Summer@ICERM 2026 Project Descriptions
Pure and Applied Mathematical Models

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Program Abstract

Mathematical modeling allows one to describe dynamics of the real world by translating the knowledge and beliefs of interactions into the language of mathematics. For this reason, mathematical modeling is not only a useful technique for describing natural occurrences, but it also allows one to address questions and test hypotheses that may not be feasible to study in reality. In general, modeling requires compromise. In order to avoid complicated systems, mathematical modelers must first identify the most important components of a system to include in the model, excluding everything else. Even with these simplifying assumptions, mathematical models can be used to develop scientific understanding, test the effect of changes in a system, and aid in decision-making. The proposed Summer@ICERM 2026 projects center around three approaches to mathematical modeling in both pure and applied mathematics spanning epidemiology, graph theory, and combinatorics.

1 Disease Transmission and Control in Local Communities

This project will investigate the community transmission of *Clostridioides difficile* (*C. difficile*) using both systems of ordinary differential equations (ODEs) and agent-based models (ABMs) in order to determine optimal strategies for mitigating the spread of this bacteria. While *C. difficile* remains one of the most common causes of healthcare-associated infections in the United States [33, 51], data from the CDC's Emerging Infections Program has shown a decrease in the overall burden of *C. difficile* in both healthcare settings and long-term care facilities (LTCFs) from 2011 to 2017. During that same period, no such decrease occurred in community-associated infections, which accounted for nearly 50% of the burden of *C. difficile* infection (CDI) in 2017 [21].

Many mathematical models using ODEs have previously been developed to represent nosocomial transmission [5, 9, 23, 24, 32, 35, 50, 58, 59, 60]; however, models of *C. difficile* community spread are scarce [33]. Furthermore, increased awareness of the role of environmental transmission in the spread of some pathogens has led to increased development of models that incorporate environmental components [4, 9, 10, 12, 32, 50, 51, 60, 66]. Our ODE model of *C. difficile* spread in a hospital ward [60] was the first of its kind that explicitly incorporated the environmental contamination of surfaces with two environmental compartments in addition to the more standard patient classes. Of those models of *C. difficile* in communities [29, 30, 41, 44, 46], only Otten et al. [46] incorporated an environmental transmission pathway; however, they have not calibrated this model with epidemiological data.

Following up our work in [60], we have since developed ABMs of *C. difficile* transmission in both hospitals [38] and LTCFs [6], along with an ODE model of its spread in LTCFs [13]. Central to our work, we have incorporated the effect that environmental surfaces contribute towards the spread of disease. In this proposed research, we aim to continue examining the impact of environmental contamination on the spread of *C. difficile* by modeling its transmission within localized communities using multiple models, such as individual community models, LTCFs in combination with hospitals, and communities in combination with hospitals and/or LTCFs. Since

we have developed mathematical models of disease spread in hospitals and LTCFs, much of the structure of the new models can be based on these past models. New parameter values will need to be collected along with updated assumptions about transmission pathways in the community to ensure that the proposed mathematical models remain feasible.

Recommendations from mathematical models regarding disease control are sensitive to underlying assumptions, and there are trade-offs when choosing different modeling techniques. Widely-used ODE models assume common behavioral interactions and typically assume direct transmission from infected to susceptible individuals. Such models typically do not account for spatial heterogeneity, a key feature of the epidemiology of a pathogen with an environmental reservoir, such as *C. difficile* [47, 57, 63, 64]. Conversely, ABMs consider the individual behaviors of system components by defining a set of rules that govern how individuals interact on a spatial grid. These types of models rely heavily on probabilities, which allow for the randomness of individual decision-making to be simulated. By developing mathematical models using both techniques, the analysis of both models can be compared to determine the most effectual strategies for mitigating the spread of *C. difficile* in communities, especially with movement between a hospital and LTCF.

After developing the system of ODEs, we will use a combination of literature review and estimation techniques, such as the method of least squares, to determine appropriate parameter values for our model. We will then analyze the ODE model with a global sensitivity analysis [43] using Latin Hypercube Sampling and Partial Rank Correlation Coefficients to determine which parameters lead to the greatest changes in the incidence of colonization. The results of the sensitivity analysis will inform potential control strategies to mitigate disease spread and be the basis for applying Optimal Control Theory, a method that will allow us to determine time-optimal varying parameters that most effectively reduce incidence of colonized and diseased [37]. Model simulations and analysis will be completed using MATLAB. Students with knowledge of calculus and the interpretation of derivatives can succeed in this project even without explicit study of differential equations. Programming experience is a bonus but is not required for successful completion of this project.

