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MCTDH Quantum Dynamics in EGEE: Advances Made and Improvements needed

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Our communication provides a detailed description of the present performance of grid-Fluss and grid/MCTDH, tools for the direct quantum-mechanical calculation of kinetic coefficients, implemented on the section of the production computing Grid of EGEE accessible to the COMPCHEM virtual organization. The performance and reliability of the method is illustrated by presenting the results of two computational campaigns: the N + N2 reaction and the CH4 + Ni(111) dissociative sticking process.

Impact

The flux correlation method employed in our work can make quantum calculations suitable for implementation on computing grid and distributed computing. This possibility is exploited by propagating separately the several quantum state basis functions using the grid-MCTDH tool. In this way, an increase of the quantum dynamics basis to be propagated is transformed into a computational effort associated to the number of concurrent processes that need to be distributed.
The present state of the grid-Fluss and grid-MCTDH tools will be presented, focussing on two realistic applications. Special attention will be paid to the advantages provided by the
distributed nature of the grid-tools and the possible strategies for improvement.

Keywords

quantum dynamics

URL for further information

http://www.ub.edu/gdrq

Detailed analysis

The direct calculation of chemical reactions thermal rates coefficients k(T) has increasingly attracted theoretical and computational work. The computation of reliable thermal rate
values can be of great use in several realistic multiscale simulations of complex Systems.
Whenever an elementary chemical reaction occurs through a reaction barrier and no long-living complex is formed, a rigorous method of calculating k(T) in a direct way by means of flux correlation functions. The method is based on a dynamics simulation confined in the region around the saddle point and has the advantage of decreasing significantly the numerical effort with respect to a full scattering simulation. The MCTDH scheme offers an
additional numerical advantage to the approach by expanding the time-dependent multidimensional wavefunction onto a basis of time-dependent functions.

Conclusions and Future Work

Grid computing infrastructures offer new possibilities for Quantum Dynamics calculations, provided that the appropiate workflows are applied. The EGEE production section accessible to the COMPCHEM virtual organization has been employed to calculate thermal rate coefficients for the N + N2 reaction and and sticking probabilities of CH4 + Ni(111) .

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