbf{x})|}$ for known $\mathbf{x}(0) = \mathbf{x}_0$.
- Map $t \mapsto f(\mathbf{x}(t))$ characterizes f on $\{f^{-1}\left(f(\mathbf{x}(t))\right)\}_{t \in T}$.
- If $\mathbf{y} \notin \{\mathbf{x}(t)\}$, $f(\mathbf{y}) = f(P(\mathbf{y})) = f(\mathbf{x}(t))$.
  - Projection $P(\mathbf{y})$ constructed by "walking level sets".
- AM works well:
  - in low dimensions; when data is available.
  - Drawback is online cost: ODE for each evaluation.



R. Bridges, A. Gruber, C. Felder, M. Verma, C. Hoff, ICML 2019

Nonlinear Level set Learning

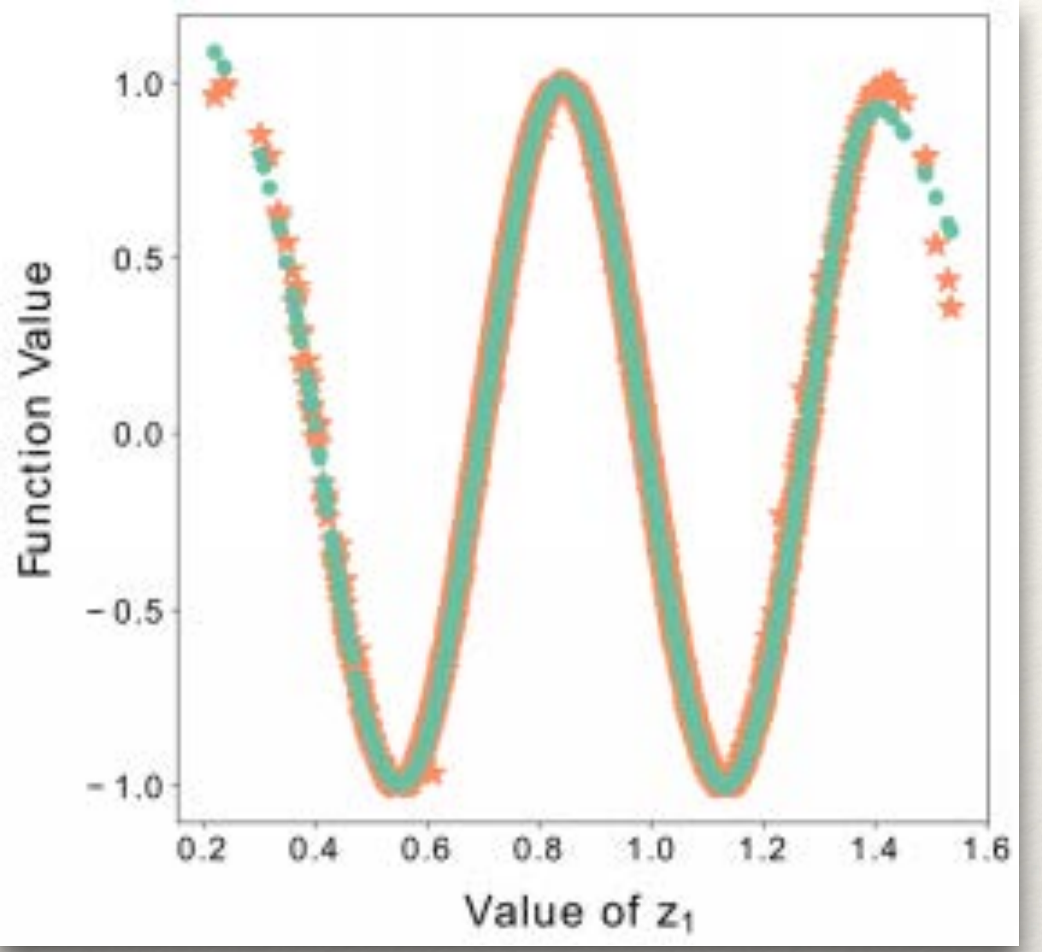
- ANN-based method for EDR.
    - Introduced (NIPS 2019) by G. Zhang, J. Zhang, J. Hinkle.
    - Improved (NMTMA 2021) by our group.
- Seek invertible transformation (RevNet) $\mathbf{z} = \mathbf{g}(\mathbf{x}),\ \mathbf{h} \circ \mathbf{g} = \mathbf{I}$.
    - Splits domain of $f \circ \mathbf{h}$ into $\mathbf{z} = (\mathbf{z}_A, \mathbf{z}_I)$.
- $\mathbf{z}$-domain truncated by $\mathbf{z}_A$.
- Ridge regression $\hat{f}(\mathbf{z}_A) \approx f(\mathbf{x})$.

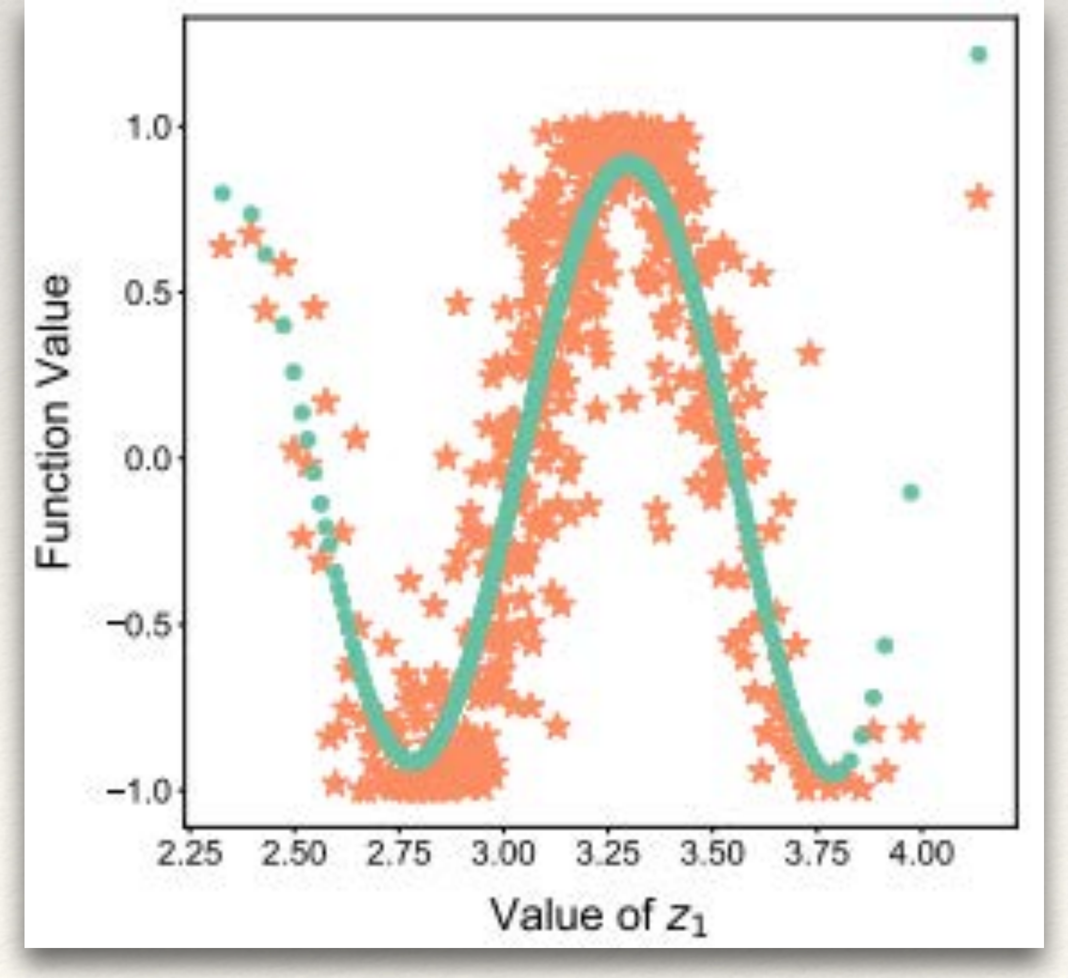
$$
\begin{tikzcd}
& X \arrow[rr, shift right, "\mathbf{g}(x)"'] \arrow[dl, "f(x)"] & & Z \arrow[ll, shift right, "\mathbf{h}(z)"'] \arrow[r, "\pi_1"] \arrow[dl, "f \circ \mathbf{h}(z)"] & Z_{red} \arrow[dllll, bend left, "\hat{f}(z_1)"] \\
{} & & {} & &
\end{tikzcd}
$$

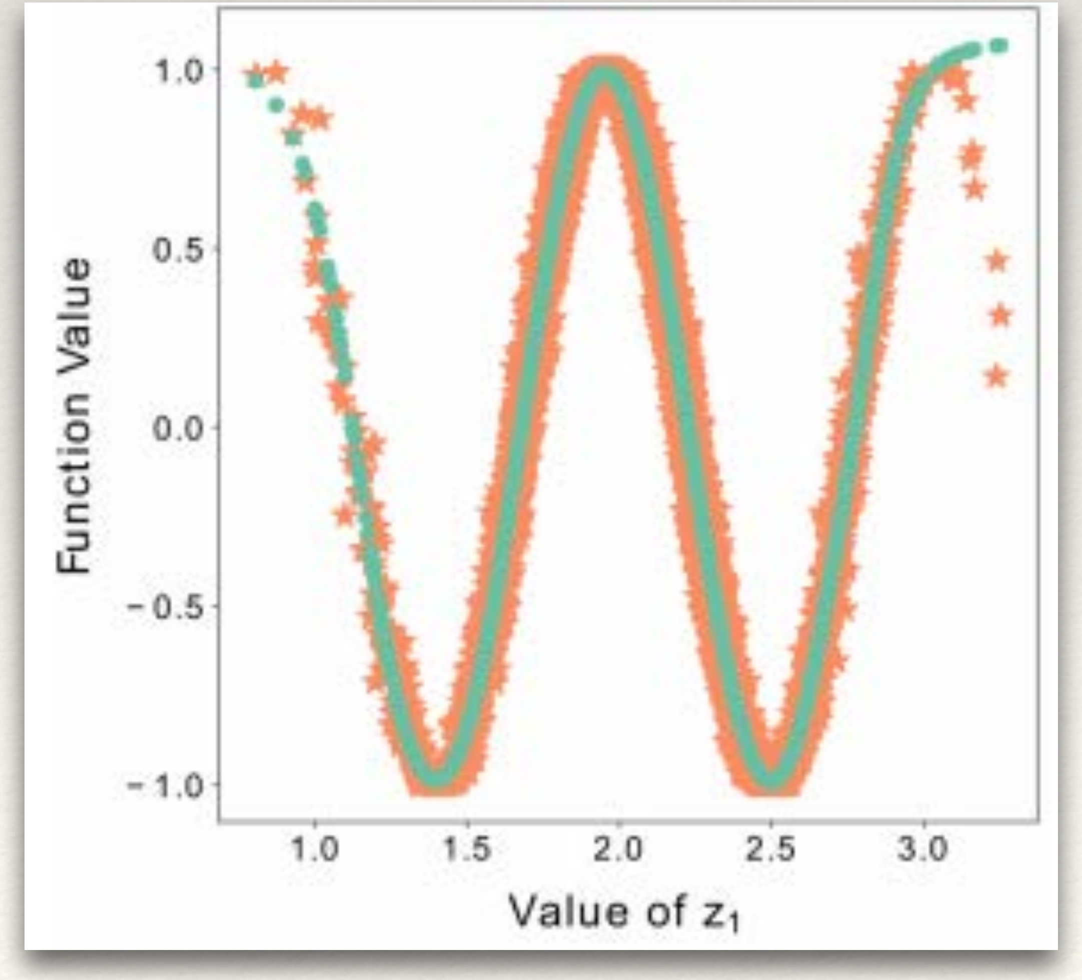
$$\int_U |(f \circ \mathbf{h})'|_{\perp}^2 \, d\mu^n = \sum_{i \in I} \int_U \left(\nabla f(\mathbf{x}) \cdot \mathbf{h}_i(\mathbf{z}) \right)^2 d\mu^n$$

