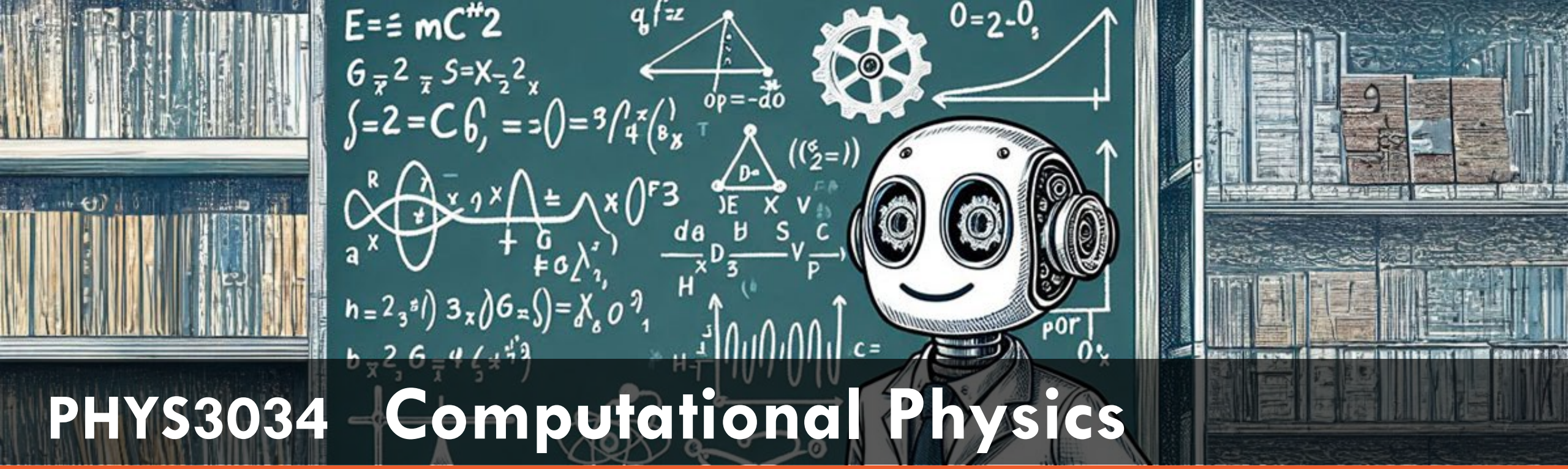


PHYS3034 Computational Physics

A/Professor Sveta Postnova

svetlana.postnova@sydney.edu.au

THE UNIVERSITY OF SYDNEY

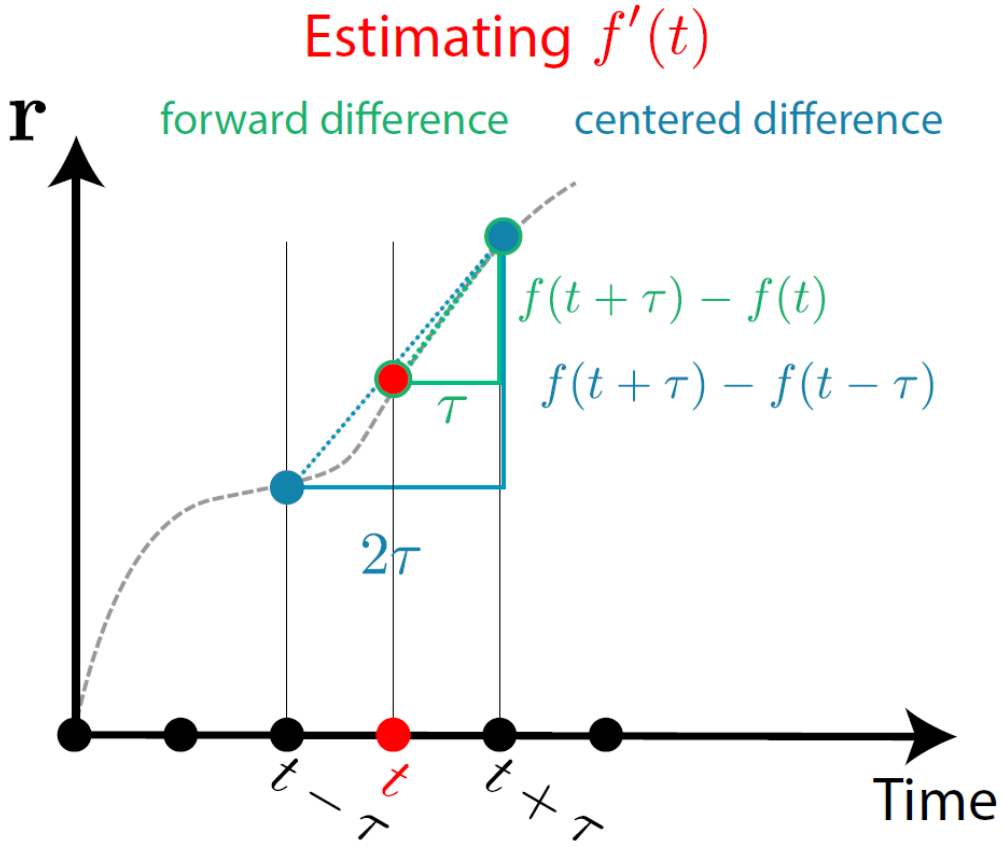
Recap Week 2

- Introduced the *Kepler problem*
- *Non-dimensionalisation* simplified the formulation.
- Introduced the *centred-difference approximation* to overcome the limitations of the scheme based on the forward difference approximation (Euler).
- Yields a new method, *Verlet*, which exhibits better accuracy for Keplerian orbits with near conservation of energy

Recap weeks 1&2:
How to step forward in time, given a gradient dr/dt?

- *Euler*: use *forward difference* approximation
  - The velocity at the current time step to extrapolate forward in time.

- *Verlet* (for solving a dynamics problem): use *centred difference* approximation for the second derivative
  - So can use the acceleration and two previous values to make the update.



Lecture 3: Outline

- Our last lecture on ODEs (PDEs from next week!)
- *General form of ODEs* suitable for numerical solution.
  - Dynamics equations we've considered so far are a special case (Verlet).
- Introduce *Runge-Kutta (RK)* (Taylor series) methods:
  - Can be applied to the general form for ODEs.
  - Euler's method is the first-order RK scheme.
- Simulate motion of a *simple pendulum*.
  - Illustrate the general form and a vector ODE *right-hand side function*.

General form of ODEs

General form of a system of ODEs

- $\boxed{\frac{d\mathbf{x}}{dt} = \mathbf{f}\left[\mathbf{x}(t), t\right]}$.
  - N coupled first order ordinary differential equations (ODEs).
  - t is the *independent* variable (often time, but could be anything).
- $\mathbf{x}$ is a vector of the *dependent* variables, $\mathbf{x}(t) = [x_1(t), x_2(t), \ldots, x_N(t)]$.
- $\mathbf{f}$ is a vector function called the *right-hand side* (RHS):
