COST STSM report

Warsaw 05.03.2007

The aims of this STSM project were:

- to upgrade the existing time-dependent wave-packet propagation algorithms based on the split-operator method and on the fast-Fourier-transform (FFT) method, in order to run them in a parallel way on a Linux cluster of computers.
- to investigate the wave-packet dynamics on the electronically excited coupled potential-energy surfaces of the water dimer – the simplest generic model to study the photodynamics of bulk water.

During the STSM, I was able to encode a parallel version of the wave-packet propagation algorithm and to carry out the first test runs (simulating the parallel behavior of the code). However, the program could not be executed to produce required results during the STSM because of a long waiting queue at the Linux cluster of the Bavarian Computer Center (LRZ).

With the help of Dr. Zhenggang Lan, I have fixed and corrected several errors in my code, one of which was found in the construction of the kinetic-energy operator of the described (water-dimer) system.

The 3D potential-energy surface (PES) of the water-dimer system investigated is spanned by two tuning and one coupling vibrational modes. As the ab initio determined 3D-PES's of the water dimer was supplied in the last days of my STSM, the investigation of the desired 3D water-dimer system will be carried out shortly after the STSM. However, several test-runs in serial mode of the 3D water-dimer system have been already carried out to simulate the systems behavior with certain coupling mode models.

Thanks to the cooperation with prof. Domcke's group, it will be possible for me to use the computational resources at the TUM and at the LRZ computer center. As a result of this STMS there exists the possibility of implementation of a similar parallel environment (OpenMP) on the Linux cluster of computers in my home institute.

The program developed during the STSM and the computational resources acquired thanks to the inter-institute cooperation which resulted from the STSM will allow us to investigate the described water-dimer system and other molecular complexes (the pyridine-pyrrole complex, for instance) to investigate photophysical dynamics of hydrogen-bonded systems.

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