Computational Physics

Lecture-01

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Contents

- Basis Concepts

Basic Concepts

- Computational Physics aims at **solving physical problems** by means of **numerical methods developed** in the field of numerical analysis

- In most cases it **is not possible to find analytic solutions** and one must rely on good approximations.

$$\int_a^b e^{-x^2}\mathrm{d}x$$

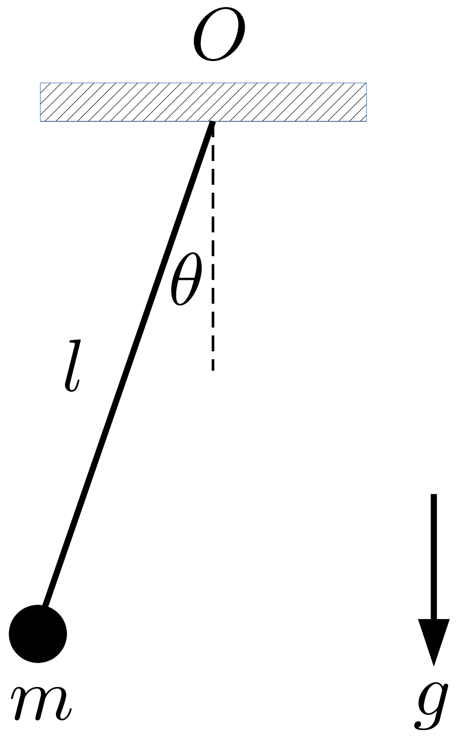
- In contrast to the much simpler integral

$$\int_a^b e^{x}\mathrm{d}x = e^a - e^b$$

- Hence, we have to approximate this integral in such a way that the approximation is accurate enough for our purpose.

$$\int_a^b e^{-x^2}\mathrm{d}x \approx \cdots$$

Basic Concepts



- We know from basic mechanics that the time evolution of a frictionless pendulum of mass m and length l in a gravitational field is modeled by the differential equation

$$\ddot{\theta} + \frac{g}{l}\sin\theta = 0$$

$$\theta(t=0) = \theta_0 \text{ and } \dot{\theta}(t=0) = 0$$

$$\theta \ll 1 : \ \sin\theta \approx \theta \qquad \ddot{\theta} + \frac{g}{l}\theta = 0$$

$$\theta = \theta_0 \cos(\omega t), \qquad \omega = \sqrt{\frac{g}{l}}, \qquad T_0 = 2\pi\sqrt{\frac{l}{g}}$$

Basic Concepts

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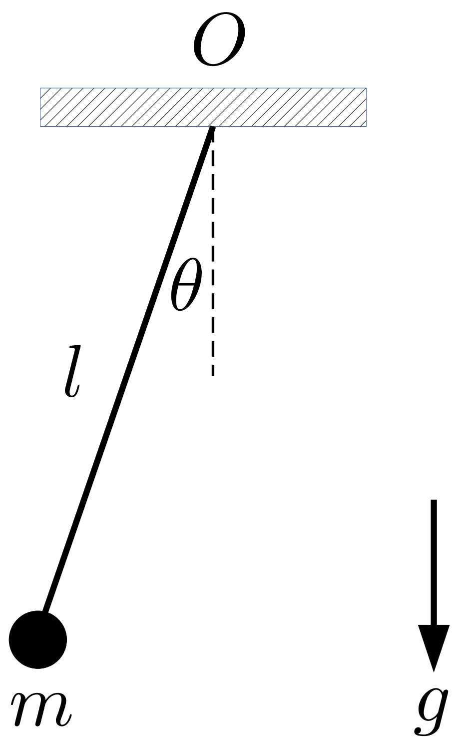


