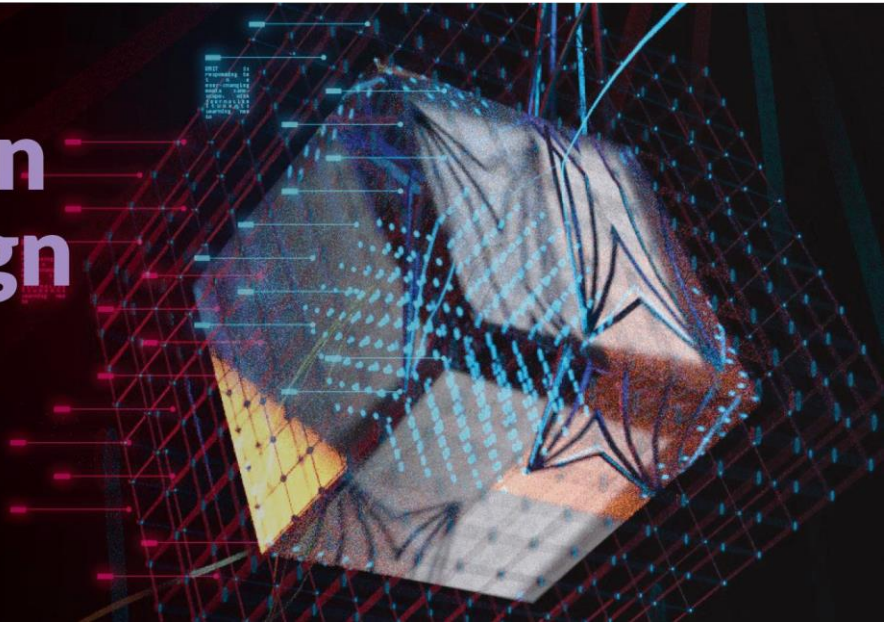
HPC and Data in Materials Design and Discovery

Course Outline



The course curriculum is fashioned from the contributions and insights of prominent professors and scientists, with a view to supporting graduate students and ECRs in Australia who are working in the space between HPC and Data in materials design and discovery.

Contributing Lecturers

Prof Debra Bernhardt (UQ)

Prof Ben Corry (ANU)

Prof Maria Forsyth (Deakin)

Prof Julian Gale (Curtin)

A/Prof Amir Karton (UWA)

Prof Shyue Ping Ong (UCSD)

A/Prof Alister Page (Newcastle)

Prof Katya Pas (Monash)

Prof Sean Smith (ANU)

Prof Tiffany Walsh (Deakin)

Dr Asaph Widmer-Cooper (USyd)

HPC Facility Introduction and Hands-on Tutorials

Dr Sherif Abdulkader Tawfik (Deakin)

Dr Maciej Cytowski (Pawsey)

Dr Jingbo Wang (NCI)

And other supporting team members

Target Audience

Graduate students, ECRs and beyond in fields relating to computational materials science.

Lectures
This course will be taught live online via Zoom Webinar platform and will be available also for subsequent streaming for registered participants. There will be two 60-minute lectures weekly on Wednesday and Friday from 1 to 2 pm (AEST) for 12 weeks starting Wednesday 1/9/2021 and ending Friday 26/11/2021.

Tutorials
If applicable, weekly exercises will be posted online prior to the tutorial hands-on sessions. An Eventbrite registration for each separate tutorial topic will be sent out in advance, in order to plan logistics according to the number of students participating.

Technology
To participate in this course minimally, all you need is a web browser with Eventbrite and Zoom app.

Prerequisites
Knowledge Base: Undergraduate study in physical science or engineering are generally recommended and assumed as prior academic training in order to make most of the lectures.

Computing Skills: To benefit most from the hands-on tutorial training sessions, some familiarity with Linux would be strongly recommended. Admission for tutorials will be more selective than the larger lecture course for reasons of accessibility and teachability.

Resources for basic research computing skills such as Unix and general guide for getting started with HPC can be found on Intersect website, in addition to other resources. Further resource materials are listed at the bottom of this document.

Literature
Some reading recommendations are listed at the last page below.

Learning Support Group
To facilitate general announcements to the cohort, exchanges of ideas, comments, Q&A and so on, all registrants and lecturers will be invited by the course Coordinator to join a Slack group prior to the start of the course.

Semester Break
One week break is scheduled between Week 4 and 5.

Organizing Committee
Prof Debra Bernhardt (UQ)

Prof Julian Gale (Curtin)

Prof Sean Smith (ANU)

Prof Tiffany Walsh (Deakin)

Dr. Asaph Widmer-Cooper (USyd)

Dr. Meiyun Chang-Smith (Intersect Australia), Coordinator

Reading

Michael P Allen and Dominic J Tildesley (2017). *Computer Simulation of Liquids* (2nd Ed), Oxford University Press (ISBN-13: 9780198803195. DOI:10.1093/oso/9780198803195.001.0001)

Daan Frenkel and Berend Smit (2002). *Understanding Molecular Simulation: From Algorithms to Applications* (2nd Edition), Academic Press (ISBN: 978-0-12-267351-1. DOI https://doi.org/10.1016/B978-0-12-267351-1.X5000-7).

Andrew Leach (1996). *Molecular Modelling: Principles and Applications* (2nd Edition), Glaxo Smith Kline Research and Development Ltd, UK.

Resources

Programming (Basic to advanced)

- Thinking like a Computer: The fundamentals of programming (Intersect webinar - recordings are available)
- Programming with Python (software carpentry course materials)
- Learn to Program: Python (Intersect training)
- Data Manipulation & Visualisation in Python (Intersect training)
- Series of Machine Learning Using Python: Linear Regression, Classification, SVM & Unsupervised Learning (Intersect training)

Research Computing

- Linux Command Guide
- Unix Shell and Command Line Basics (Intersect training)
- The Unix Shell (software carpentry course materials)
- From PC to Cloud or High-Performance Computing (Intersect webinar - recordings are available)
- Getting started with HPC using PBS Pro (Intersect training)
- Version Control with Git (software carpentry course materials)

NCI Documentation

- Gadi User Guide
- Gadi Supported Software Application

Pawsey Documentation & Training

- Pawsey Training, including Supercomputer training
- Training to Accelerate your Code

Videos

- Introduction to Gadi (Roger Edberg - NCI)