

# Homework 3

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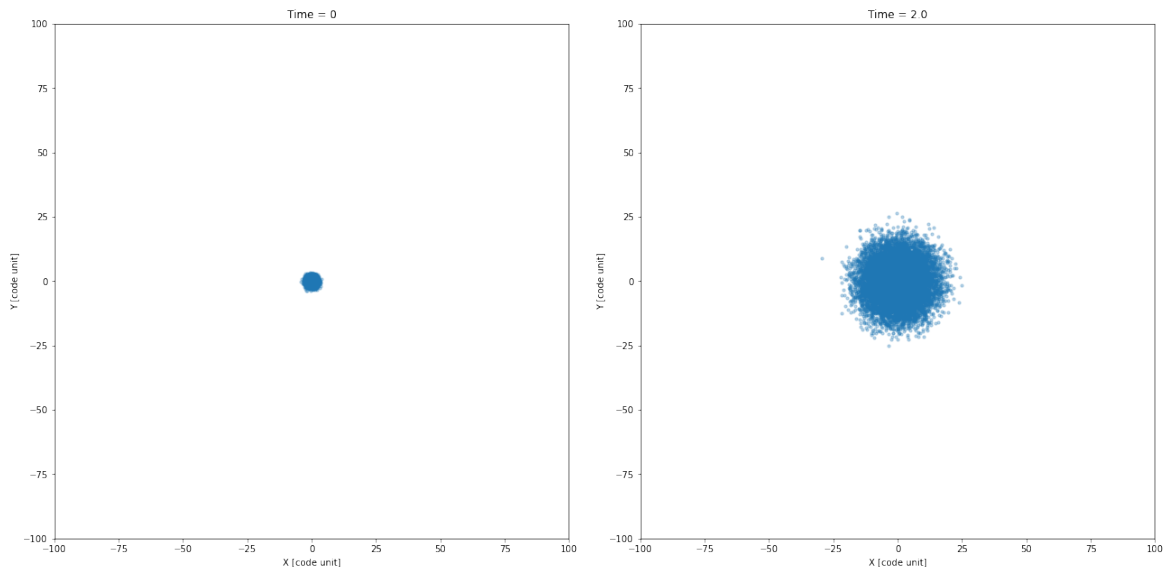
Hsinchu, Taiwan

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## 1 Programming Assignments

### 1.1 (1) Normal Cloud

In this section, in the beginning, we create a cloud of particles ( $N = 10^4$ ) distributed by a normal distribution with zero mean and one variance (or in other words,  $s.d. = 1$ ) in 3D Cartesian coordinates. Additionally, we set the initial particle velocities, and accelerations are distributed by the same normal distribution and the system's total mass is 20. We, afterward, use our N body simulation code from  $t = 0$  up to  $t = 10$  with a constant time step  $\Delta t = 0.01$  and a soften length  $r_{soft} = 0.01$ . We, meanwhile, implement numba @njit with 8 cores to accelerate the loop speed (@jit (nopython=True) have spent more time so I discard to use it). Besides, I, firstly, set the particle's number  $= 10^5$  tried to use either @jit or @njit to accelerate the code; however, with RK4 it takes no lowering than 800 minutes! Therefore, I use  $10^4$ , instead. Figure1 is the group of snap-shot of the normal cloud distribution with the RK4 method and with the extended boundary from -50 to +50. This is a time-consuming task, for orders of 4, RK4, it took 42015 [s]; for orders of two, RK2 and Leapfrog, they took 29506 and 18009 [s], respectively. The last order of one, Euler, took 17794 [s].



