Supplemental Material

von Arnim and Missra

Supplemental Material

von Arnim, A.G. & Missra, A. (2017) Graduate Training at the Interface of Computational and Experimental Biology - An Outcome Report from a Partnership of Volunteers between a University and a National Laboratory. CBE-Life Science Education.

Contents

A. Learning goals of the GST program

Learner outcome	Assessment method(s)
I. Analytical thinking Students will synthesize information from the published literature. Students will draft hypotheses to guide further study, and plan experiments. Students will formulate compelling arguments supporting the validity of their conclusions.	**Progression in the program from first to second year**
	Comprehensive examination The exam is designed to measure the student's ability for rigorous and independent analytical thinking in the area of their specialization.
II. Research competence Students will demonstrate their ability for original scientific investigation.	**Peer reviewed publications at graduation** Number of publications per student at graduation and other relevant time points.
III. Teamwork and professional development Students will demonstrate their ability to formulate and communicate, discuss, and solve scientific questions in a collaborative context.	1. **Conference participation** Number of conference attendances, poster presentations and oral talks per student. 2. **Teamwork** Analysis of students' resume for quantifiable data at the time of their graduation. 3. Activity in the scholarly community (research colloquium, interactions with external speakers, the annual symposium, or outreach)
IV. Teaching Students will demonstrate competency as teachers.	**Teaching experience** Analysis of resume for number and diversity of class sections taught, attendance of teacher development workshops, and leadership in developing new curricular materials.
V. Communication skills Students will create effective written reports and oral presentations.	**Dissertation committee meetings with faculty members** Qualitative scores (scale 1= fair; 2=good; 3=excellent) extracted from committee meeting reports.
	Comprehensive exam Qualitative scores (scale 1-3) extracted from comprehensive exam reports.

B. Supplemental DIscussion

1. Institutional Change

The following section provides additional context to the institutional environment in which the GST program is operating, in the hope that this information may help readers to implement appropriate innovations in graduate training at their own institution. We note that some of the contextual circumstances mentioned below are based on personal experience, and the inferences and ideas drawn from them have not been tested. For this reason we refrain from making specific recommendations.

The GST program was developed during a period of a substantial transformation in the life sciences. At its inception, computational biology was a fringe discipline, and most experimental research was still data-poor and not highly quantitative. Now, most research groups at UT and ORNL are accustomed to large datasets (genomics, structural biology, imaging) and have at least basal expertise in extracting meaning from such data, but most labs would like to have more expertise. The GST program has accompanied this transformation at UT, and having grown over the years, we like to think that it has in small part accelerated it. GST recruits a special class of students, scientists who are motivated to develop their computational skills and are intrigued by the opportunity to conduct research at a National Lab. Many faculty members are eager to recruit these students to their labs.

GST was the intellectual home for an NSF graduate training grant, which operated between 2008 and 2014. This grant stimulated the creation of the Interdisciplinary Graduate Minor in Computational Science. The Minor in turn spawned three new courses, a service course taught by the Computer Science Department entitled Programming for Scientists and Engineers as well as GST's computer programming course, both of which are well subscribed. Another cross-training course entitled Biology for Computational Scientists was created and taught for several years by GST students and faculty, although demand for it has waned in recent years. Furthermore, the former Director of GST was also the project director of an ongoing NIH R25 predoctoral training program designed to augment the recruitment, retention and professional development of underrepresented minorities and women in quantitative biomedical science. Finally, a few years ago, UT and ORNL created a second inter-campus degree program in Energy Science and Engineering, which now trains over 130 students, and a third inter-campus program in Data Science is about to be launched. In summary, although it is impossible to quantify the degree to which GST stimulated these and other institutional changes, it may have played a part in shaping them.

2. Benefits and Challenges of the GST Model

As a degree-granting intercollegiate graduate program, GST enjoys substantial autonomy in setting its own curriculum. The GST curriculum does not need to be coordinated with that of other departments. This is a substantial advantage, as it eliminates a source of friction and underscores the benefits of GST's presence to our campus.

At UT, the faculty is organized into departments and colleges, which are defined primarily by their responsibility for undergraduate instruction and which each host their own graduate program. As the only interdepartmental graduate program in the life sciences, GST competes for resources and recognition with the departments. GST does not have faculty positions, and therefore most of the teaching and committee work by GST faculty is voluntary, is incentivized because the faculty member enjoys teaching his expertise to students who are receptive to it, and this occurs at the discretion of the head in whose department the GST faculty member's line resides. This limits what the program can accomplish.

GST spans two institutions with distinct scientific cultures, the University of Tennessee, and the Oak Ridge National Laboratory. Many of our applicants list this aspect of the program as particularly attractive; and we are grateful that ORNL scientists participate in the graduate training enterprise. While GST was becoming more data-driven, many of its founding computational biologists at ORNL departed for professional opportunities elsewhere. In their place came new investigators, several of who have since trained the bulk of GST alumni in high-performance supercomputing and related areas. Faculty turnover has been an occasional challenge, yet as a result the GST program is continually evolving.

GST is financially independent from other departments. Although its assets and resources pale with those of the academic departments, it has been able to assist in focused ways that are generally appreciated by the campus community, by sponsoring students' attendance of conferences, honoraria for classroom teaching, visits by invited speakers, site licenses for computer software, and the like. As a result of GST's business model, GST students are more expensive for the UT faculty members than students in other programs. This limits the number of students that GST can admit, train, and graduate, and also deters

some faculty members with appropriate expertise from participating in the program. Given the career tracks of GST alumni in the US and beyond, these financial constraints may also hamper the development of the workforce in computationally enabled life science.

Because faculty lines are housed in departments, and teaching credit accrues to departments rather than GST, the substantial depth of graduate training in computational life science that is offered on our campus appears dispersed, as it is not clearly associated with one specific program. This is a lost opportunity for graduate recruiting. GST tries to remedy this by publishing a list of courses every semester to orient the UT community about what courses are available.

The title Genome Science and Technology is perceived as a handicap by a few of our colleagues because it does not accurately capture the breadth of the program, yet it would be counterproductive to continually change the name of a program. Therefore, the program is not as visible worldwide as programs in traditional disciplines such as Microbiology, Biochemistry, or Computer Science. We suspect that the name limits the size of the applicant pool and in turn limits the number of students that can be trained in this emerging area of science.

Genome Science and Technology I - Genetics and Genomics

Life Sciences 520

4 credits

Fall 2016

WF (9:05-11:00 am) Hesler 427

Instructors: Loren Hauser, UT (lhauser@tennessee.edu; 607-7143)

Michael Gilchrist, EEB, UT (mikeg@utk.edu; 974-6453)

Tim Sparer, Micro, UT (tsparer@utk.edu; 974-3800)

Albrecht von Arnim, BCMB, UT (vonarnim@utk.edu; 974-6206)

Hwa-Chain Wang, Vet Medicine, UT (hcrwang@utk.edu; 974-3846)

Course Outline

GST I is the entry-level course in the graduate program in Genome Science and Technology. The course aims to lay a solid foundation of the current state of biological concepts, primarily at the organismal and cellular levels. Thoroughly covered areas include genome structure, mutation, gene expression, metabolism, regulation, signal transduction, development, and disease. At the upper end of biological organization, the course reaches into population genetics, evolution, and ecology; at the lower end, it touches on molecular and structural biology.

It is understood that students enter the course with widely different backgrounds. There will be a certain amount of in-class review, but mostly to 'refresh your memory'. Students who enter the class with little background in biology should be prepared to develop those underlying concepts (Genetics, Cell Biology, and Biochemistry) through background reading.

Activities

- In-class lecture
- In-class projects, including discussion of the primary literature and other topics
- Homework, including readings of the primary literature and writing assignments
- Independent study
- Exams

Learning goals

* Ability to define the state-of-the-art in microbial genomics, plant, and biomedical research.
* Understand the techniques for both genome-scale and classical small-scale investigation through
        Lectures

Readings of the primary literature and their discussion in class

Homework and take-home exam assignments

* Appreciate the opportunities (and pitfalls) inherent in genome-scale investigation, including the value of genome sequence data, and of genome-wide datasets such as microarrays, association studies and QTL mapping, genetic screens, proteomics and metabolomics.

* Designing future research projects

Synthesizing existing data into a coherent model

Identifying a solvable problem

Assembling an experimental plan

Justifying the experimental approach

* Developing a perspective of the current status of biology in a historical context.

* Communicating orally.

Rule of thumb: Everyone is expected to contribute orally to every class period.

* Laying a foundation for competent scientific writing (homework, take-home exam).

Expectations and tips

* *Regular class attendance*. If you cannot attend class for whatever reason, please email the instructor, preferentially ahead of time.

* *Preparation.* Instructors will assign readings prior to class and expect you to be prepared to discuss ('flipped classroom').

* *Oral class participation* will contribute to your grade. The more fully you are engaged in the class, the more you will get out of it.

* *Do your own work.* The instructors will explain whether and when teamwork is expected.

* *Manage your time*. Turn in assignments on time, and don't wait until the last evening to prepare for class the next day.

* Q*uality over quantity.* What you learn should be integrated into your conceptual framework of Biology.

Resources for background reading

There is no textbook for GST I. However, you will probably need backup access to textbooks in undergraduate-level genetics/cell biology.

* Griffiths et al. Introduction to Genetic Analysis (text used in undergraduate Genetics at UT).

