COSC3011 Scientific Computing
COSC3911 Scientific Computing Advanced – Semester 2, 2011

UNIT OUTLINE

Unit Description

COSC 3011/3911 Scientific Computing is a 6-credit point unit for Senior students. (The Advanced version of the unit, COSC3911, is also available to Physics Honours and PhD students in a 4 credit point form.) COSC3011/3911 is a core unit of the Computational Science (COSC) major. The unit provides a Senior-level treatment of scientific problem solving using computers, and students in this unit learn to apply a wide range of numerical schemes for solving ordinary and partial differential equations. Emphasis is placed on the suitability of particular methods to particular problems, and on the understanding of numerical accuracy and stability. A variety of scientific problems are considered, including planetary motion, population age structure, heat diffusion, traffic flow and quantum mechanics. Coding is performed with MATLAB, and basic programming experience is assumed. Example codes are provided which implement the methods and solve science problems. The lab sessions, assignments, and a project provide practical experience in scientific programming and in implementing numerical methods to solve science problems.

Students enrolled in the Advanced unit encounter a selection of more challenging laboratory and assignment questions, and the written examination contains a question for the Advanced students only. Physics Honours/PhD students must take the Advanced unit.

Unit Details

Credit points 6 (4 for Physics Honours/PhD students in COSC 3911)
Offered Semester 2
Classes Two 1-hour lectures per week and one 3-hour computational lab per week for 10 weeks
Assumed knowledge Programming experience in MATLAB
Prohibitions COSC3011 (for COSC3911), COSC3911 (for COSC3011), COSC 3001, COSC 3301, COSC3901
Assessment 2-hour final examination, two assignments, completion of computational lab sessions and a project (the project is omitted for Physics Honours/PhD students in COSC3911)
Lecturer A/Prof. Mike Wheatland (michael.wheatland@sydney.edu.au)

Class timetabling

There are two lectures per week, plus a three-hour computational laboratory class. The lectures are during weeks 1-11, and the labs are during weeks 2-11. There are no lectures in week 10 due to Labour Day. Weeks 12 and 13 are dedicated to the project (described below). Any changes to the schedule of lectures and labs will be advised in class.

<table>
<thead>
<tr>
<th>Time</th>
<th>Class</th>
<th>Location</th>
</tr>
</thead>
<tbody>
<tr>
<td>Monday 9am</td>
<td>Lecture</td>
<td>LT1</td>
</tr>
<tr>
<td>Monday 1pm</td>
<td>Lecture</td>
<td>LT1</td>
</tr>
<tr>
<td>Friday 9am-12pm</td>
<td>Computational Laboratory</td>
<td>Rm 359</td>
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Study resources

There is no textbook for the unit.

The book *Numerical Methods for Physics* (Second Edition) by Alejandro Garcia is a recommended reference, and sections of this text are followed by parts of the unit, as indicated in the week-by-week outline below. However, the unit contains additional material and the lecture presentation is self-contained. Students are not expected to buy this book, although copies are available at the CoOp book shop. A copy is also on Reserve at the SciTech Library.
The recommended reference on numerical methods is any of the *Numerical Recipes: The Art of Scientific Computing* books (second editions). Chapters of these books, which are also referred to in the week-by-week outline, are available for download (subject to some restrictions) at [www.nrbook.com/a](http://www.nrbook.com/a).

This unit uses MATLAB for computation, and basic programming experience in MATLAB is assumed. MATLAB is available on the computers in the Computational Science Laboratory (Room 359 in the School of Physics). If you wish to purchase your own copy of MATLAB, a student version is available from the Co-op book store for $99, including documentation on DVD. However, students are not expected to buy a copy. A variety of reference material is available online for MATLAB, including the documentation accessible via the helpbrowser command in MATLAB or online at the MathWorks site ([www.mathworks.com](http://www.mathworks.com)).

The eLearning pages for this unit provide access to lecture and lab notes, codes, and additional material.

### Assessment

<table>
<thead>
<tr>
<th>Item</th>
<th>Senior students in COSC3011/3911 (6 credit point unit)</th>
<th>Physics Honours/PhD students in COSC 3911 (4 credit point unit)</th>
<th>Weighting</th>
</tr>
</thead>
<tbody>
<tr>
<td>Laboratory</td>
<td>10%</td>
<td>Laboratory</td>
<td>14%</td>
</tr>
<tr>
<td>Assignments</td>
<td>25%</td>
<td>Assignments</td>
<td>36%</td>
</tr>
<tr>
<td>Project</td>
<td>30%</td>
<td>Omitted</td>
<td>-</td>
</tr>
<tr>
<td>Written exam</td>
<td>35%</td>
<td>Written exam</td>
<td>50%</td>
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### Laboratory

The laboratory sessions consist of sets of exercises requiring you to modify the codes introduced in the lectures (available via the eLearning site), and to write your own codes, to implement numerical methods and solve science problems. The laboratory sessions support the lecture material, and are a crucial part of the unit. Students work individually, with assistance from tutors and a supervisor. You will be provided with swipe-card access to the Computational Laboratory (Room 359 in the School of Physics) which will give you access during normal building hours. This will provide you with additional time using the lab computers to work on your assignments and the project.

The lab sessions account for 10% of the course mark (14% of the course mark for Physics Honours/PhD students). The mark is based on satisfactory completion of the exercises for each week. The work must be done during the lab class: work done outside the lab class time will not be marked. The tutor or supervisor will assess completion of the exercises, and record this during the laboratory class. You must get the tutor or supervisor to sign off on your work and record a mark to receive the marks for the week.

You are required to keep an A4-sized logbook recording the results of your computations. Your logbook need only be hand-written, but should include derivations, numerical results, explanatory text, and sketches of important graphs. The tutor or supervisor will determine and record completion based on discussion with you and reference to your logbook, during the class. You need to supply the logbook.

### Assignments

The assignments consist of a number of questions, requiring you to write codes to solve science problems. There are two assignments, worth a total of 25% (36% for Honours/PhD students) of the total mark. Assignments must be done individually and handed in to the Student Services Office.

1. Assignment 1 is due at 5pm on Friday 26 August (end of week 5).
2. Assignment 2 is due at 5pm on Friday 14 October (end of week 11).

### Project

The project is a substantial part of the unit, involving three weeks of work (there are no lectures in weeks 11-13, to allow work on the project), and comprising 30% of the mark (Honours/PhD students do not do the project). The project is due Friday 28 October at 5pm, i.e. the end of week 13, and should be handed in to the Student Services Office in the School of Physics. A one paragraph summary of the project topic is due Friday 14 October, i.e. the end of week 11. You may revise the topic at a later date, but failure to submit a one-paragraph summary on time may result in a deduction of 5% from your project mark.

**Project scope and the choice of a topic**

The project is an opportunity for you to extend the skills developed in the laboratory sessions, and to pursue your own interests. You are encouraged to design your own topic, using your general scientific knowledge, or by drawing on one of the suggestions below. However, please ensure that the scientific model you are solving makes sense. Do not construct your own model, unless you are sure that it is correct. The project must use MATLAB and should apply and/or extend upon the material covered in lectures. The project must involve numerical solution of ODEs or...
PDEs. The project should be associated with a problem in science, although the emphasis may be more towards the science or towards the numerical methods applied. The report must provide references, listing any resources or materials used.

The one-paragraph summary (due 14 October) is a chance to obtain initial feedback about the suitability and difficulty of your chosen topic. The summary should be e-mailed to the lecturer, who will provide some preliminary advice, recommendations for reading, etc. However, after that initial feedback the project choice and the work itself should be your own. The level of help provided in the lab sessions is not provided for the project work.

Assessment of the project is via a written report that should be not more than 15 pages in length, excluding appendices. It may be shorter. The report should introduce the scientific area, explain the modelling and numerical methods applied, and present a discussion of the results obtained. You should include, as an appendix to the report, all relevant MATLAB codes. If you use codes other than ones you write yourself, this must be acknowledged and explained. The lecturer will provide examples of excellent past student project reports for inspection during the Computational lab sessions.

As part of your project submission, you may perform a demonstration of your codes in the laboratory during week 13. Please arrange with the lecturer if you want to do this.

The project accounts for 30% of the unit mark (Honours/PhD students do not do the project), and is assessed according to: clarity of presentation (20%); understanding of topic and methods (30%); quality of results (30%); difficulty/novelty of topic (10%); and on a brief self-reflective statement (10%). Note that the ‘difficulty/novelty’ category rewards projects involving a significant extension beyond the course material.

Past student projects have covered diverse topics including the motion of charged particles in specified electromagnetic fields (orbit theory), solution of the Black-Scholes equation describing financial markets, the three-body problem for orbital motion, solution of Burger’s equation describing nonlinear advection, solution of the Korteweg-de Vries equation describing solitons, solution of the wave equation in 2-D to describe a vibrating drum skin, multigrid methods, the Generalised Minimum Residual method, and Chebyshev methods. Other possibilities include modeling the spread of a disease, modeling the evolution of the age structure of a population (using a more realistic model than the Leslie model), investigating a particular nonlinear system, and investigating symplectic methods.

