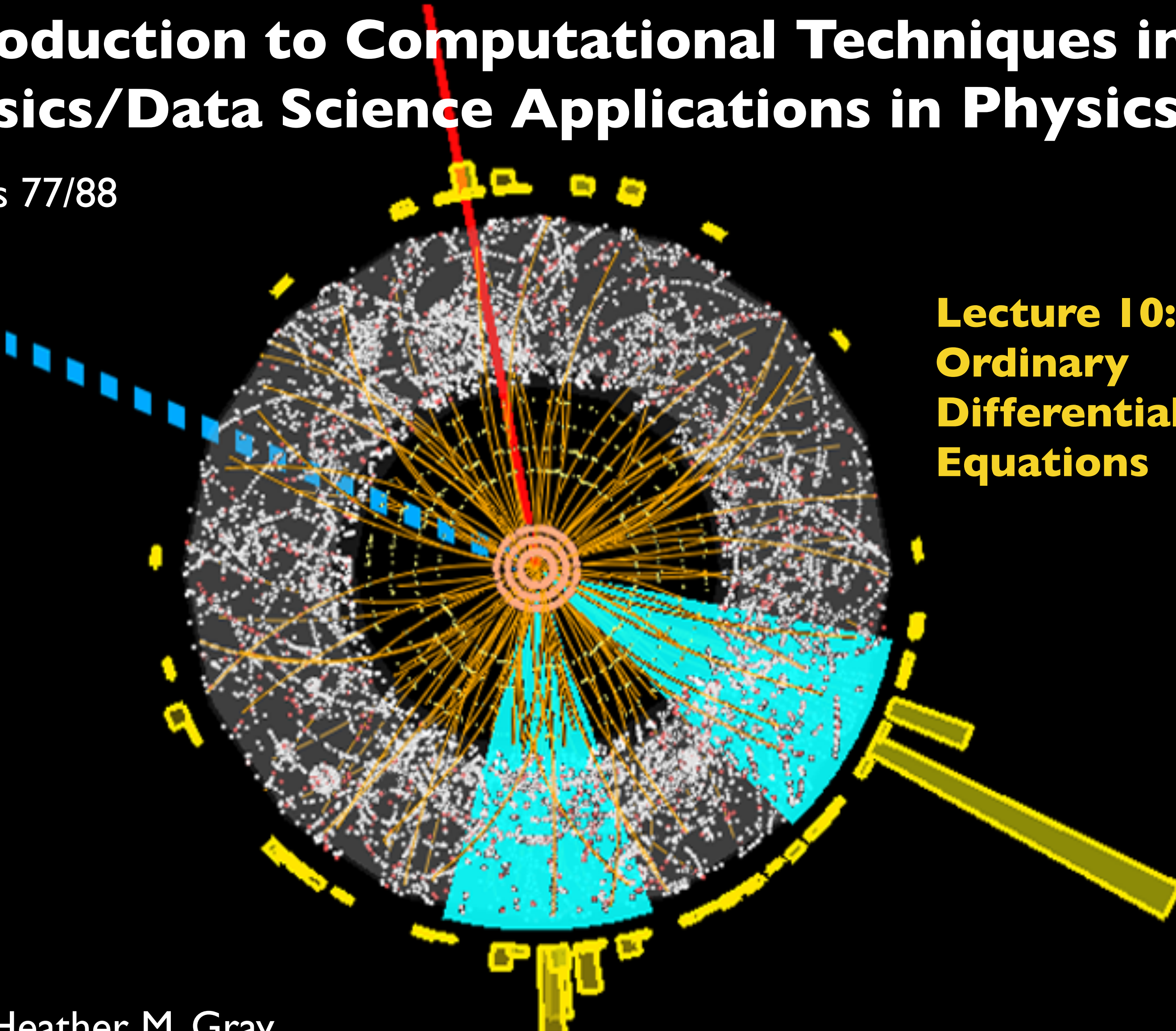
Introduction to Computational Techniques in Physics/Data Science Applications in Physics

Physics 77/88



Lecture 10: Ordinary Differential Equations

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Many thanks to Yury Kolomensky for material used in this course

Differential Equations

- Equations that are composed of unknown function(s) and their derivative(s) are called differential equations

$$\frac{dv}{dt} = g - \frac{c}{m} v$$

  - v: dependent variable
  - t: independent variable
- Fundamental importance in physics:
  - Dynamical problems: naturally formulated in terms of rate of some changes of some
    - Equations of motion: relate acceleration to forces
    - Thermodynamics: temperature gradient to heat flow
    - E&M: divergence of field to charge distribution

Ordinary Differential Equations (ODEs)

- Most physical systems are described by a (set of) differential equations
  - e.g. $F(x, t) = m\ddot{x}$
- Solutions are not always analytical
  - Only for the simplest cases you find in a textbook
    - e.g. $x(t) = x_0 + v_0 t + \frac{a}{2} t^2$
- We will consider the most generic
  - Numerical solutions