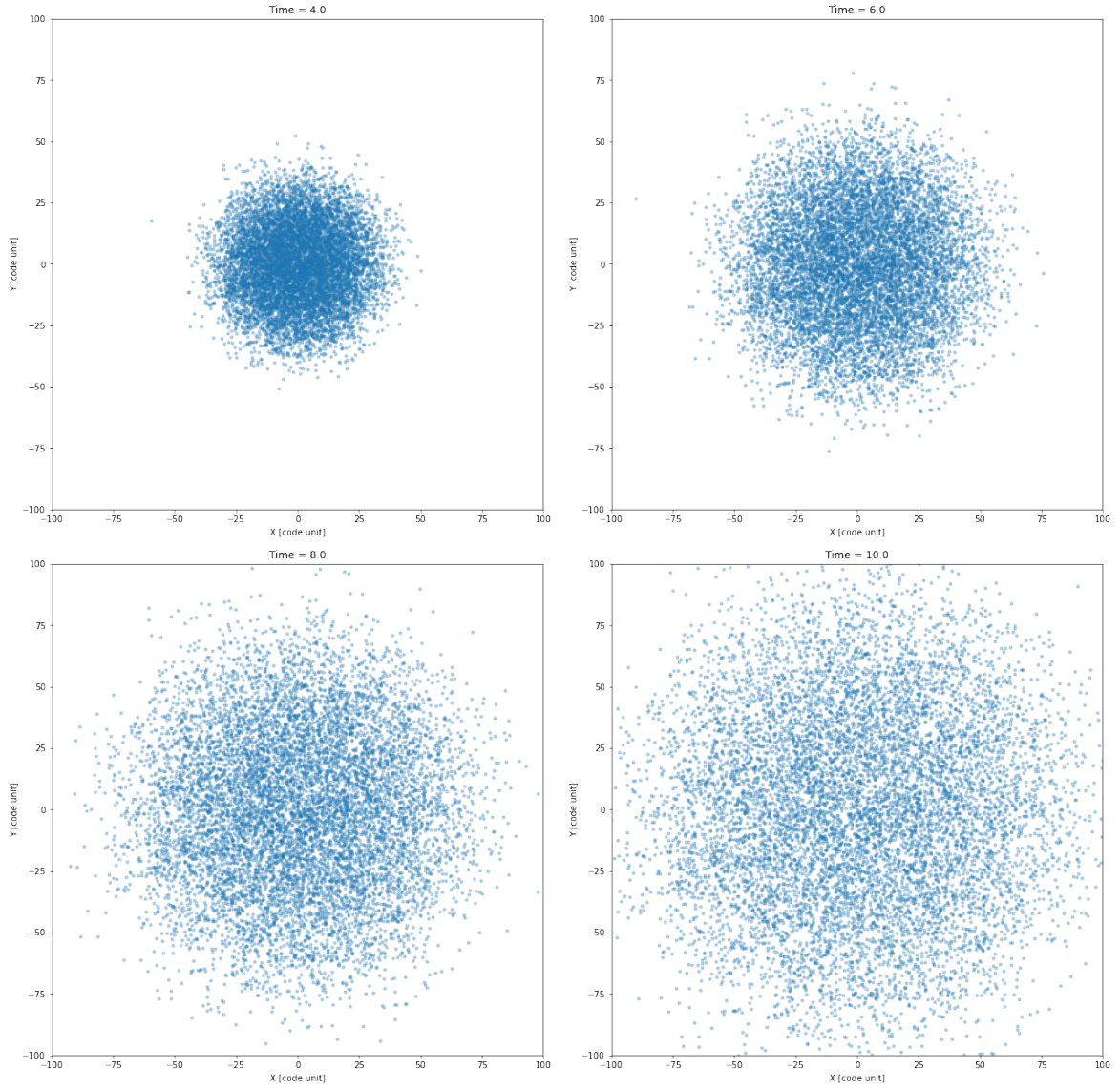


Figure 1: This the normal cloud with RK4, from  $t = 0$  to  $t = 10$  and  $dt = 0.01$ . One run took: 18009 [s]

## 1.2 (2) Leapfrog method

The leapfrog method is a second-order method for solving an initial value problem. The main idea in this is divided into three parts, kick-drift-kick. For each time step  $dt$ , each particle receives a half-step kick,

$$v_{i+1/2} = v_i + a_i \frac{dt}{2}$$

and use the above half-step velocity, and followed by a full-step drift,

$$x_{i+1} = x_i + v_{i+1/2} dt$$

and lastly, use the above drift, and followed by another half-step kick,

$$v_{i+1} = v_{i+1/2} + a_{i+1} \frac{dt}{2}$$

In the next subsection, we will discuss and compare the Leapfrog method with Euler, RK2, and RK4 as well.

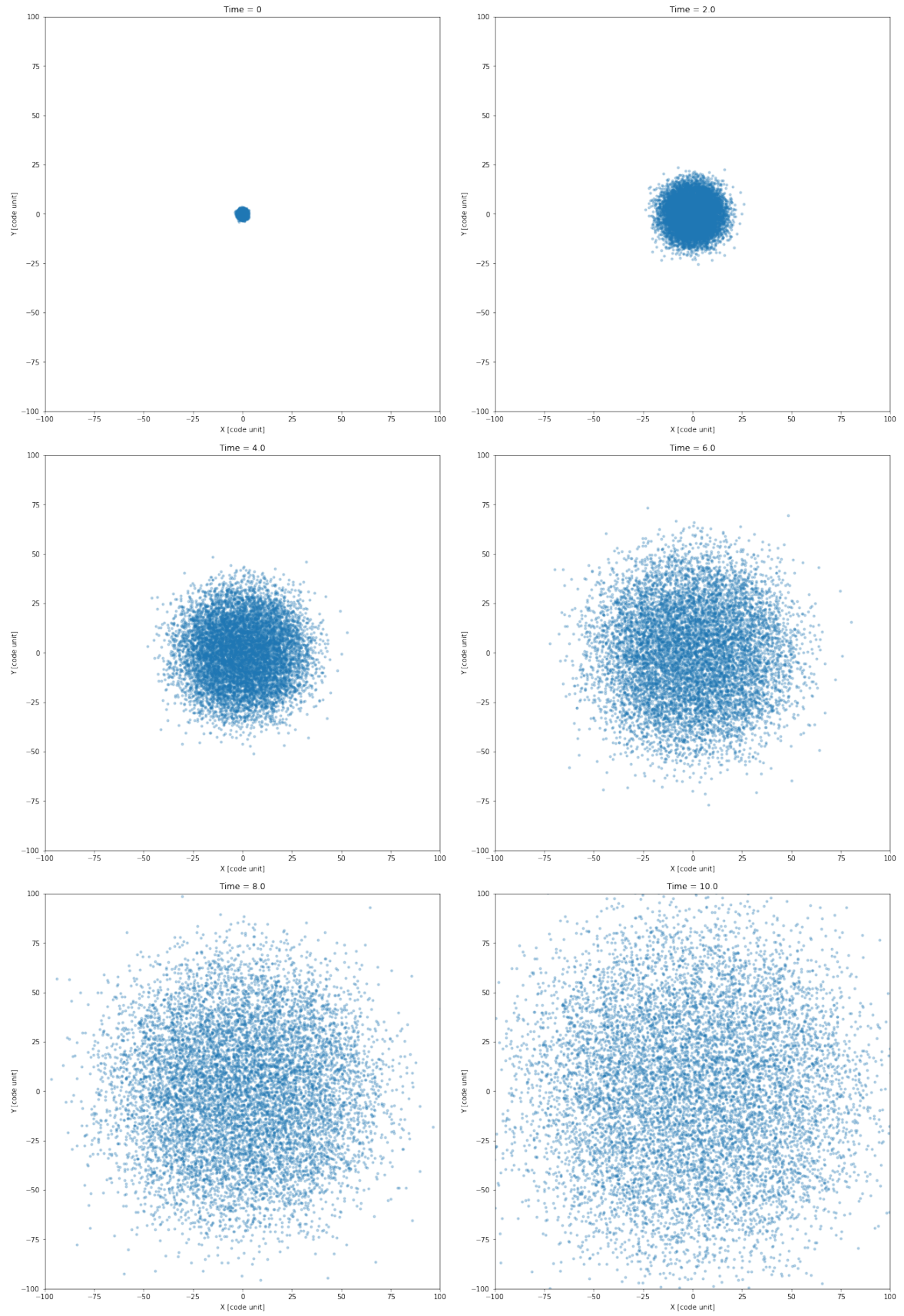


Figure 2: This the normal cloud with Leapfrog, from  $t = 0$  to  $t = 10$  and  $dt = 0.01$ . One run took: 18009 [s]

