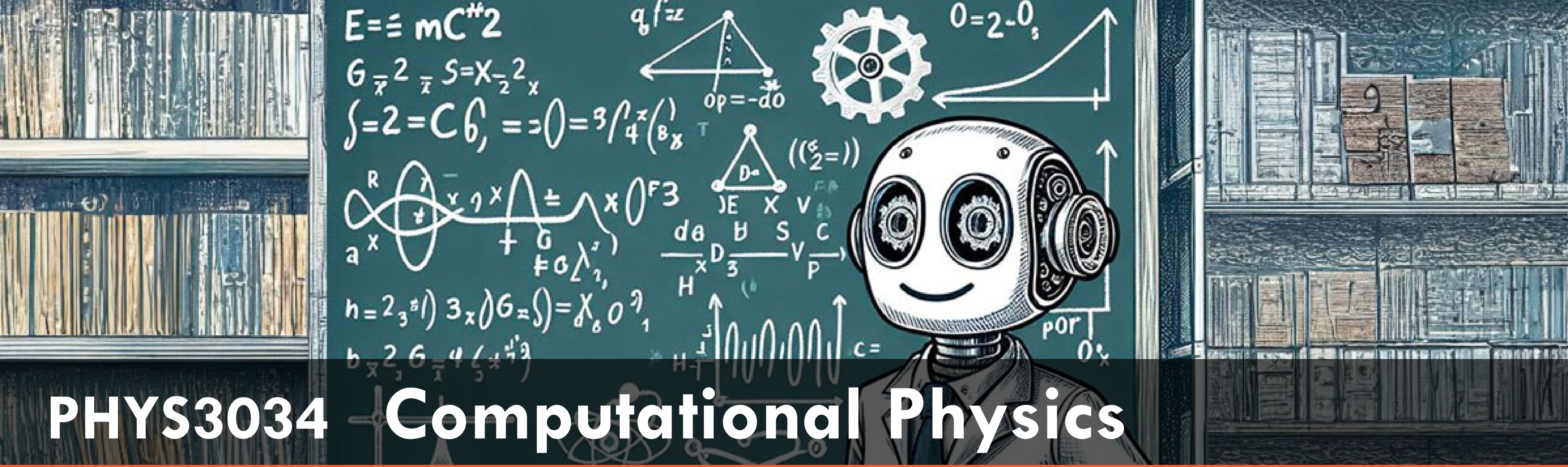

PHYS3034 Computational Physics

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Recap: Week 1

- Errors: *floating point* and *truncation*.
- Simple projectile motion problem.
- Introduced *non-dimensionalisation*, a standard procedure for numerical methods.
- Introduced *Euler's method*, a simple forward difference approximation to the derivative.
  - $\mathbf{r}_{n+1} = \mathbf{r}_n + \tau \mathbf{v}_n \,, \qquad \mathbf{v}_{n+1} = \mathbf{v}_n + \tau \mathbf{a}_n \,.$

Computer Lab (Lab 1)

- Evaluated how local and global errors scale with τ.
- Euler's method worked ok!
- Implemented(!) the *midpoint method*, which provides an exact numerical method for the constant acceleration case.
  - $\mathbf{v}_{n+1} = \mathbf{v}_n + \tau \mathbf{a}_n \,, \mathbf{r}_{n+1} = \mathbf{r}_n + \frac{1}{2}\tau \left(\mathbf{v}_n + \mathbf{v}_{n+1}\right)$
  - Requires the velocity update to be done before the position update.

Lecture 2: Verlet integration

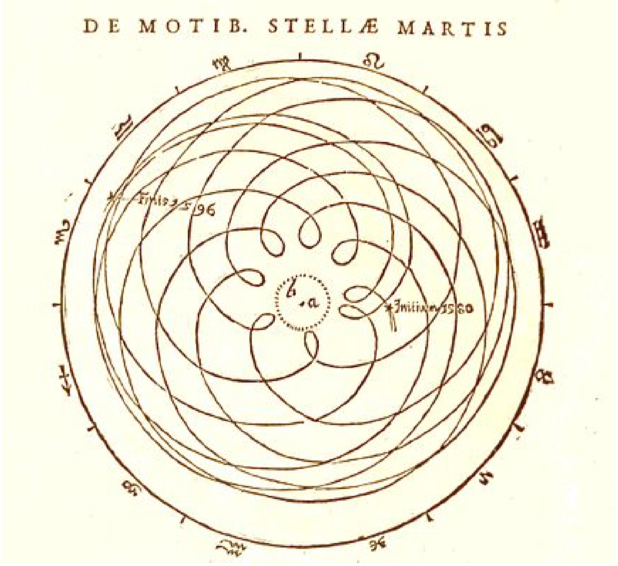
✅ Euler method works well for simple, non-stiff, slowly varying systems over short times

❌ Euler performs poorly for stiff, oscillatory, chaotic, or long-time Hamiltonian systems
Examples: harmonic oscillator, Lorenz system, orbital motion

Today's example: the Kepler Problem

- Special case of the two-body problem
- Orbital motion

Check out some orbits around Earth.



