MONASH University
Information Technology

FIT3139
Computational science

Unit Guide

Semester 2, 2011

Last updated: 22 Aug 2011

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FIT3139 Computational science - Semester 2, 2011

The unit provides an overview of computational science and an introduction to the central methods in this field. While it is not tied to any particular field of scientific study, it requires a general scientific background at advanced introductory level.

Topics include: the role of computational tools and methods in 21st century science; modelling and simulation; continuous vs discrete models; analytic versus numeric models; deterministic versus stochastic models; Monte-Carlo methods; epistemology of simulations; visualisation; high-dimensional data analysis; optimisation; limitations of numerical methods; high-performance computing and data-intensive research.

Each topic area will be introduced with a general overview followed by a discussion of one or a few selected methods in full technical detail. These will be practiced in tutorials and laboratories, which will also acquaint the students with standard software packages for scientific computing (for example, Mathematica, Matlab, Maple, Sage).

Seminars and guest lectures will present case studies and link to current topics in research.

Applications examples will be drawn from Physics, Biology, Bioinformatics, Chemistry, Social Science, etc.

Mode of Delivery

Clayton (Day)

Contact Hours

2 hrs lectures/wk, 3 hrs lab/wk, 1 hr tutorial alternating fortnightly with attendance at Monash University Research Projects Abroad (MURPA) seminars.

Workload

Workload Commitments:

Students will be expected to spend a total of 12 hours per week during semester on this unit.

This includes:

2 hours of lectures per week

3 hours of lab session per week

1 hour of tutorial/MURPA seminar per week (Note: MURPA seminars and tutorials roughly alternate). However, due to speaker availability for MURPA seminars, there is a slight change to the sequence of weeks the class is required to attend the seminars. Specifically: attendance to MURPA seminars is required for weeks: 2,4,6,7,8,11. The tutorials will go on every alternate week as scheduled: weeks 1,3, 5,7,9,11. Refer moodle course page for details.

Up to an additional 6 hours of personal self-study, completeting lab and assignment work and revision.

Unit Relationships

Prerequisites

One of MAT1841, MAT2003, ENG1091, MTH1030 or equivalent plus any introductory programming unit (eg FIT1002, ECE2071, TRC2400, or equivalent)

Chief Examiner

Dr Arun Konagurthu

Campus Lecturer

Clayton

Arun Konagurthu

Contact hours: Monday 3pm - 4pm

Academic Overview

Learning Objectives

Upon successful completion of the unit students will -

- understand the role of computational tools and methods in modern science;
- understand the process of model construction, model fitting, model verification and analysis in scientific problem solving;
- understand the differences between the core modelling approaches (numeric versus analytic; continuous versus discrete; linear versus non-linear; deterministic versus stochastic);
- understand the implications of choosing a particular modelling approach;
- understand central computational methods for the analysis of models in each of these classes
- understand the role of simulation and visualisation;
- be introduced to at least one standard scientific software package for model construction and analysis;
- have an general overview of high-performance techniques in scientific computing and of methods for data-intensive research (storage, archiving etc).

Graduate Attributes

Monash prepares its graduates to be:

1. responsible and effective global citizens who:

a. engage in an internationalised world
b. exhibit cross-cultural competence
c. demonstrate ethical values

critical and creative scholars who:

a. produce innovative solutions to problems
b. apply research skills to a range of challenges
c. communicate perceptively and effectively

Assessment Summary

Examination (3 hours): 50%, In-semester assessment: 50%

Assessment Task	Value	Due Date
Assignment 1	15% (Part 1 = 5%, Part 2 = 10%)	2 September 2011
Assignment 2	10%	7 October 2011
Pracs during Labs (1 and 1/2 hours each)	25% (2.5% for each assessable prac)	Weekly in Labs
Examination 1	50%	To be advised

Teaching Approach

Lecture and tutorials or problem classes

This teaching and learning approach provides facilitated learning, practical exploration and peer learning.

Students first encounter the information at lectures, discuss and explore them at length during tutorials, and practice them in a hands-on environment during labs.

Feedback

Our feedback to You

Types of feedback you can expect to receive in this unit are:

- Informal feedback on progress in labs/tutes
- Graded assignments with comments
- Test results and feedback
- Solutions to tutes, labs and assignments

Your feedback to Us

Monash is committed to excellence in education and regularly seeks feedback from students, employers and staff. One of the key formal ways students have to provide feedback is through SETU, Student Evaluation of Teacher and Unit. The University's student evaluation policy requires that every unit is evaluated each year. Students are strongly encouraged to complete the surveys. The feedback is anonymous and provides the Faculty with evidence of aspects that students are satisfied and areas for improvement.