  - $\mathbf{f}[\mathbf{x}(t), t] = \{f_1[\mathbf{x}(t), t], f_2[\mathbf{x}(t), t], \ldots, f_N[\mathbf{x}(t), t]\}$.
- General *Initial Value Problem* (IVP):
  - Given $\mathbf{x}(t_1)$, calculate $\mathbf{x}(t)$ for $t > t_1$.
- Writing ODEs in this form makes it easy for us to apply general numerical methods
  - Just need to specify the *RHS function* $\mathbf{f}\left[\mathbf{x}(t), t\right]$.

Dynamics problems in general form

Motion problems are a *special case*:

- $\frac{d^2\mathbf{r}}{dt^2} = \mathbf{a}$ can be written $\frac{d\mathbf{r}}{dt} = \mathbf{v}$, $\frac{d\mathbf{v}}{dt} = \mathbf{a}$.
- Position $\mathbf{r} = (x, y, z)$, velocity $\mathbf{v} = (v_x, v_y, v_z)$, and acceleration, $\mathbf{a} = (a_x, a_y, a_z)$.

We can write them in the *general form*, $\frac{d\mathbf{x}}{dt} = \mathbf{f}(\mathbf{x}, t)$, by identifying $\mathbf{x} = (x, y, z, v_x, v_y, v_z)^T$ and $\mathbf{f} = (v_x, v_y, v_z, a_x, a_y, a_z)^T$:

$$\frac{d}{dt}\begin{pmatrix} x \\ y \\ z \\ v_x \\ v_y \\ v_z \end{pmatrix} = \begin{pmatrix} v_x \\ v_y \\ v_z \\ a_x \\ a_y \\ a_z \end{pmatrix}.$$

Writing higher-order ODEs in general form

- A similar trick can get any high-order ODE into the general form 🐛
  - ❓ Where did we do this already?
- Consider Nth-order linear ODE in y_1: $a_1 y_1 + a_2 \frac{dy_1}{dt} + a_3 \frac{d^2 y_1}{dt^2} + \cdots + a_{N+1} \frac{d^N y_1}{dt^N} = 0$.
- We can always *replace higher derivatives by new variables*, y_2, y_3, ...:
  - $y_2 = \frac{dy_1}{dt}$, $y_3 = \frac{dy_2}{dt} = \frac{d^2 y_1}{dt^2}$, $\cdots$ $y_N = \frac{dy_{N-1}}{dt} = \left(\frac{d}{dt}\right)^{N-1} y_1$.
- So now we can rewrite the Nth-order ODE equivalently in *general form*, $\frac{d\mathbf{x}}{dt} = \mathbf{f}$, by identifying:
  - $\mathbf{x} = (y_1, y_2, \ldots, y_N)$, and $\mathbf{f} = \left[y_2, y_3, \ldots, -\frac{1}{a_{N+1}}(a_1 y_1 + a_2 y_2 \cdots + a_N y_N)\right]$.
- *You need to know how to apply this procedure*