$$\ddot{\theta} + \frac{g}{l}\sin\theta = 0$$

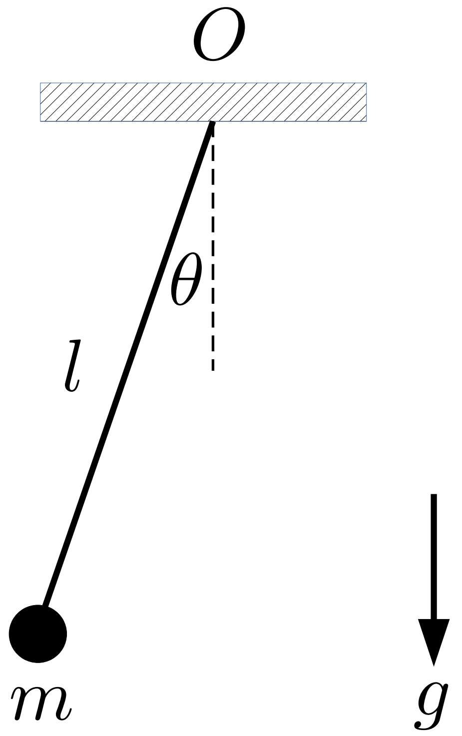
$$\theta(t=0) = \theta_0 \text{ and } \dot{\theta}(t=0) = 0$$

$$\ddot{\theta} = \frac{\mathrm{d}\dot{\theta}}{\mathrm{d}t} = \frac{\mathrm{d}\dot{\theta}}{\mathrm{d}\theta}\frac{\mathrm{d}\theta}{\mathrm{d}t} = \dot{\theta}\frac{\mathrm{d}\dot{\theta}}{\mathrm{d}\theta}$$

$$\dot{\theta}\frac{\mathrm{d}\dot{\theta}}{\mathrm{d}\theta} + \frac{g}{l}\sin\theta = 0 \Rightarrow \dot{\theta}\mathrm{d}\dot{\theta} = -\frac{g}{l}\sin\theta\mathrm{d}\theta \Rightarrow \int_0^{\dot{\theta}}\dot{\theta}\mathrm{d}\dot{\theta} = -\frac{g}{l}\int_{\theta_0}^{\theta}\sin\theta\mathrm{d}\theta$$

Basic Concepts

- We know from basic mechanics that the time evolution of a frictionless pendulum of mass m and length l in a gravitational field is modeled by the differential equation



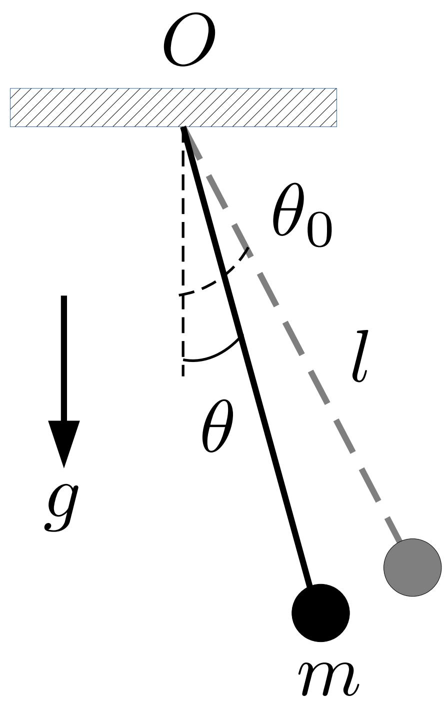
$$\int_0^{\dot\theta} \dot\theta \mathrm{d}\dot\theta = -\frac{g}{l}\int_{\theta_0}^{\theta} \sin\theta \mathrm{d}\theta$$

$$\frac{1}{2}\dot\theta^2 = \frac{g}{l}\left(\cos\theta - \cos\theta_0\right) = \frac{g}{l}\left(1 - 2\sin^2\frac{\theta}{2} - 1 + 2\sin^2\frac{\theta_0}{2}\right)$$

$$\frac{1}{2}\dot\theta^2 = 2\frac{g}{l}\left(\sin^2\frac{\theta_0}{2} - \sin^2\frac{\theta}{2}\right) \Rightarrow \dot\theta = 2\sqrt{\frac{g}{l}}\sqrt{\sin^2\frac{\theta_0}{2} - \sin^2\frac{\theta}{2}}$$

Basic Concepts

- We know from basic mechanics that the time evolution of a frictionless pendulum of mass m and length l in a gravitational field is modeled by the differential equation



