



Collaborative Graduate Specialization in Computational Science and Engineering

WEEKLY COLLOQUIUM

Tuesday, 21 November 2006

2:30-3:30 in Goodes 303

Speaker: TUCKER CARRINGTON
Professor, Department of Chemistry
Université de Montréal

Title: New tools for studying the dynamics of small molecules: ideas and applications

Abstract: I shall review theoretical and computational techniques used to solve the Schrodinger equation to study the motion of atoms in molecules and reacting systems. A new method for using contracted basis functions in conjunction with the Lanczos algorithm to calculate vibrational energy levels of methane will be presented. As basis functions we use products of eigenfunctions of reduced-dimension Hamiltonians obtained by freezing coordinates at equilibrium. The basis functions represent the desired wavefunctions well, yet are simple enough that matrix-vector products may be evaluated efficiently. We propose a compaction technique to reduce the memory required to store the basis functions used in the final calculation. I shall also discuss a scheme for extracting a smaller basis from a huge direct product basis by removing some of the product functions. The 1-D functions from which we build the direct product basis are chosen to satisfy two conditions: (1) they nearly diagonalise the full Hamiltonian matrix; (2) they minimize off-diagonal matrix elements that couple basis functions with diagonal elements close to those of the energy levels we wish to compute. We assess the usefulness of our basis by applying it to model 6, 8, and 16-D Hamiltonians with various coupling strengths. We find approximately linear scaling.

About the speaker:

Professor Carrington received his Ph.D. in theoretical chemistry from the University of California at Berkeley under the direction of Professor William H. Miller. After graduating in 1985 he took up a postdoctoral fellowship at the Physical Chemistry Laboratory of the Eidgenoessische Technische Hochschule Zurich where he stayed until 1987. From 1987 to 1988 he was a research associate at the Herzberg Institute of Astrophysics. He has been professor in the Department of Chemistry of the Université de Montréal since September 1988.