Lecture 2: Outline

- The Kepler problem as a *dynamical system*.
- *Non-dimensionalisation* of the Kepler problem.
- Euler's method (forward-difference) is unsatisfactory.
- *Centred-difference approximation*.
  - Yields a new method: *Verlet integration*.
  - Accurately integrates Keplerian orbits with near-conservation of total energy!
- *Codes*: kepler_verlet.ipynb,

  kepler_dynamics.ipynb

The Kepler problem as a dynamical system

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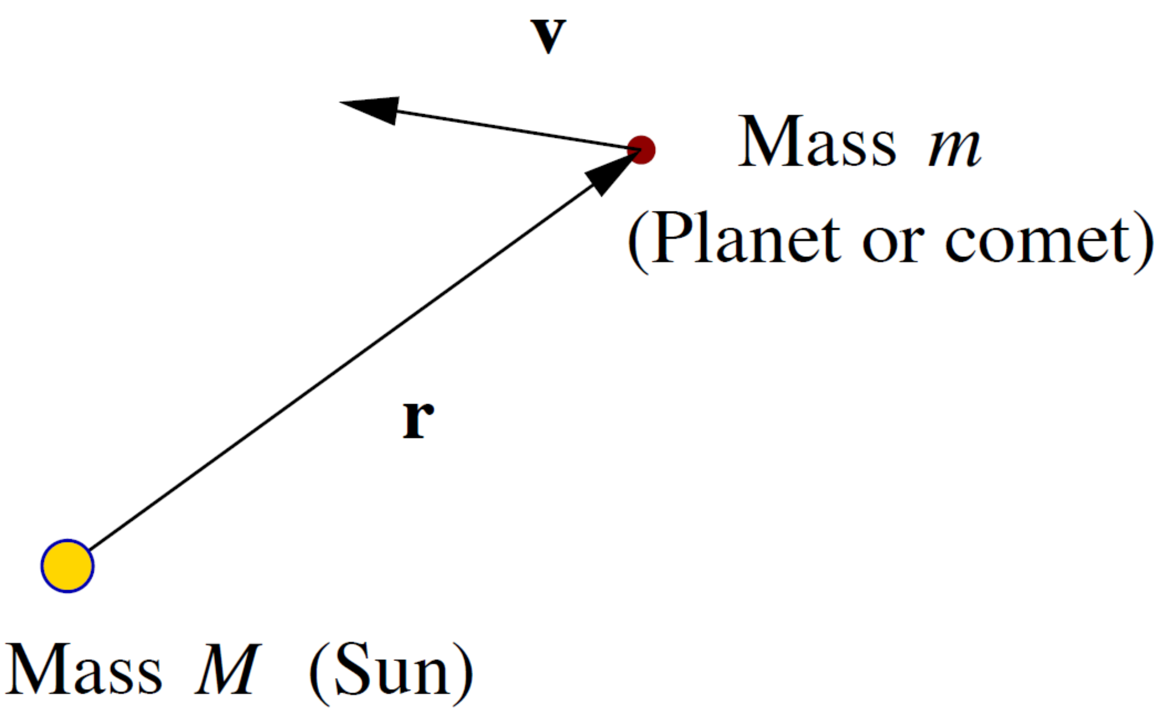
Recall: Dynamics problems

$$\frac{d\mathbf{r}}{dt} = \mathbf{v}\,, \qquad \frac{d\mathbf{v}}{dt} = \mathbf{a}(\mathbf{r},\mathbf{v},t)\,.$$

- Describe the motion of particle(s).
- Numerical methods (e.g., Euler) allow us to step forward in time (time step of size τ) and piece together an approximate trajectory:
  - $(\mathbf{r}_1\,,\mathbf{v}_1) \xrightarrow{\tau} (\mathbf{r}_2\,,\mathbf{v}_2) \xrightarrow{\tau} \cdots$
  - Local truncation error in each step.

The Kepler problem

- Dynamics of some object (e.g., a planet) of mass, $\boldsymbol{m}$, under the gravitational force of the Sun.
- Assume the Sun (mass $\boldsymbol{M} \gg \boldsymbol{m}$) is fixed at the origin.
- Paths followed are called *orbits*.
- Stable orbits trace out ellipses with the Sun at a focus.



Gravitational acceleration and the Kepler problem

A particle of mass *m* moves under Newtonian gravity: $\mathbf{F} = -\frac{GMm}{r^2}\hat{\mathbf{r}}$

$G \approx 6.67 \times 10^{-11}\,\mathrm{kg^{-1}m^3s^{-2}}$.

The equation of motion is then: $m\ddot{\mathbf{r}} = -\frac{GMm}{r^2}\hat{\mathbf{r}} \Rightarrow \mathbf{a}(\mathbf{r}) = -\frac{GM}{r^2}\hat{\mathbf{r}} = -\frac{GM}{|\mathbf{r}|^3}\mathbf{r}$

The acceleration depends only on position r, and points towards the origin (Newton, 1687)

So the *Keplerian equations of motion*:

$$\boxed{\frac{d\mathbf{r}}{dt} = \mathbf{v}\,, \qquad \frac{d\mathbf{v}}{dt} = -\frac{GM}{r^2}\hat{\mathbf{r}}}$$

- Equivalent second-order ODE: $\frac{d^2\mathbf{r}}{dt^2} = -\frac{GM}{r^3}\mathbf{r}$

Solving the Kepler problem

$$\boxed{\frac{d\mathbf{r}}{dt} = \mathbf{v}\,, \qquad \frac{d\mathbf{v}}{dt} = -\frac{GM}{r^2}\hat{\mathbf{r}}}$$

Our goals:

1. *Solve these ODEs* to numerically compute planetary orbits.
   - Given some initial conditions $\mathbf{r}(0) = \mathbf{r}_1$, and $\mathbf{v}(0) = \mathbf{v}_1$

