CFEL SCIENCE

SEMINAR

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CFEL – Building 49a, seminar room 204 (2nd floor)

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A parallel algorithm for Hamiltonian matrix construction in electron-molecule collision calculations: MPI-SCATCI

Construction and diagonalisation of the Hamiltonian matrix is the rate-limiting step in most low-energy electron – molecule collision calculations. Tennyson (J Phys B, 29 (1996) 1817) implemented a novel algorithm for Hamiltonian construction which took advantage of the structure of the wavefunction in such calculations.

A new parallel algorithm to make use of distributed computer clusters with any MPI diagonaliser is considered. Test calculations demonstrate that significant speed-ups can be gained using multiple CPUs. This opens the way to calculations which consider higher collision energies, larger molecules and / or more target states. The methodology, which is implmented as part of the UK molecular R-matrix codes (UKRMol and UKRMol+) can also be used for studies of bound molecular Rydberg states and photoionisation.

Host: Jochen Küpper/ CFEL Molecular Physics Seminar