JASPER Communications

Quantum Monte Carlo Volunteer Project

Further develop the Quantum Monte Carlo method for general use in quantum chemistry

QMC Goal

Futher develop the QMC method

QMC@home Scientific Research (qah.uni-muenster.de)

We live...
... in a world full of molecules: Molecules constitute our bodies and reactions between molecules are the essential phenomena behind all life processes. We breath, eat and wear molecules every day.

With this in mind...
... one can imagine the great importance that knowledge about molecular structure inheres, and also the usefulness of the ability to make accurate predictions about molecular reactivity.

Quantum Theory
- in principle allows us to predict the structure and reactivity of all molecules, but the equations of Quantum Theory become intractable complex with increasing system size. Exact analytical solutions are only possible for the smallest systems and for almost all molecules of interest in chemistry and life sciences no such solutions are known to us.

Quantum Chemistry
- is the science that invents smart approximations to Quantum Theory to predict molecular information with high accuracy. Nevertheless the solving of even approximated quantum chemical equations for real life systems require huge amounts of computing power.

Quantum Monte Carlo (QMC)
- is a very promising method new to Quantum Chemistry. One of the major advantages of QMC is the ability to perform massively parallel calculations, which can be utilized to broaden the horizon of calculable systems by distributing the work over hundreds or even thousands of processors.

Quantum Monte Carlo At Home (QMC@HOME)
- is a project designed to further develop the Quantum Monte Carlo method for general use in Quantum Chemistry. With the help of volunteers all over the world we want to aquire the computing power that is needed to test and further develop the opportunities of the promising new approach of Quantum Monte Carlo.

Why does it matter?

The ability to accurately predict molecular structure and reactivity is of importance to the whole of chemistry and life sciences. Quantum Chemistry is a vital field of theoretical research into these phenomena. A very promising new Quantum Chemistry method is Quantum Monte Carlo (QMC). Our project Quantum Monte Carlo At Home (QMC@HOME) is dedicated to the further development of QMC for general use in Quantum Chemistry, to predict the structure and reactivity of molecules important to chemistry and life sciences.

What is Quantum Theory?

Quantum Theory was developed in the first half of the 20th century by Planck, Einstein, Bohr, Schrödinger, Born, Heisenberg, Pauli, Dirac and others. It replaced newtonian mechanics and classical electromagnetism, as it can explain observations at atomic and subatomic levels which cannot be explained by these classical theories.

What is Quantum Chemistry?

Based on the theoretical fundament of Quantum Theory Quantum Chemistry tries to give predictions on all what is important to Chemistry. Quantum Theory equations are intractable for most of the systems of concern to chemistry, therefore smart approximations have to be made. Even with these approximations quantum chemical calculations need a lot of computing power. The only Quantum Chemistry method which is suitable for massively parallel calculations is Quantum Monte Carlo (QMC), but up to now, little is known about the performance of QMC for real life problems. Within our project we want to test and further develop the opportunities of QMC for quantum chemical calculations.

Project Specific System Requirements – (QMC@home website)

- 20 MB of free disk space
- 64 MB of RAM
- 233MHz processor
- Project time of roughly 2 weeks with check pointing every 5 – 20 minutes