CS-7863: Scientific and Statistical Computing
Homework #1
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1.a)

```
## Part A: compute binding energy
computeBindingEnergy <- function(A, Z){
  if (A %% 2 == 1) {
    spin <- 0
  }else if (A %% 2 == 0 && Z %% 2 == 0){
    spin <- 12
  }
  else {
    spin <- -12
  }

  return((15.67*A)-
           (17.23*(A^(2/3)))-
           ((0.75)*((Z^2)/(A^(1/3))))-
           ((93.2)*(((A-(2*Z))^2)/A))+
           (spin/(A^(1/2))))
}
```

1.b)

```
## Part B: compute Z=28 and A=58
# Nickel
bind.energy <- computeBindingEnergy(58,28)
cat(round(bind.energy,digits=2),"MeV")
```

493.94 MeV

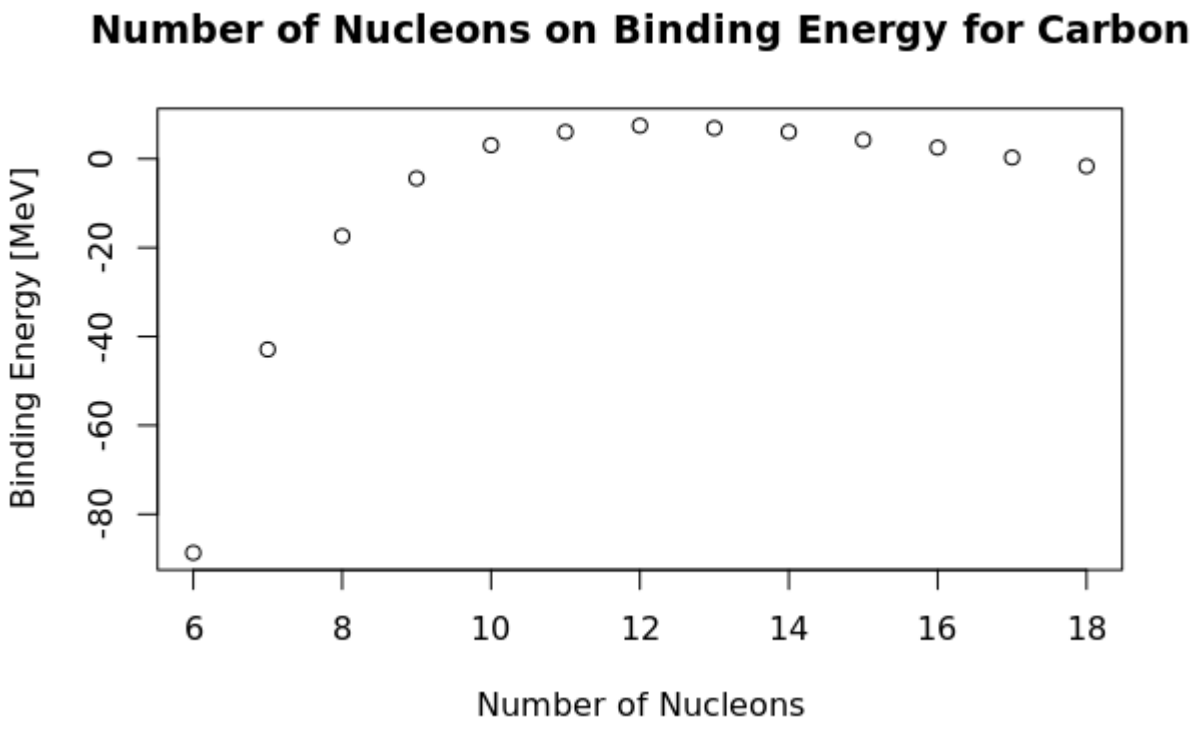
1.c)

```
## Part C: table with two columns: nucleons and binding energy per
nucleon
Z=6 # Carbon
carbon_df <- data.frame(nrow=2*Z, ncol=2)
for (i in seq(Z, 3*Z)){
  # +1 since R indexes at 1
  carbon_df[i-Z+1,] <- rbind(i, computeBindingEnergy(i, Z)/i)
}
rownames(carbon_df) <- NULL
colnames(carbon_df) <- c("A", "B/A")
print(carbon_df, row.names=FALSE)
# Get max binding energy row
print(carbon_df[which.max(carbon_df$"B/A"),], row.names=FALSE)

plot(carbon_df$A, carbon_df$"B/A", xlab="Number of Nucleons",
     ylab="Binding Energy [MeV]",
     main="Number of Nucleons on Binding Energy for Carbon")
```

```
 A        B/A
 6 -88.6719833
 7 -42.9044922
 8 -17.4021699
 9  -4.4111252
10   3.0707868
11   6.0487081
12   7.4500014
13   6.9074722
14   6.0478948
15   4.2257131
16   2.5250851
17   0.2890953
18  -1.6752533
```

```
> print(carbon_df[which.max(carbon_df$"B/A"),], row.names=FALSE)
 A      B/A
12 7.450001
```



