Developing a Bifurcation Theory of Path-Constrained Optimal Control Extremals to Support Technological Development of Carbon Nanocoils

Motivation: Carbon nanocoils have exciting technological applications in the form of chemical sensors, supercapacitors, and flexible electronics [3]. However, their dynamics are not easily observed. Highly flexible macroscopic springs, such as toy Slinkies, are governed by similar dynamics and adopt equilibria that "jump" to very different configurations after small perturbations such as twist and extension. I spent the summer of 2019 at an **NSF-funded REU** at **Cornell University** studying such springs to gain insight into analogous behavior of carbon nanocoils. Using optimal control methods, I found stable and unstable equilibrium configurations of upright springs with twisted and vertically extended ends. By plotting the displacement of the centerline from the vertical axis against the height of the free end, I discovered saddle-node bifurcations that explained observed hysteresis (Figure 1). Spurred on by this exciting discovery, **I plan to develop methods for analyzing bifurcations of extremals of optimal control problems. I will then use these tools to understand the dynamics of carbon nanocoils.**

Background: Consider the path-constrained optimal control problem:

$$\underset{x,u}{\text{minimize}} \int_{t_0}^{t_f} L\big(x(t), u(t)\big)dt$$

$$\text{subject to} \frac{dx}{dt} = f(x,u), x(t_0) = x_0, x\big(t_f\big) = x_f,$$

$$g\big(u(t)\big) \geq 0$$

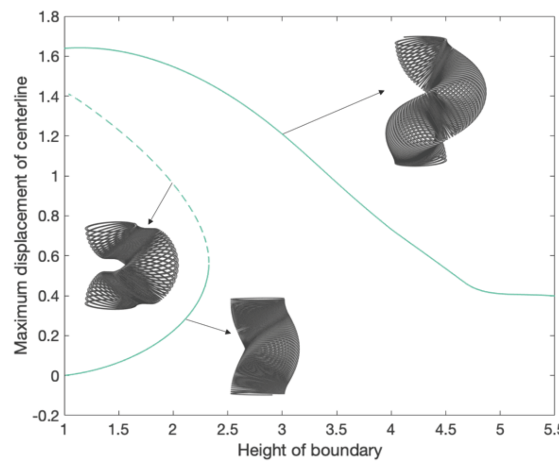

Figure 1: Stable and unstable equilibrium shapes of a spring with free end twisted 195° and raised. Once the height of the free end exceeds 2.3, the spring only adopts configurations corresponding to the top solution branch.

The Pontryagin Maximum Principle (PMP) gives extremals of the constrained cost functional, which are stable and unstable solutions of the optimal control problem. A flexible spring can be modeled as such a problem. Its equilibrium configurations maximize or minimize the potential energy L of the spring, subject to the dynamics f of the centerline, prescribed endpoints x_0 and x_f, and a nonlinear path constraint g that prohibits intersection of adjacent coils. The path constraint physically corresponds to contact between adjacent coils. This coil contact causes bifurcations and hysteresis in spring configurations (Figure 1). Path constraints vastly increase the difficulty of solving optimal control problems and preclude existing approaches for determining solution stability. Therefore, gaining a deeper understanding of unusual spring behavior requires more advanced methods for studying optimal control problems with path constraints.

Goal 1: Develop numerical methods to robustly solve path-constrained optimal control problems and determine solution stability. During my REU, I coded a MATLAB solver for the spring problem using the shooting method, but the path constraint impeded convergence. I will build on the new variational evolving method (VEM) in [2] to devise a robust VEM for solving general path-constrained problems. I previously developed numerical methods to find unstable extremals for springs, as path constraints prevent the use of existing tools for determining the stability of PMP extremals. These methods succeeded because the extremals were path-connected, which is true for any optimal control problem with a scale-invariant Hamiltonian [1]. I will extend this work by developing algorithms for path-constrained problems without the scale-invariance property and devising numerical stability conditions for general PMP extremals.

Goal 2: Develop bifurcation theory of path-constrained PMP extremals. In my previous work on twisted springs, I discovered bifurcations in the spring configurations in which the bifurcation parameter was the height of the spring's free end. Using this discovery as precedent, I want to develop a bifurcation theory of path-constrained PMP extremals. While infinite-dimensional bifurcation theory has been applied to related systems arising from the Euler-Lagrange equations [4], no analogous theory exists for path-constrained problems, which are more naturally studied using optimal control and the PMP. I plan to use the numerical methods developed in Goal 1 to find extremals of specific path-constrained problems and characterize their stability. Using these examples, I will develop analytical bifurcation conditions for path-constrained problems and implement this work in a robust software package.

Goal 3: Use the new numerical tools and bifurcation theory to predict behavior of carbon nanocoils. I will apply the optimal control spring model to carbon nanocoils by changing physical parameters in the energy function L and the path constraint g, and will use the numerical methods developed in Goal 1 to explore their configurations. I will validate the model and new numerical tools by comparing predicted configurations to those determined experimentally via a precisely controlled robot. I will then use the theory developed in Goal 2 to identify and classify bifurcations in the configurations of carbon nanocoils. In doing so, the following three objectives will be pursued: (i) predict continuous movements of the endpoints that lead to hysteresis, as carbon nanocoils must be able to reversibly deform to perform their functions; (ii) find continuous movements that cause the nanocoils to jump between qualitatively distinct configurations, as such jumps adversely impact nanocoil functions and are difficult to model precisely; (iii) find unstable extremals of the optimal control problem, as these extremals denote a dangerous unstable boundary between stable configurations. These predicted configurations and bifurcation analyses will support further technological applications of carbon nanocoils by avoiding undesired behavior.

Intellectual Merit: My proposed work will produce a robust optimal control method for path-constrained problems, expand the reach of bifurcation theory into the field of optimal control, and illuminate the dynamics of carbon nanocoils. As bifurcation theory predicts the effects of parameters on long-term solution behavior of dynamical systems, an analogous theory for extremals of optimal control problems will be an invaluable tool for multiple applications. I have the mathematical background to investigate such problems and the computational skill to develop software implementing the novel bifurcation analysis.

Broader Impacts: A bifurcation theory for extremals will explain unique behaviors, such as hysteresis, in any phenomenon that can be modeled as an optimal control problem. Identifying bifurcations of configurations is especially important for carbon nanocoils, which have exciting technological applications in the form of chemical sensors, fuel cells, supercapacitors, and flexible electronics [3]. In addition, the necessary experimental validation opens doors for interdisciplinary collaborations, such as with chemists synthesizing carbon nanocoils and engineers developing precise methods of robot control. Finally, many of the diverse tools and concepts involved in this work are accessible to motivated students of all ages, making it ideal for introducing them to new applications of mathematics and computation. I will encourage undergraduate involvement in my research, and I will use toy Slinkies to demonstrate this work in K-12 outreach settings, thereby helping to inspire the next generation of scientists.

References:

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