### 1.3 (3) Energy comparison

In this section, we will discuss kinetic energy, potential energy, and total energy. The definitions are below:

$$U = -\frac{Gm_i m_j}{r + r_{soft}}$$

$$K = \frac{1}{2}m_i v_i^2$$

$$E = U + K$$

where the subscriptions indicate which particles;  $G$  is the gravitational constant, here we set it to 1;  $m$  is the mass of each particle;  $r$  and  $r_{soft}$  is the distance between two particles and the tolerance of distance, which can avoid the nominator equal to zero. After defining all the parameters, we use four different methods, Euler, RK2, RK4, and Leapfrog, and implement the initial conditions as in section 1 to rerun the codes.

See in Figure 3~6, we can find out that the potential energy is much smaller than the kinetic energy owing to the small masses of particles. On the other hand, the total energy is dominated by the kinetic part, which makes sense to us. In Figure 3~6, we can also see the total energy is not the “constant” at the beginning because we initially set the normal random accelerations to each particle which can be regarded that there are other forces applied to the particles. Nevertheless, in the wake of a little period, the total energy will gradually be in a stable stage because of no external force. These phenomena not merely can see in the Euler but in others as well. Compare this with the stable speed, which means how long to be stable. We use RK4 as the theoretical benchmark. It is obvious that Euler (first order) is the slowest one; in the other words, it is the most distorted one; for the second order, RK2 is shapeless at the beginning, and Leapfrog is the most similar one with the benchmark. Therefore, we can conclude that if individuals want to calculate a large number of particles problem, they can choose the Leapfrog method because it has not merely high speed but also high accuracy. (detail of accuracy can see in the next section, the accuracy compared with the benchmark is within one order.)

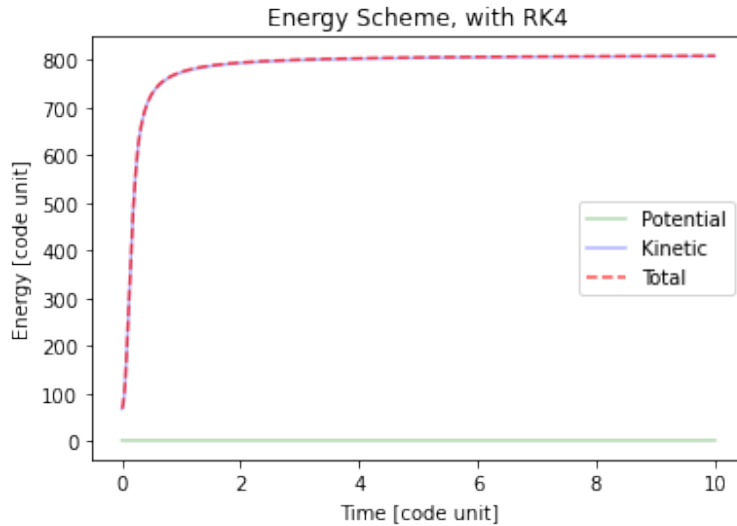


Figure 3: RK4, y-axis is Energy; x-axis is time.

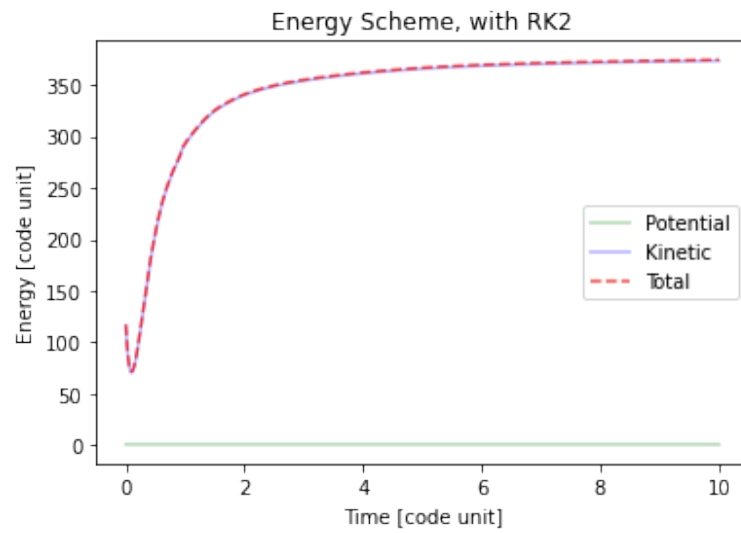


Figure 4: RK2, y-axis is Energy; x-axis is time.

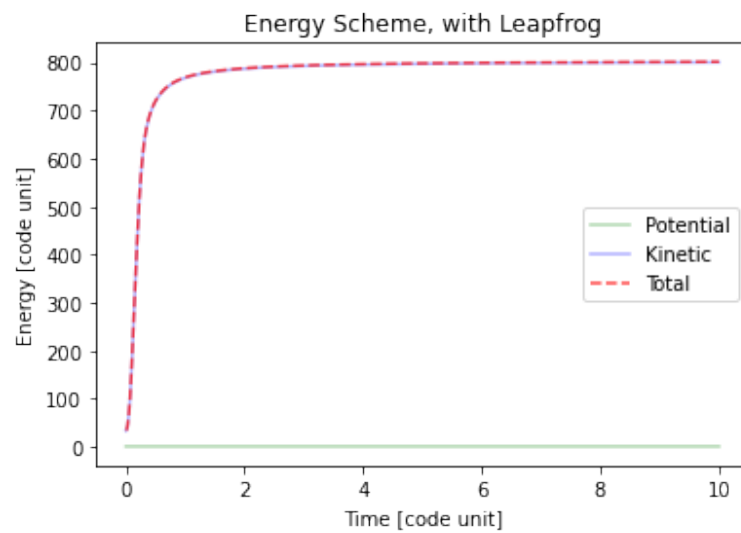


Figure 5: Leapfrog, y-axis is Energy; x-axis is time.

