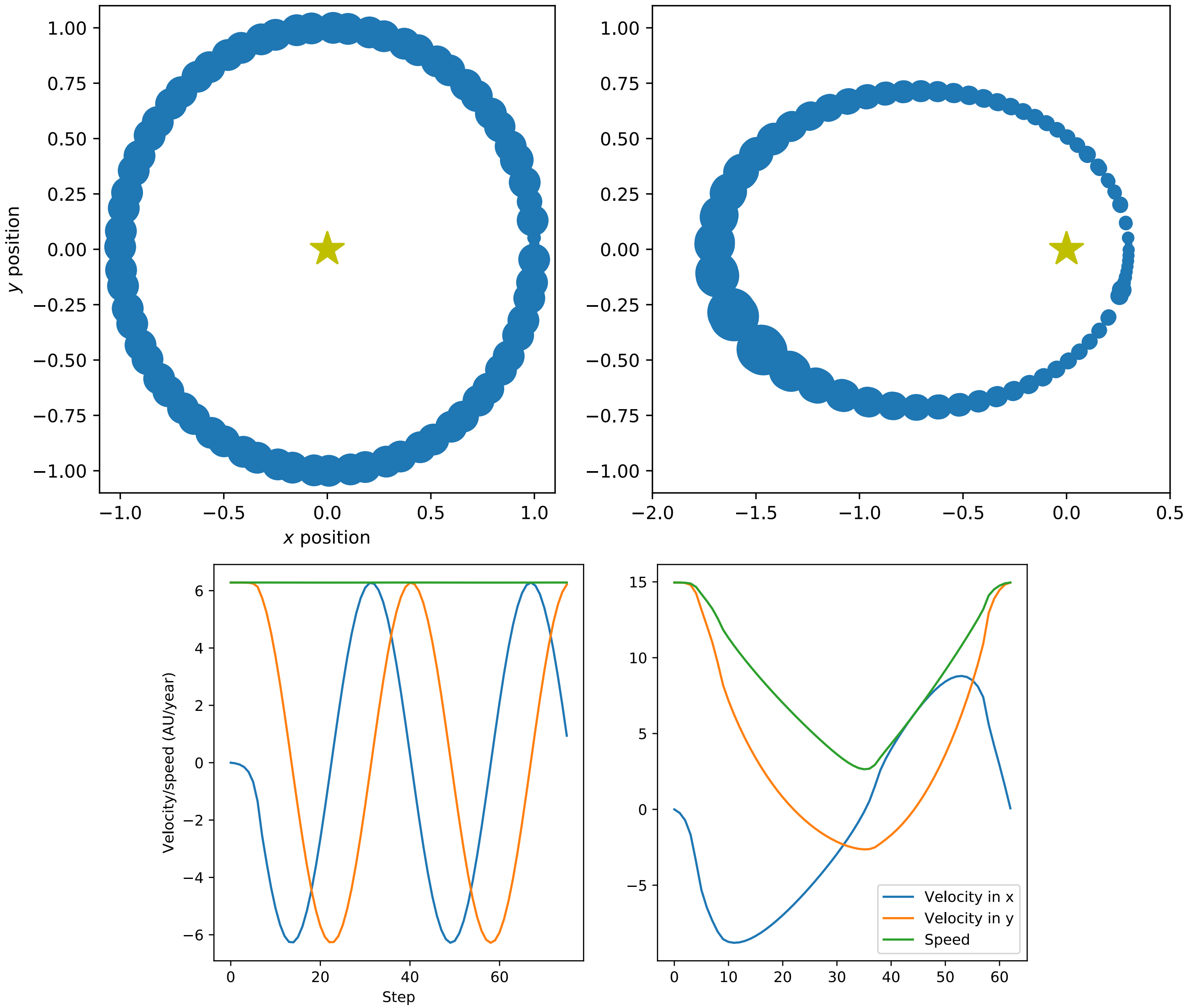
PHY604 Lecture 9

October 3, 2023

Review: Elliptical orbit with adaptive 4^{th}-order RK

<u>Circular</u>:
x_0= 1 AU
v_{y0} =6.283185 AU/year