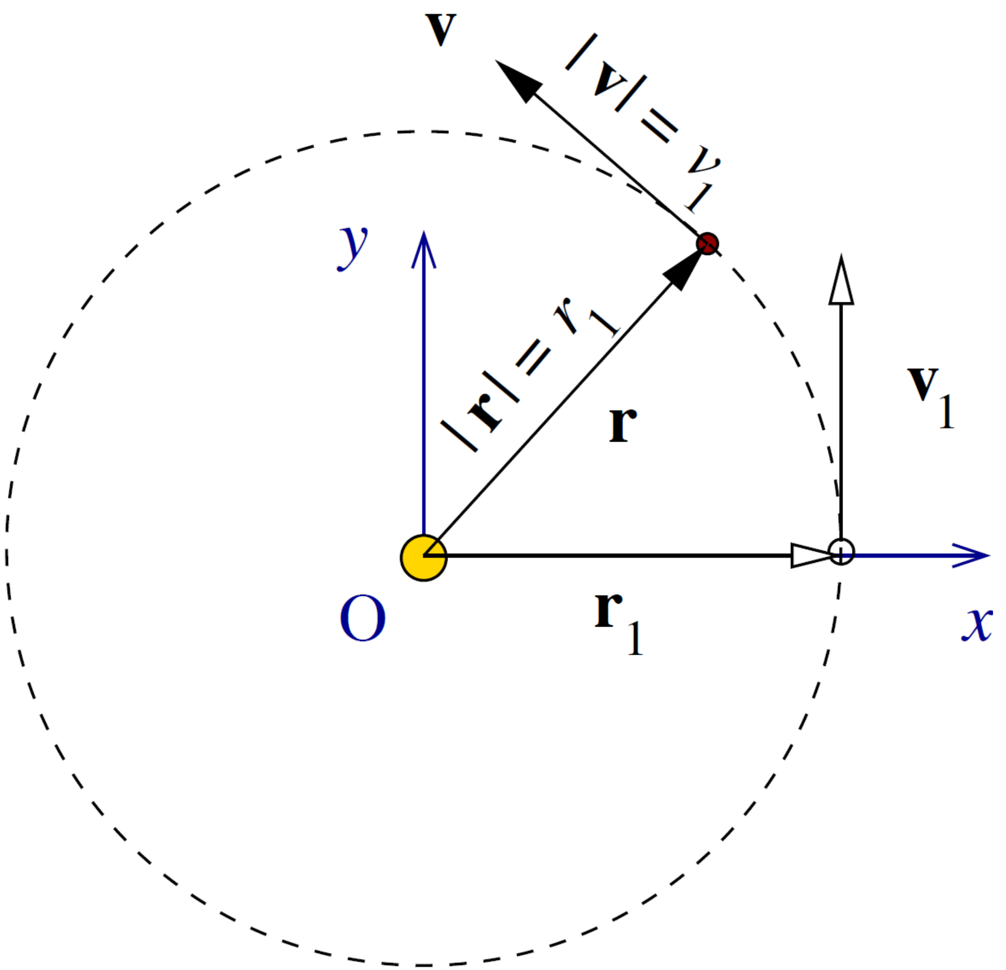
2. *Assess the accuracy* of numerical solutions against known quantities:
   - Test the *conservation* of physical quantities that we know should be conserved.
     - Angular momentum: $\mathbf{L} = \mathbf{r} \times m\mathbf{v}$
     - Total energy: $E = \frac{1}{2}mv^2 - \dfrac{GMm}{r}$
     - [**Exercise**: Prove $\dfrac{dL}{dt} = 0$ and $\dfrac{dE}{dt} = 0$].
   - Compare the simulated trajectory against an *analytic solution*.

Special case: the Circular Motion Solution

- We can parametrize the *circular motion solution* as $\mathbf{r}_\mathrm{c}(t) = r_1\left[\cos(\omega t), \sin(\omega t)\right]$.
  - Can solve (e.g., using 2nd-order ODE) for the angular frequency, $\omega = \omega_\mathrm{c} = \dfrac{(GM)^{1/2}}{r_1^{3/2}}$.
  - And so the period, $T_\mathrm{c} = \dfrac{2\pi}{\omega} = \dfrac{2\pi r_1^{3/2}}{(GM)^{1/2}}$.
- Circular motion is a *good test case* to evaluate numerical methods
  - Because it's easy to see when we wobble off course 🙈
- We should obtain circular motion from $\mathbf{r}(0) = (r_1, 0)$ and $\mathbf{v}(0) = (0, v_1)$, with $v_1 = \omega r_1 = \sqrt{\dfrac{GM}{r_1}}$.
  - **Exercise**: Show that these choices reproduce the requirement $\mathbf{r}_\mathrm{c}(t) = r_1\left[\cos(\omega t), \sin(\omega t)\right]$.

Circular Motion

- We start at $\mathbf{r}(0) = (r_1, 0)$ and $\mathbf{v}(0) = (0, v_1)$.
  - $v_1 = \omega r_1 = \sqrt{\dfrac{GM}{r_1}}$.
- This is our circular motion test solution ⚪.



Non-dimensionalisation of the Kepler problem

Non-dimensionalisation

- We *rescale variables* to form new dimensionless versions by dividing by dimensional constants $\bar{\mathbf{r}} = \dfrac{\mathbf{r}}{L_s}$, $\bar{t} = \dfrac{t}{t_s}$, $\bar{\mathbf{v}} = \dfrac{\mathbf{v}}{L_s/t_s}$.
- Rewriting the second-order equation of motion: $\dfrac{d^2\mathbf{r}}{dt^2} = -\dfrac{GM}{r^3}\mathbf{r} \quad \Rightarrow \quad \dfrac{d^2\bar{\mathbf{r}}}{d\bar{t}^2} = -\dfrac{GMt_s^2}{L_s^3}\dfrac{\bar{\mathbf{r}}}{\bar{r}^3}$
  - ❓ What's a convenient choice for t_s?
    - 👀 $t_s = \sqrt{\dfrac{L_s^3}{GM}}$, which gives $\dfrac{d^2\bar{\mathbf{r}}}{d\bar{t}^2} = -\dfrac{\hat{\mathbf{r}}}{\bar{r}^2} = -\dfrac{\bar{\mathbf{r}}}{\bar{r}^3}$
  - So we get $\boxed{\dfrac{d\bar{\mathbf{r}}}{d\bar{t}} = \bar{\mathbf{v}}\,, \qquad \dfrac{d\bar{\mathbf{v}}}{d\bar{t}} = -\dfrac{\bar{\mathbf{r}}}{\bar{r}^3}\,.}$
    - Thanks non-dimensionalisation: no more G and M to worry about 🆒

Conserved quantity: total energy

$$E = \tfrac{1}{2}mv^2 - \frac{GMm}{r}.$$

- We can also write down a non-dimensional form for the total energy, $\overline{E} = \dfrac{E}{E_s}$.
- A natural choice: $E_s = \dfrac{GMm}{L_s}$
- Yields $\overline{E} = \dfrac{1}{2}\overline{v}^2 - \dfrac{1}{\overline{r}}$.