The ABM will be built in NetLogo which works on a grid where each patch on the grid can be labeled to represent its type. The considered communities will be gridded and translated into the NetLogo Graphical User Interface (GUI). After developing the foundation of the ABMs, we will incorporate agents with individualized characteristics. Every ABM consists of submodels that dictate the movement between agents. To replicate interactions within the community, we will code procedures that dictate how an individual operates daily. Due to the stochasticity embedded in ABMs and to best assess the impact of the control intervention strategies, we will run 100 iterations over a one-year simulated time period with each combination of parameter values (representing different control strategies). The model will be run on a fifteen-minute time-step using the BehaviorSpace tool in NetLogo, which allows us to specify the various parameter combinations we want to simulate and the resulting outputs of interest. Because of the computing power required to run these simulations, we will utilize parallel processing and high performance computing. These simulations will aid in evaluating effective interventions for reducing disease and colonization incidence. Students do not need programming experience to be successful in this project, but it is a bonus.

2 Graph Theoretical Modeling of DNA Self-Assembly

DNA self-assembly is a rapidly advancing field with the unique properties of double-stranded DNA molecules making DNA a valuable structural material from which to form nanostructures, a process integral to the field of DNA nanotechnology [48, 56, 55], including numerous polyhedra [8, 22, 25, 61, 69], arbitrary graphs [27, 52, 65], and a variety of DNA and RNA knots [39, 40, 62]. This project explores the graph theoretical and combinatorial properties of DNA self-assembly which are used to form nanostructures. These nanostructures offer promise for emergent applications in nanoelectronics, biosensors, biomolecular computing, drug delivery systems, and directed organic synthesis, which lead to more effective diagnosis and treatment of illness [1, 14, 16, 17, 20, 28, 31, 42, 45, 55, 67, 68]. The introduction of a graph theoretical formalization for exploring the combinatorial properties of self-assembly of DNA molecules was first introduced by Jonoska et al. [26]. A *branched junction molecule* whose flexible k-arms are strands of DNA is represented in the abstract as a *tile*, which becomes a vertex of degree k in a graph. We represent the complementary cohesive-ends or *bond-edges* of these tiles using letter labels. For example, bond-edge types a and $\hat{a}$ represent complementary sequences of bases (see Figure 1). This allows us to combinatorially represent a k-armed branched-junction molecule with bond-edge types $a_1, ..., a_k$ using a tile $t = \{a_1, ..., a_k\}$. We call a collection of tiles (each of which can theoretically be used "infinitely many" times) a *pot*.

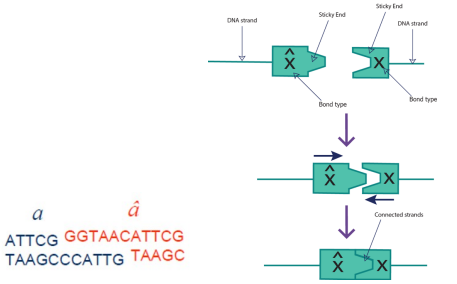

Figure 1: Representation of the complementary cohesive end types (left) and the formation of bond-edges (right).

The central focus of research with the flexible-tile model of DNA self-assembly is the efficient construction of certain target complexes (see Figure 2). This generally involves finding accurate bounds for the number of tile types and bond-edge types in pots constructing selected graphs. Given a target graph G, one can seek to determine the minimum numbers of tile and bond types needed to construct the graph under various constraints [15]. This application of graph theory is both relevant and enticing given the wide range of uses DNA self-assembly has in biomedical applications. These research projects revolve around the exploration of the graph theoretical and combinatorial properties of DNA self-assembly, as well as the development of computational tools to aid in answering fundamental questions that arise. This project lends itself well to computational experimentation. In particular, linear algebra and programming are used to help answer our fundamental questions. Given a pot P of tiles, in order for a complete complex to be formed and no smaller graph to be formed, the proportions of different tile types must satisfy a system of equations often represented as an augmented matrix called the *construction matrix*, denoted $M(P)$ [15, 26]. The construction matrix is a useful way to determine whether pots can generate graphs smaller than the target graph.

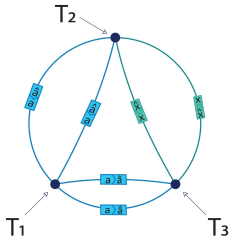

Figure 2: Example of a graphical representation of a complete complex constructed from pot $P = \{T_1 = \{a^4\}, T_2 = \{\hat{a}^2, x, \hat{x}\}, T_3 = \{\hat{a}^2, x, \hat{x}\}\}$.

There is also a need for exhaustive searches for specific solutions and for creating algorithmic approaches to solutions, such as those found in [3, 14, 15, 18, 19, 49]. This particular program will build off the progress from the 2023 Summer@ICERM Program and focus on the exploration of the graph theoretical and combinatorial properties of DNA self-assembly, as well as the development of computational tools to aid in answering fundamental questions that arise. Students do not need programming experience nor have any experience in graph theory or linear algebra to be successful in this project, but having experience in an introduction to proofs course would be very helpful for this project.

We expect students in this project to create, expand, and improve current software and proof methods used to find and check optimal solutions for k-regular graphs and graphs which exhibit multi-dimensional growth. Additional information can be found below.

