Honours Biophysics – Semester 2, 2016

COURSE OUTLINE

Biophysics is one of the latest branches of physics that has been growing fast in the last few decades. Experimental methods from physics have been used in studies of biomolecules from the early days but use of computational methods is relatively new (thanks to the cheap HPC systems), and they are expected to play a crucial role in turning molecular biology into a hard science like physics and chemistry. This course will provide an introduction to the computational methods used in description of biomolecules. Fundamental problems in molecular biology as well as applications in biotechnology and pharmacology will be considered.

The Details

| Credit points | 1 halfHonours course |
| Offered | Semester 2 |
| Assumed knowledge | Senior Statistical Mechanics |
| Classes | 10 hours of lectures |
| Assessment | 1 assignment and a 1.5-hour final exam |
| Lecturer | A/Prof. Serdar Kuyucak, School of Physics, room 438, Phone: 9036 5306, Email: serdar@physics.usyd.edu.au |

Unit of study goals

(a) To present a comprehensive introduction to molecular dynamics (MD) simulations of biomolecules, discussing the strong and weak points of currently used force fields.
(b) To discuss applications of MD simulations to several biomolecular systems, pointing the limitations of brute-force MD and how they can be overcome using sampling techniques.
(c) To generate a critical appreciation of what is currently feasible using MD simulations. To drive home that accuracy of the results is the main goal of current efforts.

Your learning commitments

The final exam will be on the material presented in the lectures. Assignment will be based on performing literature search on application of MD simulations to a particular biomolecular system and writing a report on the current state of research. The report should critically examine the work done so far and suggest potential avenues of research that could advance the field.

Texts and reference books

There is no set textbook for the course. Lecture notes will be provided during the course via the web page (see the table above). Some useful books for further reading are:
T. Schlick, Molecular modeling and simulation, 2002.

Assignment and Assessment

Assessment will be based on a 1.5-hour final examination (60 marks) and one assignment (40 marks) due on Aug. 29. Assignments should be submitted to the Student Office on the due date by 5pm.
Lecture Content (weekly) and Specific Objectives

   **Specific objectives:** Learn about various biomolecules in cells and identify proteins as the main functional elements. Consider quantum, classical and stochastic description of biomolecules and rationalise classical MD simulations as the standard model of biomolecules.

2. Basics of MD simulations: Discuss the basic ingredients of MD simulations; empirical force fields, integration algorithms, constrained dynamics, boundaries, handling of long range forces, constant temperature and pressure ensembles, molecular mechanics, equilibration.
   **Specific objectives:** Understand how an MD code works by examining its basic ingredients. Critically examine the force fields currently used in MD simulations and appreciate their strengths and weaknesses.

3. Analysis of trajectory data from MD simulations: RMSD, pair distribution functions, conformational analysis, time correlation functions and transport coefficients, free-energy calculations using free energy perturbation, thermodynamic integration, umbrella sampling, and steered MD simulation methods.
   **Specific objectives:** Learn the basic computational tools used in analysing the trajectory data generated from MD simulations. Recognize the use of different methods in free energy calculations.

4. Applications of MD simulations to ion channels and transporters: Role of the ion channels and transporters in the nervous system, MD simulations of gramicidin A and potassium channels, structure and function of glutamate transporter.
   **Specific objectives:** Learn how MD simulations have been used to investigate the function of channels and transporters using the crystal structure (or a homology model) of the corresponding protein. Appreciate what is feasible at present, and what will be achievable in near future.

5. Applications of MD simulations to protein-ligand interactions: Two fundamental problems in description of ligand binding to proteins: i) determination of the complex structure, ii) calculation of free energy of binding, applications to rational drug design from toxin peptides.
   **Specific objectives:** Learn how the docking methods can be used in combination with MD simulations to generate accurate structures for protein-ligand complexes. Appreciate problems of low affinity and lack of selectivity in drug development, and learn how these problems can be resolved using computational methods.
Generic Details for Honours Courses

Academic Dishonesty/Plagiarism
We will NOT accept assessments that are simply copied. Copying the work of another person without acknowledgment is plagiarism and contrary to University policies on Academic Dishonesty and Plagiarism (http://sydney.edu.au/ab/policies/Academic_Honesty_Cwk.pdf).