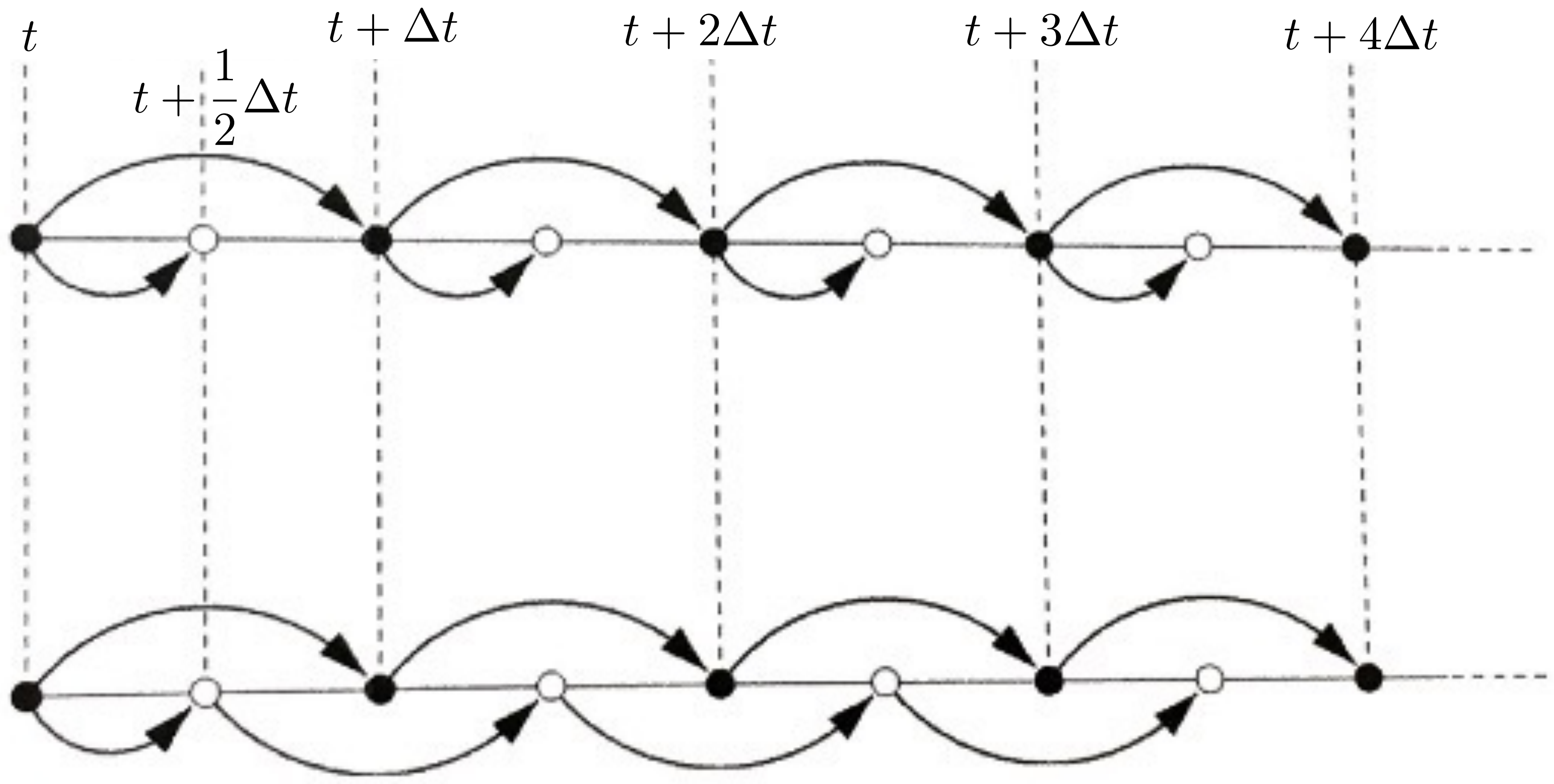


<u>Elliptical</u>:
x_0= 0.3 AU
v_{y0} =14.955378 AU/year

Review: Leapfrog method versus 2nd order RK

2nd order RK:

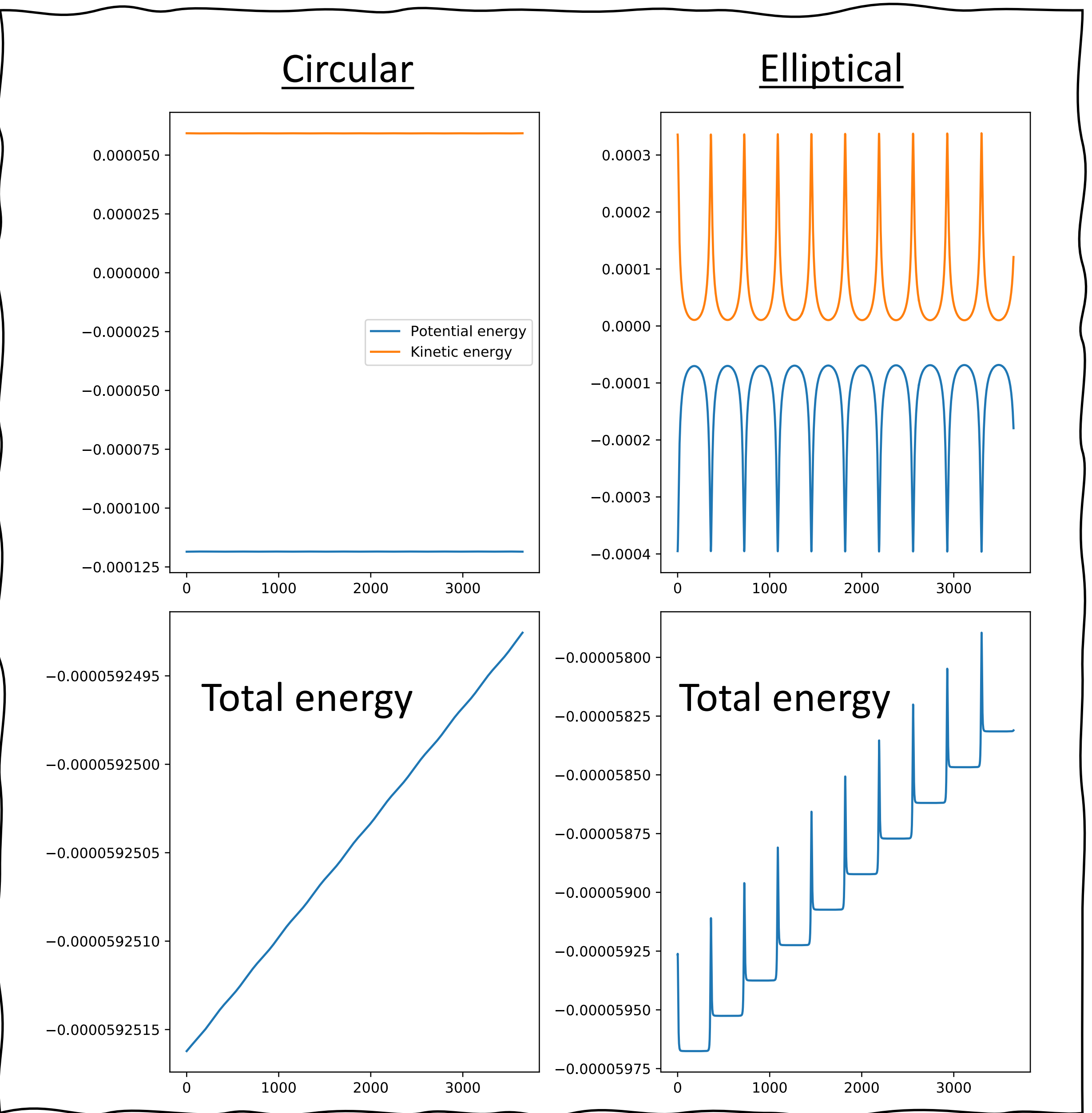
Leapfrog:



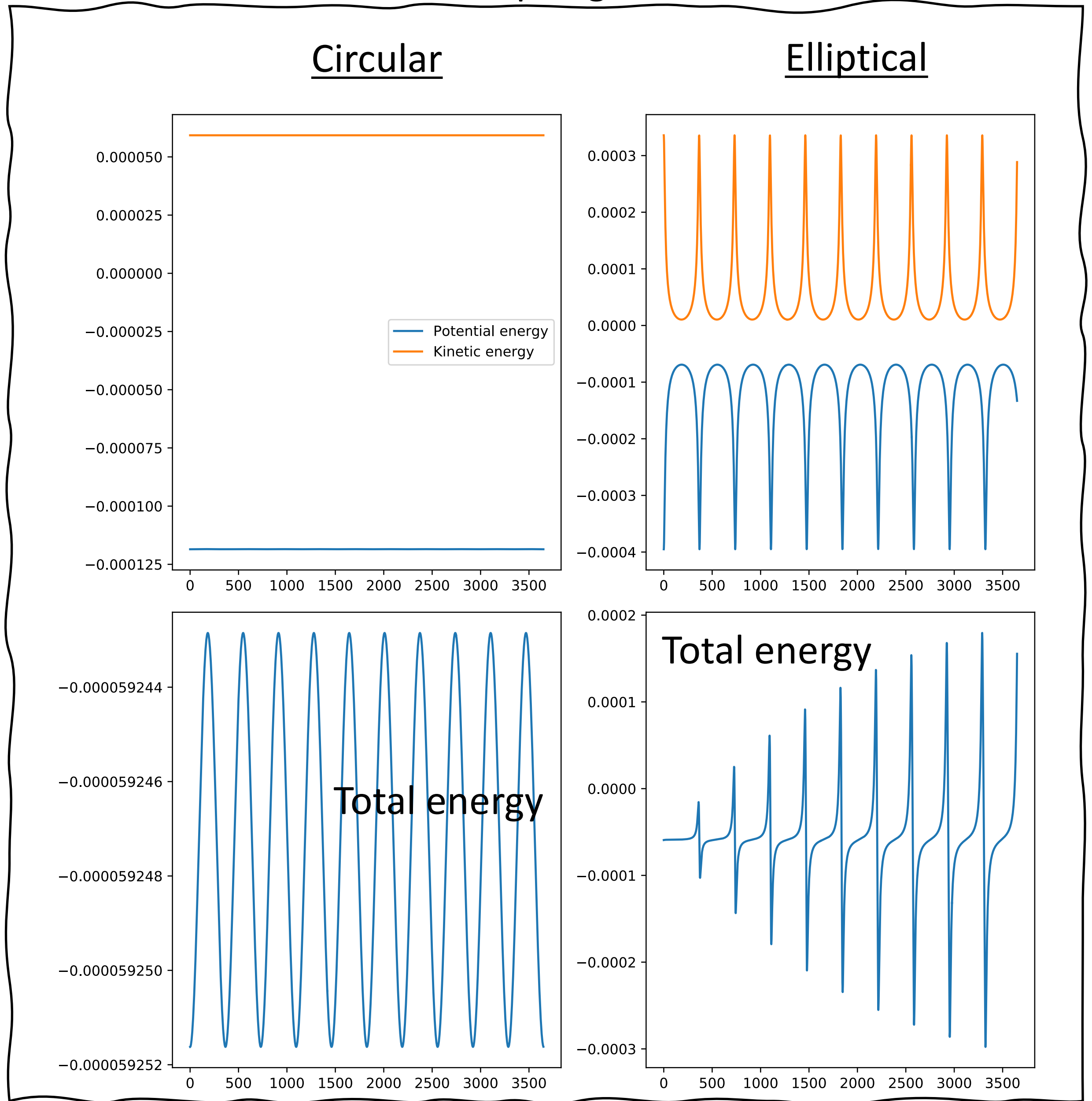
(Newman)

Review: Time-reversal symmetry and energy conservation!

