Homework 2 Write Up

Intro Computational Materials Modeling

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October 4, 2024

Problem 1. Carbon Dating

Analytical solution.

The radioactive decay equation is given by eq. 1, where the amount of parent nuclei decreases exponentially with time.

$$N(\Delta t) = N_0 e^{-t/\tau} \tag{1}$$

The half-life ($T_{1/2}$) is given by eq. 2. which is the time when half of the original amount of nuclei have decayed.

$$N(T_{1/2}) = \frac{N_0}{2} \tag{2}$$

Eq. 2 is put into eq.1 to find the relationship between half-life and the decay constant.

$$\frac{N_0}{2} = N_0 e^{-} T_{1/2}/\tau$$
$$\frac{1}{2} = e^{-} T_{1/2}/\tau$$
$$\ln(\frac{1}{2}) = -T_{1/2}/\tau$$
$$\tau(-\ln 2) = -T_{1/2}$$
$$\boxed{\tau \ln 2 = T_{1/2}}$$

Python code development.

Step 1. Setting variables:

- $M_i * M_{^{14}_{2}C} * N_A = N_0$
  - N_0 - The number of initial $^{14}_{2}$C nuclei before decaying begins
  - N_A - Avogadro's Number $\frac{6.022*10^{23} \text{ nuclei}}{\text{mol}}$
  - $M_{^{14}_{2}C}$ - Molar mass of Carbon isotope $\frac{14\text{g}}{\text{mol}}$
  - M_i - Initial mass of sample 10^{-12} kg
- $\tau \ln 2 = T_{1/2}$
  - τ - The time constant for the decay
  - $T_{1/2}$ - Half life decay 5700 years
- T - The total duration of decay $20,000$ years
- Δt - Time step for the calculation $10, 100$ and 1000 years

Step 2. Creating an array for time steps/spacing and initial condition:

- A numpy 1D array of time points from $t = 0$ to $t = T$ at steps of Δt.
- The initial boundary of $N_U(0) = N_0$ when $t = 0$.

- The final boundary condition when $t = T$

Step 3. Iterative calculation using Euler method approximation:

- From eq. 3, we can know the amount of undecayed nuclei as a function of time.

$$\frac{dN_U}{dt} = -\frac{N_U}{\tau} \tag{3}$$

- Using the Euler method approximation and eq. 3, we can calculate the number of undecayed nuclei (N_U) at each time step (Δt).

$$N_U(t + \Delta t) \approx N_U(t) - \frac{N_U(t)}{\tau}\Delta t$$

- Starting at the initial boundary condition, the Euler approximation formula updates $N_U(t)$ at each continuous time step $t + \Delta t$ until the final boundary condition.

Step 4. Activity Calculation:

- The activity is calculated as the rate of change of undecayed nuclei from eq. 5.

$$R(t) = -\frac{dN_U}{dt} \tag{4}$$

- We also know from eq. 3 the amount of undecayed nuclei as a function of time. Equating these two equations to each other gives us the activity at each time step after $N_U(t)$ is calculated.

$$R(t) = \frac{N_U}{\tau}$$

Step 5. Plot:

- Plot the activity $R(t)$ as a function of time t.
- Compare the activity calculated from the Euler approximation to the exact activity on a single plot.

$$R_{\text{Exact}}(t) = -\frac{dN}{dt} = \frac{1}{\tau}N_0 e^{-t/\tau}$$

Results and Discussion

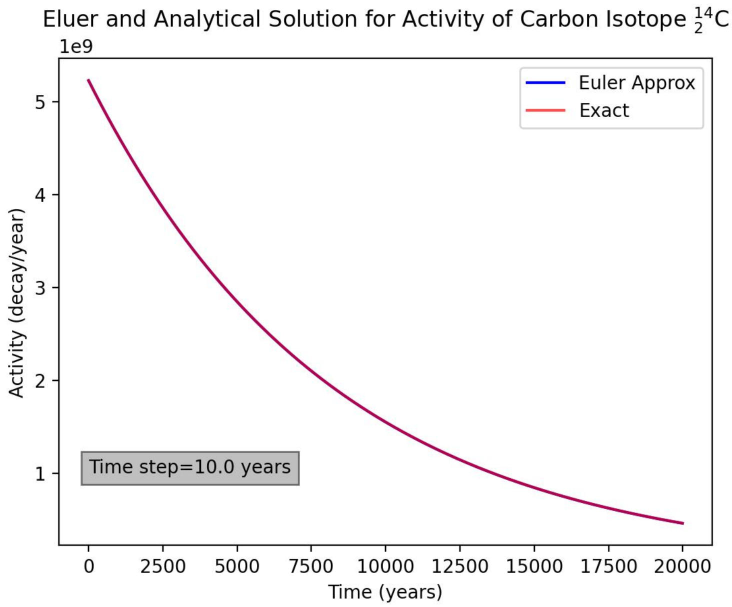


Figure 1: The activity of the sample over 20,000 years at a **time step of 10 years**.

