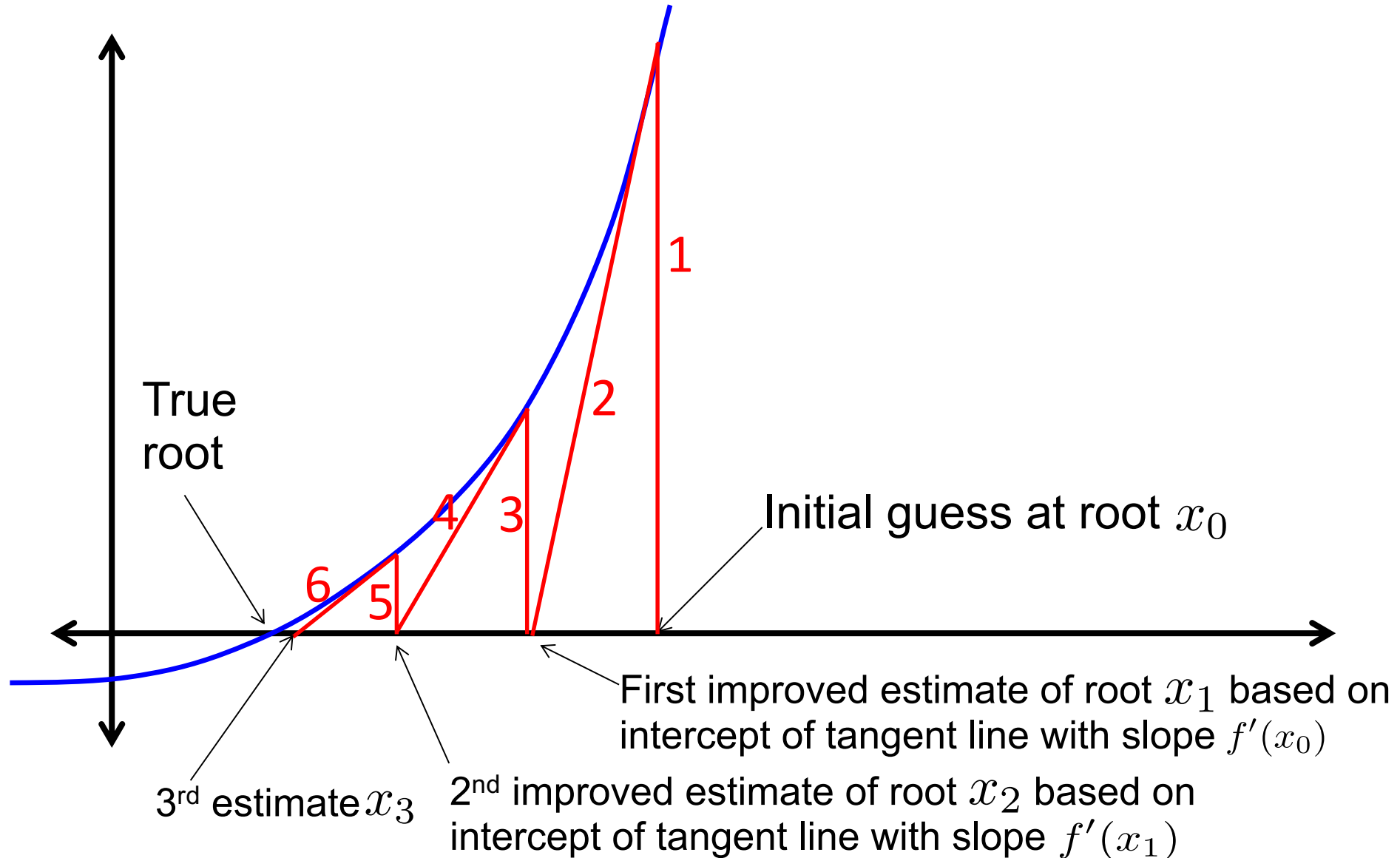


# PHY604 Lecture 7

September 14, 2021

# Review: Geometrical Interpretation of Newton-Raphson Iteration



# Review: Pseudocode of Newton-Raphson Algorithm

- 1. Choose initial guess at the root ( $x_0$ ), and the convergence tolerance ( $\epsilon$ ).
- 2. Loop through  $n$  up to a maximum number  $N_{\max}$  (exit and tell the user that the root finding has failed if it reaches  $N_{\max}$ )
- 3. Make sure  $f'(x) \neq 0$
- 4. Compute new estimate of root:  $x_n \simeq x_{n-1} - \frac{f(x_{n-1})}{f'(x_{n-1})}$
- 5. Check convergence criteria:

$$|x_{n+1} - x_n| < \begin{cases} \epsilon|x_n|, & \text{when } |x_n| \neq 0 \\ \epsilon, & \text{when } |x_n| = 0 \end{cases}$$

# Review: Summary of root-finding methods

- Bisection:
  - Robust (with appropriate initial guesses)
  - Slow, each iteration reduces error by a factor of two
  - Need to make sure root is within initial guesses
- Newton-Raphson:
  - Fast: often only takes a few iterations
  - Need to know derivative of function, and they must exist
  - Can diverge, e.g., in cases with small second derivatives
- Secant method
  - Similar convergence speed as NR method
  - Don't need analytical derivatives
  - Same divergence properties as NR method
  - Numerical derivatives may be noisy

# Review: Differential equations (Newman Ch. 8)

- One of the major applications of computation to science and engineering is solving differential equations
  - Even for very simple-looking equations if they are “nonlinear,” they are difficult or impossible to solve analytically
- Classifications:
  - Initial value problems
  - Boundary value problems
  - Eigenvalue problems
- Often problems are described by **systems of coupled differential equations**
- As with the other topics, there are many different methods
  - We just want to see the basic ideas and popular methods

# Review: Runge-Kutta methods

- Euler method can be thought of as the first-order RK method
  - Accurate to first order in  $\Delta t$ , i.e., error is order  $\Delta t^2$
- Second-order RK method accurate to  $\Delta t^2$ , so error  $\Delta t^3$
- Fourth-order RK method accurate to  $\Delta t^4$ , so error  $\Delta t^5$ 
  - By far the most common method for the numerical solution of ODEs
  - Balances accuracy and complexity
- **Quoted accuracies are for one step**, errors accumulate over the number of steps needed in the calculation, usually lose an order of accuracy (see Newman)

# Review: The fourth-order Runge-Kutta method

- In practice, the workhorse algorithm for first-order sets of ODEs is the **fourth-order Runge-Kutta** algorithm which (we state here without derivation)

- Step 1:  $\mathbf{k}_1 = \Delta t \mathbf{f}(\mathbf{y}^n, t^n)$

- Step 2:  $\mathbf{k}_2 = \Delta t \mathbf{f}\left(\mathbf{y}^n + \frac{1}{2}\mathbf{k}_1, t^n + \frac{1}{2}\Delta t\right)$

- Step 3:  $\mathbf{k}_3 = \Delta t \mathbf{f}\left(\mathbf{y}^n + \frac{1}{2}\mathbf{k}_2, t^n + \frac{1}{2}\Delta t\right)$

- Step 4:  $\mathbf{k}_4 = \Delta t \mathbf{f}(\mathbf{y}^n + \mathbf{k}_3, t^n + \Delta t)$

- Step 5:  $\mathbf{y}^{n+1} = \mathbf{y}^n + \frac{1}{6} (\mathbf{k}_1 + 2\mathbf{k}_2 + 2\mathbf{k}_3 + \mathbf{k}_4)$