For more information on Monash's educational strategy, and on student evaluations, see:
http://www.monash.edu.au/about/monash-directions/directions.html
http://www.policy.monash.edu/policy-bank/academic/education/quality/student-evaluation-policy.html

Previous Student Evaluations of this unit

If you wish to view how previous students rated this unit, please go to
https://emuapps.monash.edu.au/unitevaluations/index.jsp

Required Resources

MATLAB programming environment will be used in Pracs. However, since MATLAB is not freely available students should use GNU Octave (a freely available MATLAB-like numerical programming language) for self-study. GNU Octave source as well as binaries (for various operating systems) can be downloaded from this link:

http://www.gnu.org/software/octave/download.html

Unit Schedule

Week	Activities	Assessment
0	Download GNU Octave (see Required Resources). Familiarise with MATLAB using Octave. Links to the documentation (for both Octave and MATLAB) are given in the Reading list section below)	No formal assessment or activities are undertaken in week 0
1	Introduction to Computational Science + Tute + Prac (Lab)	Prac 1 (formative feedback only)
2	Lectures on solving linear models + MURPA Seminar + Prac (Lab)	Prac 2 (formative feedback only)
3	Lectures on solving non-linear models + Tute + Prac (Lab)	Prac 3
4	Lectures on Continuous and discrete models + MURPA Seminar + Prac (Lab)	Prac 4
5	Lectures on solving ordinary differential equations + Tute + Prac (Lab)	Prac 5
6	Lectures on Static and Dynamic Simulations + MURPA Seminar +Prac (Lab)	Prac 6 + Assignment 1 due 2 September 2011
7	Lectures on Monte Carlo Approach + Tute + Prac (Lab)	Prac 7
8	Lectures on Linear Optimisation + MURPA Seminar + Prac (Lab)	Prac 8
9	Lectures on non-linear optimisation + Tute + Prac (Lab)	Prac 9
10	High dimensional data analysis + MURPA Seminar + Prac (Lab)	Prac 10 + Assignment 2 due 7 October 2011
11	High dimensional data visualisation + Tute + Prac (Lab)	Prac 11
12	Overview of High-Performance Computing + MURPA Seminar + Prac (Lab)	Prac 12
	SWOT VAC	No formal assessment is undertaken SWOT VAC
	Examination period	LINK to Assessment Policy: http://policy.monash.edu.au/policy-bank/academic/education/assessment/assessment-in-coursework-policy.html

*Unit Schedule details will be maintained and communicated to you via your MUSO (Blackboard or Moodle) learning system.

Assessment Requirements

Assessment Policy

To pass a unit which includes an examination as part of the assessment a student must obtain:

- 40% or more in the unit's examination, and
- 40% or more in the unit's total non-examination assessment, and
- an overall unit mark of 50% or more.

If a student does not achieve 40% or more in the unit examination or the unit non-examination total assessment, and the total mark for the unit is greater than 50% then a mark of no greater than 49-N will be recorded for the unit

Assessment Tasks

Participation

Students should attend at least 4 out of the 6 MURPA seminars (this is a hurdle). As part of Assignment 2, you will be required to summarise in detail 1 MURPA seminar.

Students must actively participate in 4 out of the 6 tutorials. Participation includes contributing opinions to a discussion, providing an answer to questions/exercises, or posing a unit related question.

Students must attend at least 8 out of the 12 pracs sessions (labs).

A student who does not meet all these hurdles can only get a maximum of 49-N for the unit.

For applying for special consideration refer to the link provided under 'Extensions and penalties' at the end of this section.

- **Assessment task 1**

Title:
Assignment 1
Description:
This assignment is about computational problem solving and has two parts.

Part 1 - The assignment will consist of questions and problems designed to evaluate your understanding of the material provided during the first six weeks of the semester.

Part 2 - Additionally, a short paper discussing a computational technique will be provided. The students are required to read the paper and summarise it. They will also be expected to write a MATLAB program that implements the technique.
Weighting:
15% (Part 1 = 5%, Part 2 = 10%)
Criteria for assessment:
Part 1 - Ability to answer the questions and solve the stated problems correctly

Part 2 - Ability to read and clearly summarise the computational technique, ability to code the technique, and correctness of the program on sample data sets
Due date:

2 September 2011

- **Assessment task 2**

Title:

Assignment 2

Description:

Problems will be given relating to the material learnt in the first 10 weeks of the semester.

Weighting:

10%

Criteria for assessment:

Demonstrate abilities in modelling the problems and using the right computational/simulation techniques to solve them.

Due date:

7 October 2011

- **Assessment task 3**

Title:

Pracs during Labs (1 and 1/2 hours each)

Description:

Each week you will need to complete a prac assignment using MATLAB independently. NOTE: MATLAB WILL NOT BE TAUGHT IN LECTURES. Students are required to self-learn MATLAB. GNU-Octave (see Required Resources section above) is a freely available MATLAB-like programming environment. Students should use GNU-Octave during self-study for preparation and solving the prac assignments. Pointers where needed will be provided in lectures and tutorials.

Prac assignments are composed of several computer-based problems. The solutions to the problems are expected to be primarily designed and developed (using GNU Octave) during your 6 hours of "self-study" period every week. This means that you must have a significant proportion of the prac prepared and sorted out before attending the scheduled computer lab and testing it on the available MATLAB environment.