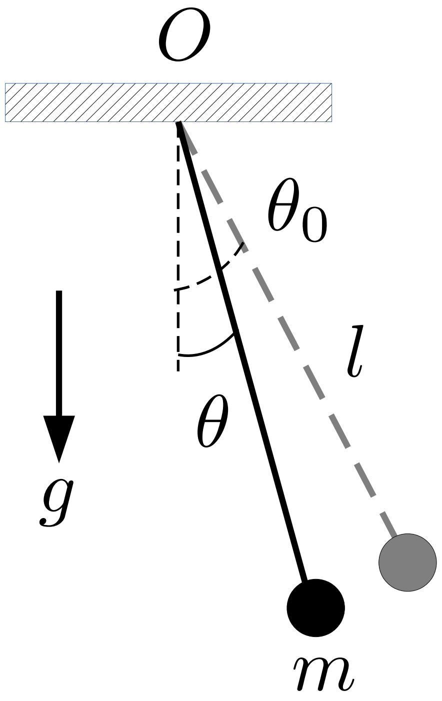
$$\dot{\theta} = 2\sqrt{\frac{g}{l}}\sqrt{\sin^2\frac{\theta_0}{2} - \sin^2\frac{\theta}{2}}$$

$$\frac{\mathrm{d}\theta}{\mathrm{d}t} = 2\sqrt{\frac{g}{l}}\sqrt{\sin^2\frac{\theta_0}{2} - \sin^2\frac{\theta}{2}} \Rightarrow \mathrm{d}t = \frac{1}{2}\sqrt{\frac{l}{g}}\frac{\mathrm{d}\theta}{\sqrt{\sin^2\frac{\theta_0}{2} - \sin^2\frac{\theta}{2}}}$$

$$\frac{1}{4}\int_0^T \mathrm{d}t = \frac{1}{2}\sqrt{\frac{l}{g}}\int_0^{\theta_0}\frac{\mathrm{d}\theta}{\sqrt{\sin^2\frac{\theta_0}{2} - \sin^2\frac{\theta}{2}}}$$

Basic Concepts

- A frictionless pendulum

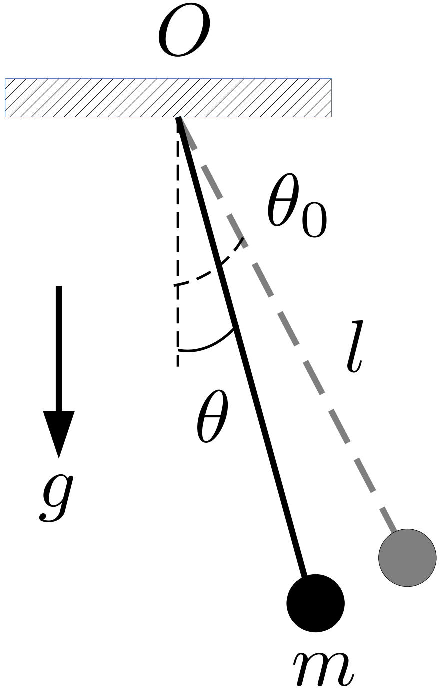


$$T = 2\sqrt{\frac{l}{g}}\int_0^{\theta_0} \frac{\mathrm{d}\theta}{\sqrt{\sin^2\frac{\theta_0}{2} - \sin^2\frac{\theta}{2}}}$$

$$k = \sin\frac{\theta_0}{2}: \quad T = \frac{2}{k}\sqrt{\frac{l}{g}}\int_0^{\theta_0} \frac{\mathrm{d}\theta}{\sqrt{1 - \frac{1}{k^2}\sin^2\frac{\theta}{2}}}$$

Basic Concepts

- A frictionless pendulum



$$T = \frac{2}{k}\sqrt{\frac{l}{g}}\int_0^{\theta_0} \frac{\mathrm{d}\theta}{\sqrt{1-\frac{1}{k^2}\sin^2\frac{\theta}{2}}}$$

$$k\sin\alpha = \sin\frac{\theta}{2}, \qquad 0 \le \sin\frac{\theta}{2} \le \sin\frac{\theta_0}{2} \Rightarrow 0 \le \alpha \le \pi/2$$