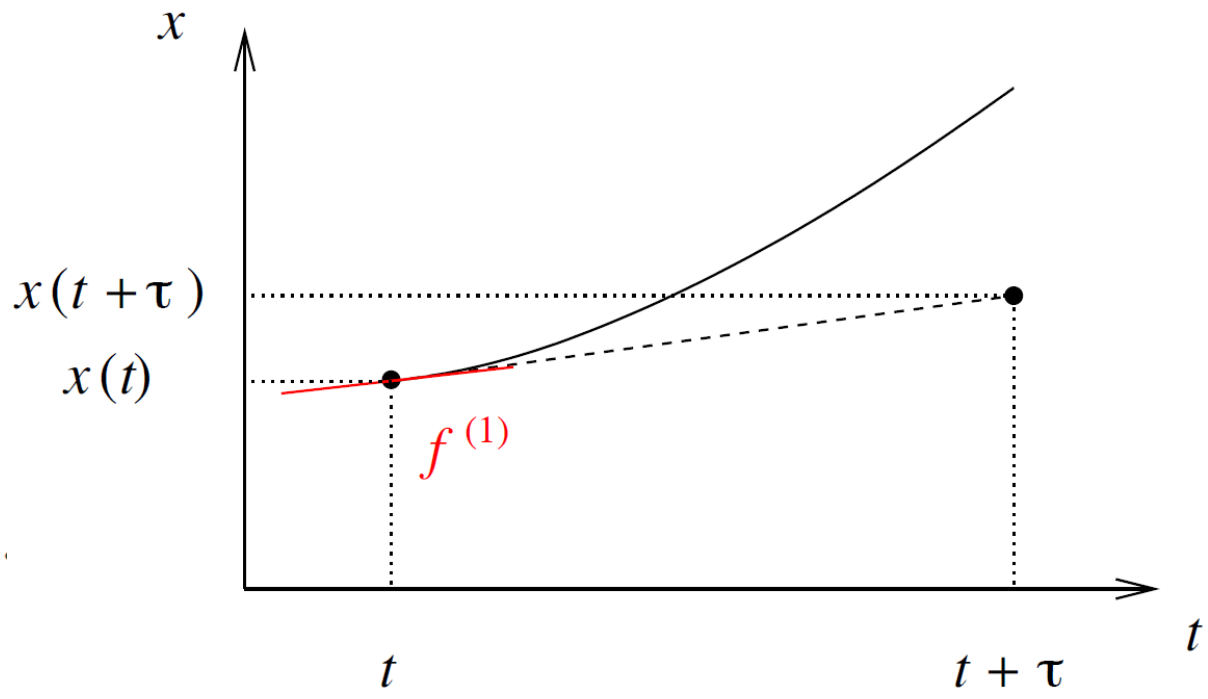
Euler method for the general form

Euler's method for the general form

- *Taylor-series* expansion (using $\frac{d\mathbf{x}}{dt} = \mathbf{f}[\mathbf{x}(t), t]$):
  - $$\mathbf{x}(t+\tau) = \mathbf{x}(t) + \tau\frac{d\mathbf{x}}{dt} + O(\tau^2)\,,$$
    $$= \mathbf{x}(t) + \tau\mathbf{f}[\mathbf{x}(t), t] + O(\tau^2)\,.$$
- *Euler's method* matches the Taylor series to $O(\tau)$:
  - $\mathbf{x}(t+\tau) = \mathbf{x}(t) + \tau\mathbf{f}^{(1)}$, where $\mathbf{f}^{(1)} = \mathbf{f}[\mathbf{x}(t), t]$.
  - For Euler, $\mathbf{f}^{(1)}$ is the *right-hand side (RHS)* of the ODE.
- Euler for dynamics problems is a special case.

An Euler step in 1-D

- $x(t+\tau) = x(t) + \tau f^{(1)}$,
  - with $f^{(1)} = f[x(t), t] = \dfrac{dx}{dt}$.
- $f^{(1)}$ is $\dfrac{dx}{dt}$ evaluated at $(t, x(t))$:
  - the gradient of the tangent (red).
- Euler extrapolates forward τ along the tangent line.



Testing Euler on a simple exponential case

- *Simple ODE/IVP:* $\frac{dx}{dt} = x$ with $x(0) = 1$.
  - Analytic solution is $x(t) = e^t$ so integrating to $t = 1$ the final value should be ≈ 2.71828.

- `expproblem.ipynb` solves this by defining a function rhs_exp(x) that returns the same input, x.
- ❓ Why is RHS $f^{(1)} = x$ here?