* Lodish et al. Molecular Cell Biology (text used in graduate Advanced Cell Biology)

* Watson et al. Molecular Biology of the Gene (text used in graduate Advanced Molecular Biology).

* Online: Wikipedia is usually accurate, though not always balanced.

-> *ask Albrecht von Arnim if you would like to borrow a textbook.*

Evaluation and grading

*** 600 points total. 200 points per Segment I, II and III. ***

a) The major assignments in Segment I-III will be take-home exams that are worth up to 150 points each.

b) In-class participation yields up to 50 points per segment.

c) Homework assignments may be counted as 'extra credit' or may be part of the 150 points under (a).

GST I
Syllabus Fall 2016

August 17 - September 9	**Microbial Genetics and Genomics** (Hauser)
	Biological Sequences as Information; Three Generations of DNA Sequencing; Genome, Gene and Operon Structure; Genome Annotation; Transcription and Gene Regulation; Systems Biology; Comparative Genomics; Genome Manipulation.
September 14	RNA-based Regulation (Fozo)
September 16	Microbial Metagenomics (deBruyn)
	TEST I (Take home, due Sep 23)

September 21 - October 5	**Plant Genetics and Genomics** I (von Arnim)
	Introduction to Eukaryotic Genetics; Rice model system, Life cycle, Domestication; Molecular Markers, mapping and positional cloning; Structural genomics and genome browser; Recombinant DNA in crop improvement; Agrobacterium; Golden rice; Gene X Environment Interactions - Ethylene.
October 7	Fall Break
October 12 - October 21	Plant Genetics and Genomics II (von Arnim)
	Gene X Environment - Flowering; Heterosis , genetics and epigenetics; Genes-to-Traits - Domestication genes; Complex traits - Genetic analysis, QTLs; Complex Traits - (Nested) Association Mapping.
	TEST II (Take home, due October 28)

October 26 - November 4	**Biomedical Science and Population Genetics**
	Molecular Oncology & Signal Transduction (Wang)
Nov. 9 - Nov. 11	Biomedical Science: Cancer Genomics and Immune Therapy (Sparer)
Nov. 16 - Nov. 18	Population Genetics, Genome Evolution (Gilchrist)
November 23	Final Project (von Arnim)
	TEST III (Take home, due December 2)

Genome Science and Technology II - Analytical Technologies

Life Sciences 521
4 credits
Spring 2017

MWF (9:05-9:55 am) WLS M415 (Fridays 8:00-8:50 am, Discussion M 415)

Coordinator: Robert Hettich (ORNL) (hettichrl@ornl.gov, 574-4968)
Instructors: Elias Fernandez (BCMB) (efernan1@utk.edu, 974-4090)
               Nitin Jain (BCMB) (njain@utk.edu, 974-4045)
               Steven Brown (ORNL) (brownsd@ornl.gov, 576-2368)
               Edward Wright (BCMB) (edwright@utk.edu. 974-2530)

Schedule:

Jan. 11	General Introduction (Hettich)
Jan. 13	X-Ray Crystallography (Fernandez)
Jan. 16	Martin Luther King Holiday
Jan. 18 – Feb 10	X-Ray Crystallography (Fernandez)
Feb. 10	TEST I (Take home, Crystallography, due Feb 17)
Feb. 13 – Mar. 6	Mass Spectrometry (Hettich)
Mar. 8 – Mar. 10	Spectroscopy (Jain)
Mar.13 – Mar. 17	Spring Break
Mar.20	TEST II (Take home, Spectroscopy and MS, due Mar. 27)
Mar.20 – Apr. 10	Nuclear Magnetic Resonance Spectroscopy (NMR) (Jain)
Apr. 12	Electron Paramagnetic Resonance Spectroscopy (EPR) (Wright)
Apr. 14	Spring Recess
Apr. 17	Surface Plasmon Resonance (Wright)
Apr. 19	Calorimetry (Wright)
Apr. 21	Calorimetry (Wright)
Apr. 24	Analytical Ultracentrifugation (AUC) (Wright)
Apr. 26	DNA Sequencing (Brown)
Apr. 26	TEST III (Calorimetry, AUC, NMR, EPR, due May 3)
Apr. 28	Overall Review and Discussion (Hettich)

The central objective of this course is to teach main principles of several experimental techniques, data collection and interpretation and their application to biological problems. The techniques discussed include, mass spectrometry, uv-vis and fluorescence spectroscopy, DNA

sequencing technologies, calorimetry, nuclear magnetic resonance spectroscopy and X-ray crystallography.

Any minor revisions to syllabus and other announcements will be posted on the Blackboard course website and sent to students as email through Blackboard.

Lectures will be posted on the Blackboard site as power point presentations. Please print three figures per page to allow room for notes. Additional paper copies of lecture notes will be given for some of the topics.

Each exam constitutes $1/3^{rd}$ of the total grade. Letter grading will be determined by curving the class average. The class average receives the grade "B". Tests are to be submitted electronically to either the instructor or to dropbox on the Blackboard course site. Late submissions will be penalized by 10% reduction of the grade per half hour. Make up exams can be given only in case of sickness and family emergencies in documented cases.

Attendance to lectures is required. Exceptions are sickness, conference attendance, and family emergencies with documentation. Plagiarism will result in a failing grade. Description and examples of plagiarism can be seen at :
http://www.indiana.edu/~wts/pamphlets/plagiarism.shtml or
http://plagiarism.org/. These links are posted on the course Blackboard site.

Additional policies on UTK academic honesty and accommodation for disabilities that restrict learning are at:
http://tenntlc-utk-edu.wpengine.netdna-cdn.com/files/2012/11/CAMPUS-SYLLABUS1.pdf

LFSC507 Programming for Statistical and Graphical Analysis of Biological Data

Syllabus

Fall 2016

Textbooks and Materials

Biostatistical Analysis by Jerrold Zar, fourth edition
Computational Notebook 75 sheets, 4x4 Quad, 11 3/4'' x 9 1/4'' page size
Installed on your laptop: Linux, Pgplot libraries for Fortran (for gfortran compiler, see
http://www.dur.ac.uk/physics.astrolab/ppgplot.html) and Perl (will be installed on the first Lab
class if you cannot do it earlier, which is ok).

Schedule, subject to change depending on class dynamics

Date	Section	Title
8/19/2015 W	Lecture 1	Operating systems. Orientation in Linux. Basic commands. Emacs. Access. Environmental variables.
8/24/2015 M	Lab 1	**Orientation in Linux command line and installation of Python (Windows/Mac/Linux)** ● *In lab class, Linux is the default development environment.* ● *All the assignments could be finished by using just Python, without limitation of development environment.* ■ Basic Linux command ■ Basic Python functions such as print
8/26/2015 W	Lecture 2	"Welcome" quiz. Data sample: basic statistics. Programming in Fortran: Types of variables, mathematical operations and functions, compiling, arrays, loops
8/31/2015 M	Lab 2	**Python Basics: Types and Operations** ● *Numbers, Strings, Lists, Dictionaries, Tuples and Files* ■ Type casting ■ Operations on data types
9/2/2015 W	Lecture 3	Fortran: Logical Expressions if-then-endif, user written subroutines. Libraries of subroutines.
9/07/2015 M	Lab 3	**Python Basics: Statements and Syntax** ● *Assignments, Expressions, and Prints* ● If/Else ● While and for loops

		○ E.g. Fibonacci
9/9/2015 W	Lecture 4	Fortran: Writing to Files and Functions. Using Pgplot library for drawing.
9/14/2015 M	Lab 4	**Input/Output** ● Built-in open() and close() functions 　○ use of the "*with*" statement ● Reading a file 　○ readline() and similar functions ● Creating own files ● Appending and writing to a file ● File Paths (Mac/Linux/Windows)
9/16/2015 W	Lecture 5	Drawing with PgPlot. Distributions. Cumulative distribution function, cdf. Five distributions that most often occur in biology. Four distributions that are statistical tools. Sample, population. Statistical analysis. On the sample size.
9/21/2015 M	Lab 5	**Functions and Program Structure** ● *How to write functions* ● *Scopes* ● Pass by reference *vs.* Pass by copy
9/23/2015 W	Lecture 6	Getting comfortable with data distribution. More programming: implicit declaration. Graphic file formats. Postscript. Creating printable files using pgplot. Converting to PDF. Distribution of means. Drawing curves y=f(x) using pgplot. Normal distribution. Data with true intrinsic zero.
9/28/2015 M	Lab 6	**Build-in Modules** ● *How to install modules* ● *How to use modules* ● Regular Expression (import re)
9/30/2015 W	Lecture 7	The 30 points discussion, Z score. Common blocks in Fortran. Numerical Recipes Library. Random numbers. Nested loops. Fitting histogram with the distribution curve.
10/05/2015 M	Lab 7	**Statistical Modules (I)** ● Numpy ● Scipy ● Pandas
10/07/2015 W	Lecture 8	Fortran: common blocks again, passing variables to subroutine, operator goto. Taming Lognormal Distribution. Null hypothesis. Student's t-test. F test. Chi-square test.