2nd order RK



Leapfrog



Today’s lecture:
ODEs and Linear Algebra

- Beyond RK: Other methods for ODEs
  - Verlet method
  - Bulirsch-Stoer Method

- Boundary Value problems

- Eigenvalue problems

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:

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

- (i.e., where the RHS of the first equation does not depend on **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

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

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

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

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

- Rearrange to get:

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

- 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:

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

- Then repeatedly apply:

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

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

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

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

Error of leapfrog/Verlet is even in step size

- Error for a single step is proportional to Δt^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:

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

- 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:

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

Wait, what about initial Euler half step?

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

- 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:

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

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

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

$$\vdots \qquad\qquad \vdots$$

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

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

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 Δt_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: $c_2 \Delta t_3^4 = \dfrac{16}{65}(R_{3,2} - R_{2,2})$

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

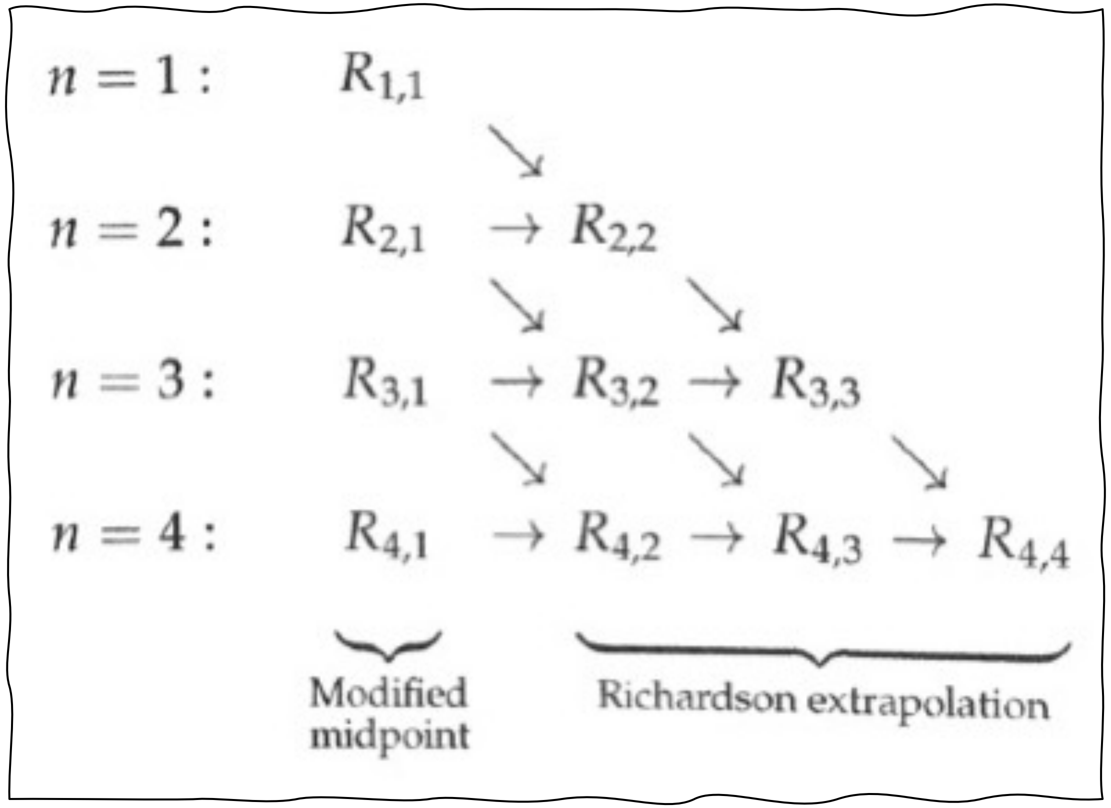
- n is the number of modified midpoint steps, which gives us $R_{n,1}$
  - Can obtain $R_{n,m}$ for $m < n$

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

  - See Newman Sec. 8.5

- Which gives an estimate of the result:

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



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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 $x(t+\mathrm{t}_f)$
  - At intermediate points, we just get raw midpoint method estimates (accurate to Δt^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

- Can give better accuracy with less work then 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 δ 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 $R_{\mathrm{n},1}$ with the modified midpoint method
- 3. Calculate the "row" via Richardson extrapolation, i.e., $R_{n,2} \ldots R_{n,n}$
- 4. Compare the error to the target accuracy δt_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.

