MOLCAS Workshop Intro

Roland Lindh

Department of Theoretical Chemistry

Chemical Center

Lund University
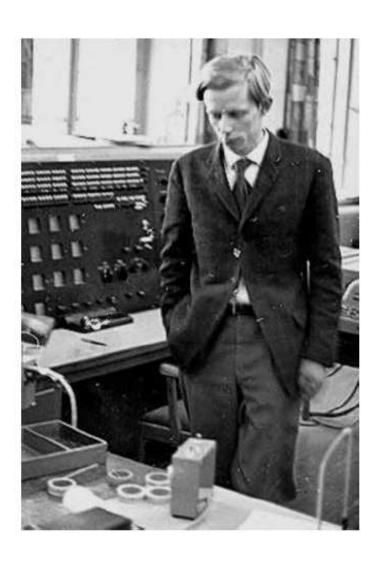
Sweden

April 14, 2009

Once upon a time...

MOLCAS History

Status late 1980'ies

- Björn Roos: CASSCF / multi configurational methods

- Jan Almlöf: MOLECULE / 2-electron integrals

- Per Siegbahn: MRCI / dynamic electron correlation

- Ulf Wahlgren: Relativistic effects

MOLCAS History

- From only point energy calculations (MOLECULE/CASSCF/MRCI)

- MOLCAS Version 1 ('89), 2 ('91), 3 ('93), 4 ('97), 5 ('00), 6 ('03), and 7 ('07)

- Parallelization

- More general (DFT, CC, Opt., Freq., exc. states, and SO)

- 2006 1st MOLCAS workshop, Valencia

- 2007 2nd MOLCAS workshop, Villars

- 2008 3rd and 4th MOLCAS worshops, Lund and Bojnice.

- Cholesky decomposition and RI technique for all wfn models

- Version 7.4 April, 2009

- GUI, fall 2009

What is MOLCAS?

Software for Quantum Chemistry

- for ground and excited states,

- for molecular structure, chemical and photochemical reactions,

- for solution chemistry, chemical bonding, and much more,

- for all elements of the periodic table.

Developed by quantum chemists at the Lund University + many external developers

Features and methods

- Electronic structure methods

  - Hartree-Fock and DFT for closed and open shell systems.

  - Møler-Plesset second order perturbation theory.

  - Multiconfigurational SCF: CASSCF and RASSCF.

  - Multiconfigurational second order perturbation theory CASPT2.

  - Multi-reference CI MRCI.

  - Coupled-cluster methods CCSD, CCSD(T).

- **Geometry optimization**

  - Analytical gradients for SCF/DFT and RASSCF.

  - Numerical gradients for CASPT2, Coupled-Cluster methods

  - Automatic geometry optimization of equilibrium geometries, transition states, intersystem crossing, conical intersections, etc.

  - Vibrational frequencies and thermodynamic quantities.

- Excited States and and Electronic Spectra

    – Electronic Spectroscopy with vibrational resolution.

    – Photochemical reactions,
      locating (CIs and) ISCs.

    – Geometries and vibrational frequencies
      for excited states.

    – Spin-orbit coupling and spin-forbidden transitions
      and reactions.

- **Environmental Effects**

  – Solvent effects using the Onsager spherical cavity
    model or the Polarizable Continuum Model (PCM).

  – Combined QM and molecular Mechanics (MM) calculations.

Typical applications with MOLCAS

- Accurate Potential Energy Curves

- Molecular spectroscopy

- Reaction mechanisms

- Biochemistry

- Heavy element chemistry

WELCOME to the 5th MOLCAS workshop!

We are pleased to see you here. We hope that both you, the students, and we, the teachers, will learn from this experience.

We will be using MOLCAS 7.4!

Diploma and Evaluation.