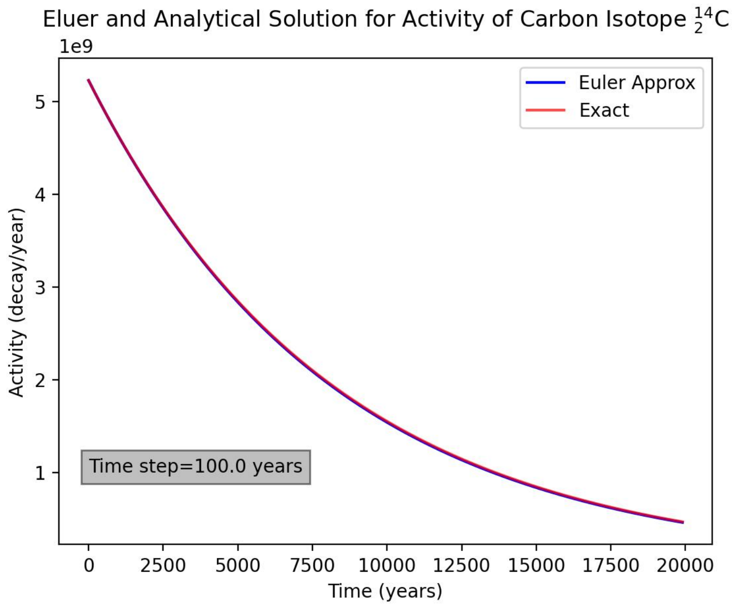


Figure 2: The activity of the sample over 20,000 years at a **time step of 100 years**.

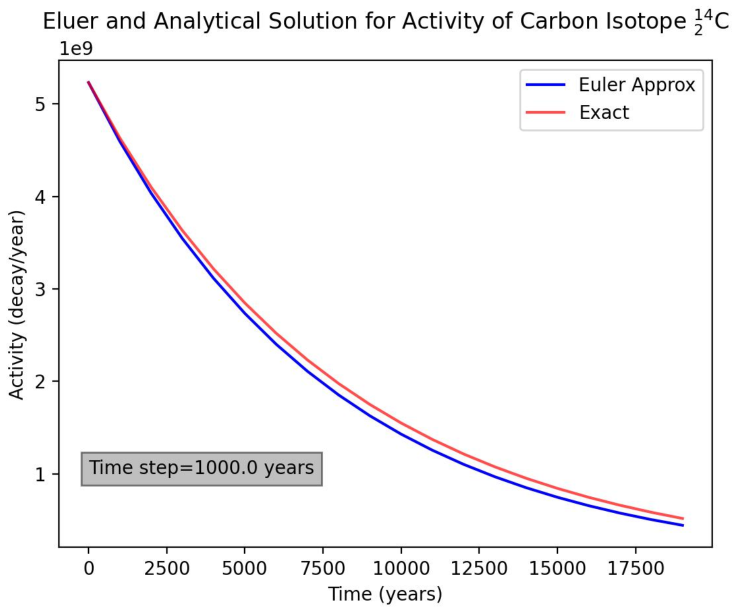


Figure 3: The activity of the sample over 20,000 years at a **time step of 1000 years**.

When using a time-step of 1000 years, after 2 half-lives, the **percent deviation from the exact result is 9.21**%. The deviation is as large as I would expect from the neglected second-order term because the second-order term increases with larger time steps, creating more error.

Problem 2. Golf Ball Code

Python Code Development.

Setting (global) variables:

- m - The mass of the golf ball 46 grams
- θ - The angle of the golf ball trajectory 45°, 30°, 15°, and 9°.
- v_i - The initial velocity $70\frac{\text{m}}{\text{s}}$
- ρ - Density of air (at sea level) $1.29\frac{\text{kg}}{\text{m}^3}$
- A - Frontal area of the golf ball $0.0014\ \text{m}^2$
- g - Gravity $9.8\ \frac{m}{s^2}$

Case 1. Solving for x, y, v_{mag}, C, v_x, and v_y for a golf ball with **ideal trajectory with no drag and no spin**.

