NDnano
Notre Dame Nanoscience and Technology

NDnano Undergraduate Research Fellowship (NURF)
2024 Project Summary

1. Student name & home university: Abbass H. Mourtada | University of Notre Dame

2. ND faculty name & department: Professor Dervis Vural | Physics department

3. Summer project title: Complex Systems and the Life and Death of Strongly Interacting Populations

4. Briefly describe new skills you acquired during your summer research:

- Gained the ability to read and write code in Python and Mathematica
- Exposed to conducting firsthand research
- Practiced reading scientific articles and writing literature reviews
- Learned theory in evolutionary thermodynamics and information theory

5. Briefly share a practical application/end use of your research: This research allows development in ecosystem dynamics meaning producing better management strategies for sustainable use of natural resources and conservation of endangered species. Another example is disease modeling, where pathogen evolution and antibiotic resistance can be simulated giving a deeper understanding of the illness and thus providing insights to combat illnesses and develop more effective treatments. A third of the numerous applications is its use in industry for optimizing biological processes such as fermentation and biofuel production by applying thermodynamic models, enhancing efficiency and yield.

6. 50- to 75-word abstract of your project: On the path of modeling biological processes through transcribing them to mathematical systems, one might encounter difficulty in producing analytical results due to the complexity of the math in use. To avoid such a hindrance, the utilization of thermodynamics comes in handy. This research provides an application of thermodynamics to evolutionary biology. This application answers the question: What is the change in the phenotype distribution of a species due to a change in entropy from the sun?

7. References for papers, posters, or presentations of your research: NDNano presentation.pdf

One-page project summary that describes problem, project goal and your activities / results:

Applying mathematical models to biology can be surprisingly difficult due to the complexity of biological systems. Analytical results often become nearly impossible to produce because of the intricate mathematics involved. Thermodynamics offers a solution, especially in modeling evolutionary biology. Its principles, rooted in energy and matter transformations, provide a framework that accommodates the dynamic nature of biological systems. This approach helps understand energy flows and transformations driving evolutionary processes.

The research I am conducting, under the provision of Prof. Vural, entails building a “thermodynamically realistic” model of basic evolutionary dynamics. This would allow us to formulate tools like the first law of thermodynamics to answer the question: What is the change in the phenotype distribution of a species due to a change in entropy incoming from the sun?

After a series of lectures by Prof. Vural on the basics of the field, I had to work with a version of the Kolmogorov-Chapman equation known as the Kolmogorov forward equation or Fokker–Planck equation. My task was to solve the partial differential equation both analytically and using Mathematica to find a general solution for the probability density of a phenotype distribution at a certain time. I am still currently working on this Mathematica code and the purpose of this is to take the solution and input it into Shannon's entropy equation. This entropy would be used to model a special first law of thermodynamics that describes the energy dynamics of a population.

The other half of my research entailed creating a Python simulation of the Wright-Fisher model which describes the evolution of the frequencies and fixation probabilities of two alleles of a gene in a population. My first simulation described a population of two types of cells that have equal chances of making it into the following generations. For the second version of this code, I created a black box model for the so-called cells from the first code such that they have maintenance input energy and mass they have to keep up with to reproduce and survive making for a more realistic simulation of the Wright-Fisher Model. The code currently runs for two different phenotypes of different survival and reproduction requirements outputting distribution probabilities, entropy values for different initial conditions, and heat loss in the system. My next task is to debug the flaws in the code and generalize it for n phenotypes.

My research, guided by Prof. Vural and focusing on applying thermodynamic principles to evolutionary biology by examining how changes in entropy from the sun affect the phenotype distribution of species, has been a blessing and an eye-opening experience. From solving the Fokker–Planck equation to derive probability densities and using these results in Shannon's entropy equation to modeling energy dynamics in populations, I’ve earned much knowledge. Additionally, developing the Python simulation of the Wright-Fisher model to study cell frequency evolution under more realistic conditions, incorporating maintenance energy and mass requirements for cell survival and reproduction, took my coding ability from being virtually non-existent to functional and capable of growth. Moving forward, my work will focus on refining this code and the Mathematica code and extending their applicability to multiple phenotypes, thereby contributing to a deeper understanding of evolutionary dynamics through the lens of thermodynamics.