PHYS703
Computational Science
S1 Day 2015
Dept of Physics and Astronomy

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General Information

Unit convenor and teaching staff

Unit Convenor
Jason Twamley
jason.twamley@mq.edu.au
Contact via jason.twamley@mq.edu.au
E6B 2.612
Thursdays 10--11am; other times by appointment.

Lecturer
David Spence
david.spence@mq.edu.au
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E6B 2.709

Credit points
4

Prerequisites
Admission to MRes

Corequisites

Co-badged status
Unit description
Computational techniques are a critical aspect of modern physics, science and engineering. They sit apart from theoretical and experimental physics but borrow characteristics from both. The aim is to turn a computer into a virtual laboratory for research, that allows breakthroughs and insights from what would otherwise be intractable problems by analytical methods. This unit focuses specifically on the computational techniques for solving problems in physics, engineering and science in general. It is not a course in programming though a low level of programming ability will be required to practice the techniques. Topics to be covered: o Introduction to Python and the Python scientific environment. o ODEs: Euler, Runge-Kutta and adaptive techniques, examining accuracy and stability with examples drawn from planetary science and chaotic systems. o Spectral methods: systems of linear equations, spectral analysis and analysis of normal modes. o PDEs: Initial and boundary conditions, discretisation. Relaxation and implicit schemes. Examples of Poisson, diffusion and wave equations. o Monte Carlo methods: random numbers, Monte Carlo integration, random walks, Metropolis algorithm. Examples of Ising model and phase transitions. o Convex optimisation: convex sets and functions, optimisation problems, linear and quadratic programming, duality.

Important Academic Dates
Information about important academic dates including deadlines for withdrawing from units are available at https://students.mq.edu.au/important-dates

Learning Outcomes
1. This unit is designed to give the students a tool set of computational techniques that will be useful in their research and future careers. Students will be able to:
2. understand the framework of techniques and which techniques would be most applicable to a given problem.
3. demonstrate an understanding of the methods covered.
4. apply their knowledge to solve computational problems, creating and testing the necessary routines.
5. understand how to analyse and evaluate the accuracy of a computational routine.
6. develop skills in basic programming, code organisation
7. understand at an introductory level key concepts in modern scientific programming - classes, parallel techniques

Assessment Tasks

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**Assignments**

**Due:** TBA  
**Weighting:** 25%

The assignments will comprise of 3-4 questions designed to engage the students with the material as it's covered. The difficulty of the questions will be set so that the assignment would take on average around 7 hours to complete; mix of theory and programming work.

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**In-Lab Assessment**

**Due:** Weekly  
**Weighting:** 25%

Laboratory exercises (computer laboratory; based on structured class work sheets and note books)

This Assessment Task relates to the following Learning Outcomes:

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  - demonstrate an understanding of the methods covered.
  - apply their knowledge to solve computational problems, creating and testing the necessary routines.
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Project
Due: **Week 12**
Weighting: **25%**
Individual projects - 4 weeks at the end of the semester with close supervision and a final report/in class presentation

This Assessment Task relates to the following Learning Outcomes:
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Final Examination
Due: **Exam Weeks**
Weighting: **25%**
Final exam based on a combination of written and oral examination

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Delivery and Resources

- New and Improved Unit Description available HERE.
- Textbook required is called "Introduction to Computational Science", Angela B. Shiflet and George W. Shiflet, and is available in the on-campus bookstore.
- All the material will be available via iLearn.
- Course will use Matlab and Vensim (Systems Dynamics simulation: free for educational use).

Unit Schedule

Monday 16:00-18:00 Location EMC G240
Tuesday: 14:00-17:00 Location: EMC G210

All contact hours are a combination of lecture and interactive labs.

The course will start in Week w of S1 for the Labs to be setup.

