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GRID CALCULATION OF REACTION KINETIC COEFFICIENTS: A QUANTUM MECHANICAL APPROACH

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No, poster or oral communication if planned for Applications

Project(s) or EGEE activity presenting the demo or poster (project or activity names only)

COMPCHEM VO

Special requirements other than the set up mentioned in the CfA text.

no

Abstract

Our communication provides a detailed description of the gridification of a quantum method for the direct calculation of kinetic coefficients by means of flux correlation functions and the Multiconfigurational time-dependent Hartree (MCTDH) scheme for the wavefunction. The methodology has been implemented and made available to the COMPCHEM VO within EGEE.

It is accepted that the parametric nature of classical and semiclassical trajectory calculations makes these intrinsically suitable for implementation on computing grid and distributed computing naturally beneficial for related techniques. What is a new outcome of our work is that the flux correlation method can play an equivalent role for quantum calculations.

The performance and realiability of the method is illustrated by presenting the results of a computational campaign aimed at the calculation of the N + N2 reaction rate coefficients using on the LAG3 potential energy surface.

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