EPSRC Centre for Doctoral Training in Theory and Simulation of Materials

MSc Course Handbook
2016–17
Foreword

The MSc in Theory and Simulation of Materials (TSM) runs under the auspices of the Centre for Doctoral Training (CDT) in TSM. The course is the brainchild of Prof. Adrian Sutton FRS, founding Director and member of the Strategic Advisory Team of the CDT, who had long foreseen the need for a mathematically rigorous and multidisciplinary training in the theory of materials and the methods used to simulate them. The course therefore spans many orders of magnitude in length- and time-scales: from the quantum-mechanical treatment of electrons, through phase-field models of microstructure, to finite element calculations for the continuum limit. It covers topics traditionally confined to the territory of single disciplines: chemistry, physics, materials science and engineering. Whatever your own background, this course will expose you to subjects you have never encountered before. Graduates of this MSc will be more thoroughly equipped than ever before to tackle the complex, multiscale materials problems that arise in modern technologies from nuclear reactors to mobile phones.

Originally established in 2009 by a grant from the Engineering and Physical Sciences Research Council (EPSRC), in 2013 the TSM-CDT was awarded funding to train a further five cohorts of students. As part of the proposal for continued funding, this MSc has been reviewed and revised, with the following aims in mind:

i. to maintain the ethos of continuous innovation;
ii. to increase the engagement of our external partners in the delivery of the training;
iii. to promote the development of students’ self-reliance and independence in learning, in preparation for research;
iv. to provide more opportunities for peer learning, e.g. through group projects;
v. to introduce a more comprehensive training in computational methods;
vi. to facilitate the involvement of a wider range of academic staff in the delivery; and
vii. to create more time for the research project and particularly for the literature review.

Our goal is to make the TSM-CDT an enriching, challenging and supportive environment that is conducive to learning and scholarship. We hope, therefore, that all of you will engage constructively with us as partners to help us identify problems, devise solutions and ensure that we continue to deliver a cutting-edge training experience that provides the best possible preparation for research in TSM.

The TSM-CDT, and our MSc students in particular, are currently housed in the Whiteley Suite (RCS building) alongside the CDT in Controlled Quantum Dynamics. Interest in the TSM-CDT has been registered by over 80 academics at Imperial from the nine Departments of Aeronautics, Chemical Engineering, Chemistry, Civil & Environmental Engineering, Earth Science & Engineering, Materials, Mathematics, Mechanical Engineering and Physics across the Faculties of Engineering and Natural Sciences. This reflects the strength and breadth of expertise in the College on TSM and the wide range of research topics that will be available to you.

The TSM-CDT also benefits from the Thomas Young Centre (www.thomasyoungcentre.org), the London Centre for TSM. The TYC is a federation of research groups involved in TSM at Imperial, King’s College, UCL and Queen Mary. It provides an outstanding program of seminars, workshops, conferences, distinguished visitors, and short courses by experts from around the world, all of which are available to everyone in the TSM-CDT. You are strongly encouraged to participate in the events organised by the TYC to further enrich your educational and social experience.

We hope our course will prove attractive to mathematically oriented students of physical sciences and engineering around the world. For more information about the CDT visit www.tsmcdt.org.

Arash Mostofi (MSc Director)
a.mostofi@imperial.ac.uk
# Table of Contents

1 **Introduction** ........................................................................................................................................ 6  
1.1 About This Handbook .......................................................................................................................... 6  
1.2 Aims and Objectives of the MSc in Theory and Simulation of Materials ........................................... 6  
1.3 The Centre for Doctoral Training on Theory and Simulation of Materials ........................................ 7  
1.4 Lines of Communication ....................................................................................................................... 7  
1.5 Student Representation ........................................................................................................................ 8  
1.6 Yearly Calendar ....................................................................................................................................... 8  

2 **General Information on the Course** .................................................................................................. 10  
2.1 Administration ......................................................................................................................................... 10  
2.2 Timetables and the Working Day ........................................................................................................ 10  
2.3 Safety .................................................................................................................................................... 10  
2.4 Cohort Mentors ..................................................................................................................................... 11  
2.5 The Curriculum ..................................................................................................................................... 11  
2.6 Student Feedback ................................................................................................................................... 13  

3 **Assessment of the Course Components** ............................................................................................ 15  
3.1 Overview ............................................................................................................................................... 15  
3.2 In detail ............................................................................................................................................... 16  
3.3 Written Examinations .......................................................................................................................... 19  
3.4 Oral (viva voce) examinations for Advanced Options ......................................................................... 19  
3.5 Literature Review and Research Project ............................................................................................. 20  
3.6 Transferable skills ................................................................................................................................... 20  
3.7 Letter Grades ........................................................................................................................................ 20  
3.8 Requirements for Passing the MSc ..................................................................................................... 21  
3.9 Sutton Prize .......................................................................................................................................... 21  

4 **Academic Support** .............................................................................................................................. 22  
4.1 Absences and Illness ............................................................................................................................. 22  
4.2 Disabilities, specific learning difficulties and long-term health issues ......................................... 23  
4.3 Blackboard ......................................................................................................................................... 24  
4.4 Outreach .............................................................................................................................................. 24  

5 **General Information about Life in the Centre for Doctoral Training** ............................................ 25  
5.1 Before you Arrive .................................................................................................................................. 25  
5.2 Where to Find Us .................................................................................................................................. 25  
5.3 When you Arrive .................................................................................................................................. 25  
5.4 ID Cards ............................................................................................................................................... 25  
5.5 Mail ..................................................................................................................................................... 25  
5.6 Telephones ......................................................................................................................................... 26  
5.7 Security and Emergencies .................................................................................................................. 26  
5.8 Library Facilities .................................................................................................................................. 26  
5.9 Accommodation ................................................................................................................................... 26  
5.10 Food and Drink ................................................................................................................................... 26  
5.11 Health ................................................................................................................................................ 27  
5.12 Sports Facilities .................................................................................................................................. 28  
5.13 Banking ............................................................................................................................................. 28  
5.14 Parking .............................................................................................................................................. 28  
5.15 Travel and Travel Insurance ............................................................................................................. 28  
5.16 Life in London .................................................................................................................................... 28  
5.17 Moving on from Imperial .................................................................................................................... 28  
5.18 And When You Leave Imperial ......................................................................................................... 28
Appendix 1  Synopses of courses ................................................................. 29
Mathematics for the Theory of Materials (MTM1 and MTM2) ................. 31
Equilibrium in Materials (EQM1) ............................................................... 33
Transformations of Materials (TM1) ......................................................... 35
Electronic Structure of Materials (ESM1) ................................................ 37
Classical Field Theory of Materials (CFTM1) ......................................... 39
Methods of Simulating (MSM1 and MSM2) .............................................. 41
Equilibrium in Materials (EQM2) ............................................................... 44
Transformations of Materials (TM2) ......................................................... 45
Electronic Structure of Materials (ESM2) ................................................ 46
Classical Field Theory of Materials (CFTM2) ......................................... 48
Matlab Primer [Computational Methods Hub] ........................................... 51
Introduction to Linux ............................................................................... 51
Introduction to C++ ................................................................................. 51
Numerical Methods ................................................................................ 52
Group Research Strategy Project (GRSP) ............................................... 55
Appendix 2  Guidelines for the Conduct and Assessment of Research Projects .... 58
1 Introduction

1.1 About This Handbook

The purpose of this handbook is to provide current students and staff with a detailed description of the MSc in Theory and Simulation of Materials (TSM) course run by the EPSRC Centre for Doctoral Training (CDT) in TSM, including assessment and feedback mechanisms (where appropriate).

This edition of the handbook applies to the academic year 2016–17. An electronic copy of this handbook will be provided to every student at the start of the academic year and any significant changes to its content will be communicated to them. A copy of the current handbook will be made available online at the course Blackboard site and on the CDT web site www.tsmcdt.org.

The MSc course usually has a relatively small number of students (in comparison to many undergraduate courses) and they have extensive access to the academic and support staff of the TSM-CDT. Students therefore should not hesitate to approach the MSc Director or any member of staff for advice or assistance.

This handbook describes the framework of the course and its assessment but the MSc Director and/or Course Committee may make changes to detailed procedures if the circumstances indicate that this is desirable. Similarly, the Board of Examiners has absolute discretion to modify the criteria described in this handbook, although in practice this would only occur in exceptional circumstances. Students will be notified of any changes prior to their introduction.

1.2 Aims and Objectives of the MSc in Theory and Simulation of Materials

The formal aim of the MSc in Theory and Simulation of Materials is “to train students in the core concepts and methods of theoretical and computational materials physics necessary for doctoral study in the field or for a technical career outside academia.”

This aim is fulfilled via the following formal objectives. The MSc in TSM will:

- attract well-qualified Bachelor level students and provide an intellectually challenging degree programme;
- provide high quality advanced education in materials theory and simulation beyond Bachelor level within an environment with considerable teaching and research experience in the field;
- give students the experience of undertaking a major, individual project and reporting the results in a full scientific report and presentation;
- give students training in appropriate research methods, including comprehensive training in computational methods;
- develop students’ skills of communication, both written and oral, peer learning and teamwork;
- equip students for further academic study at doctoral level in materials physics and subjects where this is an important enabling science, such as aerospace, automotive transport, renewable energy, health-care and construction.

The key elements of the course that support these objectives are:

- about 100 lectures and 50 tutorials, rapid feedback sessions and computational classes in core and optional subjects in the first two terms, assessed by written and oral examinations, as well as assessed exercises and problem-solving;
- courses offered by the Graduate School, which are optional during the MSc;
- a four-month individual research project, assessed by an oral presentation and written report.

The course is delivered according to the Imperial College Student Charter: https://www.imperial.ac.uk/students/student-support/our-principles/
1.3 The Centre for Doctoral Training on Theory and Simulation of Materials

The Engineering and Physical Sciences Research Council (EPSRC) established the TSM-CDT in 2009, with the intention of training a cadre of physical scientists and engineers with advanced skills in TSM, an area in which there is recognised to be a national and international shortage of trained people. Funding for a further five cohorts was awarded in 2013. The CDT draws upon the expertise of the Departments of Physics, Materials, Chemistry, Mechanical Engineering, Aeronautics, Chemical Engineering, Mathematics, Earth Science & Engineering and Civil & Environmental Engineering at Imperial College plus academic staff at UCL and King’s College London via the Thomas Young Centre. The CDT works closely with the other Centres based in the College and with other academic departments working in TSM.

For administrative purposes, including quality assurance and oversight, students are registered for the MSc degree in the Department of Physics where they have full access to departmental support structures in addition to those provided by the CDT. These include Dr Andrew Williamson and Ms Loli Sanchez Rey in the postgraduate administration office, and Professor Stefan Maier the Director of Postgraduate Studies. The Department of Physics taught Masters webpages may be found here: https://www.imperial.ac.uk/natural-sciences/departments/physics/students/current-students/taught-postgraduates/

1.4 Lines of Communication

A list of all academic staff involved in the CDT may be found on our web site: http://www.imperial.ac.uk/theory-and-simulation-of-materials/people/staff/ and most contribute to the MSc course either directly or indirectly. The following table lists those with administrative responsibility.

<table>
<thead>
<tr>
<th>Responsibility</th>
<th>Person</th>
<th>Room No.</th>
<th>Tel.</th>
</tr>
</thead>
<tbody>
<tr>
<td>CDT Director</td>
<td>Dr Arash Mostofi</td>
<td>332, Bessemer</td>
<td>48154</td>
</tr>
<tr>
<td>CDT Assistant Director</td>
<td>Dr Johannes Lischner</td>
<td>342, Bessemer</td>
<td>49949</td>
</tr>
<tr>
<td>Strategic Advisory Team</td>
<td>Professor Peter Haynes</td>
<td>201B, Royal</td>
<td>45158</td>
</tr>
<tr>
<td></td>
<td></td>
<td>School of Mines</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Professor Adrian Sutton</td>
<td>807, Blackett</td>
<td>47540</td>
</tr>
<tr>
<td>Admissions Tutor</td>
<td>Professor Dimitri Vvedensky</td>
<td>813, Blackett</td>
<td>47605</td>
</tr>
<tr>
<td>Cohort Mentor (2012 entry)</td>
<td>Dr Arash Mostofi</td>
<td>332, Bessemer</td>
<td>48154</td>
</tr>
<tr>
<td>Cohort Mentor (2013 entry)</td>
<td>Dr Daniel Balint</td>
<td>513, MechEng</td>
<td>47084</td>
</tr>
<tr>
<td>Cohort Mentor (2014 entry)</td>
<td>Dr Mike Bearpark</td>
<td>265, Chemistry</td>
<td>45727</td>
</tr>
<tr>
<td>Cohort Mentor (2015 entry)</td>
<td>Dr Andrew Horsfield</td>
<td>331 Bessemer</td>
<td>46753</td>
</tr>
<tr>
<td>Cohort Mentor (2016 entry)</td>
<td>Dr Kim Jelfs</td>
<td>134C, Chemistry</td>
<td>44338</td>
</tr>
<tr>
<td>CDT Senior Administrator</td>
<td>Miss Miranda Smith</td>
<td>115, Whiteley</td>
<td>40709</td>
</tr>
<tr>
<td>CDT Administrator</td>
<td>Miss Veena Dhulipala</td>
<td>115, Whiteley</td>
<td>45609</td>
</tr>
<tr>
<td>Postgraduate Administrator in Physics</td>
<td>Ms Loli Sanchez Rey</td>
<td>316, Blackett</td>
<td>47512</td>
</tr>
<tr>
<td>Postgraduate Development Officer in Physics</td>
<td>Dr Andrew Williamson</td>
<td>316, Blackett</td>
<td>47632</td>
</tr>
<tr>
<td>Postgraduate Welfare Advisor in Physics</td>
<td>Dr Arnaud Czaja</td>
<td>726, Huxley</td>
<td>41789</td>
</tr>
<tr>
<td>Careers Advisor in Physics</td>
<td>Professor Mark Neil</td>
<td>608, Blackett</td>
<td>47611</td>
</tr>
<tr>
<td>Director of Postgraduate Studies in Physics</td>
<td>Professor Stefan Maier</td>
<td>903, Huxley</td>
<td>46063</td>
</tr>
<tr>
<td>External Examiner</td>
<td>Professor Graham Ackland</td>
<td>University of</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>Edinburgh</td>
<td></td>
</tr>
</tbody>
</table>

The MSc Director and other staff will provide information to students through one of several channels, depending upon the nature of the information (e.g. confidential or not):

- e-mail;
- via the MSc course Blackboard site;
• on the notice boards in the Whiteley Suite;
• letter delivered by internal mail;
• letter to your home address;
• personal communication before/after lectures or during classes.

In particular, students are expected to check their College email account at least once a day during term and while undertaking the research project.

Further information about roles and responsibilities of staff members can be found here: http://www.imperial.ac.uk/staff/tools-and-reference/quality-assurance-enhancement/good-practice/

1.5 Student Representation

There is one elected student representative from each cohort who serves on the CDT Operations Board, usually for a fixed term of one year. The representative from the cohort currently undertaking the MSc will also serve as the student representative on the MSc Course Committee in the Department of Physics, and students are encouraged to raise general or specific matters through this channel as well.

Any concerns of a more urgent or personal nature should be discussed with the appropriate Cohort Mentor or the CDT Director.

The College has an online mechanism to evaluate each and every course called PG SOLE: Postgraduate Student On Line Evaluation. Each student is asked to complete this survey about the course towards the end of Terms 1 and 2. The results are discussed at the MSc Course Committee with a view to addressing any concerns in the future.

1.6 Yearly Calendar

Term dates may be found at http://www.imperial.ac.uk/admin-services/registry/term-dates/. The course is described in more detail in §2.5. The following outline is approximate: lectures and classes may need to be rescheduled due to staff absence etc.

TERM 1

Week 1  Introduction to the MSc (9.30am, Monday)
      Provost’s welcome address (2.45pm, Monday)
      Group project (cohort challenge)
      Safety briefing and reception in Physics (2pm, Wednesday)
      TSM welcome lunch (midday, Friday)

Week 2  Election of Student Representative for the new cohort
Weeks 2–5 Lectures and classes for core courses
Week 6  Reading week*
Weeks 7–10 Lectures and classes for core courses
Week 11 Revision week*

TERM 2

Week 1  Written Examinations – all courses delivered in Term 1
      Group projects commence
Weeks 2–5 Lectures and classes for core and advanced courses
Week 6  Reading week*
Weeks 7–10 Lectures and classes for core and advanced courses
Week 11 Oral Examinations – courses delivered in Term 2

TERM 3 and SUMMER VACATION
April
  Literature review starts
May
  Start of research project
  Presentations/interviews for group projects
  E-MRS Spring Meeting in Strasbourg (22-26 May 2016)**
June/July
  Industrial site visit
Early September
  Project presentations
Mid-September
  Project report submission
Late September
  Examiners' Meeting
Day of Examiners' Meeting
  Informal Notice of Results (usually around 4pm)

* We endeavour to keep Reading and Revision weeks free from timetabled commitments, but this is usually not possible in practice and students should expect there to be some timetabled classes, though much fewer than in other weeks during term.

** This is just one suggestion of a possible cohort conference trip. The actual conference attended will be decided through discussion with the Cohort Mentor and may occur earlier or later in the year.
2 General Information on the Course

2.1 Administration

The MSc in TSM is administered day-to-day by the CDT Administrators, Miss Miranda Smith and Miss Veena Dhulipala, working closely with the CDT Director and academic and administrative staff in the Departments participating in the CDT. The CDT Operations Board and the MSc Course Committee of the Department of Physics oversee the course and make changes to the course content and organisation as appropriate. The CDT Operations Board meets weekly through term time and at least monthly out of term time. The MSc Course Committee of the Department of Physics meets once a term. The members of the CDT Operations Board are:

- Dr Arash Mostofi (CDT Director and Chair)
- Dr Johannes Lischner (Assistant CDT Director)
- Student Representatives and Cohort Mentors
- Dr Simon Foster (Outreach Officer)
- Miss Miranda Smith (Senior Administrator)
- Miss Veena Dhulipala (Administrator)

The members of the MSc Course Committee of the Department of Physics from the CDT are:

- Dr Arash Mostofi
- Student Representative of the MSc cohort

2.2 Timetables and the Working Day

The MSc term dates are the same as those for undergraduate courses at Imperial College – see https://www.imperial.ac.uk/admin-services/registry/term-dates/ – except for the summer term. Lecture courses run during the first two terms. Examinations and major assessments are held at the start and end of the second term and start of the third term. Work on the literature review starts after Easter as an introduction to the research project that follows. The project continues through the rest of the summer term and into the undergraduate summer vacation, finishing in mid-September. Timetables for each term are prepared in time for the start of term and are distributed to all students. These contain details of all lectures, rapid feedback (problem) classes, computational classes, examinations, presentations and deadlines. If an examination or major assessment is scheduled to clash with a religious obligation, please consult the CDT Director. The College’s policy is online: http://www.imperial.ac.uk/student-records-and-data/for-current-students/undergraduate-and-taught-postgraduate/exams-assessments-and-regulations/exams-and-religious-obligations/

The College standard working day is used, with 50-minute lectures commencing on the hour, starting at 9am each day. In Term 1, there are 16 timetabled hours a week on average during the eight main teaching weeks (weeks 2–5 and 7–10). During week 1 students undertake a "cohort challenge", week 6 is a reading week and week 11 is intended for revision. In Term 2, there are approximately 10 timetabled hours during the eight main teaching weeks. Written examinations are held in week 1, week 6 is a reading week and week 11 is intended for revision and oral examinations. An attempt is made to keep Wednesday afternoons free for other activities. Lectures and rapid feedback classes (i.e. problem classes) are usually held in the Whiteley Suite, room 113 and occasionally in 114. Some lectures may be held elsewhere, e.g., in the Department of Physics.

2.3 Safety

Although most of your MSc is class-based, you should be mindful of safety considerations at all times, not least because the Whiteley Suite is adjacent to experimental labs. All students are issued with the current version of the Blackett Laboratory Safety Booklet at the start of the MSc course, and all students are required to attend the Health and Safety Induction in the Physics Department and to complete the online Risk Assessment Foundation Training (RAFT). See http://www.imperial.ac.uk/natural-sciences/departments/physics/safety and www3.imperial.ac.uk/safety for more information.
The Evacuation Signal in the Whiteley Suite is a continuous alarm. In the Blackett Laboratory the Evacuation Signal is an announcement “to leave the building”. Upon hearing the Evacuation Signal everyone must leave immediately by the nearest fire exit and assemble at the muster point.

2.4 Cohort Mentors

Each cohort of students has a mentor appointed to accompany them through the MSc and continues with those who stay on for the PhD. In the event of a large number of MSc students, the MSc Director may act as mentor to students taking the MSc course only. The role of the mentor is to be a point of contact for each student within a cohort throughout the course; to offer advice on the selection of options and projects; to help with career decisions; to be available for writing references; and to help with any matters of a non-academic nature that may arise. During the MSc, the cohort mentor also fulfils the crucial role of providing virtually instant feedback from MSc students about any aspect of their courses. This feedback is reported to the Operations Board, which normally meets weekly during term time. This has already proved to be an extremely effective way of identifying and solving problems before they become serious.

The College has a web-site http://www.imperial.ac.uk/student-space/ providing access to advice on a very wide range of welfare and other issues.

2.5 The Curriculum

2.5.1 Overview

There are two main elements to the MSc course, with the following contributions to the final mark:

- **Taught courses.** These are assessed by written and oral examinations, problem sets, computational classes and other exercises. They count for 60% of the overall mark (defined in detail in §3.7).
- **Research project.** This is assessed by literature review, a presentation and a written report at the end of the project, and counts for 40% of the overall course mark.

To be awarded an MSc, students are required to satisfy the requirements explained in §3.7. This section also explains the requirements for the award of a “Merit” and “Distinction”.

An illustration of the MSc is shown below:

<table>
<thead>
<tr>
<th>Week</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
<th>8</th>
<th>9</th>
<th>10</th>
<th>11</th>
</tr>
</thead>
<tbody>
<tr>
<td>Term 1</td>
<td>Cohort challenge</td>
<td>MTM 1 – core</td>
<td>EQM 1 – core</td>
<td>ESM 1 – core</td>
<td>CMM – core</td>
<td>Reading week</td>
<td>MTM 2 – core</td>
<td>TM 1 – core</td>
<td>CFTM 1 – core</td>
<td>CMM – core</td>
<td>Revision</td>
</tr>
<tr>
<td>Term 3</td>
<td>Literature review</td>
<td>GRSP – core</td>
<td>Research project</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
2.5.2 Taught courses

All students must take the compulsory parts of the core courses. These six subjects are:
- Mathematics for Theory of Materials (MTM);
- Equilibrium in Materials (EQM);
- Transformations of Materials (TM);
- Electronic Structure of Materials (ESM);
- Classical Field Theory of Materials (CFTM);

During Term 1 all courses are compulsory, and comprise six parts:
- Mathematics for Theory of Materials: Parts 1 and 2 (MTM1 and MTM2);
- Equilibrium in Materials: Part 1 (EQM1);
- Transformations of Materials: Part 1 (TM1);
- Electronic Structure of Materials: Part 1 (ESM1);
Each part consists of 16 lectures with four rapid feedback classes, with the exception of MTM, which in total (ie, Parts 1 & 2) consists of 24 lectures and 7 rapid feedback classes.

During Term 2 all students take the compulsory sixth subject:
- Methods for Simulating Materials (MSM1 and MSM2).
This course is delivered through 16 lectures and 16 hours of hands-on computational classes and feedback sessions.

In addition, during Term 2, students select two advanced courses, which comprise the second parts of four subjects:
- Equilibrium in Materials: Part 2 (EQM2);
- Transformations of Materials: Part 2 (TM2);
- Electronic Structure of Materials: Part 2 (ESM2);
These courses will be delivered through directed reading, and about eight discussion classes.

During Term 2 students also take the Group Research Strategy Project. Further details will be given in a briefing meeting towards the end of Term 1.

2.5.3 Rapid Feedback Classes

Rapid feedback classes are held approximately every week for each of the standard lecture courses. They may consist of problems that are worked through during the class, discussions or further explanation of the material. Students are encouraged to liaise with the lecturer to help set the agenda for these classes.

2.5.4 Computational Methods

Training in computational methods is given during Terms 1 and 2 consisting of a general introduction to tools for programming, Python and C/C++, followed by training in numerical methods. There are approximately two hours of classes per week during the main teaching weeks.
2.5.5 Industrial engagement

An appreciation of the role of materials in industry, and TSM in particular, is an important part of the training provided by the CDT. To this end there will be a number of “Materials Challenge” lectures delivered by external partners during the year and an industrial site visit. All students are expected to attend all of these events.

2.5.6 Literature review

The literature review begins after the conclusion of the oral exams at the end of Term 2 as a prelude to the research project (on the same topic). This must be submitted electronically as a report in PDF format (3,000 words maximum) by 5pm on 12 May 2017 to the CDT Senior Administrator. The literature review accounts for 10% of the total marks available in the MSc.

2.5.7 Research project

The research element of the project starts in the summer term. Each student is required to give an oral presentation about the project at the MSc conference on 1 September 2017. The project report must be submitted electronically in PDF format (5,000 words maximum, excluding appendices) by 5pm on 8 September 2017 to the CDT Senior Administrator.

The research project may be carried out at Imperial College or at a partner institution of the CDT or another academic institution, where appropriate arrangements exist. All students have a project supervisor at Imperial College and any student carrying out the project elsewhere must also have an Imperial College supervisor.

The research project (excluding the literature review) accounts for 30% of the total marks available in the MSc. One fifth of the marks for the project are assigned to the oral presentation and four fifths to the written report. The report is marked independently by two members of staff.

Further details about the research project and its assessment are provided in Appendix 2.

2.6 Student Feedback

Your feedback is important to the CDT, the College and Imperial College Union. The primary mechanism for passing on your comments, concerns and suggestions to the Operations Board of the CDT is to speak to your Cohort Mentor. In the past this has proved to be a very effective way of tackling problems that have arisen during the course. The CDT Director is also happy to speak to you.

In addition, the following College-wide surveys give you regular opportunities to reflect on the shape of the courses and overall programme and your experience as a student in the CDT:

- PG SOLE lecturer/module
- Student Experience Survey (SES)

The PG SOLE lecturer/module survey runs at the end of Terms 1 and 2. This survey is your chance to comment on the courses you have attended and the lecturers who taught them. Run at the same time as the Term 1 PG SOLE is the Union’s Student Experience Survey (SES). This survey will cover your induction, welfare, pastoral and support services experience. During December you will receive an email in your Imperial College account with a link to the survey. Both of these surveys are anonymous and the more students that take part the more representative the results so please take a few minutes to give your views.

As a result of student feedback received in the past, the CDT has made major changes to the delivery of the course including the introduction of foundation courses and group projects, the coordination of coursework deadlines and changes to our assessment and feedback processes.
To find out more about any of these surveys or to see the results from previous surveys, visit: http://www.imperial.ac.uk/students/academic-support/student-surveys/pg-student-surveys/
For further information on surveys please contact the Registry’s Surveys Team at surveys.registrysupport@imperial.ac.uk
3  **Assessment of the Course Components**

3.1  **Overview**

This section details the assessment procedures for each element of the MSc course. The distribution of marks between the different elements of assessed work is summarised below.

<table>
<thead>
<tr>
<th>Activity</th>
<th>Total marks</th>
<th>Written Exam</th>
<th>Oral Exam or Presentation</th>
<th>Assessed Coursework</th>
<th>Written Report</th>
</tr>
</thead>
<tbody>
<tr>
<td>Compulsory core (MTM1&amp;2, EQM1, TM1, ESM1, CFTM1, MSM1&amp;2)</td>
<td>320 (35.6%)</td>
<td>192 (21.3%)</td>
<td>24 (2.7%)</td>
<td>104 (11.6%)</td>
<td></td>
</tr>
<tr>
<td>Advanced core (two of EQM2, TM2, ESM2, CFTM2)</td>
<td>80 (8.9%)</td>
<td>40 (4.4%)</td>
<td></td>
<td>40 (4.4%)</td>
<td></td>
</tr>
<tr>
<td>Computational methods</td>
<td>60 (6.7%)</td>
<td>6.6 (0.7%)</td>
<td></td>
<td>49.2 (5.5%)</td>
<td>4.2 (0.5%)</td>
</tr>
<tr>
<td>Group project</td>
<td>80 (8.9%)</td>
<td>26.7 (3.0%)</td>
<td></td>
<td></td>
<td>53.3 (5.9%)</td>
</tr>
<tr>
<td>Literature review</td>
<td>90 (10%)</td>
<td></td>
<td></td>
<td></td>
<td>90 (10%)</td>
</tr>
<tr>
<td>Research project</td>
<td>270 (30%)</td>
<td>54 (6.0%)</td>
<td></td>
<td>216 (24%)</td>
<td></td>
</tr>
<tr>
<td>Total</td>
<td>900 (100%)</td>
<td>192 (21.3%)</td>
<td>151.3 (16.8%)</td>
<td>193.2 (21.5%)</td>
<td>363.5 (40.4%)</td>
</tr>
</tbody>
</table>

For each of the compulsory core courses MTM1&2, EQM1, TM1, ESM1 and CFTM1, 20% of the marks come from assessed coursework and 80% from the written examinations in January. For MSM the whole mark comes from assessed coursework, including an oral presentation.