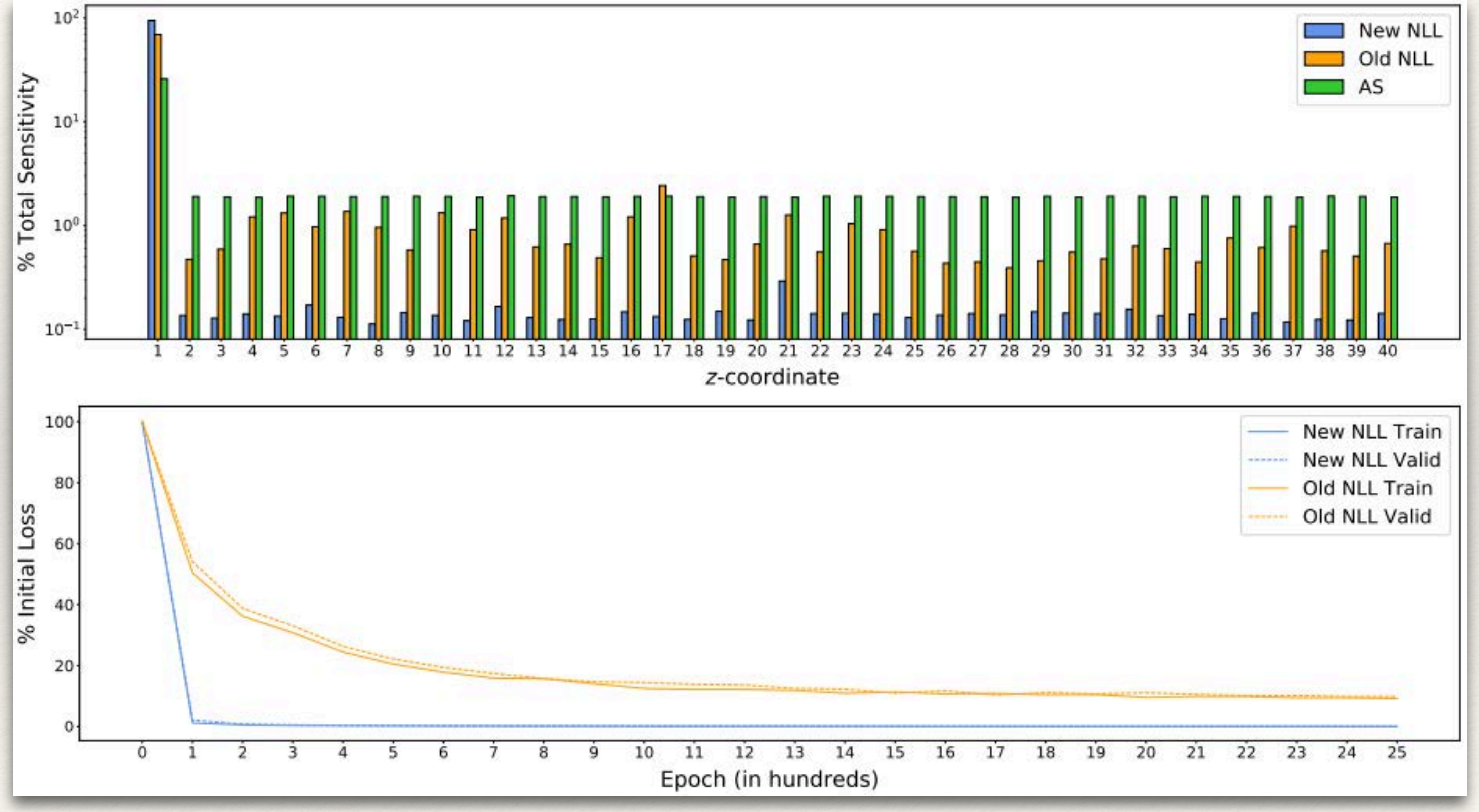
Results on Toy Examples

- On 40-dim $\sin\left(|\mathbf{x}|^2\right)$
- Only 100 data





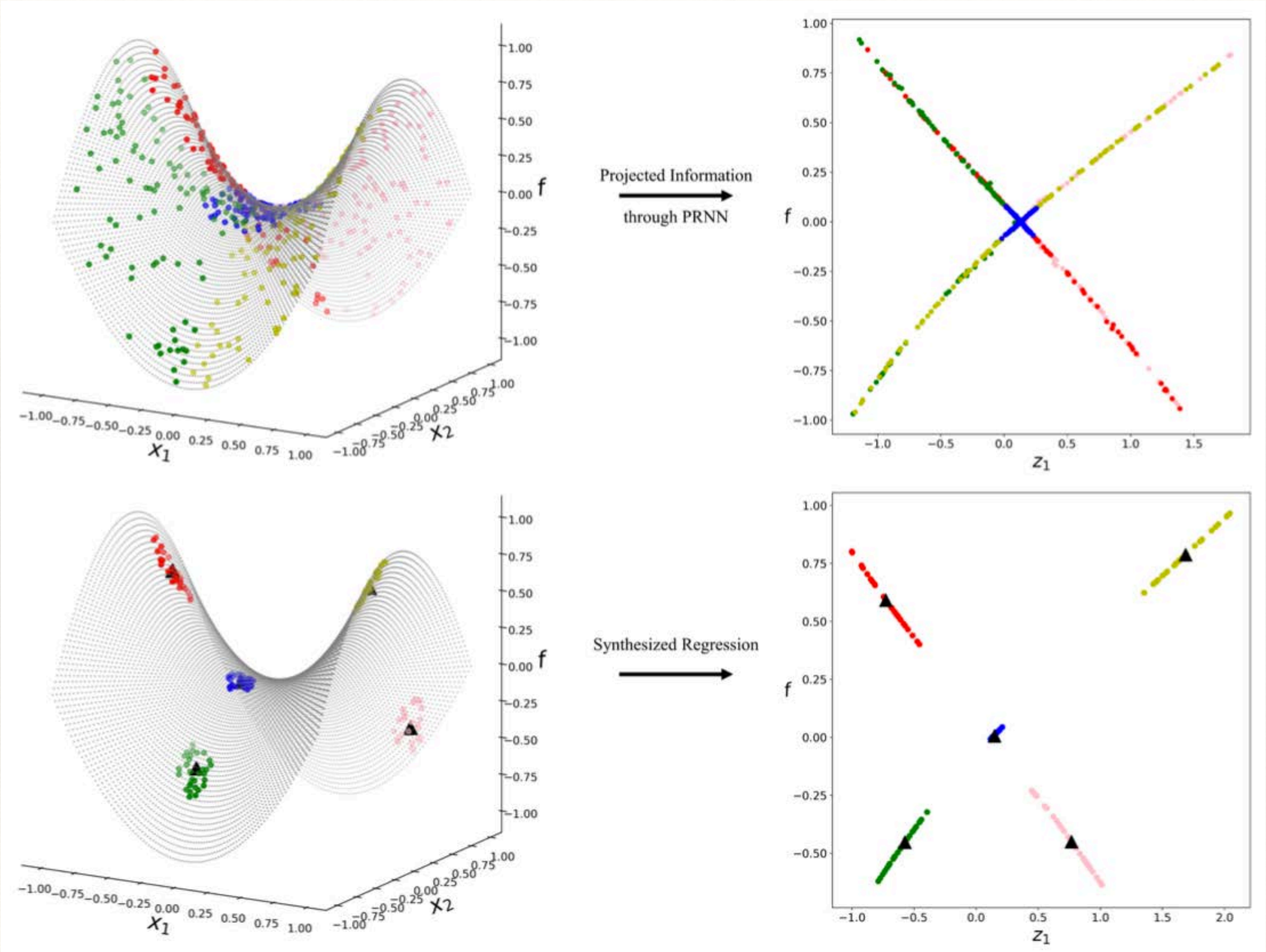




A. Gruber, M. Gunzburger, L. Ju, Y. Teng, Z. Wang.
Numer. Math. Theor. Meth. Appl. (2021)

NLL with Pseudo-Reversible NNs

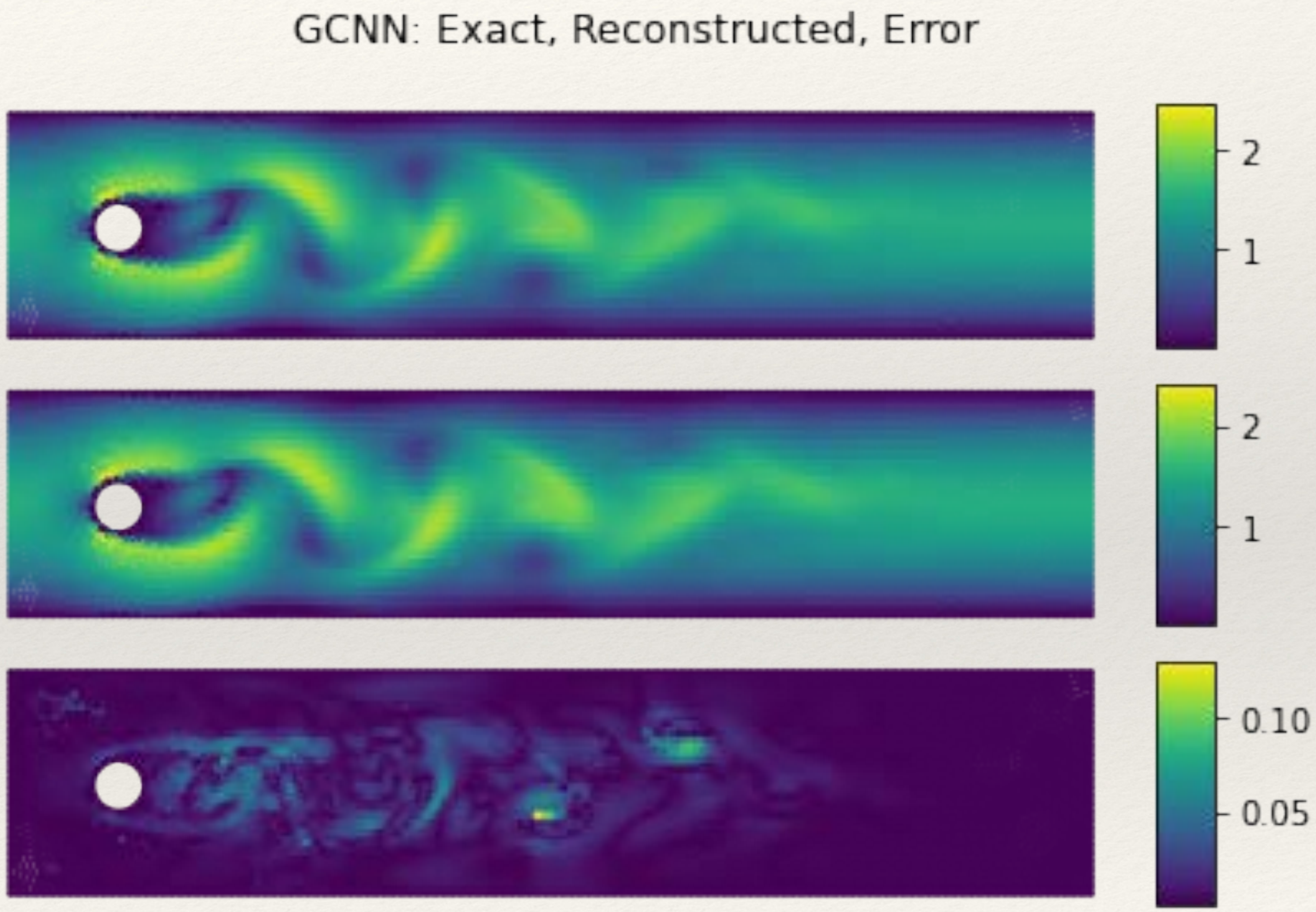
- Reversibility of RevNet can create issues.
  - What if level sets are closed?
- Can consider pseudo-reversible network.
- Local regression based on neighbors in input space.
- Fixes some issues with NLL.
  - **BUT:** Needs more data.



Y. Teng, Z. Wang, L. Ju, A. Gruber, G. Zhang (under review)

Intrinsic DR: Reduced-order Modeling

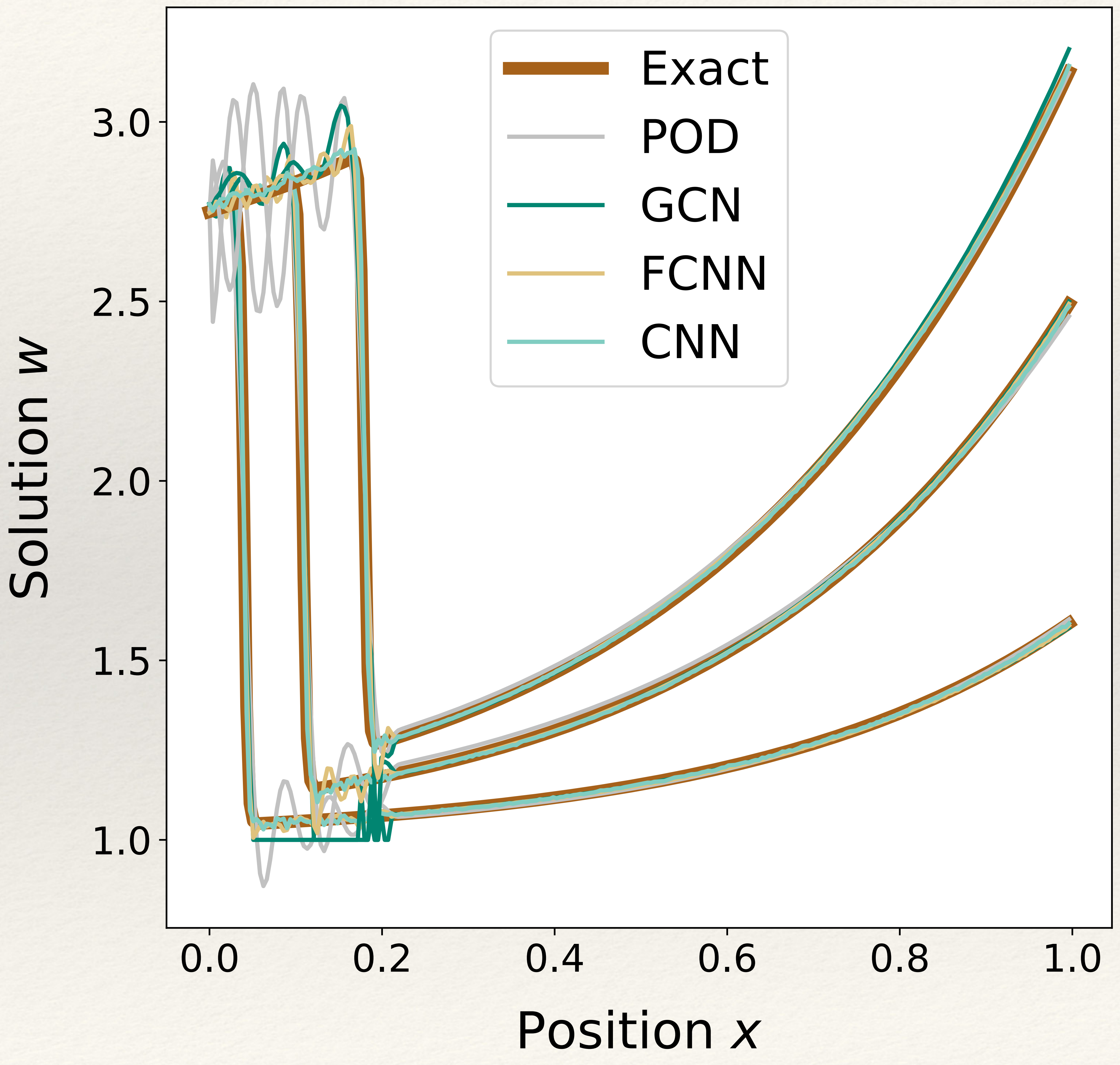
- Semi-discretization $u(x, t) =: \mathbf{u}(\mathbf{x}, t)$
  - Creates *a lot* of dimensionality.
- Can we approximate the solution without solving the full PDE?
- Standard is to **encode -> solve -> decode.**
  - PDE solving is low-dimensional.



A. Gruber, M. Gunzburger, L. Ju, Z. Wang, *CMAME* (pending revision)

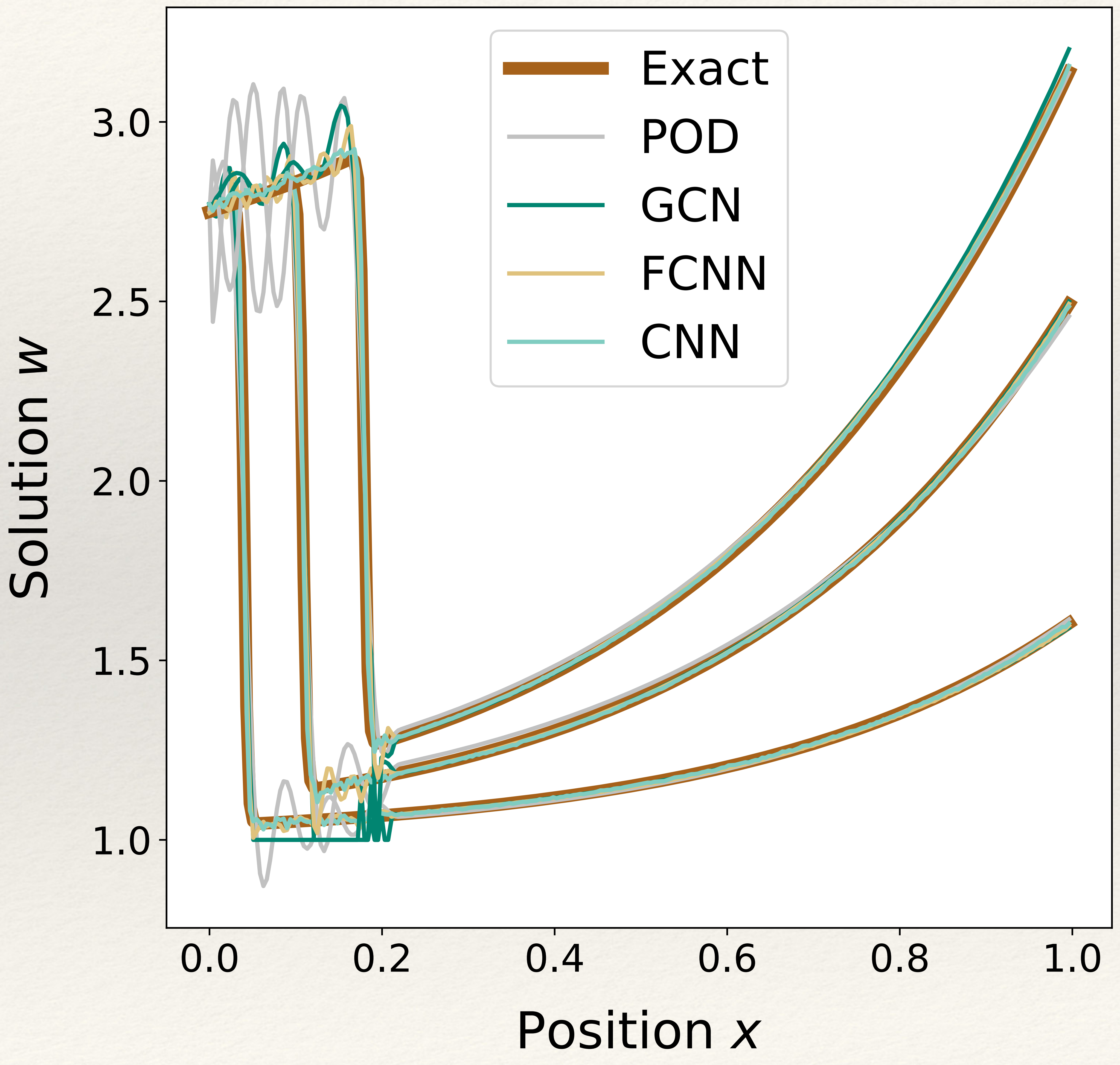
Common ROM Methods

- Most popular (until recently): proper orthogonal decomposition (POD).
- PCA on solution *snapshots* $\{\mathbf{u}(\mathbf{x}, t_j)\}_{j=1}^{N}$, generate $\mathbf{S}$.
- SVD: $\mathbf{S} = \mathbf{U}\boldsymbol{\Sigma}\mathbf{V}^\top$.
  - First n cols $\mathbf{U}_n$: reduced basis.
- $\mathbf{U}_n\dot{\hat{\mathbf{u}}} = \mathbf{f}(t, \mathbf{U}_n\hat{\mathbf{u}})$ replaces $\dot{\mathbf{u}} = \mathbf{f}(t, \mathbf{u})$.



