课程名（Coursename）  
Computer Simulation Methods in Chemistry and Physics  
  
课程代码（Coursenumber）  
M6  
  
课程对象（Audience）  
Graduates  
  
开课教师（Teacher）  
Dr R. Best and Dr M. Vendruscolo  
  
学期（Semester）  
  
课程描述（Description）  
In the last few decades computer simulations have emerged as a new scientific methodology – sandwiched between mathematical theories and experiment – with applications across the sciences and engineering. Because the parameters can be carefully controlled, these “theoretical experiment” provide powerful ways to develop fundamental understanding of the connection between microscopic models of the interactions between atoms and molecules and observable properties of many-particle systems.  
This course is an introduction to the two basic simulation techniques, namely molecular dynamics, in which the equations of motion are solved step by step, and Monte Carlo, in which configuration space is explored by a series of “smart” random steps. We will emphasise the basic techniques and their statistical mechanical origins instead of attempting to cover the vast array of special tools now available. Knowledge of computer language or program skills are not required. Instead, concepts will be detailed in “pseudo code”, describing the steps involved in setting up a simulation for simple model systems.  
Topics Molecular Dynamics basics: Verlet algorithm, time and ensemble averages, temperature scaling, force calculation under periodic boundary conditions.  
Monte Carlo Basics: Importance sampling, Metropolis algorithm.  
Calculation of properties of a system: radial distribution function, virial pressure, velocity autocorrelation function.  
Advanced Monte Carlo methods: Calculations in Different Ensembles, Biased Monte Carlo Simulations.  
Advanced molecular dynamics methods: Temperature control using Nose thermostats, method of constraints.  
Equilibrium and Non-Equilibrium Processes: Free Energy Calculations, Simulations of Phase Equilibria, Simulations of Non-Equilibrium Processes.  
  
课时信息（Totalhours）  
  
教参信息（Textbookinfo）  
1 Coarse-Graining of Condensed Phase and Biomolecular Systems by Gregory A. Voth (Hardcover - Sept. 22, 2008)  
ISBN-13: 978-1420059557  
世界各地拥有馆藏的图书馆（OCLC）:80  
2 Ab Initio Molecular Dynamics: Basic Theory and Advanced Methods by Dominik Marx and Jürg Hutter (Hardcover - May 25, 2009)  
ISBN-13: 978-0521898638  
世界各地拥有馆藏的图书馆（OCLC）:143  
3 Advanced Computer Simulation Approaches for Soft Matter Sciences II (Advances in Polymer Science) (v. 2) by Christian Holm and Kurt Kremer (Hardcover - Dec. 14, 2005)  
ISBN-13: 978-3540260912  
世界各地拥有馆藏的图书馆（OCLC）:48  
4 Statistical Mechanics of Nonequilibrium Liquids by Denis J. Evans and Gary Morriss (Hardcover - June 2, 2008)  
ISBN-13: 978-0521857918  
世界各地拥有馆藏的图书馆（OCLC）:133  
5 Hybrid Methods of Molecular Modeling (Progress in Theoretical Chemistry and Physics) by Andrei L. Tchougréeff (Hardcover - Aug. 6, 2008)  
ISBN-13: 978-1402081880  
世界各地拥有馆藏的图书馆（OCLC）:40  
6 Molecular Dynamics Simulation: Elementary Methods (Wiley Professional) by J. M. Haile (Paperback - Mar. 14, 1997)  
ISBN-13: 978-0471184393  
7 Mathematical Methods using Mathematica by Sadri Hassani (Paperback - June 11, 2003)  
ISBN-13: 978-0387955230  
世界各地拥有馆藏的图书馆（OCLC）:229  
8 Noise in Semiconductor Devices: Modeling and Simulation (Springer Series in Advanced Microelectronics) by Fabrizio Bonani and Giovanni Ghione (Hardcover - Sept. 6, 2001)  
ISBN-13: 978-3540665830  
世界各地拥有馆藏的图书馆（OCLC）:143  
9 Molecular Description of Biological Membrane Components by Computer Aided Conformational Analysis, Volume I by Robert Brasseur (Hardcover - Sept. 25, 1990)  
ISBN-13: 978-0849363757