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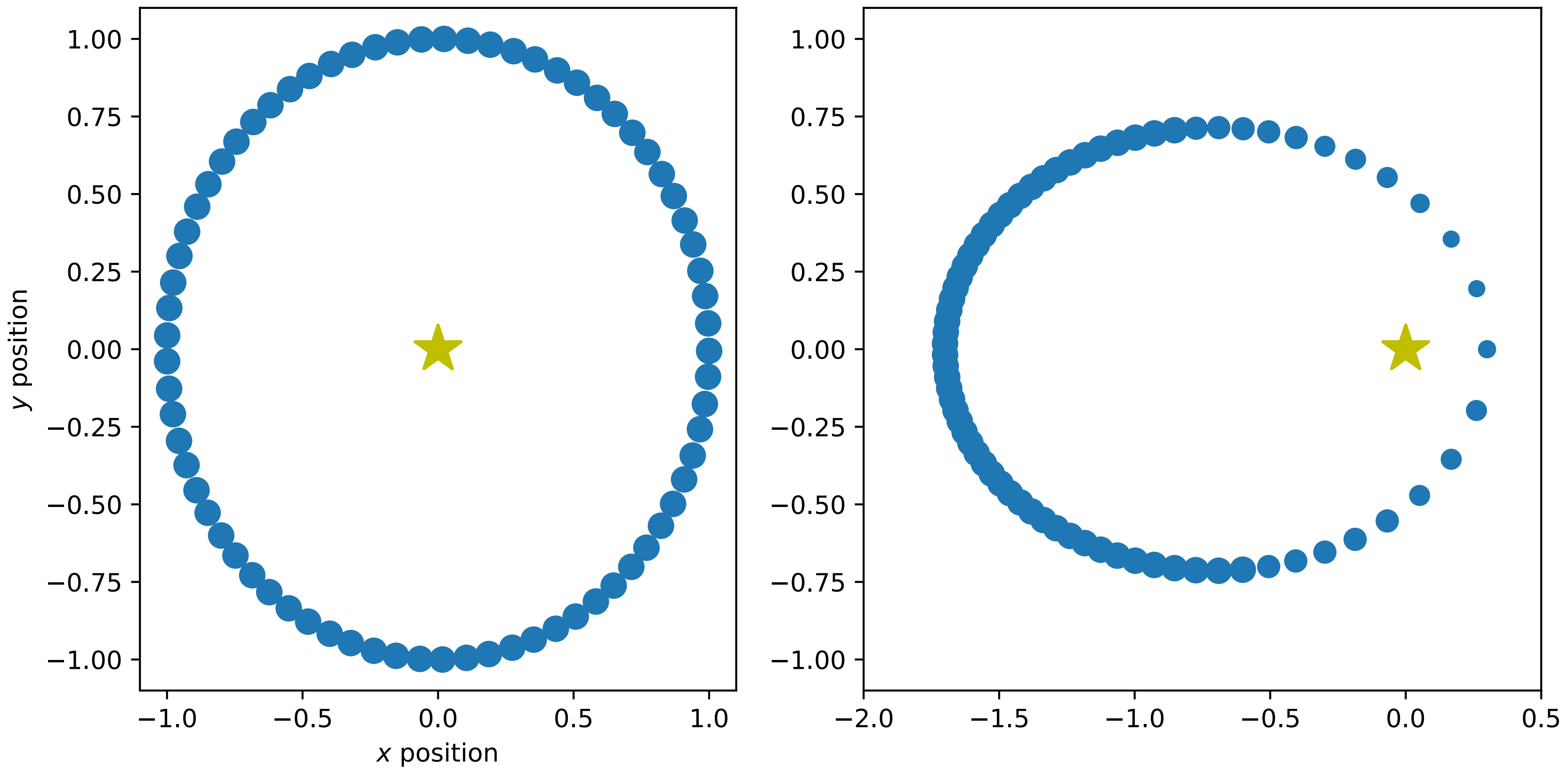
Example: Orbits with the Bulirsch-Stoer method