The aim of the 1 and 1/2 hour computer lab practical is to iron out any bugs, ask any questions about the prac you have not been able to solve on your own, and improve the parts that your demonstrator points out as lacking (including comments, algorithms, etc). If you do nothing before the 1 and 1/2 hours scheduled, you will soon realise that you do not have enough time to complete the assignment. The prac sheets will be released (every Thursday) and made available on the unit's web page on Moodle.

Each prac will be marked during the hour-and-a-half immediately after the first hour-and-a-half of that lab session. You must remain in the lab session until your prac is marked.

Every prac sheet contains the assessment criteria used to assess that prac. In addition, demonstrators carry with them a marking guide prepared by the lecturer which indicates how exactly to mark each prac question. You can request the demonstrator to show you the marking guide after he/she has marked your prac.There is a prac every week.

The first two practical sessions will not be assessed. Only formative feedback will be given where required.

Weighting:

25% (2.5% for each assessable prac)

Criteria for assessment:
Quality of completed assignments.
Due date:
Weekly in Labs

Examinations

- **Examination 1**

Weighting:
50%
Length:
3 hours
Type (open/closed book):
Closed book
Electronic devices allowed in the exam:
None

Assignment submission

It is a University requirement (http://www.policy.monash.edu/policy-bank/academic/education/conduct/plagiarism-procedures.html) for students to submit an assignment coversheet for each assessment item. Faculty Assignment coversheets can be found at http://www.infotech.monash.edu.au/resources/student/forms/. Please check with your Lecturer on the submission method for your assignment coversheet (e.g. attach a file to the online assignment submission, hand-in a hard copy, or use an online quiz).

Extensions and penalties

Submission must be made by the due date otherwise penalties will be enforced.

You must negotiate any extensions formally with your campus unit leader via the in-semester special consideration process: http://www.infotech.monash.edu.au/resources/student/equity/special-consideration.html.

Returning assignments

Students can expect assignments to be returned within two weeks of the submission date or after receipt, whichever is later

Other Information

Policies

Monash has educational policies, procedures and guidelines, which are designed to ensure that staff and students are aware of the University's academic standards, and to provide advice on how they might uphold them. You can find Monash's Education Policies at: http://policy.monash.edu.au/policy-bank/academic/education/index.html

Key educational policies include:

- Plagiarism (http://www.policy.monash.edu/policy-bank/academic/education/conduct/plagiarism-policy.html)
- Assessment (http://www.policy.monash.edu/policy-bank/academic/education/assessment/assessment-in-coursework-po
- Special Consideration (http://www.policy.monash.edu/policy-bank/academic/education/assessment/special-consideration-policy.h
- Grading Scale (http://www.policy.monash.edu/policy-bank/academic/education/assessment/grading-scale-policy.html)
- Discipline: Student Policy (http://www.policy.monash.edu/policy-bank/academic/education/conduct/student-discipline-policy.html)
- Academic Calendar and Semesters (http://www.monash.edu.au/students/key-dates/);
- Orientation and Transition (http://www.infotech.monash.edu.au/resources/student/orientation/); and
- Academic and Administrative Complaints and Grievances Policy (http://www.policy.monash.edu/policy-bank/academic/education/management/complaints-grievance-policy.
- Codes of Practice for Teaching and Learning (http://www.policy.monash.edu.au/policy-bank/academic/education/conduct/suppdocs/code-of-practice-tea

Student services

The University provides many different kinds of support services for you. Contact your tutor if you need advice and see the range of services available at www.monash.edu.au/students The Monash University Library provides a range of services and resources that enable you to save time and be more effective in your learning and research. Go to http://www.lib.monash.edu.au or the library tab in my.monash portal for more information. Students who have a disability or medical condition are welcome to contact the Disability Liaison Unit to discuss academic support services. Disability Liaison Officers (DLOs) visit all Victorian campuses on a regular basis

- Website: http://adm.monash.edu/sss/equity-diversity/disability-liaison/index.html;
- Telephone: 03 9905 5704 to book an appointment with a DLO;
- Email: dlu@monash.edu
- Drop In: Equity and Diversity Centre, Level 1 Gallery Building (Building 55), Monash University, Clayton Campus.

Reading list

1. Scientific Computing: An Introductory Survey (second edition) Michael T. Heath. Publisher: McGraw-Hill

2. Introduction to Computational Science: Modelling and Simulation for Sciences. Angela B. Shiflet and George W. Shiflet. Publisher: Princeton University Press

3. Applied Numerical Methods with MATLAB for Engineers and Scientists. Steve C Chapra, McGraw-Hill

4. Insight Through Computing: A MATLAB introduction to Computational Science and Engineering. Charles F. Van Loan and K.-Y. Daisy Fan

5. Computational Science and Engineering. Gilbert Strang Publisher: Wellesley-Cambridge Press

6. Getting started with MATLAB: A Quick introduction for scientists and Engineers. Rudra Pratap. Publisher: Oxford University Press

7. Wiki resource on GNU Octave: http://wiki.octave.org/

8. MATLAB documentation: http://www.mathworks.com/help/techdoc/learn_matlab/bqr_2pl.html