Classification of ODEs

- ODE can be classified in different ways
  - Order
    - first
    - second
    - nth
  - Linearity
    - Linear
    - Nonlinear
  - Auxiliary conditions
    - Initial value problems
    - Boundary value problems

Order of ODE

- The order of an ordinary differential equation is the order of the highest order derivative
  - Examples
    - $\frac{dy}{dx} - y = e^x$: first order ODE
    - $\frac{d^2y}{dx^2} - 5\frac{dy}{dx} + 2y = \cos x$: second order ODE
    - $(\frac{d^2y}{dx^2})^3 - \frac{dy}{dx} + 2y^4 = 1$: second order ODE

Linear vs Nonlinear ODEs

- An ODE is linear if the unknown function and its derivatives appear to power one
  - And there is no product of the unknown function and/or its derivatives
  - $a_n(x) y^n(x) + a_{n-1}(x) y^{n-1}(x) + \dots + a_1(x) y'(x) + a_0 y(x) = g(x)$
  - Examples
    - $\dfrac{dy}{dx} - y = e^x$ linear ODE
    - $\dfrac{d^2y}{dx^2} - 5\dfrac{dy}{dx} + 2x^2y = \cos(x)$ linear ODE
    - $(\dfrac{d^2y}{dx^2})^3 - \dfrac{dy}{dx} + \sqrt{y} = 1$ non-linear ODE

Initial Conditions

- Initial-value problems
  - The auxiliary conditions are at one point of the independent variable
    - e.g. $y'' + 2y' + y = e^{-2x}$
      - $y(0) = 1$; $y'(0) = 2.5$
- Boundary-value problems
  - The auxiliary conditions are not at one point of the independent variable
    - e.g. $y'' + 2y' + y = e^{-2x}$
      - $y(0) = 1$; $y'(1) = 2.5$ $\rightarrow$ $y(1) = 2.5$

Analytical vs Numerical Solutions

$F = ma$

$$\frac{dv}{dt} = g - \frac{c}{m}v$$

$$v = \frac{gm}{c}\left(1 - e^{-(c/m)t}\right)$$

Analytical

$$v_{i+1} = v_i + \left(g - \frac{c}{m}v_i\right)\Delta t$$

Numerical

Physical Law

ODE

Solution

Visualization: Direction Fields

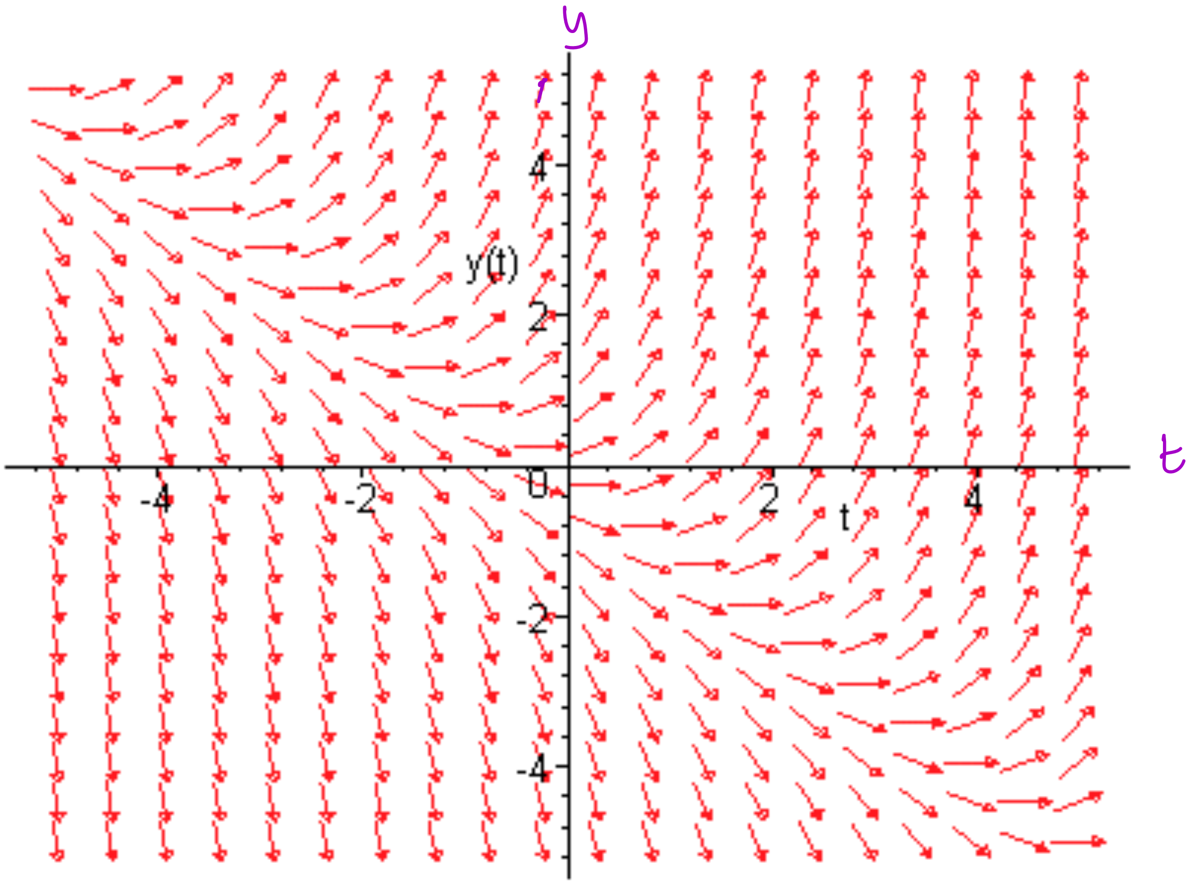
- Consider the first order differential equation