- The Euler approximation gives us the ball's x and y positions where Δt is a given time step.

$$x(t + \Delta t) = x(t) + v_x(t)\Delta t$$
$$y(t + \Delta t) = y(t) + v_y(t)\Delta t$$

- The velocity magnitude is found by using the x and y components of velocity.

$$v_{mag} = |\vec{v}| = \sqrt{v_x^2 + v_y^2}$$

- For the drag-free problem, there is no drag coefficient.

$$C = 0$$

- The Euler approx velocity components of x and y where the derivative of position with respect to time is taken.

$$v_x(t + \Delta t) = v_x(t)$$
$$v_y(t + \Delta t) = v_y(t) - g\Delta t$$

Case 2. Solving for x, y, v_{mag}, C, v_x, and v_y for a **smooth golf ball with drag**.

- The Euler approx calculations for the position values of x and y don't change with drag being considered, so the Euler approx equations stay the same as they were in case 1.
- To add drag into the system, we are given the drag coefficient (which will be a local variable).

$$C = \frac{1}{2}$$

- For drag, the general form is used.

$$F_{\text{drag}} = -C\rho A v^2$$

- The drag in the x and y direction are vectors with a magnitude and direction that is always opposite the velocity where $|\vec{v}|$ is the magnitude of the velocity.

$$\vec{F}_{\text{Drag},x} = -C\rho A|\vec{v}|v_x$$
$$\vec{F}_{\text{Drag},y} = -C\rho A|\vec{v}|v_y$$

- The Euler approx calculations now factor in drag moving in the opposite direction of the velocity.

$$v_x(t + \Delta t) = v_x(t) - \frac{C\rho A|\vec{v}|}{m}v_x(t)\Delta t$$
$$v_y(t + \Delta t) = v_y(t) - g\Delta t - \frac{C\rho A|\vec{v}|}{m}v_y(t)\Delta t$$

Case 3. Solving for x, y, v_{mag}, C, v_x, and v_y for a **dimpled golf ball with drag**.

- Now that the golf ball has dimples, there is a transition in the drag coefficient to a reduced value because of turbulent flow.
- For speeds up to $|\vec{v}| = 14\frac{m}{s}$.

$$C = \frac{1}{2}$$

- For speeds greater than $|\vec{v}| = 14\frac{m}{s}$.

$$C = \frac{7.0}{|\vec{v}|}$$

- The Euler approx equations from case 3 are still the same, but the code will contain an if statement to determine which drag coefficient to use based on the magnitude of the velocity.

Case 4. Solving for x, y, v_{mag}, C, v_x, and v_y for a **dimpled golf ball with drag and spin**.

- The magnus force $\vec{F}_{magnus}$ acts on a rotating object due to spin. It is perpendicular to the object's velocity and its axis of rotation.

$$\vec{F}_{magnus} = S_0\omega \times v$$

- The spin vector $S_0\omega$ has a magnitude proportional to the to the (back)spin rate of the ball and the direction is along the axis of rotation.

$$\frac{S_0\omega}{m} = 0.25s^{-1}$$

- The Euler approx for the position of x and y are the same as Case 1.
- The drag coefficient considerations are the same as in case 3.
- The Euler approx for the velocity components now factor in the $\vec{F}_{magnus}$.

$$v_x(t + \Delta t) = v_x(t) + \Big(- \frac{C\rho A|\vec{v}|}{m} - \frac{S_0\omega}{m} v_y(t)\Big)\Delta t$$
$$v_y(t + \Delta t) = v_y(t) + \Big(- \frac{C\rho A|\vec{v}|}{m} - \frac{S_0\omega}{m} v_x(t) - g\Big)\Delta t$$

Initializing code for each case using Euler approx:

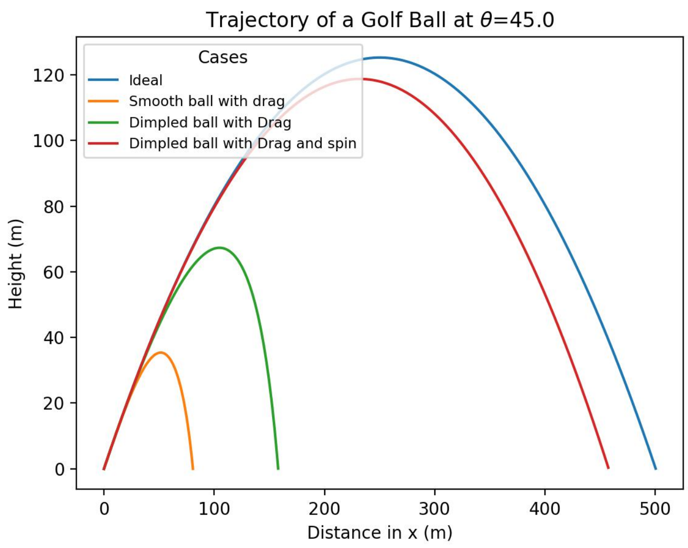
- The initial position in the x and y is set to 0 when time is 0.
  $x_0 = 0$ and $y_0 = 0$
- The initial velocity x and y components in terms of the angle when t=0 are set.
  $v_{x_0} = v_0 cos(\theta)$ and $v_{y_0} = v_0 sin(\theta)$
- The first boundary condition is when $t = 0$.
- At each time step Δt the x and y position values are calculated.
- At each time step using the results from the x and y calculations v_{mag} is calculated.
- Then using the results from the x and y calculations the v_x and v_y at each time step Δt.
- The final boundary condition is when the ball touches the ground when the y position component is 0.

Plotting trajectories:

- To plot the ball's trajectory for the cases, y in meters is plotted with respect to x also in meters.

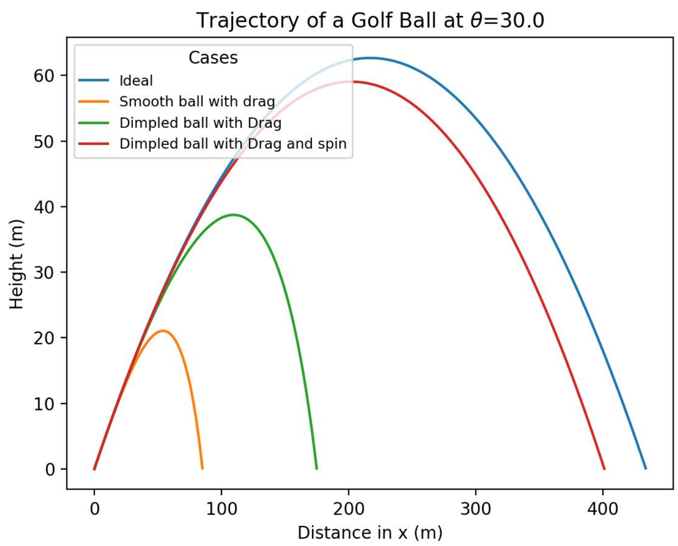
Results and Discussion.
The time step used was **0.01 seconds**
$\theta = 45°$

	Final Velocity before Impact (m/s)	Total Time of Flight (s)
Case 1	70.06	10.12
Case 2	19.63	5.28
Case 3	25.92	7.63
Case 4	68.17	9.59



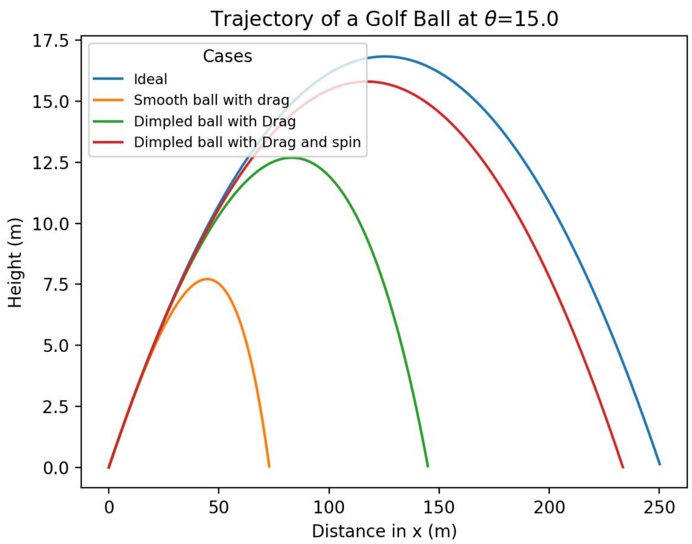
$\theta = 30°$

	Final Velocity before Impact (m/s)	Total Time of Flight (s)
Case 1	70.04	7.16
Case 2	18.18	4.03
Case 3	24.47	5.72
Case 4	68.44	6.75



$\theta = 15°$

	Final Velocity before Impact (m/s)	Total Time of Flight (s)
Case 1	70.01	3.71
Case 2	18.59	2.45
Case 3	30.92	3.24
Case 4	69.10	3.49



$\theta = 9°$

	Final Velocity before Impact (m/s)	Total Time of Flight (s)
Case 1	70.01	2.25
Case 2	22.34	1.65
Case 3	40.38	2.06
Case 4	69.44	2.11