		K-S test. Experimental error.
10/12/2015 M	Lab 8	**Statistical Modules (II)** ● Numpy ● Scipy ● Pandas
10/14/2015 W	Lecture 9	Hypotheses testing. Experimental error. Term paper.
10/19/2015 M	Lab 9	**Sorting Algorithm**
10/21/2015 W	Lecture 10	A few words on ANOVA, one-way ANOVA, F-statistics. Remaining Fortran: parameter, format, implicit loops. Modeling. Fitting data, merit function, and linear regression.
10/26/2015 M	Lab 10	**Statistical Analysis by using Python (II)** ● ANOVA o Knowledge and Practice
10/28/2015 W	Lecture 11	Modeling. Fitting data: general linear least square. Goodness of fit. Programming in C. First picture for the term paper is due.
11/02/2015 M	Lab 11	**Statistical Assessment of Proteins (I)** **Mass Spectrometry**
11/04/2015 W	Lecture 12	Programming in C
11/09/2015 M	Lab 12	**Statistical Assessment of Proteins (II)** **Mass Spectrometry**
11/11/2015 W	Lecture 13	Programming in C
11/16/2015 M	Lab 13	**Python for Biology (I)** (Provided by Barry Bruce)
11/18/2015 W	Lecture 14	Bioinformatics and Computational Biology. Protein structure prediction
11/23/2015 M	Lab 14	**Python for Biology (II)** (Provided by Barry Bruce)
11/25/2015 W	Lecture 15	Term paper presentations
11/30/2015 M	Lab 15	**Programming Resources** Python and Beyond

GENOMICS and BIOINFORMATICS (MICR480/MICR540/LFSC517)

Spring 2017

Time: Monday and Wednesday 09:45am – 11:15pm
Location: HSS, room 51

Instructor: Prof. Igor Jouline
Office: WLS F203
E-mail: ijouline@utk.edu
Office hours: Monday 3:00pm – 4:00pm

In this course, you will learn how the whole genome sequencing technology has revolutionized biology and provided a foundation for new developments in science and medicine. You will become familiar with computational tools that are necessary to analyze genomic data and you will find out what biological questions can be answered by genomic approaches. We will use prokaryotes as the main material for genomic studies, but the core principles that you will learn are also applicable to eukaryotes including humans.

Prerequisites: Biology 240.

Textbook: No textbook is required for this course.

Attendance: Attendance is required, especially because notes taken in class will be your main source of information.

Semester outline: This is an approximate schedule for the course. Any changes to the schedule will be announced in advance and posted on the course Canvas site.

Week	Dates	Material
1	Jan 11	Course introduction and requirements. Introduction to Genomics
2	*No class on Jan 16 -* Jan 18	*MLK holiday* Introduction to Bioinformatics
3	Jan 23 & 25	Databases and information retrieval
4	Jan 30 & Feb 1	Computational gene finding and nucleotide sequence analysis

5	Feb 6 & 8	Protein sequence analysis
6	Feb 13 & 15	**TEST 1** and Basic sequence-based database searches
7	Feb 20 & 22	Multiple sequence alignment.
8	Feb 27 & March 1	Advanced sequence-based database searches
9	March 6 & 8	Advanced sequence-based database searches

No class on March 13 & 15 - Spring Break

10	March 20 & 22	**TEST 2** and Protein structure.
11	March 27 & 29	Evolutionary concepts in genomics
12	April 3 & 5	Phylogenetic trees
13	April 10 & 12	Phylogenomics
14	April 17 & 19	**TEST 3** and Whole genome reconstruction and analysis
15	April 24 & 26	Genomics and bioinformatics in medicine

Final examination is on Monday, May 8, 8:00 am to 10:00 am.

Assignments and grading: Homework assignments will be for students taking Micro540 or LFSC517. Assignments will be posted on the course Canvas site and announced in class. Due dates will be clearly indicated. No late assignments will be accepted. There will be two assignments over the course of the semester, and each will carry equal weight.

Three tests will take place during regular lecture hours as indicated. First test will cover material from weeks 1 through 5, the second test will cover material from weeks 6 to 9 and the third test will cover material from weeks 10 to 13. Final examination will cover the material from weeks 14 and 15 as well as basic, conceptual questions from the entire semester. If you are sick on test date, a make-up test will scheduled individually. You must email Dr. Jouline on the original test date to let him know that you are sick. Your final course letter grade will be computed as follows:

MICRO480

First test	20%
Second test	20%

Third test	20%
Final exam	40%

MICRO540 & LFSC517

First test	15%
Second test	15%
Third test	15%
Homework assignments	15%
Final exam	40%

Letter grades will be assigned using the following conversion table:

A	90 and higher	C+	78 to 78.9
A-	89 to 89.9	C	70 to 77.9
B+	88 to 88.9	C-	69 to 69.9
B	80 to 87.9	D	60 to 68.9
B-	79 to 79.9	F	below 60

Other important notes:

All important course-related announcements will be posted on the "Announcements" section of the course Canvas site. Students are bound by the Honor Statement found in the Undergraduate Catalog and *Hilltopics*; please, make sure to review it. All homework assignments must be completed individually.

Predicting the mechanisms of life:
An application of molecular dynamics simulation to biological problems

BCMB 420/LFSC 595
Spring 2017

Course Section:	**001/003**
Meeting Time and Place:	**T/TR 12-2:00 pm, Walters Life Sciences Building M-313**
Course Credit Hours:	**Three Credit Hours**

FACULTY CONTACT INFORMATION:

Instructor:	Dr. Quentin Johnson
Office:	Claxton 110A
Phone:	974-9448
Email:	qjohnso3@vols.utk.edu
Office hours:	T @10:00-11:50 am, TR @2:30-4:30 pm

I.   COURSE DESCRIPTION:

This course utilizes molecular biophysics to deepen students' understanding of several molecular phenomena covered in core science courses such as biology, chemistry, physics and biochemistry. In particular, molecular dynamics (MD) simulation and molecular visualization tools are used to reveal the structure and motions of biologically relevant molecules like proteins, water and drug molecules. A special emphasis is put on describing protein structure, intermolecular interactions, and free energy. Students will use MD to create a protein system, simulate that system's motions, and analyze the trajectory produced by the simulation to address a specific biological question. The graded portion of the course is derived from daily in-class contributions to the learning environment, several small "module projects" that reinforce concepts and techniques covered in class and a final project that requires students to demonstrate their mastery of all information and procedures covered throughout the semester.

II.   VALUE PROPOSITION:

In science, the microscopic world can be hard to grasp because of a lack of perspective; we can't see an atom, or feel the pull of electronegativity, we have to trust that its there without experiencing it first-hand. While we can't shrink down to a subatomic level like *Ant Man*, we can model this microscopic world on a scale more amiable to human perception. Molecular Dynamics simulation is a tool for doing just this. Through a complex mathematical calculation we can predict the structure (what they look like) and the dynamics (how they move) of atoms and molecules. Students will learn to work with supercomputers, advanced scientific software, and brilliant three-dimensional visualization tools to simulate the behavior of proteins, DNA, and lipids in microscopic environments. The intention of the course is to grant students the tools and knowledge to grasp biological events at their most basic level.

III.   LEARNING OBJECTIVES:

1. **Students will be able to articulate the concept of LIGAND BINDING**:
   Many proteins are inactive until they bind a specific ligand that is biologically tailored to fit into the binding pocket through a series of intermolecular interactions.
2. **Students will be able to articulate the concept of STRUCTURE AND FUNCTION:**

Macromolecules are able to access a variety of structures, but particular structures can correspond to a certain biological function.

3. **Students will be able to articulate the concept of DYNAMICS AND FUNCTION:**
   Though structure is important for function, everything in nature is in perpetual motion, therefore the breadth of structural fluctuation is also important for function.

4. **Students will be able to articulate the concept of FREE ENERGY:**
   All molecules have a particular energy landscape, and every possible molecular structure corresponds to a specific free energy, the probability that a molecule will be in any particular structure is inversely related to the free energy.

5. **Students will be able to:**
   a) Set up, perform, and analyze a molecular dynamics simulation
   b) Articulate the implications of structure and dynamics as they relate to ligand binding
   c) Create a hypothesis that can be tested via analysis of an MD trajectory
   d) Create and interpret figures and tables
   e) Interpret data; construct an argument from scientific data and communicate this in writing

IV.   COURSE GOALS:

The goal of this course is to teach students to use MD simulation and the associated analysis techniques to expand their understanding of core scientific concepts. The goal for those that come in with a research-oriented focus is to provide them with the skills to utilize molecular biophysics techniques in their own research.

1. **Students will understand and be able to articulate:**
   o The basics of MD simulation
   o How the structure of proteins, carbohydrates, lipids, and other biomolecules contributes to their functions
   o How free energy is affected by structure and how structures fluctuate around a minima
   o MD simulation results and the biological implications of them
   o Figures and graphs and their biological implication
   o Protein sequences and 3D protein structures

V.   LEARNING ENVIRONMENT:

Class attendance is mandatory. Most of the practical instruction on how to use software will be given during class. Additionally, the majority of class time will be used for hands-on learning, which is essential for understanding the course material and to completing module projects. Attendance to office hours is not mandatory, but is recommended. The instructor will provide one-on-one time during office hours, which can be very helpful for completing course work. Please make every effort to be prepared in the classroom before the class is scheduled to begin. Arriving late is disruptive. Much of the class will consist of working on a computer; therefore, surfing the web, engaging in social media or any other disruptive activities are prohibited and can result in deductions from students' final grade. The policy regarding incompletes is as stated in the university catalog. When a grade of incomplete is awarded; the course can be completed once the student finishes the rest of the coursework. No work completed prior to the incomplete may be repeated.