- *Testing:*
  - Let's compute the error for a 10-step integration.
  - ❓ What's your prediction for a 20-step integration...?
- Euler works ok, but *can we do better than just taking little steps forward based on extrapolating the current derivative*?

t	x
0	1
0.1	1.1
0.2	1.21
0.3	1.331
0.4	1.4641
0.5	1.6105
0.6	1.7716
0.7	1.9487
0.8	2.1436
0.9	2.3579
1	2.5937

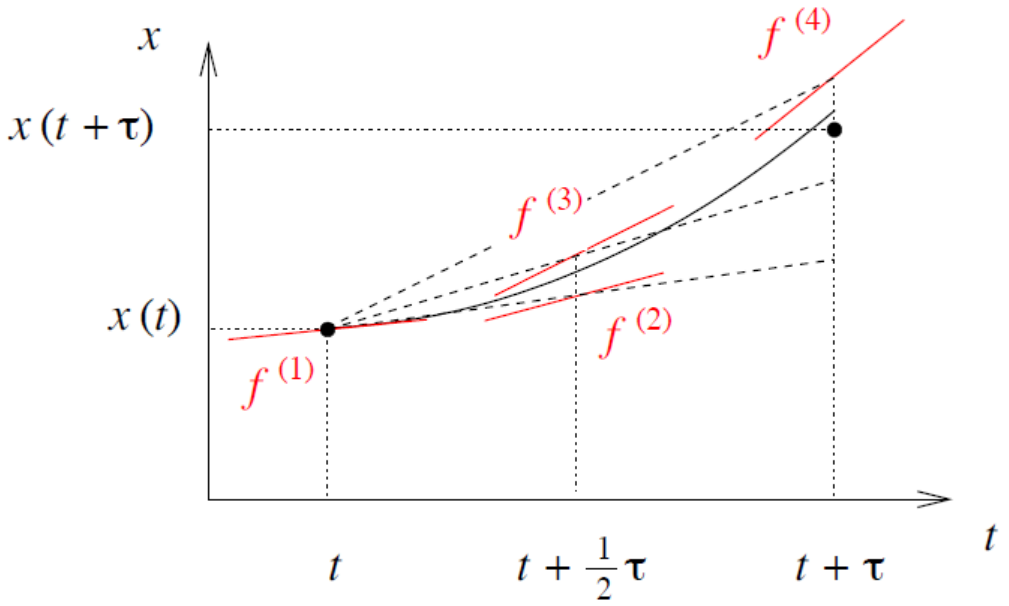
Error: 4.58155%

Runge-Kutta method

Runge-Kutta

- Carl Runge (1856-1927) and Martin Kutta (1867-1944).

- In general, we can do better than naively marching forward with a single estimate of the derivative by combining information at fractions of a step.



Runge-Kutta Methods

- Runge-Kutta methods *match the Taylor series* to a given order.
  - Euler is 'first-order Runge-Kutta': $\mathbf{x}(t+\tau) = \mathbf{x}(t) + \tau\mathbf{f}^{(1)}$.
- Higher-order schemes are more accurate.
- A *very popular* one: ⭐ ***Fourth-Order Runge-Kutta (RK4)*** ⭐:

$$\mathbf{x}(t+\tau) = \mathbf{x}(t) + \tfrac{1}{6}\tau\left[\mathbf{f}^{(1)} + 2\mathbf{f}^{(2)} + 2\mathbf{f}^{(3)} + \mathbf{f}^{(4)}\right],$$

