Research Statement

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1 Overview

My research focuses around the pure and applied questions that arise during the study of problems in computer graphics, data science, and reduced-order modeling. Particularly, I apply techniques from differential geometry, nonlinear partial differential equations, and numerical optimization to develop mathematics-informed algorithms and justify their practical behavior. As the most basic goal of my work is often to solve, simulate, or understand a system of nonlinear PDE, it is widely applicable to many areas of science and benefits from a diverse array of expertise. This has led to fruitful collaborations with mathematical biologists, high-performance computer scientists, and cybersecurity researchers which I hope to expand in the future.

Coming from a background in differential geometry, my projects often involve interesting combinations of rigorous geometric theory with modern scientific computing techniques. Leveraging programming ability in Python and C++, I employ finite element and artificial neural network methods to minimize the various functionals that arise when approximating PDE solutions or visualizing geometric phenomena. I enjoy that these problems require a collaborative environment and diversified skillset, as I am constantly learning from others and refining my research process. The remainder of this statement provides some examples of past, current, and continuing work.

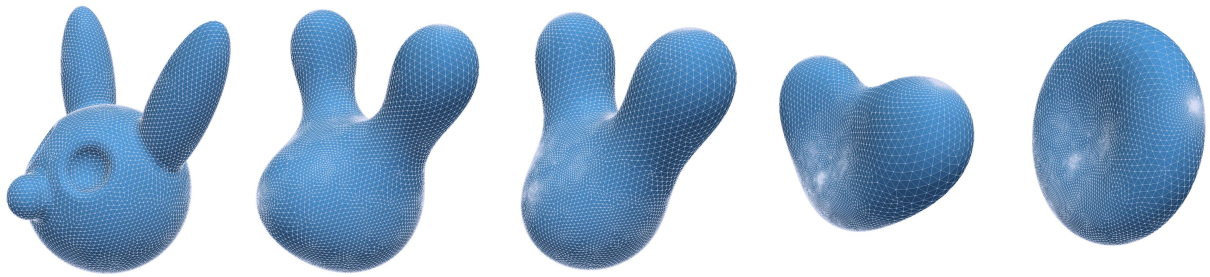

FIGURE 1: Willmore L^2-gradient evolution of a rabbit mesh, constrained by both surface area and enclosed volume. Here appears the biconcave discoid shape characteristic of genus 0 minimizers of the constrained Helfrich energy such as red blood cells (c.f. [26]).

2 Geometric PDEs in Computer Graphics

Some of the most interesting and physically relevant nonlinear PDEs are posed on domains in motion. To understand least-action principles in physical systems, for example, it is necessary to understand the formation of minimal surfaces such as those approximated by the soap films spanning a wire loop (see e.g. [1]). Similarly, phenomena such as the growth of biological tumors and the evolution of fluid interfaces are best understood in the context of nonlinear PDEs on evolving surfaces [10]. Therefore, it is not surprising that these PDE systems are also some of the most difficult to rigorously analyze, as the equations to solve are defined on an object which is determined by their solution.

As it turns out, certain nonlinear PDE are also quite useful for computer graphics applications. Indeed, curvature flows—Hilbert space gradient flows of functionals depending on surface curvature—are frequently employed in the graphics literature for the purposes of animation, mesh editing, and surface denoising (see e.g. [8, 4] and Figure 1). As such, it is important to have a variety of accurate and efficient algorithms available to simulate gradient flows. In [13] we develop and investigate a finite element method for the p-Willmore flow, which is a generalization of the usual Willmore flow (c.f. Section 4) to higher powers of the mean curvature. Making use of a clever operator splitting technique due to Dziuk [9], our scheme includes optional constraints on surface area and enclosed volume and is provably energy decreasing. In addition, we

develop a procedure based on quaternionic conformal geometry (see e.g. [22, 23]) which keeps mesh elements close-to-conformal as they evolve, yielding high-quality discrete surfaces and preventing artificial numerical failure along the flow.

Inspired by the success of our regularization procedure mentioned above, we challenged ourselves in [14] to consider computing quasiconformal mappings with the goal of producing surface deformations with prescribed boundary. A common problem in graphics applications, it is well known that conformal mappings between surfaces cannot satisfy a pointwise boundary correspondence (c.f. Figure 2). On the other hand, if the class of allowable mappings is relaxed to include those with bounded shearing distortion, this requirement is not difficult to satisfy. The contribution of [14] is a genus-agnostic algorithm (to our knowledge, the first) for computing Teichmüller mappings from immersed Riemann surfaces with boundary into $\mathbb{R}^3$ satisfying a prescribed boundary correspondence. As before, the key component to this is an extension of the quaternionic conformal machinery to the quasiconformal case. We show that computational Teichmüller mappings can be computed via the minimization of a certain energy functional, and demonstrate their effectiveness in surface deformation and remeshing applications.

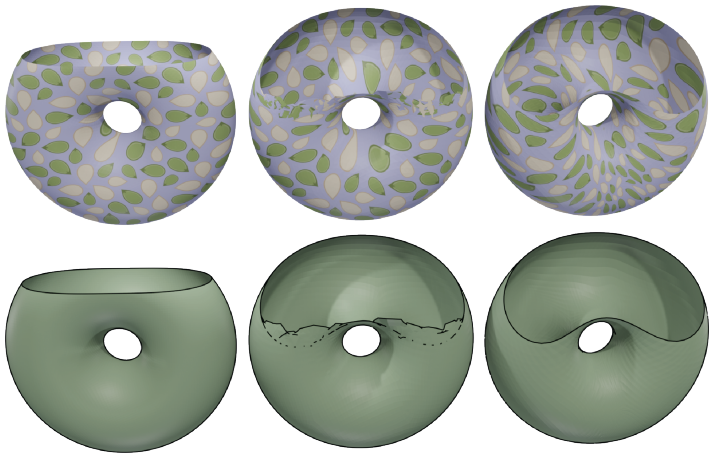

FIGURE 2: Comparison of least-squares conformal mapping (mid) and Teichmüller quasiconformal mapping (right) from one open torus to another. Note that the LSCM does not remain injective as the boundary is slid along the surface, despite producing lower average texture distortion.

Continuing and Future Work: As the intrinsic-to-extrinsic technology provided by quaternionic surface theory has been highly useful in mesh editing applications, future projects will consider other ways to improve or extend existing mesh manipulation technologies by reformulating them in these terms. On the other hand, there is now also significant interest in mesh-free methods for scientific computing, including neural network and point cloud techniques. Since the set of two-layer ReLU neural networks is known to include the set of linear finite elements as a special case (see e.g. [2]), it would be interesting to consider network-based quaternionic algorithms for surface editing applications. Due to the large interest by the NSF and other organizations into machine learning methods for scientific pursuits (e.g. NSF CDS&E meta-program), this work has strong potential to receive external funding.

3 Data-Driven Function Approximation and Reduced Order Modeling

It is frequently the case that scientists or engineers need to draw conclusions about the output of a function based on limited or incomplete data. Such situations arise, for example, when the output depends on the solution of expensive differential equations, or when lack of time and resources precludes the collection of suffcient high-quality samples. When this occurs, it becomes critical to maximize the value of the limited resources at hand, which requires informed algorithms for dimension reduction. Our work in [5] addresses this problem through an application of the Implicit Function Theorem. In particular, we show that by calculating an integral curve of the gradient vector field and a suitable projection mapping to this curve, one can recover the value of an unknown function at any regular point in its high-dimensional parameter space. After computing the integral curve through straightforward gradient descent, we provide an algorithm for projection based on traversing the level sets of the function. This method is shown to be direct and effective, but comes with the drawback of a relatively high online cost.