The percentage (which has been rounded to the nearest 0.1%) under each heading indicates the weighting used in calculating the overall course mark. These notes are intended to assist students, by showing the basis and criteria on which marks are awarded, and staff in standardising the assessment procedures as applied from student to student, and from year to year.

*The Examiners nevertheless reserve the right to make adjustments to the procedures given in this section in exceptional circumstances.*

Formal feedback to the students in each activity is by way of a letter grade indicating the percentage band of their attainment. The definition of the letter grades is given in §3.6 below.

All of the marks are reviewed at a meeting of a sub-board of the Board of Examiners, usually comprised of the CDT Director, Assistant Director and Cohort Mentor. This sub-board is informed by staff involved in the MSc course, who may suggest that the examiners take into account any special factors. This board also acts as the Mitigation Advisory Panel that takes into account any mitigating circumstances that have been submitted by students (see §4.1 below). The marks are then forwarded to the External Examiner for information. The Board of Examiners, comprised of the External Examiner and all staff involved in the delivery of the course, meets in late September or early October to review all the marks and make final recommendations to the College. It is
traditional to send a copy of the project reports to the External Examiner in advance of this meeting, to provide additional information that might assist the decision process. The marks presented before the Board of Examiners for the MSc in TSM is not anonymous (i.e., student names appear with the marks that are being considered).

3.2 In detail

The marks available

There are TWO assessed elements of the MSc:

1. the taught courses, consisting of SEVEN components (combinations of courses):
   
   (a) Mathematics for Theory of Materials (MTM1 and MTM2)
   (b) Equilibrium in Materials (EQM1) and Transformations of Materials (TM1)
   (c) Electronic Structure of Materials (ESM1) and Classical Field Theory of Materials (CFTM1)
   (d) Methods of Simulating Materials (MSM1 and MSM2)
   (e) advanced parts of the core courses, TWO chosen from the following FOUR options:
       Equilibrium in Materials (EQM2)
       Transformations of Materials (TM2)
       Electronic Structure of Materials (ESM2)
       Classical Field Theory of Materials (CFTM2)
   (f) Group Research Strategy Project (GRSP)
   (g) Computational Methods – numerical methods (CMM)

2. the research element, consisting of TWO components:
   
   (h) Literature Review
   (i) Research Project

The marks (credits) available for each component are as follows:

(a) MTM1 and MTM2: 80 marks (8 ECTS) in total – 16 marks for assessed problems, 64 marks from the written examination
(b) EQM1 and TM1: 80 (8 ECTS) in total – 16 marks for assessed problems and 64 marks from the written examination
(c) ESM1 and CFTM1: 80 (8 ECTS) in total – 16 marks for assessed problems and 64 marks from the written examination
(d) MSM1 and MSM2: 80 marks (8 ECTS) in total – 56 marks for assessed coursework and 24 marks from an oral presentation
(e) advanced parts (two chosen from EQM2, TM2, ESM2, CFTM2): 80 marks (8 ECTS) in total – 40 marks for assessed coursework and 40 marks from the oral examinations
(f) group project (GRSP): 80 marks (8 ECTS) in total – 53.3 marks for a written proposal, 26.7 marks for a presentation and panel interview. A proportion of these marks is awarded by peer-to-peer allocation (see Appendix for more details)
(g) CMM: 60 marks (6 ECTS) in total – for assessed coursework, a presentation and a written report on numerical methods
(h) literature review: 90 marks (9 ECTS) in total – assessed by a written report of no more than 3,000 words, excluding appendices
(i) research project: 270 marks (27 ECTS) in total – 216 marks for the written report and 54 marks for the oral presentation

---

1 Further information about reporting progress during the research project, the assessment criteria, the structure of the report, and marking of the report are provided in §3.4 and Appendix 2.
For the elements as a whole:
(1) taught courses (a)–(g): 540 marks (54 ECTS) in total
(2) research element (h)–(i): 360 marks (36 ECTS) in total

Totals for the course: 900 marks (90 ECTS)

Schedule of examinations

Written examinations for the six compulsory parts of the core courses taught in Term 1 will take place in the first week of Term 2. Written examinations normally last 2 hours. Rubrics will be circulated to students during Term 1.

Oral examinations for the advanced parts of core courses taught in Term 2 will normally take place in the last week of Term 2. The oral presentation/examination for the group projects will normally be held during Term 3.

Marking of problem sets

For many courses assessed problems will be set weekly while lecture courses are running. They will be graded either by the lecturer or by teaching assistants. Students will receive feedback including a letter grade for each problem set, according to the following criteria:

α (alpha): mostly correct with only a little wrong
β (beta): slightly more correct than wrong
γ (gamma): some correct elements but mostly wrong
δ (delta): almost entirely wrong
ø (null): did not hand in the problems on time, or entirely wrong

Each assessed problem set should take you around 2 hours to complete. If it is taking you significantly longer please speak to the lecturer or your cohort mentor.

Deadlines for handing in assessed coursework are indicated on the course timetable. Unless the course lecturer makes alternative arrangements or another time is specified, work should be handed in to the CDT Administration Office by 5pm on the day of the deadline. Late submissions will be refused if there are no extenuating circumstances. Acceptable reasons for failing to hand in work on time are the usual ones such as illnesses or significant personal problems. If you know you are going to miss a deadline you must complete a minor mitigating circumstances form available from the CDT Administrators, which will be considered by the Operations Board. You should also inform the lecturer concerned as a matter of courtesy. If you haven’t finished the work hand in what you have done anyway, otherwise you will receive no marks. Deadlines will only be extended in exceptional circumstances.

You are strongly encouraged to collaborate with other students in your cohort by discussing your approaches and solutions to the problems with each other. However, when you write down your solutions you must do so by yourself. Copying another student’s work and presenting it as your own constitutes cheating and is subject to the College’s disciplinary procedures.

The College statement regarding plagiarism follows. Early in the academic year you will attend a compulsory workshop on research ethics that covers plagiarism to ensure that you understand what it involves and how to avoid it. This will be followed by an opportunity to take the College’s online course and test on plagiarism that is compulsory for all Master’s students.
Imperial College Statement regarding Plagiarism

Students should be aware of the need to give proper credit for the work of others when writing papers, reports, theses, etc. This is particularly important when the work is in collaboration with other persons. The College’s advice on Examinations and academic integrity contains a section on plagiarism, which is reproduced here:

You are reminded that all work submitted as part of the requirements for any examination and assessment (including coursework) must be expressed in your own words and incorporate your own ideas and judgements.

Plagiarism, which is the presentation of another person’s thoughts, words or images and diagrams as though they were your own and which is a form of cheating, must be avoided, with particular care in coursework, essays, reports and projects written in your own time and also in open and closed book written examinations. You are encouraged to read and criticise the work of others as much as possible, and you are expected to incorporate this into your thinking and in your coursework and assessments. But you must be sure to acknowledge and identify your sources.

Direct quotations from the published or unpublished work of others, whether from the internet or from any other source, must always be clearly identified as such by the use of quotation marks, whether in coursework or in an open or closed book examination. A full reference to their source must be provided in the proper form. Remember that a series of short quotations from several different sources, if not clearly identified as such, constitutes plagiarism just as much as a single unacknowledged long quotation from a single source. Equally, if you summarise another person’s ideas or judgements, figures, diagrams or software, you must refer to that person in your text, and include the work referred to in your bibliography. Departments are able to give advice about the appropriate use and correct acknowledgement of other sources in your own work.

Where plagiarism is detected this is most usually in project work or coursework i.e. work that is submitted in the candidate’s own time but plagiarism can also occur in closed book written examinations. Such situations can arise where candidates have been able to learn text by heart [by rote] and simply reproduce what they have learnt without attribution. Where the examination is based on technical knowledge this may be acceptable and not regarded as plagiarism. In other subjects where candidates are asked to write essays the examiners may regard text reproduced without reference or critical analysis as plagiarism. Boards of Examiners are encouraged to clarify where appropriate in examination rubrics how sources should be acknowledged in those examinations.

The direct and unacknowledged repetition of your own work which has already been submitted for assessment can constitute self-plagiarism.

Where group work is submitted, this should be presented and referenced, with individual contributions recorded, in the convention appropriate to your discipline. You should therefore consult your personal or senior tutor or course director if you are in any doubt about what is permissible. You should be aware that you have a collective professional responsibility as a group for the integrity of all of the work submitted for assessment by that group. If you become aware that a member or members of the group may have plagiarised part of the group’s submission you have an obligation to report your suspicions to your personal or senior tutor or the course director.

The use of the work of another student, past or present, also constitutes plagiarism. Where work is used without the consent of that student, this will normally be regarded as a major offence of plagiarism. Giving your work to another student to use (other than in a group assessment) may also constitute an offence. The College may submit your work to an external plagiarism detection service, and by registering with the College you are automatically giving your consent for any of your work to be submitted to such a service.

The College will investigate all instances where an examination or assessment offence is reported and apply appropriate penalties to students who are found guilty. These penalties include a mark of zero for the assessment in which the examination offence occurred or a mark of zero for all the assessments in that year or exclusion from all future examinations of the University (i.e. expulsion from the university).
Use of Materials for Teaching

It is anticipated that all materials involved in the delivery of the course work will be made available to students electronically. Such materials may include lecture notes, problem sets and solutions, computational exercises and solutions, and recordings of lectures and problem classes etc. All this material is copyright, and students may not use it for any purpose other than their own private study, and they may not distribute it to anyone else in any medium. The penalties for infringing these rules are severe and they may include expulsion from Imperial College and prosecution under copyright law.

Use of Calculators in Written Examinations

The College Board of Graduate Studies has determined that only College-owned approved non-programmable calculators can be used in the written examinations. The Physics Department has approved and can provide calculators, which use algebraic logic. Appropriate arrangements will be made for students wishing to use reverse Polish notation (RPN) calculators. However, in all cases, only College-owned calculators may be used in the written examinations and therefore students are advised to either purchase an appropriate calculator or practise on a College-owned calculator before the written examinations.

Written Reports

Here are some general comments which are applicable to all MSc reports. All reports should be word processed. Margins should not be less than 20mm. Number all pages. Do not use fonts smaller than 11pt for the main text. Make sure diagrams, figures and graphs are clearly laid out with clear labels and captions.

DEADLINES: Deadlines are absolute. The Board of Assessors reserves the right not to mark reports submitted late. Computer difficulties will not be accepted as excuses for late submission. Any extenuating circumstances (e.g. illness) should be discussed with the MSc Director or Cohort Mentor immediately.

3.3 Written Examinations

Draft examination papers are prepared by the lecturer, moderated by a second member of staff and sent in advance to the External Examiner who reviews them and may suggest changes. After discussion with the course lecturers, these changes are usually incorporated into the final papers.

Each examination question is normally marked out of 25 by the course lecturer; each question is then check marked by a second marker. The total mark for each paper is converted to a percentage, the corresponding letter grade being fed back to the student.

Past examination papers will be made available on Blackboard.

The regulations concerning the conduct of examinations can be found at: http://www.imperial.ac.uk/about/governance/academic-governance/regulations/

3.4 Oral (viva voce) examinations for Advanced Options

Oral examinations for the Advanced Option courses (EQM2, TM2, ESM2, and CFTM2) take place at the end of Term 2. They are designed to test your depth of knowledge in the subject. For each course, around one week in advance of your oral examination, you will be provided with a list of three topics. You choose one out of the three topics to be the focus of the questions in the oral examination. The examination will be conducted by the course lecturer; an independent member of staff will act as an observer and moderator, who will ensure a similar standard is set across all of the Advanced Option courses. No formal presentation is required- the format will be one in which the lecturer will ask questions on the chosen topic for the duration of the viva, which will be 15
minutes. If helpful or appropriate students may use the whiteboard or write things down on paper during the discussion. The oral examination is marked out of 100 by the lecturer and independent observer.

### 3.5 Literature Review and Research Project

The literature review is assessed by a written report and marked by the principal supervisor.

The research project is assessed via oral presentation and a written report. The final mark for the project is the weighted average of the oral presentation and the written report (weighting 1:4). The project report is marked by two independent assessors, informed by a report from the supervisor about the student’s performance and any external factors that should be taken into account. In the event of significant disagreement between the marks awarded by the two markers, the markers will confer to arrive at a consensus mark. In the unlikely event that a consensus cannot be reached, the CDT Director and/or External Examiner will determine the final mark.

Guidelines for the conduct and assessment of literature reviews and research projects for the MSc in TSM may be found in Appendix 2.

### 3.6 Transferable skills

Training in professional or transferable skills is embedded within the MSc in TSM course, e.g.:

- **Writing skills**: written work is a major part of the continuously assessed coursework. Written reports account for more marks than any other form of assessment, notably the literature review and report on the research project.
- **Presentation skills**: short talks contribute to the assessment of one of the group projects and the research project. Participating in outreach activities coordinated by Simon Foster is an excellent way of developing these skills.
- **Research ethics**: a one day course on research ethics covering topics such as plagiarism, scientific misconduct, whistleblowing and open access publishing will be given in Term 1 by Marianne Talbot, Director of Studies in Philosophy at the University of Oxford.
- **Interview skills**: several components of the course, including the advanced core parts, may be assessed by interview (oral examination).
- **Computing and programming skills**: the course will ensure that you become proficient in using a UNIX-based environment and programming in Python and/or C/C++, particularly through the computational methods classes.
- **Networking and collaboration**: the cohort-based approach to the course, together with the events organised by the Thomas Young Centre, provide excellent opportunities for networking and to develop skills in collaboration.