Office Hours
Attendance at office hours is not mandatory. The class will meet as a whole during two lecture periods a week. In addition, there are optional office hours in which the instructor will be available to answer your

questions and help with your technical problems. Extra credit points will be awarded to students that attend these sessions consistently. However, those that do attend will likely do well in the class regardless of any extra credit.

VI.   TEXTS/MATERIALS/RESOURCES FOR THE COURSE:
- Students will be given access to **Blackboard** at the onset of class which will contain PPTs, assignment guidelines, tutorials, etc.
- **Slack** will be used to ask questions outside of class. This provides a message board for Q&A on a peer-to-peer and instructor-to-peer basis. You are allowed and encouraged to access **Slack** through your computer during class.

VII.   INFORMATION LITERACY/TECHNOLOGICAL RESOURCES:
Module projects will be assigned on a regular basis in class, questions regarding those projects can be addressed on **Slack**; a written version of the project requirements will also be posted there and on **Blackboard**. Services are free of charge. Students are responsible for accessing (and printing, if desired) these materials.

VIII.   COURSE REQUIREMENTS, ASSESSMENT AND EVALUATION METHODS:

Class Participation
You can earn participation points in a plethora of ways, and it will behoove you to do so. Many times, I will utilize class time to facilitate a discussion on previously assigned reading material. The purpose of these exercises is to convey the actuality of the research (tell you guys what the researchers actually did and how you can do it) and to expose students to how computational literature is written. You are expected to engage in these discussions and a portion of your participation grade can come from these activities. Also, I tend to ask questions randomly during class, you can earn participation points by giving your opinion on these questions or by just Googling it, and giving me the answer. You can also earn points by using **Slack** during class to ask questions, contribute to a discussion, or upload files. In short, there are many different ways to contribute to the learning environment and you are expected to contribute.

Module Projects and Exams
There are multiple module projects that are expected to be completed after class, and turned in at the start of class on the assigned date. Note, time will be allotted in class to work on projects with the instructor's guidance, but you should refine these projects after class. There will also be a final project that will be completed during the university's final exam week. These projects will be an expansion on what you learned in class. Students are expected to create all projects independently. This does not mean that you cannot work together, but duplicate work will result in a zero as in accordance with the university's guidelines on plagiarism. Grades on projects are final. The only situation in which I will review a project grade is if you feel **strongly** that the project has been **grossly** miss-graded. In this case, you have **one week** after the project is returned to submit a request **in writing** that you wish to have the project reviewed. Please be aware that the review can also result in a lower grade than originally assigned, so be careful in submitting review requests.

Author-Editor Grading System
I am a proponent of lifting as you climb and I believe that the true value of science is in empowering

others through the communication of your science. Therefore, many of my class activities are centered on communicating and cooperating with peers. In this sort of class there isn't a lot of actual class time available for exclusive peer communication since I will be leading the class in many instances, and will usually be the source of technical solutions. However, the class will be taught in a computer lab setting, so I encourage leaning over to click the proper sequence of buttons to catch a neighbor up with the class or saying to friend, "Hey you need a semi-colon after this line of code". Additionally, as a way to emphasize the meticulous nature of computational work and to grade students on their editing and debugging abilities, I am implementing an author-editor grading system. This system serves to simultaneously evaluate a student on their ability to author and edit code, manuscripts, and presentations, as both roles are essential in science. Since the graded portion of this class is chiefly obtained from a series of projects, each student will be the author of his own project and the editor of another student's project. Additionally, a student's final project grades will be compose of 75% of their grade as an author and 25% of their partner's grade. In this way a quarter of their grade directly depends on their ability to debug code, communicate improvements, and collaborate as a whole.

Make-ups
In general you will not be allowed to make up missed projects **except in unusual circumstances** (provided in writing ahead of time). If you are ill at the time the project is to be turned in, you can email your project directly to the instructor.

Office hours
Please respect the office hour times given for the instructor. They are **Tuesday at 10:00-11:50 am and Thursday at 2:30-4:30 pm**. If these times are inconvenient, then make an appointment. I am quite accommodating to students with the intention to learn.

Grade assignment:

	Points
Module Projects	60
Participation	20
Final Project	20
TOTAL	100

The grading scale is as follows:

A: 90 – 100	
A-: 87-89	C+: 71-75
B+: 84-86	C: 65 – 70
B: 80 – 83	D: 50 – 64
B-: 76-79	F: 0 – 49

IX.   HOW TO BE SUCCESSFUL IN THIS CLASS:
- Prepare for class. Read the assigned readings; take notes on the reading, practice skills from class, complete projects, actively collaborate with others on projects.
- Come to class. Think about the material while it is being presented, take notes, participate in the discussion, and ask questions for clarification.
- Review your notes. Think about how what you're learning connects to what you've learned in previous courses.

- Work cooperatively. This course can be overwhelming if you take in on alone, so talk to a friend, seek help from online sources, and talk with the instructor regularly.

X. COURSE FEEDBACK:

At UT, it is our collective responsibility to improve the state of teaching and learning. During the semester, you may be requested to assess aspects of this course either during class or at the completion of the class. You are encouraged to respond to these various forms of assessment as a means of continuing to improve the quality of the UT learning experience.

XI. UNIVERSITY POLICIES:

Honor Statement: *An essential feature of the University of Tennessee, Knoxville, is a commitment to maintaining an atmosphere of intellectual integrity and academic honesty. As a student of the university, I pledge that I will neither knowingly give nor receive any inappropriate assistance in academic work, thus affirming my own personal commitment to honor and integrity.*

Academic honesty practices:

Much of this course will be done with the intention to openly help your classmates. Take advantage of this group learning approach. However, any blatant duplication of code, figures, plots, etc. will be considered cheating and/or plagiarism and you will receive a zero on the assignment.

XII. STUDENTS WITH DISABILITIES POLICY:

Any student who feels he or she may need an accommodation based on the impact of a disability should contact the Office of Disability Services (ODS) at 865-974-6087 in 2227 Dunford Hall to document their eligibility for services. ODS will work with students and faculty to coordinate reasonable accommodations for students with documented disabilities.

XIII. THE INSTRUCTORS RESERVE THE RIGHT TO REVISE, ALTER AND/OR AMEND THIS SYLLABUS, AS NECESSARY. STUDENTS WILL BE NOTIFIED IN WRITING AND/OR BY EMAIL OF ANY SUCH REVISIONS, ALTERATIONS AND/OR AMENDMENTS.

XIV. PREREQUISITES

Chemistry 1 & 2
It is paramount that students possess an understanding of molecular chemistry, that is, be comfortable with concepts like molecular structure, electronegativity, and atomic interactions.

Biology 1

During this course many biological terms and concepts will come up in the reading, and in lecture. Ignorance on these subjects may prove difficult to overcome, but is doable for a determined student.

Basic computer Skills

For this type of class, it is a great advantage to be computationally savvy. This will take away the syntactical learning curve in many instances. However, an individual with basic computer knowledge and little typing skills can excel in this course. This is not a computer science class, rather it is geared towards biological scientists that wish to employ or understand a computational approach to biological systems.

XV.   TENTATIVE COURSE OUTLINE

Week 1
Module 1: Theory of MD Simulation – ½ week

The purpose of this module is to introduce students to the theory behind MD, and to explain what the computer is actually doing during a simulation. Here, students will get acquainted with terms like *forcefield*, *equations of motion*, and *trajectory*. This module will also cover the workflow of a simulation and expound upon individual steps. This section will consist of lectures, individual readings, group discussion, and a take-home module project.

Module 2: Navigating the Shell, a Linux tutorial – ½ week

This module is intended to wade students in the computational waters. Students will be introduced to a UNIX/Linux operating system and how to navigate the UNIX shell (command line interface). This section will be mostly hands-on, including following along with the instructor and executing commands from the instructor's screen.

Week 2-3
Module 3: Creating Structural Input Files with Leap – ½ week

This module is focused on understanding what the structural inputs to a simulation are, why they are needed and how to create them. This is an extremely hands-on and interactive module. Students will follow along with the instructor through a Leap tutorial, and subsequently perform the steps of the tutorial semi-independently.

Module 4: Performing an MD Simulation with NAMD – 1 ½ weeks

Here students will learn how to create the simulation input files that control all the variables of the simulation and actually run the simulation via remote submission to a cluster. This will be extremely hands-on, a packet of files will be provided by the instructor and students will follow along with the instructor to modify these files to fit their individual system. Then students will follow the instructor through a simulation submission tutorial, before they semi-independently perform a simulation on their individual systems.

Week 4-5
Module 5: Trajectory Analysis by Ptraj – 2 weeks

This module focuses on analyzing the raw data produced by the simulation to monitor specific aspects of the system to address a scientific question. Again, this will be a hands-on, tutorial driven module where the instructor will walk students through the steps and then expect them to work semi-independently on a module project.

Week 6
Module 6: Pre-processing and Formatting Data – 1 week

Here students will learn that data is not always perfect and often takes some pre-processing before statistical properties can be analyzed. This module will emphasize judging data convergence and data formatting. The instructor will provide several bash scripts that will be explained and modified in a tutorial format.

Week 7
Module 7: Statistical Analysis of Data – 1 week

This section will entail a short lecture about statistical analysis, but will mostly be composed of following the instructor as he demonstrates how to modify analysis scripts and explains the details of those scripts.

