MONASH University
Information Technology

FIT3139
Computational science

Unit Guide

Semester 2, 2015

Last updated: 23 Jul 2015

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FIT3139 Computational science - Semester 2, 2015

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)

Workload Requirements

Minimum total expected workload equals 12 hours per week comprising:

(a.) Contact hours for on-campus students:

- Two hours of lectures
- One 3-hour laboratory
- One 1-hour tutorial/seminar

(b.) Additional requirements (all students):

- A minimum of 6 hours independent study per week for completing lab and assignment work, private study and revision.

See also Unit timetable information

Additional workload requirements

Note: MURPA seminars and tutorials alternate weekly. However, due to speaker availability for MURPA seminars, there may be a slight change in the sequence of weeks the class is required to attend the MURPA seminars. The exact sequence will be made available closer to the start of the semester.

Unit Relationships

Prerequisites

One of MAT1841, MAT2003, ENG1091, MTH1030, MTH1035 or equivalent plus any introductory programming unit (eg FIT1040, FIT1002, ECE2071, TRC2400, or equivalent)

Chief Examiner

Dr Arun Konagurthu

Campus Lecturer

Clayton

Arun Konagurthu

Consultation hours: Monday 3pm - 4pm

Tutors

Clayton

James Collier

Phil Abramson

Rui Chen

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 the Student Evaluation of Teaching and Units (SETU) survey. 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, see:

www.monash.edu.au/about/monash-directions/ and on student evaluations, see:
www.policy.monash.edu/policy-bank/academic/education/quality/student-evaluation-policy.html

Previous Student Evaluations of this Unit

Feedback from previous semesters suggests that students enjoy this unit.

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

Academic Overview

Learning Outcomes

Upon successful completion of the unit, students will:

1. apply the process of computational scientific model building, verification and interpretation;
2. develop and analyse the differences between core classes of modelling approaches (Numerical versus Analytical; Linear versus Non-linear; Continuous versus Discrete; Deterministic versus Stochastic);
3. evaluate the implications of choosing a particular modelling approach over other possible approaches;
4. explain the role of simulation and data visualisation in science;
5. solve idealisations of several real-world problems across various scientific disciplines.

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)	Participation in labs and tutes weekly (5%)
2	Lectures on solving linear models + MURPA Seminar + Prac (Lab)	
3	Lectures on solving non-linear models + Tute + Prac (Lab)	
4	Lectures on Continuous and discrete models + MURPA Seminar + Prac (Lab)	
5	Lectures on solving ordinary differential equations + Tute + Prac (Lab)	
6	Lectures on Static and Dynamic Simulations + MURPA Seminar +Prac (Lab)	
7	Lectures on Monte Carlo Approach + Tute + Prac (Lab)	Assignment 1 due end of week 7 (10%)
8	Lectures on Linear Optimisation + MURPA Seminar + Prac (Lab)	
9	Lectures on non-linear optimisation + Tute + Prac (Lab)	
10	Lectures on data analysis + MURPA Seminar + Prac (Lab)	
11	High dimensional data analysis and visualization + Tute + Prac (Lab)	Assignment 2 due end of week 11 (10%)
12	High dimensional data visualization+ MURPA Seminar + Prac (Lab)	
	SWOT VAC	No formal assessment is undertaken in 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 learning system.

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.

Assessment Summary

Examination (3 hours): 75%, In-semester assessment: 25%

Assessment Task	Value	Due Date
Assignment 1	10% (Part 1 = 5%, Part 2 = 5%)	end of week 7
Assignment 2	10%	end of week 11
Active participation in labs and tutes	5%	Weekly in Labs
Examination 1	75%	To be advised

Assessment Requirements

Assessment Policy

Faculty Policy - Unit Assessment Hurdles
(http://intranet.monash.edu.au/infotech/resources/staff/edgov/policies/assessment-examinations/assessment-hurd

Academic Integrity - Please see resources and tutorials at
http://www.monash.edu/library/skills/resources/tutorials/academic-integrity/

Assessment Tasks

Participation

Students are expected to attend at least 4 out of the 6 MURPA seminars.

Students are expected to 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 are expected to attend at least 8 out of the 12 pracs sessions (labs).

