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Grid implemented quantum versus semiclassical evaluation of thermal rate coefficients

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The implementation on the grid of the programs MCTDH and SCIVR evaluating thermal rate coefficients using quantum and semiclassical approaches, respectively, can exploit concurrency at several levels. To this end the use of different models of distributions and of different types of coordinates can differently enhance the performances of the two approaches

Impact

The advantage of using direct approaches to evaluate thermal rate coefficients on the grid makes it possible to use these calculations in complex kinetics modeling in which extended matrices of those quantities are needed at different thermal conditions

URL for further information

www.compchem.unipg

Conclusions and Future Work

The calculations performed show both the efficiency of the MCTDH and the SCIVR approaches once related computer codes are implemented on the Grid.

Keywords

thermal rate coefficients, quantum methods, semiclassical approaches

Detailed analysis

MCTDH is a general quantum approach to solve the time-dependent Schrödinger equations for multidimensional dynamical systems consisting of distinguishable particles. MCTDH is designed for treating conventional way by going through the calculation of state to state S matrix elements. MCTDH can calculate thermal rate coefficients by calculating the flux correlation functions at a suitably chosen dividing surface and then integrate them over time. To this end the computational procedure is divided in three steps of which the one carrying out the propagation in time of the single body components is naturally suited for distribution on the Grid.

The MCTDH and the SCIVR codes have been developed in collaboration between Perugia and Barcelona and have been jointly implemented on the EGEE Grid. Calculations are carried out using the asymmetric (Delves) hyperspherical coordinates and the use of different coordinates has been investigated

Author: Prof. LAGANA, Antonio (Department of Chemistry, Universtiy of Perugia, Italy)

Co-authors: Dr HUARTE LARRANAGA, Fermin (Cerqt, Barcelon); Dr FAGINAS LAGO, Noelia (Department of Chmeistry)

Presenter: Prof. LAGANA, Antonio (Department of Chemistry, Universtiy of Perugia, Italy)

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