About the course

The Foundations of Molecular Simulation

This course covers the basic principles involved in simulating chemical and physical systems in the condensed phase. Simulations are a means to evaluate equilibrium properties such free energies as well as dynamical properties such as transport coefficients and reaction rates. In addition, simulations allow one to gain insight into molecular mechanisms. After presenting the theoretical basis of Monte Carlo and molecular dynamics simulations, particular attention is given to recent developments in this field. These include the hybrid Monte Carlo method, parallel tempering, and symplectic and other integration schemes for rigid, constrained, and unconstrained systems. Time permitting, techniques for simulating quantum systems and mixed quantum-classical systems are also discussed.

Organizational details

Location: WE 76 (Wetmore Hall, New College)
Dates and Time: Wednesdays, 3:00 - 5:00 pm

Instructors

- Prof. Jeremy Schofield
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- Office hours: Fridays, 3:00 pm - 4:00 pm

Grading

1. 4 problem sets 70%
2. Short literature report (3500 word limit) or simulation project 30%

Suggested reference books

- D. A. McQuarrie, *Statistical Mechanics*
- D. Frenkel and B. Smit, *Understanding Molecular Dynamics: From Algorithms to Applications* (Academic Press, 2002) 2nd ed. Through the UoT library: `www.sciencedirect.com/science/book/9780122673511` .
- D. C. Rapaport, *The Art of Molecular Dynamics Simulations* (Cambridge U. P., 2004).
- W. H. Press, S. A. Teukolvsky, W. T. Vettering, and C. P. Flannery, *Numerical Recipes: The Art of Scientific Computing* (Cambridge University Press, 1992) 2nd ed. `www.nrbook.com/a/bookcpdf.php` (c), `www.nrbook.com/a/bookfpdf.php` (fortran).