Project assessment
The project accounts for 30% of the unit mark (Honours/PhD students do not do the project), and is assessed according to: clarity of presentation (20%); understanding of topic and methods (30%); quality of results (30%); difficulty/novelty of topic (10%); and on a brief self-reflective statement (10%). Note that the ‘difficulty/novelty’ category rewards projects involving a significant extension beyond the course material.

The emphasis in assessment is on the quality of the work and not the quantity. A report may be significantly shorter than 15 pages and receive high marks. Two crucial points are that the science problem should make sense, and that you must correctly implement numerical methods. Do not invent your own model for a system unless you are certain that it provides a sensible description. It is important to get your codes to work correctly, and to provide evidence that the codes work correctly, e.g. in application to simple test cases. If there is aberrant behaviour, you need to work out what is going wrong.

Marks will be awarded in the different categories according to the general guidelines in the Table shown below. Note that not all of the points listed may be relevant for a given project, depending on the topic and methods chosen.

<table>
<thead>
<tr>
<th>Assessment guidelines</th>
<th>Description</th>
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<tbody>
<tr>
<td>Clarity of presentation (20%)</td>
<td>Are the science context, modeling, numerical methods, and results clearly presented? Is the 'jargon' of a particular field used, is it explained when first introduced? Is all notation simple, consistent and correct? Are explanations brief but sufficiently complete? Are any approximations being made adequately explained, together with their limitations? Are the figures well presented, and clearly explained? Are the codes well written, clear, and adequately documented? Is there a brief conclusion, explaining what has been found?</td>
</tr>
<tr>
<td>Understanding of topic and methods (30%)</td>
<td>Does the report demonstrate understanding of the science, the model, and the numerical methods? Are any assumptions in the model, and the basis of the numerical methods explained? Are the methods used appropriate for the problem at hand? Have alternative methods been considered? Does the report provide references for the science topic and for the numerical methods used? Are any aberrant results</td>
</tr>
<tr>
<td>Section</td>
<td>Details</td>
</tr>
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<td>------------------------------------------------------------------------</td>
<td>----------------------------------------------------------------------------------------------------------------------------------------</td>
</tr>
<tr>
<td>Quality of results (30%)</td>
<td>Does the scientific problem being solved make sense? Are the numerical methods correctly implemented? Is a solution presented to the problem at hand? Are the results related back to the problem, and explained in the context of the problem? Are the results correctly and adequately interpreted, in the context of the model? Have comparisons been made between methods, and/or with results in the literature? Has the numerical method been adequately tested e.g. on an analytic solution? Have stability and accuracy been considered?</td>
</tr>
<tr>
<td>Difficulty/novelty of the topic (10%)</td>
<td>Does the project extend beyond the material in the unit? Are new numerical methods, or new science topics (i.e. ones not covered in the unit) introduced? Does the project demonstrate reading and understanding of literature outside the lecture notes and recommended references? Does the project involve theory outside of that covered in the unit? Has the work involved significant or difficult coding?</td>
</tr>
<tr>
<td>A self-reflective statement (10%)</td>
<td>You should conclude your report with a brief (less than half a page) reflective statement, in which you describe what you have learnt from the experience of doing the project. What particular skills have you gained, if any, and what would you do differently if you did it again? Did you encounter any particular difficulties? The statement can be personal/anecdotal – it should describe your experience.</td>
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**Where to go for help**

If you need help, you can
- as a first step, always check your unit eLearning pages for information, documents and links.
- go to the Physics Student Services Office, Room 210 in the Physics building, or phone 9351 3037.
- ask the lecturer or a tutor in the lab sessions.
- ask other students using the Discussion forum provided in the Discussions link on the unit eLearning pages.
- consult one of the many services provided by the University, such as the Maths Learning Centre. These can be found at sydney.edu.au/current_students/student_services/index.shtml or through your MyUni pages sydney.edu.au/myuni.
- e-mail or visit your lecturer (A/Prof. Mike Wheatland, Rm 463, Physics Annex, michael.wheatland@sydney.edu.au)
- (for questions about the COSC program) contact the COSC coordinator Dr Pulin Gong (pulin.gong@sydney.edu.au)

**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 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 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 School of Physics Student Services Office 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.

**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/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 (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 and Special Arrangements apply throughout the University. Policies on other forms of Consideration are specific to Physics and may be different in Departments responsible for your other units of study.

**Providing us with feedback**

We welcome comments on all aspects of this unit. You should feel free to contact your lecturer, tutors or the COSC coordinator (listed under "Where to go for help" above) at any time. There is also a formal opportunity for feedback at the Senior Physics Staff-Student Liaison meeting, held one lunch time towards the end of semester with staff and student representatives from the various units of study, including this one. Your feedback helps us improve this unit.

### Changes this year

Changes this year include:

- revision of lectures to clarify many points and reduce content
- revision of assessment weighting to better reflect emphasis on practical skills
- revision of lab questions to ensure students complete labs on time
- revision of UoS outline

These changes were motivated in part by feedback received from students last year, and in previous years.

### Week-by-week descriptions

The following outline lists the topics covered each week in the lectures and labs, the science problems used to illustrate the topics, and lists the relevant sections of the recommended references.

#### Week 1

**Lectures:** Review of MATLAB; review of matrix algebra; Types of numerical error; Ordinary Differential Equations or ODEs (Euler and midpoint methods for dynamics problems)

**Science problem:** projectile motion

**Refs:** Garcia sections 1.2, 1.4, 1.5, and 2.1; Numerical Recipes sections 1.3, 2.1, 2.11, 20.1

**Lab:** There is no lab in week 1

#### Week 2

**Lectures:** Dynamical ODEs continued: the Kepler problem; Non-dimensionalisation; Elementary methods applied to the Kepler problem; New methods (Verlet and Velocity-Verlet)

**Science problem:** Keplerian orbits

**Refs:** Garcia section 3.1

**Lab:** Based on lectures in week 1
Week 3
Lectures: Adaptive time steps; General form of ODEs for numerical solution; Runge-Kutta (Taylor series) methods; Stability of ODEs; Stiff problems
Science problem: the simple pendulum
Refs: Garcia sections 2.1, 3.2, and 3.3; Numerical Recipes sections 16.0, 16.1, 16.2, 16.6
Lab: Based on lectures in week 2

Week 4
Lectures: Two-point Boundary Value Problems or BVPs; Shooting method for two-point BVPs; ODE eigenvalue problems; Quantum Simple Harmonic Oscillator or SHO; Leslie model
Science problems: quantum oscillators and population age structure
Refs: Garcia section 4.3, and pages 283–285; Numerical Recipes sections 17.0, 17.1
Lab: Based on lectures in week 3

Week 5
Lectures: Two-point BVPs and solution via finite differencing and relaxation; Eigenvalue problems; the quantum SHO revisited (inverse iteration, deflation, and over-relaxation)
Science problems: stationary states of a quantum system
Refs: Garcia pages 283–285
Lab: Based on lectures in week 4

Week 6
Lectures: Partial Differential Equations or PDEs; Classification of PDEs (Initial Value Problems or IVPs and BVPs); Parabolic PDEs and the diffusion equation; Forward-Time Centred Space discretisation, and solution for diffusion, numerical stability of FTCS for 1-D diffusion; 2-D diffusion
Science problem: the spread of heat
Refs: Garcia sections 6.1 and 6.2; Numerical Recipes section 19.0
Lab: Based on lectures in week 5

Week 7
Lectures: Hyperbolic PDEs and the wave and advection equations; FTCS applied to advection; von Neumann stability analysis; Lax and Lax-Wendroff methods for advection; Nonlinear advection
Science problem: the advection of a pulse
Refs: Garcia sections 7.1 and 9.1; Numerical Recipes sections 19.1 and 19.2
Lab: Based on lectures in week 6

Week 8
Lectures: Compressible fluid model for traffic; Analytic analysis of the traffic model (nonlinear advection speed, shock waves/traffic jams, method of characteristics); Cars starting from a set of traffic lights
Science problems: various problems to do with traffic flow
Refs: Garcia: Section 7.2
Lab: Based on lectures in week 7

Week 9
Lectures: 2-D elliptic PDEs and the Laplace and Poisson equations; Jacobi and Gauss-Seidel methods of relaxation for elliptic PDEs; Successive Over-Relaxation or SOR for elliptic PDEs; Fourier methods for elliptic PDEs; Convergence rates of elliptic methods; Fourier methods using FFTs
Science problem: the electric fields around electrical charges
Refs: Garcia sections 8.1 and 8.2; Numerical Recipes sections 19.4 and 19.5
Lab: Based on lectures in week 8

Non-teaching week

Week 10
Lectures: There are no lectures due to Labour Day
Lab: Based on lectures in week 9

Week 11
Lectures: Order/accuracy of PDE solution methods; Implicit methods for diffusion (Crank-Nicolson); More general diffusion problems; Stencils; Revisiting the (time-dependent) Schrödinger equation
Science problem: Evolution in time of a quantum wave packet
Refs: Garcia sections 9.2 and 9.3; Numerical Recipes section 19.2
Lab: Based on lectures in week 11

Weeks 12–13
There are no formal lectures or laboratory — this is time to work on the project.