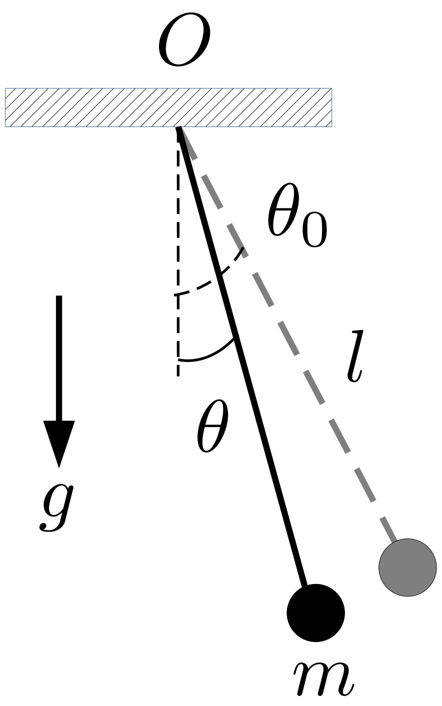
$$T = 4\sqrt{\frac{l}{g}}\int_0^{\pi/2} \frac{\mathrm{d}\alpha}{\sqrt{1-k^2\sin^2\alpha}} = 4\sqrt{\frac{l}{g}}F(k,\frac{\pi}{2})$$

$F(k,\frac{\pi}{2})$: Complete elliptic integral of the first kind

Basic Concepts

- A frictionless pendulum

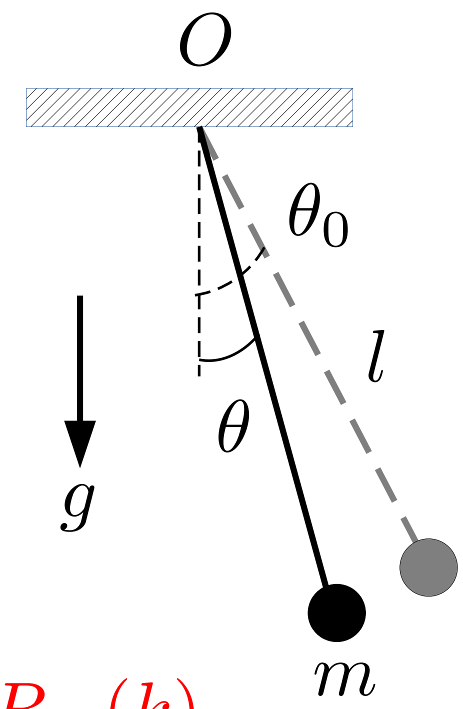
$$T = 4\sqrt{\frac{l}{g}}\int_0^{\pi/2}\frac{\mathrm{d}\alpha}{\sqrt{1-k^2\sin^2\alpha}} = 4\sqrt{\frac{l}{g}}F(k,\frac{\pi}{2})$$



Amplitude, θ_0	$k = \sin\left(\frac{\theta_0}{2}\right)$	$F\left(k, \frac{\pi}{2}\right)$	Period, T
0°	0	$1.5708 = \pi/2$	T_0
10°	0.0872	1.5738	$1.0019\ T_0$
45°	0.3827	1.6336	$1.0400\ T_0$
90°	0.7071	1.8541	$1.1804\ T_0$
135°	0.9234	2.4003	$1.5281\ T_0$
178°	0.99985	5.4349	$3.5236\ T_0$
179°	0.99996	5.2660	$4.6002\ T_0$
180°	1	∞	∞

Basic Concepts

- A frictionless pendulum



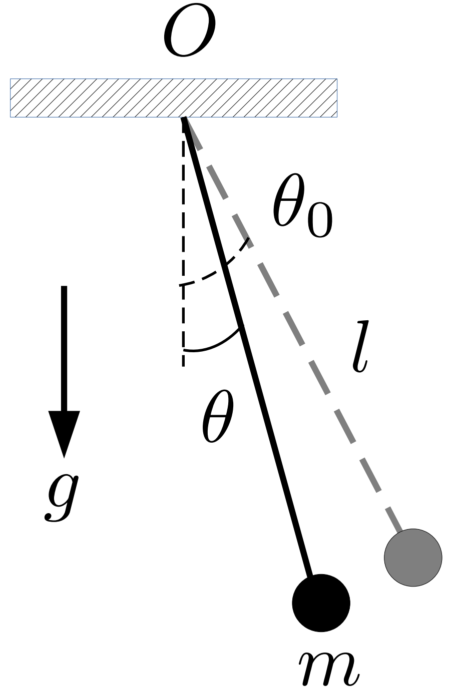
$$T = 4\sqrt{\frac{l}{g}}\int_0^{\pi/2}\frac{d\alpha}{\sqrt{1-k^2\sin^2\alpha}} = 4\sqrt{\frac{l}{g}}F(k,\frac{\pi}{2})$$