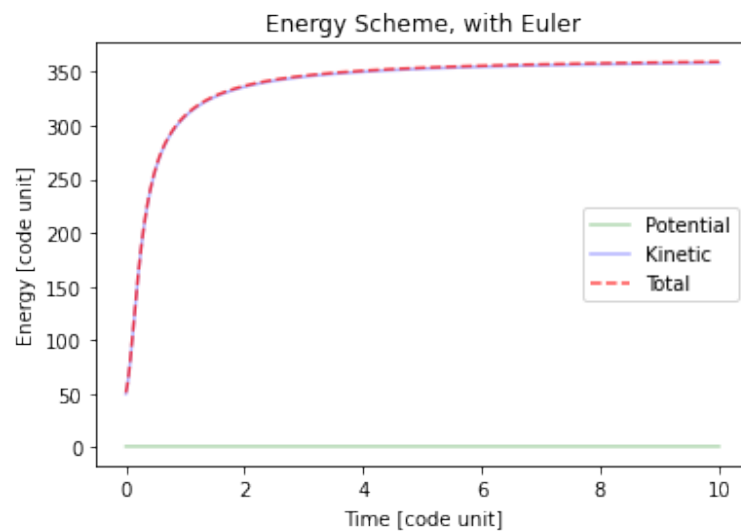


Figure 6: Euler, y-axis is Energy; x-axis is time.

So as to analyze the accuracy of the Leapfrog method, we set the RK4 (fourth order) as a benchmark. We, likewise, applied a logarithm of 10 to investigate the order of accuracy thereafter. In Figure 7, we can see the accuracy comparisons between Leapfrog methods and the benchmark.

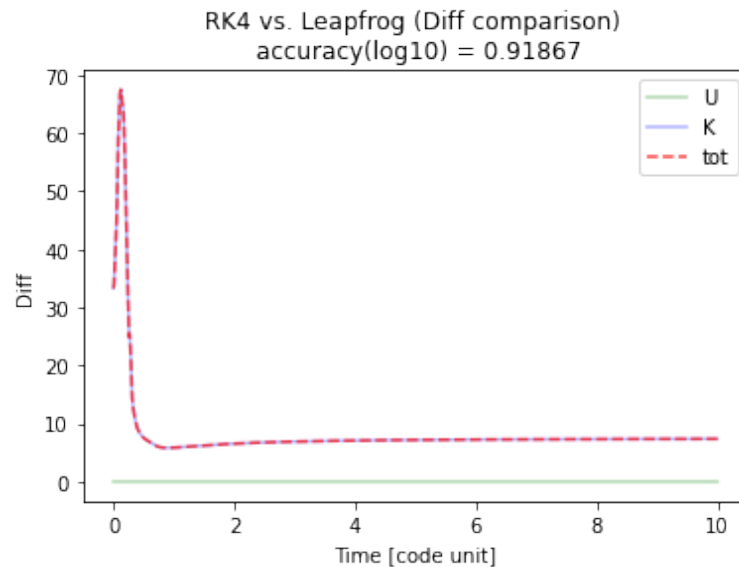


Figure 7: In the comparison of energy schemes between the RK4 and Leapfrog methods, the average accuracy is approximately 0.9 orders.

## 2 Codes

All the codes are transferred from jupyterlab or python codes; hence, if you want to re-run them, please see the source code in the attached files or my GitHub repository:

<https://github.com/gary20000915/Comphyslab-HW3.git>

### 2.1 particles.py

---

```

1 import numpy as np
2
3 class Particles:
4     """
5
6     The Particles class handle all particle properties
7
8     for the N-body simulation.
9
10    """
11    def __init__(self, N:int = 100):
12        """
13        Prepare memories for N particles
14
15        :param N: number of particles.
16
17        By default: particle properties include:
18            nparticles: int. number of particles
19            _masses: (N,1) mass of each particle

```

```

20         _positions: (N,3) x,y,z positions of each particle
21         _velocities: (N,3) vx, vy, vz velocities of each particle
22         _accelerations: (N,3) ax, ay, az accelerations of each partciel
23         _tags: (N) tag of each particle
24         _time: float. the simulation time
25
26         """
27         self.nparticles = N
28         self._time = 0 # initial time = 0
29         self._masses = np.ones((N, 1))
30         self._positions = np.zeros((N, 3))
31         self._velocities = np.zeros((N, 3))
32         self._accelerations = np.zeros((N, 3))
33         self._tags = np.linspace(1, N, N)
34         self._U = np.ones((N, 1))
35         self._K = np.ones((N, 1))
36
37         return
38
39
40     def get_time(self):
41         return self._time
42
43     def get_masses(self):
44         return self._masses
45
46     def get_positions(self):
47         return self._positions
48
49     def get_velocities(self):
50         return self._velocities
51
52     def get_accelerations(self):
53         return self._accelerations
54
55     def get_tags(self):
56         return self._tags
57
58     def get_time(self):
59         return self._time
60
61     def get_U(self):
62         return self._U
63
64     def get_K(self):
65         return self._K
66
67
68     def set_time(self, time):
69         self._time = time
70         return
71
72     def set_masses(self, mass):

```

```

73     self._masses = mass
74     return
75
76 def set_positions(self, pos):
77     self._positions = pos
78     return
79
80 def set_velocities(self, vel):
81     self._velocities = vel
82     return
83
84 def set_accelerations(self, acc):
85     self._accelerations = acc
86     return
87
88 def set_tags(self, IDs):
89     self._tags = IDs
90     return
91
92 def set_U(self, U):
93     self._U = U
94     return
95
96 def set_K(self, K):
97     self._K = K
98     return
99
100 def output(self, fn, time):
101     """
102     Write simulation data into a file named "fn"
103     """
104     mass = self._masses
105     pos = self._positions
106     vel = self._velocities
107     acc = self._accelerations
108     tag = self._tags
109     header = """
110         -----
111         Data from a 3D direct N-body simulation.
112
113         rows are i-particle;
114         coumns are :mass, tag, x ,y, z, vx, vy, vz, ax, ay, az
115
116         NTHU, Computational Physics Lab
117
118         -----
119         """
120     header += "Time = {}".format(time)
121     np.savetxt(fn, (tag[:,0], mass[:,0], pos[:,0], pos[:,1], pos[:,2],
122                    vel[:,0], vel[:,1], vel[:,2],
123                    acc[:,0], acc[:,1], acc[:,2]), header=header)
124
125     return

