

**Wednesday Nov. 27<sup>th</sup>**

**Summer School**

Instructors

A/Prof. Asaph Widmer-Cooper *University of Sydney*

Prof. David Huang *University of Adelaide*

A/Prof Toby Hudson *University of Sydney*

Schedule

9:00 Seminar on Monte Carlo Simulations and Applications

**Learning Studio 4003**

10:00 Coffee and Tea Break

**Learning Hub LG3**

10:30 Seminar on Free Energy Methods

**Learning Studio 4003**

12:30 Lunch

1:30 Computer Exercises

**Learning Hub LG3**

5:00 Finish

Syllabus

**Monte Carlo Simulations and Applications**

The Monte Carlo method

MC simulations: Classical systems, equilibrium properties

Sampling at constant NVT: Colloidal assembly, lattice models, faster equilibration

Sampling at constant NPT: Effect of shape on phase behaviour

Sampling at constant  $\mu$ VT: Adsorption

Gibbs ensemble technique: Locating critical points & Code packages

**Free Energy Methods**

Free energy perturbation

Thermodynamic integration

Umbrella sampling

Metadynamics

Steered molecular dynamics