

Quantum Monte Carlo from Minerals and Materials to Molecules

Roadmap of topics

(B. Militzer)

Geophysics:

MON, 7/9 Introduction to Geophysics (Lars Stixrude)

Density Functional Theory (DFT):

MON, 7/9 Introduction to Density Functional Theory (Ronald Cohen)

TUE, 7/17 Applications of DFT in geophysics (Renata Wentzcovitch)

MON, 7/9 LAB: Structural optimizations within DFT (R. Cohen, R. Hennig)

TUE, 7/10 Nonlocal pseudopotentials in DFT and VMC (Lubos Mitas)

WED, 7/11 LAB: Pseudopotential generation with Opium (Ken Esler)

THU, 7/12 Lattice dynamics and thermal properties of solids (Ronald Cohen)

THU, 7/12 LAB: Phonons with Espresso package (Dario Alfe)

Monte Carlo in general:

TUE, 7/10 Simulations, random walks and error analysis (David Ceperley)

TUE, 7/10 LAB: Error analysis using DATASPORK (D. Ceperley, J. Kim)

Variational Monte Carlo (VMC):

TUE, 7/10 Introduction to QMC - VMC and trial wavefunctions (Claudia Filippi)

TUE, 7/10 LAB: VMC using the QMCPACK code (Jeongnim Kim)

TUE, 7/17 Variational optimization and multi-determinants (Cyrus Umrigar)

Diffusion Monte Carlo (DMC):

WED, 7/11 Diffusion Monte Carlo - The basics (Claudia Filippi)

THU, 7/12 Selected topics in diffusion Monte Carlo (Claudia Filippi)

WED, 7/18 Reptation MC method (David Ceperley)

WED, 7/18 LAB: Ground-state QMC with QMCPACK (Jeongnim Kim)

Better fermion nodes for DMC:

WED, 7/11 Fixed-node method and geminal nodes (Lubos Mitas)

MON, 7/16 Nodes using backflow coordinate transformations (Pablo Lopez Rios)

MON, 7/16 New pairing wavefunctions and methods for nonlocal

pseudopotentials (Michele Casula)

DMC applications:

WED, 7/11 Electronic properties, band gaps, defects in silicon (Richard Hennig)

THU, 7/12 QMC on geomaterials (Dario Alfe)

MON, 7/16 Overview of Applications in the Cambridge Group (Neil Drummond)

Improving DMC methods:

FRI, 7/13 Ewald Interactions and Finite-Size Errors (Neil Drummond)

FRI, 7/13 Order(N) methods in QMC (Dario Alfe)

FRI, 7/13 Localized Orbitals, Periodic Systems and Backflow using CASINO (Neil Drummond, Pablo Lopez Rios)

Quantum Monte Carlo at finite temperature - Path Integrals MC:

TUE, 7/17 Path Integral MC for distinguishable particles (Burkhard Militzer)

THU, 7/19 Path Integral MC for bosons (Burkhard Militzer)

THU, 7/19 Bosonic Applications (David Ceperley)

TUE, 7/17 LAB: PIMC for distinguishable particle (Saad Khairallah, Burkhard Militzer)

THU, 7/19 Lab: PIMC++ and UPI codes for bosons (Bryan Clark, Ken Esler)

Advanced QMC methods:

MON, 7/16 Time dependent QMC (Nancy Makri)

WED, 7/18 Auxiliary Field Methods (Shiwei Zhang)