```

---



## 2.2 simulation.py

---

```
1 import numpy as np
2 from pathlib import Path
3 import time
4 from numba import jit, njit, prange, set_num_threads
5 from nbody.particles import Particles
6 import matplotlib.pyplot as plt
7
8 """
9
10 This program solve 3D direct N-particles simulations
11 under gravitational forces.
12
13 This file contains two classes:
14
15 1) Particles: describes the particle properties
16 2) NbodySimulation: describes the simulation
17
18 Usage:
19
20     Step 1: import necessary classes
21
22     from nbody import Particles, NbodySimulation
23
24     Step 2: Write your own initialization function
25
26         def initialize(particles:Particles):
27             ....
28             ....
29             particles.set_masses(mass)
30             particles.set_positions(pos)
31             particles.set_velocities(vel)
32             particles.set_accelerations(acc)
33
34             return particles
35
36     Step 3: Initialize your particles.
37
38         particles = Particles(N=100)
39         initialize(particles)
40
41
42     Step 4: Initial, setup and start the simulation
43
44         simulation = Simulation(particles)
45         simulation.setip(...)
46         simulation.evolve(dt=0.001, tmax=10)
47
48
49 Author: Yuan-Yen Peng (editted from Prof. Kuo-Chuan Pan, NTHU 2022.10.30)
50 Dept. of Physics, NTHU
```

```

52 Date: Npv. 28, 2022
53 For the course, computational physics lab
54
55 """
56
57 def ACC_norm(N, posx, posy, posz, G, mass, rsoft, U, K, vel_square):
58     '''
59     Acceleration with normal for loops.
60
61     :param N: number of particles
62     :param posx: position x
63     :param posy: position y
64     :param posz: position z
65     :param G: gravitational constant
66     :param mass: mass
67     '''
68
69     acc = np.zeros((N, 3))
70     for i in range(N):
71         for j in range(N):
72             if j > i:
73                 x = posx[i] - posx[j]
74                 y = posy[i] - posy[j]
75                 z = posz[i] - posz[j]
76                 r = np.sqrt(x**2 + y**2 + z**2) + rsoft
77                 theta = np.arccos(z / r)
78                 phi = np.arctan2(y, x)
79                 F = - G * mass[i, 0] * mass[j, 0] / np.square(r)
80                 Fx = F * np.cos(theta) * np.cos(phi)
81                 Fy = F * np.cos(theta) * np.sin(phi)
82                 Fz = F * np.sin(theta)
83
84                 acc[i, 0] += Fx / mass[i, 0]
85                 acc[j, 0] -= Fx / mass[j, 0]
86
87                 acc[i, 1] += Fy / mass[i, 0]
88                 acc[j, 1] -= Fy / mass[j, 0]
89
90                 acc[i, 2] += Fz / mass[i, 0]
91                 acc[j, 2] -= Fz / mass[j, 0]
92
93                 U[i] = -G * mass[i, 0] * mass[j, 0] / r
94                 K[i] = 0.5 * (mass[i, 0] * np.sum(vel_square[i, :])
95                             + mass[j, 0] * np.sum(vel_square[j, :]))
96     return acc, U, K
97
98 @jit(nopython=True)
99 def ACC_jit(N, posx, posy, posz, G, mass, rsoft, U, K, vel_square):
100     '''
101     Acceleration with numba jit for loops
102
103     :param N: number of particles
104     :param posx: position x

```

```

105 :param posy: position y
106 :param posz: position z
107 :param G: gravitational constant
108 :param mass: mass
109 '''
110 acc = np.zeros((N, 3))
111 for i in range(N):
112     for j in range(N):
113         if j > i:
114             x = posx[i] - posx[j]
115             y = posy[i] - posy[j]
116             z = posz[i] - posz[j]
117             r = np.sqrt(x**2 + y**2 + z**2) + rsoft
118             theta = np.arccos(z / r)
119             phi = np.arctan2(y, x)
120             F = - G * mass[i, 0] * mass[j, 0] / np.square(r)
121             Fx = F * np.cos(theta) * np.cos(phi)
122             Fy = F * np.cos(theta) * np.sin(phi)
123             Fz = F * np.sin(theta)
124
125             acc[i, 0] += Fx / mass[i, 0]
126             acc[j, 0] -= Fx / mass[j, 0]
127
128             acc[i, 1] += Fy / mass[i, 0]
129             acc[j, 1] -= Fy / mass[j, 0]
130
131             acc[i, 2] += Fz / mass[i, 0]
132             acc[j, 2] -= Fz / mass[j, 0]
133
134             U[i] = -G * mass[i, 0] * mass[j, 0] / r
135             K[i] = 0.5 * (mass[i, 0] * np.sum(vel_square[i, :])
136                         + mass[j, 0] * np.sum(vel_square[j, :]))
137     return acc, U, K
138
139 set_num_threads(8)
140 @njit(parallel=True)
141 def ACC_njit(N, posx, posy, posz, G, mass, rsoft, U, K, vel_square):
142     '''
143     Acceleration with numba njit for loops (parallel)
144
145     :param N: number of particles
146     :param posx: position x
147     :param posy: position y
148     :param posz: position z
149     :param G: gravitational constant
150     :param mass: mass
151     '''
152     acc = np.zeros((N, 3))
153     for i in prange(N):
154         for j in prange(N):
155             if j > i:
156                 x = posx[i] - posx[j]
157                 y = posy[i] - posy[j]