In addition the Graduate School offers a range of courses and these will be publicised during the year. Details can be found at [https://www.imperial.ac.uk/study/pg/graduate-school/](https://www.imperial.ac.uk/study/pg/graduate-school/) and [https://www.imperial.ac.uk/study/pg/graduate-school/professional-skills/](https://www.imperial.ac.uk/study/pg/graduate-school/professional-skills/)

### 3.7 Letter Grades

Letter grades are produced by the assessors for the purposes of student feedback. For major pieces of coursework the letter grade is determined from a numerical mark, $m$, according to the following scheme:

<table>
<thead>
<tr>
<th>Letter</th>
<th>Mark Range</th>
</tr>
</thead>
<tbody>
<tr>
<td>A*</td>
<td>$m \geq 80%$</td>
</tr>
<tr>
<td>A</td>
<td>$70% \leq m &lt; 80%$</td>
</tr>
<tr>
<td>B</td>
<td>$60% \leq m &lt; 70%$</td>
</tr>
<tr>
<td>C</td>
<td>$50% \leq m &lt; 60%$</td>
</tr>
<tr>
<td>D</td>
<td>$40% \leq m &lt; 50%$</td>
</tr>
<tr>
<td>E</td>
<td>$30% \leq m &lt; 40%$</td>
</tr>
</tbody>
</table>
3.8 Requirements for Passing the MSc

Classification of the MSc

0%-49% Pass
50%-59% Merit
60%-69% Distinction
70%-100% Distinction

These percentages refer to the aggregate mark for the MSc.

You must get at least 40% for every component to pass the MSc.

This is a ruling passed by the Senate of the College in 2009. More precisely, the ruling states that if you get less than 50% in any component, then you will receive a compensated pass provided (i) your aggregate mark is at least 50% and (ii) you get no less than 40% in any component.

If you get less than 40% in any component you will fail the entire MSc.

Progression onto Year 2 for CDT students on the 4-year PhD course

In order to progress to year 2 of the CDT, MSc students must gain an aggregate mark of at least 60% in the MSc.

If your aggregate mark is between 50% and 59% you will leave Imperial College at the end of year 1 with an MSc in Theory and Simulation of Materials.

Resits

There are no plans to hold any resits of examinations for the MSc.

How to complain

Imperial College aims to give the highest specialised instruction and service to all its students, however, in some cases it recognises that students may not always be satisfied with the service that they have received. If you wish to raise a concern, you should first seek advice from your student representatives and raise the matter with the individual concerned. If you are not satisfied with the outcome, you should consult the College’s Registry website which provides clear and consistent procedures that indicate how you can take your comments further:

http://www.imperial.ac.uk/students/terms-and-conditions/appeals/

3.9 Sutton Prize

A prize of £600 will be awarded to the student with the best overall performance in the MSc, as determined by the aggregate mark.
4 Academic Support

General

The academic support for the MSc students comes primarily from the course lecturers, the other academic staff associated with the CDT and project supervisors. The number of students on the MSc course is normally a small enough group that they are actively encouraged to go directly to course lecturers and other staff with academic questions on an informal basis. The College also has a Success Guide for students, available at the following link: https://www.imperial.ac.uk/students/success-guide/

Projects

For the MSc research projects, each student will have at least two supervisors allocated. For other projects such as the group projects, a member of academic staff will brief students about the work at the beginning of the project and thereafter advises the students whenever necessary.

Writing and Communication Skills

There is written support material for writing skills and for the oral presentation of coursework – courses are arranged by the Graduate School and details will be given early in the course. Communication skills are assessed continuously throughout the course and students submit written work and give public oral presentations which are assessed and whose assessment counts towards their final degree result. Feedback to students is available on all submitted work and oral presentations.

4.1 Absences and Illness

The College monitors the attendance of all its students. Students hand in their solutions to problem sets each week. This enables staff to monitor attendance. Students are requested to notify lecturers and the Senior Administrator if they become ill.

If coursework is affected students must complete a (minor) mitigating circumstances form as soon as possible.

Students are required to provide a medical certificate if they are absent for 3 days or more, including during the summer project.

If a student misses an examination because they are ill it is essential that they obtain a medical certificate and complete a (major) mitigating circumstances form as soon as possible.

Further information on the College’s policy and procedures for mitigating circumstances can be found at http://www.imperial.ac.uk/natural-sciences/departments/physics/students/current-students/student-welfare/mitigating-circumstances/

All students have access to the College Health Centre at 40 Prince’s Gardens. Details of their services can be found at www.imperialcollegehealthcentre.co.uk

Note that absences due to work commitments are not admissible as mitigating circumstances, and in general due to the demands of this course, part-time employment is strongly discouraged. The College’s policy on employment during studies may be found at https://workspace.imperial.ac.uk/registry/Public/Procedures%20and%20Regulations/Policies%20and%20Procedures/Student%20Employment%20During%20Studies.pdf
4.2 Disabilities, specific learning difficulties and long-term health issues

At Imperial College we recognise that studying at university can be a challenge, especially if you have a disability. We are keen that you have every opportunity to fulfil your potential and graduate with the degree you deserve. It is therefore important that you let us know about any disability, specific learning difficulty or health problem as soon as possible so that we can give expert advice and support to enable you to do this.

Some people never think of themselves as having a disability, but students who have experienced any of the issues listed below have found that a little extra help and support has made all the difference to their study experience.

- Specific learning difficulties (such as dyslexia, dyspraxia, AD[H]D)
- Autistic spectrum disorder (such as Asperger’s)
- Deafness or hearing difficulties
- Long term mental health difficulties (such as chronic anxiety, bipolar disorder, depression)
- Medical conditions (such as epilepsy, arthritis, diabetes, Crohn’s disease)
- Physical disabilities or mobility impairments
- Visual difficulties

Where to find help:

1. **Your Disability Liaison Officer** (Andrew Williamson: andrew.williamson@imperial.ac.uk)
   Andrew Williamson is your first point of contact within your department and is there to help you with arranging any support within the department that you need. Andrew is also the person who will apply for Special Examination arrangements on your behalf. You need to contact him without delay if you think that you may need extra time or other adjustments for your examinations.

2. **Disability Advisory Service**: [www3.imperial.ac.uk/disabilityadvisoryservice](http://www3.imperial.ac.uk/disabilityadvisoryservice)
   The Disability Advisory Service works with individual students no matter what their disability to ensure that they have the support they need. We can also help if you think that you may have an unrecognised study problem such as dyslexia. Our service is both confidential (information about you is only passed on to other people in the university with your agreement) and individual in that any support is tailored to what you need.
   Some of the sorts of things we can help with are:
   - Being an advocate on your behalf with others in the College such as your departmental liaison officer, senior tutor or exams officer, the accommodation office or the estates department
   - Checking that your evidence of disability is appropriate and up-to-date
   - Arranging a diagnostic assessment for specific learning difficulties
   - Help with applying to the College for the cost of an assessment
   - Help with your application for the Disabled Students Allowance (DSA) see below
   - Helping students not eligible for the DSA in obtaining support from other sources
   - Help with arranging extra Library support
   - Supporting applications for continuing accommodation for your second or later years

3. **Disabled Students Allowance**: [https://www.imperial.ac.uk/disability-advisory-service/support/dsa/](https://www.imperial.ac.uk/disability-advisory-service/support/dsa/)
   Students who are home for fees and who have a disability can apply for a grant called the Disabled Students Allowance which can pay any extra costs that are a direct result of disability. This fund is not means-tested and is also a grant not a loan so any home student with a disability can apply and will not be expected to pay it back. Remember students with unseen disabilities such as mental health difficulties, dyslexic type difficulties or long term health problems are also eligible for this fund.
4.3 Blackboard

Some of the material for the lecture courses may be delivered using the Blackboard Learning System, a Virtual Learning Environment (VLE), which can be used to access material, such as lecture notes and problem sheets posted by the course lecturer. Past exam papers may also be found there. Different lecture courses use Blackboard to differing degrees and you will be advised by each lecturer about the material they have made available. You will need to register with the course before you can access the material. In most cases this will be done upon your arrival but please contact andrew.williamson@imperial.ac.uk if you wish to gain access for a particular course.

Log on to Blackboard at bb.imperial.ac.uk.

4.4 Outreach

Our Outreach Officer, Dr Simon Foster, works with CDT students to help them develop and practise a range of communication skills for various audiences. Besides their presentation abilities, students also hone a capacity to structure and present complex information, which will aid them throughout their academic careers and beyond. During the MSc, participation in these activities is optional but nevertheless encouraged. If you would like to get involved then email simon.foster1@imperial.ac.uk.
5 General Information about Life in the Centre for Doctoral Training

This section is intended to supply all new MSc students with some essential information about the TSM-CDT and Imperial College.

5.1 Before you Arrive

Prior to arriving at Imperial College, you should have received joining instructions, a timetable and the details on the introductory lecture where you shall be given further details of the course, briefings and documents on your course and the CDT (such as safety information) and the opportunity to meet your colleagues. You are also encouraged to look at the web page for all new students at Imperial: www3.imperial.ac.uk/students/newstudents.

5.2 Where to Find Us

Imperial College is located just behind (south of) the Albert Hall in South Kensington. The nearest tube stations are South Kensington and Gloucester Road on the District/Circle Line and High Street Kensington on the Circle Line. South Kensington and Gloucester Road are also on the Piccadilly Line which goes directly to Heathrow Airport. Campus maps and information may be found here: http://www.imperial.ac.uk/visit/campuses/south-kensington

- The CDT on TSM is located in the Whiteley Suite in the RCS1 Chemistry building, which is opposite the Skempton building on Imperial College Road.
- The Department of Physics is located at the Blackett Laboratory, on the corner of Queen’s Gate and Prince Consort Road (the entrance is on this road).
- The Department of Mechanical Engineering is opposite the Whiteley Suite, on Imperial College Road.
- The Department of Chemistry is on Imperial College Road, opposite the Queen’s Lawn.
- The Department of Materials is based in the Royal School of Mines, the Bessemer Building and the Goldsmiths Building. These are on the corner of Exhibition Road and Prince Consort Road (the entrance is on this road).

5.3 When you Arrive

MSc students will be sent an email inviting them to register online. The induction begins at 9.30am on the first weekday of Term 1. Laptops provided for all those taking the course will be distributed on the same day.

5.4 ID Cards

One of the very first things you need to do when you arrive is obtain an identity card. Instructions on how to obtain an ID card will be sent to you in the welcome packs. The ID card is essential for a number of purposes, including access to the Central Library. It is also used as a swipe card to get in and out of the Whiteley Suite where the CDT is housed.

5.5 Mail

The CDT postal address is:

CDT in TSM, Whiteley Suite, RCS1 Building, Imperial College London, Exhibition Road, London, SW7 2AZ. UK
For deliveries of equipment or deliveries by courier it is better to use the following address:

CDT in TSM,
Imperial College London,
Whiteley Suite, RCS1 Building,
Imperial College Road,
London, SW7 2AZ, UK

In general we do not encourage students to have mail sent to them at the CDT. But if it is necessary that something is sent to you at the CDT please inform the Senior Administrator, who will pass it on to you when it arrives.

5.6 Telephones

The general college number is 020 7589 5111. The College operator may be obtained by dialling 0. Five-figure internal numbers may be dialled directly on the phone. All extension numbers prefixed with a 4 may be dialled directly by external callers using 020 7594-XXXX. Extension numbers prefixed with a 5 do not have the directly dialling facility. Use the “People” tab (top right, next to the Search textbox) on the College website to find telephone numbers and offices of members of College. Microsoft Outlook also has contact details for the staff and students.

5.7 Security and Emergencies

Emergencies of all types within College should be reported to extension 4444. Outside the College telephone network the number is 020 7589 1000 and you are encouraged to store this on your mobile. Your safety induction and literature will give you details on First Aid procedures.

Although access to the Whiteley Suite is via a swipe card it is possible that thieves may gain entry by tail-gating. Always keep your laptop locked when it is left in your office and keep the doors to the student offices closed at all times. If your laptop is stolen it is unlikely the CDT will be able to replace it. In addition, petty theft happens from time to time. Don't leave valuables lying around and always close and lock the door, even if you go out for just a short time. Unfortunately, some thefts have been from locked offices, so either take laptop home each night or lock it securely. If you see anyone at all suspicious, call security on extension 4444.

5.8 Library Facilities

The Central Library is next to the Sherfield Building. The catalogue may be accessed from terminals in the Central Library and over the web via www.imperial.ac.uk/admin-services/library. The Central Library also houses the Haldane Collection, with a good general collection (fiction and non-fiction) and a music library.

The CDT also has a small library housed in the Whiteley Suite.

Electronic journals are available via the library website: http://www.imperial.ac.uk/admin-services/library/find-books-articles-and-more/

5.9 Accommodation

The College Accommodation Office may provide you with help in finding accommodation. You may enquire at the Student Hub (ext 4-9444, student.hub@imperial.ac.uk) on level 3 of the Sherfield Building or visit the College's accommodation webpages at https://www.imperial.ac.uk/study/campus-life/accommodation/

5.10 Food and Drink
MSc students can buy lunch in the Junior Common Room off the Main Walkway. Tea and coffee making facilities are available in the Whiteley suite.

A number of sandwich shops, restaurants and pubs, at a range of prices, may be found on Gloucester Road (one block west of Queen's Gate), and around the tube station at South Kensington. Beit Quad and Eastside have student bars and catering facilities.

There is a kitchen in the CDT with a microwave and fridge. Please keep this area clean and fresh at all times. Be very careful not to spill any drinks onto computers.

5.11 Health

The College Health Service may be found at 40 Prince’s Gardens. Their telephone number is extension 4-9375/6. For emergencies call extension 4444. Students, local residents and visitors from overseas may all use the Health Service free of charge. The Health Service is open from 8am to 6pm weekdays during term time (but it is closed after 1pm on Tuesdays), and 8am to 5pm out of term. Appointments may be made by calling the above number. In addition to General Practitioners, an extensive range of services are offered, including free condoms, physiotherapy, acupuncture, herbal medicine, osteopathy, massage, psychotherapy, vaccinations and treatment for sports injuries. Dental treatment is also provided at the Health Service. It is open from 9am to 6pm. Appointments are usually necessary (call 020 7589 6623). It is generally necessary to pay for dental treatment, although students and those on income support can obtain subsidies.

If travelling elsewhere in the European Union, you would be advised to obtain an EHIC card [www.ehic.org.uk/Internet/home.do](http://www.ehic.org.uk/Internet/home.do) prior to your travel, as this will enable you to receive medical treatment at reduced cost. The EHIC is available to all persons resident in the United Kingdom, but non European Union students will need longer to apply.