$$F(k,\frac{\pi}{2}) = \frac{\pi}{2}\sum_0^{\infty}\left[\frac{(2n)!}{2^{2n}(n!)^2}\right]^2 k^{2n} = \frac{\pi}{2}\sum_0^{N}\left[\frac{(2n)!}{2^{2n}(n!)^2}\right]^2 k^{2n} + R_N(k)$$

$R_N(k)$: Truncation Error

Basic Concepts

- A frictionless pendulum



$$T = 2\pi\sqrt{\frac{l}{g}}\sum_{0}^{\infty}\left[\frac{(2n)!}{2^{2n}(n!)^2}\right]^2 k^{2n} = T_0\sum_{0}^{\infty}\left[\frac{(2n)!}{2^{2n}(n!)^2}\right]^2 k^{2n}$$

$$\sum_{0}^{\infty}\left[\frac{(2n)!}{2^{2n}(n!)^2}\right]^2 k^{2n} = \frac{T}{T_0} \Rightarrow k =? \text{ or } \theta_0 =?$$

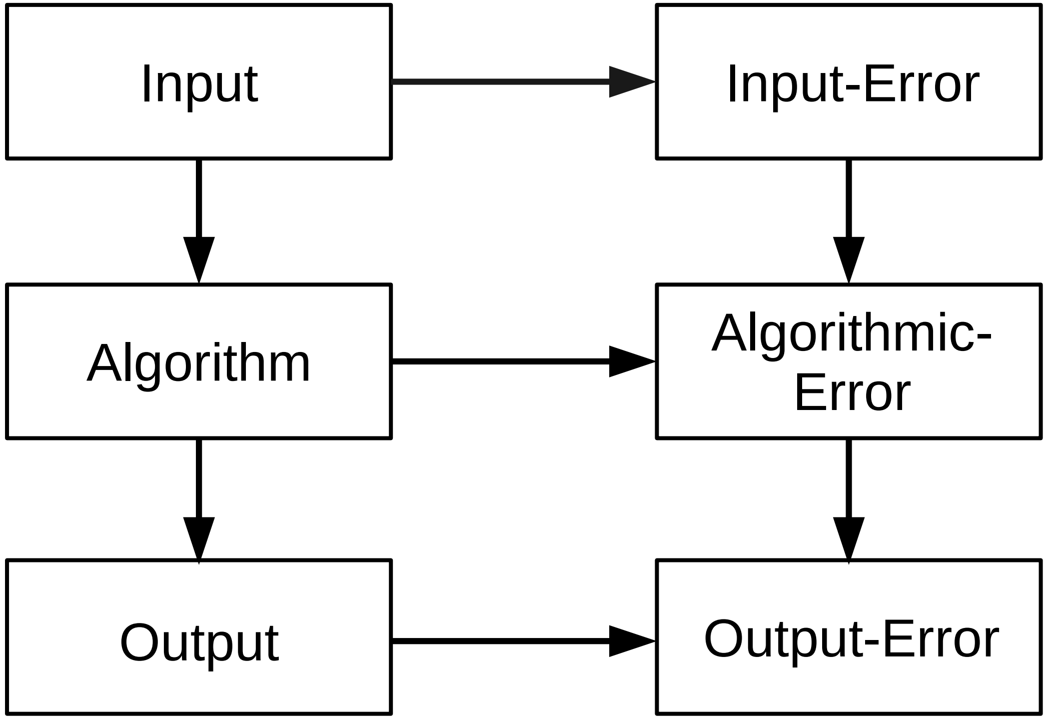
However, such an approach would be very inefficient due to two reasons:

- We are confronted with the **impossibility of finding analytically the roots** of a polynomial of order *N*>4.
- At which value should we **truncate the power series**?

Basic Concepts

- Classify the occurring errors based on the structure every numerical routine.