```

```

158         z = posz[i] - posz[j]
159         r = np.sqrt(x**2 + y**2 + z**2) + rsoft
160         theta = np.arccos(z / r)
161         phi = np.arctan2(y, x)
162         F = - G * mass[i, 0] * mass[j, 0] / np.square(r)
163         Fx = F * np.cos(theta) * np.cos(phi)
164         Fy = F * np.cos(theta) * np.sin(phi)
165         Fz = F * np.sin(theta)
166
167         acc[i, 0] += Fx / mass[i, 0]
168         acc[j, 0] -= Fx / mass[j, 0]
169
170         acc[i, 1] += Fy / mass[i, 0]
171         acc[j, 1] -= Fy / mass[j, 0]
172
173         acc[i, 2] += Fz / mass[i, 0]
174         acc[j, 2] -= Fz / mass[j, 0]
175
176         U[i] = - G * mass[i, 0] * mass[j, 0] / r
177         K[i] = 0.5 * (mass[i, 0] * np.sum(vel_square[i, :])
178                     + mass[j, 0] * np.sum(vel_square[j, :]))
179     return acc, U, K
180
181 class NbodySimulation:
182     """
183
184     The N-body Simulation class.
185
186     """
187
188     def __init__(self, particles: Particles):
189         """
190         Initialize the N-body simulation with given Particles.
191
192         :param particles: A Particles class.
193
194         """
195
196         # store the particle information
197         self.nparticles = particles.nparticles
198         self.particles = particles
199
200         # Store physical information
201         self.time = 0.0 # simulation time
202
203         # Set the default numerical schemes and parameters
204         self.setup()
205
206     return
207
208     def setup(self, G=1,
209              rsoft=0.01,
210              method="RK2",

```

```

211         io_freq=10,
212         io_title="particles",
213         io_screen=True,
214         visualized=False):
215     """
216     Customize the simulation enviroments.
217
218     :param G: the graivtational constant
219     :param rsoft: float, a soften length
220     :param meothd: string, the numerical scheme
221                   support "Euler", "RK2", and "RK4"
222
223     :param io_freq: int, the frequency to outupt data.
224                   io_freq <=0 for no output.
225     :param io_title: the output header
226     :param io_screen: print message on screen or not.
227     :param visualized: on the fly visualization or not.
228
229     """
230     # TODO:
231     self.G = G
232     self.rsoft = rsoft
233     self.method = method
234     self.io_freq = io_freq
235     self.io_title = io_title
236     self.io_screen = io_screen
237     self.visualized = visualized
238     return
239
240 def evolve(self, dt:float=0.01, tmax:float=1):
241     """
242
243     Start to evolve the system
244
245     :param dt: time step
246     :param tmax: the finial time
247
248     """
249     # TODO:
250     method = self.method
251     if method=="Euler":
252         _update_particles = self._update_particles_euler
253     elif method=="RK2":
254         _update_particles = self._update_particles_rk2
255     elif method=="RK4":
256         _update_particles = self._update_particles_rk4
257     elif method=="Leapfrog":
258         _update_particles = self._update_particles_lf
259     else:
260         print("No such update meothd", method)
261         quit()
262
263     # prepare an output folder for lateron output

```

```

264 io_folder = "data_"+self.io_title
265 Path(io_folder).mkdir(parents=True, exist_ok=True)
266 io_folder_fig = "fig_" + self.io_title
267 Path(io_folder_fig).mkdir(parents=True, exist_ok=True)
268
269 # =====
270 #
271 # The main loop of the simulation
272 #
273 # =====
274
275 # TODO:
276 particles = self.particles # call the class: Particles
277 n = 0
278 t = self.particles.get_time()
279 t1 = time.time()
280 step = int(tmax / dt) + 1
281 UU = np.ones((step, 1))
282 KK = np.ones((step, 1))
283 EE = np.ones((step, 1))
284 for i in range(step):
285     # update particles
286     particles = _update_particles(dt, particles)[0]
287     UU[i] = _update_particles(dt, particles)[1]
288     KK[i] = _update_particles(dt, particles)[2]
289     EE[i] = UU[i] + KK[i]
290     # update io
291     if (n % self.io_freq == 0):
292         if self.io_screen:
293             # print('n = ', n, 'time = ', t, 'dt = ', dt)
294             # output
295             fn = io_folder+"/data_"+self.io_title+"_"+str(n).zfill(5)+".txt"
296             print(fn)
297             self.particles.output(fn, t)
298
299             # savefig
300             scale = 100
301             fig, ax = plt.subplots()
302             fig.set_size_inches(10.5, 10.5, forward=True)
303             fig.set_dpi(72)
304             ax.set_xlim(-1*scale, 1*scale)
305             ax.set_ylim(-1*scale, 1*scale)
306             ax.set_aspect('equal')
307             ax.set_xlabel('X [code unit]')
308             ax.set_ylabel('Y [code unit]')
309             pos = particles.get_positions()
310             plt.title(f'Time = {np.round(t, 0)}')
311             FIG = f'{io_folder_fig}/fig_{self.io_title}_{str(int(0.01 *
312                 n)).zfill(1)}.png'
313             ax.scatter(pos[:, 0], pos[:, 1], s = 10, alpha = .3)
314             plt.savefig(FIG)
315             plt.show()

