Molecular dynamics and its applications
CHEM 440 and 740/74100
Winter 2012

Class Time: Tuesday and Thursday, 13:00-14:20

Instructor	Pierre-Nicholas Roy
Office	ESC 330A
Office Hours	Tuesday and Thursday from 11:00 to 12:00 AM (or by appointment)
Phone	(519)-888-4567 ext. 38640
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Useful references:

1. Allen and Tildesley, *Computer Simulation of Liquids*, Oxford, 1987.
2. Chandler, *Introduction to Modern Statistical Mechanics*, Oxford, 1987.
3. McQuarrie, *Statistical Mechanics*, Harper and Row, 1976.
4. K. Hinsen, *The molecular modeling toolkit: A new approach to molecular simulations*, J. Comp. Chem. 21(2), 79-85 (2000).

Grade Distribution:

Problem Sets (approximately 5)	15%
Midterm Exam (February 28; in class)	25%
Report and oral presentation (based on the critical assessment of a literature article)	10%
Final Exam	50%
Total	100%

Examinations:
Excused absences from examinations will be given only if a completed Verification of Illness Form is provided. The form can be obtained from the Health Services web-site.[1,2] The completed form must first be registered with the Science Undergraduate Office (ESC 253). Absence for any other reason will result in a grade of ZERO. In the case of an excused absence on a midterm examination, the credit for the midterm will be transferred to the final examination.

[1] http://www.healthservices.uwaterloo.ca/
[2] See equivalent service at Guelph

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Proposed Course Outline

1. Introduction: The purpose of molecular simulations
2. Statistical Mechanics primer
    a. Ensembles, distributions, and partition functions
    b. Properties: Ensemble averages
3. Interactions and force fields
4. Equilibrium
    a. The Ergodic hypothesis
    b. Molecular dynamics simulations
        i. Classical Equations of motion
        ii. Constraints
        iii. Constant Energy simulations
        iv. Constant temperature simulations
    c. Monte Carlo simulations
        i. Importance sampling (Metropolis method)
    d. Structural properties and distribution functions
        i. The structure of liquids
        ii. Solvation
    e. Quantum effects
        i. Path Integral methods
        ii. Application: equilibrium aspects of proton transfer
5. Dynamics
    a. Onsager's regression hypothesis and time correlation functions
        i. Green-Kubo relations and connection to transport properties
        ii. Diffusion in liquids
        iii. Reaction rate constants
    b. Quantum effects
        i. Wave-packet propagation
        ii. Calculation of spectra