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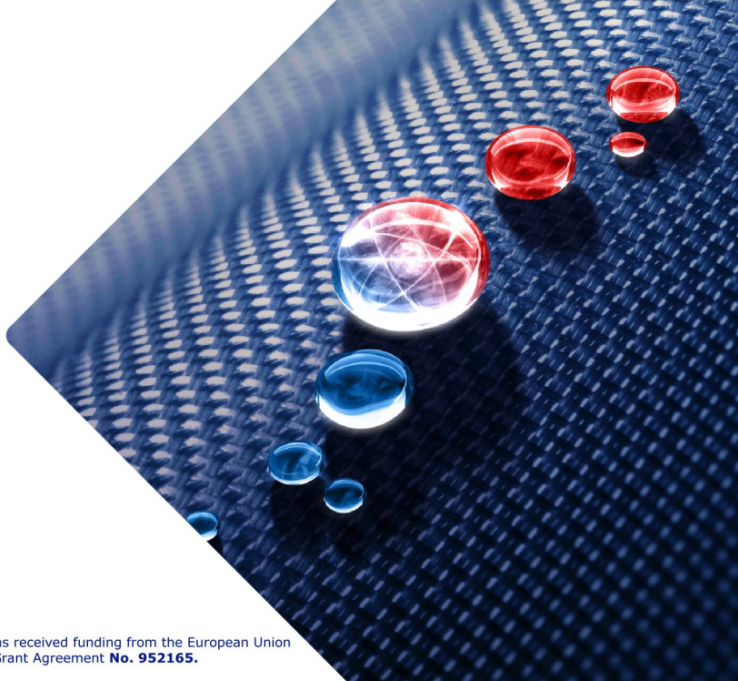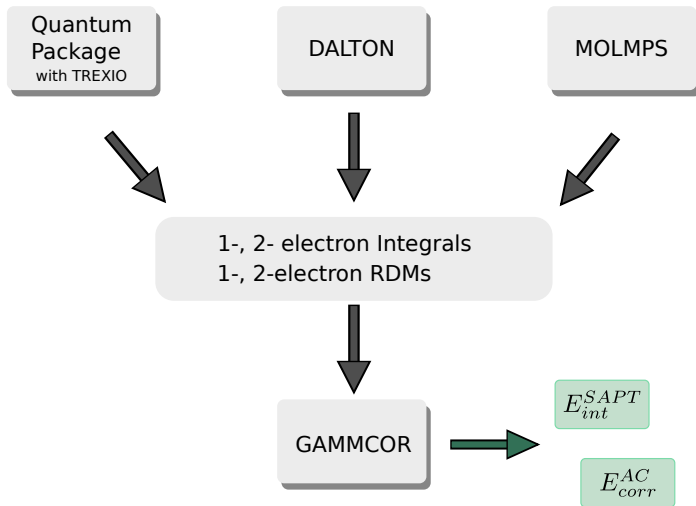
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1 Install GammCor code
2 Run tests
3 Do exercises and discuss the results
   - SAPT (Quantum Package)
   - AC (MOLMPS)

EXERCISES

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

GET THE CODE →

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

INSTALLATION GUIDE →

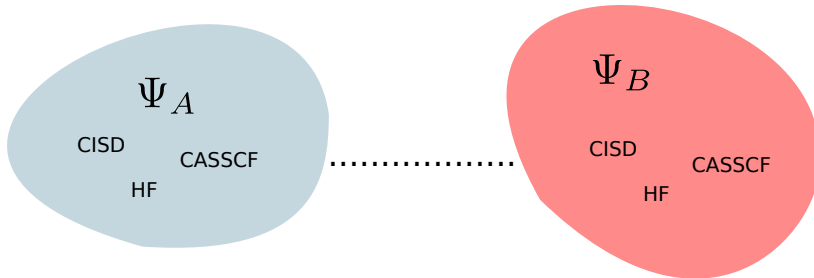https://qchem.gitlab.io/gammcor-manual/

INSTALLATION
AT DRAGON

```
git clone https://github.com/pernalk/GAMMCOR.git
cd GAMMCOR
git checkout workshop2023
env FC=gfortran CXX=g++ CC=gcc cmake -S. -Bbuild -Cconfig_gnu
cd build
make -j 4
ctest -V
```