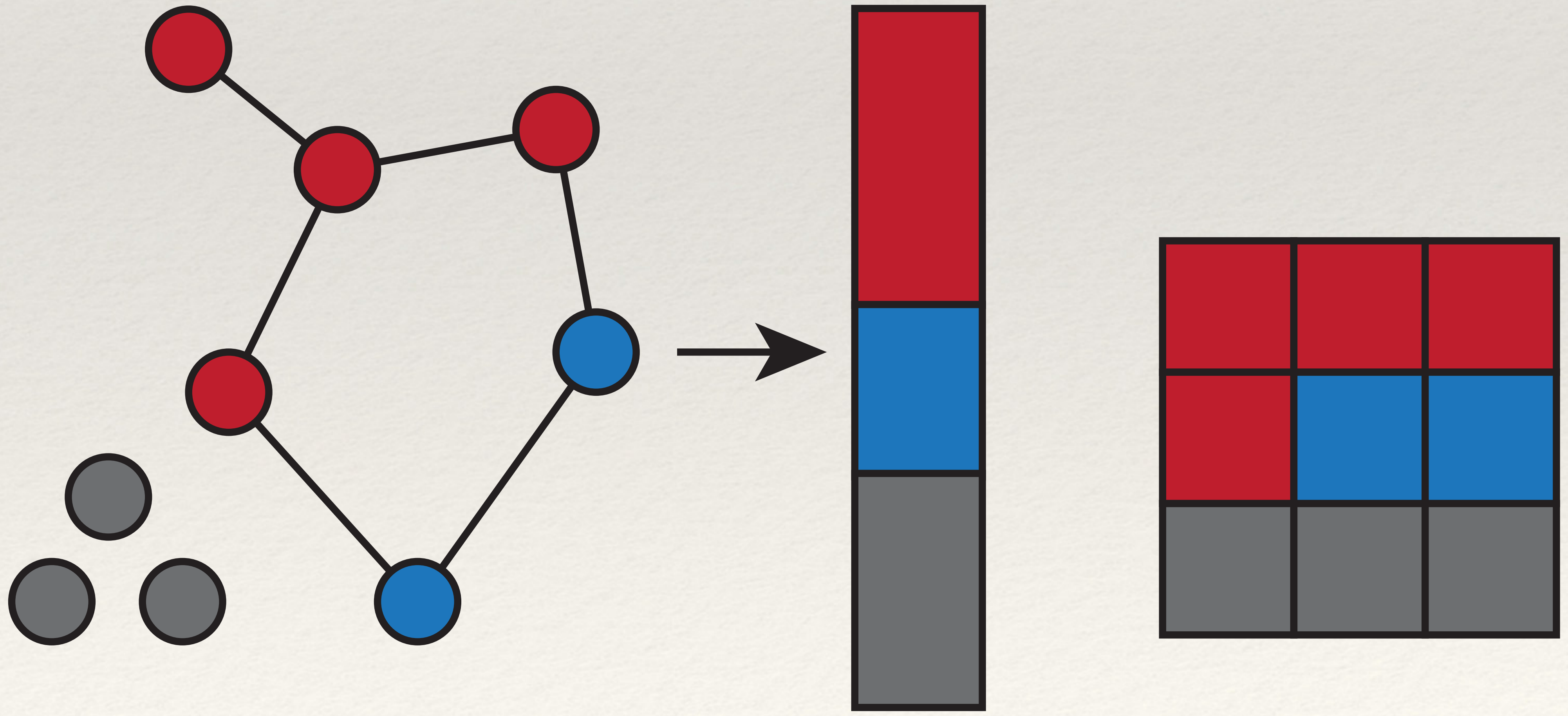
Common ROM Methods

- Next most popular: Convolutional neural network (CNN) autoencoder.
- Improved performance over POD**.
  - ** (In some cases)
- **BUT** slower and more difficult to train.
  - Also more memory consumptive!
- Now often used "by default".



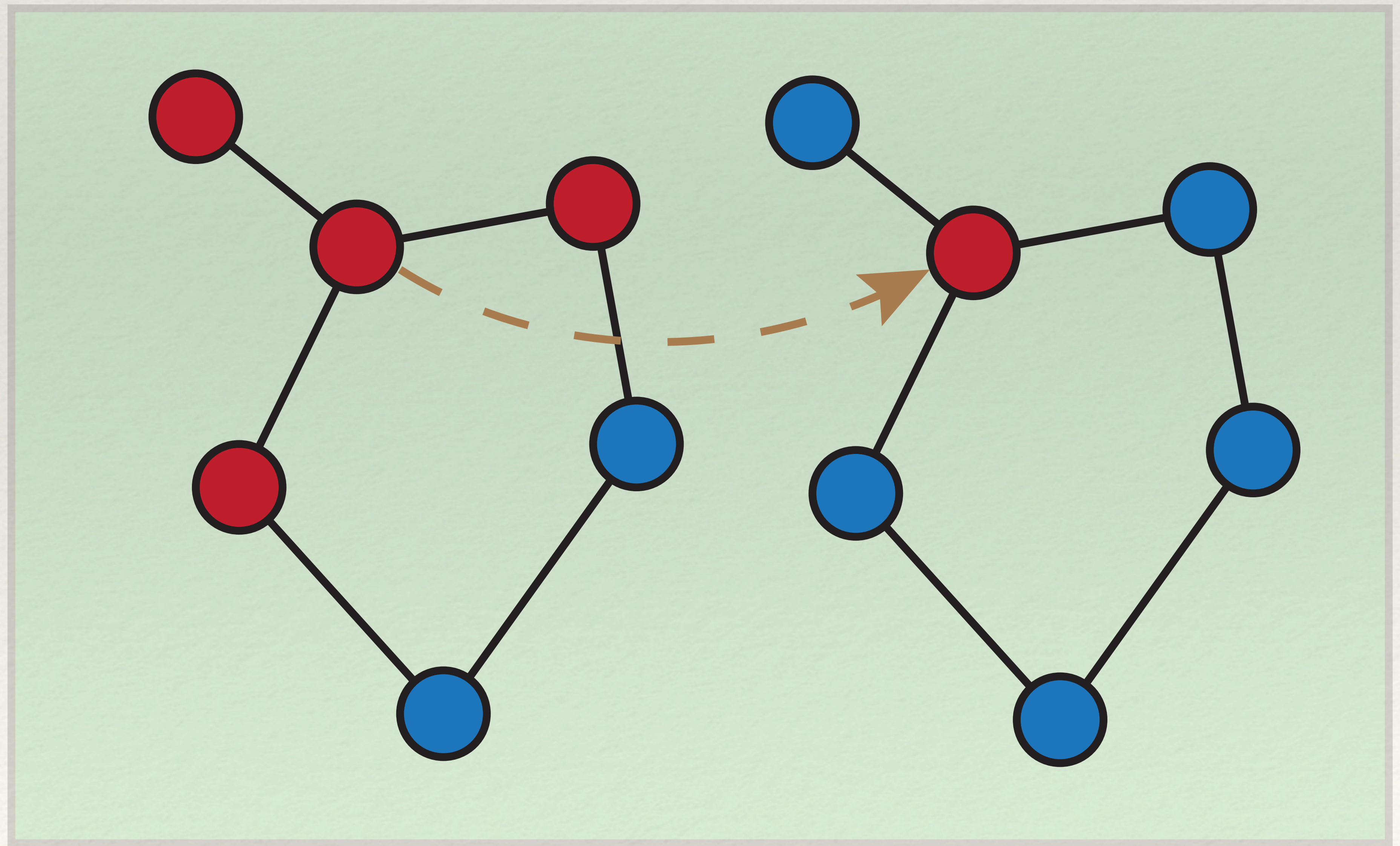
Disadvantage of CNN ROMs

- Standard CNN: not well defined for irregular data. How to use?
- **Option 1:** *Ignore the issue!*
  - Pad inputs with fake nodes until square-able.
  - Convolve square-ified input.
  - Reassemble at end; fake nodes ignored.
- Works surprisingly well!
  - But, not very meaningful.



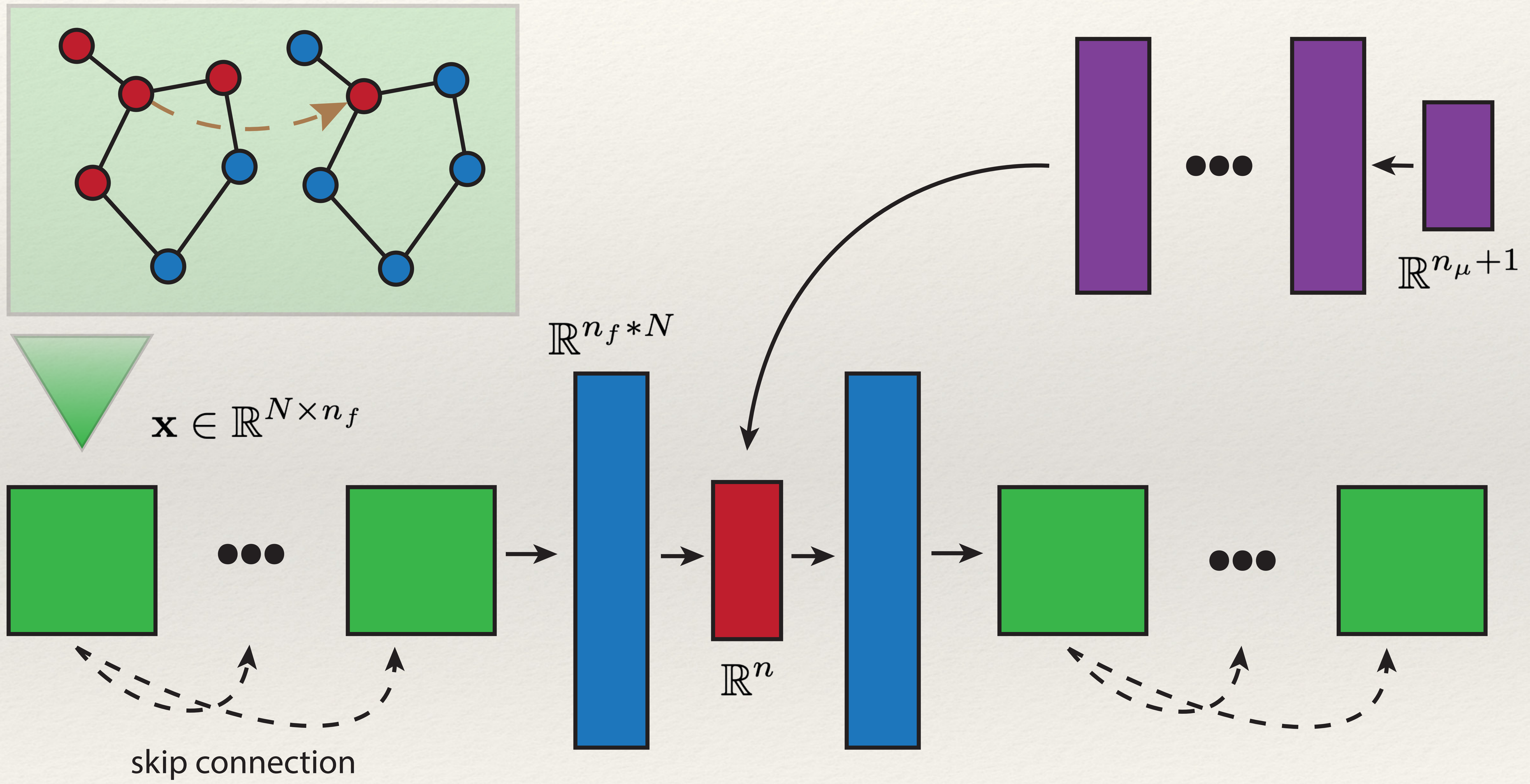
Graph Convolutional Networks

- **Option 2:** *Use a graph convolutional network!*
- $\mathscr{G} = (\mathscr{V}, \mathscr{E})$ undirected graph; adj. matrix $\mathbf{A} \in \mathbb{R}^{|\mathscr{V}| \times |\mathscr{V}|}$.
- $\mathbf{D}$: degree matrix $d_{ii} = \sum_j a_{ij}$.
- Laplacian of $\mathscr{G}$: $\mathbf{L} = \mathbf{D} - \mathbf{A} = \mathbf{U}\boldsymbol{\Lambda}\mathbf{U}^\top$.
  - Columns of $\mathbf{U}$ are Fourier modes of $\mathscr{G}$.
  - Discrete FT / IFT: multiply by $\mathbf{U}^\top / \mathbf{U}$.



GC Autoencoder ROM

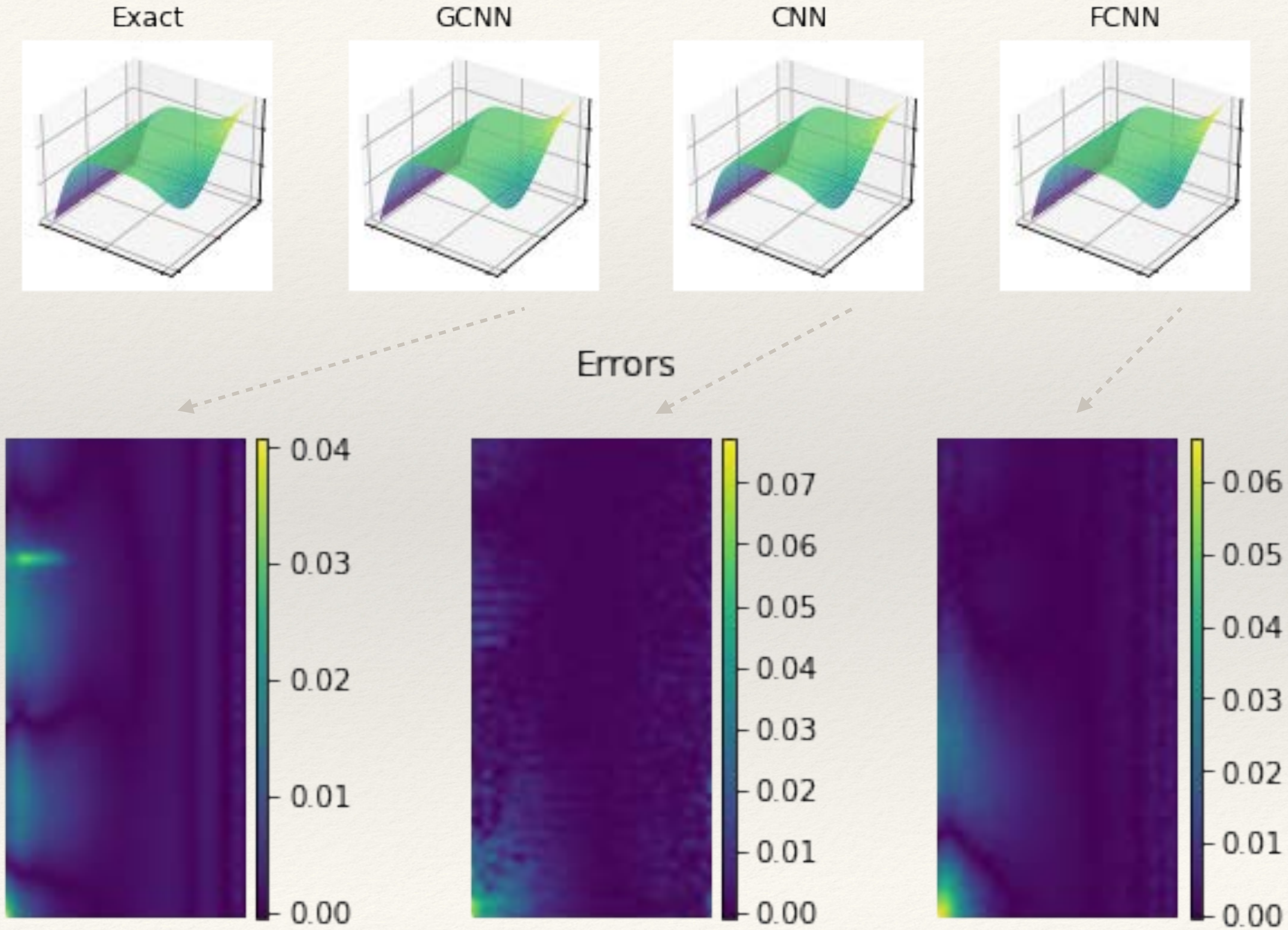
- GCN2 layers (Chen et al. 2020) encode-decode.
- Blue layers are fully connected.
- For ROM: purple network simulates low-dim dynamics.
- Split network idea due to (Fresca et al. 2020).



A. Gruber, M. Gunzburger, L. Ju, Z. Wang, *CMAME* (pending revision)

2-D Parameterized Heat Equation: Results

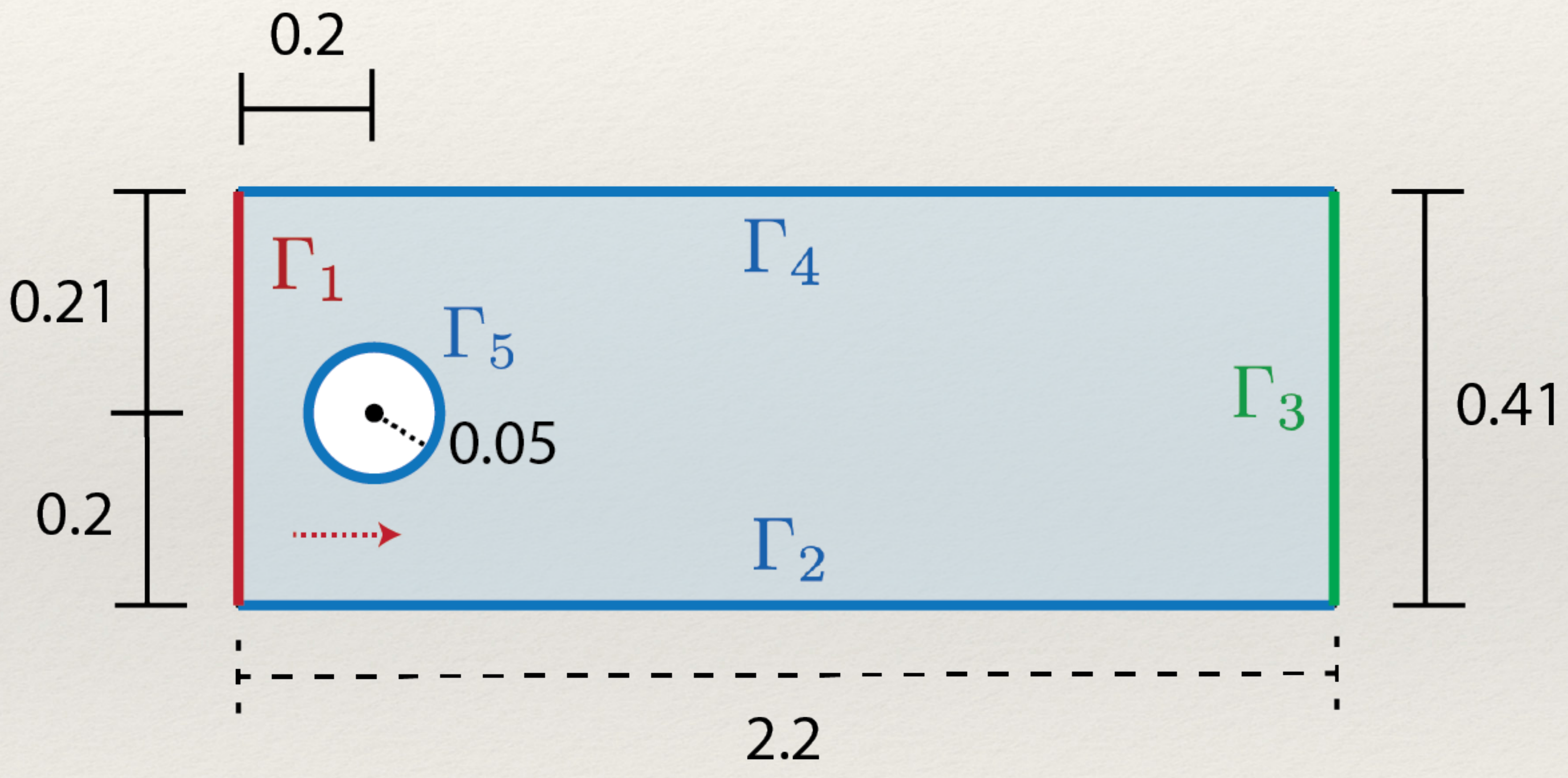
- Results shown for $N = 4096$, $n = 10$.
- GCNN has lowest error and least memory requirement (by >10x!)
- CNN is worst..
  - Cheap hacks have a cost!



Unsteady Navier-Stokes Equations

- Consider the Schafer-Turek benchmark problem:

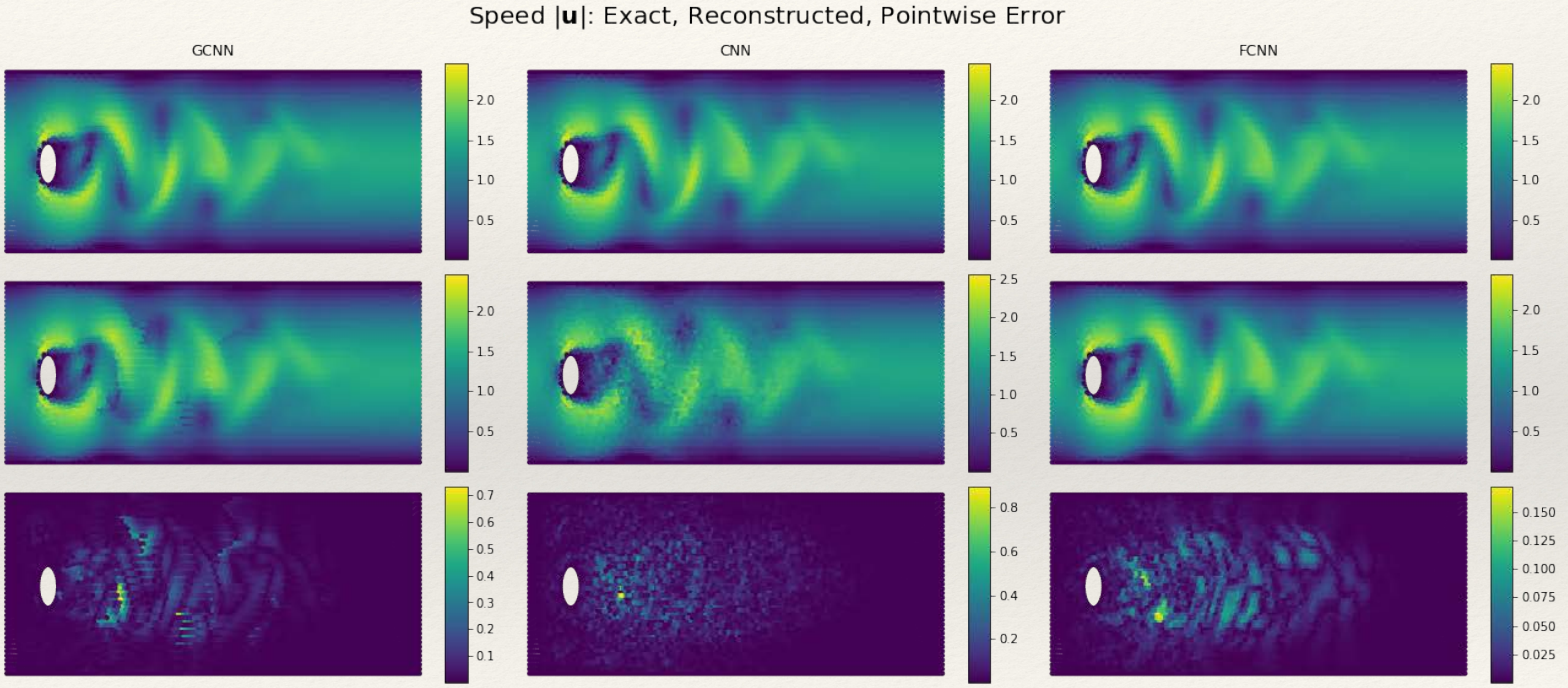
$$\dot{\mathbf{u}} - \nu\Delta\mathbf{u} + \nabla_{\mathbf{u}}\mathbf{u} + \nabla p = \mathbf{f},$$
$$\nabla \cdot \mathbf{u} = 0,$$
$$\mathbf{u}\big|_{t=0} = \mathbf{u}_0\,.$$



- Impose 0 boundary conditions on $\Gamma_2, \Gamma_4, \Gamma_5$. Do nothing on Γ_3. Parabolic inflow on Γ_1.

Navier-Stokes Equations: Full ROM

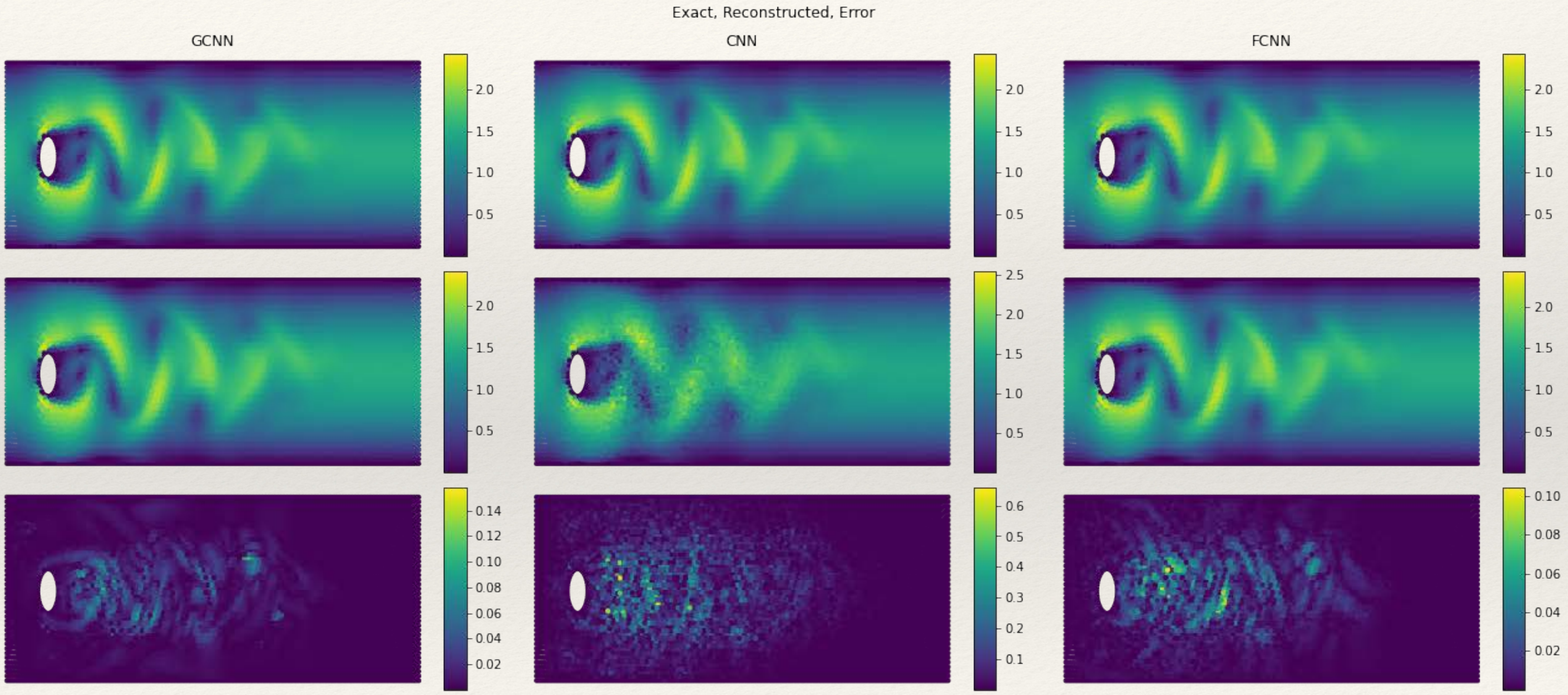
- $N = 10104$
- $n = 32$
- Reynolds number 185.
- FCNN best.
- GCNN still beats CNN.



A. Gruber, M. Gunzburger, L. Ju, Z. Wang, (under review)

Navier-Stokes Equations: Enc/Dec only

- GCNN matches FCNN in accuracy
- GCNN memory cost **>50x less** than FCNN
- ***(FCNN best on full ROM)



A. Gruber, M. Gunzburger, L. Ju, Z. Wang, (under review)

PDE on Moving Domains

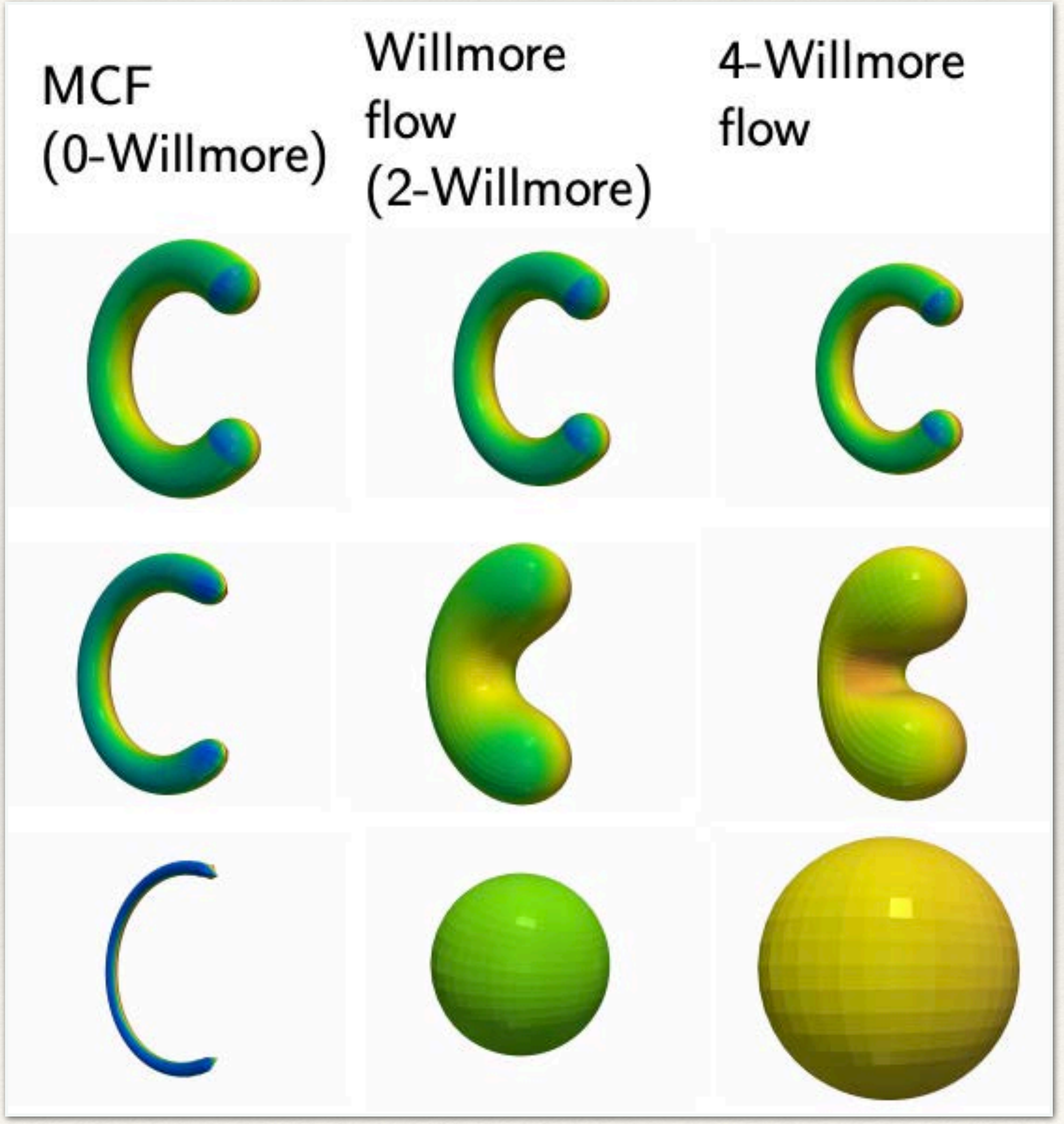
- Many natural phenomena modeled by conservation laws on moving surfaces.
  - Surface dissolution (pictured).
  - Motion of surfactant films between media.
- Various methods of solution:
  - Level set methods.
    - Generally implicit, stable, hard to formulate.
  - Finite difference methods
    - Implicit or explicit, easy to formulate, poor convergence.
  - **Evolving surface FEM.**
    - Implicit or explicit, versatile, can be delicate.

