CHEMICAL ENGINEERING 512

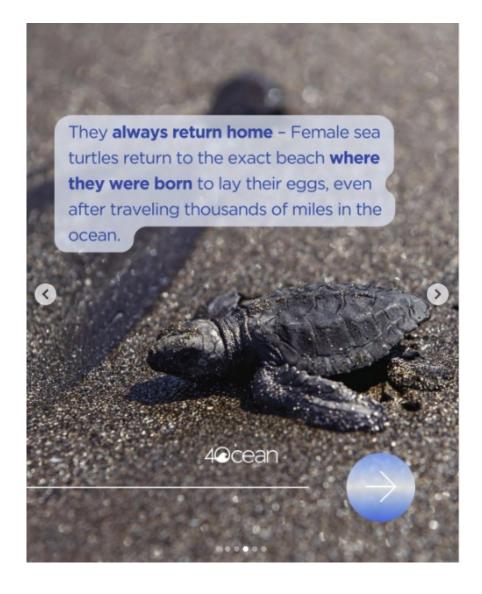
RELAP5-3D

Lecture 12
Batch Files and Python Interfacing





Spiritual Thought



My dear brothers and sisters, my dear friends, I testify that God sees us as we truly are—and He sees us worthy of rescue.

You may feel that your life is in ruins. You may have sinned. You may be afraid, angry, grieving, or tortured by doubt. But just as the Good Shepherd finds His lost sheep, if you will only lift up your heart to the Savior of the world, He will find you.

He will rescue you.

He will lift you up and place you on His shoulders.

He will carry you home.

- Dieter F. Uchtdorf, April 2016



Objectives

- Batch Files
- Practice Problem
- Python Interfacing



Batch Files – What They Are

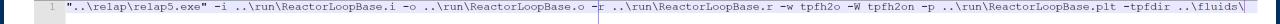
- A Microsoft Windows script file
- File extension .bat
- Can be written with Notepad ++ (or any other text editor)
- Command line script can be used





Batch Files and RELAP5-3D

- The RGUIStationJar is an interface to allow you to input file names and then runs a batch file
- RELAP/r3d434ie/relap/relapcommand.bat
- Batch files can be used to run multiple RELAP runs much more quickly





Create a batch file to run RELAP

- RELAP command (if preformed in the relap folder)
- "relap5.exe" -i file.i -o file.o -r file.r -w tpfh2o –W tpfh2on p file.plt -tpfdir ../fluids/

- Delete a file in windows command line
- del /f file.o

How does Python come into all of this

- We can rapidly create multiple RELAP input decks, run them, and pull in results data all in one python script
- Why is this valuable?

Python Integration Practice

- Write a python script to do the following:
 - Delete output file
 - Execute RELAP command

RELAP command (if preformed in the relap folder)
"relap5.exe" -i file.i -o file.o -r file.r -w tpfh2o -W tpfh2on -p
file.plt -tpfdir ../fluids/

