Final Project Presentation: Extension of CNDO/2 to large molecules

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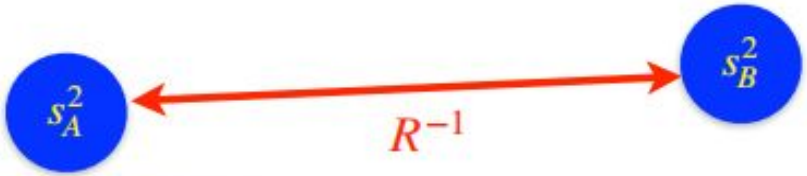
Outlines

- Recap: CNDO/2 (Briefly as 2 minutes)
- Coding plan to improve the efficiency of the original CNDO/2 (About 2 minutes)
- Runtime comparison before and after the optimization (3 minutes)
- Possible Improvements (2 minutes)
- References
- Acknowledgements (30 seconds)

Recap: CNDO/2

- A (quite drastic) simplification of ab initio HF theory
- (i) Use a valence minimal basis (like EHT) so no core 1s electrons for C, N, O, etc.
- (ii) "Zero differential overlap" (ZDO) approximation to simplify 2-electron integrals
  - Like $S_{\mu\nu}$, ERIs decay exponentially with distance between ω_μ and ω_ν (& likewise ω_λ and ω_σ)
  - But decay only as R^{-1} with distance between $(\mu\nu)$ and $(\lambda\sigma)$
  - Motivates the ZDO approximation for ERIs: $(\mu\nu\,|\,\lambda\sigma) \approx (\mu\mu\,|\,\lambda\lambda)\delta_{\mu\nu}\delta_{\lambda\sigma}$
- Approximate retained ERIs so as to preserve rotational invariance of $E_{\text{CNDO/2}}$
  - $(\mu\mu\,|\,\lambda\lambda) \leftarrow \gamma_{AB}$ where ω_μ is on atom A, and ω_ν is on atom B
  - $\gamma_{AB} = \int d\mathbf{r} \int d\mathbf{r}' [s_A(\mathbf{r})]^2 |\mathbf{r} - \mathbf{r}'|^{-1} [s_B(\mathbf{r}')]^2$



Coding plan to improve the efficiency of the original CNDO/2

- Reorganization of the Memory we implemented.
- Optimization of Mathematical Part like Linear Algebra
- Balance between Runtime with Theory Level
- Modification on the previous coding
- Make sure it works

Runtime comparison before and after the optimization

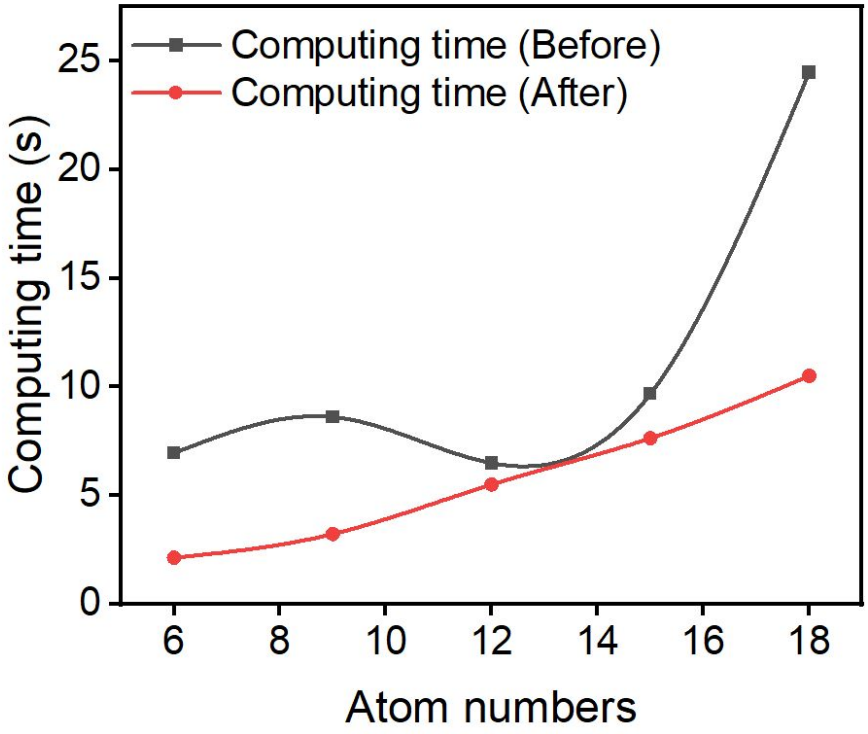
Initially, how can we do to monitor the runtime of our coding?

Option 1: Obviously, you can code your own method to monitor the runtime as many people do.

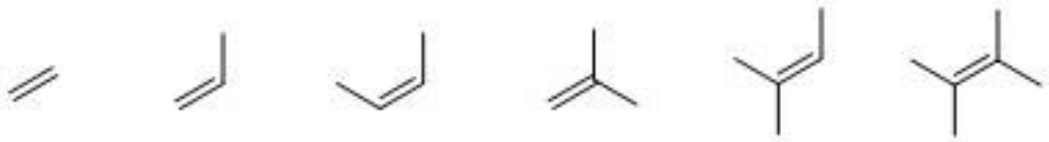
Option 2: Here is a tricky way to do it as well: Using the Visual Studio tools, you can get your own runtime, EVEN CPU and MEMORY occupation.

Runtime with different number of atoms

- The black line with square markers represents the computing time before the change. This line shows a non-linear increase in computing time as the number of atoms increases. After an initial plateau between 8 and 12 atoms, the computing time rapidly increases, particularly from 14 to 18 atoms.
- The red line with circular markers represents the computing time after the change. This line shows a more linear and gradual increase in computing time as the number of atoms increases, remaining consistently lower than the computing time before the change across the range of atom numbers.



Computing time before and after



	Computing time					
	Total (s)	main (s)	Fock Matrix (s)	Hamiltonion (ms)	Density Matrix (s)	
C2H4	2.134	2.19	0.22	79.56	1.72	after
	6.948	6.51	5.5	185.96	5.97	before
C3H6	3.223	1.92	1.56	167.29	2.46	after
	8.615	8.39	6.35	344.65	7	before
C4H8	5.501	5.02	3.42	343.17	3.23	after
	6.491	6.19	2.78	644.23	3.73	before
C5H10	7.632	7.38	5.05	463.88	5.3	after
	9.675	9.4	4.22	944.77	5.73	before
C6H12	10.503	10.41	7.11	638.78	7.18	after
	24.483	24.51	16.54	1390	19.18	before

Possible improvements

1, It takes me nearly 56 minutes to get the result from the around 700 atoms, which is probably needed to improve.

2, The code monitor shows the high occupation of CPU while taking calculations on the large molecules.

References

[1]https://blog.csdn.net/qq_36549611/article/details/107293258

[2]Duke, C.B. (1979), Electronic structure of large molecules: CNDO/S3 model. Int. J. Quantum Chem., 16: 267-281. https://doi.org/10.1002/qua.560160828

[3]https://www.chemeurope.com/en/encyclopedia/Computational_chemistry.html#Methods_for_solids

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