```

```

316         # update time
317         if t + dt > tmax:
318             dt = tmax - t
319         t += dt
320         n += 1
321
322     T = np.linspace(0, tmax, step)
323     plt.plot(T, UU, 'g', alpha = .3, label = 'Potential')
324     plt.plot(T, KK, 'b', alpha = .3, label = 'Kinetic')
325     plt.plot(T, EE, '--r', alpha = .7, label = 'Total')
326     plt.xlabel('Time [code unit]')
327     plt.ylabel('Energy [code unit]')
328     plt.title(f'Energy Scheme, with {method}')
329     plt.legend()
330     plt.show()
331     t2 = time.time()
332     print("Time diff: ", t2 - t1)
333     print("Done!")
334
335     return [UU, KK]
336
337 def _calculate_acceleration(self, mass, pos):
338     """
339     Calculate the acceleration.
340     """
341     # TODO:
342     particles = self.particles
343     G = self.G
344     rsoft = self.rsoft
345     posx = pos[:, 0]
346     posy = pos[:, 1]
347     posz = pos[:, 2]
348     N = self.nparticles
349     U = particles.get_U()
350     K = particles.get_K()
351     vel_square = np.square(particles.get_velocities())
352     # return ACC_jit(N, posx, posy, posz, G, mass, rsoft, U, K, vel_square)
353     return ACC_njit(N, posx, posy, posz, G, mass, rsoft, U, K, vel_square)
354
355 def _update_particles_euler(self, dt, particles:Particles):
356     # TODO:
357     mass = particles.get_masses()
358     pos = particles.get_positions()
359     vel = particles.get_velocities()
360     acc = self._calculate_acceleration(mass, pos)[0]
361     y0 = np.array([pos, vel])
362     yder = np.array([vel, acc])
363
364     y0 = np.add(y0, yder * dt)
365
366     U = np.sum(self._calculate_acceleration(mass, y0[0])[1])
367     K = np.sum(self._calculate_acceleration(mass, y0[0])[2])
368

```

```

369     particles.set_positions(y0[0])
370     particles.set_velocities(y0[1])
371     particles.set_accelerations(acc)
372
373     return particles, U, K
374
375 def _update_particles_rk2(self, dt, particles:Particles):
376     # TODO:
377     mass = particles.get_masses()
378     pos = particles.get_positions()
379     vel = particles.get_velocities()
380     acc = self._calculate_acceleration(mass, pos)[0]
381
382     y0 = np.array([pos, vel])
383     yder = np.array([vel, acc])
384     k1 = yder
385     y_temp = y0 + dt * k1
386     acc = self._calculate_acceleration(mass, y_temp[0])[0]
387     k2 = np.array([y_temp[1], acc])
388     y0 = np.add(y0, (dt / 2) * (k1 + k2))
389
390     acel = self._calculate_acceleration(mass, y0[0])[0]
391     U = np.sum(self._calculate_acceleration(mass, y0[0])[1])
392     K = np.sum(self._calculate_acceleration(mass, y0[0])[2])
393
394     particles.set_positions(y0[0])
395     particles.set_velocities(y0[1])
396     particles.set_accelerations(acel)
397     return particles, U, K
398
399 def _update_particles_rk4(self, dt, particles:Particles):
400     # TODO:
401     mass = particles.get_masses()
402     pos = particles.get_positions()
403     vel = particles.get_velocities()
404     acc = self._calculate_acceleration(mass, pos)[0]
405
406     y0 = np.array([pos, vel])
407     yder = np.array([vel, acc])
408     k1 = yder
409     y_temp = y0 + 0.5 * dt * k1
410     acc = self._calculate_acceleration(mass, y_temp[0])[0]
411     k2 = np.array([y_temp[1], acc])
412     y_temp = y0 + 0.5 * dt * k2
413     acc = self._calculate_acceleration(mass, y_temp[0])[0]
414     k3 = np.array([y_temp[1], acc])
415     y_temp = y0 + dt * k3
416     acc = self._calculate_acceleration(mass, y_temp[0])[0]
417     k4 = np.array([y_temp[1], acc])
418
419     y0 = np.add(y0, (1/6) * dt * (k1 + 2*k2 + 2*k3 + k4))
420
421     acel = self._calculate_acceleration(mass, y0[0])[0]

```



```

422     U = np.sum(self._calculate_acceleration(mass, y0[0])[1])
423     K = np.sum(self._calculate_acceleration(mass, y0[0])[2])
424
425     particles.set_positions(y0[0])
426     particles.set_velocities(y0[1])
427     particles.set_accelerations(accel)
428     return particles, U, K
429
430 def _update_particles_1f(self, dt, particles:Particles):
431     # TODO:
432     mass = particles.get_masses()
433     pos = particles.get_positions()
434     vel = particles.get_velocities()
435
436     acc = particles.get_accelerations()
437     vel_prime = vel + acc * 0.5 * dt
438     pos = pos + vel_prime * dt
439     acc = self._calculate_acceleration(mass, pos)[0]
440     vel = vel_prime + acc * 0.5 * dt
441
442     U = np.sum(self._calculate_acceleration(mass, pos)[1])
443     K = np.sum(self._calculate_acceleration(mass, pos)[2])
444
445     particles.set_positions(pos)
446     particles.set_velocities(vel)
447     particles.set_accelerations(acc)
448     return particles, U, K
449
450
451 if __name__=='__main__':
452
453     # test Particles() here
454     particles = Particles(N=10)
455     # test NbodySimulation(particles) here
456     sim = NbodySimulation(particles=particles)
457     sim.setup(G = 6.67e-8, io_freq=2, io_screen=True, io_title="test")
458     sim.evolve(dt = 1, tmax = 10)
459     print(sim.G)
460     print("Done")

```

---

## 2.3 NormalCloud.ipynb

---

```

1 # %% [markdown]
2 # ## Homework 3
3 # ### Programming Assignment 1
4 # ### 111 Computational Physics Lab
5 # >Author: Yuan-Yen Peng 108000204
6 # >Email: garyphys0915@gapp.nthu.edu.com
7 # >Date: Nov. 11, 2022
8 # >LICENCE: MIT
9
10 # %%