# Today's lecture:

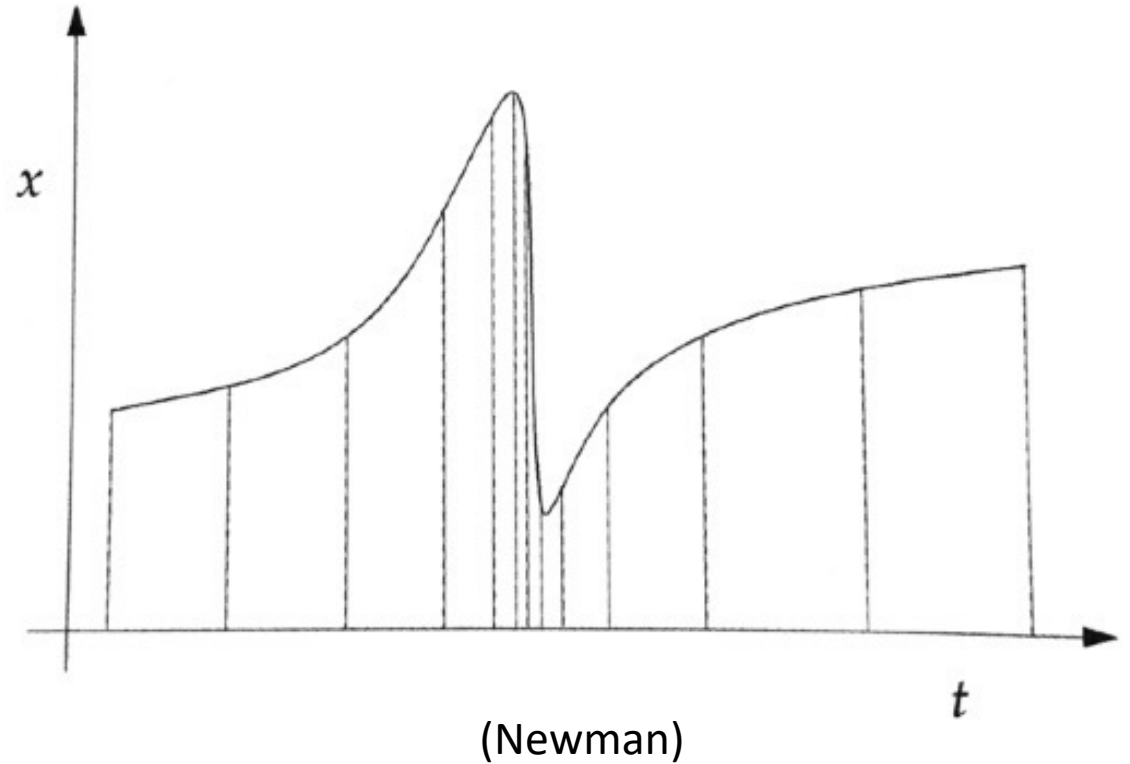
## More on ordinary differential equations

- Adaptive Runge-Kutta method
- Beyond RK: Other methods for ODEs
  - Leapfrog/Verlet/modified midpoint
  - Bulirsch-Stoer Method
- Boundary Value problems
- Eigenvalue problems



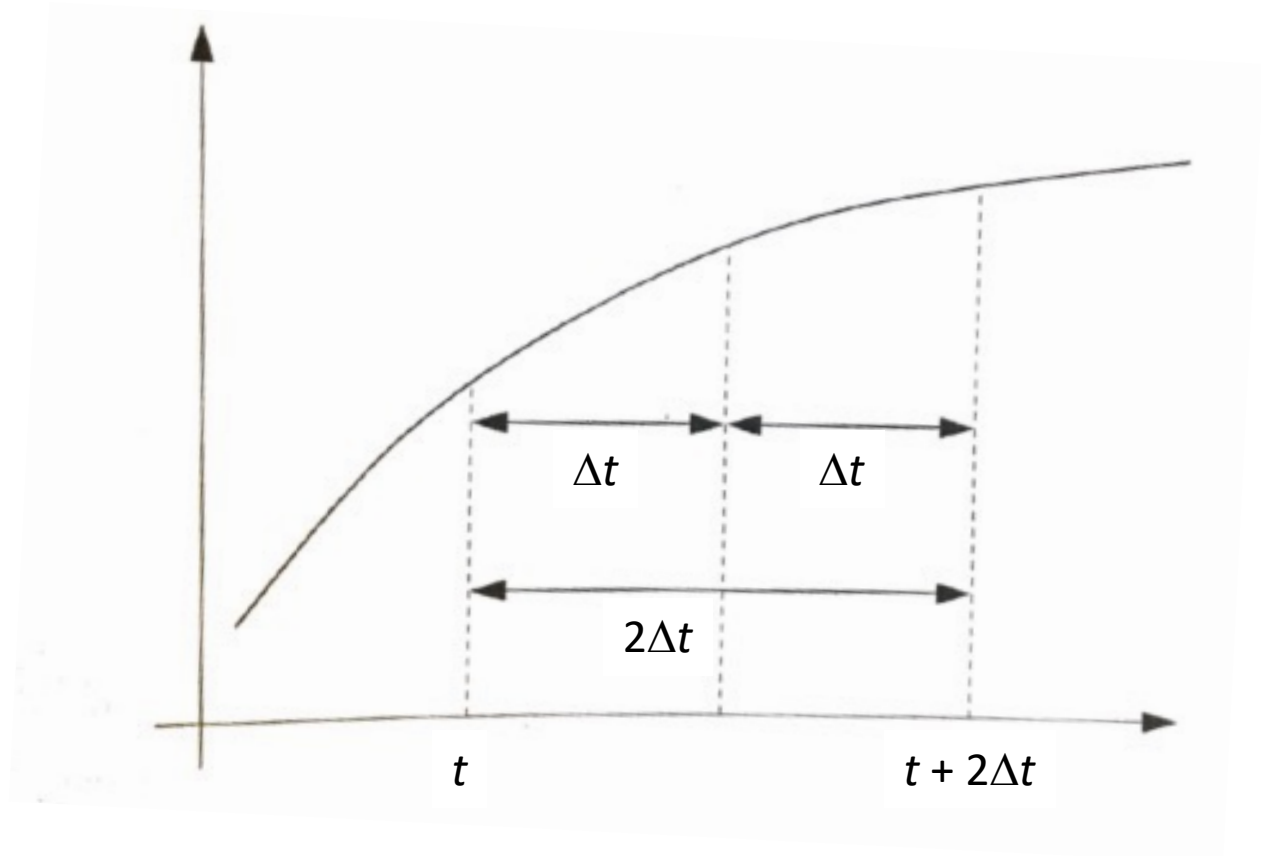
# Adaptive step size

- So far, we have set by hand a constant step size  $\Delta t$
- Often, we can get better results by varying the step size
  - Increase in regions where function varies rapidly, decrease where it varies slowly
- Approach: Vary  $\Delta t$  so the error introduced per unit interval is roughly constant
  - First, we need to estimate the error in the steps



# Adaptive step size: Estimating the error

- 1. Choose initial (small)  $\Delta t$
- 2. Use RK method to do two  $\Delta t$  steps of the solution
- 3. Go back to initial  $t$  and do an RK step with  $2\Delta t$
- 4. Compare the results to estimate the error



# Adaptive step size: Estimating the error

- True value of function related to estimate  $y_{\Delta t}$ :

$$y(t + 2\Delta t) = y_{\Delta t} + 2c\Delta t^5$$

- For doubled step size  $y_{2\Delta t}$ :

$$y(t + 2\Delta t) = y_{2\Delta t} + 32c\Delta t^5$$

- So, per-step error is:

$$\epsilon = c\Delta t^5 = \frac{1}{30}(y_{\Delta t} - y_{2\Delta t})$$

- Take  $\delta$  to be the target accuracy per step. Then the step size necessary to get that accuracy is:

$$\Delta t' = \Delta t \sqrt[4]{\frac{30\Delta t\delta}{|y_{\Delta t} - y_{2\Delta t}|}}$$

# Adaptive step size: Complete approach

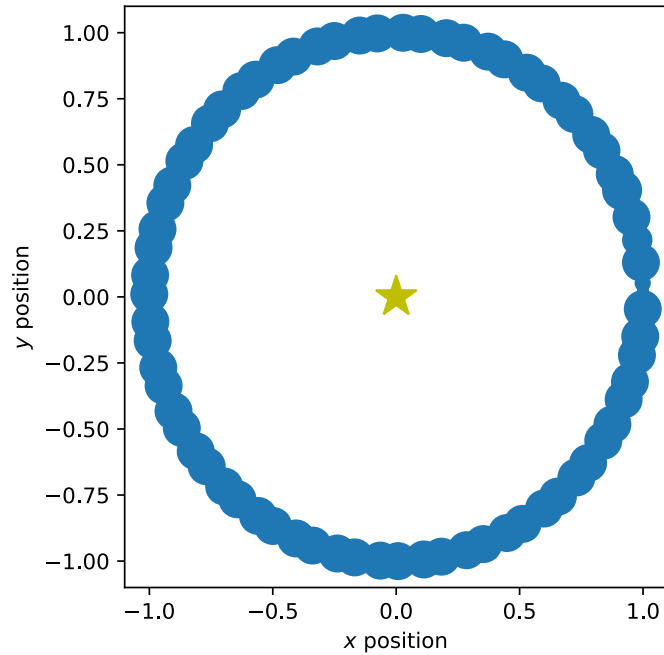
- 1. Choose initial (small)  $\Delta t$
- 2. Use RK method to do two  $\Delta t$  steps of the solution
- 3. Go back to initial  $t$  and do an RK step with  $2\Delta t$
- 4. Compare the results to estimate the error
- 5. Calculate ideal step size  $\Delta t'$ 
  - If  $\varepsilon > \delta$ , then redo the calculation with  $\Delta t'$
  - If  $\varepsilon < \delta$ , take the results obtained using  $\Delta t$  and move on to time  $t + \Delta t$ . In the next iteration use  $\Delta t'$  as the timestep
- Requires at least 3 RK steps for every two actually used, but usually results in an overall speedup for a given accuracy
- Usually limit how much  $\Delta t'$  can differ from  $\Delta t$  (e.g., by less than a factor of two) in case the denominator happens to diverge