Another approach to this problem pioneered in [29] and improved by our work in [14] is known as Nonlinear Level set Learning (NLL), which uses advances in machine learning technology to address the

problem of function prediction in the presence of sparse data. Similar to the well known linear method of Active Subspaces [7], NLL learns a transformation of the input data so that the sensitivity of the function is concentrated in the span of only a small number of active variables. This allows for the nonlinear projection of the sampled data into the span of the active variables, naturally increasing its density and enabling ridge regression approximation of the original function. We show that computing this mapping through the minimization of a particular Dirichlet-type energy functional leads to improved training performance of the reversible neural network (RevNet [12]) architecture which parameterizes it. This in turn leads to faster, more stable convergence than the original method and improved sensitivity concentration in the active directions. Moreover, we demonstrate that our procedure combined with ridge regression against one active variable is already enough to produce relative errors of within 10% even in the presence of very sparse sampling (e.g. 100 samples in 40 dimensions), and this error decreases to less than 1% with the addition of more data.

While the methods described so far are primarily designed for quantities of interest that arise from parameterized PDEs, it is crucial in high-performance computing applications to have approximation methods which can directly predict PDE solutions. In particular, simulations which are real-time or many-query in nature rely heavily on reduced-order models (ROMs) to provide fast and accurate approximations to the high-fidelity solution, which is often too expensive to enable such applications. To that end, ongoing work involves developing and comparing convolutional and graph convolutional autoencoder networks for the approximation of PDEs on irregular grids and finite element domains (e.g. our work in [15]). Reduced-order models based on deep convolutional autoencoders have recently gained in popularity due to their ability to break the Kolmogorov width barrier which significantly limits the power of linear ROMs like proper orthogonal decomposition (POD). In [15], we propose a novel graph convolutional autoencoder based on the operation from [6] and compare its performance to both the deep CNN-autoencoder most commonly employed for nonlinear ROM (e.g. [24, 11]) as well as a basic fully connected autoencoder. The proposed architecture is seen to have significant advantages over the others in accuracy and memory efficiency provided the dimension of the reduced latent space is not too small. An example illustration is shown in Figure 3.

Continuing and Future Work: We are aware of several ways in which the NLL algorithm for function approximation on sparse data can be improved. As the invertibility requirement enforced by the RevNet is somewhat artificial in this context, it remains highly relevant to construct a robust and efficient network architecture which does not enforce this constraint explicitly. Moreover, the energy functional that is currently minimized is not coercive over the entire input space, and therefore allows many nonunique solutions. So, it would be highly beneficial to have a modification which produces unique solutions while maintaining the numerous benefits of the present algorithm. Regarding the work on graph autoencoder-based ROM, there are similar avenues for improvement. For one, it remains to determine the optimal way to simulate the reduced dynamical system that results after the input is encoded. The data-driven approach in [15] is seen to bottleneck the accuracy of the ROM in some cases, so it would be interesting to compare this with an approach based on standard Newton or quasi-Newton methods which may perform better. Note that the reduced-order modeling of PDEs is a well funded area; since our present work is funded through DOE grant DE-SC0020418, it is reasonable to expect that future projects in this area will also be of interest to the U.S. Department of Energy or other governmental organizations.

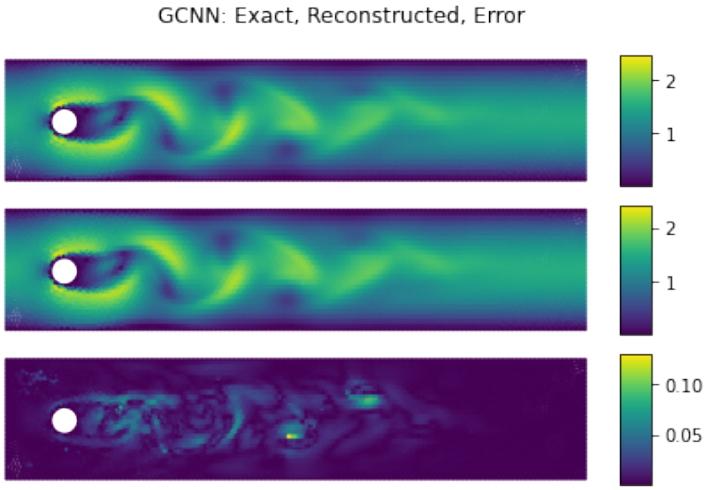

FIGURE 3: Speed profile of a solution to the Navier-Stokes equations (top) with 20208 degrees of freedom which is compressed via a novel graph autoencoder to 32 degrees of freedom and reconstructed (mid), along with the pointwise reconstruction error (bottom).