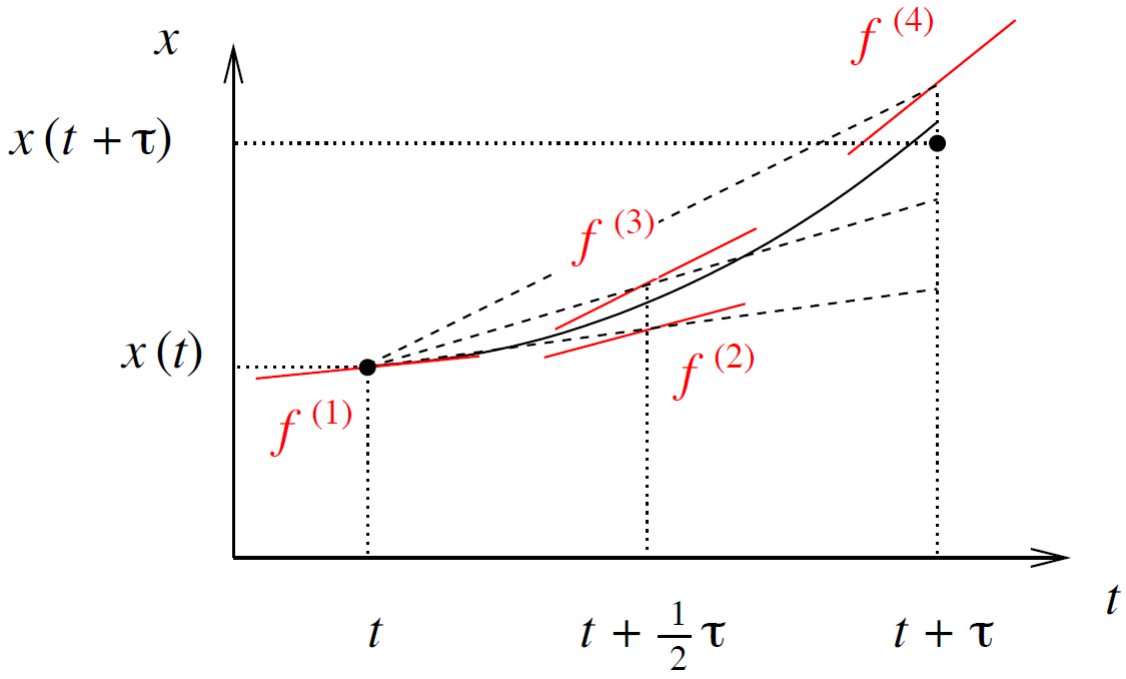
$$\mathbf{f}^{(1)} = \mathbf{f}[\mathbf{x}(t), t],$$
$$\mathbf{f}^{(2)} = \mathbf{f}[\mathbf{x}(t) + \tfrac{1}{2}\tau\mathbf{f}^{(1)}, t + \tfrac{1}{2}\tau],$$
$$\mathbf{f}^{(3)} = \mathbf{f}[\mathbf{x}(t) + \tfrac{1}{2}\tau\mathbf{f}^{(2)}, t + \tfrac{1}{2}\tau],$$
$$\mathbf{f}^{(4)} = \mathbf{f}[\mathbf{x}(t) + \tau\mathbf{f}^{(3)}, t + \tau].$$

Fourth-Order Runge-Kutta (RK4)

- Four RHS/gradient evaluations:
  - two at a half step $(t + \frac{1}{2}\tau)$
  - two at a full step $(t + \tau)$.
- Extrapolates forward to $t + \tau$ along a complicated average gradient line.

$$\mathbf{x}(t+\tau) = \mathbf{x}(t) + \tfrac{1}{6}\tau\left[\mathbf{f}^{(1)} + 2\mathbf{f}^{(2)} + 2\mathbf{f}^{(3)} + \mathbf{f}^{(4)}\right],$$

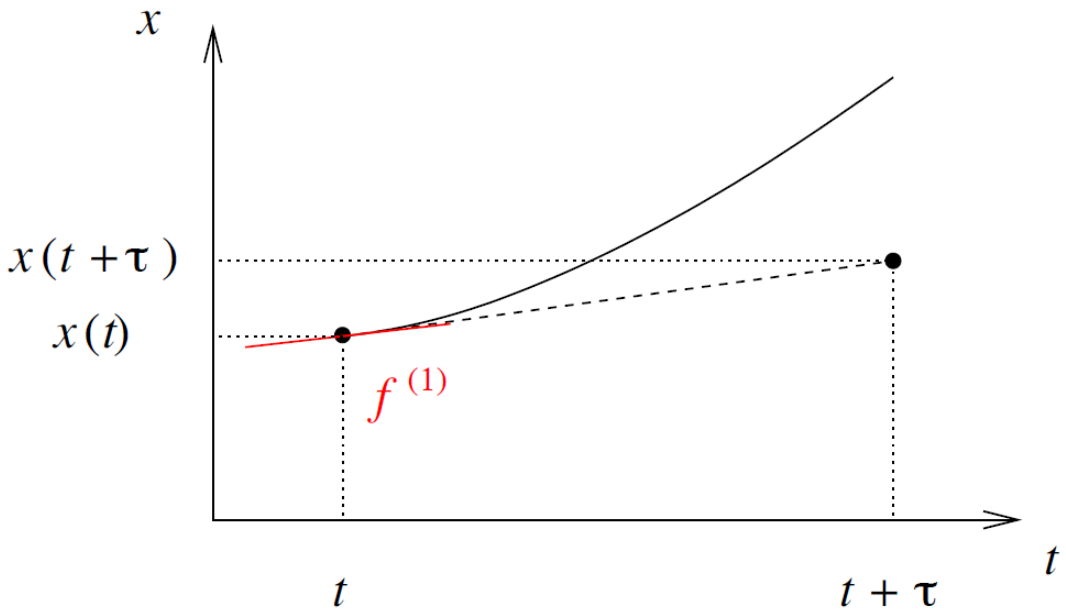
$$\mathbf{f}^{(1)} = \mathbf{f}[\mathbf{x}(t), t],$$
$$\mathbf{f}^{(2)} = \mathbf{f}[\mathbf{x}(t) + \tfrac{1}{2}\tau\mathbf{f}^{(1)}, t + \tfrac{1}{2}\tau],$$
$$\mathbf{f}^{(3)} = \mathbf{f}[\mathbf{x}(t) + \tfrac{1}{2}\tau\mathbf{f}^{(2)}, t + \tfrac{1}{2}\tau],$$
$$\mathbf{f}^{(4)} = \mathbf{f}[\mathbf{x}(t) + \tau\mathbf{f}^{(3)}, t + \tau].$$