Academic Dishonesty means seeking to obtain or obtaining academic advantage (for example, in assessments) by dishonest or unfair means or knowingly assisting another student to do so. Academic Dishonesty includes, but is not limited to:

(a) recycling – that is, the resubmission for assessment of work that is the same, or substantially the same, as work previously submitted for assessment in the same or in a different unit of study (except in the case of legitimate resubmission with the approval of the examiner for purposes of improvement);
(b) fabrication of data;
(c) the engagement of another person to complete or contribute to an assessment or examination in place of the student, whether for payment or otherwise or accepting such an engagement from another student;
(d) communication, whether by speaking or some other means, to other candidates during an examination;
(e) bringing into an examination forbidden material such as textbooks, notes, calculators or computers;
(f) attempting to read other student’s work during an examination;
(g) writing an examination or test paper, or consulting with another person about the examination or test, outside the confines of the examination room without permission;
(h) copying from other students during examinations;
(i) Inappropriate use of electronic devices to access information during examinations.

Plagiarism means presenting another person’s work as one’s own work by presenting, copying or reproducing it without acknowledgement of the source. Plagiarism is a form of Academic Dishonesty, but is treated separately. Plagiarism includes presenting work for assessment, publication, or otherwise, that includes:

(a) phrases, clauses, sentences, paragraphs or longer extracts from published or unpublished work (including from the Internet) without acknowledgement of the source; or
(b) the work of another person, without acknowledgement of the source and presented in a way that exceeds the boundaries of legitimate cooperation.

Where to go for help
If you need help, as a first step you should ask the lecturer. For general help with Honours, please see the Honours Coordinator.

Providing us with feedback
We welcome comments on all aspects of this unit. You should feel free to contact the lecturer / honours coordinator at any time. There is also a formal opportunity for feedback at the Honours Staff-Student Liaison meeting.

Consideration of factors affecting your study
If your academic performance in a Science Faculty unit of study is adversely affected by illness or some other serious event, such as an accident, you should notify both:

- the Honours Co-ordinator
- the Faculty of Science Student Information Office (level 2 of the Carslaw building)

within 7 days after the period for which consideration is sought, by completing an Application for Special Consideration with accompanying documentation. This is especially important if you miss an examination.

If you have another reason for the Science Faculty to take account of your circumstances - religious commitments, legal commitments (e.g. Jury duty), elite sporting or cultural commitments (representing the University, state or country), or Australian Defence Force commitments (e.g. Army Reserve) - you should notify both:

- the Honours Co-ordinator
- the Faculty of Science Student Information Office (level 2 of the Carslaw building)

at least 7 days BEFORE the period for which consideration is sought, by completing an Application for Special Arrangements with accompanying documentation.

These two forms of Consideration should cover most allowable circumstances. However, if you have another reason for requiring the School of Physics to take account of your circumstances, you should notify the Honours Co-ordinator immediately.

You should not submit an application of any type if

- there is no assessment associated with a missed class, or
- you have a reasonable opportunity to make up any work you missed.

If, for example, you miss an assignment, an application for appropriate Consideration is required to allow late submission, but we do expect the assignment to be submitted. Sometimes catching up may be impossible, in which case we will consider a pro-rata adjustment of your marks on the basis of an application for Consideration.

Note: all applications for Special Consideration in Physics Honours are considered by a Special Considerations Committee at the end of your Honours year. We will not necessarily adjust your mark for a
specific Honours course (as such marks are not officially reported) but will take into account any application for special consideration in the assignment of a final Honours mark and grade.

Special Consideration or Special Arrangements
To submit an application for *Special Consideration* or *Special Arrangements* you should:

1. Obtain the appropriate Application pack from the Student Information Office of the Faculty of Science, the Faculty website at http://sydney.edu.au/science/cstudent/ug/forms.shtml, or the Physics Student Services Office.
2. Complete the forms and obtain whatever original documentary evidence is appropriate. Note especially that the Professional Practitioner's Certificate is essential for Special Consideration on grounds of serious illness - Medical Certificates will NOT be accepted.
3. Take the original copy of all forms and documents, plus sufficient copies for each unit of study affected and yourself, to the Faculty of Science Student Information Office (NOT any other Faculty Office if you are seeking Consideration in a unit taught by Physics). They will sign/stamp both the original application form and the copies. In the case of Physics units, one copy of the documentation must then be submitted to the Physics Student Services Office. Keep one copy yourself. A formal decision on your application will be sent to your university email address within 14 days.

Further details on University policy regarding Considerations can be found in policy documents entitled *Assessment and Examination* at the University Policy web site (http://sydney.edu.au/policy/).

Students unsure what type of Consideration is appropriate, or unhappy with a Consideration decision, should consult the Physics Student Services Office.

It is important to realise that the policies on *Special Consideration* apply throughout the University. However, actions in response to requests for Consideration may be specific to Physics and may be different in Departments responsible for your other units of study.