# Example: Circular orbit with adaptive 4<sup>th</sup>-order RK

Circular:

$x_0 = 1$  AU

$v_{y0} = 6.283185$  AU/year

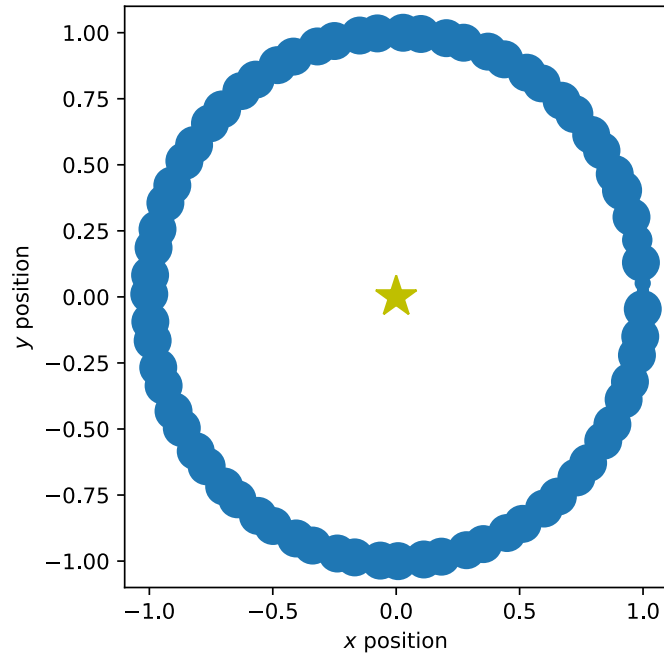


# Example: Elliptical orbit with adaptive 4<sup>th</sup>-order RK

Circular:

$x_0 = 1$  AU

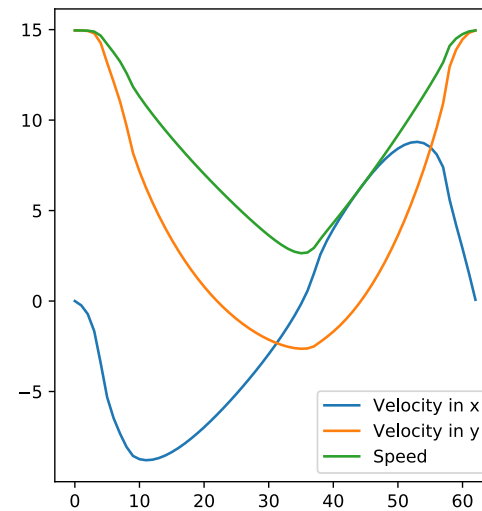
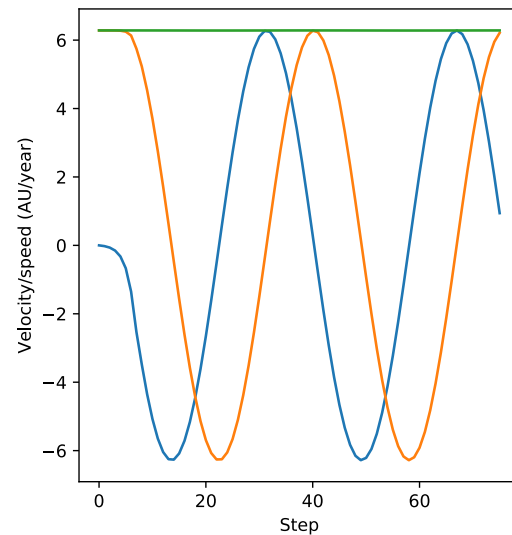
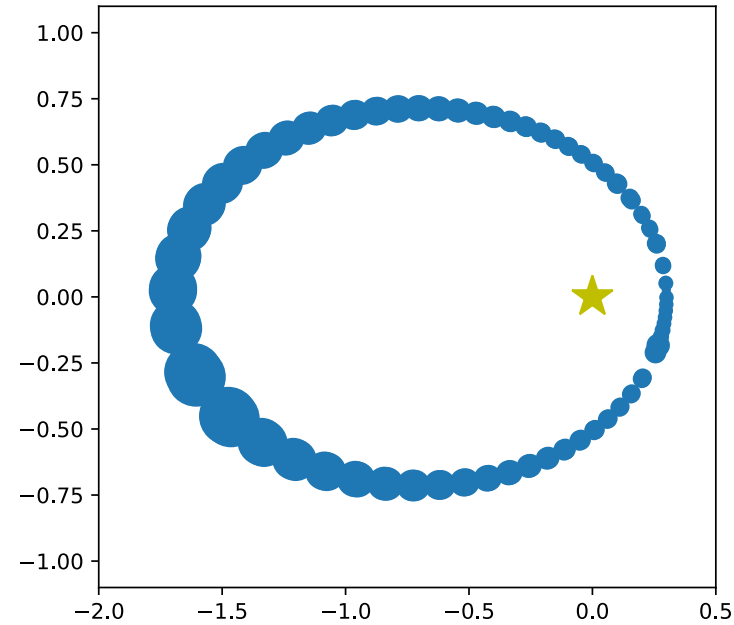
$v_{y0} = 6.283185$  AU/year



Elliptical:

$x_0 = 0.3$  AU

$v_{y0} = 14.955378$  AU/year



# Improving the results with local extrapolation

- We can use our knowledge of the error to improve our estimate for  $y(t+\Delta t)$  recall that:

$$y(t + 2\Delta t) = y_{\Delta t} + 2c\Delta t^5$$

- And:

$$\epsilon = c\Delta t^5 = \frac{1}{30}(y_{\Delta t} - y_{2\Delta t})$$

- So:

$$y(t + 2\Delta t) = y_{\Delta t} + \frac{1}{15}(y_{\Delta t} - y_{2\Delta t}) + \mathcal{O}(\Delta t^6)$$

- No estimate of the error but presumably better than previous 4<sup>th</sup> order result

# Today's lecture:

## More on ordinary differential equations

- Adaptive Runge-Kutta method
- Beyond RK: Other methods for ODEs
  - Leapfrog/Verlet/modified midpoint
  - Bulirsch-Stoer Method
- Boundary Value problems
- Eigenvalue problems