Euler vs Runge-Kutta

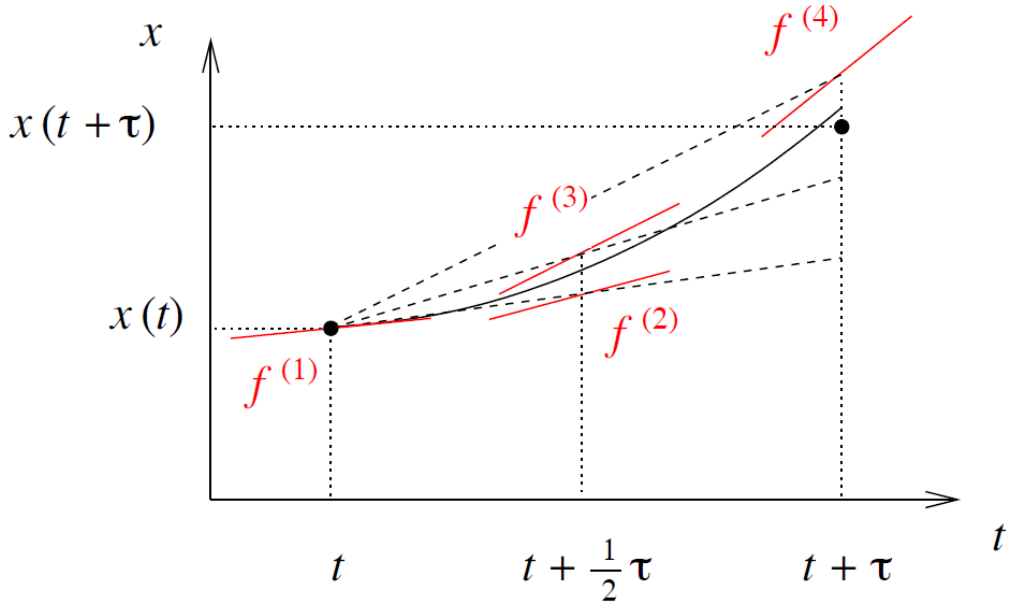
Euler (RK1)

$$\mathbf{x}(t+\tau) = \mathbf{x}(t) + \tau \mathbf{f}^{(1)}.$$



Fourth-Order Runge-Kutta (RK4)

- $\mathbf{x}(t+\tau) = \mathbf{x}(t) + \frac{1}{6}\tau\left[\mathbf{f}^{(1)} + 2\mathbf{f}^{(2)} + 2\mathbf{f}^{(3)} + \mathbf{f}^{(4)}\right]$
  - $\mathbf{f}^{(1)} = \mathbf{f}[\mathbf{x}(t), t]$
  - $\mathbf{f}^{(2)} = \mathbf{f}[\mathbf{x}(t) + \frac{1}{2}\tau\mathbf{f}^{(1)}, t + \frac{1}{2}\tau]$
  - $\mathbf{f}^{(3)} = \mathbf{f}[\mathbf{x}(t) + \frac{1}{2}\tau\mathbf{f}^{(2)}, t + \frac{1}{2}\tau]$
  - $\mathbf{f}^{(4)} = \mathbf{f}[\mathbf{x}(t) + \tau\mathbf{f}^{(3)}, t + \tau]$



Understanding Runge-Kutta methods

- We're given a function, $\mathbf{f}\left[\mathbf{x}(t), t\right]$ and we have to try to work out how make a good step forward in time 😵
- Consider a *Taylor-series expansion* of the dependent variables:
  - $\mathbf{x}(t+\tau) = \mathbf{x}(t) + \tau\frac{d\mathbf{x}}{dt} + \frac{\tau^2}{2!}\frac{d^2\mathbf{x}}{dt^2} + \frac{\tau^3}{3!}\frac{d^3\mathbf{x}}{dt^3} + \ldots$
- The Runge-Kutta approach is to *reproduce this series to a certain order*.
- *Euler matches to first order* (is 'RK1')
  - Uses RHS directly: $\frac{d\mathbf{x}}{dt} = \mathbf{f}\left[\mathbf{x}(t), t\right]$.
- Fourth-order Runge-Kutta (RK4) *matches the Taylor series to* $O(\tau^4)$.
  - i.e., local truncation error $O(\tau^5)$: *very accurate* 💪💪💪
  - *Very commonly used* and can get you far: Matlab has RK4 `ode45` (but we will write our own version 😆)
- The derivation is complicated (cf. Appendix for RK2).