Delete a file in windows command line del /f file.o





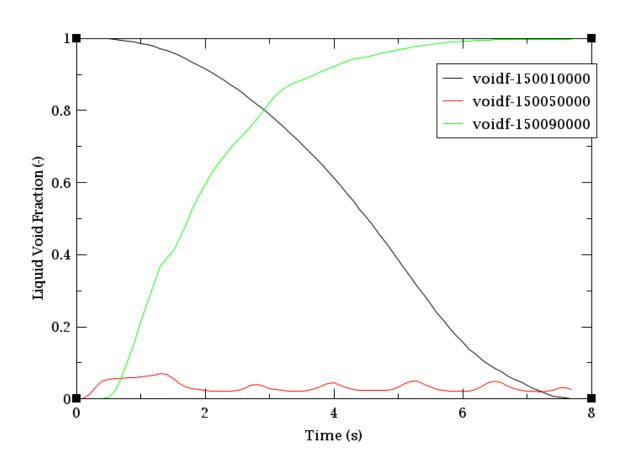
Python Integration Practice

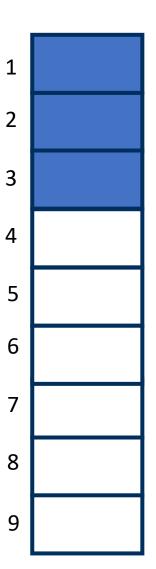
```
import subprocess
import os
# Get the filename from the user
filename = input("Enter a filename (without extension): ")
# Define the input and output filenames
input file = f''{filename}.i"
output_file = f"{filename}.o"
relap5 command = f'relap5.exe -i {input file} -o {output file} -r {filename}.r -w tpfh2o -W tpfh2on -p {file
# Check if the output file exists and delete it
if os.path.exists(output file):
    os.remove(output file)
    print(f"Deleted {output file}")
try:
    subprocess.run(relap5_command, shell=True, check=True)
except subprocess.CalledProcessError as e:
    print(f"Command execution failed with error code {e.returncode}")
except Exception as e:
    print(f"An error occurred: {str(e)}")
else:
    print("Command executed successfully")
```



Practice: Nodalization Study

• Remember HW 2?







Practice: Nodalization Study

- What is the optimum number of volumes?
- Time step has already been set to be less than Courant limit
- To compare results we will plot the time it takes for all of the water to leave the top 1/3 of the pipe

- $(19 \text{ RELAP experts})^*(10 \text{ min}) = 3.17 \text{ hours of manpower}$
- $(1 \text{ python script})^*(18 \text{ sec}) = 0.005 \text{ hours of machine power}$



Let's take a look at the code

```
1 %%capture
 2 # Import needed packages
 3 import numpy as np
 4 import os
 5 %matplotlib inline
   import matplotlib.pyplot as plt
 8 # Create arrays to store data
 9 Volumes = np.zeros(17)
   Times = np.zeros(17)
11
12 # Starting number of Volumes
13 j = 3
14
   for i in range(17):
16
       # Initial Parameters
17
       NoV = j # Number of Volumes
18
       pipe length = 4.16448 # meters
19
20
       name = 'lecture12'
21
       # Calculated Parameters
       minor edit vol = int(NoV*2/3+1) # Minor edit volume of interest (used to see when top 1/3 of the pipe is 99.9% empty)
23
24
        param = "{:02d}".format(minor_edit_vol) # placed in 2 digit form for input into deck
25
```



Creating an input deck

```
# Create Input File
26
       file_name = f'''{name}.i'''
27
28
29
       input_deck = f'''* Title Of Deck
30
        = {name}
31
32
                               Miscellaneous Control Cards
33
34
35
36
37
                       Option
               Type
38
       100
              new
                       transnt
39
               Inp-Chk/Run
40
       101
41
               Input-Units
                              Output-Units
                               si
42
       102
43
                                  CPUalloted
44
              5.0
                         6.0
                                   1000.0
       105
               Noncondensables
45
46
47
               Ref-Vol
                                     Fluid
                             Elev
                                              Name
                                             'Primary'
48
       120
              140010000
49
50
51
52
                                    Time Step Control Cards
53
54
55
56
               TimeEnd MinStep MaxStep Ssdtt MinorEditFreq MajEditFreq
57
                                                                             30000
```



Changing values in the input deck

```
************************
59
60
62
      *************************
63
                        Parameter
                        140{param}0000
      *************************
      **********
      *********
             Name Type
             pipe pipe
             NumOfVolumes
            {int(NoV)}
             Area
                               VolNum
      1400101
                               {int(NoV)}
             Length
                               VolNum
             {pipe_length/NoV}
                                      {int(NoV)}
             InclAng
                               VolNum
                                {int(NoV)}
              ElevationChange
                               VolNum
             {pipe_length/NoV}
                                 {int(NoV)}
              Roughness HydraulicDiam VolNum
                                {int(NoV)}
                                VolNum
             00000000
                                {int(NoV)}
91
                                {int(NoV-1)}
             Ebt Initial-Conditions
     1401201 004 101325. 298. 0. 0 0 {int(NoV*2/3)}
            003 101325. 298. 0. 0 0 {int(NoV)}
             Vel/Mfr
      1401300
             1
             Liquid Vapor Interface JunNum
                                {int(NoV-1)}
99
100
101
```

