Python for Physicist

Lecture Note - 4

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List and Arrays

- List:
  - x = [a, b, c]
  - y = [1, 2, 4, 7, 2, 5, 9]
  - z = log(y)
  - y.append(10)
  - y.pop()
- Arrays:
  - Number of elements are fixed
  - Same data type
  - n-dimensional matrix
  - Arithmatics of arrays are like matrix operation in mathematics
  - The package 'numpy' is very efficient with the arrays

Simple Physics Problem

- Problem:
  - If a ball falls from a tower (Height = H) freely, what would the height (h) after each second before reaching the ground.
- Analysis:
  - Similar to the earlier problem. **Save height and time in an array.**
- The Python code:

```
before loop:

    save_h = []
    save_t = []

within loop:

    save_h.append(H-s)
    save_t.append(t)
```

Plotting by python

matplotlib as package for plotting graph in a desirable way

```
import matplotlib.pyplot as plt
x = [1, 2, 3, 4, 5]
y = [1, 3, 4, 2, 5]
plt.plot(x,y)
plt.show()
```

Try:

```
plt.plot(x,y, 'ro')
plt.xlabel('x axis with unit')
plt.ylabel('y axis with unit')
```

http://matplotlib.org/1.3.1/gallery.html

Reading data from a file

- 'numpy' can be used to read data file as

```
from numpy import loadtxt
a = loadtxt(“data.txt”, float)
print(a)
```

Example for testing programming performance

- Printing 0 to 99 by using **for-loop** statement

```
for n in range(100):
    print(n)
```

- Emission lines of hydrogen atom:
  - $\frac{1}{\lambda} = R\left(\frac{1}{m^2} - \frac{1}{n^2}\right)$

  Code:

```
R = 1.09e-2
for m in [1, 2, 3]:
    print("Series for m = ", m)
    for k in [1, 2, 3, 4, 5]:
        n = m + k
        invlambda = R * (1/m**2 - 1/n**2)
        print(" ", 1/invlambda, " nm")
```

Exercise: Can you simplify the above code?

Exercise

Calculate the Madelung constant

In the case of table salt, sodium and chlorine are sturcted in a cubic arrangement with the alternating position.

Consider

- For the co-ordinate system (i, j, k) the position is defined as
  - sodium at $i + j + k = even$ and chlorine at $i + j + k = odd$
  - sodium reside at the origin $(i = j = k = 0)$

Analysis

- For lattice spacing, a, the distance between atom at (i,j,k) from origin will be $\sqrt{(ia)^2 + (ja)^2 + (ka)^2} = a\sqrt{i^2 + j^2 + k^2}$
- So, the potential at origin will be $V(i, j, k) = \pm \frac{e}{4\pi\epsilon_0 a\sqrt{i^2+j^2+k^2}}$.
- Thus the total potential at the origin will be $V_{total} = \sum_{i,j,k=-L}^{L} v_{i,j,k} = \frac{e}{4\pi\epsilon_0 a} M$
- where M is the Madelung constant

Exercise Write a program to calculate the Madelung constat for table salt.