Summary: non-dimensional circular motion test

- We have $\bar{v}_1 = \bar{r}_1^{-1/2}$, $\bar{\omega}_c = t_s\omega_c = \bar{r}_1^{-3/2}$, and $\bar{T}_c = 2\pi\bar{r}_1^{3/2}$.
- If we set the characteristic length scale for the problem, $L_s = r_1$ (the initial distance of the body from the origin), then…
  - Initial conditions: $\mathbf{r}(0) = (1, 0)$ and $\mathbf{v}(0) = (0, 1)$ yield *circular motion* with $r_c = 1$.
  - Orbits trace out the *unit circle* with period $T_c = 2\pi$.

Euler method for the Kepler problem

Euler method for the Kepler problem

kepler_dynamics.ipynb

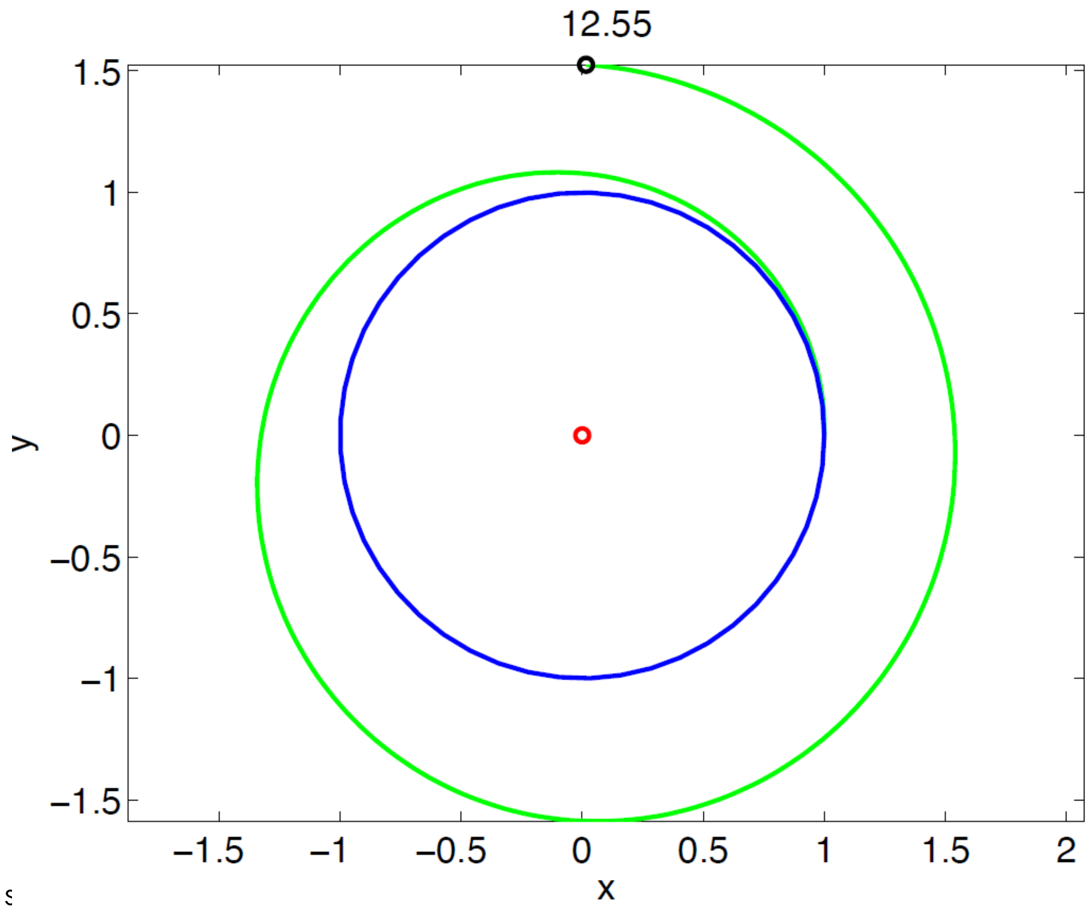
$$\mathbf{r}_{n+1} = \mathbf{r}_n + \tau \mathbf{v}_n \,,$$
$$\mathbf{v}_{n+1} = \mathbf{v}_n + \tau \mathbf{a}_n \,.$$

- Time steps forward discretely, as $t_n = (n-1)\tau$
- The Euler method (forward-difference approximation) worked ok for projectile motion…
  - What about for the Kepler problem?!

- Euler scheme for the Kepler problem is implemented in: kepler_dynamics.ipynb:
  - Integrates for a total time 4π(should be two orbits).
  - Default (non-dimensional) time step is $\tau = 0.05$
  - Code plots the orbit and the analytic solution (unit circle).
  - Calculates non-dimensional $E(t)$ at each time step.
- Let's test it!

Euler on Kepler

- *It doesn't go well at all* !
  - The orbit spirals out and the total energy increases.
  - Smaller time steps, τ, only delay the inevitable.