<table>
<thead>
<tr>
<th>Emergency assistance (Medical, Security and Fire, Police, Ambulance)</th>
<th>Telephone</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>4444 (internal)</td>
</tr>
<tr>
<td></td>
<td>020 7589 1000</td>
</tr>
<tr>
<td>The Health Centre</td>
<td>49375 or 49376</td>
</tr>
<tr>
<td>(<a href="http://www.imperialcollegehealthcentre.co.uk">www.imperialcollegehealthcentre.co.uk</a>)</td>
<td>020 7584 6301</td>
</tr>
<tr>
<td>The Student Accommodation Office</td>
<td>49444</td>
</tr>
<tr>
<td>(<a href="https://www.imperial.ac.uk/study/campus-life/accommodation/">https://www.imperial.ac.uk/study/campus-life/accommodation/</a>)</td>
<td></td>
</tr>
<tr>
<td>The Student Counselling and Mental Health Advice Service</td>
<td>49637</td>
</tr>
<tr>
<td>(<a href="http://www3.imperial.ac.uk/counselling">www3.imperial.ac.uk/counselling</a>)</td>
<td></td>
</tr>
<tr>
<td>Careers Service</td>
<td>48024</td>
</tr>
<tr>
<td>(<a href="http://www3.imperial.ac.uk/careers">www3.imperial.ac.uk/careers</a>)</td>
<td></td>
</tr>
<tr>
<td>Chaplaincy (Religious support, including other major faiths)</td>
<td>49600</td>
</tr>
<tr>
<td>(<a href="http://www3.imperial.ac.uk/chaplaincy">www3.imperial.ac.uk/chaplaincy</a>)</td>
<td></td>
</tr>
<tr>
<td>Students Union</td>
<td>48060</td>
</tr>
<tr>
<td>(<a href="http://www.imperialcollegeunion.org">www.imperialcollegeunion.org</a>)</td>
<td></td>
</tr>
<tr>
<td>Student Financial Support</td>
<td>48122</td>
</tr>
<tr>
<td>(<a href="http://www3.imperial.ac.uk/studentfinance">www3.imperial.ac.uk/studentfinance</a>)</td>
<td></td>
</tr>
</tbody>
</table>

More information is available at the College’s Student Support webpages: [http://www.imperial.ac.uk/student-space/](http://www.imperial.ac.uk/student-space/)
5.12 **Sports Facilities**

The College Sports Centre can be found at 7 Prince’s Gardens. Details of facilities, opening time, etc can be found at [www3.imperial.ac.uk/sport](http://www3.imperial.ac.uk/sport).

5.13 **Banking**

Students are recommended to open a bank account in London. The four largest banks in the UK are National Westminster, Barclays, Lloyds and HSBC. Many banks are attentive to the special needs of students. There is a branch of Santander on the walkway. Students opening accounts should bring a Certificate of Registration at Imperial College. Students from abroad should also bring their passport.

5.14 **Parking**

Parking is extremely limited in the College. Permits for short visits (a day or so) can sometimes be obtained.

5.15 **Travel and Travel Insurance**

All staff and students travelling on College business are automatically covered by the College’s insurance policy if they register their trip in advance— see

[https://www.imperial.ac.uk/finance/financial-services/insurance/](https://www.imperial.ac.uk/finance/financial-services/insurance/)

It is worth taking with you a copy of the cover note, which may be downloaded from the above page. You should also register before you leave by following the link at

[https://wiki.imperial.ac.uk/display/FKB/Overseas+Travel](https://wiki.imperial.ac.uk/display/FKB/Overseas+Travel)

If you do plan to go away during term time, even if only for a few days, please speak to your Cohort Mentor beforehand and leave details indicating where you can be contacted.

5.16 **Life in London**

*Time Out*, published weekly, has extensive listings of much that is going in London. It can be bought at a discount at the student shop on the walkway outside the Sherfield Building.

The Student Union organises many events, details of which can be found at [www.imperialcollegeunion.org](http://www.imperialcollegeunion.org) or from posters on the notice boards.

5.17 **Moving on from Imperial**

The Careers Advisory Service [www3.imperial.ac.uk/careers](http://www3.imperial.ac.uk/careers) provides training on important skills like CV writing and interview techniques as well as careers advice and information from potential employers.

5.18 **And When You Leave Imperial...**

Make sure you return all keys, copy cards, ID card, books and other College material. Please either provide details of how you can be contacted or monitor your College email account as we may need to contact you afterwards (with your final result, for instance).
Appendix 1  Synopses of courses

The following brief descriptions of the content of the courses are indicative and changes may be made by the lecturer before each course starts. The descriptions given here may not always match the College Prospectus, since the Prospectus is prepared up to 18 months before a course is given.
Compulsory core courses
Mathematics for the Theory of Materials (MTM1 and MTM2)
Dr Gunnar Pruessner (GP) and Prof. Matthew Foulkes (WMCF)

24 one-hour lectures and 7 rapid feedback sessions in Term 1

Items in italics are pre-requisite knowledge.


II. Green’s Functions [3 lectures & 1 RF, GP]. Dirac delta function. Variation of parameters method for inhomogeneous ODEs. Green’s functions for initial value and boundary value problems.

III. Hilbert Spaces [3 lectures & 1 RF, GP]. Definition of a Hilbert space; dimensionality, orthogonality, linear dependence, Wronskian. Sturm-Liouville Theory; self-adjoint operators, eigenfunctions, eigenvalues, weight function. Eigenfunction expansions, completeness. Examples of orthogonal functions to include Bessel functions, spherical harmonics and Legendre polynomials, including solution of Laplace’s equation in spherical polar coordinates by separation of variables and series solution of Legendre’s equation.

IV. Integral Transforms [3 lectures & 1 RF, GP]. Continuous Fourier transforms: Parseval’s theorem and convolution theorem; bandwidth theorem and connection to quantum mechanics; application to Fraunhofer diffraction and heat diffusion. Laplace transforms: convolution theorem; application to ordinary differential equations. (Pre-requisite knowledge: Fourier series, orthogonality of cos and sin, Gibbs phenomenon, Parseval’s theorem and Bessel’s inequality for Fourier series, odd and even functions, Kronecker delta).

V. Complex Analysis and Contour Integration [7 lectures & 2 RF, WMCF]. Functions of a complex variable. Cauchy-Riemann relations, analytic functions, Cauchy’s theorem, Laurent’s theorem. Order of poles. Residue theorem. Principal values and the Kramers-Kronig relation. Jordan’s lemma. Contour integration. Inverse integral transforms; Bromwich integral. (Pre-requisite knowledge: complex numbers; Argand diagram; modulus and argument; Cartesian and polar form; \(z^n\), with \(n\) not necessarily an integer; multi-variate real calculus; vector calculus; line integration; Taylor and Maclaurin series; Laplace transform; Dirac delta function.)

Continuous Assessment
- For sections I to IV, there are four problem sheets, one per week, with one long question assessed each.
- For sections V and VI, there are three problem sheets, one per week, with 4-5 assessed problems each.
- The problem sheets also contain other problems that are not assessed.
Equilibrium in Materials (EQM1)
Professor Dimitri Vvedensky

16 one-hour lectures and 4 rapid feedback sessions in Term 1

Outline

1. Elements of Thermodynamics
   a) Basic concepts
   b) The laws of thermodynamics
   c) The fundamental equation
   d) Equations of state

2. Thermodynamic Potentials
   a) Isothermal processes: The Helmholtz function
   b) Isothermal and isobaric processes: The Gibbs function
   c) Isobaric processes: The enthalpy
   d) Spontaneous processes

3. Chemical Potential and Phase Equilibria
   a) Mixtures of ideal gases
   b) The chemical potential
   c) Gibbs’ phase rule

4. Solid Solutions
   a) The ideal solution model
   b) The free energy of solid solutions
   c) The stable state of an alloy
   d) Variation of solubility with temperature

5. Phase diagrams
   a) Reference states and general features
   b) Binary phase diagrams with two competing phases
   c) Miscibility gaps and spinodal decomposition
   d) Two-phase regions

Recommended Textbooks

D. A. Porter and K. E. Easterling, Phase Transformations in Metals and Alloys (Taylor & Francis, 2004), Ch. 1.

Course Administration and Learning Support

Lecture notes: Comprehensive notes will be provided for all the material covered in the lectures. The material for each lecture will be made available prior to that lecture. In addition to providing a written record of the course material, this will allow the lectures to focus on important points, rather than routine calculations. The presentations of each lecture will also be made available.

Homework and Rapid Feedback: Problem sets will be assigned each week. The lectures and problem sets are to be regarded as an organic whole. Accordingly, the assignments will include
problems that illustrate concepts and methods covered in the lectures as well as those that extend these discussions. The solutions of the problems will be covered in separate weekly problem-solving sessions.

*Office hours:* Office hours provide the opportunity for students to meet face-to-face with the lecturer to discuss any aspect of the course. These will be announced at the beginning of the first lecture.
Transformations of Materials (TM1)
Professor Peter Haynes

16 one-hour lectures and 4 rapid feedback sessions in Term 1

The aim of this course is to cover the background theory necessary for understanding phase transformations in materials. It will therefore focus primarily on theoretical concepts, but illustrate them by application to real materials wherever possible. Thermodynamics applies to systems in equilibrium e.g. we can use it to calculate the relative stability of two phases. However in order to calculate the rate with which one phase will transform into another we need to study kinetics, which are often determined by diffusion processes. This is crucial for understanding how the processing of a material affects its microstructure, which in turn determines its properties. The concepts taught in this course will be picked up and applied to specific types of transformations in the advanced course TM2.

The continuous assessment for this course will take the form of four assessed problem sheets containing a total of ten questions. One question from each sheet will be selected for assessment.

Prerequisites

This course assumes familiarity with the material covered in EQM1.

Synopsis

0. Microstructure
   Examples of different microstructures and their influence on materials properties; control by processing and the central role of kinetics.

1. Driving forces and fluxes for diffusion (PES chapter 1, BAC chapters 2 & 3)
   a. The role of Gibbs free energy in thermodynamics (equilibrium condition \( dG = 0 \)) and kinetics (activation free energy and Arrhenius laws).
   b. Regular solution model of binary substitutional alloy: derivation of the free energy of mixing for a random alloy (configurational entropy from Stirling’s approximation, enthalpy from the quasichemical approach); connection between plots of \( G \) versus composition and binary phase diagrams for both exothermic and endothermic mixing at high and low temperatures; miscibility gap, common tangent construction and lever rule to determine equilibrium composition; nucleation versus spinodal decomposition; chemical potentials and their interpretation using plots of \( G \) versus composition; departure from ideal behaviour due to ordering or clustering of atoms, activities and activity coefficients, Henry’s law and Raoult’s law for dilute solutions.
   c. Driving forces for diffusion: fundamental role of chemical potential gradient (illustrated using \( G \) versus composition plots) and the possibility of ‘uphill’ diffusion against a concentration gradient; additional driving forces from interfacial energy (Gibbs-Thomson effect), electrostatic potential gradient for charged species and stress (formation of Cottrell atmospheres and creep)
   d. Fluxes and conjugate forces: derivation of Fick’s first law and the analogy with current flow (Ohm’s law) and heat flow (Fourier’s law); coupling of fluxes and Onsager’s symmetry principle as seen in the Seebeck and Peltier effects and electromigration; network constraints and vacancies.

2. The diffusion equation (PES chapter 2, BAC chapters 4 & 5, BB)
   a. Derivation and simplification of the diffusion equation from Fick’s first law and conservation of matter.
b. Steady-state solutions (harmonic functions) for planar, cylindrical and spherical geometries.
c. Linearity of the diffusion equation: superposition and the uniqueness theorem for the diffusion equation (proof not required).
d. Separation of variables: solution of the diffusion equation in a finite spatial domain; treatment of the initial condition using orthogonal functions (e.g., Fourier series).
e. Fundamental solution: derivation for the infinite spatial domain using integral transforms; superposition of solutions for the semi-infinite spatial domain by analogy with the method of images in electrostatics; derivation of error function solutions by superposition of point sources.
f. Scaling: characteristic diffusion length and solution method for a 1D semi-infinite spatial domain through conversion to an ordinary differential equation; re-derivation of error function solutions; re-derivation of the fundamental solution by superposition.
g. Precipitate growth: Stefan (moving) boundary conditions; solution for planar and spherical geometries (recall of the form of the solution is not required).

3. Atomic mechanisms for diffusion in solids (PES chapter 2, BAC chapters 7–9, BB)
a. Random walks: derivation of diffusivity in $d$ dimensions; re-derivation of fundamental solution in one dimension.
b.Interstitial diffusion: octahedral interstitial sites in bcc and fcc, re-derivation of Fick’s first law for cubic lattices, migration free energy barrier and jump rate.
c. Substitutional diffusion in a pure metal: vacancy mechanism: derivation of equilibrium vacancy, activation energy for diffusion and its correlation with melting temperature; direct exchange, ring and interstitialcy mechanisms.
d. Substitutional diffusion in a binary alloy: Kirkendall effect; derivation of Darken’s equations; dislocation kinks as sources/sinks of vacancies.
e. High-diffusivity paths: grain boundaries and dislocations; estimation of their relative importance at high and low temperatures relative to lattice diffusion.

4. Interfaces and microstructure (PES chapter 3, BAC appendix B)
a. Classification of interfaces: sharp versus diffuse; singular, vicinal and general; homophase versus heterophase; coherent, semi-coherent and incoherent.
b. Interfacial free energy: effect on nucleation; $\gamma$-plot and Wulff construction.
c. Instabilities in solidification fronts: undercooling in pure liquids and constitutional supercooling of alloys; Mullins-Sekerka linear stability analysis for spherical interfaces.

References and recommended reading


BB – additional material on Blackboard site
Electronic Structure of Materials (ESM1)
Johannes Lischner (8 lectures) and Paul Tangney (8 lectures)

16 one-hour lectures and 4 rapid feedback sessions in Term 1

The aim of this course is to introduce students to some fundamental concepts of the electronic structure of materials. The course consists of two parts: i) concepts for understanding interacting many-electron systems (taught by Paul Tangney) and ii) applications of electronic structure theory to materials (taught by Johannes Lischner).

Prerequisites:
The course assumes familiarity with basic concepts of quantum mechanics, such as operators, wave functions, solutions of the Schrödinger equation for simple systems (free particle, simple harmonic oscillator, hydrogen atom).

Synopsis:

Part 1: Making quantum mechanics tractable for many-electron systems: the simplifying assumptions and approximations (PT).

Statement of the problem.
Many electrons and many nuclei; Schrödinger's time-dependent equation and the meaning of the wave function; stationary states; time-independent Schrödinger equation; variational principle; Hohenberg-Kohn theorems; observables
\[ \langle \hat{O} \rangle = O[n] \].

Mathematically separating electrons and nuclei
Adiabatic and Born-Oppenheimer approximations; classical nuclei; Hellman-Feynman theorem.

