What I learned in implementing CCSD with Ambit

Tianyuan (Sam) Zhang

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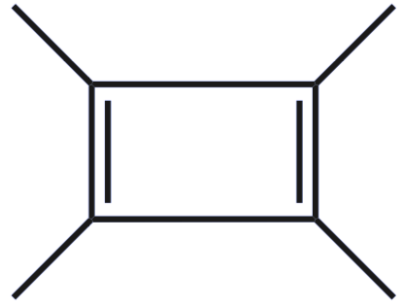
First version: dictating Crawdad project

$$\mathcal{F}_{me} = f_{me} + \sum_{nf} t_n^f \langle mn \| ef \rangle$$



Cyclobutadiene
C1 symmetry, freeze core

```
W1_["me"] = F_["me"];
W1_["ME"] = F_["ME"];

W1_["me"] += T1_["nf"] * V_["mnef"];
W1_["me"] += T1_["NF"] * V_["mNeF"];
W1_["ME"] += T1_["nf"] * V_["nMfE"];
W1_["ME"] += T1_["NF"] * V_["MNEF"];
```

Time/iteration

	cc-pVDZ	cc-pVTZ
uhf-CCSD (Psi4)	1.65s	35.8s
ambit-CCSD	2.56s	120s

http://sirius.chem.vt.edu/wiki/doku.php?id=crawdad:programming:project5

J.F. Stanton, J. Gauss, J.D. Watts, and R.J. Bartlett, *J. Chem. Phys.* **1991**, 94,4334-4345

Second version: Remove explicit W_{abef} intermediate

$$\mathscr{W}_{abef} = \langle ab \| ef \rangle - P_{-}(ab) \sum_{m} t_{m}^{b} \langle am \| ef \rangle$$

$$t_{ij}^{ab} D_{ij}^{ab} \longleftarrow \frac{1}{2} \sum_{ef} \tau_{ij}^{ef} \mathscr{W}_{abef}$$

cc-pVDZ, 10 iter total

```
W2_["abef"] = V_["abef"];                                  0.170s
W2_["abef"] -= T1_["mb"] * V_["amef"];                     1.824s
W2_["abef"] += T1_["ma"] * V_["bmef"];                     0.150s

T2D["ijab"] += 0.5 * tau_["ijef"] * W2_["abef"];           0.639s
```

```
T2D["ijab"] += 0.5 * tau_["ijef"] * V_["abef"];            0.648s
T2D["ijab"] += 0.5 * tau_["ijef"] * T1_["ma"] * V_["bmef"];  0.110s
T2D["ijab"] -= 0.5 * tau_["ijef"] * T1_["mb"] * V_["amef"];  0.102s
```

O^3V^3 OV^4

Third version: Optimized permutation

$$t_{ij}^{ab} D_{ij}^{ab} \longleftarrow P_{-}(ij) \sum_{e} t_{i}^{e} \langle ab \| ej \rangle$$

cc-pVTZ, 54 iter total

```
T2D["ijab"] -= T1_["je"] * V_["abei"];      55.6s
T2D["iJaB"] += T1_["JE"] * V_["aBiE"];       7.8s
```

```
T2D["ijab"] -= T1_["je"] * V_["abie"];       7.2s
T2D["iJaB"] += T1_["JE"] * V_["aBiE"];       8.0s
```

Version	Description	Time/iteration
1	dictating	120s
2	Remove W_{abef}	52.3s
3	Optimized permutation	34.2s
uhf-CCSD(Psi4)		35.8s

- Ambit can provide reasonable intermediates automatically.
- Move the summed up indices to the outer most or inner most position.

Thanks!