

6. In the following URLs, the atomic radii are given as a list that you can readily copy paste into a csv file: [Link 1](#) or [Link 2](#), skip empty rows as needed. Pick an element that has the atomic number ending with the same digit as your roll number and list all elements whose atomic radii are within a certain percentage. Choose this percentage to be 10% to start with and increase if needed to be able to list at least 3 elements that are of comparable size.

The solution includes your script, the element chosen, its radius in picometers, criterion for closeness in size and the list of elements that are close in size. [3 Marks]

Hint: First create a csv file for input data and try a mix of shell and awk scripts.

Application: Analysis of data available in the open domain in not so readily usable form is part of scientific computing research. Webpage scraping, scripts to automate it and storing historical data is part of research.

Link to the GitHub repository for this question: [GitHub](#)

This awk script takes in the Atomic Radii data and outputs the elements whose radii is close to the selected element.

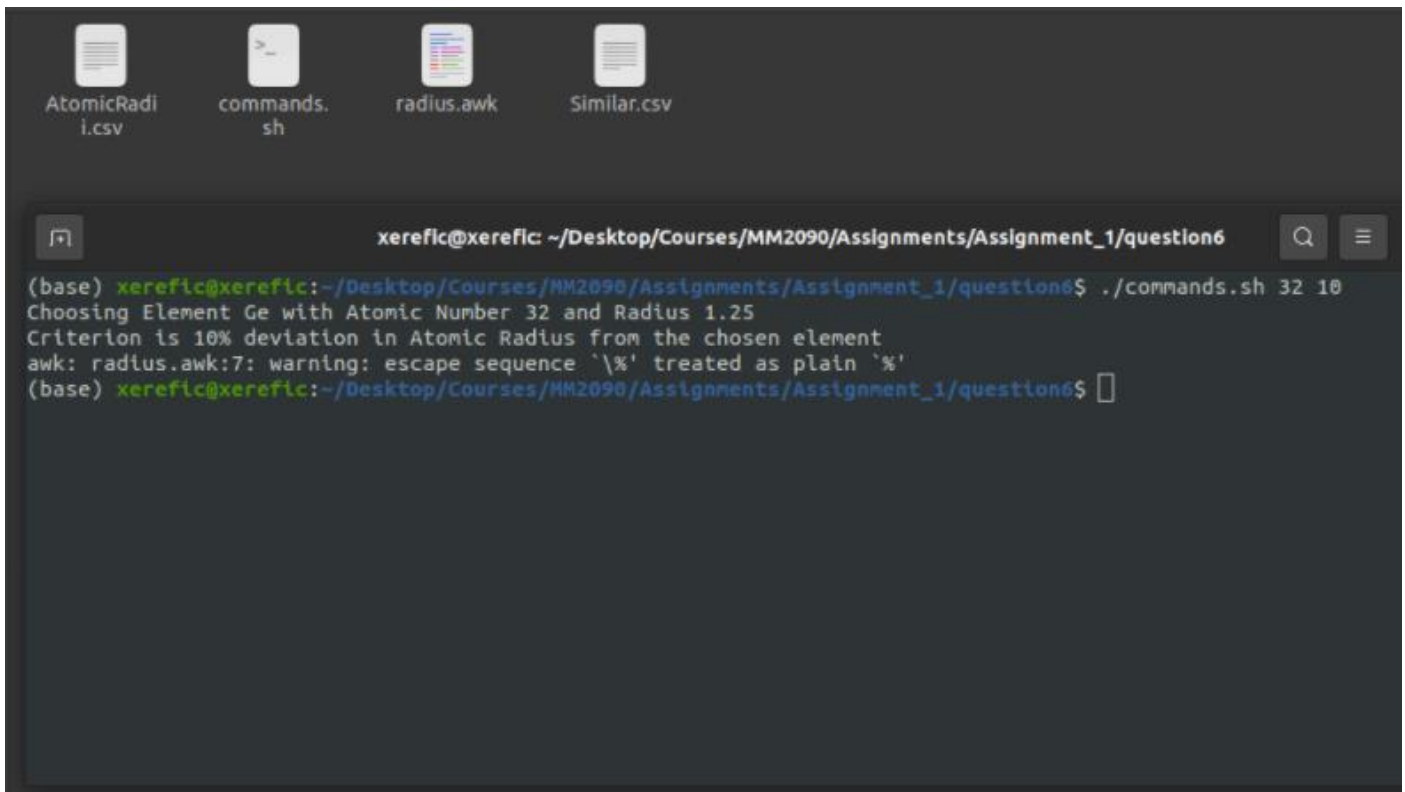
```
1. #!/usr/bin/gawk -f
2. BEGIN{
3.     FS = "\t";
4.     criterion = criterion/100;
5.     # Printing the header
6.     printf("Atomic Number,Element,Atomic Radii,Deviation\n")
7.     printf("%d,%s,%.2f,0%\n", atomic, element, key);
8. };
9.
10. {
11.     # Getting the absolute difference in atomic radii between the chosen element and iterated
12.     diff = $3-key;
13.     if (diff<0) diff = -1*diff;
14.
15.     # Checking if the deviation is <10% and outputting if True
16.     if (diff<=key*criterion && $1!=32) printf("%d,%s,%.2f,%.2f%\n", $1, $2, $3,diff/key*100);
17. };
18.
19. END{
20. };
21.
```