Week 8-9
Module 8: Creating Publication Quality Figures – 2 weeks

Here the focus is on creating effective illustrations of data. This section centers on using the VMD and Grace programs to create figures and plots that clearly display data. Students will follow the instructor's tutorial on how to use the software to manipulate and render figures.

Week 10-11
Module 9: Mock Poster Presentation of Research/ Mock Publication – 2 week

As final project, students will apply all the skills they have learned throughout the semester to create a mock research poster (undergrad) or a mock publication (grad). The instructor will present an actual poster in class to demonstrate how such a presentation is done, and assist students in making their own poster. This module will also contain a "journal club" like discussion, and a mini workshop on scientific writing.

Tentative Course Schedule

Date	Topic	Reading Assignment	Due
TR, Jan 12	Introduction		
TU, Jan 17	1:Theory of MD Simulation	Protein background	
TR, Jan 19	2: Linux/VI Tutorial	Protein background	MP 1
TU, Jan 24	2: Linux/VI Tutorial	Protein background	
TR, Jan 26	3: Leap Tutorial	Protein background	MP2
TU, Jan 31	3: Leap Tutorial	Protein background	
TR, Feb 2	4: NAMD Tutorial	Protein background	
TU, Feb 7	4: HPC Tutorial	Sim paper methods	MP3
TR, Feb 9	4: HPC Methods Disc/Catch-up	Sim paper methods	
TU, Feb 14	5: Ptraj Tutorial	Sim paper results	
TR, Feb 16	5: Ptraj Disc/Catch-up	Sim paper results	MP4
TU, Feb 21	5: Bash Scripting Tutorial	Sim paper results	
TR, Feb 23	5: Bash Scripting Tutorial	Sim paper results	
TU, Feb 28	5: Analysis Workshop	Sim paper results	
TR, Mar 2	5: Analysis Workshop	Sim paper conclusion	
TU, Mar 7	6: Data Formatting Workshop	Sim paper conclusion	MP5
TR, Mar 9	6: Data Formatting Workshop	Sim paper conclusion	
Mar 13-17	**Spring Break**	**How to have fun**	**Relaxation**
TU, Mar 21	6: Analysis Disc/ Catch-up	Sim paper conclusion	
TR, Mar 23	7: Statistical Analysis Workshop	Sim paper conclusion	MP6
TU, Mar 28	7: Statistical Analysis Workshop	Sim paper figures	
TR, Mar 30	8: Figure Creation Workshop	Sim paper figures	
TU, Apr 4	8: Figure Creation Workshop	Sim paper figures	MP7
TR, Apr 6	8: Overall Catch-up	Sim paper figures	
TU, Apr 11	8: Figure Creation Workshop	Sim paper figures	
TR, Apr 13	8: Figure Creation Workshop	Presentation	
TU, Apr 18	9: Presentation Workshop	Presentation	MP8
TR, Apr 20	9: Presentation Workshop	Presentation	
TU, Apr 25	9: Presentation Practice Day	Presentation	
TR, Apr 27	9: Presentation Workshop	Presentation	
April 28	**Last day of classes**		
TU, May 2	Final Project		Final project

<div align="center">

Syllabus
EPP 622 /LFSC 696 Bioinformatics Applications, Fall 2016
University of Tennessee, Knoxville

</div>

Course sections: EPP 622-50557, LFSC 696-50332
Meeting Time: MW 1:25-3:20
Meeting Place: Plant Biotechnology Building, Room 160
Course Credit Hours: 3
Couse website: http://epp.agbioinfo.utk.edu/

Intructor
Meg Staton   Email: mstaton1@utk.edu
Assistant Professor   Office: PBB 154
Entomology and Plant Pathology   Office hours: MW 3:25-4:30 and by appointment

The instructor reserves the right to revise, alter or amend this syllabus as necessary. Students will be notified by email of any such changes.

Teaching Assistant
Ming Chen   Email: mchen33@vols.utk.edu
Graduate Research Assistant   Office: PBB 153

I. Course Description

Fundamental bioinformatics concepts, principles and techniques with a focus on the application of bioinformatics to problems in agriculture. Laboratory practical will be taught within a LINUX computational environment where students will gain basic skills in bash and python scripting and construct open-source software workflows to analyze genomic data.

II. Value Proposition

The discipline of bioinformatics is one of the most effective and promising tools for generating biological research discoveries, but it requires robust training in order to apply the principles correctly. This course will provide students with bioinformatic skills for processing and understanding of large datasets such as genome and transcriptome sequences, gene and protein expression measurements, and heritable genomic variations. These skills will enhance student's research efficiency and scope and, long-term, will position students to be more effective and competitive in the technology-driven biomedical and agricultural science industries.

III. Student Learning Outcomes/Objectives

A. Students will be able to apply basic bioinformatic theory and tools to analyze biological datasets
B. Students will be able to effectively communicate and critically assess the application of bioinformatic tools to a variety of biological problems
C. Students will have basic competence in the UNIX shell, python scripting, and usage of bioinformatic tools from the command line

IV. Learning Environment

Class meets MW 1:25 - 3:20 and will consist of an hour of lecture/discussion followed by computer laboratory exercises.

A classroom is a collaborative environment, and both the instructor and the students have a shared responsibility to ensure a successful learning experience. Students should be prepared for all classes, be respectful of others, actively contribute to the learning activities in class and abide by the UT Honor Code. The teaching assistants and I will be prepared for all classes, evaluate learners fairly and equally, be respectful of all students, create and facilitate meaningful learning activities and follow University codes of conduct.

V. Course Communication
Outside of class and the website, the instructor and TA will utilize email to communicate course information, such as additional readings, changes to the syllabus, answering questions relevant to all students, etc. All students are responsible for checking their university email accounts and reading all emails regarding the class.

VI. Texts/Resources/Materials
The course website will be used to distribute reading materials, links to references, lecture slides, and laboratory exercises (https://github.com/mestato/epp622/wiki). There is not a required textbook to purchase. Readings for each class period can be found on the course website. Blackboard will be used to turn in homework assignments, keep track of grades, and possibly to distribute a mid-semester survey (http://bblearn.utk.edu).

VII. Required Equipment
Students are required to bring their own laptops (and power cord if needed) to class.

VIII. Course Evaluation
The final grade for each student will be on an A-F scale:

A	93-100 points
B+	88-92 points
B	80-87 points
C+	77-79
C	70-76
F	below 70

Points will be accrued through laboratory homework assignments, three tests and a final project. The final grade will be weighted as follows

Lab Homework	30%
Test 1	20%
Test 2	20%
Final Project	30%

Lab Homework Grading – Laboratory homework assignments will be distributed during each labortory class period (see schedule below). Submissions will be accepted through blackboard until midnight on the due date (http://bblearn.utk.edu). Assignments turned in up to 1 week late will receive a 20% grade reduction. Assignments turned in more than 1 week late will not be graded. The lowest lab grade for the semester will be dropped.
Tests - Tests will be given in class and will review material covered in both lecture and laboratory exercises. Extra credit questions will cover the literature readings provided.
Final Project – Each student will prepare a final project. This project requires that the student identify a bioinformatics research goal and appropriate dataset, execute the project, and prepare a written report with supporting data, analysis methods, code and other

documentation. Each student will give a final oral presentation of 15 minutes or prepare a blackboard wiki page on their work. Final project grades are based on a 100 point scale:

- One page project proposal – 10 points
- Final oral presentation – 10 points
- Final written report – 30 points
- Code and methodology documentation ("lab notebook") – 30 points
- Grade from peers – 10 points
- Providing feedback for other student's projects – 10 points

IX. Attendance

Attendance is the responsibility of each student. Presence during lecture and lab is essential for a students to achieve success in the class, but it will not be formally recorded or graded. Absences due to special circumstances should be discussed with the instructor prior to the absence via email or in person. Missed tests may not be made up unless the instructor has previously discussed the absense with the student and made those arrangements.

X. How to Be Successful in This Course

- <u>Do the readings and exercises during the week they are assigned</u>. Many of the concepts and practical exercises build on the material covered in prior lessons, so it is essential to try to attend all classes and to keep up with the subject matter. Getting behind can cause major setbacks for the rest of the semester.
- <u>Get help early with problems</u>. The instructor and TA are there to help and want you to be successful. If something is not making sense or you are unable to complete a lab exercise, seek help immediately through email and/or in-person meetings. This will prevent you from falling behind during this fast-paced class. Requests for help the night before a test or lab are due are not acceptable and may not be answered.
- <u>Use lab time wisely.</u> The hands-on lab time is your opportunity to explore the assigned exercise and ask any questions about it to the instructor and TAs. If you can complete the lab during the time slot, that means you won't have to worry about turning it in later. If not, try to make sure you have the basic concepts down and a plan for completing the work. This will save you time and frustration later.
- <u>Select a final project that is of a proper scope to accomplish in 4-5 weeks and work on it</u> **before** <u>and during dedicated class time.</u> Five class periods are devoted to working on the final project; this time is an opportunity to get help from the instructor and TA on any problems you encounter. The scope of the project should be sufficient to demonstrate mastery of a particular bioinformatic skillset, but should be accomplished in this short time frame. **Starting on the project prior to these classes and then attending the project classes** will ensure that you make regular progress on the project instead of procrastinating, and if roadblocks do arise, you can get help well before the due date.