Potential Copyright Issue

G. Dziuk, C. M. Elliott, *Acta Numer.* (2013)

Modeling p-Willmore Flow

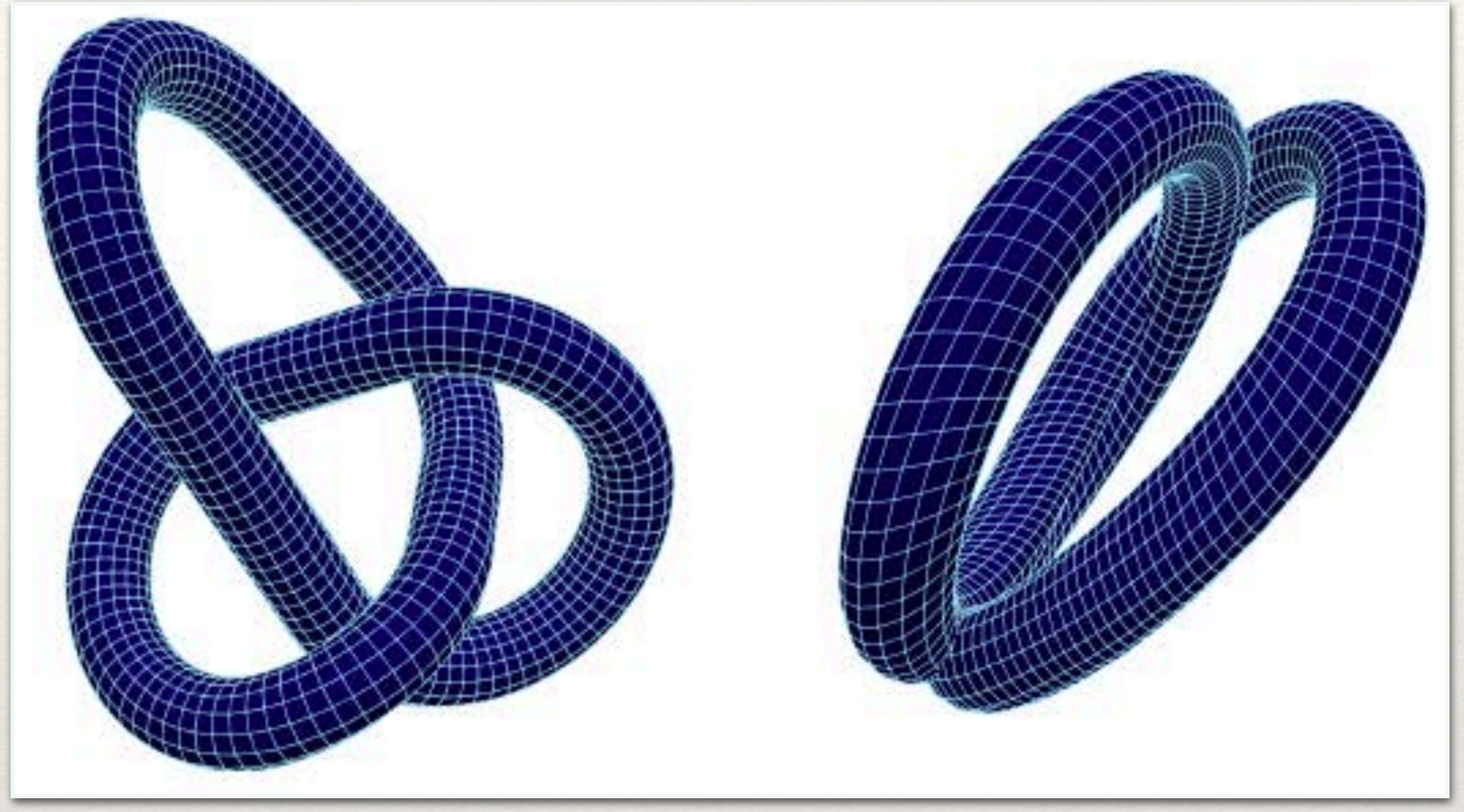
- p-Willmore energy: $\mathscr{W}^p(\mathbf{X}) = \int_M |H|^p \, d\mu_g$.
  - membrane biology, molecular entropy, liquid crystallography
- E-L equation 4^{th}-order QL degenerate elliptic.
  - How to model with p.w. linear FEM?
- (G. Dziuk 2012) $\mathbf{Y} := \Delta_g \mathbf{X} = 2HN$.
  - Willmore flow becomes coupled pair of 2^{nd}-order PDEs for X (weakly 1^{st}-order).

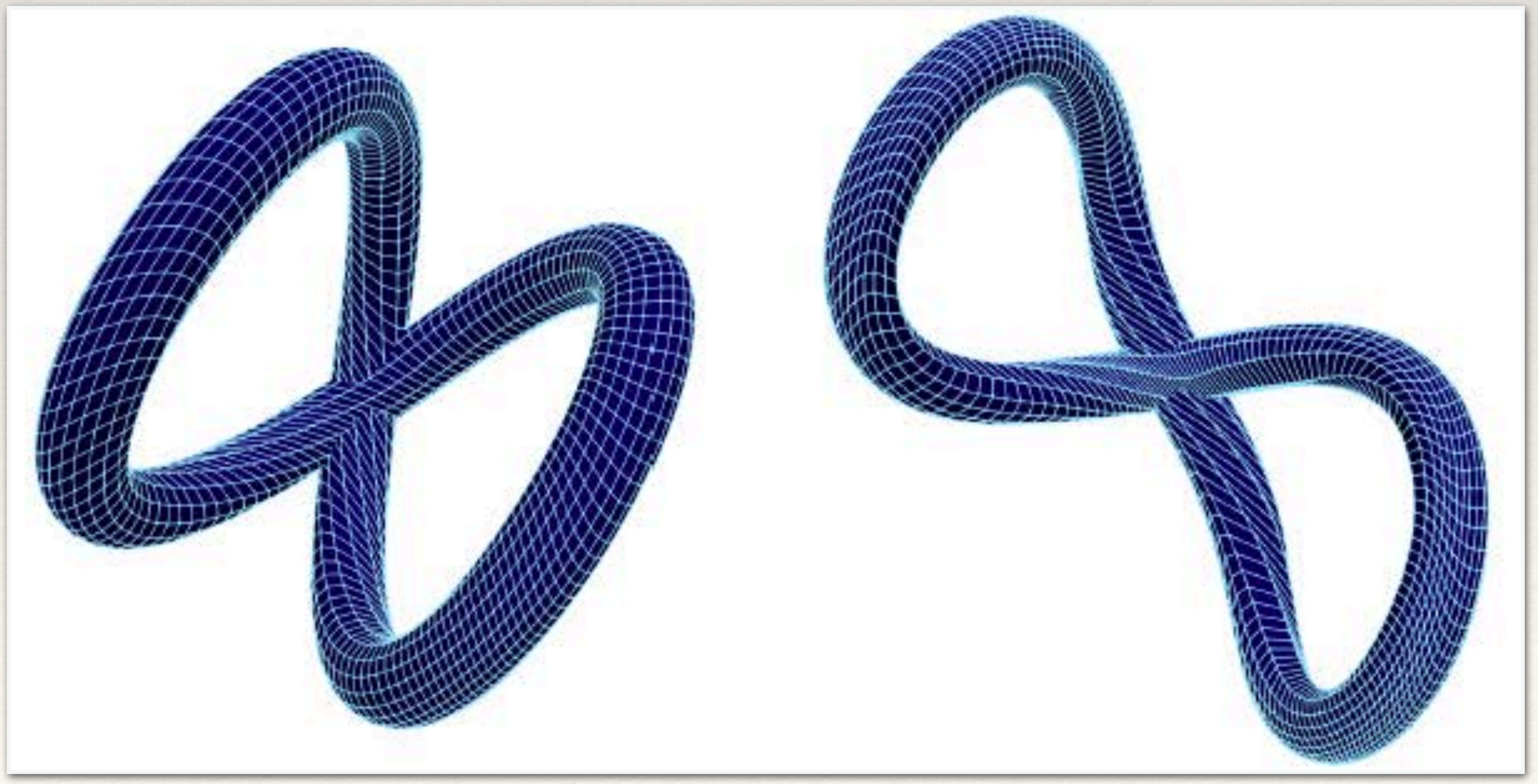


A. Gruber, E. Aulisa, *ACM Trans. Graph.* (2020)

Modeling p-Willmore Flow

- Trick works for p-Willmore, too!**
  - (with some modification)
- Yields provably dissipative scheme.
  - Including area/volume constraints.
- **Bad news:** mesh degenerates with large motion…
  - Parametrization invariance of $\mathscr{W}^p$ is a negative here.
- How can we fix it?

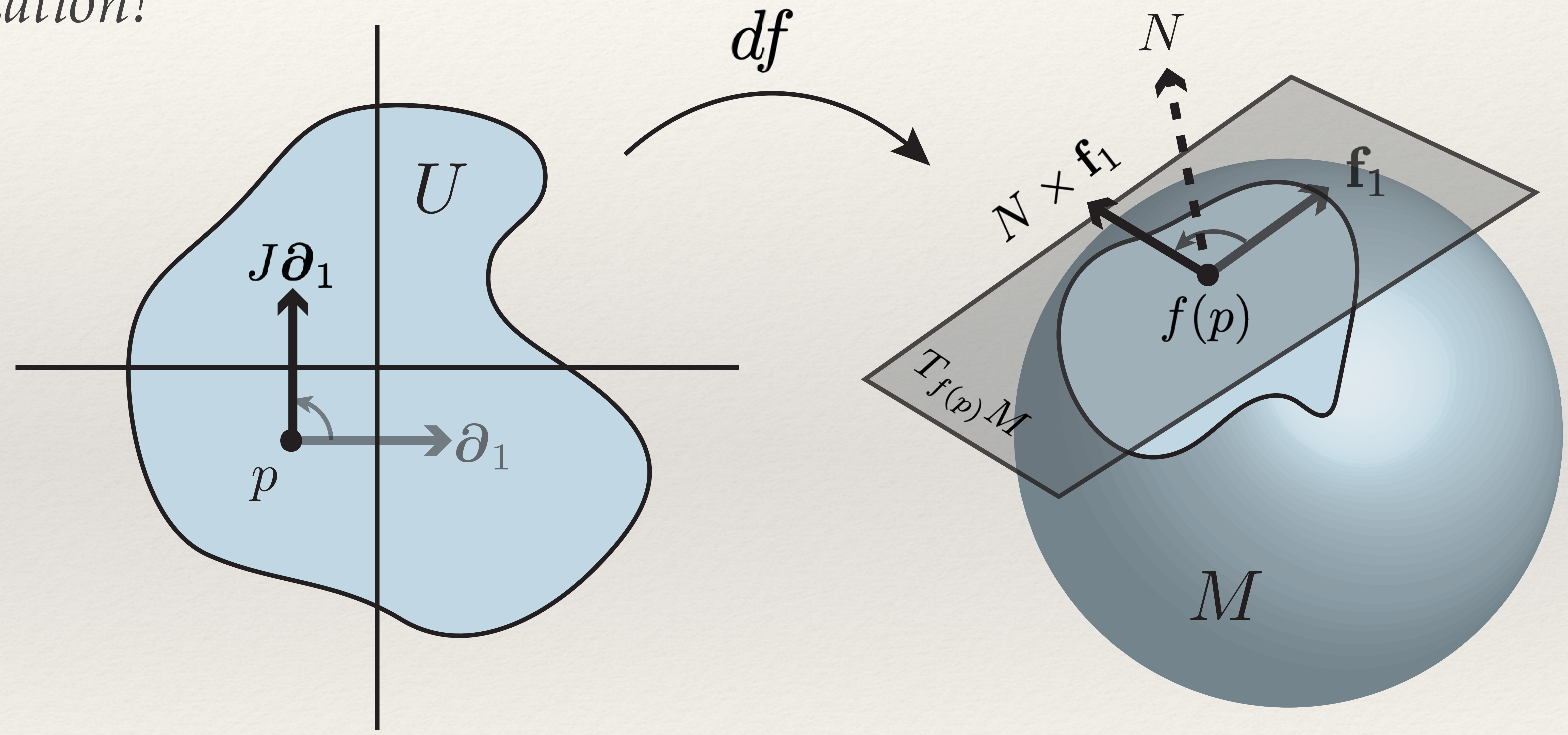




What about the Mesh?

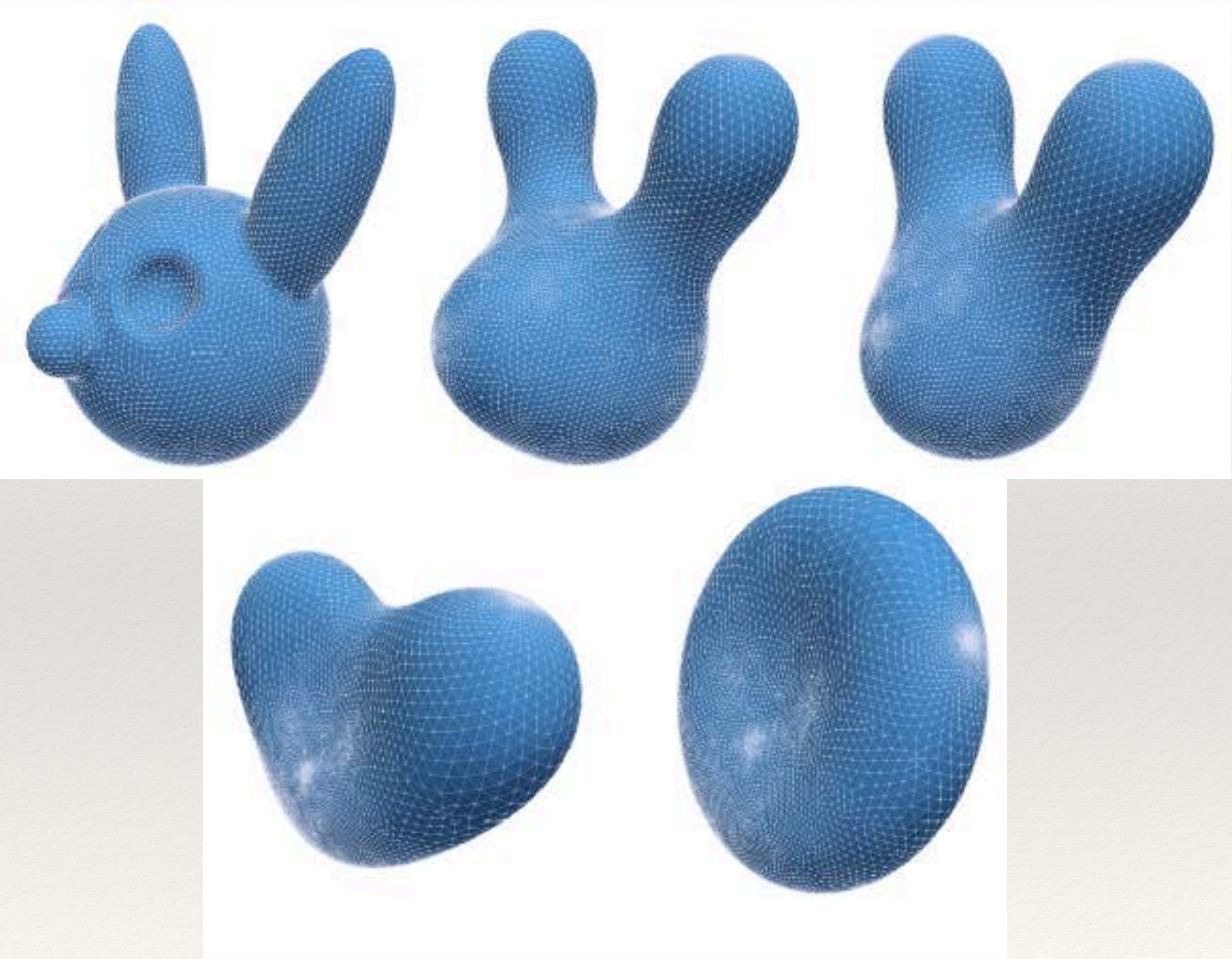
- *Least-squares conformal regularization!*
- $f : (M, g) \to (P, h)$ is conformal if $f^*h = e^{2\phi} g$.
- Think $f : M \to \operatorname{Im} \mathbb{H}$.
  - $\exists N$ s.t. $\star\, df = N\, df$.

    (Kamberov, Pedit, Pinkall 1996).
- Implementable.
- No explicit reference to metric!! (wrapped in $\star$).