  * **Input-Error**
    - □ Roundoff errors in input data
  * **Algorithmic-Error**
    - □ Roundoff errors during evaluation
    - □ Methodological errors due to mathematical approximations
  * **Output-Error**
    - □ Roundoff errors



Basic Concepts

- Roundoff errors

Since every number is stored in **a computer using a finite number of digits**, we have to **truncate** every non-terminating number at some point.

$$\frac{2}{3} = 0.666666666666\cdots \xrightarrow{\text{stored}} \overbrace{0.6666666667}^{\text{Ten digits}} \quad \text{truncated}$$

floating-point form $\mathrm{FL}\left(\frac{2}{3}\right) = 0.6666666667$

This has the consequence: $\mathrm{FL}(\sqrt{3})\mathrm{FL}(\sqrt{3}) \neq \mathrm{FL}(\sqrt{3}\sqrt{3}) = 3$

Basic Concepts

- Roundoff errors

  * Absolute error

$$\epsilon_a = \mid y - \bar{y} \mid$$

True value y
Approximate value $\bar{y}$

  * Relative error

$$\epsilon_r = \left| \frac{y - \bar{y}}{y} \right| = \frac{\epsilon_a}{\mid y \mid}$$

In most applications, the **relative error is more significant**.

	y	$\bar{y}$	ϵ_a	ϵ_r
(1)	0.1	0.09	0.01	0.1
(2)	1000.0	999.99	0.01	0.00001

Basic Concepts

- Roundoff errors

True value $y = 0.d_1 d_2 d_3 \cdots d_k d_{k+1} \cdots \times 10^n$

Approximate value $\bar{y} = 0.d_1 d_2 d_3 \cdots d_k \times 10^n$

$d_1 \neq 0$

$$\epsilon_r = \left| \frac{0.d_1 d_2 d_3 \cdots d_k d_{k+1} \cdots \times 10^n - 0.d_1 d_2 d_3 \cdots d_k \times 10^n}{0.d_1 d_2 d_3 \cdots d_k d_{k+1} \cdots \times 10^n} \right|$$

$$\epsilon_r = \left| \frac{0.d_{k+1} d_{k+2} \cdots \times 10^{-k}}{0.d_1 d_2 d_3 \cdots d_k d_{k+1} \cdots} \right| = \left| \frac{0.d_{k+1} d_{k+2} \cdots}{0.d_1 d_2 d_3 \cdots} \right| 10^{-k} < \frac{1}{0.1} 10^{-k} = 10^{-k+1}$$

$$d_1 \neq 0 : \; 0.d_1 d_2 d_3 \cdots \geq 0.1, \qquad 0.d_{k+1} d_{k+2} \cdots < 1$$

Basic Concepts

- Roundoff errors

  * Particular care is required

    when two nearly identical numbers are subtracted

    or

    when a large number is divided by a small number.

  increase in the relative error.

  * In such cases the **roundoff error will increase** dramatically.

  * We note that it might be necessary to avoid such operations in our aim to design an algorithm which is required to produce reasonable results.

Basic Concepts

- Roundoff errors

* The **machine-number** is smallest positive number which can be added to another number, such that a change in the result is observed.

$$\eta = \min_{\delta}\{\delta > 0 | 1 + \delta > 1\}$$

* A typical value for **double-precision** in FORTRAN or C is

$$\eta \approx 10^{-16}$$

Basic Concepts

- Methodological Errors

    * A **methodological error** is introduced whenever
    a complex mathematical expression is replaced by an approximate,
    or
    we have to deal with expressions we cannot evaluate analytically.

$$\sum_{0}^{\infty}\left[\frac{(2n)!}{2^{2n}(n!)^2}\right]^2 k^{2n} \approx \frac{\pi}{2}\sum_{0}^{N}\left[\frac{(2n)!}{2^{2n}(n!)^2}\right]^2 k^{2n}$$

$$f'(x_0) = \left.\frac{\mathrm{d}f}{\mathrm{d}x}\right|_{x_0} = \lim_{h\to 0}\frac{f(x_0+h)-f(x_0)}{h} \xrightarrow{\text{Finite difference}} \left.\frac{\mathrm{d}f}{\mathrm{d}x}\right|_{x_0} \approx \frac{f(x_0+h)-f(x_0)}{h}$$