XI. Course Feedback

A committee of 3 faculty members other than the instructor will be attending some classes and will be surveying the students in person at some point during the semester. You will receive more information about this during class. The instructor will leave the room while students fill out any surveys or answer questions. A final course evaluation will be provided to each student at the end of the course through the Student Assessment of Instruction System (SAIS). Each student will receive an email toward the end of the semester providing a link to the survey.

Course Schedule

Class Num.	Day	Date	Lecture Topic	Lab Topic
1	W	August 17th	Syllabus and Introduction to Linux	Shell Lab I
2	M	August 22nd	Bioinformatics	Shell Lab II (HW1 assigned)
3	W	August 24th	HPC Resources and Newton	Shell Lab III
4	M	August 29th	Unix Shell IV	Programming with Python I (HW2 assigned, HW1 due)
5	W	August 31st	Online resources and databases	Programming with Python II
	M	September 5th	Labor Day Holiday	
6	W	September 7th	Overview of high-throughput sequencing	Programming with Python III (HW3 assigned, HW2 due)
7	M	September 12th	Pairwise sequence alignments & BLAST	BLAST
8	W	September 14th	Applications of DNA sequencing	Programming with Python IV (HW4 assigned, HW3 due)
9	M	September 19th	Short Read QC and Mapping	DNASeq Lab I
10	W	September 21st	Short Read Mapping and Visualization	DNASeq Lab II (HW5 assigned, HW4 due)
11	M	September 26th	Test 1 (all material through 9/19 included)	
12	W	September 28th	Genome Assembly	DNASeq Lab III
13	M	October 3rd	Genome Annotation	Biopython (HW6 assigned, HW5 due)
14	W	October 5th	RNAseq Intro	RNASeq Lab I – Mapping and Visualization
15	M	October 10th	Differential Expression Statistics	RNASeq Lab II – Counting and DE analysis (HW7 assigned, HW6 due)
16	W	October 12th	Transcriptome Assembly	RNASeq Lab III – Transcriptome

				Assembly
17	M	October 17th	Work on Project	Work on Project (Project Proposal Due)
18	W	October 19th	HMMs and Gene Networks	RNASeq Lab IV – ORF finding, functional annotation (HW8 assigned, HW7 due)
19	M	October 24th	Metagenomics and 16S Amplicon Sequencing	16S Lab I
20	W	October 26th	Version Control with Github	16S Lab II (HW8 due)
21	M	October 31st	Work on Project	Work on Project
22	W	November 2nd	Test 2 (all material through 10/26 included)	
23	M	November 7th	Work on Project	Work on Project
24	W	November 9th	Work on Project	Work on Project
25	M	November 14th	Work on Project	Work on Project
26	W	November 16th	Work on Project	Work on Project
27	M	November 21st	Project Final Presentations	Project Final Presentations
28	W	November 23rd	Project Final Presentations	Project Final Presentations
29	M	November 28th	Project Final Presentations	Project Final Presentations

UNIVERSITY POLICIES

Dear Student,

The purpose of this Campus Syllabus is to provide you with important information that is common across courses at UT. Please observe the following policies and familiarize yourself with the university resources listed below. At UT, we are committed to providing you with a high quality learning experience.

I wish you the best for a successful and productive semester.

Provost Susan Martin

Academic Integrity:
"An essential feature of the University of Tennessee, Knoxville is a commitment to maintaining an atmosphere of intellectual integrity and academic honesty. As a student of the university, I pledge

Science Ethics

Life Sciences 615 / BCMB 614
1 credit (Pass / No pass)
Fall 2016

Tuesdays (3:40-5:00pm) WLS D205

Instructors: Dr. Liz Howell (lzh@utk.edu) WLS F 327B
Dr. John Koontz (jkoontz@utk.edu) WLS F213

Date:	Topic
August 23	Introduction to course format: answering the question– what is ethics? Reading: Module from Thomas Regan entitled "Introduction to Research Ethics." Read 2 Science articles on Driverless cars.
August 30	Ethical theories, which do you prefer and why? Readings: chapters from James Rachels on Cultural Relativity, Utilitarian, Kant and Virtue ethics. As an example of cultural relativity, read the case studies on Teaching Evolution vs. Creationism and be prepared to discuss.
Sept 6	Publications and authorship. Read the module by Jim Wilson on "Responsible Authorship and Peer Review." Read the paper on Photoshop alteration of scientific figures.
Sept. 13	Mentors and Being Mentored. Read the module by Margaret King on "Responsible Mentoring." Additional articles on BB on the Elizabeth Goodwin case. Also look at the recent article by Alberts et al on "Rescuing US biomedical research from its systemic flaws."
Sept 20	Session with students and their mentors. Please consider inviting your mentor to this class where they may be asked to share their mentoring philosophy. We will also do a role play exercise. Another excellent source of information and case studies is the "Entering Mentoring" workbook, posted on BB.
September 27	Use of Animals in Research (Guest, Patti Coan, UTK Veterinarian, Director of Animal Care and IACUC member). Read: Module on "Animal Subjects in Research."
October 4	Conflicts of Interest. Several readings posted on BB. Also go to the following site which has many different tests for unconscious bias. Take a few of the tests and be ready to discuss. https://implicit.harvard.edu/implicit/
October 11	Animal research debate. Two groups will present both sides to the following resolutions: 1) (from the chapter on Utilitarian Ethics, Rachels p97-98) "Because humans and nonhumans can suffer, we have the same reason for not mistreating both. If a human is tormented, why is it wrong? Because s/he suffers. Similarly, if a nonhuman is tormented, s/he also suffers, and so it is equally wrong for the same reason."

2) (from http://en.wikipedia.org/wiki/Tom_Regan regarding Tom Regan's position) "We each experience being the "subject-of-a-life." If this is the true basis for ascribing inherent value to individuals, to be consistent we must ascribe inherent value, and hence moral rights, to all subjects-of-a-life, whether human or non-human. The basic right that all who possess inherent value have, he argues, is the right never to be treated merely as a means to the ends of others. In Regan's view, not to be used as a means entails the right to be treated with respect, which includes the right not to be harmed."

The intention of the debate is to get both sides talking to each other to understand the issues more fully, it is not to "win." Also the 2 sides need to talk and decide which side is which. One year, both sides thought they were defending animal rights and were presenting the same arguments. Also in a debate, if you understand the arguments for one side, you should be able to understand and anticipate the reverse arguments for the other side. Thus it is possible that we could ask you to switch sides at the last minute. Be prepared for this possibility.

October 18	Patents and Intellectual Property: Read Module on "Introduction to Intellectual Property, Copyright Issues "on BB. Additional readings on Supreme Court decision on BRCA. Guest visitor, Maha Krishnamurthy, a UTK licensing manager who has done license transactions of IP and patents).
October 25	Use of humans in research, Henrietta Lacks - ethics in biomedical settings: Readings posted on BB. Guest visitor, Annette Mendola, Chief, Division of Clinical Ethics, Division of Clinical Ethics at UT Medical Hospital
November 1	Genetically Modified Organisms. Readings posted on BB.
November 8	Environmental Ethics: Several reading are posted on BB on intrinsic worth. Guest visitor, Daniel Simberloff, Gore Hunger Professor of Environmental Science from the EEB dept).
November 15	Stephen J. Gould and History of Science. Readings: three articles are posted on BB. Also, there is a Philosophy Experiment website that leads you through a series of questions that can be interesting and helpful in terms of asking about ethical dilemmas and whether one is consistent in thinking about situations. It may help you clarify your thinking with respect to Kant vs. Utilitarian ethics. When you get to the site, please take the "Should you kill the fat man?" test, also the "Morality play" and then the "Would you eat your cat?" tests. The site is: http://www.philosophyexperiments.com/
November 22	Institutional Review Board (IRB). Guest visitor, Colleen Gilrane, chair of UTK's IRB.
November 29	Course evaluation by all participants

This schedule is tentative and subject to change!

Go to "Online@UT" to login to Blackboard. Readings are to be found posted on Blackboard. The main readings are from a series of modules written and edited by Thomas Regan, emeritus professor at NC State. Additional readings are from the science literature.

I.   **HOW TO BE SUCCESSFUL IN THIS CLASS:** Most importantly, be an active participant. The course is set up to encourage your persistent and continued participation. Pre-class exercises are to encourage you to come to class having thought about and prepared to participate in a discussion about the topics to be addressed in the next class period.

- This course is graded as satisfactory or no credit. We make the decision based upon active participation in the classroom. It is not enough to do the readings and submit your wiki in anticipation of class. We want your voice to be heard while in class. That is the major reason we restrict enrollment.

- We expect adherence to the following code of conduct in class:
     1. Attend all sessions
     2. Give and accept feedback
     3. Don't hesitate to ask hard questions
     4. Make it safe to talk about what we don't know: there are no stupid questions
     5. If you have issues with topics raise them publicly and not within a small group: i.e. only one discussion stream at a time.
     6. Seek multiple perspectives: listen to what others are saying
     7. Disagree without being disagreeable: i.e. be respectful of others
     8. See humor in things
     9. Give everyone the opportunity to speak
     10. No electronic devices while in meetings
     11. Different cultures/disciplines/ethnic groups may have different points of view: no right answers

II.   Format of the course. Do the readings each week and post a wiki on BB which contains your thoughts on the topic. Examples from past years are posted so you will have an idea of interesting wikis. Generally, a discussion that draws on your experience and makes connections is strong. Don't summarize what you have read, bring your thoughts and experience to the wiki.

