

REU Seminar Series

Wednesday 2:30pm, Nesbitt Room

July 26

Daniel Solano

(Mentor: Silas Alben)

Title: *Long-time Simulations of Vortex Sheet Dynamics*

Abstract: We use unsteady two-dimensional vortex sheets to represent large-scale separated flows such as the vortex wake behind an airplane. In our computations, a continuous vortex sheet is approximated by an array of Lagrangian points whose motions are governed by the discretized Birkhoff-Rott integral. During the simulation, we use an Adaptive Mesh Refinement (AMR) technique to help resolve the dynamics of the vortex sheet; new points are inserted when adjacent Lagrangian points move far apart. However, the computational cost increases rapidly as more Lagrangian points are added. The aim of this work is to explore effective point insertion & deletion algorithms that make the computation efficient while maintaining sufficient accuracy of the vortex sheets to perform long time simulations.

Adam Holeman & Jennifer Natalia Jones Baro

(Mentor: Harrison Bray & Caleb Ashley)

Title: *Random Walks on the Fundamental Group of the Once Punctured Torus*

Abstract: We will give an introduction to random walks on groups. Of primary interest is the long term behavior of a random walk on the fundamental group of the punctured torus; in particular, the average amount of time a random walk spends near the puncture. By introducing a systematic way of symbolically representing geodesics in the universal covering space of the punctured torus, we aim to better understand the asymptotic behavior of random walks. Using these symbolic codings of geodesics we prove that a random walk associated to a simple closed curve on the once punctured torus on average spends no time in the cusp. The talk will conclude with one or more conjectures.

Jingzhen Hu

(Mentor: Robert Krasny)

Title: *Computation of pKa based on Poisson-Boltzmann equation*

Abstract: Protein molecules in the human body are naturally surrounded by water containing dissolved salt. The ability of a protein active site to exchange protons with the surrounding solvent is characterized by the acid dissociation constant pKa. The pKa value can be obtained from the electrostatic free energy of the system by solving the Poisson-Boltzmann equation (PBE) for the electrostatic potential with appropriate boundary conditions. We use the treecode-accelerated boundary integral (TABI) solver which employs a well-conditioned boundary element formulation on the linearized PBE, and GMRES iteration to solve the linear system with matrix-vector product cost reduced from $O(N^2)$ to $O(N \log N)$. The computed pKa of ovomucoid third domain (OMTKY3) is close to the experimental result.

Ben Gould

(Mentor: Wouter van Limbeek)

Title: *Right-angled Artin subgroups of mapping class groups*

Abstract: Right-angled Artin groups (RAAGs) are simple examples of groups obtained from graphs: the RAAG associated to a graph G is generated by the vertex set of G , and two generators commute when their corresponding vertices are adjacent. RAAG subgroups of mapping class groups, the group of orientation-preserving homeomorphisms of a surface up to isotopy, form a rich class of algebraic and geometric objects. Some well-known constructions for embedding RAAGs into mapping class groups will be discussed, along with our research to find "better" embeddings by bounding topological invariants of the surface into whose mapping class group we are embedding RAAGs.