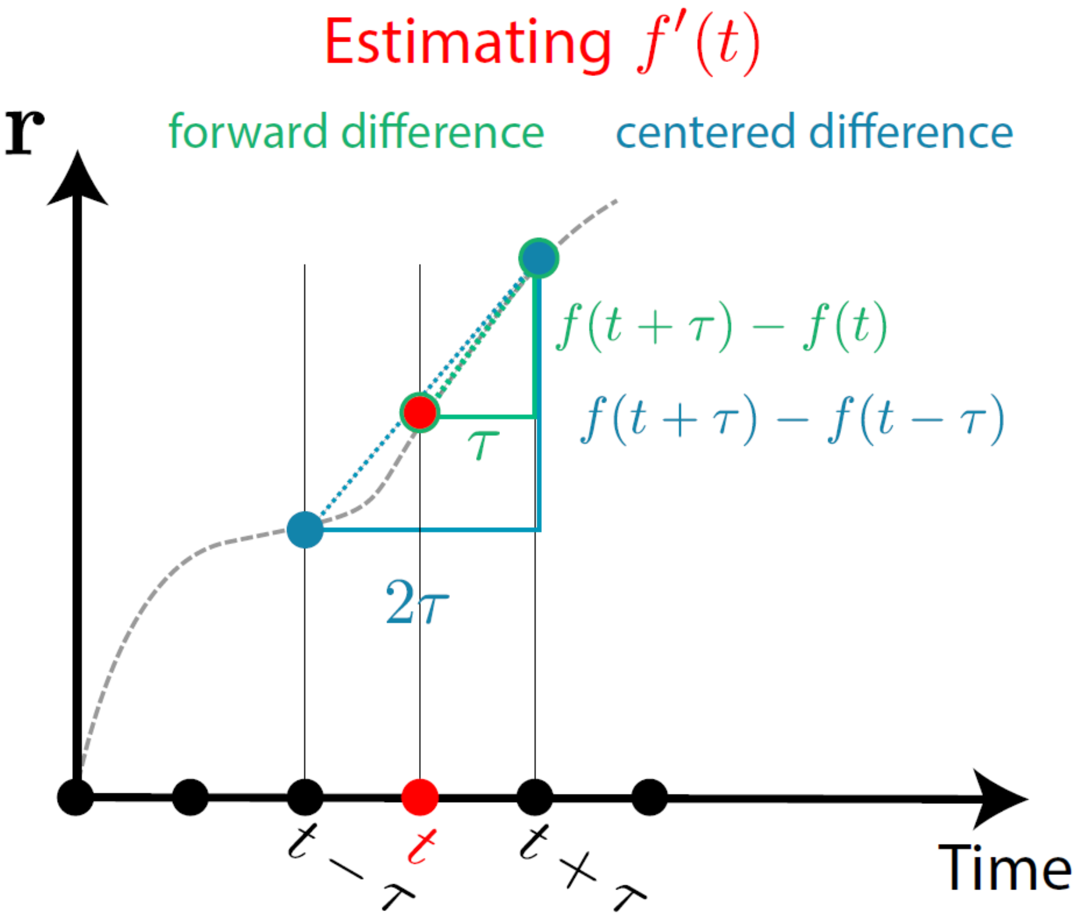


Without testing against known cases, we never know whether we're off track!

Centred difference approximation and Verlet

Centred difference approximation

- Euler uses the *forward difference approximation*:
  - $f'(t) = \dfrac{f(t+\tau) - f(t)}{\tau} + O(\tau).$
- Consider an alternative: the *centered difference approximation*
  - $f'(t) = \dfrac{f(t+\tau) - f(t-\tau)}{2\tau} + O(\tau^2).$
- ❓ Does the higher-order truncation error–$O(\tau^2)$ instead of $O(\tau)$–mean more or less accurate?



Derivation: the centred difference approximation

- Comes from manipulating the Taylor series:
  - $f(t \pm \tau) = f(t) \pm \tau f'(t) + \frac{1}{2!}\tau^2 f''(t) \pm \frac{1}{3!}\tau^3 f^{(3)}(t) + \dots$
- Even powers of τ cancel when you compute $f(t+\tau) - f(t-\tau)$.
- We get $f'(t) = \dfrac{f(t+\tau) - f(t-\tau)}{2\tau} - \dfrac{1}{6}\tau^2 f^{(3)}(t) + \dots$
  - Which we can write as $f'(t) = \dfrac{f(t+\tau) - f(t-\tau)}{2\tau} + O(\tau^2)$
- Truncation errors $O(\tau^2)$ are pretty good 😋

Centred difference approximation: 2nd derivative

$$\boxed{f''(t) = \frac{f(t+\tau) - 2f(t) + f(t-\tau)}{\tau^2} + O(\tau^2)\,.}$$

- A workhorse in this unit! 🐴🐴🐴
  - (we use this alot)

A sketch on how to get it

- Decompose the second derivative as: $\frac{\partial^2 f}{\partial x^2} = \frac{\partial}{\partial x}\left(\frac{\partial f}{\partial x}\right)$.
- For the first derivative: let $g(x) = \frac{\partial f}{\partial x} \approx \frac{f(x) - f(x-h)}{h}$
- We can do a forward difference approximation to g as: $\frac{\partial g}{\partial x} \approx \frac{g(x+h) - g(x)}{h}$.
- Putting them together:
$$\frac{\partial^2 f}{\partial x^2} \approx \frac{f(x+h) - f(x)}{h^2} - \frac{f(x) - f(x-h)}{h^2} = \frac{f(x+h) - 2f(x) + f(x-h)}{h^2}$$
- **Exercise**: Derive it fully from the Taylor-series expansion
  - By expanding about x at $f(x+h)$ and $f(x-h)$.

Centred difference approximation for dynamics

- *Dynamics equations*: $\dfrac{d^2\mathbf{r}}{dt^2} = \mathbf{a}$ and $\dfrac{d\mathbf{r}}{dt} = \mathbf{v}$.
- Apply centered difference approximations to $\left.\dfrac{d^2\mathbf{r}}{dt^2}\right|_{t=t_n}$ and $\left.\dfrac{d\mathbf{r}}{dt}\right|_{t=t_n}$
  - For $t_n = (n-1)\tau$.
- Yields the *Verlet Update Equations*:
  - $\mathbf{r}_{n+1} = 2\mathbf{r}_n - \mathbf{r}_{n-1} + \tau^2\mathbf{a}_n + O(\tau^4)$
  - $\mathbf{v}_n = \dfrac{\mathbf{r}_{n+1} - \mathbf{r}_{n-1}}{2\tau} + O(\tau^2)$.