- Write a weekly wiki and post on BB. This is due the day before class , ie Monday at 5. Before you have done any of the readings for a particular topic describe your views on the topic. Then complete the readings. Your wiki should be your reaction to the readings for that particular week in a context related to what you view as your own personal ethics. Have your views changed as a result of what you read? If so, how have they changed? If not, then how have the readings reinforced or clarified your views? While you may refer to specific parts of the text, it is not acceptable to simply provide a summary of what you read.

- If you are facilitating a group discussion for the week, you are exempt from writing a wiki that week.

- Find one current example in Science, Nature, etc magazines of a scientific ethics issue.   Post on BB in your wiki by Nov 14th. This will let us identify your interests as well as provide future topics. Recent examples include:
  http://news.sciencemag.org/brain-behavior/2014/05/u.s.-brain-initiative-gets-ethical-advice
  http://pipeline.corante.com/archives/2014/05/06/crispr_in_the_courts.php 2 different groups participated in the development of CRISPR but are independently filing patents
  http://www.sciencemag.org/content/344/6187/960.full Should congress require NSF to curb wasteful and unwise research?

- For the class meeting, two students will facilitate the discussion. Below are some ideas for class engagement.
  - ➢ Use case studies from the readings.
  - ➢ Break the class up into smaller groupings and invite discussion on a topic. This would then be followed by the small groups reporting to the larger class. Similarities as well as differences in discussion can be identified and further considered.
  - ➢ Include everyone by going around the room and asking everyone to provide their thoughts on a topic.
  - ➢ Get other ideas from science ethics internet sites. Pat Marsteller from Emory has given us a bunch of interesting sites via Harry Richards.   They are listed below so they will be available to you for browsing.
  - ➢ Think of leading questions that perhaps others have not considered. Think of 2-3 questions and then bring them to class for discussion.
  - ➢ Ask students who were raised in different cultures for their thoughts and experiences. How do they contrast with your experiences?
  - ➢ Read the wikis and look for underlying themes. Did any comment surprise you? What did you learn from reading them?
  - ➢ Invite quiet students to share their thoughts. Being quiet does not mean not being engaged.

Course Description: Journal club in Science ethics. Topics include basic ethical theory including cultural relativity, Utilitarianism, Kant, and virtue ethics. Issues include scientific fraud, mentorship, the use of animals in research, Intrinsic Worth, Institutional Animal Care and Use Committee (IUCAC), the use of humans in research, Institutional Review Board (IRB), Patents, Intellectual Property, Conflicts of Interest (COI), Genetically Modified Organisms (GMOs), Environmental Science.

Value proposition/course goals: Ethical dilemmas abound in science. This class will give you tools to use in considering dilemmas you may encounter during your scientific career.

Student learning outcomes: at the end of this course you should be able to:
  - ➢ Differentiate between Utilitarian, Kantian and Virtue models of ethics.
  - ➢ Understand what makes an argument fallacious, see for example: http://en.wikipedia.org/wiki/List_of_fallacies
  - ➢ Provide compelling arguments to support the validity of your conclusions

Course announcements will be sent to your UTK email account. You are responsible for monitoring your UTK e-mail account. To send us email, put Sci Ethics Journal Club in the header.

III.   **UNIVERSITY POLICIES: It is important for you to know about some of the support systems and university policies that apply to all courses.**

If you need course adaptations or accommodations because of a documented disability of if you have emergency information to share, please contact the office of disability services at 974-6087.

 "An essential feature of the University of Tennessee, Knoxville, is a commitment to maintaining an atmosphere of intellectual integrity and academic honesty. As a student of the university, I pledge that I will neither knowingly give nor receive any inappropriate assistance in academic work, thus affirming my own personal commitment to honor and integrity." [*Undergraduate Catalog*]

 "Students are also responsible for any acts of plagiarism. Plagiarism is using the intellectual property of someone else without giving proper credit. The undocumented use of someone else's words or ideas in any medium of communication (unless such information is recognized as common knowledge) is a serious offense, subject to disciplinary action that may include failure in a course and/or dismissal from the university. Specific examples of plagiarism are:

- Copying without proper documentation (quotation marks and a citation) written or spoken words, phrases, or sentences from any source;
- Summarizing without proper documentation (usually a citation) ideas from another source (unless such information is recognized as common knowledge);
- Borrowing facts, statistics, graphs, pictorial representations, or phrases without acknowledging the source (unless such information is recognized as common knowledge);
- Collaborating on a graded assignment without the instructor's approval;
- Submitting work, either in whole or in part created by a professional service and used without attribution (e.g., paper, speech, bibliography, or photograph)."

Office of Research Integrity Internet sites include:

http://ori.dhhs.gov/education/
http://scholarworks.umass.edu/esence/

Lots of downloadable materials and cases:
http://www.umass.edu/sts/ethics/cases.html
http://guides.library.iit.edu/content.php?pid=31717&sid=301097

Role plays for RCR:
http://www.onlineethics.org/Topics/RespResearch/ResCases/RCRroleplays.aspx

Ethical dilemmas in research:
http://nationalethicscenter.org/
http://www.ethicsresearch.com/freeresources/rrwresearchwrongdoing.html

Blog by a Philosopher on Recent Science Ethics Issues
http://scientopia.org/blogs/ethicsandscience/
http://blather.scientopia.org/

Site that monitors retraction of scientific papers
http://retractionwatch.com/

Special Topics - Advanced Mass Spectrometry
Life Sciences 695
3 credits
Fall 2015

TR 11:10 - 12:25pm WLS M401

Lead Instructor: Robert L Hettich, ORNL (hettichrl@ornl.gov)

Lecture #	Date	Topic	Lecturer
1	Aug. 20	Class overview *Overall goals and lecture schedule* *What is mass spectrometry?* *Applications of MS*	**Hettich**
2	Aug. 25	Basic Aspects of MS *General features of mass spectrometers and spectra* *Nomenclature, customary units, and figures of merit* *Isotopic contributions and mass defects*	**Hettich**
3	Aug. 27	Ionization #1 *Electron ionization; Chemical ionization* *Ion source loss processes*	**Hettich**
4	Sept. 1	Ionization #2 *Electrospray ionization* *Matrix-assisted laser desorption ionization* *Ion transport from atmosphere to vacuum*	**Hettich**
5	Sept. 3	Mass analyzers #1 *Ions manipulation via fields* *Static field mass analyzers* *Performance figures of merit*	**Hettich**
6	Sept. 8	Mass analyzers #2 *Fundamentals of dynamic field mass analyzers* *Linear quadrupole mass filters* *3-D quadrupole ion trap* *Linear quadrupole ion trap* *Performance figures of merit*	**Hettich**
7	Sept. 10	Tandem MS overview *Basic processes* *Ion activation methods* *Instrument configurations*	**Hettich**

8	Sept. 15	Proteins: Overview *Capabilities of MS for proteins* *What information does MS give?* *Choosing the best MS tool* *Overall flow chart for protein characterization*	**Hettich**
9	Sept. 17	Proteins: Digestion *Why digest proteins to give peptides?* *Common proteases and protocols* *Peptide identification*	**Abraham**
10	Sept. 22	Proteins: Tandem MS of pept #1 *Nomenclature; Principles of fragmentation*	**Hettich**
11	Sept. 24	Proteins: Tandem MS of pept #2 *Example mass spectra*	**Hettich**
12	Sept. 29	Proteins: Chromatographic separations *Basics of protein chromatography* *Types of stationary phases, gradients, etc.*	**Abraham**
13	Oct. 1	Proteins: Sepn with MS (off-line, on-line) *Compatibility with MS; Sensitivity, solvents, etc.*	**Abraham**
14	Oct. 6	Proteins: Sep with MS (multi-LC) *Online and offline MudPIT; other variations*	**Abraham**
15	Oct. 8	Proteins: Sep with MS (applications) *Model system examples* *Hi pH-low pH combination*	**Abraham**
16	Oct. 13	Proteins: Database searching *Mass mapping: Sequest et. al. and de novo*	**Giannone**

Fall Break   Oct. 15-16

17	Oct. 20	Proteins: Automated MS/MS proc. I *It takes a process: linking steps, linking experiments* *What does it mean?False-positive and false-negative rates* *Database issues*	**Giannone**
18	Oct. 22	Proteins: Automated MS/MS proc. II	**Giannone**

		Normalization; Spectral balancing;	
		Redundancy; ScanRanker	
19	Oct. 27	Proteins: Quantitation	**Giannone**
		Relative; Labeling vs. label-free	
20	Oct. 29	Proteins: Quantitation	**Giannone**
		Relative vs. absolute; AQUA, SILIC, etc.	