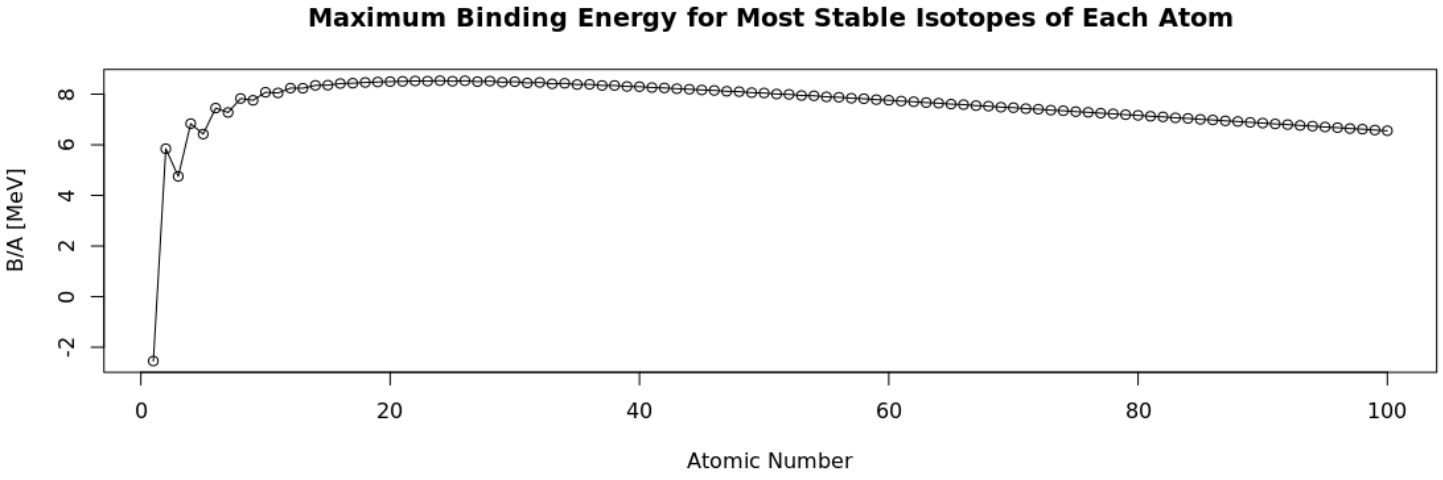
1.d)

```
## Part D: find the value of A that gives the maximum binding energy
computeMaxBind <- function(Z){
  maxBind <- -Inf
  A.maxBind <- -Inf
  for (i in seq(Z, 3*Z)){
    bindE <- computeBindingEnergy(i, Z)/i
    if (bindE > maxBind){
      maxBind <- bindE
      A.maxBind <- i
    }
  }
  return(c(A.maxBind, maxBind))
}
```

1.e)

```
bounds <- 100
binding_df <- data.frame(nrow=bounds, ncol=2)
for (i in seq(1, bounds)){
  binding_df[i,] <- c(i, computeMaxBind(i)[2])
}

plot(binding_df, xlab="Atomic Number", ylab="B/A [MeV]", type="o",
     main="Maximum Binding Energy for Most Stable Isotopes of Each
Atom")
```




```
# Z with largest binding energy
print(binding_df[which.max(unlist(binding_df[2])),], row.names=FALSE)
```

```
nrow     ncol
  24 8.532623
```