# Leapfrog method

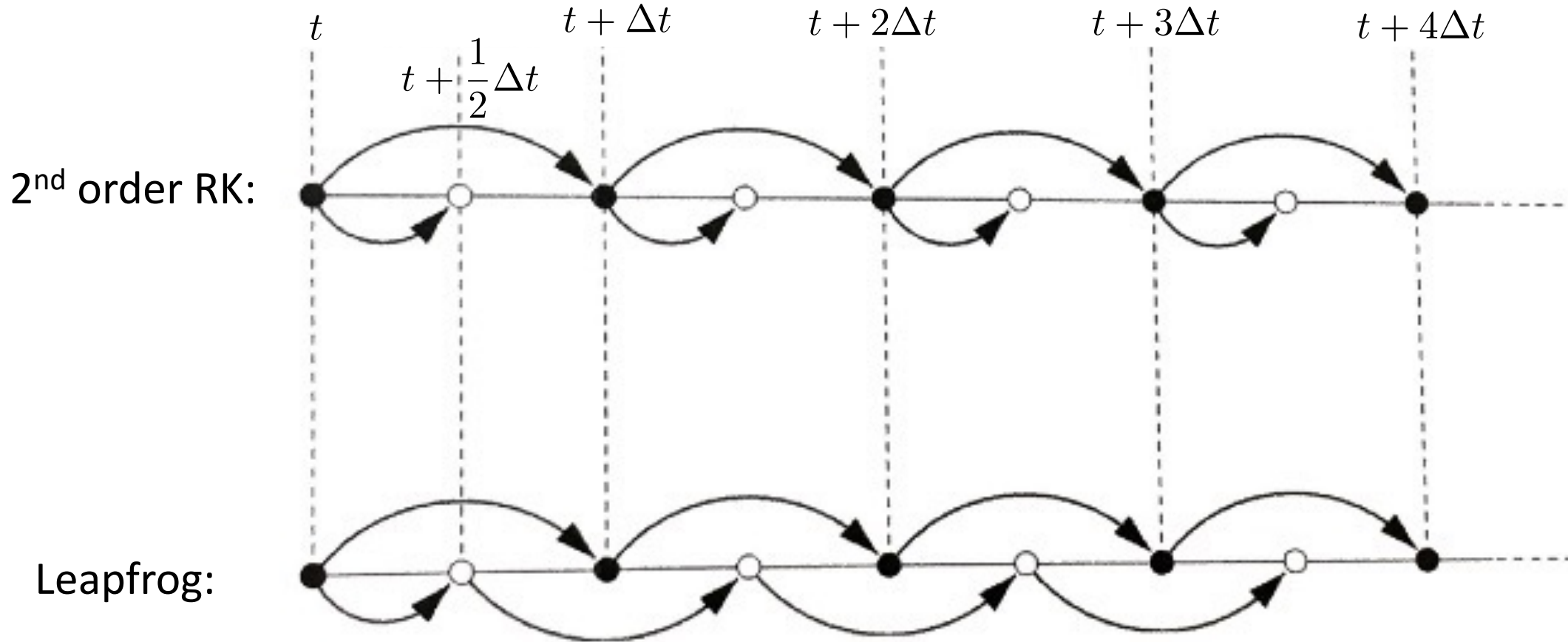
- Recall the second-order RK method:
  - Using the Euler method applied to  $t$  to estimate the value of a variable at the midpoint of the interval  $t + 1/2\Delta t$

$$y\left(t + \frac{1}{2}\Delta t\right) = y(t) + \frac{1}{2}\Delta t f(y, t)$$

$$y(t + \Delta t) = y(t) + \Delta t f\left[y\left(t + \frac{1}{2}\Delta t\right), t + \frac{1}{2}\Delta t\right]$$

- Leapfrog method uses a similar approach, except calculates the next midpoint by using the Euler method evaluated at **the previous midpoint**

# Leapfrog method versus 2<sup>nd</sup> order RK



(Newman)

# Leapfrog method

- Starts out the same as RK:

$$y(t + \frac{1}{2}\Delta t) = y(t) + \frac{1}{2}\Delta t f(y, t)$$

$$y(t + \Delta t) = y(t) + \Delta t f \left[ y(t + \frac{1}{2}\Delta t), t + \frac{1}{2}\Delta t \right]$$

- Then:

$$y(t + \frac{3}{2}\Delta t) = y(t + \frac{1}{2}\Delta t) + \Delta t f [y(t + \Delta t), t + \Delta t]$$

$$y(t + 2\Delta t) = y(t + \Delta t) + \Delta t f \left[ y(t + \frac{3}{2}\Delta t), t + \frac{3}{2}\Delta t \right]$$

# Why the leapfrog method?

- Time reversal symmetric
  - Useful for physics problems where energy conservation is important
- Error is even in step size
  - Ideal starting point for Richardson extrapolation for Bulirsch-Stoer

# Leapfrog method is “time-reversal symmetric”

- If we use  $-\Delta t$  instead of  $\Delta t$ , we should retrace our steps
- To see this, start with the equations we repeatedly apply for the Leapfrog method:

$$y(t + \Delta t) = y(t) + \Delta t f \left[ y(t + \frac{1}{2} \Delta t), t + \frac{1}{2} \Delta t \right]$$

$$y(t + \frac{3}{2} \Delta t) = y(t + \frac{1}{2} \Delta t) + \Delta t f [y(t + \Delta t), t + \Delta t]$$

- Set step size to  $-\Delta t$  :

$$y(t - \Delta t) = y(t) - \Delta t f \left[ y(t - \frac{1}{2} \Delta t), t - \frac{1}{2} \Delta t \right]$$

$$y(t - \frac{3}{2} \Delta t) = y(t - \frac{1}{2} \Delta t) - \Delta t f [y(t - \Delta t), t - \Delta t]$$

# Leapfrog method is “time-reversal symmetric”

- Now make a trivial shift in time:  $t \rightarrow t + \frac{3}{2}\Delta t$
- To get:

$$y(t + \frac{1}{2}\Delta t) = y(t + \frac{3}{2}\Delta t) - \Delta t f [y(t + \Delta t), t + \Delta t]$$

$$y(t) = y(t + \Delta t) - \Delta t f \left[ y(t + \frac{1}{2}\Delta t), t + \frac{1}{2}\Delta t \right]$$

- Same as the original: (but moving backwards)

$$y(t + \Delta t) = y(t) + \Delta t f \left[ y(t + \frac{1}{2}\Delta t), t + \frac{1}{2}\Delta t \right]$$

$$y(t + \frac{3}{2}\Delta t) = y(t + \frac{1}{2}\Delta t) + \Delta t f [y(t + \Delta t), t + \Delta t]$$

# What about 2<sup>nd</sup> order Runge-Kutta?

- Original expressions:  $y(t + \frac{1}{2}\Delta t) = y(t) + \frac{1}{2}\Delta t f(y, t)$

$$y(t + \Delta t) = y(t) + \Delta t f \left[ y(t + \frac{1}{2}\Delta t), t + \frac{1}{2}\Delta t \right]$$

- Set step size to  $-\Delta t$ :  $y(t - \frac{1}{2}\Delta t) = y(t) - \frac{1}{2}\Delta t f(y, t)$

$$y(t - \Delta t) = y(t) - \Delta t f \left[ y(t - \frac{1}{2}\Delta t), t - \frac{1}{2}\Delta t \right]$$

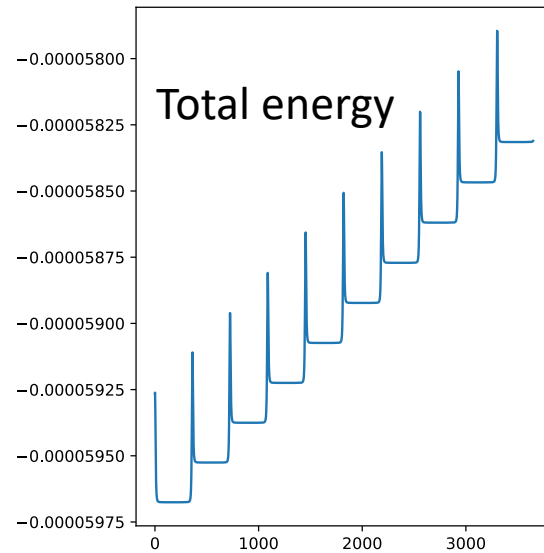
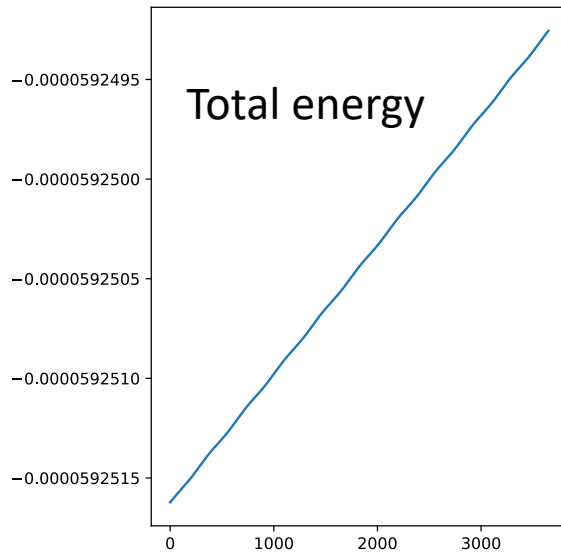
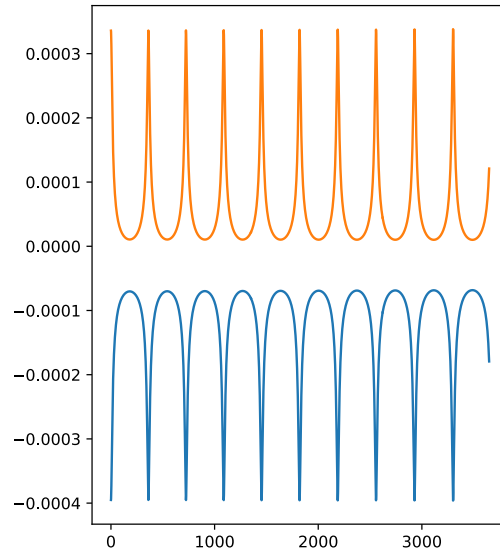
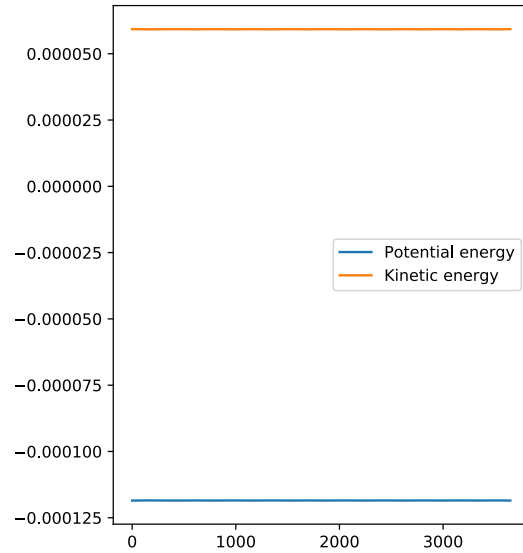
- No way to, e.g., make a shift in  $t$  to get back to original operations in the opposite direction
  - Errors will result in broken time-reversal symmetry