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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)

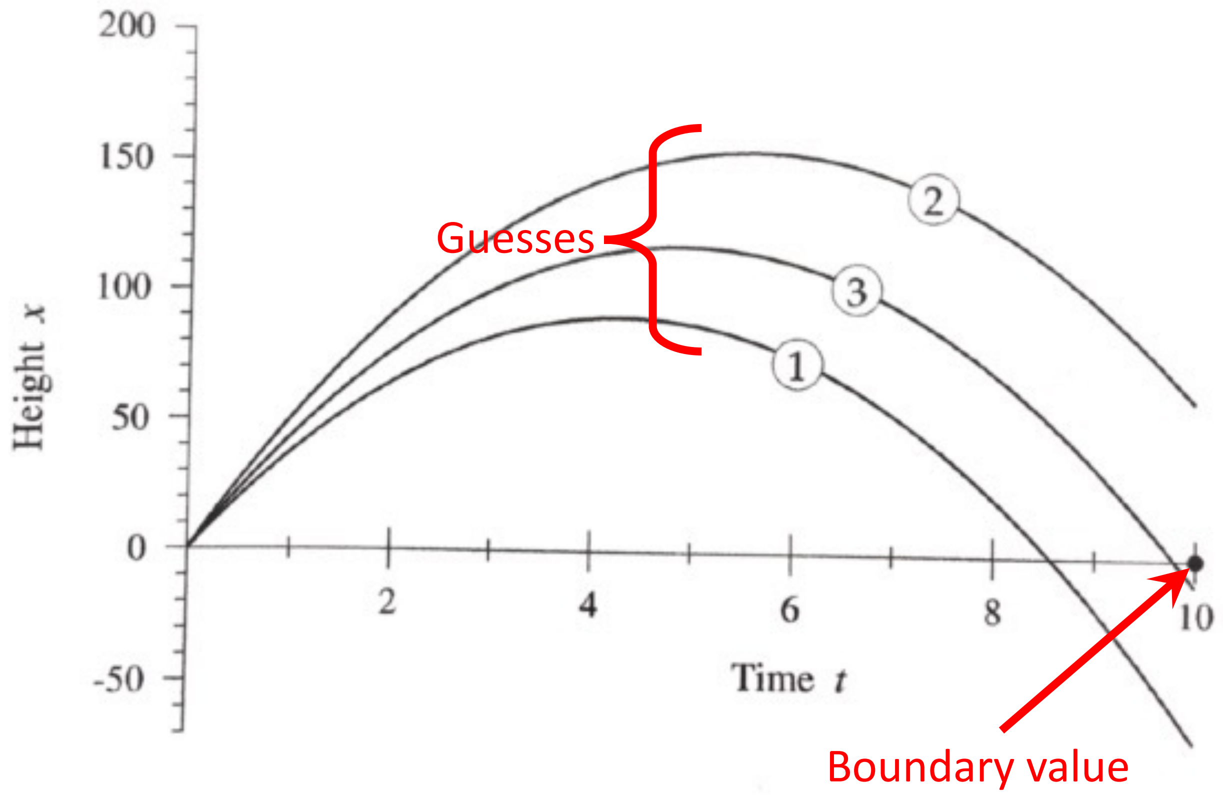
Shooting method example: Ball thrown in the air

- "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.

