BME 450: Numerical Methods for Computational Modeling in Biomedicine

Course goals
Advanced computational methods are required for the creation of biological models, from protein folding to whole-organ function. Students will be introduced to the process of model development from beginning to end, which includes model formulation, how to solve and parameterize equations, and how to evaluate model success. To illustrate the potential of these methods, participants will systematically build a model to simulate a "real-life" biological system that is applicable to their research or interest. A mechanistic appreciation of the methods will be gained by programming the methods in a low-level language (C++) in a Linux environment.

Prerequisites
Some programming knowledge (e.g. familiarity with conditional statements, loops, etc.)

Corequisites
None.

Credits
3.0 total credits. 1.0 Design credit.

Location
Whitaker 218.

Schedule
Tues and Thurs, 1:00-2:30 pm.

Ethics
All students are expected to comply with the Washington University in St. Louis student code of conduct. In particular, all work turned in must be your own. It is acceptable to obtain help from a classmates, but it is not acceptable to copy their code, digitally or manually. All assignments will be checked with SafeAssign on Blackboard to ensure that no code is copied from the internet. Any code that is not original must be attributed to its source. Plagiarism will be vigorously and unapologetically enforced via grades of zero, and reported as appropriate.

Resources
Website:
Blackboard class page: bb.wustl.edu

Computing:
shell.cec.wustl.edu – can login from home to implement/run code
Engineering Computer Lab – Lopata 400.

Office Hours:
Tuesdays and Thursdays 2:30-4:00 pm in Whitaker 290G

Contact:
email: jonsilva@wustl.edu

Grading
1. Homework: 60%
2. Final Project: 35%
3. Class Attendance/Participation: 15% (On-time for class, participate in discussions, provide helpful comments to classmates.)
**Requirements**

**Homework**
Homework will be assigned weekly and graded out of ten points.

Points: Out of 10
- 2 – Attempting all problems (Was a worthy effort made to complete each problem?)
- 4 – Succeeding (Does the code do what is supposed to?)
- 2 – Creativity (Did you do something novel, more than simply following instructions?)
- 2 – Execution (Comments, proper indentation, use of object-oriented principles?)

**Final Project**
The goal of the final project will be to identify an ion channel of interest and to create a novel model of that channel. Criteria for grading are novelty of the model, complexity, use of methods and concepts taught in class, and quality of the code. In addition to the code, a 2-4 page report will be required. The report should include a description of the physiological relevance of the channel, a statement of what data needed to be fit, a demonstration of how well the model fits this data, and a section that details insights derived from the model. The model itself will comprise 70% of the grade and the report 30%.

**Topics**
Week of:

1/13: C++ programming syntax, streams, flow control, containers.
1/20: Introduction to object-oriented concepts.
2/3: Equations that are used to describe ion channels.
2/10: Random number generators, Monte Carlo simulation of ion channels.
2/17: Individual meetings to define class projects.
3/10: Spring Break!
3/17: Ion channel model outputs and protocols.
4/7: Peer-to-peer discussion of final projects.
4/14: Optimization and Parallelization.
4/21: Short presentation of final projects.