Franklin W. Olin College of Engineering

Special Topics in Bioengineering: Biological Thermodynamics for Engineers Spring 2009

MODULE 2

2nd Law, Free Energy, and Molecular Dynamics Simulations

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Issued: Tuesday, February 10, 2009

Goals and Objectives for Module 2:

- Become acquainted with and understand the basics of the 2nd Law of Thermodynamics.
- Be familiar with the concepts of Entropy and Free Energy, and their application in solving problems of equilibrium.
- Become acquainted with the Boltzmann Distribution, its assumptions and limitations, and how to apply it to quantitative problem solving.
- Know and understand the basic assumptions of Molecular Dynamics (MD) simulations, the capabilities and limits of MD, and examples of how MD is used in research.
- Perform preliminary research and write a research proposal incorporating MD simulations and basic concepts of thermodynamics to investigate a problem in Bioengineering or Medicine.

Reading:

- Haynie, Ch. 1, 2, 3, 4, and 6C
- Selected articles
- Google and Wikipedia

Module 2 Final Paper: Research Proposal

This paper will give you the opportunity to show how basic principles of thermodynamics are applied to biomedical research, and how molecular dynamics (MD) can be used to approach a research problem.

Your paper should be no more than 4 pages and include the following sections:

Abstract—Overview of the proposal in 150 words or fewer.
Introduction—State the problem you are trying to solve. Give background literature and show where the current state of knowledge is incomplete.
Aims—State in bullet form specifically what you wish to accomplish with your research.
Methods—Describe the methods you will use to accomplish the stated aims.
Preliminary results
Discussion and Conclusions—Discuss how your preliminary results and theoretical framework fit into the existing literature, and summarize your conclusions.
References—A list of references for articles cited in the proposal.

You may optionally include other sections as well to describe anticipated problems or constraints, budget and schedule information, and/or expected results that would substantiate a specific hypothesis. *Your overall goal should be to clearly communicate where there is a gap in the current knowledge, why filling that gap is important, and how you propose to do it.*

You should use what you have learned in the labs to generate graphics of proteins, observations of their structure, and preliminary MD results. Feel free to consult with me (nhammond@mit.edu) if you would like to explore another approach to obtaining preliminary results. You can do almost anything you can imagine with MD: simulate mutations to an existing protein, alter the pH, temperature, or salt concentration of the environment, apply forces or constraints to specific atoms, observe the interactions between two proteins, construct entirely new peptides (although they may not be folded correctly), etc.

Remember to cast your problem in terms of free energy or other thermodynamics concepts.

A full draft of the paper is due on 3/6, and we will review the papers and give feedback in class. The instructors will read over the drafts and return them on 3/10. The revised paper is due 3/13.