Policies and Procedures

Macquarie University policies and procedures are accessible from Policy Central. Students should be aware of the following policies in particular with regard to Learning and Teaching:

Academic Honesty Policy http://mq.edu.au/policy/docs/academic_honesty/policy.html
Disruption to Studies Policy http://www.mq.edu.au/policy/docs/disruption_studies/policy.html The Disruption to Studies Policy is effective from March 3 2014 and replaces the Special Consideration Policy.

In addition, a number of other policies can be found in the Learning and Teaching Category of Policy Central.

Student Code of Conduct

Macquarie University students have a responsibility to be familiar with the Student Code of Conduct: https://students.mq.edu.au/support/student_conduct/

Results

Results shown in iLearn, or released directly by your Unit Convenor, are not confirmed as they
are subject to final approval by the University. Once approved, final results will be sent to your student email address and will be made available in eStudent. For more information visit ask.mq.edu.au.

Student Support
Macquarie University provides a range of support services for students. For details, visit http://students.mq.edu.au/support/

Learning Skills
Learning Skills (mq.edu.au/learningskills) provides academic writing resources and study strategies to improve your marks and take control of your study.

- Workshops
- StudyWise
- Academic Integrity Module for Students
- Ask a Learning Adviser

Student Enquiry Service
For all student enquiries, visit Student Connect at ask.mq.edu.au

Equity Support
Students with a disability are encouraged to contact the Disability Service who can provide appropriate help with any issues that arise during their studies.

IT Help
For help with University computer systems and technology, visit http://informatics.mq.edu.au/help/

When using the University's IT, you must adhere to the Acceptable Use Policy. The policy applies to all who connect to the MQ network including students.

Graduate Capabilities
PG - Discipline Knowledge and Skills
Our postgraduates will be able to demonstrate a significantly enhanced depth and breadth of knowledge, scholarly understanding, and specific subject content knowledge in their chosen fields.

This graduate capability is supported by:

Learning outcomes

- This unit is designed to give the students a tool set of computational techniques that will be useful in their research and future careers. Students will be able to:
- understand the framework of techniques and which techniques would be most applicable
Learning outcomes

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  • understand at an introductory level key concepts in modern scientific programming - classes, parallel techniques

PG - Effective Communication

Our postgraduates will be able to communicate effectively and convey their views to different social, cultural, and professional audiences. They will be able to use a variety of technologically supported media to communicate with empathy using a range of written, spoken or visual formats.

This graduate capability is supported by:
Learning outcomes

- This unit is designed to give the students a tool set of computational techniques that will be useful in their research and future careers. Students will be able to:
  - apply their knowledge to solve computational problems, creating and testing the necessary routines.
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PG - Research and Problem Solving Capability

Our postgraduates will be capable of systematic enquiry; able to use research skills to create new knowledge that can be applied to real world issues, or contribute to a field of study or practice to enhance society. They will be capable of creative questioning, problem finding and problem solving.

This graduate capability is supported by:

Learning outcomes

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PG - Engaged and Responsible, Active and Ethical Citizens

Our postgraduates will be ethically aware and capable of confident transformative action in relation to their professional responsibilities and the wider community. They will have a sense of connectedness with others and country and have a sense of mutual obligation. They will be able to appreciate the impact of their professional roles for social justice and inclusion related to national and global issues

This graduate capability is supported by:

Learning outcomes

- This unit is designed to give the students a tool set of computational techniques that will be useful in their research and future careers. Students will be able to:
be useful in their research and future careers. Students will be able to:
• apply their knowledge to solve computational problems, creating and testing the necessary routines.
• understand at an introductory level key concepts in modern scientific programming - classes, parallel techniques

PG - Capable of Professional and Personal Judgment and Initiative

Our postgraduates will demonstrate a high standard of discernment and common sense in their professional and personal judgment. They will have the ability to make informed choices and decisions that reflect both the nature of their professional work and their personal perspectives.

This graduate capability is supported by:

Learning outcomes

• This unit is designed to give the students a tool set of computational techniques that will be useful in their research and future careers. Students will be able to:
• understand at an introductory level key concepts in modern scientific programming - classes, parallel techniques