Calculating electronic properties using the wave function, \( \Psi \):
Meanings of “exchange” and “correlation”; Hartree approximation; Hartree-Fock approximation; Beyond Hartree-Fock – what would an exact solution look like? Systematic improvements to Hartree-Fock.

Calculating electronic properties using the density, \( n \):
Density functional theory (DFT); Kohn-Sham approach to partitioning the total energy and calculating the ground state density; the Local Density Approximation (LDA); successes and failures of DFT; justification for (quasi-) independent electron models of materials.

Part 2: Using quantum mechanics to compute the properties of materials (JL).

Using quantum mechanics to solve mysteries of metals:
Failure of classical statistical mechanics to explain specific heat of metals; Sommerfeld theory of metals; periodic boundary conditions; total energy; density of states and bulk modulus of the electron gas; Sommerfeld expansion.

Electrons in crystals:
Crystal lattices; Wigner-Seitz cell; periodicity; lattice Fourier series; Schrödinger's equation in a periodic potential; Bloch’s theorem; crystal momentum; the nearly-free electron gas; metals; semiconductors and insulators; the role of symmetry.

From atoms to crystals:
Core and valence electrons; many-electron atoms; Aufbau principle and the periodic table; shell structure of atoms; electronegativity; bonding (van der Waals, ionic, covalent, metallic, hydrogen); tight-binding method; one-dimensional chain of hydrogen atoms.
Beyond the rigid ion approximation:
Failures of the rigid ion approximation; vibrations of a chain of atoms; physics underlying the Lennard-Jones potential; small deviations from equilibrium; normal modes; speed of sound; vibrations of a three-dimensional crystal; acoustic and optical modes; quantum theory of lattice vibrations; phonons; specific heat; Debye temperature.

Continuous assessment
There will be four assessed problem sets.

Books

This is a new book that was written with materials scientists in mind. It covers most of the topics taught in this course.

A classic textbook of solid-state physics. A good source for band theory, phonons, tight binding, etc.

Another classic textbook of solid-state physics.

More advanced books

This book introduces electronic structure theories for many-electron systems in atoms and molecules, such as Hartree-Fock, configuration interaction and coupled cluster theory.

This book explains well the foundations of density-functional theory and its application to atoms and molecules.

This book introduces advanced techniques for the treating interacting many-electron systems in solids and nanostructures.
Classical Field Theory of Materials (CFTM1)
Professor Adrian Sutton

16 one-hour lectures and 4 rapid feedback sessions in Term 1

Synopsis

- Structural vs. functional materials. Mechanical properties are determined by physics across length and time scales.
- Defects in crystals: point, linear and planar defects.
- The geometry of the elastic field: displacement vector, distortion tensor, symmetric and antisymmetric components corresponding to strains and rotations respectively. Force and stress, and the stress field. The symmetry of the stress tensor. Invariants of the stress tensor. Linear elasticity, Hooke’s law and the elastic constants as material parameters. Voigt (engineering) notation. The three independent elastic constant of cubic crystals and two of isotropic materials, and elastic anisotropy ratio in cubic crystals. The energy of the elastic field.
- The equilibrium condition for the stress field and body forces. Surface tractions. Application of Gauss’s theorem to determine the average stress tensor within a body.
- The misfitting sphere as a model of point defects. Elastic solution in an infinite isotropic medium and in a sphere of finite radius.
- The elastic Green’s function.
- Application of the elastic Green’s function to point defects with non-spherical symmetry, and connection with atomistic simulation.
- Application of the elastic Green’s function to dislocations: Volterra’s formula, Mura’s formula.

Continuous assessment
2 or 3 problems and/or short essays will be set for each of the 4 rapid feedback sessions.

Books
Elasticity
- C Teodosiu, Elastic models of crystal defects, Springer (1982). This is an excellent book on elasticity oriented towards defects in solids. It has just been brought back into print and three copies have been ordered for the CDT library. It is a good book to learn from because it is rigorous without being pedantic, and it is a book you will return to in later years because it is a mine of information.

Dislocations
- D Hull and D J Bacon, Introduction to Dislocations, Pergamon (1992). This is a very readable introduction to dislocations in solids.

Elasticity, defects
- A H Cottrell, The mechanical properties of matter. This is a very clear introduction to the subject, written by possibly the finest metallurgist of all time.
More advanced books


- T Mura *Micromechanics of defects in solids*, Kluwer (1991). This is an advanced text, but very useful and well written, and directly related to Eshelby’s work.


Methods of Simulating (MSM1 and MSM2)
Prof Daniele Dini (organiser), Dr Andrew Horsfield, Dr Johannes Lischner, Dr Paul Tangney

32 hours of lectures and classes in Term 2

Course Overview
There will be eight topics, each lasting one week. For each topic there will be two hours of lecture and two hours of problem solving / feedback. The topics and associated exercises will be:

<table>
<thead>
<tr>
<th>Topic</th>
<th>Lecturer</th>
<th>Exercises</th>
<th>Homework</th>
</tr>
</thead>
<tbody>
<tr>
<td>1. Introduction</td>
<td>Daniele Dini &amp; Andrew Horsfield</td>
<td>Multiscale Simulations Overview &amp; MATLAB program</td>
<td>N/A</td>
</tr>
<tr>
<td>2. Density functional theory</td>
<td>Johannes Lischner</td>
<td>Hydrogen atom</td>
<td>1</td>
</tr>
<tr>
<td>3. Energy landscapes</td>
<td>Paul Tangney</td>
<td>Static relaxation calculations</td>
<td>2</td>
</tr>
<tr>
<td>4. Molecular dynamics</td>
<td>Paul Tangney</td>
<td>Molecular dynamics simulations</td>
<td></td>
</tr>
<tr>
<td>5. Kinetic Monte Carlo</td>
<td>Andrew Horsfield</td>
<td>Hopping of disks between bins</td>
<td>3</td>
</tr>
<tr>
<td>6. Metropolis Monte Carlo</td>
<td>Andrew Horsfield</td>
<td>1D equilibration</td>
<td></td>
</tr>
<tr>
<td>7. Finite Elements</td>
<td>Daniele Dini</td>
<td>1D and 2D finite elements of simple engineering structures</td>
<td>4</td>
</tr>
<tr>
<td>8. Crystal Plasticity</td>
<td>Daniele Dini</td>
<td>Plasticity in crystalline structures</td>
<td></td>
</tr>
</tbody>
</table>

Assessment
1. Four problem sets (one per lecturer) based on the exercises. This is worth 70%.
2. An eight minute prepared talk by each student. The students will be given a choice of four topics to choose from, of which they choose one. The presentations will take place in the first week of Term 3. This is worth 30%.
3. The topics for the talks are:
   - Using kinetic Monte Carlo to solve the diffusion equation. Discuss the simulations you performed (NOT including the advanced tasks), offering answers to the questions asked in the description of the exercises.
   - Computing the ionization potential of atoms with DFT. Discuss how DFT can be used to compute total energies and ionization potentials of atoms and describe the results obtained in class and in the assessed problem. What are the problems of this approach, what are its merits?
   - Molecular Dynamics simulation of polymer dynamics. Discuss Langevin Dynamics and what it can tell you about the dynamics of a polymer in solution.
   - Finite Element Method for Solids and Structures. Discuss the steps required to build up a 2D finite element model to calculate displacement and forces in bodies subjected to external loads.

Contact details

<table>
<thead>
<tr>
<th>Name</th>
<th>E-mail</th>
<th>Phone</th>
</tr>
</thead>
<tbody>
<tr>
<td>Daniele Dini</td>
<td><a href="mailto:d.dini@imperial.ac.uk">d.dini@imperial.ac.uk</a></td>
<td>4-7242</td>
</tr>
<tr>
<td>Andrew Horsfield</td>
<td><a href="mailto:a.horsfield@imperial.ac.uk">a.horsfield@imperial.ac.uk</a></td>
<td>4-6753</td>
</tr>
<tr>
<td>Johannes Lischner</td>
<td><a href="mailto:j.lischner@imperial.ac.uk">j.lischner@imperial.ac.uk</a></td>
<td>4-9949</td>
</tr>
<tr>
<td>Paul Tangney</td>
<td><a href="mailto:p.tangney@imperial.ac.uk">p.tangney@imperial.ac.uk</a></td>
<td>4-8155</td>
</tr>
</tbody>
</table>

Syllabus

Introduction
Overview of what computer modelling of materials is for, and can achieve. Survey of length and time scales and the methods appropriate to each.
Density-functional theory
Atomic length and time scales; fundamental theorems of density-functional theory; deriving the Kohn-Sham equations; approximate DFT: the local density approximation and beyond; exchange-correlation hole; spin polarization; Kohn-Sham equation for atoms; spherical symmetry; pseudopotentials; computing total energies and ionization potentials of atoms; the problem of self-interaction.

Energy landscapes
Describing energy landscapes: the potential energy function \( U(\{R\}) \); ab initio methods (quantum mechanics for electrons and the connection to N-body classical potential energy functions for ions, Born-Oppenheimer approximation); pair potentials (Lennard-Jones, Born-Mayer); semiconductors and metals (angular terms, bond-order potential, embedded-atom); molecular mechanics; induced dipoles in ionic systems; parameterization and force fitting. Exploring energy landscapes: molecular dynamics (basic concept, Verlet algorithm); finding minima (steepest descent, conjugate gradients, Newton methods).

Molecular Dynamics
Tricks of the trade: periodic boundary conditions; Ewald summation; neighbour lists; thermostats; barostats. Case studies to illustrate: Accessible time and length scales; Fluctuations and their explanation in terms of basic statistics; Correlation functions; Exploiting the fluctuation-dissipation theorem; Using atomistic simulations to provide a) ideas and b) numbers (with the help of DFT).

Kinetic Monte Carlo
Slow processes and local equilibrium; master equation; detailed balance. Link to diffusion equation and chemical rate equations. N-Fold Way Monte Carlo algorithm. Example applications.

Metropolis Monte Carlo
Review of statistical mechanics; computing averages. The Metropolis algorithm (NVT); Extensions to other ensembles (NPT, \( \mu \)VT). Free energy calculations. Example applications.

Finite elements
Basic principles of Finite Elements for frames and continua; 1D Finite Element definition, 2D local and global coordinates; Linear shape function in 1D; Determination of Forces, Stress and Strain Energy; 1D Example application. 2D beam elements; Constant Strain Triangle; Jacobian matrix and Stiffness matrix; Assembly of matrix equation of equilibrium.

Crystal plasticity
Advanced core courses
**Equilibrium in Materials (EQM2)**  
**Professor Mike Finnis**

8 hours of classes in Term 2

**Prerequisites:**  
Core courses EQM1 and TM1

**Continuous assessment:**  
- 2 problem sheets to be handed in  
- 1 essay

**Examination:**  
- Viva voce examination

The overarching theme of this module will be 'Atomistic Thermodynamics', or modern approaches to calculating thermodynamic properties by studying the energies and dynamics of collections of atoms, either quantum mechanically or classically. We shall study two broad themes as described below. Besides the sources noted below, my 2013-14 Lecture Notes for EQM and S&I could be useful.

**Indicative syllabus** (time may not permit all of the topics to be covered)

1. **The thermodynamics of planar, line and point defects:**

   We shall study a rigorous thermodynamic treatment of surface energy, surface tension, segregation and other properties that play no part in the usual thermodynamics of bulk materials, with particular emphasis on how they can be calculated with atomistic models. The extension to line defects (dislocations) and point defects (e.g. vacancies) will be studied.


2. **CALPHAD: CAleulation of PHase Diagrams:**

   It is a major concern in the design of new materials and their production and characterisation to understand the occurrence and stability of all kinds of solid phases that might be formed. In the past this process has been very empirical, but increasingly electronic structure calculations (Density Functional Theory – DFT) are providing data that is inaccessible to experimentalists. This topic is about the principles of modern phase diagram calculation. A particularly general problem we shall address is how to calculate the free energy up to the melting point of a simple element or compound, which includes contributions from vibrations, electronic excitations and point defects.

Transformations of Materials (TM2)
Dr Chris Gourlay

8 hours of classes in Term 2

This course builds an understanding of phase transformations as the origin of microstructure in materials.

Prerequisites:
- Transformations of Materials Part 1
- Equilibrium in Materials Part 1

Continuous assessment:
- Presentation
- Problem sheets

Examination:
- Viva voce examination

Indicative syllabus (time may not permit all of the topics to be covered)

The aim of this course will be to study the underlying theoretical concepts associated with the following topics in order to connect them with practical computational methods for simulating transformations in materials.

1. Nucleation
   a. Classical nucleation theory (homogeneous and heterogeneous)
   b. Stochastic and deterministic nucleation
   c. Grain refinement (nucleant potency and the role of solute)
   Key questions include: Can we control grain size in a phase transformation? What makes a potent nucleant? Does easy nucleation mean many nucleation events? What is the link between nucleation undercooling and grain size? How does nucleation in a liquid compare with nucleation in a solid? How could you model nucleation?

2. Eutectic and eutectoid transformations
   a. Jackson-Hunt theory of regular eutectic growth (diffusion versus curvature)
   b. Growth at the extremum and spacing adjustment mechanisms
   c. Influence of faceting on eutectic growth
   Key questions include: Why are eutectic spacings usually about 1-10μm? Why is there no general theory for eutectic growth in real engineering alloys? Why is a theory of eutectoid growth a challenge?

3. Martensitic transformations
   a. Diffusionless transformations
   b. Martensitic transformation in carbon steel
   c. Shape memory effect
   Key questions include: What determines whether atomic motion is ‘civilian’ and ‘military’? What are the conditions required for a Martensitic transformation? Why is the crystallography of Martensite transformations important?
Electronic Structure of Materials (ESM2)
Dr Arash Mostofi

8 hours of classes in Term 2

Prerequisites:
- Electronic Structure of Materials Part 1

Continuous assessment:
- 1 set of hands-on practical computational exercises associated with modules 1-2
- 1 set of hands-on practical computational exercises associated with module 3
- 1 written essay associated with module 4

Examination: Viva voce examination

Synopsis
This course builds upon the material covered in the core course ESM1. The overall aim is for students at the end of this course to be confident about the background theory and practical application of modern electronic structure methods for calculating the ground and excited state properties of materials.

The course is structured in four modules. The reading for each module is meant to act as a springboard for further self-study.