4 Optimality and Rigidity of Curvature Functionals

As previously mentioned, naturally encountered surfactant films and material interfaces often present themselves scientifically in accordance with physical conservation laws and least-action principles. When these ideas are translated to a mathematical setting, standard techniques in the calculus of variations can be used to describe such objects in terms of the minimizing critical points of a energy functionals that act on surface immersions. Of particular relevance to these problems are functionals which depend on the curvature of a surface, more specifically on its rigid-motion-invariant mean curvature H and Gauss curvature K. Originating with Poisson and Germain in the 1820s, the study of curvature functionals has led to a robust theory of elasticity which is applicable to physical quantities such as the holographic entanglement entropy in string theory [21], the free energy in liquid crystallography [28], and the Helfrich energy of biomembranes [20].

Due to the prevalence of curvature functionals throughout mathematics and physics, it is useful to have a general analytical framework which can facilitate a greater understanding of these objects while also streamlining some of the basic ad-hoc calculations repeated many times with minor variations in the literature. To that end, our work in [18] provides concrete expressions for the first and second variations of a generic curvature functional in a three-dimensional space of constant sectional curvature, as well as some rigidity results in the special case of the p-Willmore energy. The p-Willmore energy is a signed extension of the "L^p curvature functional" idea investigated in [25] which has significant utility in connecting important geometric functionals such as the area, total mean curvature, and Willmore functionals which appear as $p = 0, 1, 2$, respectively. Our general expressions specialize to a large number of functionals including these and are expressed in terms of only basic quantities coming from the first and second surface fundamental forms, making them usable to interested researchers without expert knowledge of geometric analysis.

Study of generic curvature functionals is continued in [19] with an increased emphasis on immersions of compact surfaces with nontrivial boundary. Motivated again by considerations from physics, we compute a conservation law which characterizes critical surfaces, as well as prove rigidity results for various boundary-value problems. As in [3, 27], our conservation law effectively reduces the order of the PDE for criticality, which should allow for the demonstration of existence results under lower regularity requirements (an avenue for future work). Interestingly, it is also seen that curvature functionals which remain invariant under dilation are (in some sense) significantly more rigid with respect to their critical surfaces, as a free-boundary critical surface which is rotationally-symmetric must either be spherical or satisfy very restrictive conditions on its first partial derivatives (c.f. [19, Theorem 1.1]). Applied to the case of the p-Willmore energy, this yields some surprising consequences. For one, it follows that round spheres are not minimizing for the p-Willmore energy when $p > 2$, though they are known to be globally minimizing for the usual Willmore energy. Even more surprisingly, it is seen that any p-Willmore surface with mean curvature zero along its boundary must be minimal when $p > 2$. This shows that there can be no closed p-Willmore surfaces when $p > 2$, and yields an interesting connection to minimal surfaces that is worth exploring in future work.

Another robust line of research in this area involves coupling the area functional with an elastic energy term at the boundary. This is known as the Euler-Plateau problem, which can be understood as looking for the soap films which span a pliable loop of "fishing line", and models the competition between the surface tension of the film and the buckling of the line induced at the boundary. In [17] we study a variation of this problem which includes an elastic modulus term in the interior, and prove that axially symmetric critical immersions and immersions of disk type are necessarily planar domains bounded by area-constrained elasticae. The key to this result is an argument based on the holomorphicity of the Hopf differential.

Continuing and Future Work: Ongoing work including [16] examines more general functions which couple interior and boundary behavior, with the goal of understanding their extrema. As mentioned above, it is also worth investigating in more detail the connection between minimal and p-Willmore surfaces, which may yield interesting insights into other physically relevant curvature functionals. Funding for work related to this area has previously been obtained (by mentors and collaborators) from the NSF and the Simons foundation.

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