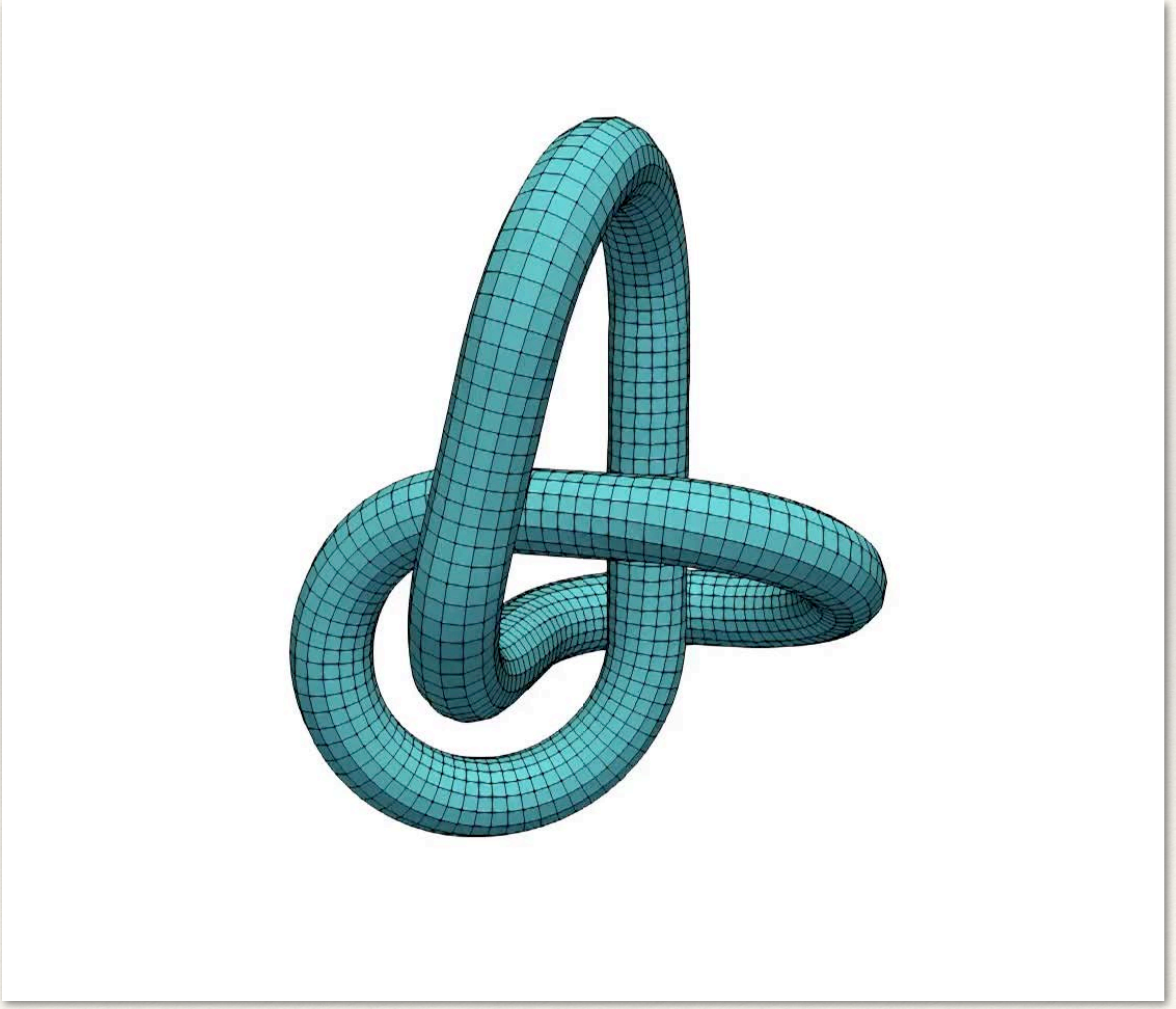
Modeling p-Willmore Flow

- Can minimize integral of $|\star dX - N\,dX|^2$ with constraint.
  - Yields least-squares conformal maps.
- Applied as subsystem in $\mathscr{W}^p$-flow reparametrizes surface.
- Keeps mesh stable along the evolution.



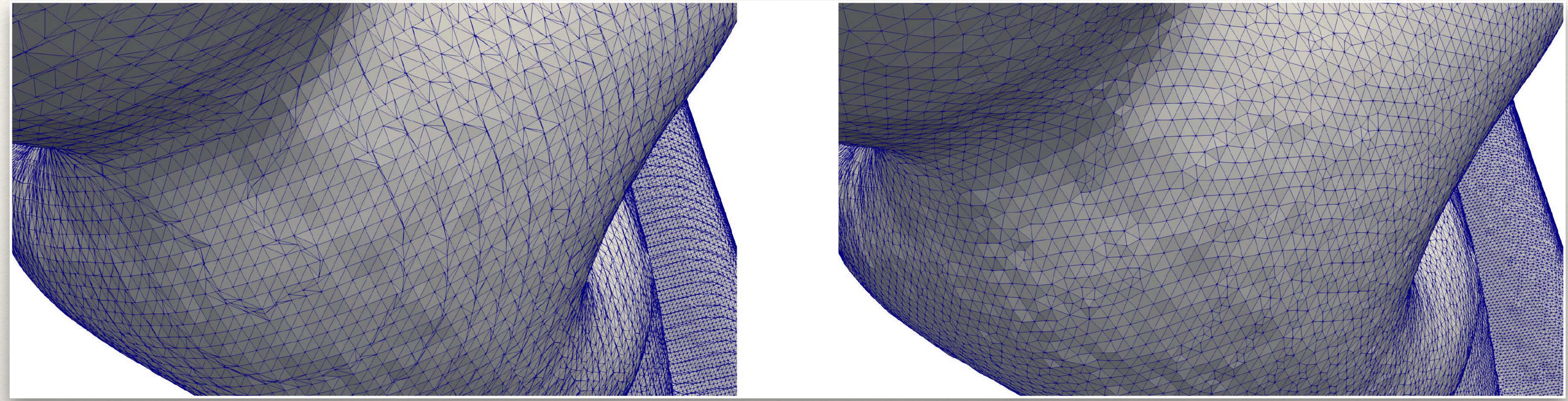
- A. Gruber and E. Aulisa, *ACM Trans. Graph.* (2020)

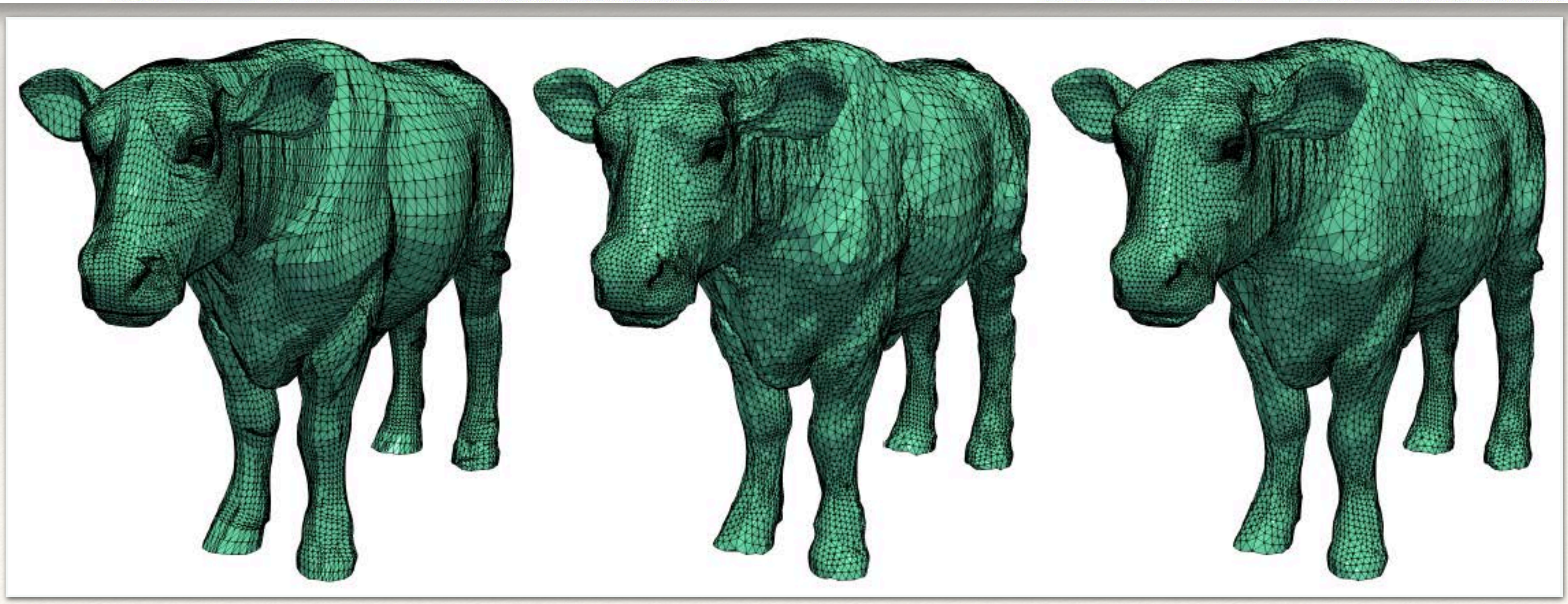
Torus Knots Unwinding



LSCM Reparametrization: Results

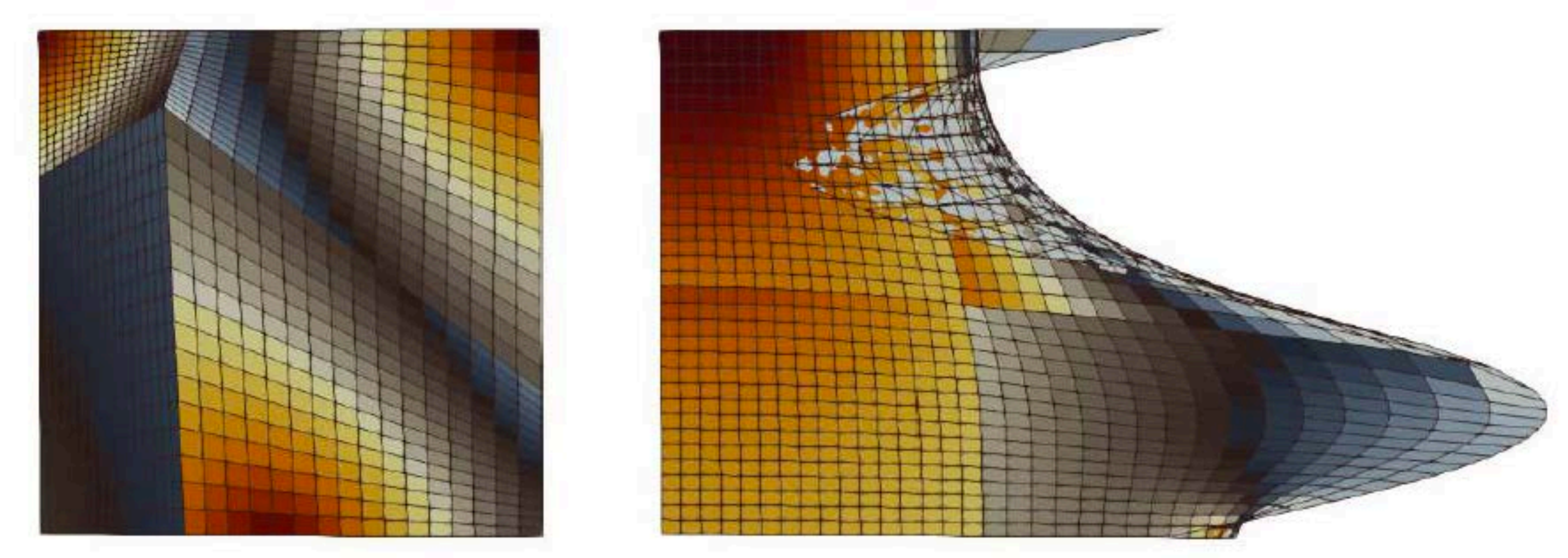
- Can also run LSC regularization on stationary surfaces.
- Makes discretizations much nicer.
- Useful for preprocessing before sci. comp. simulations





Problems with LSCM

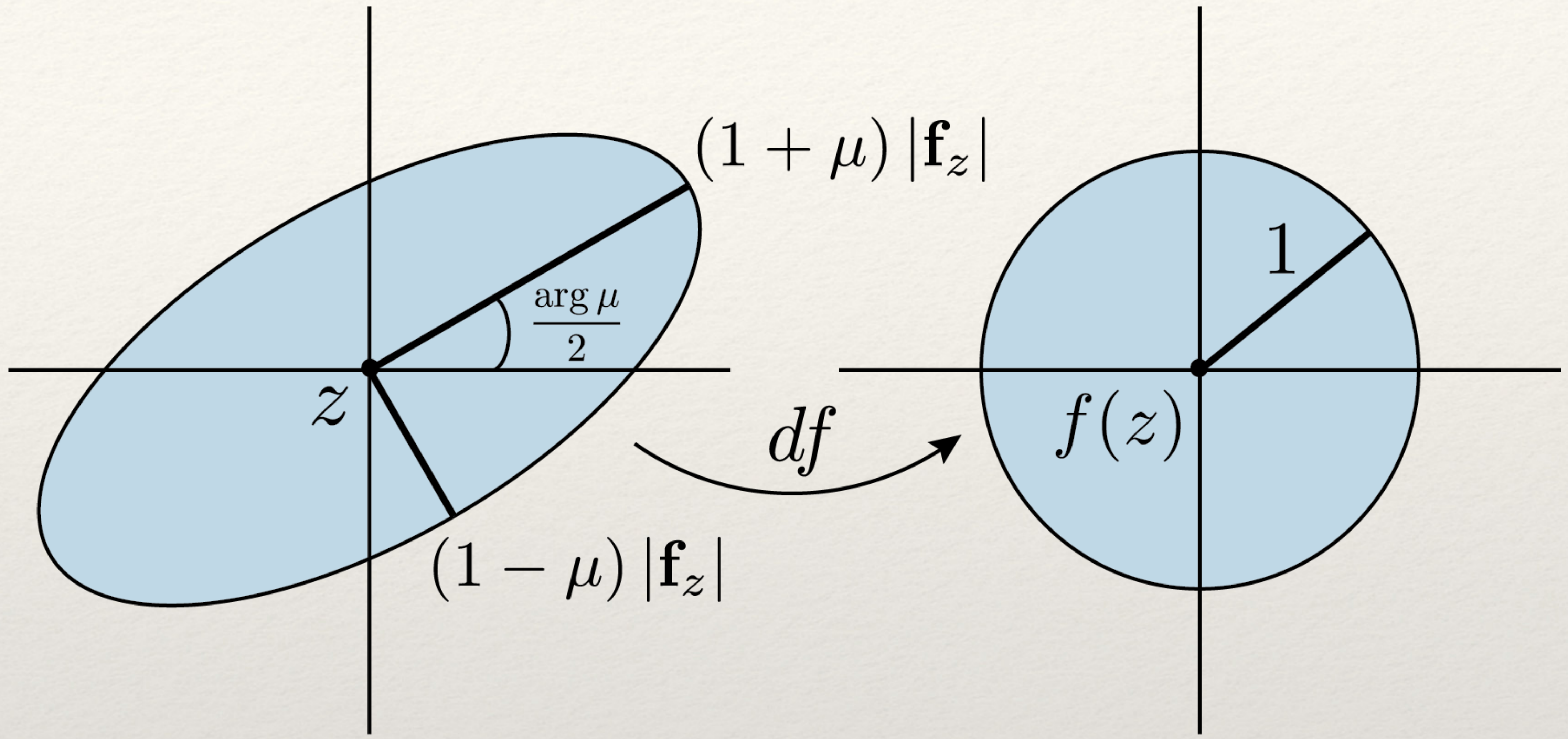
- Fails for explicit boundary correspondence!
- Not enough conformal maps available.
- Need to widen the search space.

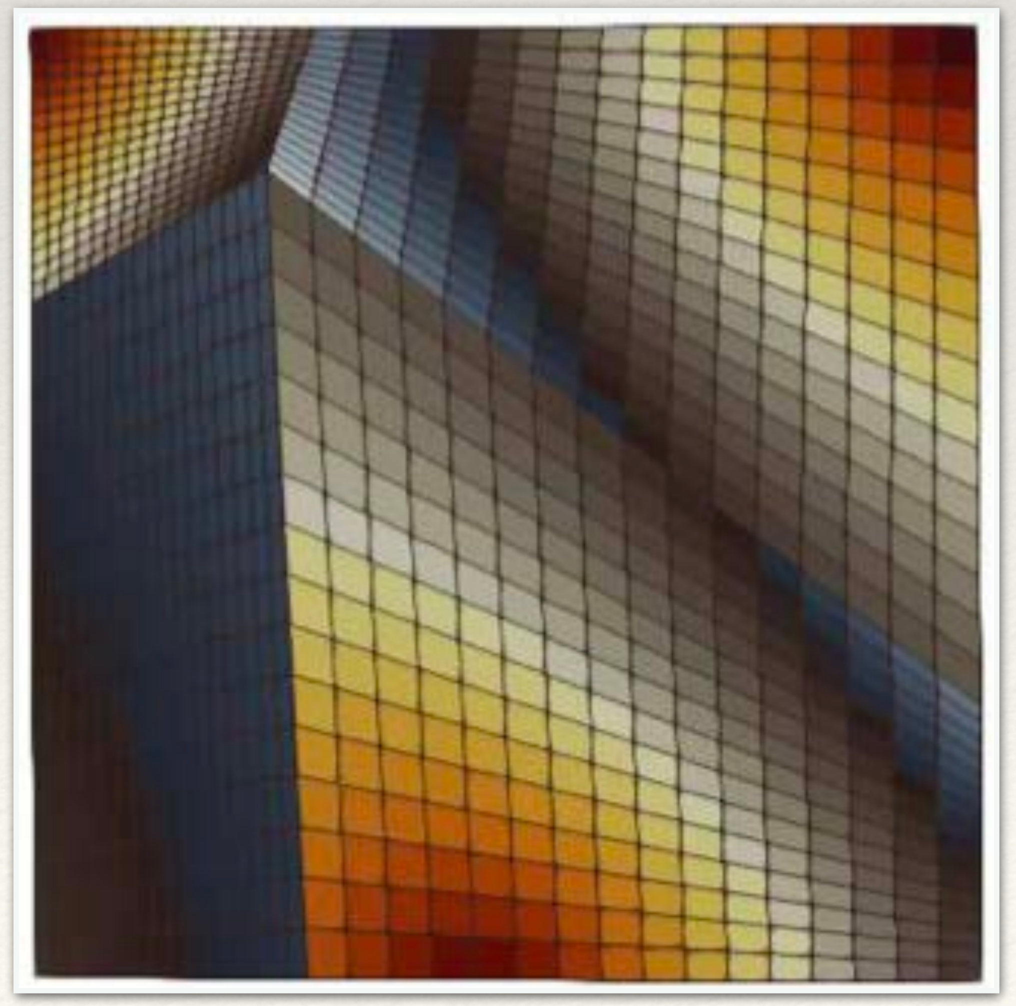


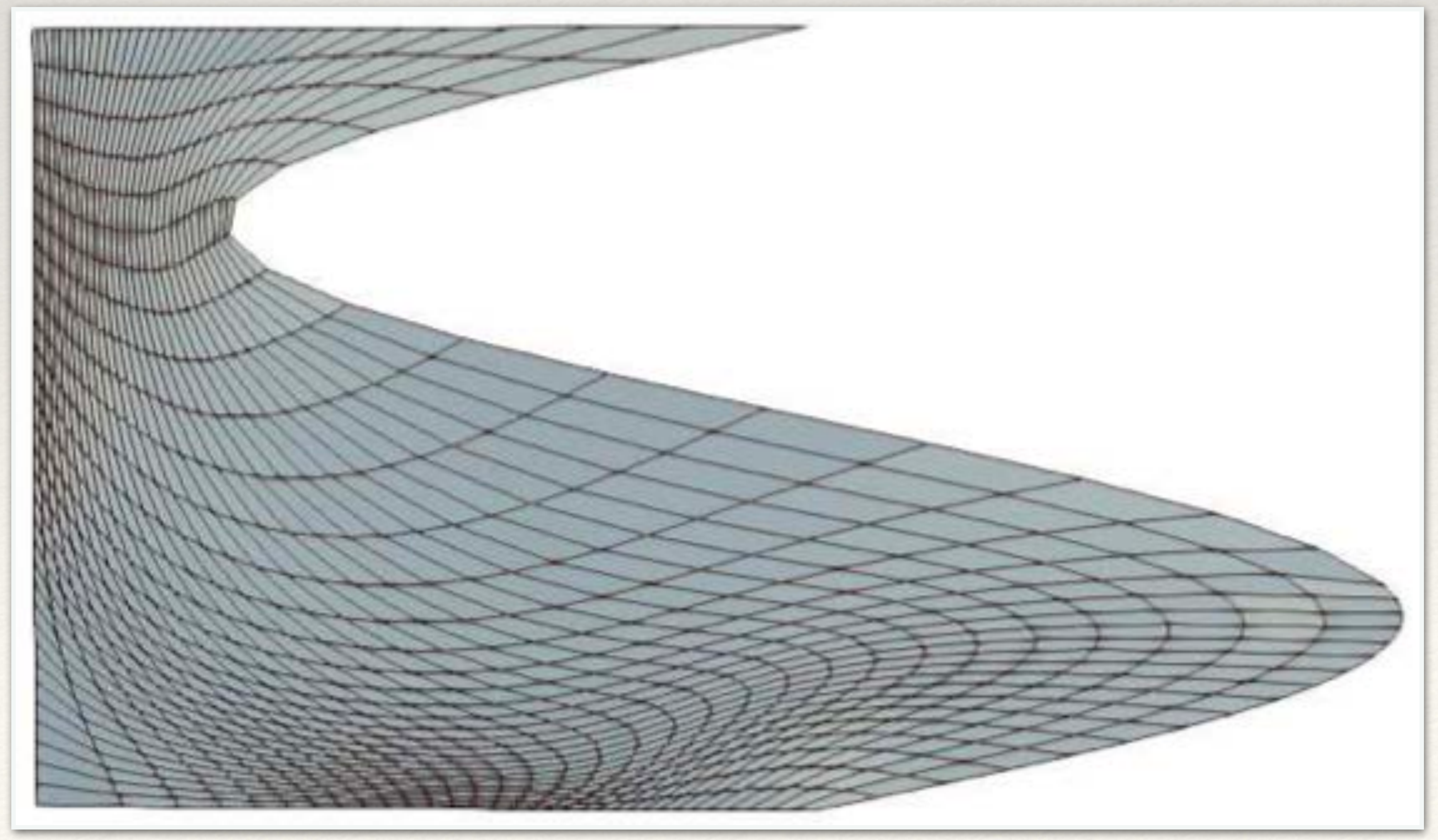
Conformal vs. Quasiconformal

- Quasiconformal mappings: $\bar{\partial} f = \partial f \circ \mu$
  - $\mu : TM \to TM$ $\mathbb{C}$-antilinear
- Small *circles* map to small *ellipses*.
  - What is the advantage?
- QC mappings are always (locally) invertible!

$$\mathrm{Jac}(f) = \left|\mathbf{f}_z\right|^2 - \left|\mathbf{f}_{\bar{z}}\right|^2$$
$$= \left|\mathbf{f}_z\right|^2 \left(1 - \left|\mu\right|^2\right) > 0$$

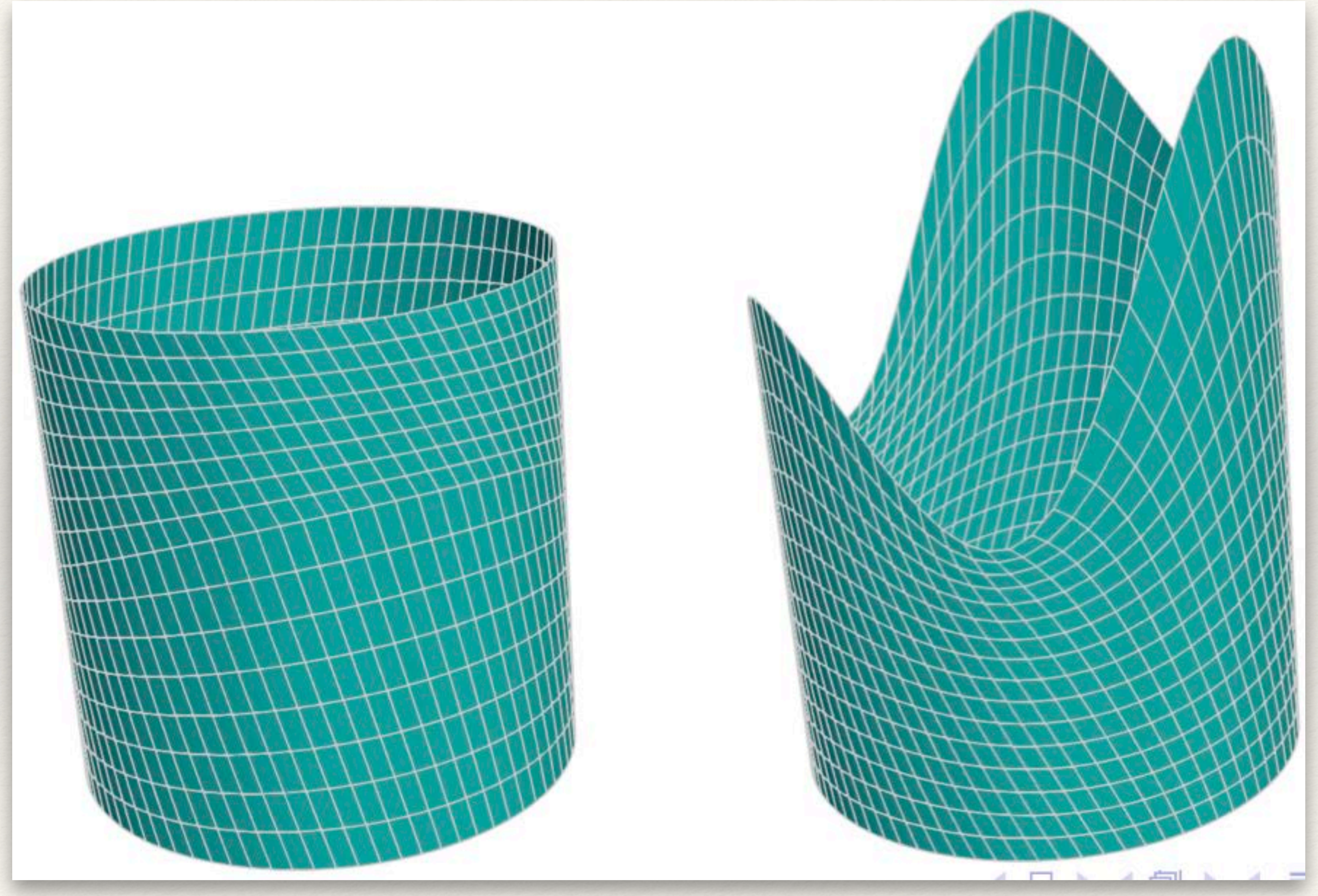






Immersed Surfaces in $\mathbb{R}^3$

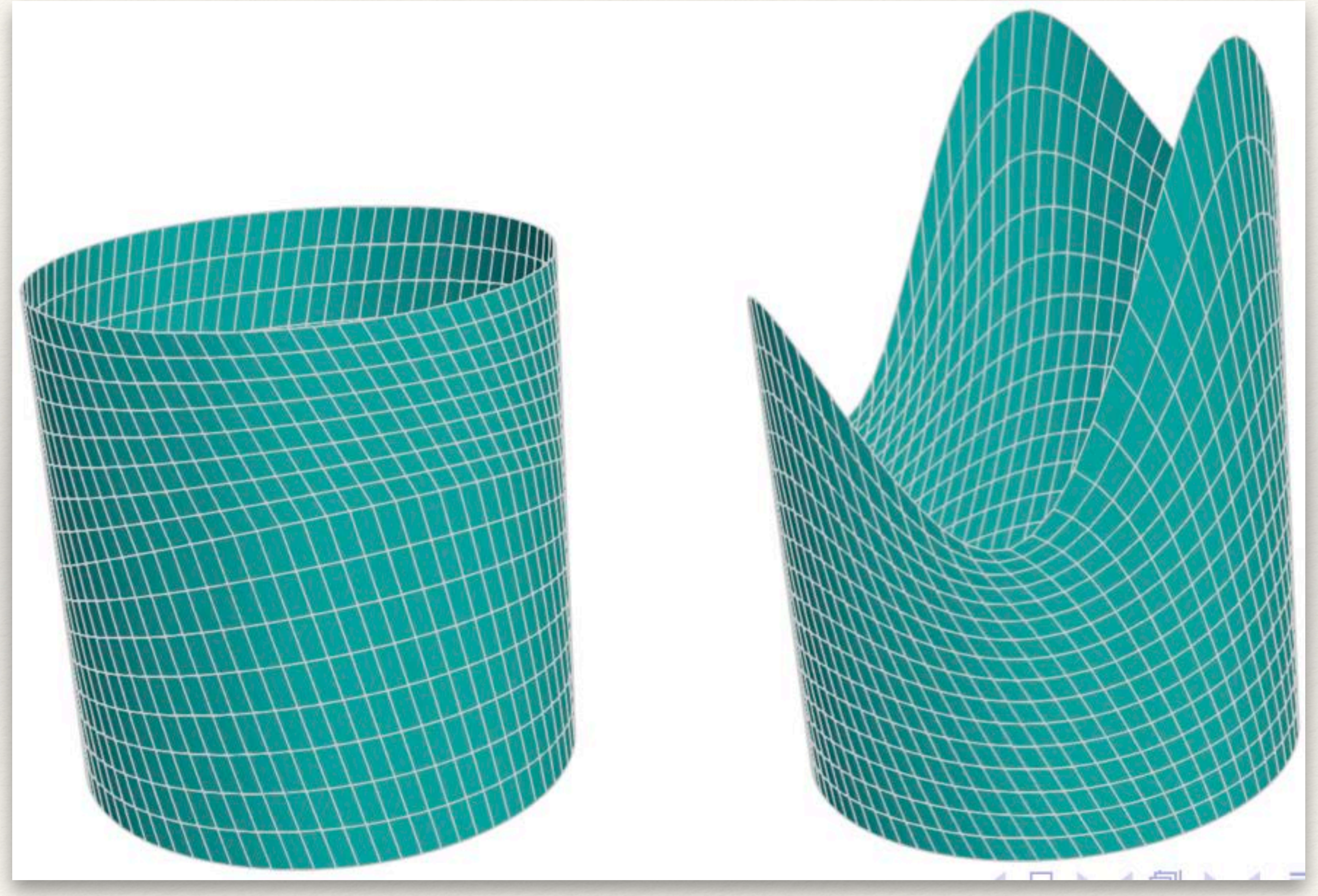
- Conformal / anticonformal parts $f : M \to \operatorname{Im}\mathbb{H}$:
  $$df^{\pm} = \frac{1}{2}\left(df \mp N \star df\right)$$
- Quasiconformal iff
  $$df^{-} = \mu\, df^{+}.$$
- BC $\mu : TM \to \mathbb{R} \oplus \mathbb{R}N$.
  - normal-valued "(-1,1)-form".



Optimal Teichmuller Mappings

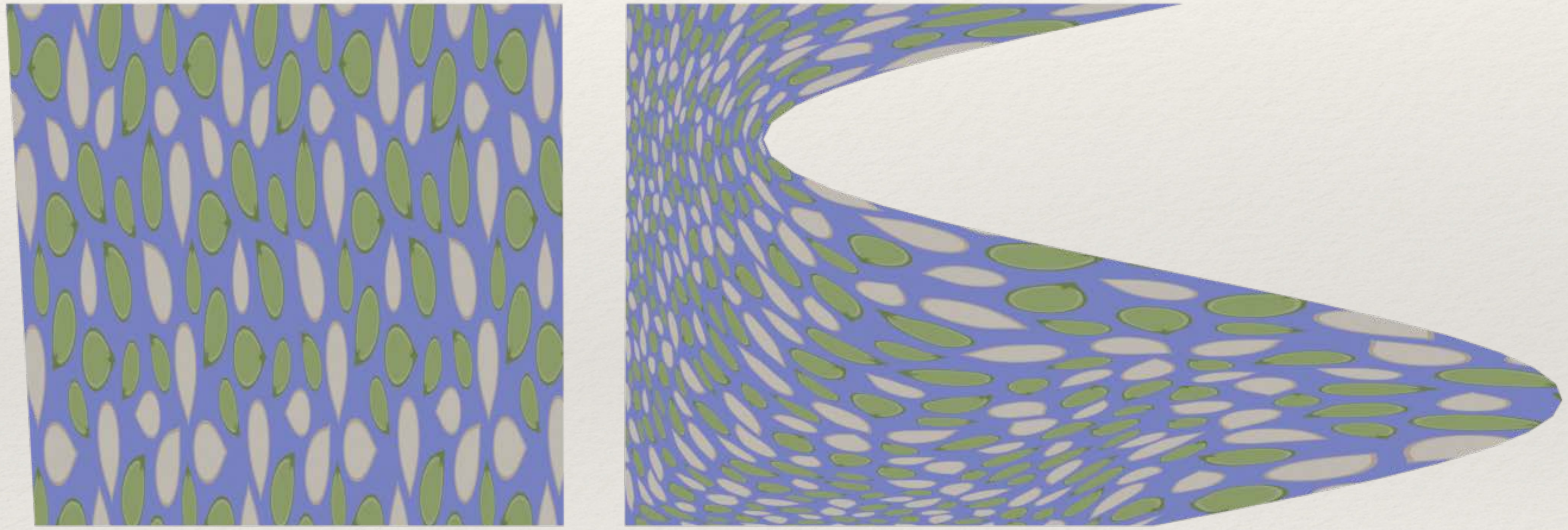
- What is the "best" QC map in a given homotopy class?
- Let $H([f]) = \inf_{h \in [f]} \left\{ \inf_{C \in M} K\left(h|_{M \setminus C} \right) \right\},$

  where $K(f) = \dfrac{1 + |\mu|_\infty}{1 - |\mu|_\infty}.$
- *(Strebel 1984)* If $H([f]) < K(f)$ then $[f]$ contains a unique Teichmuller mapping.
- TM mappings have constant $|\mu|$ and min-maxed conformality distortion.

