Research Statement
Theory and Computation of Optimal Geometry

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My research in optimal geometry involves a unique combination of mathematical theory and numerical experiments. Traditionally, pure mathematics has proceeded from examples computed with pencil and paper; its progress has been measured entirely by theorems proved. Applied mathematics has dealt with numerical simulations of differential equations arising outside mathematics. I am in the vanguard of a new effort to use such numerical modeling techniques to solve problems in pure geometry. This involves careful computer experiments to generate and test conjectures about geometrical objects too intricate to explore by hand, followed by traditional formal proofs of these conjectures.

The mathematics I am interested in involves shapes of curves and surfaces, often in our ordinary three-dimensional space, which minimize different geometric energies. Of course, many real-world situations can be cast in the form of optimizing some feature of a shape; mathematically, these become variational problems for geometric energies. Thus most of the problems I have pursued for their intrinsic mathematical interest also turn out to be of interest to other scientists, including those studying foams, lipid vesicles, knotted DNA, crystal structures, and computer-aided design. The optimal geometries I discover often have aesthetically pleasing shapes, which can be illustrated well by computer graphics.

For the simplest geometric optimization problems, like the soap bubble which minimizes its area while enclosing a fixed volume, there is extensive classical theory. But for the more intricate problems I have studied, computer simulations are essential to gain insight, before a full mathematical theory can be developed. For my simulations, I have often used (and extended) Brakke's Evolver, which is an excellent software tool for shape optimization. It was originally designed for computing minimal surfaces by minimizing area; I have added features to allow it to minimize other quantities, such as Willmore's elastic bending energy and various knot energies.

Bubble clusters are examples of constant-mean-curvature (CMC) surfaces. My recent work with Große-Brauckmann and Kusner (to appear in *Crelle's Journal*) has classified the space of all complete embedded CMC surfaces with three ends and genus zero. This, we found, is naturally equivalent to the space of triples of points on the sphere. Our next project is to extend these results to CMC surfaces with more than three coplanar ends. My *PhD* student Pavel Groisman is currently working on a dissertation extending these results further, to handle certain symmetric surfaces with noncoplanar ends.

Foams can be thought of as infinite clusters of soap bubbles, and they minimize interface area while fixing certain enclosed volumes. Lord Kelvin proposed a candidate for the equal-volume foam of least interface area; in 1993, physicists Weaire and Phelan discovered a better solution. With Almgren and Kusner, I gave a rigorous proof that their foam indeed has less area than Kelvin's candidate, but a proof that it is optimal seems difficult. Many interesting related questions remain open. A large class of foams (including the Weaire/Phelan example) can be generated from the known chemical structures of transition metal alloys. I have undertaken numerical simulations of the foams in this family. The possibility of beating Weaire/Phelan seems remote, but these foams are related to many other intriguing mathematical problems regarding good triangulations of three-manifolds.

At Illinois, I have been involved in a joint project on foams (funded by NASA) with Aref, head of the mechanics department (TAM). With my *PhD* student Wacharin Wichiramala, I have run Evolver simulations (correlated with lab experiments at TAM) for foams with varying ambient pressure, applied shearing, gas diffusion, or moving obstacles. In May 2002, Wichiramala completed his PhD, having proved the planar triple bubble conjecture: the standard cluster does minimize perimeter. His new stability component bound will be a powerful tool for future work on bubble clusters.

Foams in three dimensions exhibit the Plateau singularities of soap films. For foams in higher dimensions, or foams with imposed symmetry, the possible singularities have not been classified. I have listed candidates in higher dimensions, and plan to do computations to decide which are successful: most will be ruled out by comparison surfaces, while the rest can be shown to work by numerically integrating calibrations. Kusner and I are working together to classify the singularities for symmetric foams, in different orbifolds; this will lead to a better characterization of the Kelvin foam.

More complicated than area-minimizing foams are surfaces which minimize an elastic bending energy. Mathematically, this is the integral of mean curvature squared, usually known as the Willmore energy. Cell membranes are complicated bilayer surfaces and seem to minimize this; for instance, the shape of a red blood cell can be explained by minimizing this energy while fixing both the surface area and the volume enclosed. The Willmore energy is invariant under conformal transformations of space, and biophysicists familiar with our work have observed lipid vesicles undergoing these nonrigid motions in the laboratory.

We have used the same energy to drive a minimax sphere eversion, from a round sphere, through a Willmore-critical halfway model, to the inside-out sphere. With Brakke, Francis and Kusner, I generated a series of minimax eversions with different symmetry. These were then illustrated in the computer graphics video *The Optiverse* which I produced at the NCSA with Francis and Levy. The Willmore flow is expected to be more stable than mean-curvature flow, and in our sphere eversions, the flow never pinches off any necks.

Loops of wire in space (which may be knotted) might be driven by the analogous bending energy for curves, but one can also imagine an energy resulting from spreading electric charge along the wire. An especially interesting modification of this electrostatic energy uses a nonphysical power in Coulomb's law, and has been shown to be (like the Willmore energy) conformally invariant. Global minimizers are known to exist for prime knot types, but little is known about their structure or about possible other critical points.

My experiments (with Kusner) on the conformal knot energy failed to find any unknot which does not evolve to the global minimum, a round circle. This leaves open the intriguing possibility that the energy-minimizing flow could provide a new proof of the Smale conjecture, untangling any unknot. But more experiments are needed; perhaps a more tangled starting configuration could get stuck. Kusner and I are have also looked into theoretical methods for renormalizing analogous energies for embedded surfaces, which we have already implemented numerically.

If we consider in particular the knot energy for geometric Hopf links, it reduces to an energy on finite configurations of points in the two-sphere, which turns out to be exactly the Coulomb potential. Therefore, understanding the Morse theory of this potential led us to discover the first example of a link type with two different local energy minima.

This equivariant Morse theory also gives a fascinating insight into the topology of the configuration spaces of points on the sphere, and we expect to be able to prove that the Coulomb potential is a perfect Morse function for up to six points, but not for more.

Our energy computations also suggest that the ordering of knot types by conformal energy agrees closely with the ordering found by biologists through gel electrophoresis on knotted DNA strands. With Kusner and Cantarella, I am examining other geometric quantities for space curves, also of interest to biologists, including various notions of thickness.

Perhaps an optimal shape for a knot is that which can be tied with the shortest length of rope; we have worked to make such a notion mathematically precise. Our preliminary report on this work in geometric knot theory was published in *Nature*. Our new paper, just published in summer 2002 in *Inventiones Math.*, proves the existence of ropelength minimizers for each knot type, and characterizes the shape of the minimizers for certain links. In future work we will define a notion of criticality for this nonsmooth energy, and demonstrate the existence of more than one critical point for certain knots.

In the course of studying these thick knots, we were led to define the second hull of a space curve, as the set of points doubly enclosed by the curve, in a certain precise sense. In a separate recent paper (to appear in *Amer. J. Math*), we show that any knotted curve has a nonempty second hull. This has beautiful connections to the Fáry/Milnor result on the total curvature of a knot, and to the study of minimal surfaces spanning the knot. My *PhD* student Elizabeth Denne is working on proving new results about quadrisecants of knots, which will give another proof of the second hull result, as well as better lower bounds for ropelength.

Whenever one performs computer simulations, one must worry about the accuracy of the numerical methods. Usually, the polyhedral surfaces used are thought of as approximations to smooth surfaces. But often notions from differential geometry can be given exact interpretations for polyhedra, like Gauss curvature which is the angle defect at vertices. Such geometric insights can lead to better numerical methods, and thus are of interest in computer-aided design. At Illinois, I have been the lead mathematician in the interdisciplinary Center for Process Simulation and Design (CPSD) funded by an ITR grant from NSF and led by Haber of TAM. The Center uses geometry to improve methods for meshing and numerics in engineering calculations.

In continuing to study geometric optimization problems, my research will explore the frontier of modern geometry. Problems that may be physically natural are still challenging from both theoretical and computational standpoints. The interplay between numerical experiments and rigorous proofs is what allows progress on both fronts. Those areas with greatest mathematical interest because of their intrinsic elegance (like CMC surfaces, Willmore surfaces and knot energies) also turn out to be important outside mathematics. I am just starting, with my collaborators, to explore this new territory; each discovery therefore presents many new avenues for further fruitful investigation. With the proper resources and opportunities, I intend to bring optimal geometry, and computational math in general, into its proper place in the forefront of mathematics in the twenty-first century.