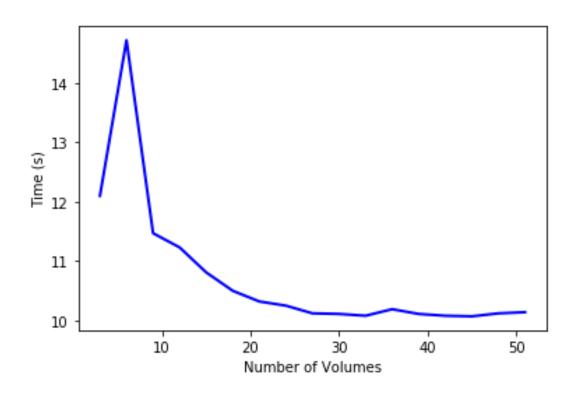


Write deck, run deck, read results

```
# Write deck to input file
103
        with open(file name, 'w') as test file:
104
             test_file.write(input_deck)
105
106
107
         # Run RELAP5-3D
108
         !del /f lecture12.o
109
         !"./relap5.exe" -i lecture12.i -o lecture12.o -r lecture12.r -w tpfh2o -W tpfh2on -p lecture12.plt -tpfdir ../fluids/
110
111
         # Read Output File
        with open("lecture12.0", "r") as a file:
112
         for line in a_file:
113
             stripped_line = line.strip()
114
             a_list = stripped_line.split()
115
116
117
             try:
118
                 map object = map(float, a list)
119
120
                 list of floats = list(map object)
121
                 if(len(list_of_floats) ==2):
122
                    if(list of floats[1] >= 1.0000):
123
124
                         ans = list_of_floats[0]
125
                         break
126
127
             except:
128
                 pass
129
         # Store data from run
130
        Volumes[i] = NoV
131
        Times[i] = ans
132
133
134
        j = j + 3
```



Results





Brainstorming

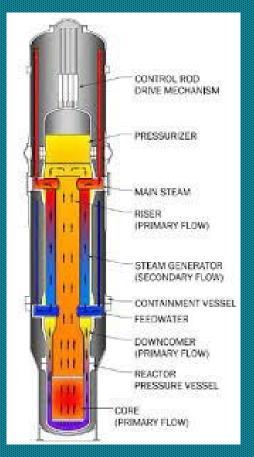
• If this is possible, what else is possible?

```
def update(prev C, prev D, prev J, C,D,J,time step):
    time = time step*900
    a_{file} = open(f''\{n_o_r\}.i'', ''r'')
    list_of_lines = a_file.readlines()
    #valve 785 cv change min and max and scaling factor based on C
    #valve 805 cv change min and max and scaling factor based on D
    list of lines[29] = f'9300201
                                    {float(time)-900}
                                                             {1388.0*prev J}
                                                                                  0.0
                                                                                          0.0\n'
    list of lines[42] = f'9600201
                                     {float(time)-900}
                                                             {1388.0*prev D}
                                                                                          0.0\n'
    list_of_lines[83] = f'6350201
                                                            {100.0*prev_J}
                                     {float(time)-900}
                                                                                0.0 0.0\n'
    list of lines[30] = f'9300202
                                    {float(time)-840}
                                                            {1388.0*J}
                                                                             0.0
                                                                                     0.0\n'
    list of lines[43] = f'9600202
                                    {float(time)-840}
                                                            {1388.0*D}
                                                                             0.0
                                                                                     0.0\n'
    list of lines[84] = f'6350202
                                    {float(time)-840}
                                                            {100.0*J}
                                                                                   0.0\n'
   if prev_C > Cs[i]:
        print('prev_C > Cs')
        list of lines[88] = f'20500100
                                         var1 integral
                                                           -0.005 {0.785*prev C} 0 3 {.784*C}
        list of lines[96] = f'20500110
                                               integral 0.005
                                                                  {0.785*prev D} 0 3 0.0 {.785}\
    elif prev C < Cs[i]:</pre>
        print('prev C < Cs')</pre>
        list of lines[88] = f'20500100
                                               integral -0.005 {0.785*prev C} 0 3 0.0 {.785*
        list of lines[96] = f'20500110
                                                integral
                                                           0.005 {0.785*prev D} 0 3 0.0 {.785}
        print('prev C = Cs')
        list_of_lines[88] = f'20500100
                                                integral
                                                           -0.005
                                                                   {0.785*prev_C} 0 3 {0.785*C-
        list of lines[96] = f'20500110
                                                integral
                                                           0.005
                                                                   {0.785*prev D} 0 3 {.785*D-.001
    list of lines[10] = f"201
                                {float(time)}
    a file.close()
    a file = open(f"{n o r}.i", "w")
    a file.writelines(list of lines)
    a file.close()
```