# Why is time-reversal symmetry important? Energy conservation!

2<sup>nd</sup> order RK

Circular

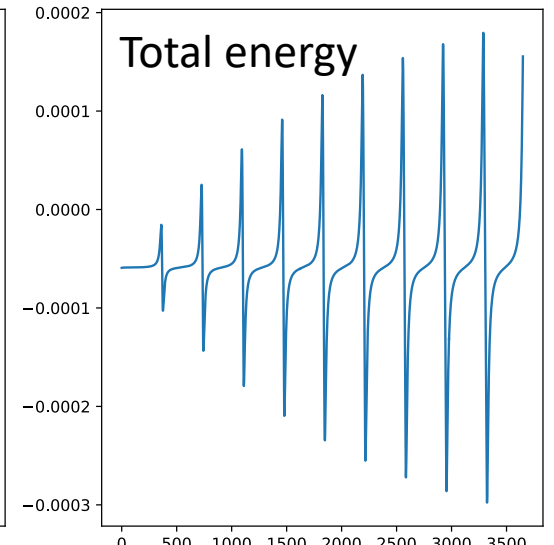
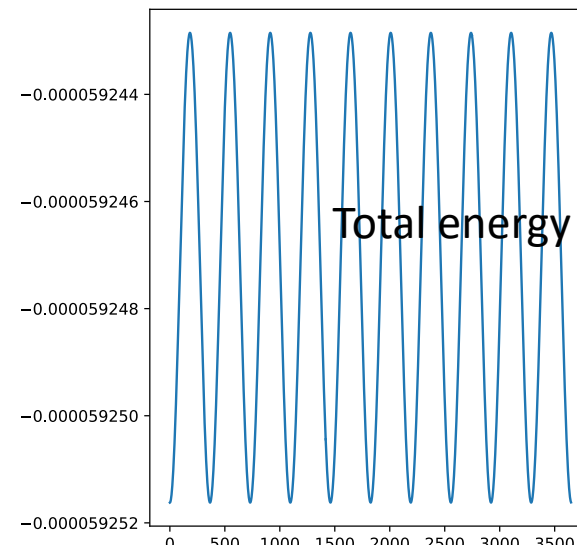
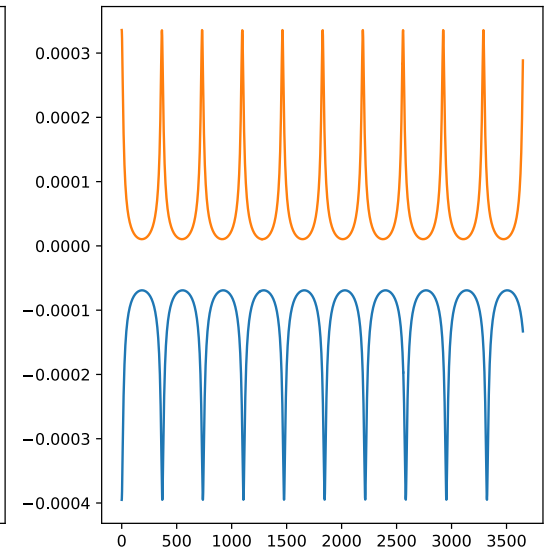
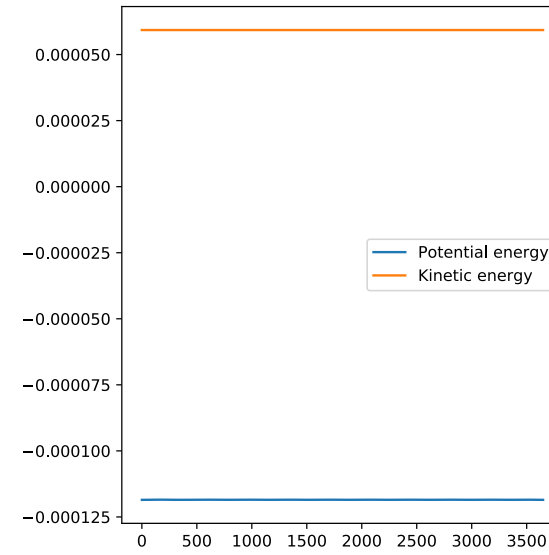
Elliptical



Leapfrog

Circular

Elliptical






# Verlet method for equations of motion using leapfrog method

- For this method we will limit ourselves to ODEs of the form of equations of motion:


$$\frac{d\mathbf{x}}{dt} = \mathbf{v}(t), \quad \frac{d\mathbf{v}}{dt} = \mathbf{f}(\mathbf{x}, t)$$

- (i.e., where the RHS of the first equation does not depend on  $\mathbf{x}$ )
- In that case, we can do the leapfrog method with two equations

Position only at integer steps


$$\mathbf{x}(t + \Delta t) = \mathbf{x}(t) + \Delta t \mathbf{v} \left( t + \frac{1}{2} \Delta t \right)$$

Velocity only at half-integer steps


$$\mathbf{v}(t + \frac{3}{2} \Delta t) = \mathbf{v}(t + \frac{1}{2} \Delta t) + \Delta t \mathbf{f}[\mathbf{x}(t + \Delta t), t + \Delta t]$$

What if we want to know, e.g., the total energy at a point?

- Total energy requires knowing  $\mathbf{x}$  and  $\mathbf{v}$  at the same point
- Let's just step the velocity back half a step with Euler's method:

$$\mathbf{v}(t + \frac{1}{2}\Delta t) = \mathbf{v}(t + \Delta t) - \frac{1}{2}\Delta t \mathbf{f}[\mathbf{x}(t + \Delta t), t + \Delta t]$$

- Rearrange to get:

$$\mathbf{v}(t + \Delta t) = \mathbf{v}(t + \frac{1}{2}\Delta t) + \frac{1}{2}\Delta t \mathbf{f}[\mathbf{x}(t + \Delta t), t + \Delta t]$$

- Gives velocity at integer points from quantities we have already calculated

Verlet method: Leapfrog in this specific situation of, e.g., EOM:

- First do an initial half step:

$$\mathbf{v}(t + \frac{1}{2}\Delta t) = \mathbf{v}(t) + \frac{1}{2}\Delta t \mathbf{f}[\mathbf{x}(t), t]$$

- Then repeatedly apply:

$$\mathbf{x}(t + \Delta t) = \mathbf{x}(t) + \Delta t \mathbf{v}\left(t + \frac{1}{2}\Delta t\right)$$

$$\mathbf{k} = \Delta t \mathbf{f}[\mathbf{x}(t + \Delta t), t + \Delta t]$$

$$\mathbf{v}(t + \Delta t) = \mathbf{v}(t + \frac{1}{2}\Delta t) + \frac{1}{2}\mathbf{k}$$

$$\mathbf{v}(t + \frac{3}{2}\Delta t) = \mathbf{v}(t + \frac{1}{2}\Delta t) + \mathbf{k}$$

# Error of leapfrog/Verlet is even in step size

- Error for a single step is proportional to  $\Delta t^3$  to leading order
- What about the other orders? Time reversal symmetry gives:

$$\epsilon(-\Delta t) = -\epsilon(\Delta t)$$

- So, the error is an odd function:

$$\epsilon(\Delta t) = c_3\Delta t^3 + c_5\Delta t^5 + c_7\Delta t^7 + \dots$$

- But total error is one order less when we accumulate over all steps:

$$\epsilon_{\text{tot}}(\Delta t) = \epsilon(\Delta t) \times \frac{t_f - t_0}{\Delta t}$$

- So:

$$\epsilon_{\text{tot}}(\Delta t) = b_2\Delta t^2 + b_4\Delta t^4 + b_6\Delta t^6 + \dots$$

# Wait, what about initial Euler half step?

$$\mathbf{v}(t + \frac{1}{2}\Delta t) = \mathbf{v}(t) + \frac{1}{2}\Delta t \mathbf{f}[\mathbf{x}(t), t]$$

- Introduces odd (and even) higher-order errors
- We can get rid of these errors with the following procedure.

