Simulation Tutorials
Lecture 1

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1.1. Purpose and Important Points of This Tutorial

Purpose:

- The purpose of this tutorial is to acquire practical knowledge and skills in computer simulations, which are essential in various aspects of scientific research.
- To achieve this goal, the lectures and exercises will cover a wide range of practical numerical calculation methods, from basic programming for **analysis** and **plotting** using C (C++) and Python to practical numerical simulation techniques such as the Monte Carlo method and molecular dynamics, with a focus on their broad application in scientific research.

Important Points:

- A self-study assignment will be given after each tutorial session.
- The main computations in this tutorial will be demonstrated using C (C++), and the plotting will be done using Python, with explanations provided.
- However, you are free to use other languages or adjust the division of tasks (e.g., writing everything in Python) for the self-study and report assignments.

Sample Programs:

- Sample programs will be stored in the following GitHub repository, so please download them as needed. [**Link**][1]

1.2. Syllabus

The following topics are planned to be covered in this tutorial (subject to change depending on the progress).

1. Introduction
   - Basics of C (C++) (mainly for numerical calculations)
   - Basics of Python (for data analysis and plotting)
   - Concepts of numerical calculations
   - Loss of significance
   - Non-dimensionalization in scientific calculations
2. Numerical solutions of ordinary differential equations: Examples with harmonic oscillators and damped oscillations
   - Numerical integration of differential equations
   - Stability and conservation laws of orbits
3. Brownian motion of a single particle
   - Langevin equation (stochastic differential equation)
   - Generation of normal random numbers
   - Euler-Maruyama method
   - Time averaging and ensemble averaging
4. Brownian motion of multi-particle systems
   - Calculation methods for interaction forces
   - Non-equilibrium system simulations: Example with phase separation
5. Molecular dynamics simulation of multi-particle systems
   - Position Verlet method and velocity Verlet method
   - Conservation laws in multi-particle systems
6. Monte Carlo method
   - Review of statistical mechanics
   - Markov chain Monte Carlo method
   - Metropolis algorithm

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2.1. Setting up the C(C++) Environment

- In this tutorial, the primary numerical calculations will be done using C(C++), and plotting will be done using Python.
- Setting up the C(C++) environment:
  - **Windows:** Installing Ubuntu Dr. Yoshii's manual (in Japaneses): [**Link**] [2]
  - **mac:** Installing Homebrew [**Homebrew Official Link**] [2]

List 1: (On terminal) (For mac) Installing emacs (terminal editor) using Homebrew.

```
brew install emacs
```

Common Unix Commands

- cd (directory name): Change directory
- mkdir (directory name): Create a directory
- rm (directory name): Remove a directory
- touch (file name): Create a file
- ls: List files and directories

2.2. Compiling C(C++) Programs

This section explains how to compile and run the following C(C++) program (pi.cpp) on your computer.

- **C Compiler:**

Various Compilers

- gcc: GNU C compiler collection.
- g++: GNU C++ compiler collection.
- clang: An alternative to gcc — the default compiler on macOS.
- clang++: An alternative to g++ — the default compiler on macOS.
- icc: Intel C/C++ compiler — expensive but offers faster computation speed.

Compilation Options

- -O3: One of the optimization options (i.e., -O -O0 -O1 -O2 -O3 -Os -Ofast -Og). -O3 is most commonly used.
- -o: Specifies the name of the output file.

- Sample program “pi.cpp”

2.2. Compiling C(C++) Programs (2)

List 2: Sample program in C “pi.cpp”

```
#include <stdio.h> // for printf, etc
#include <stdlib.h> // for rand(), etc
#include <math.h> // for sin(),cos(), etc
#include <iostream>// for cout, etc
#include <iomanip>// for setprecision()
#include <fstream> // for ifstream/ofstream
#include <time.h>// for time(NULL), etc

int main(void){
  int i, count = 0, max = 1e+5;
  double x,y,z,pi;
  char fname[128];
  std::ofstream file;
  srand(time(NULL));  // "time(NULL)" as a seed of ramdom number
  sprintf(fname,"coord%d.dat",max); // Define the file name for fname[128]
  file.open(fname); // "file" with the name of fname[128]
  for(i=0;i<max;i++){
    x = (double)rand()/RAND_MAX;
    y = (double)rand()/RAND_MAX;
    z = x*x + y*y;
    if(z<1){
      count++;
```

2.2. Compiling C(C++) Programs (3)

```
      file << x <<" "<<y <<std::endl;
    }
  }
    file.close();
    pi = (double)count / max * 4.;
    printf("%.20f\n",pi); //by C, %.20f -- Displaying with 20 decimal precision
    std::cout<< std::setprecision(21) <<  pi  << std::endl; // by C++

    return 0;
}
```

- Download the program from the designated GitHub repository [**Link**] [1].
- How to download from GitHub [**Link**] [3].
- After downloading, place ‘pi.cpp‘ in an appropriate directory.
- In the directory where ‘pi.cpp‘ is located, execute the following commands.
- Compilation method:

2.2. Compiling C(C++) Programs (4)

List 3: (On terminal) Example of code compilation: (**execute each**). Use the `-o` option to specify the name of the output executable file. a.out is obtained in case of no -o option.

```
g++ -O3 pi.cpp
g++ -O3 pi.cpp -o pi.out
g++ -O3 -o pi.out  pi.cpp
clang++ -O3 -o pi.out  pi.cpp
```

- Execution method:

List 4: (Linux/Mac terminal) Running the program (pi.out).

```

./pi.out
```

- Execution result:

List 5: (On terminal) Example of program execution result. Note that the values may vary each time as the random seed is set to the current time.

```

3.14536000000000015575
3.14536000000000015575
```

2.2. Compiling C(C++) Programs (5)

Useful Editor (Optional): Visual Studio Code

Setup Manual (in Japanses, Created by Mr. Ikeda, R Lab, Nagoya):

- Win: [**Link**]
- Mac: [**Link**]

2.3. Setting up the Python Environment

- In this course, Python programs will be executed using Jupyter Notebook.
- Jupyter Notebook is included in Anaconda Navigator ([**Official Link**], see Figure **1**).
- Refer to the following for instructions on installing Anaconda Navigator.
  - **Windows/mac:** Installation of Anaconda Navigator
    [**Windows manual**] [**Mac manual**]
- The installation method for Jupyter Notebook is shown in Figure **2**.

2.3. Setting up the Python Environment (2)

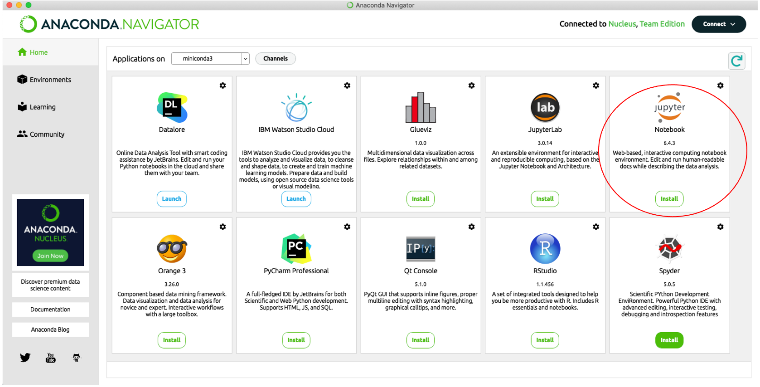
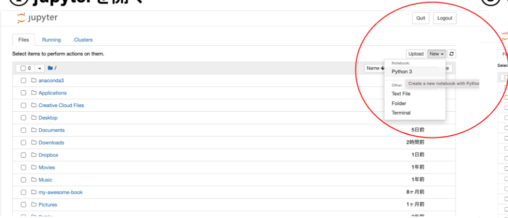


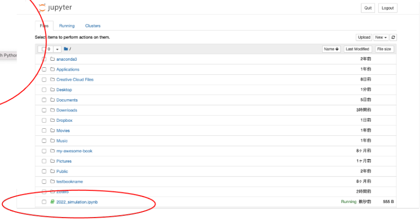
Fig 1: Install and run the Jupyter note book (circled in red) found in the Anaconda Navigator. Now you can use python.

2.3. Setting up the Python Environment (3)

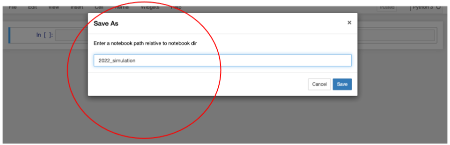
①jupyterを開く



③②で作ったnotebookを開く



②Newのタブを開きpython3を選び，新規Notebookに名前をつける．



④ グレーの箱にプログラムを書き込み，shift+enterで実行

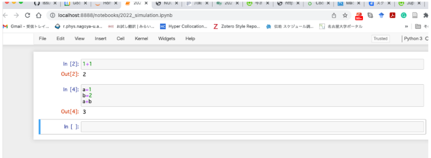


Fig 2: From the start of the Jupyter notebook to the execution of python..

2. 4. Running Python (matplotlib)

- Run the following program (plotting using matplotlib.pyplot) on Jupyter Notebook (see the execution result in Figure **3**).
- (Reference) matplotlib manual [**Link**]

Supplement on Plotting with Python [4]

- matplotlib: A graphics package for Python.
- matplotlib.pyplot: Provides various graph tools such as axes, figure, plot, scatter, etc.

List 6: Importing and using matplotlib.pyplot example

```
import matplotlib.pyplot as plt
fig = plt.figure(figsize=(7,7))
```

- NumPy: Provides fast computation. Many packages refer to NumPy. Offers various linear algebra operations, statistical operations, special functions, etc.

