Graduate Student Poster Session

AMS Central Section Meeting
University of Iowa
March 18, 2011

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Title: Spacer Sequence and DNA Topology Determine Cre-Recombination Efficiency with Symmetric Lox Sites
Exhibitor: Aarti Balasubramani, University of Texas at Dallas
Abstract: The Cre recombinase of bacteriophage P1 mediates site-specific recombination between a pair of native loxP sites. The loxP sequence consists of an 8-bp asymmetric spacer and two flanking 13-bp inverted repeats, which function as Cre-recombinase binding sites. Spacer asymmetry directs the outcome of the recombination reaction generating either deletion or inversion events exclusively with circular DNA substrates. We are interested in identifying lox sequences having symmetric spacer sequences that yield both deletion and inversion products with equal probability from the same DNA substrate in the absence of conformational constraints. We have systematically investigated the efficiency of intermolecular Cre recombination for a large subset of all possible symmetric lox sites. Recombination efficiencies vary strongly among these variant lox sites; moreover, recombination appears to be sensitive to the topology of the substrate in intramolecular reactions with circular substrates. Information about the dependence of Cre recombination on spacer symmetry, sequence, and global DNA topology is valuable in designing experimental strategies that employ Cre recombination as an assay for DNA-loop formation in vivo.

Title: Engineering Multiple Site-specific Modifications in Supercoiled DNAs
Exhibitor: Anusha Bharadwaj, University of Texas at Dallas
Abstract: Important biological processes such as DNA recombination, replication, and gene expression involve specific interactions between one or more DNA-binding proteins and multiple protein-binding sites along a single DNA molecule. Such interactions lead to the formation of a topologically closed DNA loop between protein-recognition sites, whose energetics depends on the structure and the flexibility of the intervening DNA, the degree of supercoiling, and the binding of additional proteins such as HU and Fis in bacterial systems or histones and HMG proteins in the case of eukaryotic cells. Few biophysical techniques are available for characterizing DNA looping in vitro or in vivo. We present here a novel technique for incorporating multiple modifications such as covalently attached fluorescent probes to multiple defined sites within covalently closed DNA molecules. Applications of this technology include the use of bulk and single-molecule FRET techniques to investigate the effects of DNA supercoiling on lac-repressor-mediated DNA looping both in vitro and in vivo.

Title: Modeling and Analysis of the Dynamics of the Unfolded Protein Response (UPR) in Mammalian Cells
Exhibitor: Danilo Diedrichs, University of Iowa
Abstract: The Unfolded Protein Response (UPR) is a complex dynamical mechanism present in mammalian cells, which is triggered when the cell is subjected to stress leading to an accumulation of unfolded or misfolded proteins in the endoplasmic reticulum (ER). The primary functions of the UPR are to sense any perturbation in the protein-folding capacity of the cell,

and correct the situation to restore homeostasis. A mathematical model of the UPR was developed in collaboration with experimental cell biologists and calibrated based on experimental data. This model uses a system of nonlinear ordinary differential equations (ODEs) to model the UPR as a dynamical network of interacting proteins, including the positive and negative feedback loops between them. The model tracks the concentrations of the unfolded proteins throughout the response, as well as the other UPR main proteins and complexes, such as BiP (chaperones), eIF2 (translation initiation factor), and GADD34 (growth arrest and DNA damage protein). Several types of ER stress can be assumed as input, including long-term and periodic stress. The model can be used to better understand the UPR mechanisms leading to outcomes ranging from cell survival to apoptosis.

Title: Knots Resisting Reptation
Exhibitor: Mike Dupuis, University of St. Thomas
Abstract: We have developed a model for measuring a given knot's resistance to reptation. Our approach focuses on measuring the sum of the friction generated at points of knot self-contact. These friction measurements are produced by applying a modified version of Eytelwein's Capstan equation. Our future goals include evaluating the security of physical knots in multiple contexts.

Title: A Polynomial Invariant of Spacial Graphs
Exhibitor: Egor Dolzhenko, University of South Florida
Abstract: DNA rearrangements in certain species of ciliates can be modeled by so-called assembly graphs together with a set of operations on these graphs. We use these to construct assembly polynomials. Properties of the assembly polynomials are related to the structural properties of the assembly graphs. For example, every decomposition of an assembly graph defines a factorization of the corresponding assembly polynomial. We also investigate a relationship of these polynomials with the circle graphs.

Title: Direct Entropy Calculations for Discrete Wormlike Chains
Exhibitor: Stefan Giovan, University of Texas at Dallas
Abstract: 2Molecular simulations are often aimed at calculating the free energy for a given system, $F=U-TS$. Entropy, S, is the logarithmic measure of the number of accessible microstates and is generally a difficult calculation for continuum models. Quasi-harmonic (QH) analysis is one method which has been applied to molecular dynamics (MD) trajectories to provide an upper-limit estimate for S from measured variances of atomic coordinates. For problems involving time scales much longer than those modeled by MD, Monte Carlo (MC) simulations are more suitable. Current methods of calculating F from MC ensembles are computationally expensive.2We describe a QH analysis of discrete wormlike chains (dWLCs) that provides an upper-bound estimate of S from individual MC ensembles and show how the method can be applied to simple systems (e.g., coupled harmonic oscillators and ideal dWLCs). Future applications include estimating DF of DNA looping in complex nucleoprotein assemblies.