Updating using the Verlet method

$$\mathbf{r}_{n+1} = 2\mathbf{r}_n - \mathbf{r}_{n-1} + \tau^2 \mathbf{a}_n\,, \qquad\qquad \mathbf{v}_n = \frac{\mathbf{r}_{n+1} - \mathbf{r}_{n-1}}{2\tau}\,.$$

- *Notice*: You need to update $\mathbf{r}$ before you can update $\mathbf{v}$.
- *Getting started*: Consider the first step, $n = 1$ for $\mathbf{r}$. This requires $\mathbf{r}_{n-1} = \mathbf{r}(-\tau)$: a value *before the initial condition*?! 😐
  - *Solution:* we can remove $\mathbf{r}_{n-1}$ from the Verlet method equations so that $\mathbf{r}_{n+1} = \mathbf{r}_n + \tau\mathbf{v}_n + \frac{1}{2}\tau^2\mathbf{a}_n\,.$
  - (see also the *midpoint method* from Lab 1, Q2).
  - So we can get started (for $n = 1$) using this midpoint equation, and then apply the Verlet update equations for all remaining time steps, $n \geq 2$. 🏃🏃🏃

We can simulate dynamics without computing v

$$\mathbf{r}_{n+1} = 2\mathbf{r}_n - \mathbf{r}_{n-1} + \tau^2 \mathbf{a}_n \,, \qquad \mathbf{v}_n = \frac{\mathbf{r}_{n+1} - \mathbf{r}_{n-1}}{2\tau} \,.$$

- If $\mathbf{a} = \mathbf{a}(\mathbf{r})$, the Verlet update equations allow us to evolve $\mathbf{r}$ *without ever calculating* $\mathbf{v}$:
  - $\mathbf{r}_1 \xrightarrow{\tau} \mathbf{r}_2 \xrightarrow{\tau} \mathbf{r}_3 \xrightarrow{\tau} \cdots \,.$
- Advantageous if we only want to solve for $\mathbf{r}$ 😄

Verlet method: Truncation errors

$$\mathbf{r}_{n+1} = 2\mathbf{r}_n - \mathbf{r}_{n-1} + \tau^2 \mathbf{a}_n + O(\tau^4)\,, \qquad \mathbf{v}_n = \frac{\mathbf{r}_{n+1} - \mathbf{r}_{n-1}}{2\tau} + O(\tau^2)\,.$$

- The error terms in the Verlet method equations are deceptive.
- Successive updates are not independent (each update uses the current, $\mathbf{r}_n$ and previous, $\mathbf{r}_{n-1}$ values).
  - 🔥 So you need to write *two successive updates in the form of Taylor expansions* to correctly identify the local truncation errors.
- They are $O(\tau^3)$ for both position and velocity.
  - Global error as $O(\tau^2)$: a second-order method.
- Given its simplicity, this method is quite accurate! 😊

An alternative formulation: Velocity-Verlet

- Another (equivalent) way of writing the Verlet updates is called *Velocity-Verlet*:
- $$\mathbf{r}_{n+1} = \mathbf{r}_n + \tau\mathbf{v}_n + \tfrac{1}{2}\tau^2\mathbf{a}_n \,,$$
  $$\mathbf{v}_{n+1} = \mathbf{v}_n + \tfrac{1}{2}\tau\left(\mathbf{a}_n + \mathbf{a}_{n+1}\right) \,.$$
- The position update is the midpoint method (cf. Computer Lab 1, Q2).
- Requires velocity to be calculated (the $\tau\mathbf{v}_n$ term).
- **Exercise**: Derive this scheme.