List 7: Importing NumPy

```
import numpy as np
```

2. 4. Running Python (matplotlib) (2)

List 8: Python Sample Program “matplot.py”

```
import matplotlib.pyplot as plt
%matplotlib inline
# Increase the resolution of the graph
%config InlineBackend.figure_format = 'retina'
price = [100, 250, 380, 500, 700]
number = [1, 2, 3, 4, 5]

# Plot the graph
plt.plot(price, number)

# Graph title
plt.title("price / number")

# x-axis label
plt.xlabel("price")

# y-axis label
plt.ylabel("number")

# Display the graph
plt.show()
```

2. 4. Running Python (matplotlib) (3)

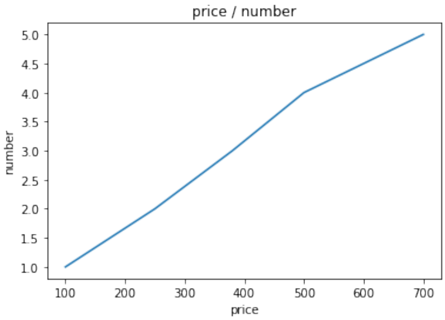


Fig 3: Execution result of matplot.py.

- Next, create a scatter plot of “coord100000.dat” generated by running the program in List 2, as shown below.
- In the sample program “coord.py,” some advanced formatting is applied, such as adjusting the size of the figure, aspect ratio, axis thickness, font size, and font (TeX). Execution result (Figure **4**):

2. 4. Running Python (matplotlib) (4)

List 9: Python Sample Program “coord.py”

```
import matplotlib
import matplotlib.pyplot as plt
%matplotlib inline
# Increase the resolution of the graph
%config InlineBackend.figure_format = 'retina'
import numpy as np
# TeX font
#plt.rcParams["text.usetex"] =True

# Change the overall size and aspect ratio of the figure
fig = plt.figure(figsize=(7,7))

# When placing multiple graphs, change this
ax = fig.add_subplot(111)

# Change the file path as needed
x, y  = np.loadtxt("./Lecture1/coord100000.dat", comments='#', unpack=True)
plt.plot(x, y, "o",markersize=0.5,color="b",label=r"$x^2+y^2\leq1$")

# Graph formatting
plt.tick_params(which='major',width = 1, length = 10)
plt.tick_params(which='minor',width = 1, length = 5)
```

2. 4. Running Python (matplotlib) (5)

```python
ax.spines['top'].set_linewidth(3)
ax.spines['bottom'].set_linewidth(3)
ax.spines['left'].set_linewidth(3)
ax.spines['right'].set_linewidth(3)
plt.xlabel(r"$x$",color='k', size=30)
plt.ylabel(r"$y$",color='k', size=30)
plt.xticks(color='k', size=25)
plt.yticks(color='k', size=25)
# Adjust the presence, position, and size of the graph legend
plt.legend(ncol=1, loc=1, borderaxespad=0, fontsize=25,frameon=True)
# Set graph margins
plt.subplots_adjust(wspace=0.0, hspace=0.25)
# Set the aspect ratio of each graph to 1:1
ax.set_aspect('equal', adjustable='box')
# Change the file path as needed.
plt.savefig('./Lecture1/coord.png')
plt.savefig('./Lecture1/coord.pdf')
```

2. 4. Running Python (matplotlib) (6)

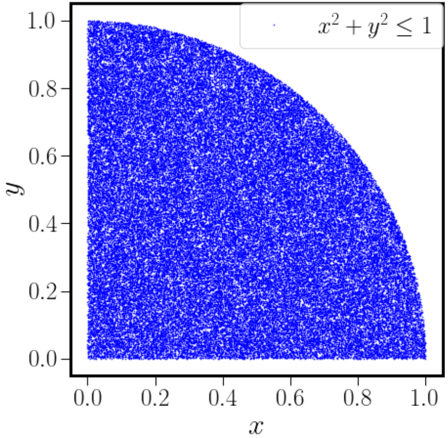


Fig 4: Execution result of coord.py.

Contents

3. First Assignment

Convergence of π (Monte Carlo Simulation)

(1) Based on the sample program in List 2, examine the convergence of the calculated value of π as the number of random samples n changes. Create a graph with n on the horizontal axis and the calculated value of $\pi(n)$ on the vertical axis. Also, plot the error $\delta(n) = |\pi(n) - \pi|$ relative to the theoretical value of π as a function of n, and evaluate the results.

(2) (Advanced Problem) In large-scale numerical simulations, the standard pseudo-random number generator rand() may occasionally cause issues due to its short period. On the other hand, the Mersenne Twister, developed by Makoto Matsumoto, is known for its high-quality pseudo-random number generation [**Reference Link**] [6]. Modify the sample program in List 2 to use the Mersenne Twister instead [**Reference Link**] [7]. The Mersenne Twister header file has been placed in the designated GitHub repository [**Link**] [1], so feel free to use it.

Contents

References and Websites

[1] Takeshi Kawasaki.
2024-simulation-tutorial (GitHub), April 2022.

[2] Homebrew (The Missing Package Manager for macOS (or Linux)).
https://brew.sh/index_ja.

[3] GitHub からファイルをダウンロードする方法【2020 年 12 月追記】.
https://tetsufuku-blog.com/github-download/, April 2020.

[4] Hiroshi Hashimoto and Koji Makino.
Python コンピュータシミュレーション入門.
オーム社, 2021.

[5] Kotaro Matsumoto.
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[6] Makoto Matsumoto.
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[7] Takahiro Ohmi.
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https://omitakahiro.github.io/random/random_variables_generation.html.