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Eigenvalue problems

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

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

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

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

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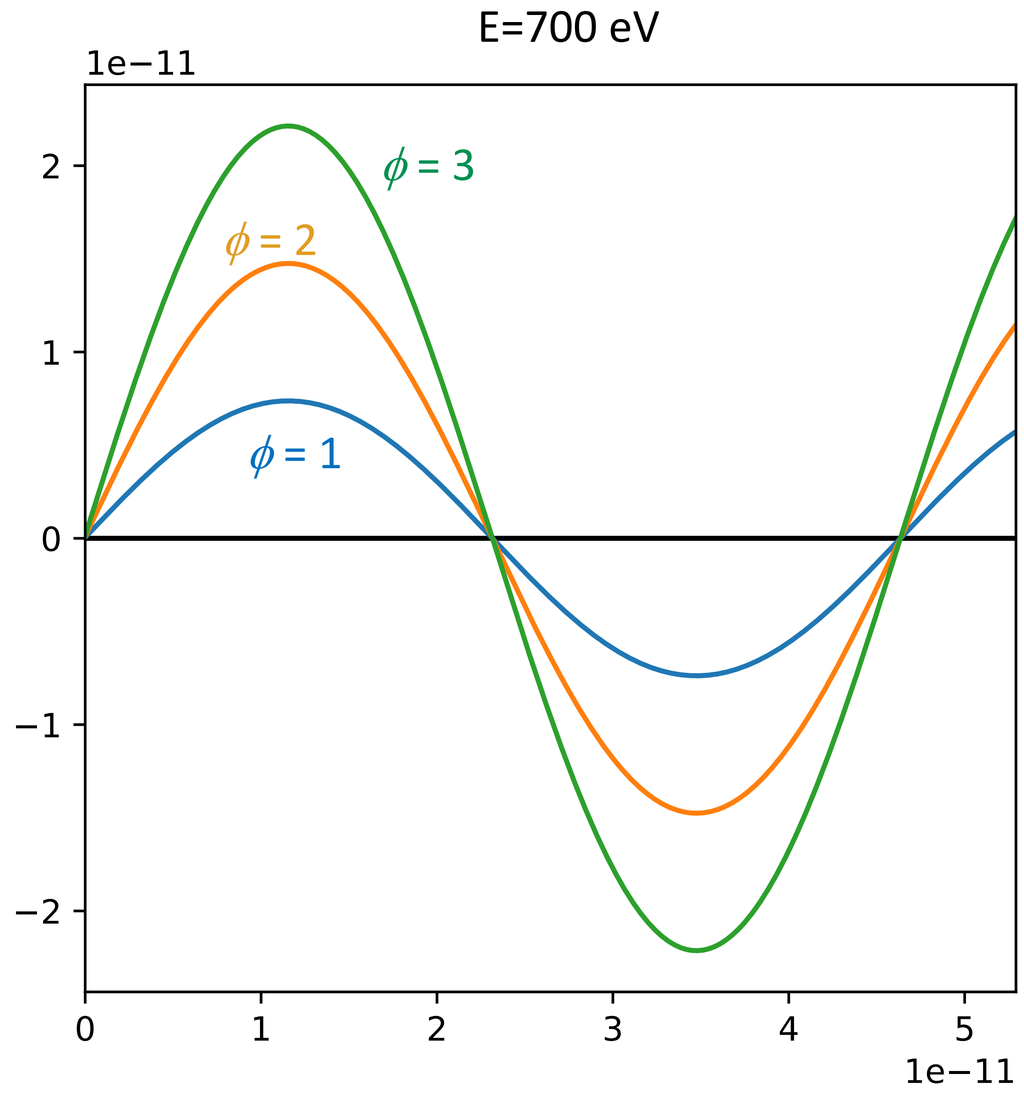
Schrodinger equation in 1D well

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

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

- Know that $\psi = 0$ at $x = 0$ and $x = L$, but don't know ϕ
- Let's choose a value of E and solve using some choices for ϕ :
- Since the equation is linear, scaling the initial conditions exactly scales the $\psi(x)$

- **No matter what ϕ, 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, ϕ can be fixed via normalization
- Same strategy, Find the E such that $\psi(L) = 0$

After class tasks

- Homework 2 due Thursday by 11pm
- Readings:
  - Newman Ch. 8
  - Garcia Ch. 4