1. Energy bands in solids [1 session] Crystal lattices; Bloch’s theorem; crystal momentum; Brillouin zone; bandstructure; calculations with energy bands.
   Reading: Foulkes, lecture 10

2. Density-functional theory [2 sessions]
   a. Theoretical concepts: Schrodinger equation; Born-Oppenheimer approximation; Hellmann-Feynman theorem; variational principle; Hohenberg-Kohn theorems; Thomas-Fermi theory; The Levy approach; Kohn-Sham mapping; exchange and correlation functionals; properties of exact DFT; Janak’s theorem; the derivative discontinuity and band-gap problem.
   Reading: Martin, chapters 6 & 7 (excluding 6.4, 7.6 & 7.7)
   b. Practical calculations: Finding the ground state; self-consistency; pseudopotentials; transferability; Brillouin zone integration; basis sets, with a focus on plane-waves.
   Reading: Martin, chapters 12 & 13 (in particular 12.1, 12.2, 12.3, 12.7, 13.1)

3. Wannier functions [2 sessions]
   a. Theoretical concepts: Wannier function for a single band and the concept of gauge freedom; Wannier functions for composite bands; criteria for choosing the gauge (including maximal-localization); exponential localization of Wannier functions in insulators; the case of entangled bands.
   Reading: Marzari, sections II and III
   b. Applications: analysis of chemical bonding; bandstructure interpolation and band derivatives; model Hamiltonians.
   Reading: Marzari, sections IV, VI, VII

4. Electronic excitations [3 sessions]
   a. Motivation from experiments involving electronic excitations.
   Reading: Onida, chapter 1
   b. Time-dependent DFT.
   Reading: Zuehlsdorff, sections 4.1 & 4.2
   c. Many-body perturbation theory, the GW method and the Bethe-Salpeter equation.
   Reading: Zuehlsdorff, sections 4.3 & 4.4
Key to references

- **Foulkes**: WMC Foulkes, Electronic Structure of Materials lecture notes (2013-14)
- **Martin**: RM Martin, Electronic Structure: basic theory and practical methods

Optional light reading for the interested

- R Jones, Psi-k Highlight 124 (2014)
- S Redner, Physics Today (2005)

More advanced texts on DFT for the interested

- Dreizler & Gross, Density Functional Theory: An Approach to the Quantum Many-Body Problem
- Fiolhais, Nogueira & Marques (Eds), A Primer in Density Functional Theory
Classical Field Theory of Materials (CFTM2)
Dr Daniel Balint

8 hours of classes in Term 2

Prerequisites:
- Mathematics for the Theory of Materials Parts 1 & 2
- Classical Field Theory of Materials Part 1

Continuous assessment:
There will be three marked assignments covering the first three units of course material, as defined below, requiring the solution (and reporting of associated background and explanation) of one problem for each unit; the fourth unit, as defined below, is an available topic for the viva (in addition to the other three) but will not be assessed via a marked assignment. Feedback will be provided during the working of the solutions and preparation of the reports, and after the reports are marked.

Examination:
- Viva voce examination

Synopsis

1. Complex variable analysis of plane isotropic linear elasticity: stress functions; derivation of the biharmonic equation; conversion of the biharmonic equation into complex space for plane strain and plane stress; derivation of the equations for the stresses, displacements and force in terms of complex potentials; solution of a point (line) load and edge dislocation in an infinite elastic space.

2. The method of analytic continuation applied to complex variable analysis of plane isotropic linear elasticity; analytic continuation of a function from one domain to another; entire functions; derivation of useful identities for complex functions on boundaries between adjacent domains of analyticity; solution of a line load and dislocation in a half space; conformal mappings.

3. The distributed dislocation technique for modelling cracks; the analogy between dislocations and cracks under mode I, II and II loading; boundary conditions in terms of Burgers vector density; formulation of the integral equations; singularities and special polynomial expansions; numerical solutions techniques.

4. Plane discrete dislocation plasticity; the linear superposition principle; plane strain slip systems and slip system definition; Frank-Read and homogeneous nucleations; annihilations, pinning events; grain boundary descriptions; computational setup; capabilities and limitations; numerical issues, including time discretisation issues such as collisions, overtaking events and special cases, and resolution of the reduced boundary conditions.

Books


Papers


Computational methods
*Matlab Primer [Computational Methods Hub]*
Dr Prasun Ray

**One 4-hour computational lab in week 1 of Term 1**

This course provides a quick, (hopefully) painless introduction to matlab for CDT students. It does not assume any prior matlab experience and should also be helpful to students who have used matlab in the past but would like a quick refresher. The course introduces students to the ‘basics’: using matlab for elementary linear algebra, programming, and data visualisation. This primer is intended to give students a head-start on their cohort challenge project in week 1 of Term 1.

**Getting started**
Students will need their CDT laptop with Matlab installed.

***

*Introduction to Linux*
Dr Éamonn Murray

**2 hands-on classes and 1 classwork session in Term 1**

This course is intended to bring students up to speed with working in a Linux environment and introducing them to common Linux tools, shell scripting and software version control. No previous experience is assumed.

**Synopsis**
1. Introduction to using the terminal. Useful commands and tools. Shell scripting.

***

*Introduction to C++*
Dr Éamonn Murray

**6 hours of hands-on classes and 3 classwork sessions in Term 1**

This course is intended to introduce students to programming in C++. Attendance of the Introduction to Linux course is prerequisite. No other previous experience is assumed. Each class consists of a set of annotated examples and exercises and provides time for questions and exploring related topics.

**Synopsis**
4. Pointers. Static and dynamic arrays.

***

*The three introductory courses above do not form part of the overall formal assessment of the MSc degree.*
Numerical Methods
Dr Pat Scott

27 hours of classes in Terms 1 and 2

Contact details:
p.scott@imperial.ac.uk
Blackett 1008
Tel. 4-5968

Description:
This course gives students a solid practical background in numerical methods required for doing
everyday research in condensed matter, materials, astrophysics, high energy (particle) physics,
and many other areas of physics. The course focuses on understanding how to implement and
effectively use the methods. The assignments involve developing a personal library of numerical
routines that students can (and should) use in their future research.

Course Outline:
Core Topics: IEEE variable types and arithmetic, interpolation, root-finding, random numbers,
umerical integration, solving differential equations, search/optimisation methods.
Advanced Topics (actual mixture depends on student interest): Splines under tension, genetic
algorithms, nested sampling, differential evolution, random forests, relaxation methods for solving
ODE boundary value problems, fast Fourier transforms (FFTs), fast wavelet transform methods,
neural networks, support vector machines, k-means and anti-k-means clustering, hierarchical
clustering, binary space partitioning, methods for creating and solving directed acyclic graphs.
Others by discussion.

Textbook:
Cambridge University Press

Languages:
A mixture of C, C++, Fortran and Python for instruction (basically pseudocode). Assignments
should use C/C++. All code must be well documented – explain what effectively every line of your
code is doing, even if it is written in very basic standard C/C++, and include a makefile so that it
can be easily compiled.

Assessment:
Continuous (no exam).
Core topics (75%): Weekly assignments addressing the contents of the lecture on the day they are
set, and due the afternoon before the next lecture. All codes (including implementations and calling
sequences, unless they are ridiculously obvious) used in the assignments should be submitted
electronically.
Advanced Topics (25%): Working in pairs, students will be asked to choose and present one of the
advanced topics to the rest of the class in 45 minutes, allowing an additional 15 minutes for
questions and discussion. Talks should outline the problem that the algorithm solves, how it
works, and give some basic examples of it in action. Assessment will be based on:
- the presentation (7%; group grade)
- a minimal working C/C++ example of the main algorithm presented (7%; group grade)
- a short academic review of the topic, including an explanation and demonstration of the
code written; roughly 10 single-spaced A4 pages long (7%; group grade)
- participation in discussions around other groups’ talks (4%; individual grade)

Schedule:
9 hours of lectures, 10 hours of tutorials, up to 8 hours of student presentations on advanced
topics.
Weekly 1-hour lectures and 1-hour tutorial / assignment help sessions in Term 1 and Term 2, covering core topics:

1. Intro, IEEE variable types and arithmetic
2. Interpolation (mostly cubic splines) Random Numbers
3. Root finding (Brent's Method, Newton-Raphson)
4. Numerical Integration I (Trapezoidal Rule, Simpson's Method)
5. Numerical Integration II (Runge-Kutta, MC integration)
6. ODEs I (Runge-Kutta)
7. ODEs II (Shooting Method for Two-Point BVPs)
8. Search/Optimisation Methods (mostly MCMCs)

Student presentations on advanced topics in up to four 2-hour sessions during Term 2 (indicative dates: Feb/Mar 2017).

**Plagiarism, etc**
For this course, you are welcome to collaborate and compare results – in fact you are encouraged to do this to cross-check your codes and identify bugs – but every student must write and comment their own code, and write up their own assignments. Where you do use some code you've gotten from elsewhere, reference it clearly in your comments. Remember though, if you don't write your own code where you're asked to, you won't really get anything out of this course.
Group project
Group Research Strategy Project (GRSP)
Dr Arash Mostofi

80 hours of contact time, collaborative work and private study in Term 2

When confronted with a complex challenge, the ability to logically analyse and break it down into manageable parts is one of the most important skills, whatever your chosen profession.

In the specific context of scientific and technological challenges, this means: (i) researching and understanding the background to the problem and the wider context in which it sits; (ii) deconstructing the problem into a hierarchy of hypotheses and questions that are each more easily amenable to scientific investigation than the broader challenge itself; (iii) designing a programme of research to test these hypotheses and questions; (iv) articulating the strategy in a scientifically sound and coherent manner and, importantly, (v) doing so a persuasive manner so that the importance and impact of the work is clear to a potential funder.

Having a good all-round knowledge of materials is an advantage, but the ability to get to the heart of a complex problem and develop a strategy to solve it is the essence of a successful research scientist. The objective of the Group Research Strategy Project (GRSP) is to enable students to experience this process, from being presented with a materials-related challenge, all the way through to writing a research proposal on how to tackle it using theory and simulation. Students will work together in groups, thereby providing direct experience of collaboration and teamwork, which are essential in modern scientific research. Note that the GRSP does not require students to solve the problem presented itself, but to develop the research strategy for doing so.

The specific problem will be suggested by one or more industrial partners of the CDT. Each group will liaise with the industrial partner to understand the problem in detail. Each group will then work towards developing a research proposal, in the style of an EPSRC Standard Grant application.

Proposals will be evaluated according to the same criteria as EPSRC Standard Grants, namely: the clarity and excellence of the proposed research and appropriateness of the methodology proposed; the importance and impact of the work; and the appropriateness of the planning and management of resources requested.

The deadline for research proposals is Friday 24th March 2017 at 4pm. Proposals should be emailed by the deadline as a single PDF document to Arash Mostofi and Miranda Smith.

The course is intended to be student-led and the students will be responsible for most aspects of the course, including setting their own goals, deadlines, and workload distribution. In addition to a weekly meeting with the member(s) of academic staff running the course, flexible office hours will be available. Organising and chairing the meetings will be a responsibility of the students.

There will be a meeting to discuss the course towards the end of Term 1.

Assessment

Written proposal (40%)
Each group’s proposal will be reviewed by at least two reviewers and according to EPSRC’s review criteria and slightly modified for the purposes of GRSP.

Panel interview (20%)
Each group will receive their anonymous reviewer reports a few days in advance of their panel interview, which will be held in Term 3 at a date to be determined. At the panel interview, each group will have the opportunity to give a 10 minute presentation about their proposal (A/V facilities will be available if required), which will be followed by up to 30 minutes of questions and discussion. In addition to exploring aspects of the proposal in more detail, the interview provides the research team the opportunity to respond to comments in the reviewer reports.
Student peer-to-peer allocation (40%)
A proportion of the marks for this option is left for the members of the group to distribute among themselves, providing an opportunity for further practical experience of the interpersonal skills involved in collaborative work (e.g., negotiation, communication and etiquette). Students may allocate marks to individual members of the research team according to the level and impact of individual contributions. The total number of marks available in this category is determined by the average obtained in the written proposal and panel interview. When deciding the distribution of marks, students are encouraged to think about how each member of the team has:
1. Contributed to the thinking in the proposal;
2. Contributed to the writing of the proposal;
3. Helped and supported other members of the team throughout the project;
4. Contributed to the planning and preparation for the interview.

EPSRC standard proposal structure

Standard EPSRC proposals have the following general structure, to which your proposal must adhere. Proposals must be on A4 paper, in Arial font (minimum size 11pt), with margins no less than 2 cm on all sides. The page limits specified below must be strictly adhered to.

- Case for Support (up to 6 pages), covering (not necessarily in this order):
  - Background
  - National Importance
  - Academic Impact
  - Research Objectives
  - Programme and Methodology
  - Timeliness
  - Risk
  - Resources and Management
- Justification of Resources (up to 2 pages)
- Workplan (up to 1 page)
- Pathways to Impact (up to 2 pages), including (not necessarily in this order):
  - Society: quality of life, policy, international development, health
  - Knowledge: scientific advances, techniques
  - People: skills
  - Economy: wealth creation, new products, new companies, inward investment

Note that the 2-page section on “Track Record” of the applicants, present in the standard EPSRC proposal structure, is not required for the purposes of GRSP, nor are CVs of named collaborators or Letters of Support.

Further resources that will be helpful when writing your proposal:
- EPSRC guidance on preparing a proposal (including advice on National Importance and Impact):
  - http://www.epsrc.ac.uk/funding/howtoapply/preparing/
  - http://www.epsrc.ac.uk/funding/howtoapply/preparing/includingnationalimportance/
  - http://www.epsrc.ac.uk/funding/howtoapply/preparing/economicimpact/
- EPSRC guidance on Pathways to Impact
  - http://www.epsrc.ac.uk/innovation/publicengagement/pathwaystoimpact/
- EPSRC (challenge) themes:
  - http://www.epsrc.ac.uk/research/ourportfolio/themes/
- The EPSRC portfolio:
  - http://www.epsrc.ac.uk/research/ourportfolio/
  - https://www.epsrc.ac.uk/funding/howtoapply/preparing/writing/
GRSP Assessment criteria

Your proposal and interview will be assessed according to EPSRC’s Standard Grant Review Criteria, modified accordingly for GRSP:

1. Quality
   a. Novelty, context, timeliness
   b. Ambition, transformative aspects
   c. Methodology

2. Importance
   a. National importance on 10-50 year timeframe in relation to other research in the area
   b. How research contributes to: other research areas; societal challenges and EPSRC challenge themes; UK economy; emerging industry

3. Impact
   a. How complete and realistic are the impacts identified?
   b. Effectiveness of activities identified to realise impacts
   c. Relevance of beneficiaries and collaborators

4. Resources and Management
   a. Appropriateness of resources requested
   b. Viability of management plans (eg, access to equipment, third-party contributions)
Appendix 2   Guidelines for the Conduct and Assessment of Research Projects

Introduction

The research project is the single most important (in terms of its contribution to your final mark), and probably the most enjoyable, component of your MSc degree. Including the literature review, it counts for 40% of your overall MSc. The assessment of the literature review accounts for 25% of these marks, the research project report forms 60% of the marks available, and the assessment of the research project presentation the remaining 15%.