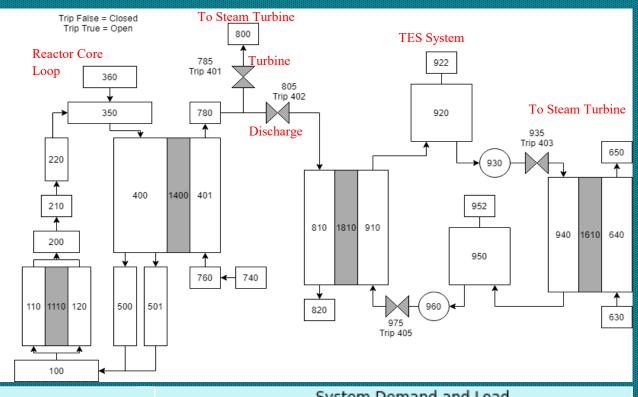


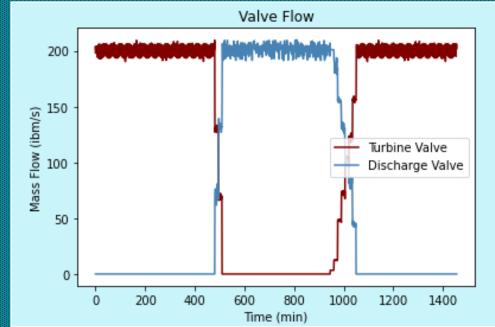
Thermal Energy Storage

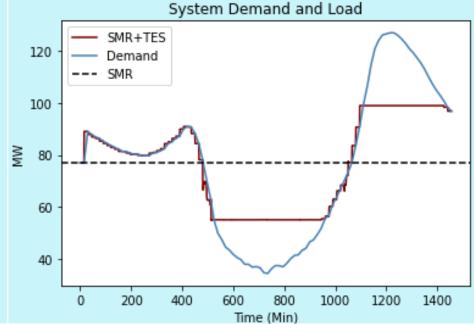
NuScale SMR



Being a baseload power, keeping up with high energy demand is a problem for nuclear reactors. Thermal energy storage systems are a proposed solution to better meet demand at all times of the day and night. The control of these systems is an important feature that requires extensive study for these reactors to be licensed with a storage system. In this work, a model predictive controller matches the load of the entire system with the demand of the power grid over a 24-hour period.

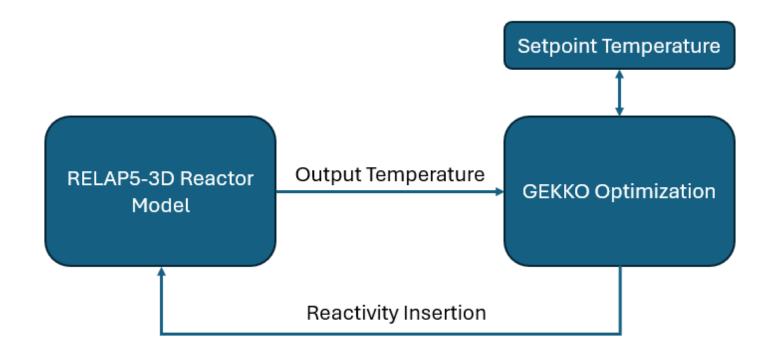






Brainstorming

 If this is possible, what else is possible?