Code: Stepping with Euler

$$\mathbf{x}(t+\tau) = \mathbf{x}(t) + \tau\mathbf{f}^{(1)}.$$

```
for n in range(numSteps):
    # One step of Explicit Euler
    f = rhs_exp(x)
    x = x + tau * f
    t = t + tau
```

Code: Stepping with RK4

- $\mathbf{x}(t+\tau) = \mathbf{x}(t) + \frac{1}{6}\tau\left[\mathbf{f}^{(1)} + 2\mathbf{f}^{(2)} + 2\mathbf{f}^{(3)} + \mathbf{f}^{(4)}\right]$
  - $\mathbf{f}^{(1)} = \mathbf{f}[\mathbf{x}(t), t]$
  - $\mathbf{f}^{(2)} = \mathbf{f}[\mathbf{x}(t) + \frac{1}{2}\tau\mathbf{f}^{(1)}, t + \frac{1}{2}\tau]$
  - $\mathbf{f}^{(3)} = \mathbf{f}[\mathbf{x}(t) + \frac{1}{2}\tau\mathbf{f}^{(2)}, t + \frac{1}{2}\tau]$
  - $\mathbf{f}^{(4)} = \mathbf{f}[\mathbf{x}(t) + \tau\mathbf{f}^{(3)}, t + \tau]$

```
for n in range(numSteps):
    # One step of RK4
    f1 = rhs_exp(x)
    f2 = rhs_exp(x + 0.5 * tau * f1)
    f3 = rhs_exp(x + 0.5 * tau * f2)
    f4 = rhs_exp(x + tau * f3)

    x = x + tau * (f1 + 2*f2 + 2*f3 + f4) / 6
    t = t + tau
```

Euler vs RK4

Let’s play with the code

`expproblem.ipynb`

Results!

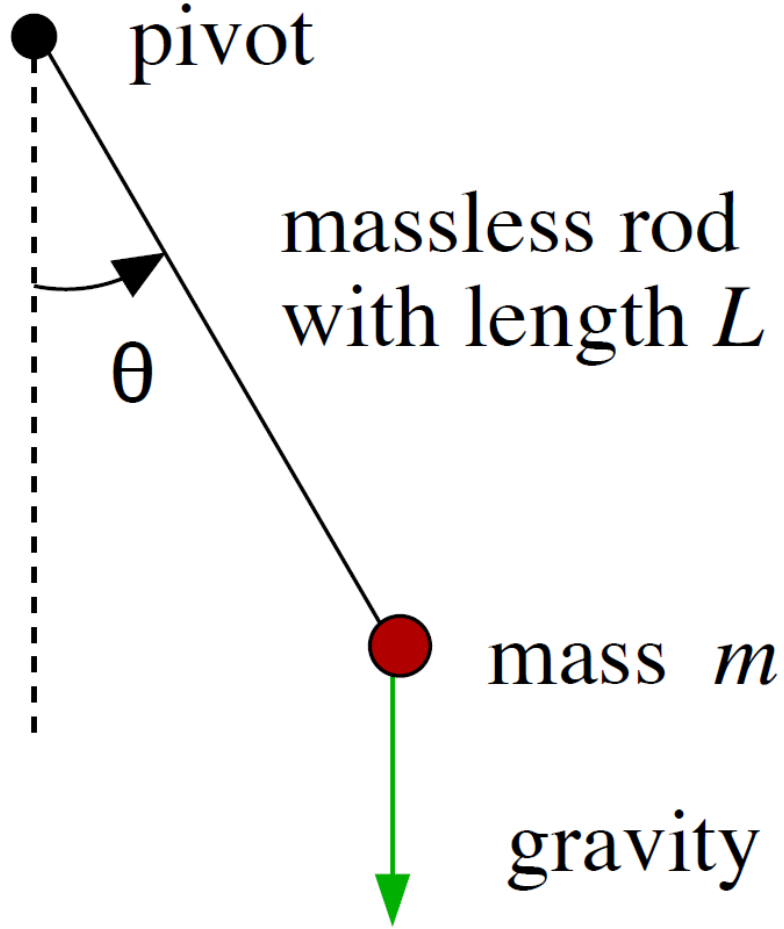
- Percentage error in $\boldsymbol{x(1)}$ after 10 steps:
  - Euler: 4.6% 😐
  - RK4: 0.000077% 😵
- With RK4, the final value is $\mathbf{2.7182797...}$ ($e = \mathbf{2.7182818...}$)
  - Can we verify the local $O(\tau^5)$?
- ❓ Why is this kind of unfair?
  - 👀😊 In each iteration, RK4 makes four RHS evaluations compared to Euler's 1...
  - *Euler*: 8 RHS calculations (8 steps): 5.6% error.
  - *RK4*: 8 RHS calculations (2 steps): 0.034% error.
- RK4 is 'smarter' at stepping forward using the same number of RHS calculations: *the increased accuracy at each step pays off!* 🐆💪🐆💪

