TREX Workshop

April 2023

1 Tchint

1.1 Input and Output

Here we will discuss the practical aspects of the evaluation of the transcorrelated integrals using TCHInt. The following files need to be provided in your working directory to run a calculation:

- *parameters.casl*: Optimized parameters of the Jastrow factor. They usually get optimized by the CASINO software [1]
- *input.molden*: Molden file which contains the information of the orbitals.
- *FCIDUMP.bare* (optional): Values of the non-TC Integrals. If not provided, they will be evaluated by pyscf before the calculation of the TC Integrals.
- *tchint.json*: Optional JSON file for configuring tchint.

The tchint.json file can have a lot of different entries, but we only need the following:

- *"grid_lvl"*: PySCF's grid density parameter, on a scale from 0 (coarse, default) to 9 (fine). A value of 2 ought to be accurate for most purposes. For demonstration purposes, we will use 0 in this tutorial.
- *"lmat_mean_field"*: Toggles use of mean-field approximation for L matrix. Defaults to false. If true, mean-field contributions are added to 0-, 1- and 2-body integrals before write of FCIDUMP. The L matrix is never be explicitly evaluated and consequently no TCDUMP will be generated. We only work with this approximation in this tutorial.

The following important output files are produced:

- *FCIDUMP*: Two-electron Integrals of the transcorrelated Hamiltonian.
- *TCDUMP*: Three-electron Integrals of the transcorrelated Hamiltonian. Only exists if *"lmat_mean_field"* is not set to *true*.
- *outfile*: Reports all the relevant steps of the calculation, ends with the transcorrelated reference energy .

1.2 Tasks

- Copy the relevant input files (see section 1.1) for the N_2 dimer from */home/ws-p.lopez/n2-tutorial* to your working directory and perform the calculation.
- To run TCHInt, execute *sbatch jobscript* in your working directory.

[1] `https://casinoqmc.net/casino_manual_dir/casino_manual.pdf`

2 e-Co.jl

e-Co.jl is a Julia implemetation of various electron correlation methods with main focus on coupled cluster using the fcidump/npy interface. Its development has started recently in our group.

2.1 Input

- The only necessary input file is a FCDIUMP containing the values of the integrals.

2.2 How to run

To run e-Co.jl, execute

- *export JULIA_DEPOT_PATH="/home/ws-d.kats/.julia:$JULIA_DEPOT_PATH"*
- srun /home/ws-d.kats/e-cojl/e-co.sh FCIDUMP $\gg$ out 2 > &1

or simply submit the file

- */home/ws-d.kats/Submit/submit.sh*

in your current working directory.

2.3 Tasks

CC-calculations should be run for the N_2 and COH_2 molecule. Therefore, copy

- The FCIDUMP of N_2 from */home/ws-p.haupt/workshop/run/n2_notc* without Transcorrelation
- The FCIDUMP of N_2 from */home/ws-p.haupt/workshop/run/n2_xtc* with the mean-field approximation from the TCHInt calculation. Note that the *"grid_lvl"* has been set to 0 in section 1.1, while it has been set to 2 to obtain this FCIDUMP.
- The FCIDUMP of COH_2 from */home/ws-p.haupt/workshop/run/coh2*

into your working directory and perform the calculation.