DIMACs REU Topics

The following projects would be supervised by Prof. Konstantin Mischaikow, Mathematics and members of his group including:

1. Prof. Marcio Gameiro
2. Prof. Ewerton Vieira
3. Hill Assistant Prof. Shane Kepley
4. Hill Assistant Prof. William Cuello
5. Postdoctoral Fellow Dr. Elena Queirolo

Studying switching systems via sloppy models

Reliably modeling the dynamics of regulatory networks is one of the most important challenges in modern systems biology. Numerous advances in molecular and systems biology has led to the identification of complex networks involving dozens of genes interacting with one another. On the mathematical side these networks are often modeled as systems of nonlinear differential equations. To analyze these networks requires a choice of nonlinearities and one popular choice involves Hill functions. A serious challenge is that the use of Hill functions for complex networks results in systems with tens to hundreds of state variables and parameters making it difficult or impossible to study the global dynamics.

This has led to the development of coarser modeling tools which incorporate combinatorial methods and algebraic topology into classical dynamical systems theory to study complex networks over large regions of parameter space. These coarse models are much more amenable to efficient, large scale computation, but at the same time, they can be systematically identified with the Hill function models.

In this project, we aim to explore computational methods for mapping between system parameters of the Hill function systems and coarse systems based on "sloppy models". Sloppy modeling is a framework for studying hierarchies of models using tools from differential geometry. In this framework, models are identified with manifolds and simplifications of these models arise naturally as boundaries of this manifold.

Our goal would be to design and implement a computational method based on sloppy modeling which provides a means for mapping parameters in coarse systems to manifolds of parameters in Hill systems which produce similar dynamics.

Domain decomposition for Taylor series ODE solvers

Solving nonlinear ODEs which arise in real world applications typically amounts to computing numerical approximations of solutions of interest. While many methods for computing these approximations exist, spectral methods are the gold standard due to the extreme precision they offer. However, this precision comes with an important trade-off. In contrast to implicit/explicit numerical integration techniques, time-stepping or *domain decomposition* for spectral methods is generally quite challenging.

One recent approach which has been successful for Chebyshev series expansions is to automatically compute an optimal domain decomposition. The approach uses techniques from functional and complex analysis to characterize optimality as a zero finding problem in an infinite dimensional Banach space which can be solved using a Newton-like iterative scheme.

This research project will focus on developing a similar technique for Taylor series expansions. We will first focus on implementing a Taylor ODE solver in Julia, Python, or MATLAB. Having finished this, our next goal is to develop a general time-stepping scheme based on adapting the approach used for Chebyshev expansions. Once this is incorporated into the Taylor ODE solver, we can explore some more sophisticated challenges, for example, extending the method to include (spatial) domain decomposition for ODEs with parameterized curves (or higher dimensional manifolds) of initial data.

Finding Hopf bifurcations in the Lorenz84 system

E. N. Lorenz produced several simple models for fluid dynamics that even today are used as conceptual models for weather. Of course, these models attained fame because they exhibit complex (chaotic) dynamics. One of the simplest hallmarks of this type of dynamics is the existence of (infinitely) many unstable periodic orbits. However, identifying the existence of these periodic obits is a challenging task for at least two reasons. First, they are unstable and so they will not be observed using direct numerical simulations. Second, their existence is parameter dependent, i.e. they exist for some parameters but not for other. In contrast, if a periodic orbit is found then a numerical technique called the continuation method allows one to track the periodic orbit as parameters are changed.

There are multiple ways in which a periodic orbit can appear or disappear as a parameter is changed. The best understood is via a Hopf bifurcation, this when a periodic orbits grows out of fixed point. Furthermore, the Hopf bifurcation can be identified by specific algebraic conditions.

We propose to study the question of the existence of periodic orbits in the Lorenz84 system. This system has 4 parameters and in Lorenzs original paper he kept three parameters fixed and varied the parameter that corresponds to asymmetric thermal forcing. Our first goal is to numerically find all Hopf bifucations when, following Lorenzs example, we only vary this one parameter and then rigorously verify this numerics. Our next goal is to build on this result. Having found a Hopf bifurcation we hope to identify hypersurfaces of Hopf bifurcations as the other parameters are allowed to vary. Finally, if these hypersurfaces of Hopf bifurcations intersect, then we obtain degenerate Hopf bifurcations that can result in much more complicated dynamics. Can we find these degeneracies and understand the resulting dynamics?

An alternative approach to predator-prey and multi-species stability analysis

Mathematical ecologists have traditionally explored predator and prey dynamics using ordinary differential equations (ODEs). These ODEs typically include functional components that capture non-linear interspecies interactions. For example, one can incorporate predator interference amongst individuals to dampen the per-capita reward of finding prey. Adding such complexity, however, can make the system harder to analyze with traditional stability analysis; the functional components are often-times parameterized with unknown quantities, and changes in these quantities can lead to qualitatively different global dynamics. Some parameter values can lead to coexistence. Others can lead to extinction of one or the other. Depending on the number of non-linearities and the number of species, completely categorizing each region of parameter space into their respective long-term dynamics can be difficult.

To address this problem, we propose that we study an approximate system. Here, we replace the non-linear, functional components with simple step functions. We can then use recently developed tools from combinatorics, algebraic topology, and dynamical systems theory to solve for long-term solutions of the system in different parameter regimes. We are then confronted with some natural questions: are the dynamics of both systems qualitatively the same under various parameter regions? Can one extend this to trophic cascades, systems of multiple species with a hierarchy of predation?

Identification of bifurcations using algebraic topology

The Conley index, an algebraic topological generalization of the Morse index, is a powerful tool for the analysis of dynamics over ranges of parameter values. The strength arises from three properties:

1. The Conley index is defined in terms of regions of parameter space and the behavior of the vector field on the boundary of the region, rather than the detailed structure of individual orbits or invariant sets.

2. Knowledge of the Conley index provides information about the existence and structure of invariant sets.

3. The Conley index remains constant under perturbations of parameters.

Because of the first property and second property, appropriate decompositions of phase space allow one to use the Conley index to obtain a characterization of the global dynamics. The second and third property allow one to identify global *bifurcations* (changes in the dynamics) over large changes in parameter by identifying changes in the Conley index information.

This index is a standard tool in the analysis of invariant sets in dynamical systems, and its significance owes partly to the fact that it is invariant under local perturbation of a flow (the continuation property). Typically, one does not investigate a single invariant set in a dynamical system but rather works with decompositions of a larger invariant set into invariant subsets and connecting orbits between them.

New computational tools based on combinatorial descriptions of dynamics are capable of identifying the appropriate decompositions and new computational homology tools can compute the Conley indices. The goal of this project is to use these tools to identify bifurcations in models of biological systems involving high dimensional parameter spaces.