Installing and running GAMESS to Excel reader

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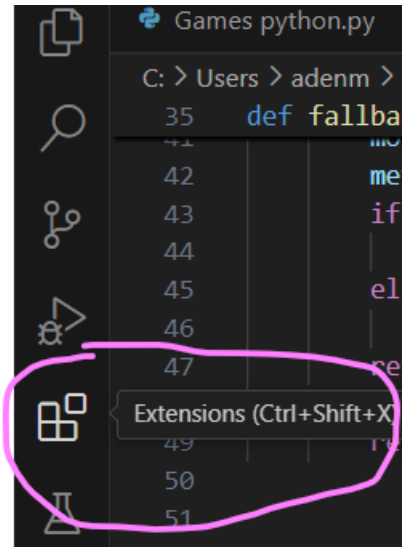
Fast tutorial:

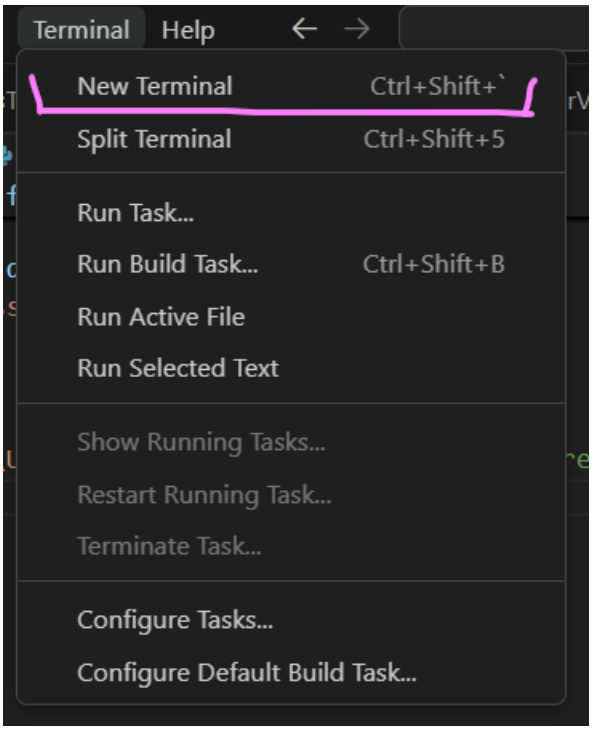
- download Visual Studio code (look up, its popular)
    - go through typical “installing” process

-add extension:



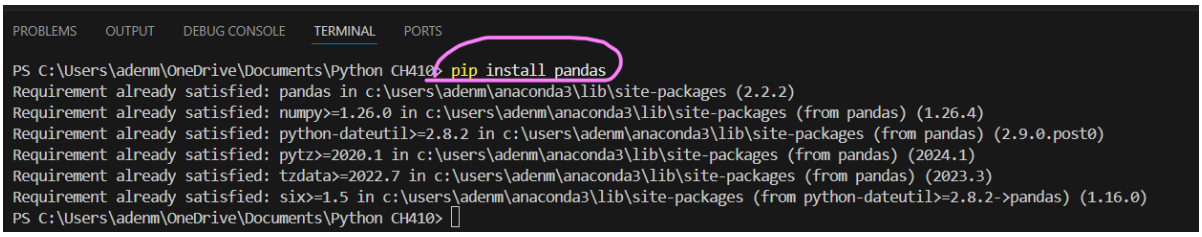
-search for “Python” and install

-open a terminal and install pandas:



While inside of terminal type:

pip install pandas



-download attached “GAMEStoExcelReaderV2” from github

-Change filepaths for input and output folders.

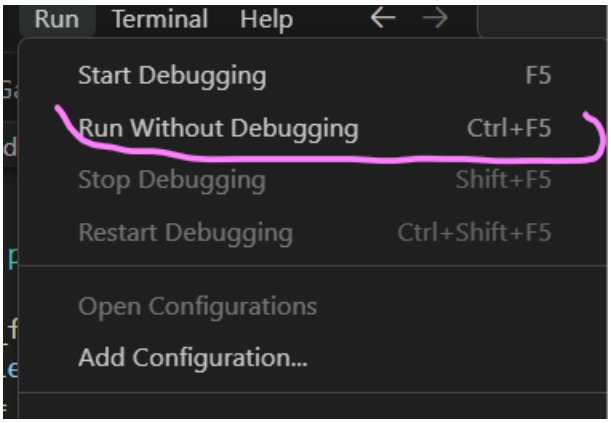
```
# === PATHS ===

input_path = Path(r'C:\Users\Public\gamess-64\outputs')
output_path = Path(r'C:\Users\Public\gamess-64\saved outputs\Python compiled csv')
output_path.mkdir(parents=True, exist_ok=True)
output_file = output_path / 'Gamess_summary.csv'

# === MAIN LOOP ===
```

These are the default directories, yours may be different. You can copy & paste your folder path by right clicking on the folder itself when in file explorer and “copy as path”

-run the code



-win

Output in Excel should look like this:

molecule	force_field	basis	comp_met	bond_lengt	heat_of_fo	Total Energy (
C4H6	MMFF94	6-311ppG	Blyp	1.337955	NA	-155.931
C4H6	MMFF94	6-311ppG	RHF	1.337887	NA	-154.962
C6H8	MMFF94	6-311ppG	Blyp	1.445278	NA	-233.313
C6H8	MMFF94	6-311ppG	RHF	1.445278	NA	-231.874
HCl	Gaff	6311pp	AM1	1.099971	-11.3595	NA
HCl	Ghemical	6311pp	AM1	1.008097	10.5191	NA
HCl	MMFF94s	6311pp	AM1	1.305786	-24.4679	NA
HCl	MMFF94	6311pp	AM1	1.305889	-24.4666	NA
HCl	UFF	6311pp	AM1	1.375697	-22.4067	NA
He-neutral	MMFF94	6311ppG2	RHF	0	NA	-2.85998