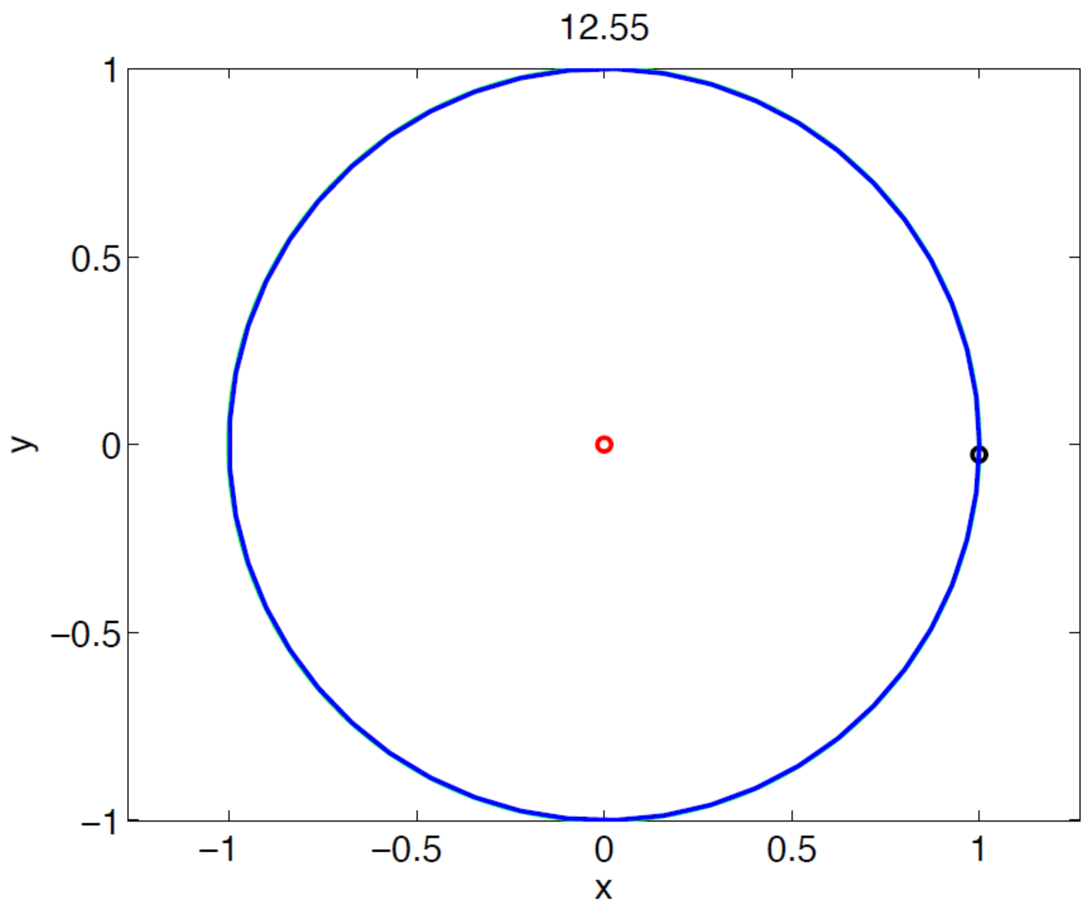
Verlet solution to the Kepler problem

kepler_verlet.ipynb

- For $n = 1$ (midpoint method to get things running 🏃), use $\mathbf{r}_{n+1} = \mathbf{r}_n + \tau\mathbf{v}_n + \frac{1}{2}\tau^2\mathbf{a}_n$.
- Then standard Verlet updates for $n > 1$:

$$\mathbf{r}_{n+1} = 2\mathbf{r}_n - \mathbf{r}_{n-1} + \tau^2\mathbf{a}_n\,,\ \mathbf{v}_n = \frac{\mathbf{r}_{n+1} - \mathbf{r}_{n-1}}{2\tau}.$$

- Accurately integrates the circular test case using $\tau = 0.05$!
- Energy is (nearly) conserved
  - (oscillates $\sim 10^{-7}$)!! 🆒🆒🆒



Let's test

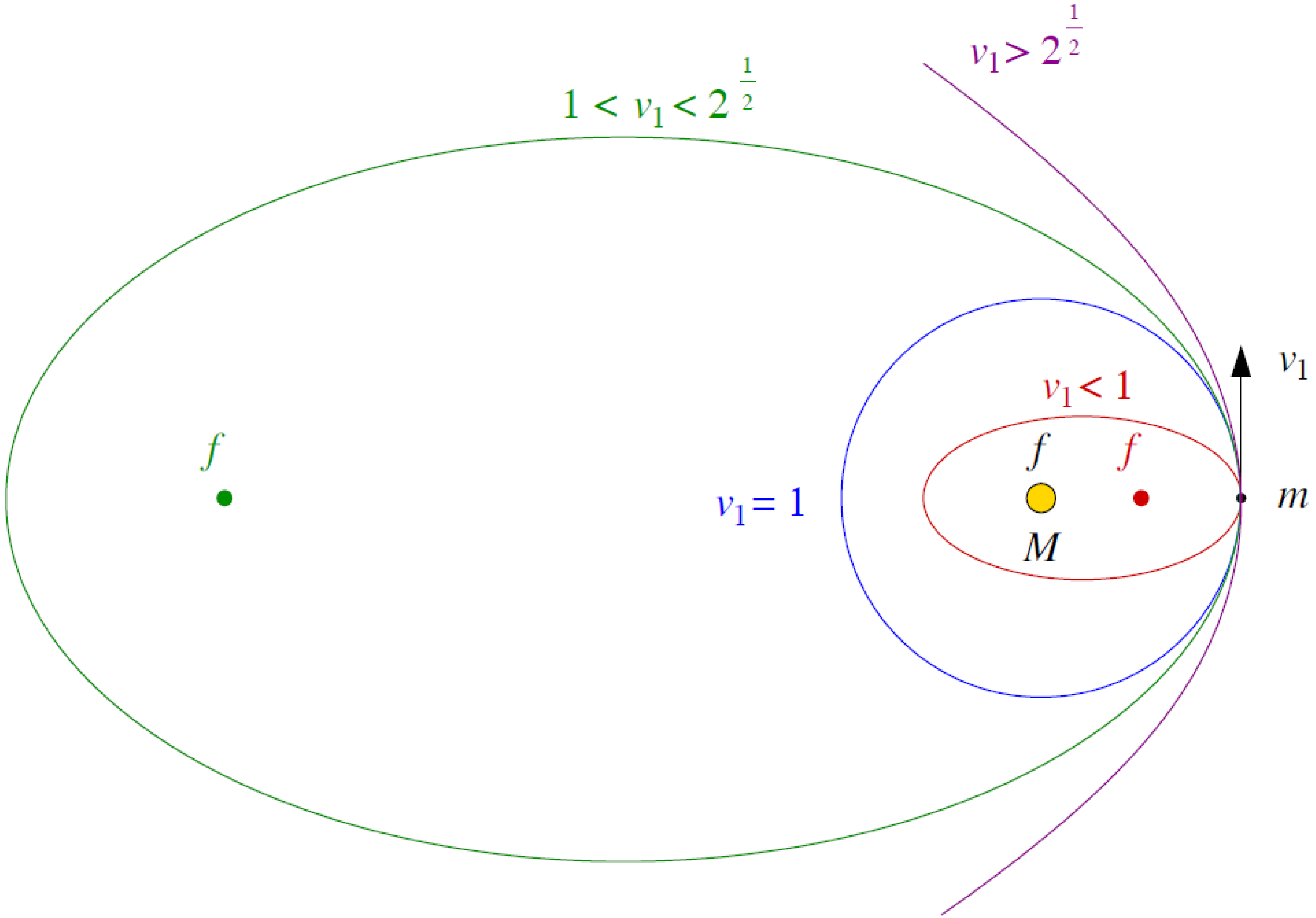
Solutions to the Kepler problem: ellipses and hyperbolae

