Targeting Real chemical accuracy at the EXascale

GammCor Code Tutorial

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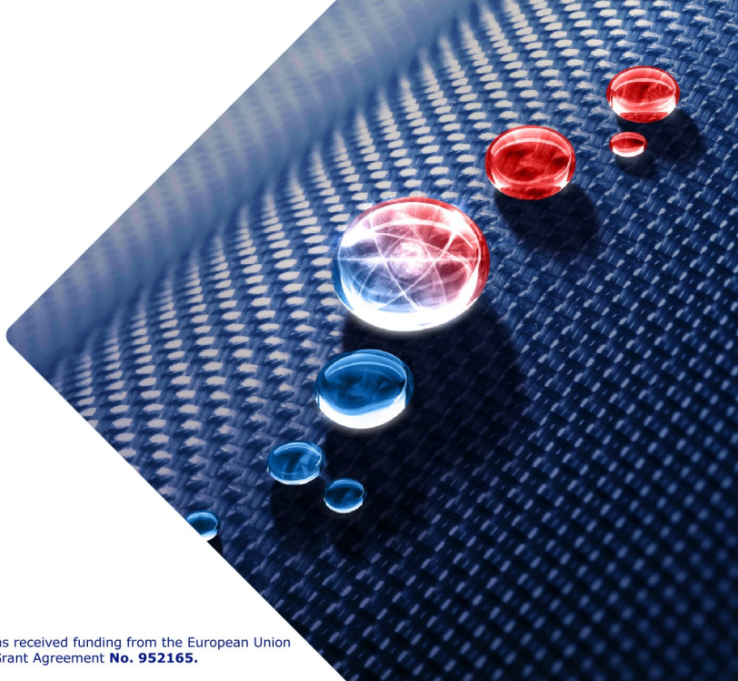

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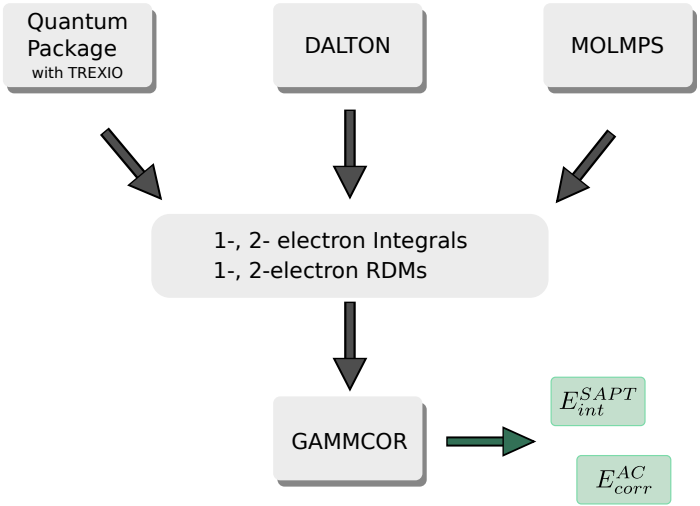
Working scheme



Plan of the tutorial

1. Install GammCor code
2. Run tests
3. Do exercises and discuss the results
   - SAPT (Quantum Package, Dalton)
   - AC (MOLMPS)

Installation of the GammCor code

GET THE CODE →

```
git clone https://github.com/pernalk/GAMMCOR.git
cd GAMMCOR
git checkout workshop2023
```

INSTALLATION GUIDE → https://qchem.gitlab.io/gammcor-manual/

EXERCISES →

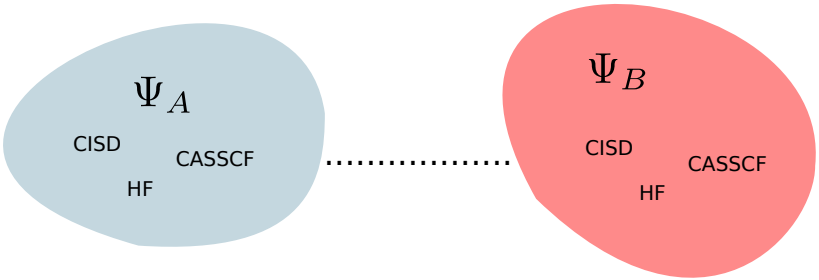
```
git clone https://github.com/michalhapka/trex_workshop2023.git
or at Dragon
cp /home/michalhapka/trex_workshop2023
```

