File operations using python example

you are given a folder gau_files which contain files having *.gau extension
these are special files in certain scientific areas
we need to modifiy these files so that lines starting with "%nproc" and "%mem" should be deleted

size * .gau uzantılı dosyaları içeren bir klasör gau_files verilir bunlar belirli bilimsel alanlarda özel dosyalardır "% nproc" ve "% mem" ile başlayan satırların silinmesi için bu dosyaları değiştirmemiz gerekiyor

```
LIG-ACC-C4.gau

LIG-ACC-C4.gau  No Selection

1   %chk=LIG-ACC-C4.chk
2   %nproc=1
3   %mem=1GB
4   # HF/6-31G* Opt=(Z-matrix,MaxCycles=100) Geom=PrintInputOrient
5
6   <qmtool> simtype="Geometry optimization" </qmtool>
7   LIG-ACC-C4
8
9   0 1
10  N1 0.8650000095367432 -0.9860000014305115 0.7519999742507935
11  C2 0.00100000000474974513 0.11500000208616257 0.2639999985694885
12  C3 -1.2949999570846558 -0.6790000200271606 0.12700000405311584
13  N4 -1.1770000457763672 -1.8220000267028809 0.9309999942779541
14  C5 -2.2869999408721924 -0.22100000083446503 -0.6449999809265137
15  C6 -2.2809998989105225 -2.680999994277954 1.065999984741211
16  C7 -3.3529999256134033 -2.493000030517578 0.18400000035762787
```

```
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4   <qmtool> simtype="Geometry optimization" </qmtool>
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```

first create new folder with a name "gau_files_modified"

In [1]:

```python
import os
```

In [2]:

```python
os.mkdir("gau_files_modified")
```

go through all the files in gau_files and modify them and copy the modified files into the "gau_files_modifie" folder

gau_files içindeki tüm dosyaları gözden geçirin ve bunları değiştirin ve değiştirilen dosyaları "gau_files_modifie" klasörüne kopyalayın

In [3]:

```python
directory="gau_files"
```

get the list of files in that folder

In [4]:

```python
filelist=os.listdir(directory)
```

In [5]:

```python
filelist
```

Out[5]:

```
['ETOH-ACC-O2.gau',
 'ETOH-DON-H11.gau',
 'ETOH-DON-H12.gau',
 'ETOH-DON-H13.gau',
 'ETOH-DON-H21.gau',
 'ETOH-DON-H22.gau',
 'ETOH-DON-HO2.gau',
 'ETOH-sp-HF.gau',
 'ETOH-sp-MP2.gau',
 'wat-sp.gau']
```

In [6]:

```python
outputdir="gau_files_modified"
```

In [7]:

```python
for file in filelist:
    if file.endswith(".gau"): # make sure that we are working only on gau files
        inputfile=open(directory+"/"+file)
        lines=inputfile.readlines()
        inputfile.close()
        outputfile=open(outputdir+"/"+file,"w")
        for line in lines:
            if line.startswith("%nproc=1"):
                pass
            elif line.startswith("%mem"):
                pass
            else:
                outputfile.write(line)
        outputfile.close()
```

In [ ]: