OpenMP/MPI threading of coupled cluster complex polarization propagator module in the Dalton program

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Background:
A recent extension of the hierarchy of time-dependent coupled cluster methods (CCS, CC2, CCSD, CCSDR(3)) has been made as to take into account relaxation effects, or the finite lifetime of the electronically excited states. This is achieved by means of the complex polarization propagator (CPP) approach which has been developed by Norman and co-workers and previously adopted to several electronic structure methods, including SCF, MCSCF, and DFT.[1,2] The extension to include the hierarchy of coupled cluster methods in the CPP framework means that theoretical simulations of electronic resonance spectroscopies (such as UV/vis and X-ray absorption as well as circular dichroism) can be made with state-of-the-art consideration of dynamic electron correlation effects.[3,4] This work represents a unique feature for the Dalton program and cannot be found in competing software.

Task:
In the CPP framework, the linear response (LR) equation needs to be solved for a grid of frequencies sampling the photon energy region of interest. This represents a computational task that is embarrassingly parallelizable. Today this step represents our bottleneck since we idle all but one core on a single node and, even for modest sized systems, quickly reach the maximum wall time limit.

Organization:
The CPP-LR module is developed by Kauczor and Norman and Kauczor will be the main contact person for the SNIC expert. The experts and authors of the original coupled cluster code in Dalton towards which the CPP-LR module is interfaced (by Coriani) are Coriani and Christiansen. There are issues with the file and memory model in the Dalton program that needs to be penetrated by the SNIC expert and Coriani and Christiansen are the relevant contact persons in this respect.

Resources:
Initially we ask for the equivalence of 10 working days of a SNIC program parallelization expert in order to analyze the problem and learn the needed program details. Our current estimate for project completion is that an additional three weeks of work is required, but this estimate is of course much dependent on the ability of the SNIC expert to get oriented in the overall program code during the initial 10 days.

References:
[1] P. Norman, D.M. Bishop, H.J.Aa. Jensen, and J. Oddershede, *Nonlinear response theory with relaxation: the first hyperpolarizability,* J. Chem. Phys. **123**, 194103 (2005)

[2] J. Kauczor, P. Jorgensen, and P. Norman, *On the efficiency of algorithms for solving Hartree-Fock and Kohn-Sham response equations*, J. Chem. Theory Comput. **7**, 1610 (2011)
[3] S. Coriani, O. Christiansen, T. Fransson, and P. Norman, *Coupled-cluster response theory for near-edge x-ray absorption fine structure of atoms and molecules*, Phys. Rev. A **85**, 022507 (2012)
[4] S. Coriani, T. Fransson, O. Christiansen, and P. Norman, *An asymmetric Lanczos-chain driven implementation of electronic resonance convergent coupled cluster linear response theory*, J. Chem. Theory Comput. **8**, 1616 (2012)

Example calculation:

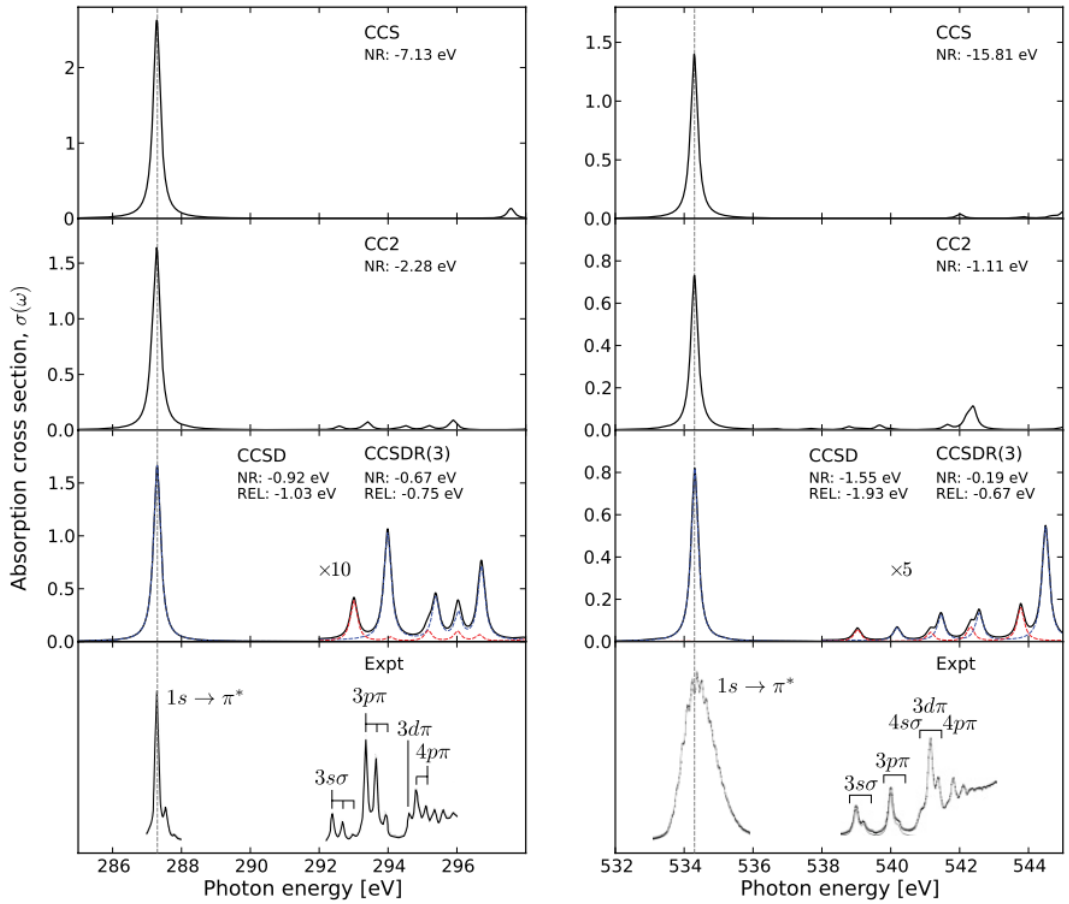

Figure 1: Illustration of coupled cluster CCP calculations in terms of the carbon and oxygen *K*-edge spectra of carbon monoxide. Taken from [3].