

# Matrix operations

# Matrix Multiplication

$$A = \begin{pmatrix} 12 & 7 & 3 \\ 4 & 5 & 6 \\ 7 & 8 & 9 \end{pmatrix} \quad B = \begin{pmatrix} 5 & 8 & 1 & 2 \\ 6 & 7 & 3 & 0 \\ 4 & 5 & 9 & 1 \end{pmatrix}$$

$$C_{ij} = A_{ik} \times B_{kj}$$

no of row =len(B)

no of column =len(B[0])

<https://github.com/ChemistryCourses/CH603/blob/master/programs/class3/matrix.py>

[https://github.com/ChemistryCourses/CH603/blob/master/programs/class3/matrix\\_big.py](https://github.com/ChemistryCourses/CH603/blob/master/programs/class3/matrix_big.py)

for logging time use time.time()

<https://github.com/ChemistryCourses/CH603/blob/master/programs/class3/matrix.f90>

# Numpy

NumPy is the fundamental package for scientific computing with Python. It contains among other things:

- a powerful N-dimensional array object
- sophisticated (broadcasting) functions
- tools for integrating C/C++ and Fortran code
- useful linear algebra, Fourier transform, and random number capabilities

Besides its obvious scientific uses, NumPy can also be used as an efficient multi-dimensional container of generic data. Arbitrary data-types can be defined. This allows NumPy to seamlessly and speedily integrate with a wide variety of databases.

**Tutorial:** <https://numpy.org/devdocs/user/quickstart.html>

**Detail Documentation:** <https://numpy.org/devdocs/>

# Matrix diagonalization

$$A = \begin{pmatrix} 12 & 7 & 3 \\ 4 & 5 & 6 \\ 7 & 8 & 9 \end{pmatrix}$$



"I climb all this way, and you tell me *THAT'S* the meaning of life?!"

# Hartree-Fock

## Resources :

1. David Sherils Lecture (<https://www.youtube.com/watch?v=6XFOF8-QkAM&feature=relmfu>, <http://www.youtube.com/watch?v=1jHkt1Qzv1A&feature=relmfu>)
2. Lecture Notes from last years CH560 course(<https://achintyachemist.wixsite.com/achintya/courses>)
3. CH560 Course

We are going to closely follow the Hartree-Fock programming tutorial developed by the group of **Prof. Daniel Crawford** at VIRGINIA TECH( <https://github.com/CrawfordGroup/ProgrammingProjects/tree/master/Project%2303>)