INSTALLATION
AT DRAGON

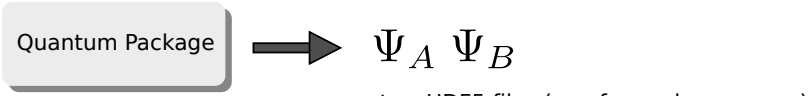
```
env FC=ifort CXX=icpc CC=icc cmake -S. -Bbuild -Cconfig_intel
cd build
make -j 4
ctest -V
```

https://qchem.gitlab.io/gammcor-manual

$$E_{int}^{SAPT} = E_{elst}^{(1)} + E_{exch}^{(1)} + E_{ind}^{(2)} + E_{exch-ind}^{(2)} + E_{disp}^{(2)} + E_{exch-disp}^{(1)}$$



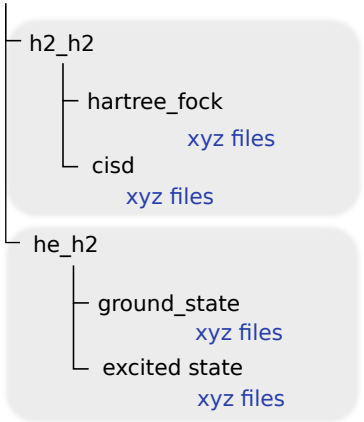
1 step



two HDF5 files (one for each monomer)

2 step

/trex_workshop2023/SAPT



EXERCISE 1

EXERCISE 2

Table 1: Results of SAPT calculations for H_2-H_2 dimer. Energy units are microhartree.

	$E^{(1)}_{\text{elst}}$	$E^{(1)}_{\text{exch}}$	$E^{(2)}_{\text{ind}}$	$E^{(2)}_{\text{exch-ind}}$	$E^{(2)}_{\text{disp}}$	$E^{(2)}_{\text{exch-disp}}$	$E^{\text{SAPT}}_{\text{int}}$
$R = 1.44$ a.u.							
HF	−62.29	89.96	−5.169	1.706	−154.2	6.911	−123.0
CISD	−52.70	88.98	−4.591	2.014	−151.5	6.111	−111.6
CAS(2,2)	−47.82	81.28	−4.030	1.637	−143.6	5.693	−106.8
CAS(2,8)	−52.61	88.43	−4.565	1.980	−151.7	6.094	−112.4
$R = 7.20$ a.u.							
HF	−185.4	445.0	−39.72	26.29	−320.6	33.55	−40.89
CISD	−47.28	210.0	−8.408	6.044	−165.6	10.45	5.193
CAS(2,2)	−44.87	201.1	−7.994	5.465	−161.1	10.15	2.748
CAS(2,8)	−47.17	209.4	−8.388	5.992	−165.9	10.43	4.335

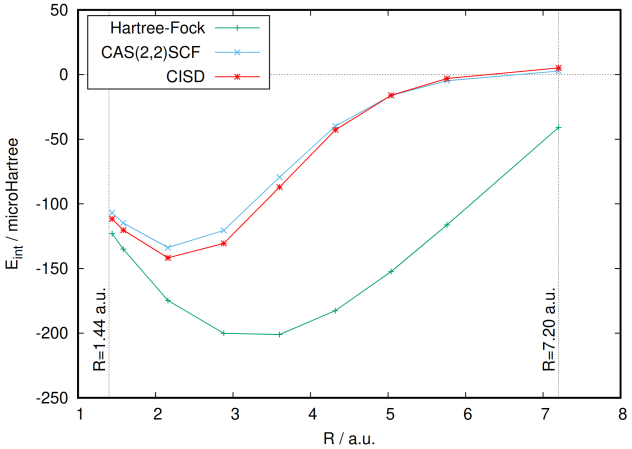


Figure 1: SAPT interaction energy curves for H_2-H_2. R denotes the covalent bond length in one the monomers.

