Computational Comparison

1. SCF Energy

Here we can see the calculated Gaussian SCF energy of both of the molecules.

Molecule	SCF Energy
Pencen	-846.741165656
Tetcen	-693.129837226

SCF energy is a measure of all of the electronic energy of a molecule from all of interactions of atoms and electrons.

The SCF energy of the “PENCEN” molecule (−846.74 Hartrees) is more negative than that of “TETCEN” molecule (−693.13 Hartrees). This is because PENCEN has more atoms and electrons, leading to more electron and nuclear interactions and electron–electron interactions. A larger molecule would result in a more negative SCF energy.

2. Computational Performance

On the following we can see a couple of tables regarding the time it took to compute a Gaussian calculation for the same molecules but each time increasing the number of CPU cores used.

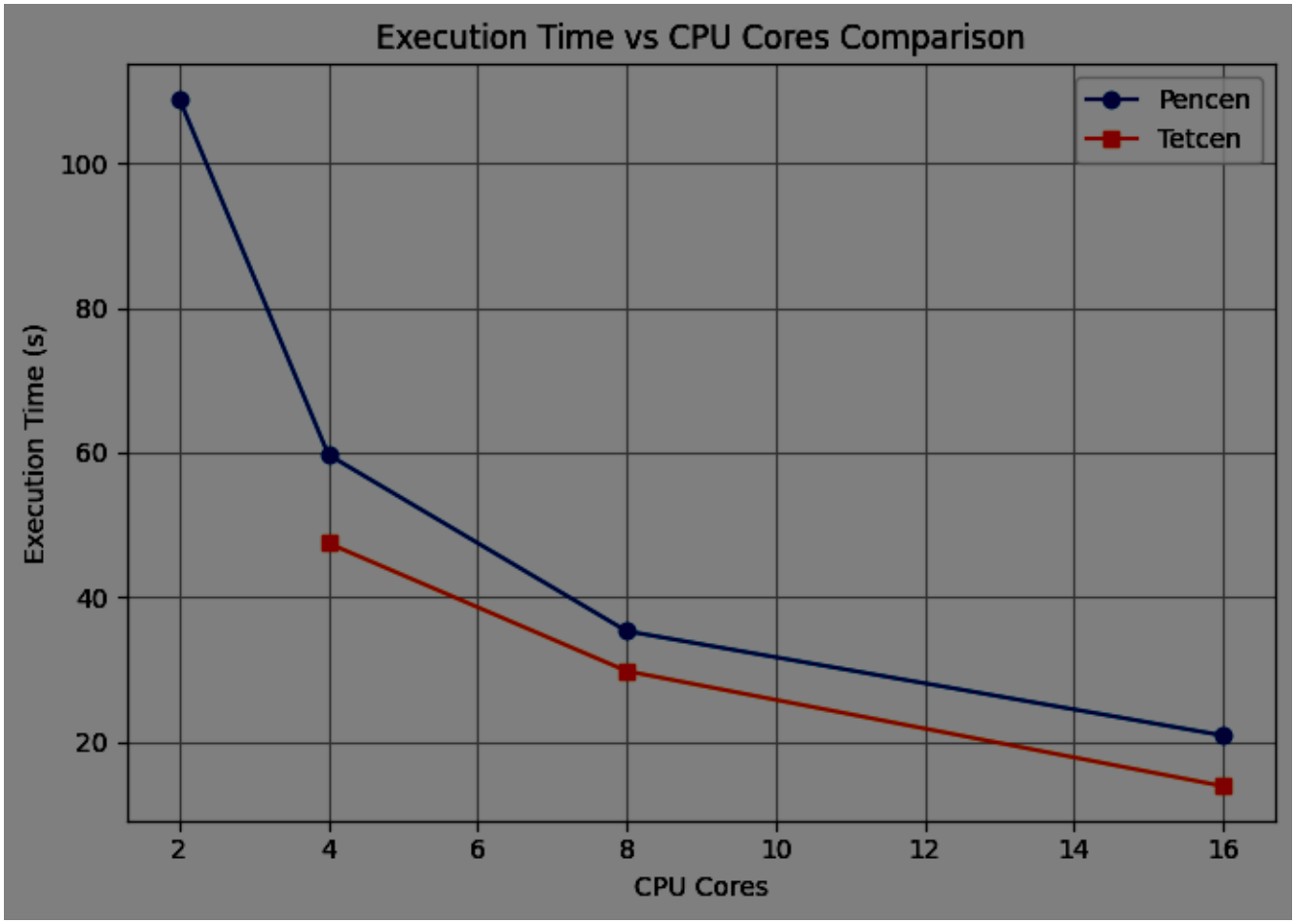
“Tetcen” Molecule

Molecule	Number of Atoms	CPU Cores	Execution Time (s)
Tetcen	30	2	-
	30	4	47.47
	30	8	29.8
	30	16	13.9

“Pencen” Molecule

Molecule	Number of Atoms	CPU Cores	Execution Time (s)
Pencen	36	2	108.9
	36	4	59.7
	36	8	35.32
	36	16	20.9

A visual representation of both tables was then plotted, where you can see the trend in time as more CPUs are used.



This reflects good computational scalability, especially in larger molecules like the one in the PENCEN file, the more CPUs involved the more calculations can be run in parallel. However, the reduction in time is not perfectly linear, indicating diminishing returns at higher core counts due to possible limit in calculation run at the same time or maybe limitations in the parallel algorithm.
The time taken does not reduce as much the more CPUs are involved. Overall, both molecules calculations show improved efficiency with more CPUs, but optimal core usage depends on the molecule size and the nature of the calculation.

3. GitHub

A repository link of GitHub is shared with all the files involved in the project.

https://github.com/kevinpinoarias/Software-Tutorial