This bash takes the element of interest and the criterion as input and calls the radius.awk wrapper to get the elements with similar atomic radii.

```
1. #!/bin/bash
2.
3. atomic=$1
4. element=`cat AtomicRadii.csv | sed 's/\t/,/g' | awk -v atomic=$atomic -F, '{if($1==atomic) print $2;}'`
5. key=`cat AtomicRadii.csv | sed 's/\t/,/g' | awk -v atomic=$atomic -F, '{if($1==atomic) print $3;}'`
6.
7. echo "Choosing Element $element with Atomic Number $atomic and Radius $key"
8. echo "Criterion is $2% deviation in Atomic Radius from the chosen element"
9. awk -v atomic=$atomic -v element=$element -v key=$key -v criterion=$2 -f radius.awk < AtomicRadii.csv >
   Similar.csv
10.
```

Element Chosen is Germanium (Atomic Number 32).

TERMINAL:



```
xereflc@xereflc: ~/Desktop/Courses/MM2090/Assignments/Assignment_1/question6
(base) xereflc@xereflc:~/Desktop/Courses/MM2090/Assignments/Assignment_1/question6$ ./commands.sh 32 10
Choosing Element Ge with Atomic Number 32 and Radius 1.25
Criterion is 10% deviation in Atomic Radius from the chosen element
awk: radius.awk:7: warning: escape sequence `\' treated as plain \'
(base) xereflc@xereflc:~/Desktop/Courses/MM2090/Assignments/Assignment_1/question6$
```

OUTPUT:

Choosing Element Ge with Atomic Number 32 and Radius 1.25  
Criterion is 10% deviation in Atomic Radius from the chosen element

Atomic Number	Element	Atomic Radii	Deviation
32	Ge	1.25	0%
13	Al	1.18	5.60%
31	Ga	1.36	8.80%
33	As	1.14	8.80%
51	Sb	1.33	6.40%
52	Te	1.23	1.60%
53	I	1.15	8.00%
84	Po	1.35	8.00%
85	At	1.27	1.60%
86	Rn	1.2	4.00%

INPUT (tab separated):

1 H 0.53 0.25 0.37 1.20 0.10
2 He 0.31 0.31 0.32 1.40
3 Li 1.67 1.45 1.34 1.82 0.90
4 Be 1.12 1.05 0.90 0.41
5 B 0.87 0.85 0.82 0.25
6 C 0.67 0.70 0.77 1.70 0.29
7 N 0.56 0.65 0.75 1.55 0.30
8 O 0.48 0.60 0.73 1.52 1.21
9 F 0.42 0.50 0.71 1.47 1.19
10 Ne 0.38 0.38 0.69 1.54
11 Na 1.90 1.80 1.54 2.27 1.16
12 Mg 1.45 1.50 1.30 1.73 0.86
13 Al 1.18 1.25 1.18 0.53
14 Si 1.11 1.10 1.11 2.10 0.40
15 P 0.98 1.00 1.06 1.80 0.31
16 S 0.88 1.00 1.02 1.80 0.43
17 Cl 0.79 1.00 0.99 1.75 1.67
18 Ar 0.71 0.71 0.97 1.88
19 K 2.43 2.20 1.96 2.75 1.52
20 Ca 1.94 1.80 1.74 1.14
21 Sc 1.84 1.60 1.44 0.89
22 Ti 1.76 1.40 1.36 0.75
23 V 1.71 1.35 1.25 0.68
24 Cr 1.66 1.40 1.27 0.76
25 Mn 1.61 1.40 1.39 0.81
26 Fe 1.56 1.40 1.25 0.69
27 Co 1.52 1.35 1.26 0.54
28 Ni 1.49 1.35 1.21 1.63 0.70
29 Cu 1.45 1.35 1.38 1.40 0.71
30 Zn 1.42 1.35 1.31 1.39 0.74
31 Ga 1.36 1.30 1.26 1.87 0.76
32 Ge 1.25 1.25 1.22 0.53
33 As 1.14 1.15 1.19 1.85 0.72