Table 2: Results of SAPT(CISD)/aug-cc-pVDZ calculations for He-H_2 and He-H_2* dimers. Energy unit is millihartree.

	$E^{(1)}_{\text{elst}}$	$E^{(1)}_{\text{exch}}$	$E^{(2)}_{\text{ind}}$	$E^{(2)}_{\text{exch-ind}}$	$E^{(2)}_{\text{disp}}$	$E^{(2)}_{\text{exch-disp}}$	$E^{\text{SAPT}}_{\text{int}}$
ground state							
$R = 4.0$ a.u.	−1.103	5.740	−0.375	0.395	−0.956	0.114	3.816
$R = 6.6$ a.u.	−0.004	0.029	−0.001	0.001	−0.050	0.001	−0.024
excited state							
$R = 4.0$ a.u.	−0.558	0.776	−1.080	0.099	−1.076	−0.003	−1.843
$R = 6.6$ a.u.	−0.026	−0.060	−0.036	−0.003	−0.204	−0.005	−0.334

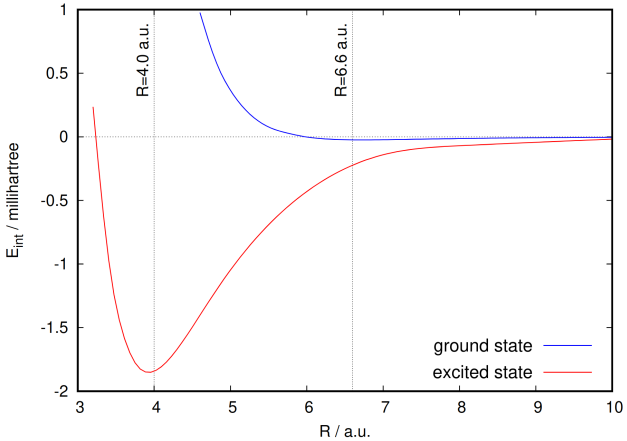
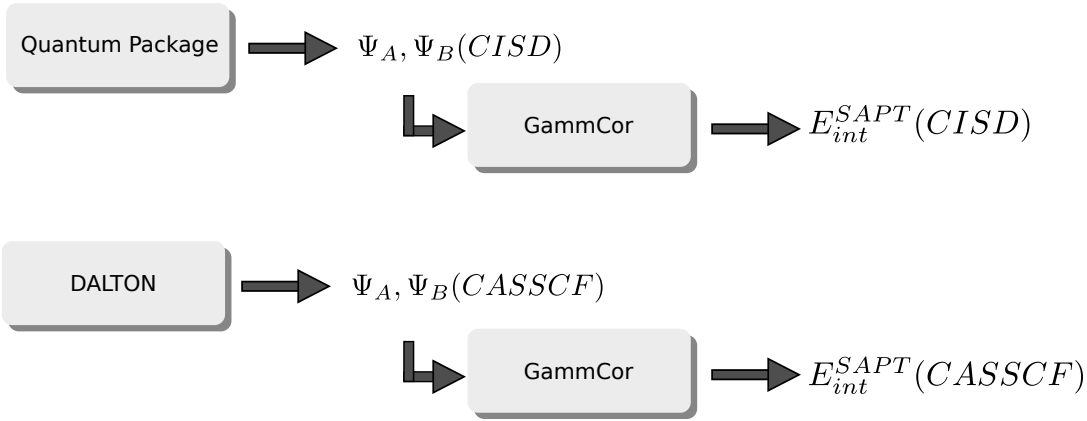


Figure 2: He-H_2 in T-shaped geometry. R denotes the distance between the He atom and COM of the H_2 molecule.


Quantum Package
$\Psi_A, \Psi_B(CISD)$
GammCor
$E_{int}^{SAPT}(CISD)$
DALTON
$\Psi_A, \Psi_B(CASSCF)$
GammCor
$E_{int}^{SAPT}(CASSCF)$