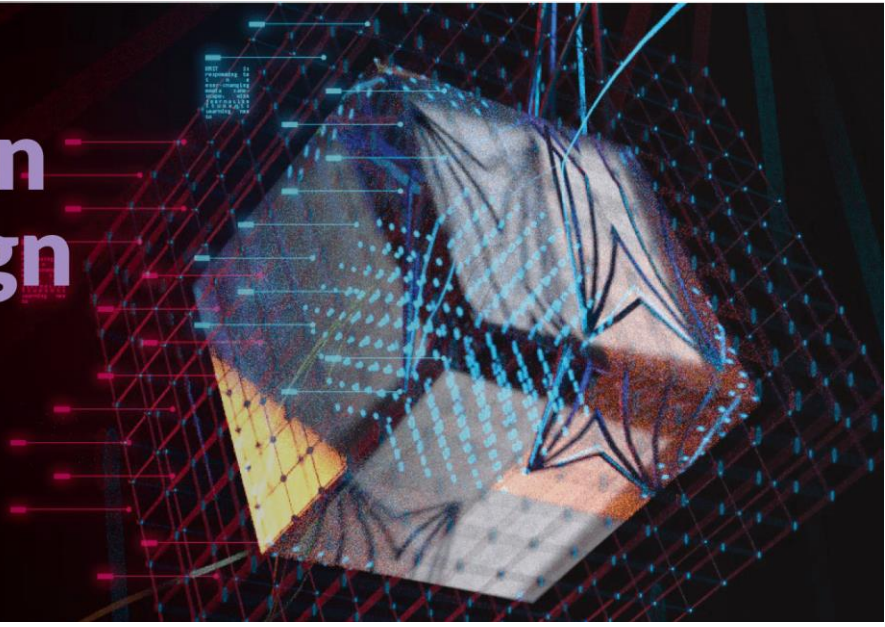
HPC and Data in Materials Design and Discovery

Syllabus



Week	Lecture	Topic	Lecturer
W1	**Introduction**		
1 Sep	Lecture 1	**Overview of HPCD in Materials Design and Discovery** • General introduction • Summary of course outline • Any additional info re the tutorials	Prof Sean Smith (ANU)
3 Sep	Lecture 2	**Overview of Australian HPC & Data Landscape** • Australia's capabilities in HPCD research • How we are positioned in the larger international environment • Tier1 Facility - NCI Gadi • Tier1 Facility - Pawsey Setonix	Overview - Prof Sean Smith (ANU) - 30 min Gadi - Dr Jingbo Wang (NCI) - 15 min Setonix - Dr Maciej Cytowski (Pawsey) - 15 min
W2	**Electronic Structure of Finite Molecular Systems - Basics**		
8 Sep	Lecture 3	**Overview of Methods Used in Electronic Structure Calculations I** • Intro to semiempirical methods • Intro to density functional theory • Intro to ab initio methods • Intro to force fields and QM/MM methods	A/Prof Amir Karton (UWA)

		• Overview of potential energy surfaces • Overview of molecular properties	
10 Sep	Lecture 4	**Overview of Methods Used in Electronic Structure Calculations II** • Intro to theory of Intermolecular interactions • Electronic structure methods for calculating intermolecular interactions • Solvation effects in computational chemistry	Prof Katya Pas (Monash)
W3	**Electronic Structure of Finite Molecular Systems – Tutorials on Gadi**		
15 Sep	Tut 1	• Calculate a potential energy surface for a simple reaction	A/Prof Karton + NCI Training
17 Sep	Tut 2	• Examples of SAPT with Psi4 to extract four fundamental forces in intermolecular complexes • Examples of BSSE calculations with Psi4 & G16 with both MP2 & DFT • Examples of CCSD(T)/CBS with Orca (through DLPNO-CCSD(T)) • Examples of implicit solvation calculations in G16	Prof Pas + NCI Training
W4	**Electronic Structure of Solids – Basics**		
22 Sep	Lecture 5	**Introduction to the Electronic Structure of Solids** • Bloch's theorem • The Brillouin zone • Band structure • Density of states • Integrating across the Brillouin	A/Prof Alister Page (Newcastle)
24 Sep	Lecture 6	**Introduction to Practical Electronic Structure Calculations for Solids** • Choice of basis set • The pseudopotential approximation • Choice of functionals for solids • Car-Parrinello and adiabatic methods	Prof Julian Gale (Curtin)