# Removing errors from initial Euler half step

- Define variable at integer and half steps:
$$x_0^{\text{int}} = x(t)$$
$$x_1^{\text{half}} = x_0^{\text{int}} + \frac{1}{2}\Delta t f(x_0^{\text{int}}, t)$$

- Then:

$$x_1^{\text{int}} = x_0^{\text{int}} + \Delta t f(x_1^{\text{half}} + \frac{1}{2}\Delta t)$$

$$x_2^{\text{half}} = x_1^{\text{half}} + \Delta t f(x_1^{\text{int}}, t + \Delta t)$$

$$x_2^{\text{int}} = x_1^{\text{int}} + \Delta t f(x_2^{\text{half}} + \frac{3}{2}\Delta t)$$

⋮

⋮

$$x_{m+1}^{\text{half}} = x_m^{\text{half}} + \Delta t f(x_m^{\text{int}}, t + m\Delta t)$$

$$x_{m+1}^{\text{int}} = x_m^{\text{int}} + \Delta t f(x_{m+1}^{\text{half}} + (m + \frac{1}{2})\Delta t)$$

# Removing errors from initial Euler half step: Modified midpoint method

- Take  $t_f$  as the final time of the calculation, achieved at step  $n$
- We can write the final solution for  $x(t+t_f)$  in two ways:

$$x(t + t_f) = x_n^{\text{int}} = x_n^{\text{half}} + \frac{1}{2} \Delta t f(x_n^{\text{int}}, t + t_f)$$

- Or we can use the average of the two:

$$x(t + t_f) = \frac{1}{2} \left[ x_n^{\text{int}} + x_n^{\text{half}} + \frac{1}{2} \Delta t f(x_n^{\text{int}}, t + t_f) \right]$$

- This cancels the error from the initial Euler step!
  - Proved by mathematician William Gragg in 1965
- Modified midpoint method: Using the iterative steps from the previous slide and the above expression for  $x(t+t_f)$

# Bulirsch-Stoer Method

- Why do we care about the modified midpoint method and even-powered errors? They are the basis of the **Bulirsch-Stoer Method**
- This method combines the modified midpoint method with Richardson extrapolation (e.g., the Romberg method for integrals)



# Simple example of Bulirsch-Stoer: First order ODE with one variable

- Equation:  $\frac{dx}{dt} = f(x, t)$
- We would like to solve from  $t$  to  $t_f$ , with  $x(t)$  given
- Start by using the modified midpoint method with a single step  $\Delta t_1 = t_f$ 
  - More specifically, two half steps
  - Call this estimate  $R_{1,1}$
- Now perform the calculation for  $\Delta t_2 = 1/2 t_f$  to get  $R_{2,1}$

# Performing Richardson extrapolation

- We can write the “exact” expressions since we know the form of the errors (using  $\Delta t_1 = 2\Delta t_2$ )

$$x(t + t_f) = R_{2,1} + c_1 \Delta t_2^2 + \mathcal{O}(\Delta t_2^4)$$

$$x(t + t_f) = R_{1,1} + c_1 \Delta t_1^2 + \mathcal{O}(\Delta t_1^4) = R_{1,1} + 4c_1 \Delta t_2^2 + \mathcal{O}(\Delta t_2^4)$$

- So: 
$$c_1 \Delta t_2^2 = \frac{1}{3}(R_{2,1} - R_{1,1})$$

- And:

New estimate accurate to fourth order!

↓

$$x(t + t_f) = \underbrace{R_{2,1} + \frac{1}{3}(R_{2,1} - R_{1,1})}_{R_{2,2}} + \mathcal{O}(\Delta t_2^4)$$

# Performing Richardson extrapolation, cont.

- Let's do another step: Calculate  $R_{3,1}$  with  $\Delta t_3 = 1/3 t_f$
- Following the same steps as before:

$$R_{3,2} = R_{3,1} + \frac{4}{5}(R_{3,1} - R_{2,1})$$

- Then we can write the “exact” result:

$$x(t + t_f) = R_{3,2} + c_2 \Delta t_3^4 + \mathcal{O}(\Delta t_3^6)$$

- From what we had previously:

$$x(t + t_f) = R_{2,2} + c_2 \Delta t_2^4 + \mathcal{O}(\Delta t_2^6) = R_{2,2} + \frac{81}{16} c_2 \Delta t_3^4 + \mathcal{O}(\Delta t_3^6)$$

- Equating these gives:  $c_2 \Delta t_3^4 = \frac{16}{65}(R_{3,2} - R_{2,2})$

# Performing Richardson extrapolation, cont.

• So, we have:  $x(t + t_f) = \underbrace{R_{3,2} + \frac{16}{65}(R_{3,2} - R_{2,2})}_{R_{3,3}} + \mathcal{O}(\Delta t_3^6)$

↑  
New estimate  
accurate to sixth  
order!

• Where:  $R_{3,3} = R_{3,2} + \frac{16}{65}(R_{3,2} - R_{2,2})$

- Three modified midpoint steps, and already have a sixth-order error
  - Gain two orders of accuracy with each step

# General Richardson extrapolation

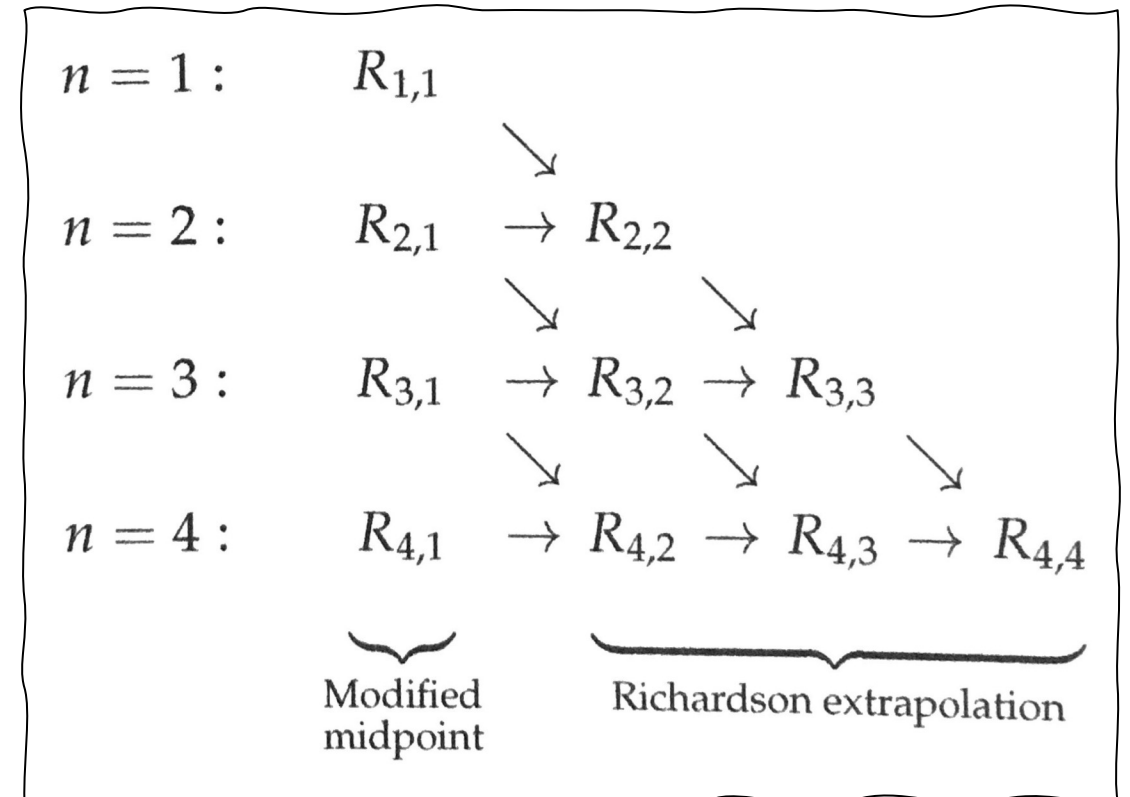
- $n$  is the number of modified midpoint steps, which gives us  $R_{n,1}$ 
  - Can obtain  $R_{n,m}$  for  $m < n$

$$R_{n,m+1} = R_{n,m} + \frac{R_{n,m} - R_{n-1,m}}{[n/(n-1)]^{2m} - 1}$$

- See Newman Sec. 8.5

- Which gives an estimate of the result:

$$x(t + t_f) = R_{n,m+1} + \mathcal{O}(\Delta_n^{2m+2})$$



(Newman)