34 Se 1.03 1.15 1.16 1.90 0.56
35 Br 0.94 1.15 1.14 1.85 1.82
36 Kr 0.88 0.88 1.10 2.02
37 Rb 2.65 2.35 2.11 1.66
38 Sr 2.19 2.00 1.92 1.32
39 Y 2.12 1.85 1.62 1.04
40 Zr 2.06 1.55 1.48 0.86
41 Nb 1.98 1.45 1.37 0.78
42 Mo 1.90 1.45 1.45 0.79
43 Tc 1.83 1.35 1.56 0.79
44 Ru 1.78 1.30 1.26 0.82
45 Rh 1.73 1.35 1.35 0.81
46 Pd 1.69 1.40 1.31 1.63 0.78
47 Ag 1.65 1.60 1.53 1.72 1.29
48 Cd 1.61 1.55 1.48 1.58 0.92
49 In 1.56 1.55 1.44 1.93 0.94
50 Sn 1.45 1.45 1.41 2.17 0.69
51 Sb 1.33 1.45 1.38 0.90
52 Te 1.23 1.40 1.35 2.06 1.11
53 I 1.15 1.40 1.33 1.98 2.06
54 Xe 1.08 1.08 1.30 2.16 0.62
55 Cs 2.98 2.60 2.25 1.81
56 Ba 2.53 2.15 1.98 1.49
57 La 1.95 1.95 1.69 1.36
58 Ce 1.85 1.85 1.15
59 Pr 2.47 1.85 1.32
60 Nd 2.06 1.85 1.30
61 Pm 2.05 1.85 1.28
62 Sm 2.38 1.85 1.10
63 Eu 2.31 1.85 1.31
64 Gd 2.33 1.80 1.08
65 Tb 2.25 1.75 1.18
66 Dy 2.28 1.75 1.05
67 Ho 2.26 1.75 1.04
68 Er 2.26 1.75 1.03

69 Tm 2.22 1.75 1.02
70 Yb 2.22 1.75 1.13
71 Lu 2.17 1.75 1.60 1.00
72 Hf 2.08 1.55 1.50 0.85
73 Ta 2.00 1.45 1.38 0.78
74 W 1.93 1.35 1.46 0.74
75 Re 1.88 1.35 1.59 0.77
76 Os 1.85 1.30 1.28 0.77
77 Ir 1.80 1.35 1.37 0.77
78 Pt 1.77 1.35 1.28 1.75 0.74
79 Au 1.74 1.35 1.44 1.66 1.51
80 Hg 1.71 1.50 1.49 1.55 0.83
81 Tl 1.56 1.90 1.48 1.96 1.03
82 Pb 1.54 1.80 1.47 2.02 1.49
83 Bi 1.43 1.60 1.46 1.17
84 Po 1.35 1.90 1.08
85 At 1.27 1.27 0.76
86 Rn 1.20 1.20 1.45
87 Fr 1.94
88 Ra 2.15 1.62
89 Ac 1.95 1.95 1.26
90 Th 1.80 1.80 1.19
91 Pa 1.80 1.80 1.09
92 U 1.75 1.75 1.86 0.87
93 Np 1.75 1.75
94 Pu 1.75 1.75 1.00
95 Am 1.75 1.75 1.12
96 Cm 1.11