PX911-15 Multiscale Modelling Methods & Applications I

23/24

Department
Physics
Level
Taught Postgraduate Level
Module leader
Nicholas Hine
Credit value
15
Assessment
60% coursework, 40% exam
Study location
University of Warwick main campus, Coventry

Description

Introductory description

an introduction to atomistic modelling techniques including DFT, classical force field methods and an appreciation of how they interact with other modelling frameworks. Students will learn how to design atomistic simulations of condensed matter or molecular systems, and how to identify simulation methodologies appropriate to bridging multiple length scales, balancing accuracy vs. cost. They will gain exposure to software packages supporting interoperability between methods, e.g. the Atomic Simulation Environment. Multiscale Modelling case studies by guest lecturers will show how problems involving heterogeneous systems are tackled at multiple length & time scales.

Module web page

Module aims

To provide students with understanding and experience of atomistic modelling techniques and an appreciation of how they interact with other modelling frameworks. This will be conveyed through lectures, tutorial workshops, case studies and web pages.

Outline syllabus

This is an indicative module outline only to give an indication of the sort of topics that may be

covered. Actual sessions held may differ.

The following syllabus is a superset of what can be covered in this module. Ideally all or most topics should be briefly touched upon, with more in-depth focus on specific parts of the syllabus as chosen by the lecturer.

1. The hierarchy of accuracy vs lengthscale for atomistic modelling techniques; links between lengthscales; advantages and disadvantages of techniques.
2. Quantum Mechanics:
   a. Aspects of single-electron quantum mechanics relevant to atomistic modelling, specifically the limits of a plane wave and an atomic orbital, and the many-body Schrodinger equation as applied to condensed matter systems;
   b. The Hohenberg-Kohn and Kohn-Sham formulations of density functional theory, and their implications for accuracy and predictive power.
   c. Methodological choices for implementing DFT: plane wave and local orbital basis sets (strengths/weaknesses of each); density functionals (hierarchy of accuracy at increasing cost); pseudopotentials/PAW. Calculation of forces via the Hellmann-Feynman Theorem.
   d. Scaling of computational effort in DFT. Linear-Scaling DFT Methods
   e. Theoretical spectroscopy: excited state dynamics via TDDFT; vibrational frequencies; Nuclear Magnetic Resonance.
3. Classical force fields and molecular mechanics
   a. Construction of force fields via parameter tuning, force-matching
   b. Essential statistical mechanics, molecular dynamics in NVT and NVE ensembles, Verlet method, MD as a sampling scheme; illustrative applications.
   c. Ab initio-based thermodynamics: free energy, reaction coordinates, potential of mean force, basic Monte-Carlo type algorithms.
4. Case studies of Multiscale Modelling: half-hour or hour-long lectures on specific cases, often by guest lecturers which will vary from year to year, examples could include:
   a. Theoretical Spectroscopy parameterisation of Hamiltonians for exciton dynamics in light-harvesting pigment-protein complexes
   b. DFT parameterisation of tight-binding models to study Anderson localisation in disordered semiconductors
   c. Machine learning for interatomic potentials
   d. QM/MM multi-scale methods
   e. Reformulation of all-atom calculations in terms of coarse-grained beads
   f. Accelerated dynamics, MTD, ABF, and related methods, advanced sampling techniques
   g. Transition state theory, MEP and MAP methods, transition path sampling

Learning outcomes

By the end of the module, students should be able to:

- Understand the context of quantum chemistry methods, density functional theory, and atomistic force-field-based modelling, and their use in a multiscale modelling context and an overview of how & why uncertainty and error can propagate between lengthscales.
- Be familiar with the common approximations and methodological choices required to implement DFT, and appreciate the widespread applications of DFT.
- Understanding of the ideas underlying classical force-fields and their applications.

- Exposure to case studies of multiscale modelling based upon atomistic calculations.
- Ability to apply the above methods in practice.
- Exposure to software environments to aid interoperability between methods (eg the Atomic Simulation Environment in Python).
- The ability to design an atomistic simulation to extract a particular property of a condensed matter or molecular system.
- The ability to identify simulation methodologies appropriate to bridging multiple lengthscales, balancing accuracy vs cost.

Indicative reading list

R. M. Martin, Electronic Structure
D. R. Bowler and V. Brázdová, Atomistic Computer Simulations: A Practical Guide
G.H. Grant & W. G. Richards, Computational Chemistry.
A. R. Leach, Molecular Modelling, Principles and Applications.
D. Frenkel and B. Smit, Understanding Molecular Simulation.

Subject specific skills

Understand the context of quantum chemistry methods, density functional theory, and atomistic force-field-based modelling, and their use in a multiscale modelling context and an overview of how & why uncertainty and error can propagate between lengthscales
Be familiar with the common approximations and methodological choices required to implement DFT, and appreciate the widespread applications of DFT
Understanding of the ideas underlying classical force-fields and their applications
Exposure to case studies of multiscale modelling based upon atomistic calculations

Transferable skills

Exposure to software environments to aid interoperability between methods (eg the Atomic Simulation Environment in Python)
The ability to design a simulation to extract a particular property of a condensed matter or molecular system.
The ability to identify appropriate simulation methodologies, balancing accuracy vs cost.

Study

Study time

Type	Required
Lectures	10 sessions of 2 hours 30 minutes (100%)
Practical classes	(0%)
Total	25 hours

Type	Required
Supervised practical classes	(0%)
Total	25 hours

Private study description

Further reading and quantum mechanics background revision.

Costs

No further costs have been identified for this module.

Assessment

You must pass all assessment components to pass the module.

Assessment group D

	Weighting	Study time
Computational Workshops	60%	40 hours
Notebooks implementing programming and data analysis exercises based on atomistic simulations.		
Viva Voce Exam	40%	10 hours
On the core material. 30 minutes.		

Feedback on assessment

-\tWritten annotations to submitted computational notebooks\r\n-\tVerbal discussion during viva voce exam\r\n-\tWritten summary of viva performance

Past exam papers for PX911

Availability

Courses

This module is Core for:

- Year 1 of TPXA-F344 Postgraduate Taught Modelling of Heterogeneous Systems
- Year 1 of TPXA-F345 Postgraduate Taught Modelling of Heterogeneous Systems (PGDip)