```

```

11 import numpy as np
12 import glob
13 from numba import jit, njit, prange, set_num_threads
14 import matplotlib.pyplot as plt
15 from mpl_toolkits.mplot3d import Axes3D
16 import matplotlib.animation as animation
17 from nbody.particles import Particles
18 from nbody.simulation import NbodySimulation
19
20 # %%
21 problem_name = "NormalCloud"
22 Num = int(1e4)
23 tmax = 10
24 dt = 0.01
25 r_soft = 0.001
26
27 # %%
28 set_num_threads(8)
29 @njit(parallel = True)
30 def generator(N, positions, velocities, accelerations):
31     mu, sigma = 0, 1 # mean = 0; variance = 1, i.e., standard deviation =
32     sqrt(var) = 1
33     for i in prange(N):
34         positions[i] = np.random.normal(mu, sigma, 3)
35         velocities[i] = np.random.normal(mu, sigma, 3)
36         accelerations[i] = np.random.normal(mu, sigma, 3)
37
38     return [positions, velocities, accelerations]
39
40 # %%
41 def initialRandomParticles(N):
42     """
43     Initial particles
44     """
45     total_mass = 20
46     particles = Particles(N = N)
47
48     positions = particles.get_positions()
49     velocities = particles.get_velocities()
50     accelerations = particles.get_accelerations()
51     masses = particles.get_masses() # ones array (size = N)
52     mass = total_mass / particles.nparticles # single particel's mass
53
54     particles.set_masses((masses * mass))
55     particles.set_positions(generator(N, positions, velocities,
56     accelerations)[0])
57     particles.set_velocities(generator(N, positions, velocities,
58     accelerations)[1])
59     particles.set_accelerations(generator(N, positions, velocities,
60     accelerations)[2])
61
62     return particles

```

```

60
61 # %% [markdown]
62 # solve with t = 0 ~ 10 with dt = 0.01 and r_soft = 0.01.
63
64 # %%
65 # Initial particles here.
66 method = "RK4"
67 particles = initialRandomParticles(N = Num)
68 # Run the n-body simulations
69 sim = NbodySimulation(particles)
70 sim.setup(G=1,method=method,io_freq=200,io_title=problem_name,io_screen=True,visualized=False)
71 Energy_RK4 = sim.evolve(dt=dt,tmax=tmax)
72
73 # %%
74 # Initial particles here.
75 method = "RK2"
76 particles = initialRandomParticles(N = Num)
77 # Run the n-body simulations
78 sim = NbodySimulation(particles)
79 sim.setup(G=1,method=method,io_freq=200,io_title=problem_name,io_screen=True,visualized=False)
80 Energy_RK2 = sim.evolve(dt=dt,tmax=tmax)
81
82 # %%
83 # Initial particles here.
84 method = "Euler"
85 particles = initialRandomParticles(N = Num)
86 # Run the n-body simulations
87 sim = NbodySimulation(particles)
88 sim.setup(G=1,method=method,io_freq=200,io_title=problem_name,io_screen=True,visualized=False)
89 Energy_Euler = sim.evolve(dt=dt,tmax=tmax)
90
91 # %%
92 # Initial particles here.
93 method = "Leapfrog"
94 particles = initialRandomParticles(N = Num)
95 # Run the n-body simulations
96 sim = NbodySimulation(particles)
97 sim.setup(G=1,method=method,io_freq=200,io_title=problem_name,io_screen=True,visualized=False)
98 Energy_LF = sim.evolve(dt=dt,tmax=tmax)
99
100 # %%
101 TT = len(Energy_RK4[0])
102 Time = np.linspace(0, tmax, len(Energy_RK4[0]))
103 Diff_tot = np.abs((Energy_RK4[0] + Energy_RK4[1]) - (Energy_LF[0] + Energy_LF[1]))
104 Diff = np.abs(np.array(Energy_RK4) - np.array(Energy_LF))
105 avg = np.average(Diff_tot)
106 accuracy = np.log10(avg)
107 print("Average = ", avg)
108 print("Accuracy (log) = ", accuracy)
109
110 plt.plot(Time, Diff[0], "g", alpha = .3, label = "U")
111 plt.plot(Time, Diff[1], "b", alpha = .3, label = "K")
112 plt.plot(Time, Diff_tot, "--r", alpha = .7, label = "tot")

```

```

113 plt.xlabel("Time [code unit]")
114 plt.ylabel("Diff")
115 plt.title(f"RK4 vs. Leapfrog (Diff comparison) \n accuracy(log10) =
        {np.round(accuracy, 5)}")
116 plt.legend()
117 plt.show()
118
119 # %%
120 Energy_RK4 = Energy_RK2
121 TT = len(Energy_RK4[0])
122 Time = np.linspace(0, tmax, len(Energy_RK4[0]))
123 Diff_tot = np.abs((Energy_RK4[0] + Energy_RK4[1]) - (Energy_LF[0] + Energy_LF[1]))
124 Diff = np.abs(np.array(Energy_RK4) - np.array(Energy_LF))
125 avg = np.average(Diff_tot)
126 accuracy = np.log10(avg)
127 print("Average = ", avg)
128 print("Accuracy (log) = ", accuracy)
129
130 plt.plot(Time, Diff[0], "g", alpha = .3, label = "U")
131 plt.plot(Time, Diff[1], "b", alpha = .3, label = "K")
132 plt.plot(Time, Diff_tot, "--r", alpha = .7, label = "tot")
133 plt.xlabel("Time [code unit]")
134 plt.ylabel("Diff")
135 plt.title(f"RK2 vs. Leapfrog (Diff comparison) \n accuracy(log10) =
        {np.round(accuracy, 5)}")
136 plt.legend()
137 plt.show()
138
139 # %%
140 Energy_RK4 = Energy_Euler
141 TT = len(Energy_RK4[0])
142 Time = np.linspace(0, tmax, len(Energy_RK4[0]))
143 Diff_tot = np.abs((Energy_RK4[0] + Energy_RK4[1]) - (Energy_LF[0] + Energy_LF[1]))
144 Diff = np.abs(np.array(Energy_RK4) - np.array(Energy_LF))
145 avg = np.average(Diff_tot)
146 accuracy = np.log10(avg)
147 print("Average = ", avg)
148 print("Accuracy (log) = ", accuracy)
149
150 plt.plot(Time, Diff[0], "g", alpha = .3, label = "U")
151 plt.plot(Time, Diff[1], "b", alpha = .3, label = "K")
152 plt.plot(Time, Diff_tot, "--r", alpha = .7, label = "tot")
153 plt.xlabel("Time [code unit]")
154 plt.ylabel("Diff")
155 plt.title(f"Euler vs. Leapfrog (Diff comparison) \n accuracy(log10) =
        {np.round(accuracy, 5)}")
156 plt.legend()
157 plt.show()

```

---