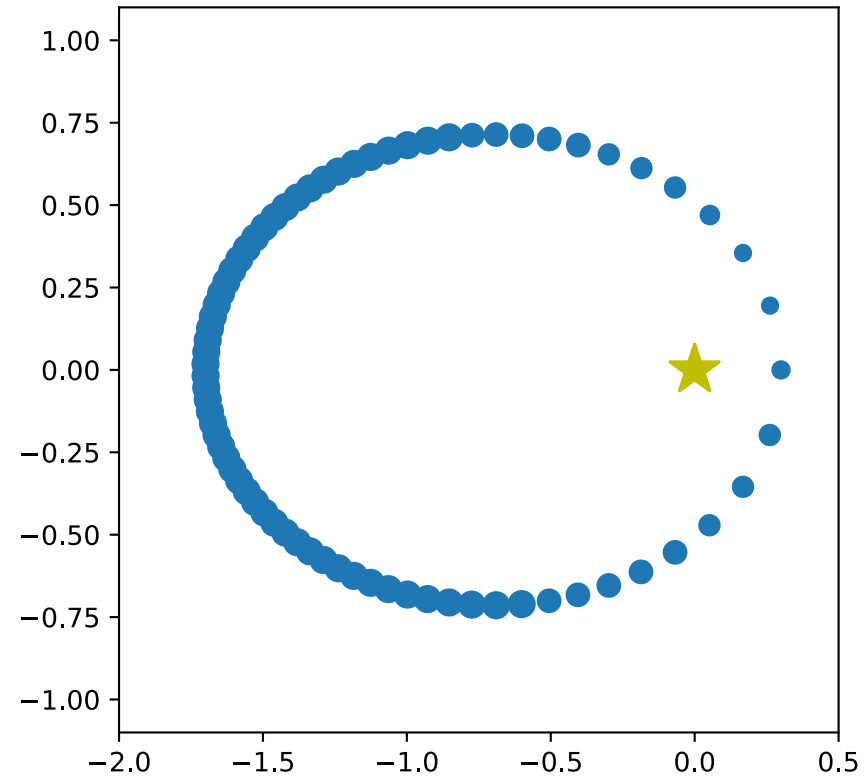
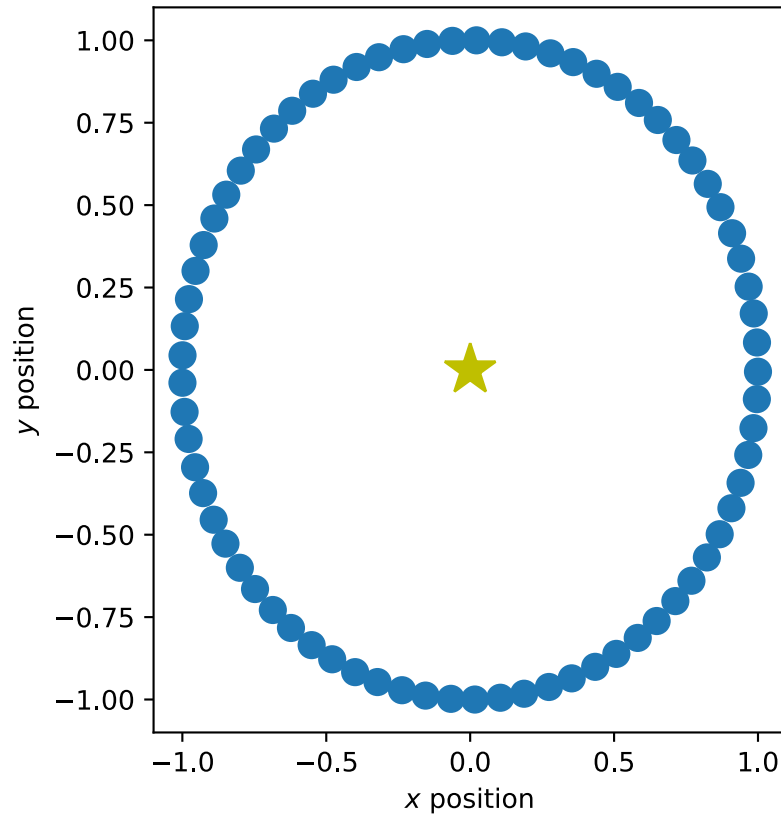
# Comments about Bulirsch-Stoer

- Adaptive method: Provides error and estimate
  - Continue until error is below a given accuracy
- Similar approach to Romberg integration with some key differences
  - Increase number of intervals by one in BS instead of doubling in Romberg
  - Not possible to “reuse” previous points like in Romberg
- Only provides accurate estimate for final result  $x(t+t_f)$ 
  - At intermediate points, we just get raw midpoint method estimates (accurate to  $\Delta t^2$ )
  - Not well suited if we need many (100's or 1000's) steps, so only for rather small regions, where we can get accuracy with  $< 8$  steps
- Can divide larger intervals into smaller ones and apply the BS method
- Often gives better accuracy with less work than RK, especially for relatively smooth functions
  - RK should be used for ODEs with pathological behavior, large fluctuations, divergences, etc.

# Bulirsch-Stoer Method: Summary

- Say we would like to solve an ODE from  $t$  to  $t_f$  up to accuracy  $\delta$  per step
- First, divide the total range into  $N$  equal intervals of length  $t_H$ . Then do the following steps for each interval:
  - 1. **Perform a modified midpoint step** with one interval from  $t$  to  $t_H$  to get  $R_{1,1}$
  - 2. **Increase the number of intervals** by one to  $n$  and calculate  $R_{n,1}$  with the modified midpoint method
  - 3. Calculate the “row” via **Richardson extrapolation**, i.e.,  $R_{n,2} \dots R_{n,n}$
  - 4. **Compare the error** to the target accuracy  $\delta t_H$ . If it is larger than the target accuracy, return to step 2. If it is less than the target accuracy, go to the next interval.

# Example: Orbits with the Bulirsch-Stoer method





# Today's lecture:

## More on ordinary differential equations

- Adaptive Runge-Kutta method
- Beyond RK: Other methods for ODEs
  - Leapfrog/Verlet/modified midpoint
  - Bulirsch-Stoer Method
- Boundary Value problems
- Eigenvalue problems