Note: 5% of the unit assessment is given for active participation in tutes and labs.

Failure to meet these expectations may cause difficulties in passing the unit.

- **Assessment task 1**

  Title:
  Assignment 1
  Description:
  This two-part assignment will consist of a practical computational problem set based on topics covered during the first half of the semester.
  As a part of this assignment, computer programs have to be written in addition to submitting a typed report analysing the given data sets.

  Weighting:
  10% (Part 1 = 5%, Part 2 = 5%)
  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:
  end of week 7
  Remarks:
  This assessment relates to Learning Outcomes 1, 2, 3, 4 and 5.

- **Assessment task 2**

Title:
Assignment 2
Description:
This assignment will contain practical problem sets based on the material covered in the second half of the semester.

Weighting:
10%
Criteria for assessment:
Correctness of modelling the given computational problems and using the right computational/simulation techniques to solving that proposed model.
Due date:
end of week 11
Remarks:
This assessment relates to Learning Outcomes 3, 4, 5, 6, 7.

- **Assessment task 3**

Title:
Active participation in labs and tutes
Description:
Each week you will need to complete a prac assignment using Python/MATLAB independently. NOTE: Python/MATLAB WILL NOT BE TAUGHT during the LECTURES. It is an expectation that students are required to self-learn Python/MATLAB if not already familiar. Since MATLAB is proprietary software, GNU-Octave (see Required Resources section above) is an equivalent open-source (freely available) MATLAB-like programming environment. Students can 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 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 scheduled labs, 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.

Your will be asked to handover your work scripts/files to your demonstrator. 5% of the unit assessment goes towards your active participation in the labs and tutes. Feedback to your lab exercises will be provided during the lab hours as well as during consultation with the lecturer (where necessary).
Weighting:
5%
Criteria for assessment:
Successfully attempt the lab and tute exercises.
Due date:

Weekly in Labs

Remarks:

This assessment relates to all Learning Outcomes

Examinations

- **Examination 1**

Weighting:

75%

Length:

3 hours

Type (open/closed book):

Closed book

Electronic devices allowed in the exam:

None

Remarks:

This assessment relates to all Learning Outcomes.

Learning resources

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

Monash Library Unit Reading List (if applicable to the unit)
http://readinglists.lib.monash.edu/index.html

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

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.monash.edu.au/exams/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.

Assignment submission

It is a University requirement (http://www.policy.monash.edu/policy-bank/academic/education/conduct/student-academic-integrity-managing-pla 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 electronic submission). Please note that it is your responsibility to retain copies of your assessments.

Online submission

If Electronic Submission has been approved for your unit, please submit your work via the learning site for this unit, which you can access via links in the my.monash portal.

Required Resources

Please check with your lecturer before purchasing any Required Resources. Limited copies of prescribed texts are available for you to borrow in the library, and prescribed software is available in student labs.

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

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: www.policy.monash.edu.au/policy-bank/academic/education/index.html

Faculty resources and policies

Important student resources including Faculty policies are located at http://intranet.monash.edu.au/infotech/resources/students/

Graduate Attributes Policy

http://www.policy.monash.edu/policy-bank/academic/education/management/monash-graduate-attributes-policy.h

Student Charter

www.opq.monash.edu.au/ep/student-charter/monash-university-student-charter.html

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 http://www.monash.edu.au/students. For Malaysia see http://www.monash.edu.my/Student-services, and for South Africa see http://www.monash.ac.za/current/.

Monash University Library

The Monash University Library provides a range of services, resources and programs that enable you to save time and be more effective in your learning and research. Go to www.lib.monash.edu.au or the library tab in my.monash portal for more information. At Malaysia, visit the Library and Learning Commons at http://www.lib.monash.edu.my/. At South Africa visit http://www.lib.monash.ac.za/.

Disability Liaison Unit

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://www.monash.edu/equity-diversity/disability/index.html
- Telephone: 03 9905 5704 to book an appointment with a DLO; or contact the Student Advisor, Student Commuity Services at 03 55146018 at Malaysia
- Email: dlu@monash.edu
- Drop In: Equity and Diversity Centre, Level 1, Building 55, Clayton Campus, or Student Community Services Department, Level 2, Building 2, Monash University, Malaysia Campus