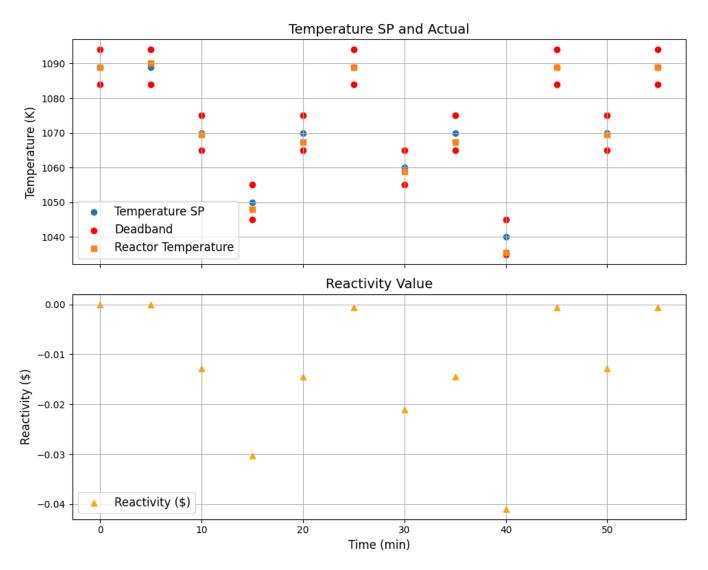


```
360203 written, block no. 25, at time=
                                                                            --- Restart Write # =
0---Restart no.
                                                                 3600.00
  MINOR EDIT
MINOR EDIT time= 3.60000000E+03 adv=360203 M.Ed. Lines
                                                           52
1 time
              cntrlvar
                           rktpow
                                        rkreac
                    82
  (sec)
                                        (dollars)
                           (Watts)
              core
              sum
                 1084.1
   3599,50
                             4.36684E+07 8.60339E-06
   3600.00
                 1084.1
                             4.36684E+07 8.53368E-06
```

```
# Read Output File
with open(output, "r") as a_file:
    for line in a_file:
        stripped line = line.strip()
                                                         def update2(s,prev_s,time_step,power,reac,p):
        a list = stripped line.split()
                                                             time = time_step*300 #Seconds
        try:
                                                             a_file = open(f"{n_o_r}.i", "r")
            map_object = map(float, a_list)
            list of floats = list(map object)
                                                             list_of_lines = a_file.readlines()
                                                             list_of_lines[26] = f'20200301 -1.0 {prev_s}\n' #Could be float_time-600, then float_time -599, then float_time
            if(len(list of floats) == 5):
                                                             list of lines[27] = f'20200302 0.0
                                                                                                    {s}\n'
                if(list of floats[0] == time):
                                                             list_of_lines[28] = f'20200303 {float(time)+.001}
                                                                                                                {s}\n'
                    temp = list_of_floats[1]
                                                             list_of_lines[37] = f'30000001 gamma-ac {float(power)} {float(reac)}
                                                                                                                                                         0.48\n'
                    power = list_of_floats[2]
                                                             list_of_lines[10] = f"201 {float(time)}
                                                                                                          1.0e-7 0.01
                                                                                                                              07003 599 60000000
                    reac = list_of_floats[3]
                                                             list of lines[55] = f'2350302 {float(p)} 1.
                                                                                                                 0.24139 4.7197997 2555.7876 32.58765 828.53474\n'
                    p = list_of_floats[4]
                                                             a_file.close()
                    print(list of floats)
                    break
                                                             a_{file} = open(f''\{n_o_r\}.i'', ''w'')
                                                             a_file.writelines(list_of_lines)
        except:
                                                             a_file.close()
            pass
```

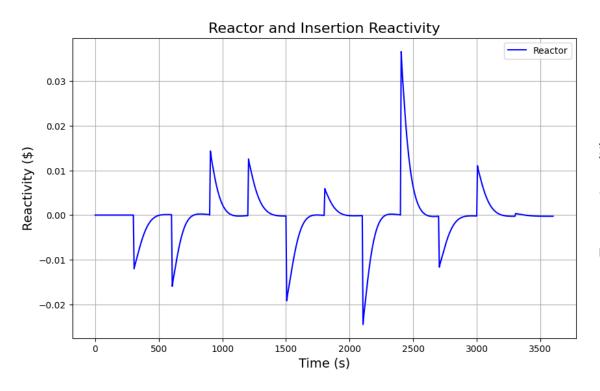
return [temp, reac, power,p]

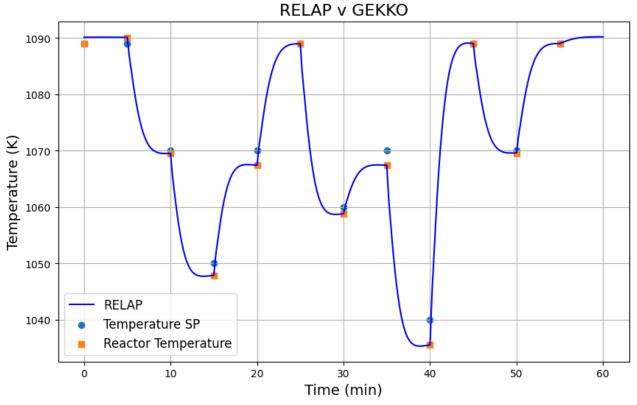
Brainstorming





Brainstorming







Assignment

- Watch DVD sections 64-71 before next class
- HW 6 due Friday (10/17)