# Boundary value problems

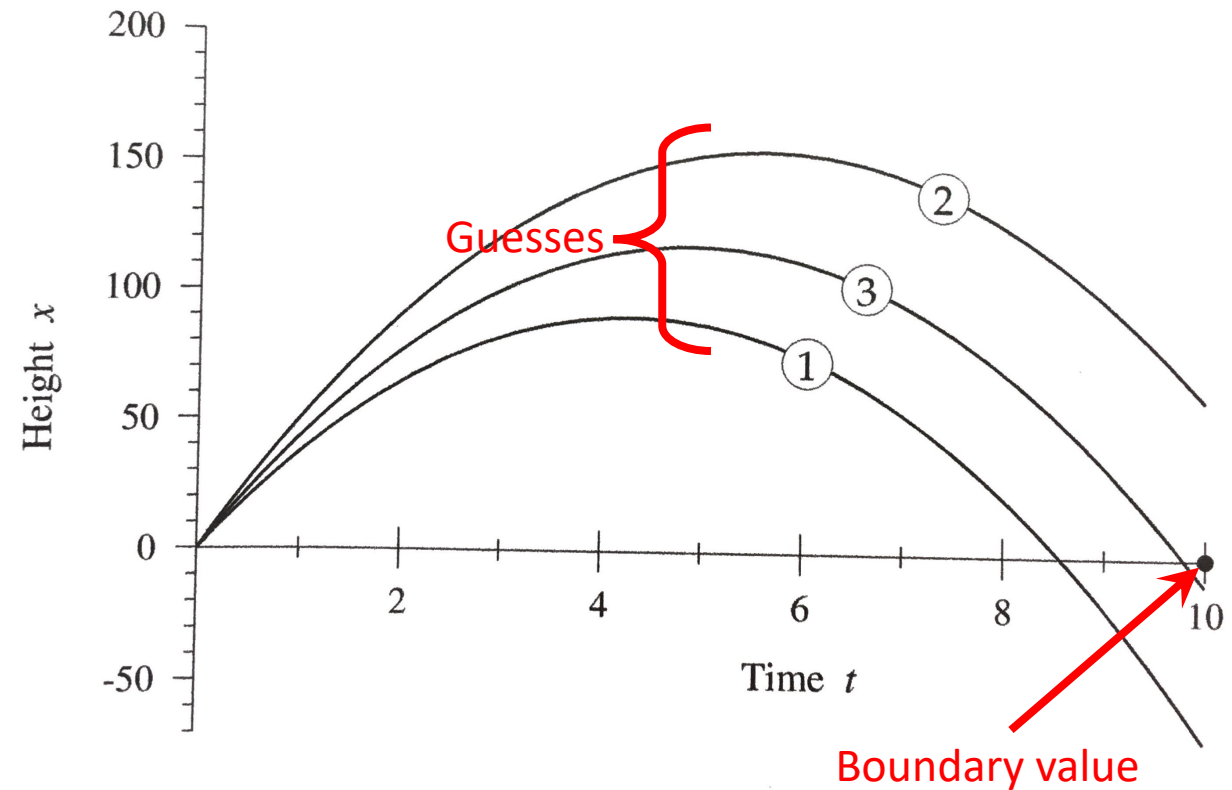
- The orbital example we have been studying is an **initial value problem**: Solving ODEs given some initial value
- **Boundary value problems**: Conditions needed to specify the solution given at some different (or additional) points to the initial point
  - E.g.: Find a solution for the EOM such that the trajectory passes through a specific point in the future
- Boundary value problems are more difficult to solve
  - Two methods: Shooting method and relaxation method (we will discuss the latter in terms of PDEs later)

# Shooting method example: Ball thrown in the air

- “Trial-and-error” method: Searches for correct values of initial conditions that match a given set of boundary conditions
- Example (from Newman Sec. 8.6): Height of a ball thrown in the air

$$\frac{d^2x}{dt^2} = -G$$

- Guess initial conditions (initial vertical velocity) for which the ball will return to the ground at a given time  $t$



# How do we modify initial conditions between guesses?

- Write the height of the ball at the boundary  $t_1$  as  $x = f(v)$  where  $v$  is the initial velocity
- If we want the ball to be at  $x = 0$  at  $t_1$ , we need to solve  $f(v) = 0$
- So, we have reformulated the problem as finding a root of a function
  - We can use, e.g., the bisection method, Newton-Raphson method, secant method
- The function is “evaluated” by solving the differential equation
  - We can use any method discussed previously, e.g., Runge-Kutta, Bulirsch-Stoer, etc.

# Today's lecture:

## More on ordinary differential equations

- Adaptive Runge-Kutta method
- Beyond RK: Other methods for ODEs
  - Leapfrog/Verlet/modified midpoint
  - Bulirsch-Stoer Method
- Boundary Value problems
- Eigenvalue problems

# Eigenvalue problems

- Special type of boundary value problem: Linear and homogeneous
  - Every term is linear in the dependent variable
- E.g.: Schrodinger equation:

$$-\frac{\hbar}{2m} \frac{d^2\psi}{dx^2} + V(x)\psi(x) = E\psi(x)$$

- Consider the Schrodinger equation in a 1D square well with infinite walls:

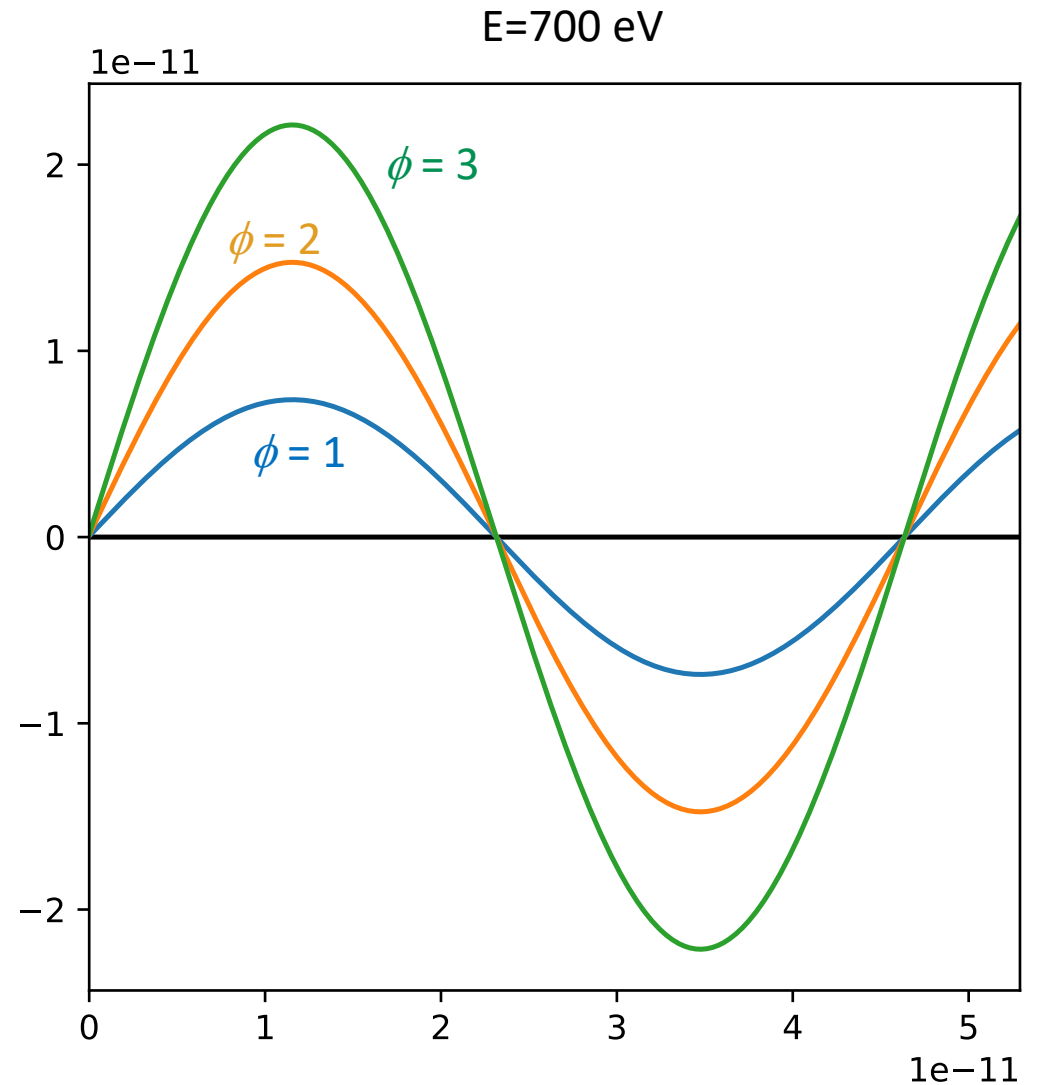
$$V(x) = \begin{cases} 0, & \text{for } 0 < x < L \\ \infty, & \text{elsewhere} \end{cases}$$

# Schrodinger equation in 1D well

- As usual, make into system of 1D ODEs:

$$\frac{d\psi}{dx} = \phi, \quad \frac{d\phi}{dx} = \frac{2m}{\hbar^2} [V(x) - E]\psi$$

- Know that  $\psi = 0$  at  $x = 0$  and  $x = L$ , but don't know  $\phi$
- Let's choose a value of  $E$  and solve using some choices for  $\phi$ :
- Since the equation is linear, scaling the initial conditions exactly scales the  $\psi(x)$
- **No matter what  $\phi$ , we will never get a valid solution!** (only affects overall magnitude, not shape)



# Only specific $E$ has a valid solution

- Solutions only exist for eigenvalues
- Need to vary  $E$ ,  $\phi$  can be fixed via normalization
- Same strategy, Find the  $E$  such that  $\psi(L) = 0$



# After class tasks

- Homework 1 due Sept. 16 by 11pm
  - Let me know if you have HW questions or questions/issues on github classroom
  - Office hours: Mondays, 3:00pm to 4:00pm; Thursdays, 11:05am to 1:00pm
    - Feel free to send me an email, and remember, if you push your changes, I should be able to see them
- Readings:
  - Newman Ch. 8