The Literature Review

Starting after the conclusion of the oral examinations at the end of Term 2, you will work on a literature review of the topic of your research project. Your supervisor will give you some suggested reading to get you started and a title for your review to give it a focus. A good literature review not only summarises what has been written about a particular topic (with comprehensive references), but compares and contrasts differing results, analyses and theories, providing a critical commentary on recent work in the field. Your literature review will take the form of a written report, not exceeding 3,000 words in length (including captions to figures and tables, but excluding any cover page, table of contents, acknowledgements, references and appendices). It will be assessed both on scientific quality and its presentation and readability. The deadline for this is 5pm on Friday 12 May 2017. The literature review will be assessed by your supervisor, who will provide feedback that should help you with your main research project report. A declaration of the word count must be included on the first or cover page of the literature review.

The Research Project Plan

The research element of your project starts after you submit your literature review. By the end of the first month of your project, you should write a short (one side A4 maximum) plan that gives:

1. a concise summary of the motivation for your project and its multiscale aspects;
2. a short project plan, stating clearly each aim and objective, and how and when you expect to achieve each one.

You should then arrange to meet with your supervisors before Friday 16 June 2017 to discuss your plan. The plan is not assessed, but it is important that it is used as an opportunity to be candid and honest so that potential problems may be identified. The template for the research plan may be found at the end of this document.

The Research Project Presentation

The project presentations will take place on Friday 1 September 2017, as part of the MSc Conference. You will be required to give a 10-minute presentation, followed by 5 minutes of questions and discussion. Your performance will be assessed by a panel of academic staff. Assessment of the project presentation will include how well you present your work in an engaging, clear and informative way and handle the discussion and questions after your presentation. The assessment form is included for information at the end of this document.

The Research Project Report

The report must be typeset using, e.g., Microsoft Word or LaTeX, and must not exceed 5,000 words in length (including captions to figures and tables, but excluding the cover page, table of contents, acknowledgements, references and appendices). It will be assessed both on scientific quality and its presentation and readability. You must submit an electronic version of your report in PDF format to the CDT Senior Administrator by 5pm on Friday 8 September 2017.
Report Structure

Try to be concise, yet complete, and to adhere in broad terms to the following structure, making allowances for the nature of your particular project:

Cover page. Include a title that clearly identifies what the report is about, the name of the author, the date of submission, and a formal statement as follows:

“A thesis submitted in partial fulfilment of the requirements for the degree of Master of Science of Imperial College London.”

A declaration of the word count must also be included.

An abstract that clearly and concisely identifies the principal features of the work, its multiscale nature, and the key results achieved (including numerical results where appropriate) and the conclusions that can be drawn, if any.

Content page(s), listing the chapters, sections, and subsections.

A formal acknowledgement section referring to the people you wish to thank. You should also clearly identify where in your project work you have received practical help and technical support from others. For example use of a pre-existing computer code, or work conducted as part of a team, etc.

An introductory chapter in which the broad aims and objectives of the project are established, the multiscale nature of the project is set out, and in which the work is clearly put into context with respect to existing work and previous literature.

Discussion of the methods employed. The methods may be computational and/or theoretical as appropriate to the project.

A clear description and presentation of the results/observations obtained. Think carefully about how to convey the results with clarity and in the most informative way. Data plots etc., which should always be referred to as figures, must have clearly labelled axes and scales and an extensive figure caption that states what is plotted and draws attention to the key points.

A critical discussion of the results, limitations and errors, and the conclusions that may be drawn from the results.

In your conclusions you should discuss the extent to which the aims of the project have been achieved and what further work would be appropriate. You should also identify clearly what your part in the work has been and acknowledge the work of others.

You must provide a clear and extensive set of references (bibliography) to which you have referred in the text. These should be in any one of the standard formats as used in scientific journals.

Lengthy mathematical derivations, computational algorithms and programs, and large quantities of data that you wish to place on record should be included as appendices and do not count towards the word limit.

It is most important that an experienced scientist should be able to read through the report and immediately be able to follow in detail what was done, to put the work into context and, in principle, be able to reproduce the project. If the project is computational, for example, exactly how the computation was approached should be described.
It must be stressed that reports must be complete and concise, and waffle must be avoided and all points made should be substantiated.

It is important to realise that most projects are never finished and the report should reflect what has been done within the limited time available. It is advisable, therefore, to plan well so as to have achieved something by the time it comes to write up. In some cases it may seem that little has been achieved; this is no reason, however, for not producing an excellent report.

**Assessment of the Report**

The project report will be marked by two independent assessors, who will be informed by a report from your supervisor, and your final mark will be an aggregate of the two. In the event that the two markers disagree by a significant margin, they will confer to arrive at a consensus mark. It may also be read and moderated by one or more members of the Board of Examiners. The assessment guidelines and assessment forms are included at the end of this document.

**A Note on Plagiarism**

Plagiarism is illegal. The penalties are severe and may include expulsion from the College. Therefore, never use the words or ideas of others from any source, e.g. published papers, the web or other student reports, without a proper attribution. For further information, see the following websites:


The electronic submission of your report may be run through software to check for plagiarism.

Please ensure that in each section of your report you state explicitly what is your own original work, what your supervisors contributed and what material is based on the literature.

**Working in an interdisciplinary research environment**

You will have more than one supervisor, but your principal supervisor will have overall responsibility for your project. You should have regular meetings with all your supervisors and you should discuss what you are doing and seek their feedback and guidance. It is quite possible that you will have to meet them separately because they are busy people. It is also quite possible that you may get conflicting advice! Don’t be worried about such conflicts – they are not uncommon in an interdisciplinary environment, and indeed they can contribute to creativity and new ways of thinking. Be open with your supervisors about any conflicts that you detect in their advice, and try to resolve them with your supervisors. If you feel you need help talk to your Cohort Mentor. If the Cohort Mentor is unavailable contact the MSc Director or the Director of the CDT. These people will help you if you ask, but don’t leave things too long before asking them.

- Don’t be afraid to tell your supervisors that you don’t know something or that you are stuck. They are there to help guide the project and need to know how things are progressing in a clear and honest manner.

- If you don’t understand something, just keep asking questions until you do. The smartest people often ask the “dumbest” questions.

- Find out where and when the research groups of your supervisors have coffee, lunch, Friday evening drinks etc. and go along as often as possible. This is where lots of problems get solved through informal discussions and the occasional back-of-the-envelope calculation.
• Keep a complete and detailed “lab book” and bring it to every meeting you attend. Your lab book will be invaluable when you write up your final report.

• Some research groups have regular progress and planning meetings. If you are asked to attend, be on time and be prepared to explain what you have done, what you plan to do next, and justify any resources you need for the next stage of your project. Take up-to-date results and your lab book with you.

• Keep backups of all your results. Keep multiple backups! Hard disk space and USB memory are both cheap, so make sure that you cannot lose your data accidentally.

• As you are writing your report keep multiple backups. If your computer crashes you will not be given an extension of the deadline for submission of your report.

• If your project needs something to progress (equipment, software, computer time etc.) prepare a realistic plan and/or budget and present this to your principal supervisor.
Research Project Plan

Student:
Project Title:
Supervisors:

Project Outline and Plan.
Please state the objectives of your project and when and how you expect them to be achieved.

Student’s signature:  Date:

Page 1/2
Student:

Comments: Please give written feedback on the student’s project plan.

Principal Supervisor’s signature:  Date:

PLEASE COMPLETE AND RETURN TO CDT ADMINISTRATION OFFICE

Page 2/2
The marking scheme uses the criteria below. It might very well be that different aspects of the report fall into different marking bands. For example, the student may give a very good account of the background material and relevant literature, but the report shows little understanding, or vice versa. In such cases, please use your discretion to assign the mark.

90 – 100 % Exceptional high quality work that clearly demonstrates a substantial independent contribution and originality at research level in addition to a thorough understanding of the topic. Comprehensive and authoritative discussion of background material and relevant literature is included. The work is of a quality that with little effort is publishable on its own or as part of an article in a peer-reviewed journal.

80 – 90 % Very high quality work that clearly demonstrates independent contributions and originality at research level in addition to an authoritative account of the work undertaken with almost no gaps in the understanding of the topic. A comprehensive discussion of background material and discussion of relevant literature is included. The work is of a quality that, with some effort, is publishable as part of an article in a peer-reviewed journal.

70 – 80 % Very good work demonstrating an authoritative account with relevant material throughout and with independent contributions by the student. There are only minor gaps in the understanding of the project work. A very good discussion of background material and relevant literature is included. Some of the work is of a quality that it could contribute to aspects of a publishable article in a peer-reviewed journal.

60 – 70 % Good work with relevant material and authoritative in most places, including some independent contributions by the student. Only a few gaps and few deficiencies in the discussion and understanding in minor parts of the report. A good discussion of background material and relevant literature is included.

50 – 60 % Satisfactory with relevant material in most places and possibly authoritative in some places. Some gaps and some deficiencies in the discussion and understanding in some parts of the report. Some background material and discussion of relevant literature is included.

40 – 50 % Adequate with relevant material in some places. Large gaps and large deficiencies in the discussion and understanding in various parts of the project. Adequate discussion of background material and relevant literature is included.

30 – 40 % Unsatisfactory but with some relevant material in some places. Of some merit but considerable gaps and considerable deficiencies in the discussion and understanding in major parts of the project. Little discussion of background material and/or relevant literature is included.

15 – 30 % Very unsatisfactory with only small amount of relevant material. Of little merit with substantial gaps and substantial deficiencies in the discussion and understanding in major parts of the project. Almost no discussion of background material or relevant literature is included.

0 – 15 % Highly unsatisfactory with almost no relevant material anywhere. Of no or very little merit. No discussion of background material or relevant literature is included.
Assessment of the literature review by the principal supervisor

Student:

1. Coverage of the Review
Mark out of 25 the extent to which the student has identified the literature relevant to the title of the review and selected pertinent issues to focus on in the review.

   0   1   2   3   4   5   6   7   8   9   10   11   12   13   14   15   16   17   18   19   20   21   22   23   24   25

2. Understanding of the Subject
Mark out of 25 for the degree of understanding shown of the literature reviewed, both of the theoretical concepts and simulation methods described.

   0   1   2   3   4   5   6   7   8   9   10   11   12   13   14   15   16   17   18   19   20   21   22   23   24   25

3. Critical Thinking
Mark out of 25 the degree of critical thinking demonstrated by the student, including the identification of conflicting points of view, weighing of the evidence on each side, judgment shown and the identification of future work required.

   0   1   2   3   4   5   6   7   8   9   10   11   12   13   14   15   16   17   18   19   20   21   22   23   24   25

4. Presentation of the Review
Mark out of 25 for the logical structure and presentation of the work, the extent to which the English is grammatical and accurate, and the quality of any figures and graphs. Consider also the overall usefulness of the review as a scientific document.

   0   1   2   3   4   5   6   7   8   9   10   11   12   13   14   15   16   17   18   19   20   21   22   23   24   25

TOTAL MARK:   out of 100.
Comments. Please give written feedback to justify the marks awarded. These written comments (which need not be typed) will be passed on to the student. Please highlight the aspects that the student did well and provide constructive criticism and advice on how to improve.

Name of principal supervisor:

Signature:                                      Date:

PLEASE COMPLETE AND RETURN TO CDT ADMINISTRATION OFFICE
Report on the research project by the principal supervisor

Student:

External factors:
Please comment on the circumstances and environment that the student experienced during the research project. This should include a description of the extent of help received from other members of your research group or the provision of simulation software to use. Please also mention any circumstances outside the student’s control that may have adversely affected their execution of the project e.g. unavailability of resources, staff absence or a bug in a code supplied to the student.

Student performance:
Please comment on the student’s performance in executing the research project, including the extent of their achievements and the level of skill in carrying out the project. This might include skills in computing, theory, novelty in bridging length or time scales, etc. – whatever is appropriate for the individual project.

Principal Supervisor’s signature:  Date:
Assessment of the research project report by an independent assessor

Student:

1. Scientific Background
Basing your judgement on the content of the report alone give a mark out of 25 for the understanding shown of the scientific background of the project, the multiscale aspects related to the project, and the motivation for the project.

2. Understanding Demonstrated by the Report
Mark out of 25 for the level of understanding demonstrated by the student in the report, including the presentation of the results and their analysis, the justification of the conclusions reached, and the identification of further work.

3. Student Achievement and Use of Skills
Basing your judgement on the contents of the student’s and supervisor’s reports give a mark out of 25 for the level of achievement and skill shown by the student. This might include skills in computing, theory, novelty in bridging length or time scales, etc. – whatever is appropriate for the individual project.

4. Presentation of the Report
Mark out of 25 for the logical structure and presentation of the work, the extent to which the English is grammatical and accurate, and the quality of the figures and graphs. Consider also the overall usefulness of the report as a scientific document.

TOTAL MARK: ________ out of 100.
Comments. Please give written feedback to justify the marks awarded. These written comments (which need not be typed) will be passed on to the student. Please highlight the aspects that the student did well and provide constructive criticism and advice on how to improve.

Name of assessor:

Signature: Date:

PLEASE COMPLETE AND RETURN TO CDT ADMINISTRATION OFFICE
Research Project Presentation Assessment Form

Student:

Did the student:
[a] explain how the work fitted into the context of related work?

0 1 2 3 4 5 6 7 8 9 10

[b] give a clear summary of the work undertaken and of the multiscale aspects of the project?

0 1 2 3 4 5 6 7 8 9 10

[c] present clearly the scientific conclusions that could be drawn?

0 1 2 3 4 5 6 7 8 9 10

[d] give a logically structured and interesting presentation with legible and informative slides?

0 1 2 3 4 5 6 7 8 9 10

[e] express themselves clearly and audibly during the presentation, and field the questions well?

0 1 2 3 4 5 6 7 8 9 10

TOTAL MARK: _______ out of 50.

Comments: Please give written feedback to justify the marks awarded. These written comments (which need not be typed) will be passed on to the student. Please highlight the aspects that the student did well and provide constructive criticism and advice on how to improve.

Assessor's name: __________________________
Signature: __________________________ Date:

PLEASE COMPLETE AND RETURN TO CDT ADMINISTRATION OFFICE