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

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

1 step

Quantum Package $\longrightarrow$ $\Psi_A \ \Psi_B$

two HDF5 files (one for each monomer)

2 step

$\Psi_A \ \Psi_B \longrightarrow$ GammCor $\longrightarrow$ E_{int}^{SAPT}

/trex_workshop2023/SAPT

├─ h2_h2

│ └─ cisd
│   xyz files   EXERCISE 1

└─ he_h2

   ├─ ground_state
   │   xyz files   EXERCISE 2
   └─ excited state
            xyz files
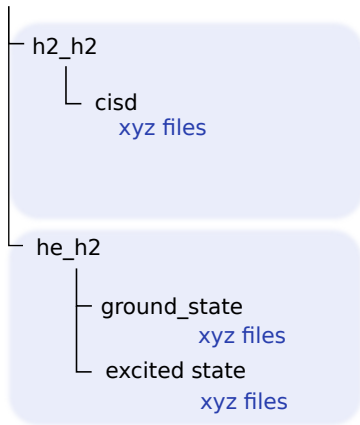
Table 1: Results of SAPT calculations for H_2-H_2 dimer. Energy units are microhartree.

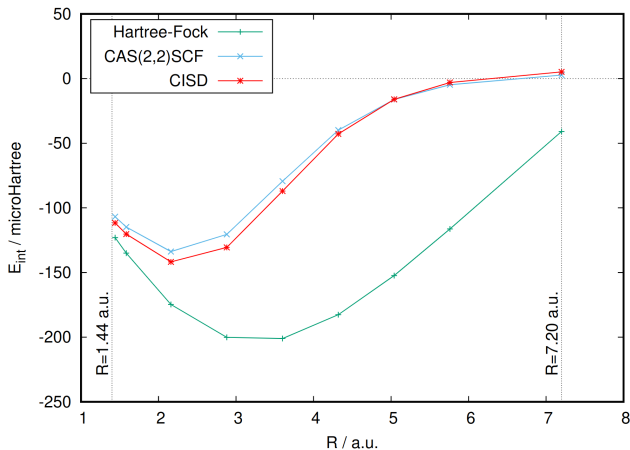|	$E_{\text{elst}}^{(1)}$	$E_{\text{exch}}^{(1)}$	$E_{\text{ind}}^{(2)}$	$E_{\text{exch-ind}}^{(2)}$	$E_{\text{disp}}^{(2)}$	$E_{\text{exch-disp}}^{(2)}$	$E_{\text{int}}^{\text{SAPT}}$
$R = 1.44$ a.u.							
HF	-62.29	89.96	-5.169	1.706	-154.2	6.911	-123.0
CISD	-52.70	88.98	-4.591	2.014	-151.5	6.111	-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.

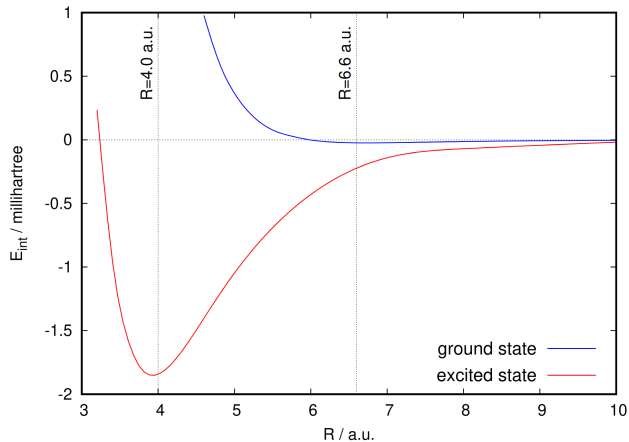|	$E_{\text{elst}}^{(1)}$	$E_{\text{exch}}^{(1)}$	$E_{\text{ind}}^{(2)}$	$E_{\text{exch−ind}}^{(2)}$	$E_{\text{disp}}^{(2)}$	$E_{\text{exch−disp}}^{(2)}$	$E_{\text{int}}^{\text{SAPT}}$
ground state							
$R = 4.0$ a.u.	−1.103	5.740	−0.375	0.395	−0.956	0.114	3.816
$R = 6.6$ a.u.	−0.004	0.029	−0.001	0.001	−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-H₂ in T-shaped geometry. R denotes the distance between the He atom and COM of the H₂ molecule.