Title: Explicit Calculation of Tight Knot Configurations
Exhibitor: Joshua Henrich, University of St. Thomas
Abstract: To date there have been no explicit characterizations of any non-planar tight knot configurations. We analyze the simplest case, that of a 6-edge trefoil knot. Using an approximately tightened configuration from the software Ridgerunner, we construct a system of equations based on the set of tube contacts to solve for the tight configuration.

Title: Tangle Equations
Exhibitor: Garrett Jones, University of Iowa

Abstract: A 2-string tangle may be thought of as a 3-ball with two arcs properly embedded. In knot theory, the use of tangles and equations involving them has been extensive. Additionally, tangle equations have been used to model physical phenomena; for example, modeling the action of specific enzymes on DNA. Solving tangle equations can be interesting and involve various concepts from topology. This poster will discuss basic ideas surrounding tangles and tangle equations with a focus on a particular type of tangle called, Eudave-Muñoz tangles.

Title: Knot Distance Calculation Using the Jones Polynomial.
Exhibitor: Hyeyoung Moon, University of Iowa

Abstract: The knot distance between two knots is defined as the minimum number of crossing changes required to convert one knot to the other. Knot distances are related to the study of topoisomerase action and the study of knot theory such as conjectures on unknotting numbers. Topoisomerases are enzymes that break one or two strands of DNA and pass another segment of DNA through the break before resealing it. In other words, these enzymes are involved in changing crossings of DNA knots. Using some mathematical theories and computer programming, knot distances have been calculated and tabulated for rational knots, composite of rational knots up to 13 crossings and 8 crossing nonrational prime knots. However, some knot distances are still undetermined. I used the Jones polynomial to improve lower bounds of signed knot distances and thus knot distances.

Title: Tight Knot Geometry and Disentanglement
Exhibitor: Jake Seltz, University of St. Thomas

Abstract: The present research investigates how Type-2 DNA topoisomerases disentangle knotted DNA strands. It is known that enzymes called topoisomerases are highly effective at disentangling DNA. Many researchers believe that topoisomerases are able to effectively unknot DNA strands by acting on specific DNA clasps which hold geometric characteristics advantageous to disentanglement.
For this project, a computer algorithm was built which mimics the hypothesized actions of Type-2 topoisomerases. The algorithm selects high curvature juxtapositions of chosen knots and attempts to disentangle them by passing the knot strands through one another at high curvature juxtapositions.

Title: Using Combinatorial Methods to Determine Universal Deformation Rings
Exhibitor: Shannon Talbott, University of Iowa

Abstract: Deformation theory studies the behavior of mathematical objects, such as representations or modules, under small perturbations. This theory is useful in pure and applied mathematics and has led to the solution of many long-standing problems. In particular, in number theory, Wiles and Taylor used universal deformation rings of Galois representations in the proof of Fermat's Last Theorem.
In this poster, we want to use combinatorial methods to determine universal deformation rings of representations. Quivers, which are directed graphs, provide a combinatorial framework for the study of representations of algebras. We consider a special class of algebras, called special biserial algebras, which are defined by certain quivers and relations, and for which all representations are given combinatorially using so-called strings and bands. We will show how to determine the universal deformation rings for certain representations given by strings.

Title: Topological Characterization of Knots and Links Arising as Products of Site-Specific Recombination Reactions on Twist Knot Substrates.
Exhibitor: Karin Valencia, Imperial College London
Abstract: This poster presents a new a model characterizing all possible knots and links arising from site-specific recombination starting with a twist knot substrate, extending previous work of Buck and Flapan. We show that all knot or link products fall into three well-understood families of knots and links. Finally, in the (common) case of twist knot substrates whose products have minimal crossing number one more than the substrate, we show that the types of products are tightly prescribed.

Title: Tangle Tabulation
Exhibitor: Guanyu Wang, University of Iowa
Abstract: A knot is the image of a circle (i.e, a closed arc) embedded in 3-dimensional space. Tangles are similar to knots, but consist of strings whose endpoints are \nailed down" on the boundary of a 3-dimensional ball. In knot tabulation, knots are tabulated using crossing number (the minimal number of crossings needed to draw the diagram of a knot/tangle). In a similar manner to knot tabulation, we are creating a table of two string tangles ordered/categorized by crossing number. A sequence of numbers is used to represent a tangle which can be visualized by using the software KnotPlot. From there, code is being implemented to generate various invariants, each of which is a quantity that is the same when computed from dierent descriptions of a knot/tangle. A webpage is being developed in which users can create a table of tangles and their dierent invariants.

Title: Modeling Almond Pollination by Two Interacting Bee species with Cross- and Self-Diffusion.
Exhibitor: Kamuela Yong, University of Iowa
Abstract: California's almond industry is one of America's4top agricultural exports valued at $1.9 billion per year. Successful production of almonds depends on the pollinator services of primarily honeybees, although pollination by wild bees is being investigated as an alternative because of recent problems with honeybees. We are modeling pollinator services of honey and wild bees, as well as4their interactions in almond orchards. We use the Shigesada-Kawasaki-Teramoto model (1979) which describes the density of two species in a two-dimensional environment of variable favorableness with respect to intrinsic diffusions and interactions of species. We apply the model to almond pollination by wild and honey bees with environmental favorableness based on empirical data measuring the attractiveness of the canopy for honey and wild bees. Using the spectral-Galerkin method in a rectangular domain, we numerically solved the 2D nonlinear parabolic PDE and examine the result of varying the parameters. We hope to determine what circumstances the presence of wild, solitary bees can increase the dispersion of honeybees, thus increasing pollination.