For initial conditions

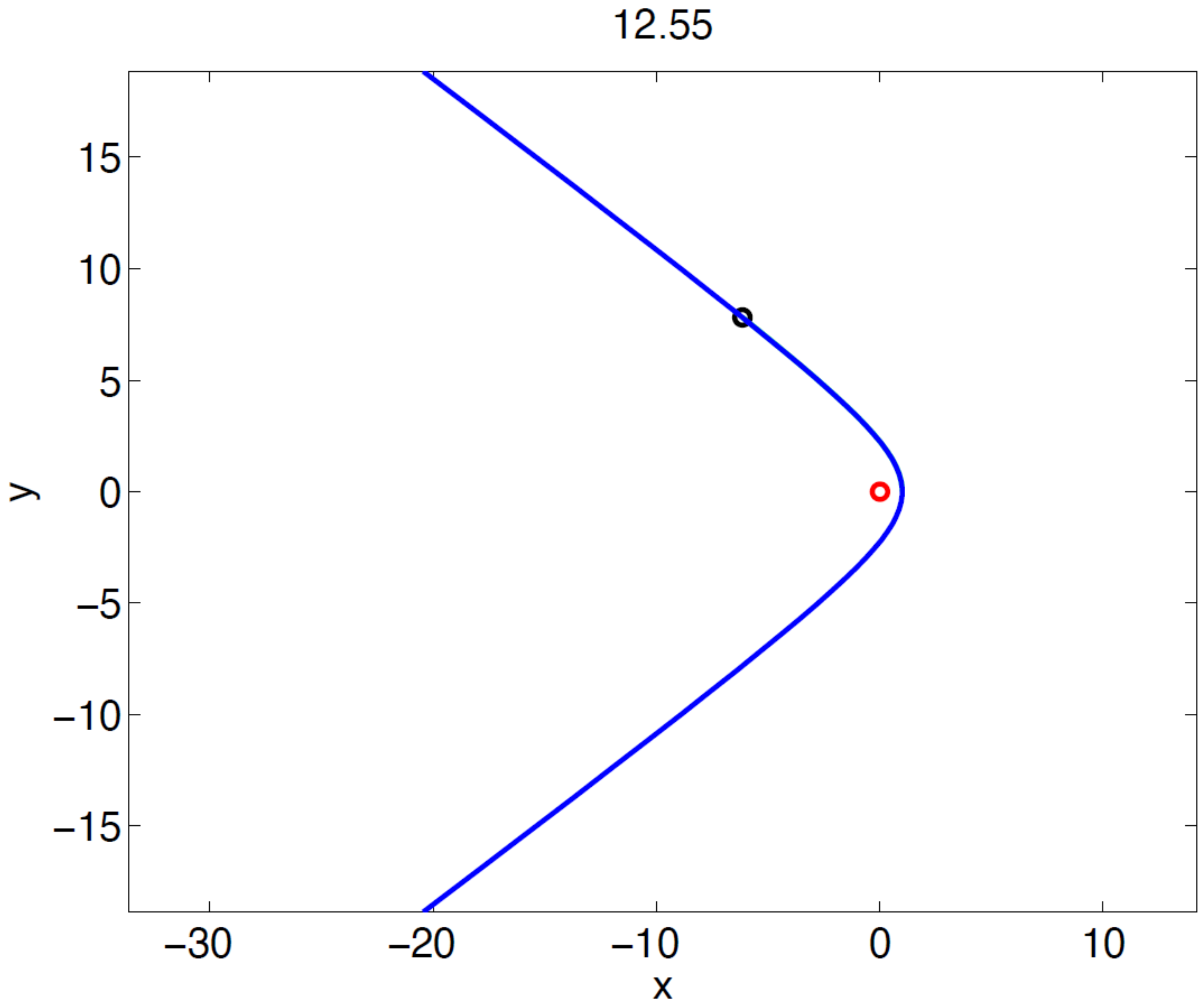
$$\mathbf{r}_1 = (1, 0)$$

$$\mathbf{v}_1 = (0, v_1)$$

we can get different types of solutions depending on v_1 :



Example: numerical solution for $v_1 = 1.5$; a hyperbolic orbit.



Appendix: Analytic solutions to the Kepler problem

- Nice to compare the performance of numerical methods to analytic solution: `kepler_analytic`.
- *Cartesian* form of (elliptic) solution for $\mathbf{r}_1 = (1, 0)$ (closest point of approach) and $\mathbf{v}_1 = (0, v_1)$:
  - $\dfrac{(x+ae)^2}{a^2} + \dfrac{y^2}{b^2} = 1$
    - eccentricity $e = v_1^2 - 1$
    - semi-major axis $a = \dfrac{1}{1-e}$
    - semi-minor axis $b^2 = a^2(1-e^2)$.

Parametric Elliptic and Hyperbolic Solutions (parametrised by θ)

- *Elliptic solutions*
  - have $e < 1$ or $v_1 < \sqrt{2}$:
  - $$x = \; - ae + a\cos\theta\,,$$ $$y = b'\sin\theta \qquad (0 \le \theta \le 2\pi)\,.$$
- Semi-major axis a
- Semi-minor axis $b' = a\sqrt{1-e^2}$.
- Focii $x_\pm = -ae \pm \sqrt{a^2 - b^2}$, so $x_\pm = 0, -2ae$
  - (the Sun is at $x_+ = 0$).

- *Hyperbolic solutions*
  - have $e > 1$ or $v_1 > \sqrt{2}$:
  - $$x = \; - ae + a\cosh\theta$$ $$y = b'\sinh\theta \qquad (-\infty < \theta < \infty)\,,$$
- Semi-minor axis $b' = a\sqrt{e^2 - 1}$.