		• How to choose the most effective code for your problem	
One week break			
W5	**Electronic Structure of Solids – Tutorials on Gadi**		
6 Oct	Tut 3	**Introduction to Electronic Structure Calculations for Solids**	Prof Gale + NCI Training
8 Oct	Tut 4	**Introduction to Electronic Structure Calculations for Solids**	
W6	**Molecular Dynamics Simulations**		
13 Oct	Lecture 7	**Introduction to MD Simulations I** • Equations of motion • Periodic boundary conditions • Thermostatting • Applications: material properties using MD simulations	Prof Debra Bernhardt (UQ)
15 Oct	Lecture 8	**Introduction to MD Simulations II** • Force fields • Advanced sampling techniques • Applications: use of force fields and advanced sampling in MD simulations	Prof Ben Corry (ANU)
W7	**Molecular Dynamics Simulations – Tutorials on Gadi**		
20 Oct	Tut 5	**Introduction to MD Simulations I**	Prof Bernhardt + NCI Training
22 Oct	Tut 6	**Introduction to MD Simulations II**	Prof Corry + NCI Training
W8	**Monte Carlo & Kinetic Monte Carlo Methods**		
27 Oct	Lecture 9	**Monte Carlo Simulations** • MC method (overview & history) • MC simulation of chemical systems (Markov chains, importance sampling, detailed balance)	

		• Sampling at constant NVT (Metropolis algorithm, use of non-physical moves) • Sampling at constant NPT (dealing with additional degrees of freedom) • Sampling at constant uVT (absorption in MOFs, systems with a single interface) • Gibbs ensemble technique (application to phase coexistence) • MC code packages	Dr Asaph Widmer-Cooper (USyd)
29 Oct	Lecture 10	**Kinetic Monte Carlo and Lattice Dynamics** • Introducing time into Monte Carlo simulation - KMC • Using molecular dynamics to obtain rate constants for KMC • Lattice vs molecular dynamics • Optimization methods for location of local minima • Static calculation of reaction barriers • Transition state theory for estimation of rate constants	Prof Julian Gale (Curtin)
W9	**AI / ML for Materials Design & Discovery**		
3 Nov	Lecture 11	**Automating Electronic Structure Calculations and Large Materials Data** • Tools to automate electronic structure calculation • Materials property databases • The Materials Project and its API	Prof Shyue Ping Ong (UC San Diego)
5 Nov	Lecture 12	**Machine Learning for Materials Design at Scale** • Introduction to machine learning (ML) and its role in materials science • Developing ML models • Challenges in ML for materials science	
W10	**AI / ML for Materials Design & Discovery Tutorial on Gadi**		
10 Nov	Tut 7	**AI and Machine Learning for Materials I**	

12 Nov	Tut 8	**AI and Machine Learning for Materials II**	Dr Sherif Abdulkader Tawfik (Deakin) + NCI Staff
W11	**Domain Application: Biomaterials**		
17 Nov	Lecture 13	**Molecular Simulations of Bio-interfaces: Fundamentals and Challenges** • Introduction to bio-interfaces & typical "simulation appropriate" research questions • Importance of interfacial structural models and understanding their limitations • Describing inter-atomic interactions across the interface • Conformational sampling at bio-interfaces • Example applications and pitfalls	Prof Tiffany Walsh (Deakin)
19 Nov	Lecture 14	**Applications and Examples of Molecular Simulations for Biomaterials** • Emphasis on connections between the purpose(s) of the investigation and the simulation techniques applied • Highlights of good practise and hazards to avoid in simulation approaches applied to biomaterials • Examples taken from sensing, health, and biotechnology applications	
W12	**Domain Application: Batteries and Hydrogen**		
24 Nov	Lecture 15	**Understanding and Design of Advanced Battery Electrolytes through Computational Modelling** Batteries and the energy transition • Examples of large-scale deployment and battery chemistry types • Is Lithium ion the best chemistry for stationary storage? • Beyond Lithium ion battery chemistries	Prof Maria Forsyth (Deakin)

		• Computational design of new electrolyte systems with properties prediction • Designing electrolyte compositions, structures, interphases to enhance battery performance	
26 Nov	Lecture 16	**The Key Role of Computational Modelling for Advancing Hydrogen Technologies** • Renewable energy storage: the gigantic challenge • Australian climate change response: economic, political and global trade implications • Why hydrogen? • Key technological challenges and why HPC modelling is critical to advancement • Examples of significant Australian contributions	Prof Sean Smith (ANU)
~ End ~			