Take-home exam #2 (50% of total grade)　　　**Oct. 29 – Nov. 9**

21	Nov. 3	Proteins: post-translation modifications	**Hettich**
		T*ypes of PTMs; phosphorylation*	
22	Nov. 5	Proteins: Intact proteins	**Hettich**
		W*hy measure intact proteins?*	
		Isotopic distributions	
		Mass accuracy and database identification	
23	Nov. 10	Protein: Higher order structure	**Hettich**
		How can MS be used for higher order structure?	
		H/D exchange, etc.	
		Surface mapping example	
24	Nov. 12	Lipids	**Campagna**
		Shotgun Lipidomics	
		Fatty Acid Methyl Ester Analyses	
		Detection of Non Polar Lipids	
25	Nov. 17	Metabolites	**Campagna**
		Targeted and untargeted metabolomics	
		The challenge of identification	
		Data processing and visualization	
		Measuring metabolic fluxes	
25	Nov. 19	Carbohydrates	**Campagna**
		Challenges: heterogeneity; lability; detection	
27	Nov. 24	MS imaging?	**Campagna**
		Overview MS imaging	
		Novel instrumentation	
28	Dec. 1	Summary of Biol MS	**Hettich**

Take-home exam #3 (25% of total grade)　　　**Dec. 1-8**

Colloquium in Genome Science and Technology
LFSC541
Spring 2016

Time: Tuesdays 3:40 - 4:55 pm
Location: M307 Walters Life Sciences
Grades: Satisfactory/No Credit, 1 credit.

Description:

This semester, the GST Colloquium will host a series of high-profile invited scientists from other research institutions in the US. Our guests are highly accomplished in the field of genome science, systems biology, or computational biology in the broader sense. The course is anchored around the lectures given by the invited speakers. Over the Fall 2015 semester, the students in the GST program formed groups. This Spring, each group is hosting one or two speakers. Each group will also introduce the research of each incoming speaker to the entire class.

Learning goals:

The course delivers professional development for all GST students. First, through the guest lectures, students are exposed to exciting advances from the forefront of genome science and related areas. Second, students will become more comfortable with communicating with external speakers, who are both colleagues and role models, on matters of scientific substance and professional development. Third, as students work with each other to select, introduce, and host the speakers, they form new ties among each other and experience the joys and pitfalls of team work. Selected students are taking on a more prominent stewardship role by chairing their teams.

Expectations:

All students are expected to participate to an approximately equal degree over the course of the semester to make the event(s) a smooth and productive experience for all. Within each host group, students will work under the guidance of their chairperson to contribute to the delivery of the introductory class and to the hosting of the speaker. Absences should be excused, preferentially ahead of time, by emailing the instructor and the group chair. Two unexcused absences are permitted per semester.

Instructor of record:

Albrecht von Arnim, Hesler 228; Email: vonarnim@utk.edu; Phone: 974-6206

LFSC 541 - Spring 2016

Month	Day	Speaker and Topic	
January	19	Introduction of Folker Meyer - The Earth Microbiome	Comparative Genomics Group
January	26	**Dr. Folker Meyer** Argonne National Laboratory *Title: Surprising Lessons Learned from a Metagenomic Investigation of a Subsurface Sample*	Comparative Genomics Group
February	2	Introduction of Adrian Elcock - The Two Faces of Proteins: Simulation and Experiment	Computational Molecular Biophysics Group
February	9	**Dr. Adrian Elcock** University of Iowa *Title: Development and Application of Molecular Simulation Methods for Modeling Macromolecular Behavior In Vivo*	Computational Molecular Biophysics Group
February	16	No class scheduled	
February	23	No class scheduled	
March	1	Introduction of Norbert Perrimon *Note unusual meeting time*	Biomedical Science Group II
March	**4**	**GST Retreat -** Guests: GST alumni Dr. Sangeetha Rajagopalan, Molecular Templates, Austin, TX. Dr. Yutao Liu, Georgia Regents University, Augusta, GA	Biomedical Science Group I
March	8	Introduction of Michael MacCoss	Proteomics Group
March	15	Spring Break – No Class	
March	22	**Dr. Michael MacCoss** University of Washington, Seattle *Topic: Proteomics from Model Organisms to Health and Disease*	Proteomics Group
March	29	**Dr. Norbert Perrimon** Harvard University Medical School *Title: Entering the Golden Age of Drosophila for Understanding and Treating Human Diseases*	Biomedical Science Group II
March	**31**	Introduction of Nikos Kyrpides *Note unusual meeting time*	Comparative Genomics Group
April	5	**Dr. Nikos Kyrpides** Lawrence Berkeley National Lab & DOE Joint Genome Institute *Topic: Microbial Metagenomics and Metabolic Pathways*	Comparative Genomics Group
April	12	Introduction of Hailing Jin	Plant and Microbial Biology Group
April	19	**Dr. Hailing Jin** University of California-Riverside *Title: Cross-Kingdom RNAi in Plant-Pathogen Interactions*	

GST Colloquium
Workshops in Bioinformatics and Computational Biology

Life Sciences 541
1 credit
Spring 2014

Time:

Plenary sessions: Tuesday 3:40pm - 4:55pm WLS M307
Workshops: 3:00pm-5:30pm Haslam Business Building Room 102

Instructor of record:

Albrecht von Arnim; Room 228 Hesler Biology; 4-6206; Email: vonarnim@utk.edu

Concept:

We often find ourselves in a situation where we need to analyze a new type of data with new tools. We would love to learn the ropes quickly for immediate payoff, but instead we are left to figure things out the hard way. On the other hand, we are sometimes wondering why other students don't know certain obvious tricks of the trade that we use in our research everyday. This semester, we will try to remove some of these barriers by organizing a series of hands-on workshops designed to teach practical skills in data analysis.

Rationale:

In order to be successful in the age of big and quantitative biological data, we need to (i) expand our technical skillset and (ii) think in an interdisciplinary way about data outside our field. (iii) We also need to know how to teach our advanced skills to others. How can a program like GST help with this? Our community has a lot of technical expertise, but we need to share it.

Logistics:

Students in the GST program will self-organize into five different teams. Each team will design, organize, and teach one workshop. The five workshops will be held at the end of the semester, once a week, in March and April 2014. The workshops will be taught to the entire class of GST. Later workshops may build on an earlier one. Students are expected to attend at least three out of the five workshops to be offered (plus one as co-instructor).

Learning goals:

1. Familiarize ourselves with commonly used and broadly applicable data analysis techniques in a hands-on, practical fashion. 2. Build on existing quantitative and computational skills formed in core courses such as LFSC507, LFSC517, BCMB510, and others. 3. Construct a peer-learning

environment where junior and senior students share expertise. 4. Gain experience with planning and implementing a successful workshop.

Format of the workshops:

All workshops should include active participation by the attendees, but will probably also include demonstrations/tutorial. A manual will be distributed one week ahead of time so that participants can come prepared. Participants should generally be working on their own laptop if at all possible. The workshops will be ~2 hours long and will be directed at all GST students.

Teams:

Each team should be about the same size (~7-9 students) and have a mix of senior and junior students. Each team will have a team leader. As these teams are quite diverse, it is clear that not every member will participate in the same way. However, every member is expected to contribute in their own way to the success of the project. It is not necessary that all team members are highly familiar with the chosen topic at the very beginning. There are other ways to contribute (define the scope, run tests prior to the live workshop, write the manual, help participants during the workshop, etc). However, 2-3 students should be sufficiently familiar to lead the project. Implementing a successful workshop requires both a broad vision and attention to detail.

Milestones:

The workshops should be of broad interest, deliver an in-depth overview over the topic at hand, and build on a broad base of expertise.

- Define the topic. What skills will be attractive to other students?
- Learning goals: What should participants be enabled to do at the end?
- Define specific tasks and techniques to be taught.
- What computer platform is needed for the workshop? What software?
- What prior knowledge is needed for participants to achieve the goal?
- Identify suitable existing datasets to be used (case study).
- Prepare workshop manual with materials for advance preparation, a script for the workshop itself, and troubleshooting tips.
- Practice the workshop >2 weeks ahead of time.

Web resources:

Outlines of 2h workshops held at a BI conference - Examples:
http://www.iscb.org/glbio2012-program/glbio2012-full-agenda

Link to BI workshops - Online and in-person
http://gettinggeneticsdone.blogspot.com/2013/04/list-of-bioinformatics-workshops-training.html

Example of an online workshop from UC Davis - Full documentation - Galaxy BI software
http://training.bioinformatics.ucdavis.edu/docs/2013/04/bootcamp/galaxy/intro-to-galaxy.html

Calendar

Groups should meet once a week ('Colloquium') to make progress on workshop planning.

January 14   Plenary session - Planning Meeting I
                Due: Teams, Selection of topics to be covered
                Homework: Define the broad concept for the workshop

January 21   Plenary session - Planning meeting II
                Due: Present broad concept to class: Learning goals, biological context
                    Schedule planning meetings

January 28   Team session I
                Due: 1st draft, Define techniques to be taught, Case study to give biological
                    context, Assign tasks to team members; Timeline with milestones

February 4   Team session II
                Due: Prerequisite skills, hardware and software requirements

February 11   Team session III
                Due: Datasets to be used in the workshop

February 18   Team session IV
                Due: 2nd draft of complete workshop

February 25   Team session V
                Due: Final set of workshop activities

March 4   Team session VI
                'First rehearsal'; Due: Draft script, troubleshooting notes

March 11   Team session VII
                'Dress rehearsal'; Due: Advertisement to GST, Workshop manual to GST

March 18   Spring Break

March 25   Workshop I - Newton HPC (3:00pm - 5:30pm)

April 1   Workshop II - Protein Sequence - Function - Evolution

April 8   Workshop III - Introduction to Statistics in R

April 15   Workshop IV - Molecular Dynamics

April 22   Workshop V - Networks

April 29   Workshop VI - Next Generation Sequencing