Simple Pendulum Problem

This week's problem: The Simple Pendulum

- $\frac{d^2\theta}{dt^2} = -\frac{g}{L}\sin\theta.$
  - angle from the vertical θ, acceleration due to gravity g, length L.
- ❓: How might we get this second-order ODE into general form (coupled first-order)?
  - 👀 Same ole trick: introduce a new variable, ω:

    $$\frac{d\theta}{dt} = \omega, \qquad \frac{d\omega}{dt} = -\frac{g}{L}\sin\theta.$$
- Easy, huh? 😌 This is the *general form*, $\frac{d\mathbf{x}}{dt} = \mathbf{f}$
  - $\mathbf{x} = (\theta, \omega)$, $\mathbf{f} = \left(\omega, -\frac{g}{L}\sin\theta\right)$.



This week's problem: The Simple Pendulum (ctnd…)

- *Initial Value Problem*: Starting from rest at an angle θ_1: $\theta(0) = \theta_1$ and $\omega(0) = \omega_1 = 0$.
- This is also a *dynamics* problem.
  - θ is angular position ($r \leftrightarrow \theta$).
  - ω is angular speed ($v \leftrightarrow \omega$).
- An *approximate* analytic solution (valid for $\theta_1 \ll 1$) is simple harmonic oscillation: $\theta = \theta_1 \cos(\Omega t)$,
  - with $\Omega^2 = \frac{g}{L}$, period $T_0 = \frac{2\pi}{\Omega} = 2\pi\sqrt{\frac{L}{g}}$, amplitude θ_1.
- For $\theta_1 \ll 1$, the period does not depend on amplitude.
  - But the general case is *nonlinear*, with no simple closed-form analytic solution 😵

Pendulum: non-dimensionalising

- θ is already non-dimensional 👍
- For time, $\bar{t} = \dfrac{t}{t_s}$, we can set our characteristic timescale, $t_s = T_0 = 2\pi\sqrt{\dfrac{L}{g}}$:
  - $\dfrac{d^2\theta}{dt^2} = \dfrac{1}{T_0^2}\dfrac{d^2\theta}{d\bar{t}^2} = \dfrac{g}{4\pi^2 L}\dfrac{d^2\theta}{d\bar{t}^2}.$
  - $\dfrac{d^2\theta}{dt^2} = -\dfrac{g}{L}\sin\theta$ becomes $\boxed{\dfrac{d^2\theta}{d\bar{t}^2} = -4\pi^2 \sin\theta}$ (no more g or L!)
- This natural timescale, T_0, yields a non-dimensional period (for $\theta \ll 1$), $\bar{T}_0 = \dfrac{T_0}{T_0} = 1.$
- In general form, $\dfrac{d\mathbf{x}}{dt} = \mathbf{f}$, we have $\mathbf{x} = \begin{pmatrix} \theta \\ \omega \end{pmatrix}$, and $\mathbf{f} = \begin{pmatrix} \omega \\ -4\pi^2 \sin\theta \end{pmatrix}$.

Pendulum Problem with RK4

simplependulum.ipynb

- The general form advantage: we write our *RHS function* and let standard numerical methods (like RK) do the rest.

- The code applies RK4 to solve the pendulum initial value problem and animates the motion of a pendulum.

- Let's play with some different settings
  - low θ_1 (e.g., 50°) recovers oscillation?
  - predictions for $\theta_1 = 180°$...?!

? What's this doing?:

```
# One step of RK4
f1 = rhs_pend(x)
f2 = rhs_pend(x + 0.5*tau*f1)
f3 = rhs_pend(x + 0.5*tau*f2)
f4 = rhs_pend(x + tau*f3)
x = x + tau*(f1 + 2*f2 + 2*f3 + f4)/6
```

? What's this doing?:

```
def rhs_pend(x):
    rhs = np.zeros(2)
    theta = x[0];
    omega = x[1];
    rhs[0] = omega;
    rhs[1] = -4*np.pi**2*np.sin(theta)
```

? What's this doing?:

```
# Update the pendulum position:
# Co-ordinates of the pendulum bar
xPendArray[n+1] = [0, np.sin(x[0])]
yPendArray[n+1] = [0, -np.cos(x[0])]
```

Computational Lab 3

Comp Lab 3

- Play with the simple pendulum code and compare Runge–Kutta to the Velocity–Verlet method.

- Adapt an implementation of RK4 to solve the Kepler problem from last week!
  - This may be your biggest challenge yet...
  - If you don't have much experience coding, you can get one-on-one help from tutors during the Lab time!

- *Next week:* We move on to PDEs!