Potential Project Descriptions

Finding Optimal Pots for k-Regular Graphs: In 2014 Ellis-Monaghan et al. [15] showed that for any k-regular graph G, $T_1(G) = 1$ or 2 if k is even or odd, respectively. Some examples of k-regular graphs have been explored in Scenarios 2 and 3, such as cycle graphs, Platonic Solid graphs, and the Rook's graph [2, 15, 18]. However, no overarching theory regarding general optimization strategies for k-regular graphs in Scenarios 2 and 3 exists. One of our research goals is to find explicit pots of tiles for certain families of k-regular graphs and search for patterns common to pots of tiles for k-regular graphs and establish conjectures regarding bounds for bond-edge and tile types in Scenarios 2 and 3.

Determine Optimal Pots for Graph Families Exhibiting Multi-Dimensional Growth: Families of graphs that exhibit growth in two or more distinct ways or "dimensions" have proven especially challenging when determining optimal pots for Scenarios 2 and 3. For example, in [19] it is shown that for the Lollipop and Tadpole graph families the values for Scenario 2 have nuanced dependence on both the order of the complete or cycle subgraph and the extending path subgraph. We aim to find explicit pots of tiles for certain graph families with multi-dimensional growth, such as lattice graphs, fan graphs, Mongolian tent graphs, and stacked book graphs.

List of Proposed Research Topics

1. Optimize design structures for families of graphs such as graphs with multiple growth patterns and k-regular graphs.

2. Create, expand, and improve the current software used to find and check optimal solutions.

3 Combinatorial Models for Kostka-Foulkes Polynomials

In the field of algebra, we often use certain polynomials to classify, or even just count, abstract structures. Kostka-Foulkes polynomials count certain multiplicities in representation theory, and they come in four classical types: A, B, C, and D, corresponding to root systems of the same names. It has long been known that these polynomials have non-negative integer coefficients. This was explicitly shown for the Kostka-Foulkes polynomials of type A through the use of a statistic

called *charge* [34]. However, it has been a long standing problem to explicitly show this non-negativity in types B, C, and D. In this project, we will consider a recently developed statistic on Kostka-Foulkes polynomials that is equivalent to the charge in type A but was designed to extend to the other types more easily [36].

As opposed to the previous attempts using tableau models, this new statistic is based on the definition of a Kostka-Foulkes polynomial as an alternating sum over certain vectors called *Kostant partitions*. The new statistic constructs, via *crystals graphs* (combinatorial models for representations of quantum groups in the form of colored directed graphs [7]), a sign-reversing involution which cancels all the negative terms in the alternating sum mentioned above. The resulting positive expansion expresses the corresponding Kostka-Foulkes polynomial in terms of a simple statistic on the uncanceled Kostant partitions (namely, the number of *parts* of the Kostant partition).

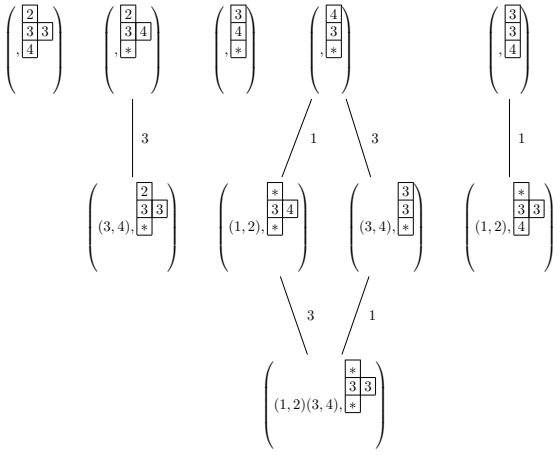

Figure 3: An example corresponding to a type A Kostka-Foulkes polynomial $t^2+t^3+t^2+t^3+t^4-t^2-t^3-t^2-t^3+t^2$ which simplifies to t^4+t^2, whose terms correspond to the two singleton components with four and two filled values, respectively.

In practice, this is done by modifying the associated crystal graphs in such a way that the vertices correspond to the terms in the Kostka-Foulkes polynomials. Each vertex comprises of a Symmetric group element and a combinatorial interpretation of a Kostant partition which together correspond to a term in the original polynomial (the number of filled boxes is the power of the term with its coefficient being the sign of the symmetric group element). A matching on each connected component corresponds to the cancellation of terms in the polynomial. The singleton components of the graph then give way to the simplified version of the polynomial (see Figure 3). The important aspect of this new model is that it relies on the underlying crystal theory, which is primarily independent of the crystal type (referring to the types A, B, C, and D).

Students will learn about root systems in all four classical types (visualizing them as vectors in $\mathbb{R}^n$), the associated Weyl groups (viewed as signed permutations), and their associated crystal structures (certain colored directed graphs with Kostant partitions as vertices). They will then build off existing Python code that extends the type A model from [36] to types B, C, and D using crystal structures which were developed in [11, 53, 54]. The heart of the project will be to discern a matching on these encoded crystal graphs which successfully describe the desired cancellation of terms in the corresponding Kostka-Foulkes polynomials in types B, C and D. Students do not need programming experience to be successful in this project, but it is a bonus. Having had a semester of Linear Algebra or Multivariable Calculus prior the program would be beneficial.

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