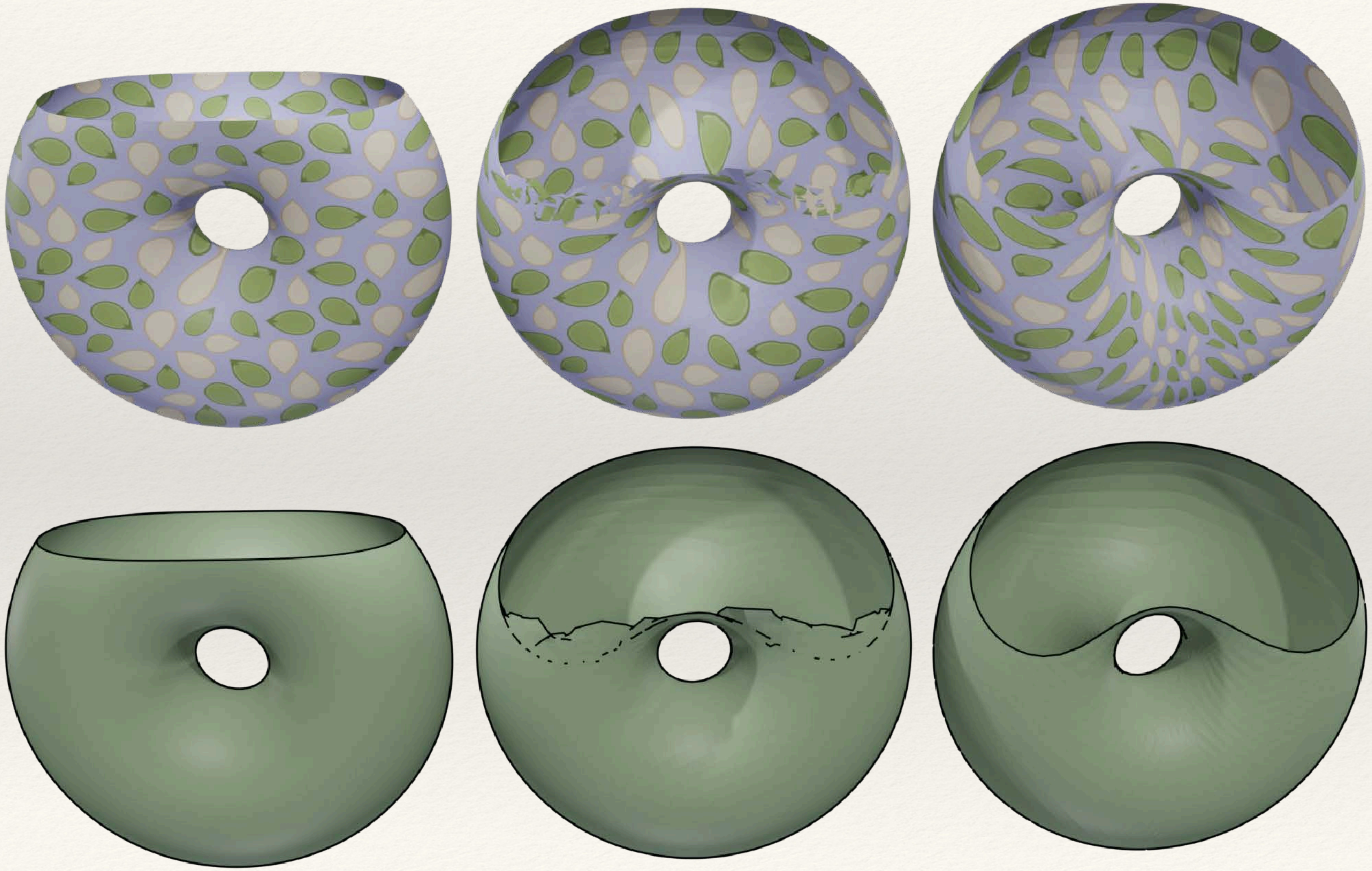


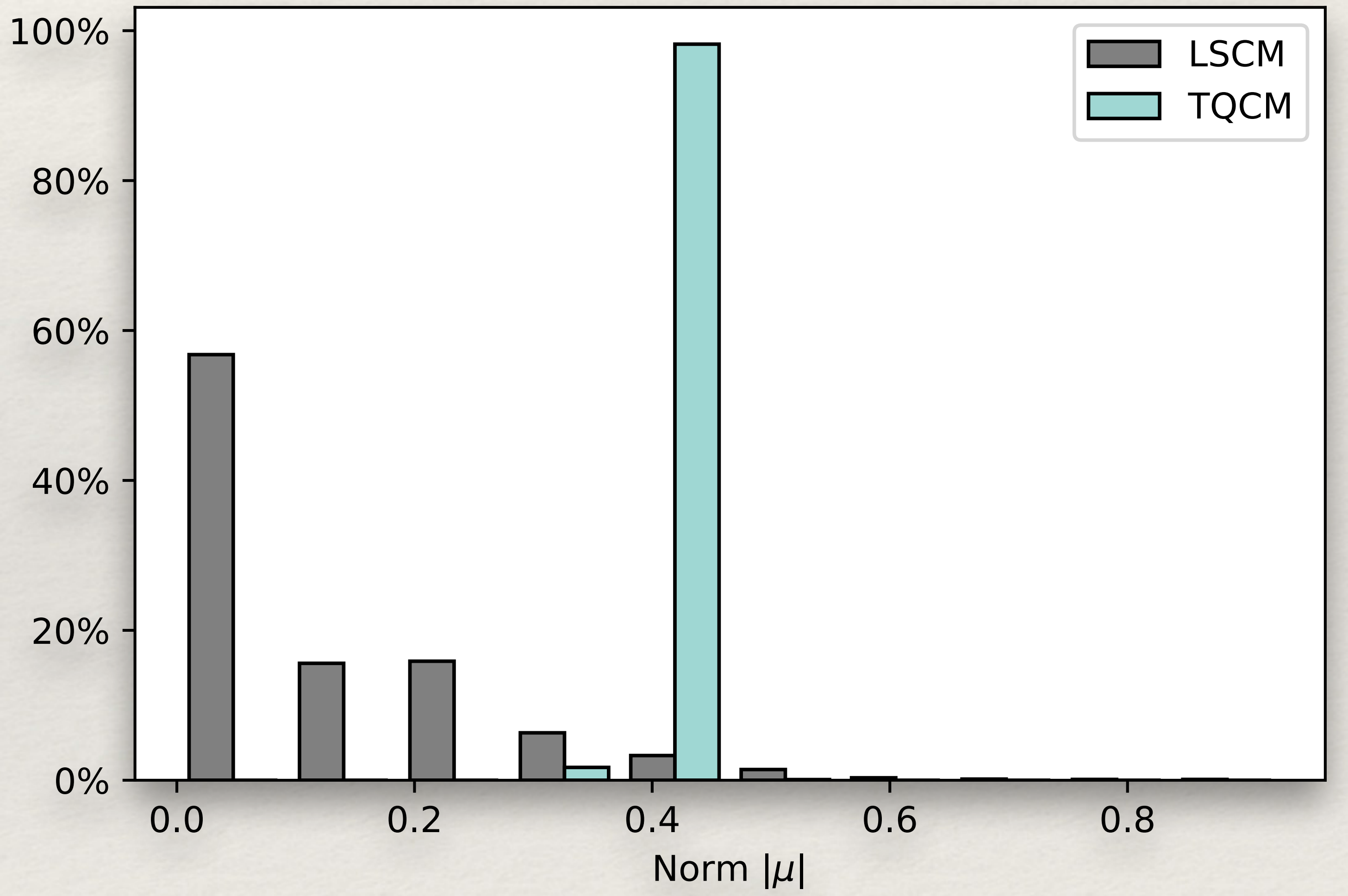
Computing TM mappings

- Minimize
  $$\mathcal{QC}(f) = \int_M |\, df^- - \mu\, df^+ |^2 \, d\omega_g$$
  alternatively over f, μ.
  - 1) Minimize for f given μ.
  - 2) Compute $\mu = df^- \left(df^+\right)^{-1}$.
  - 3) Locally adjust μ, moving it toward TM form.
  - Repeat steps 1-3 until convergence.



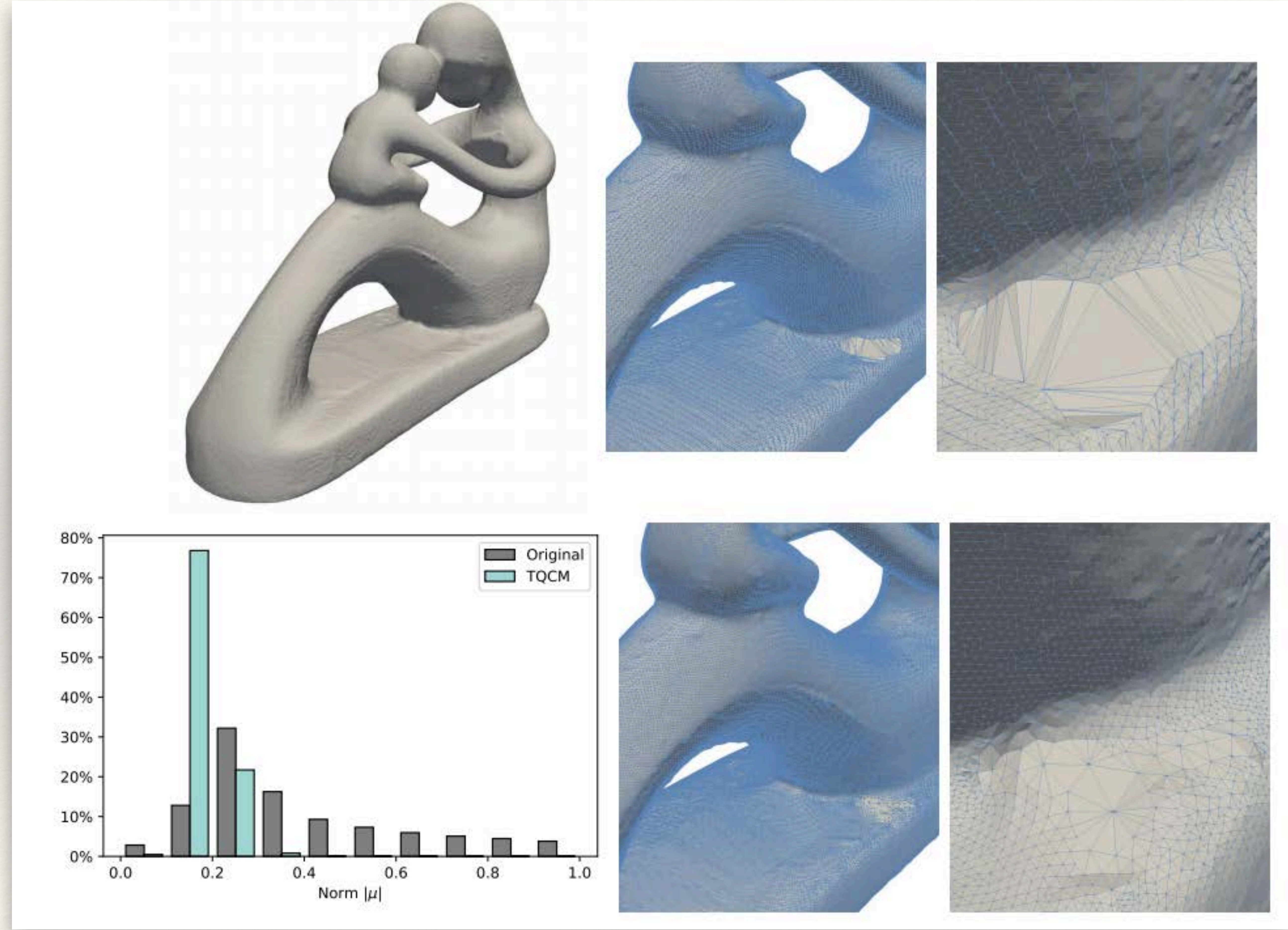
Comparison: TM vs. LSCM

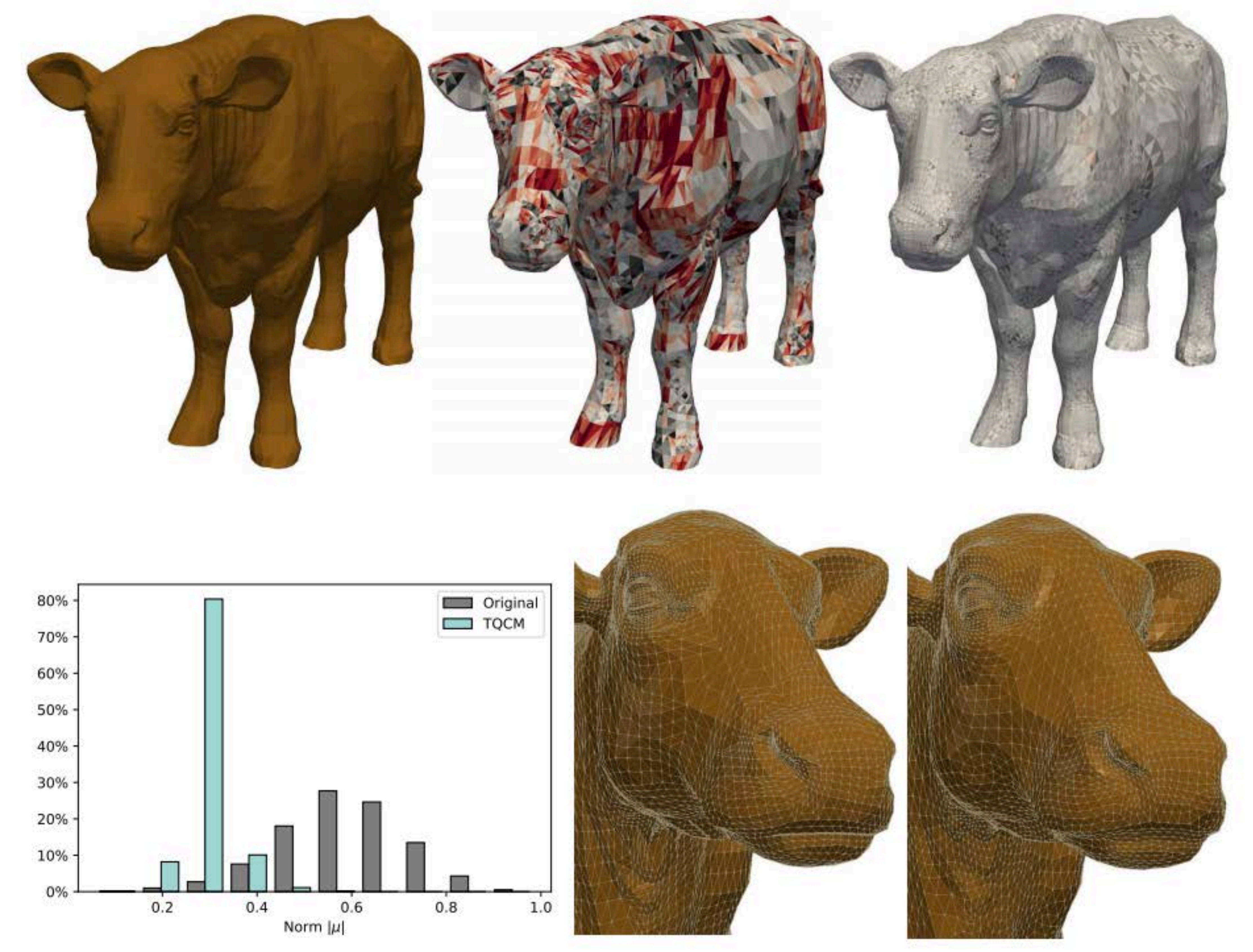




- A. Gruber, E. Aulisa (under review)

More Examples





Conclusions

- *Geometric relationships matter* for computation!
- My work:
  - Informs *concrete* problems with *abstract* ideas.
  - Investigates *rigorous solutions/algorithms* validated by simulations.
  - Benefits from *collaboration* and a diverse array of expertise.
- Projects often receive external funding.
  - Can be expected to continue.

Thank You!