  $$\frac{dy}{dx} = f(x, y)$$

- Equation specifies slope at each point in the x-y plane
- Gives the direction that a solution to the equation must have at each point
- A plot of short line segments drawn at various points in the $x - y$ plane showing the slope of the solution curve
  - Direction field
- Direction field gives the flow of solutions

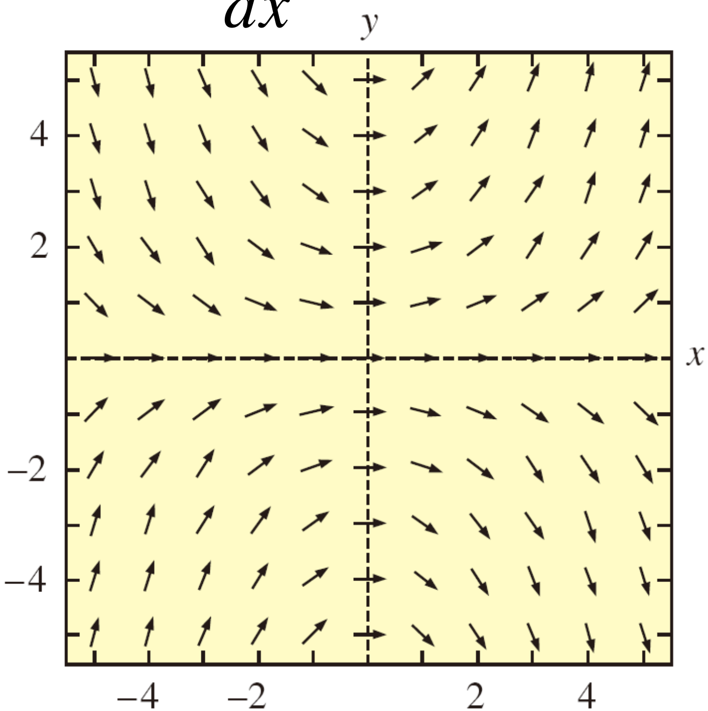
Example

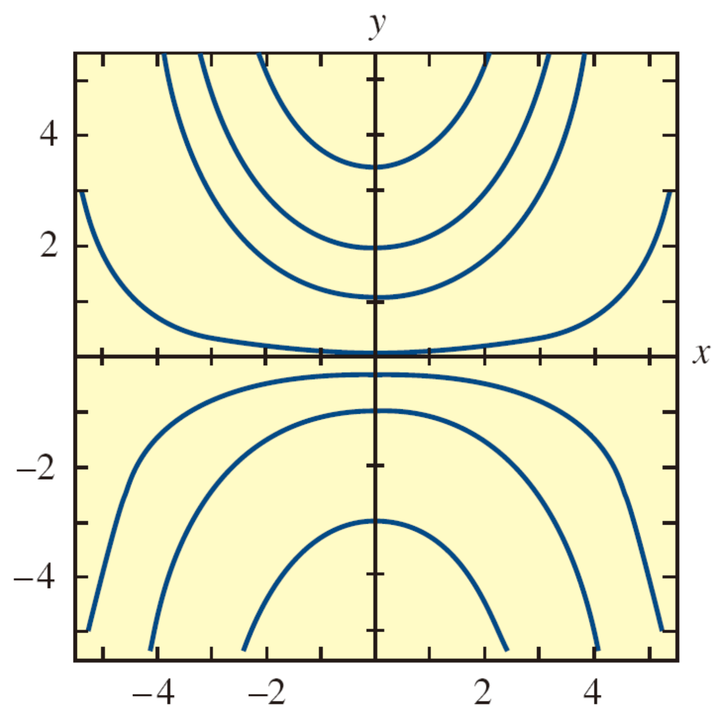
$$f(t, y) = t + y$$



Example

$$\frac{dy}{dx} = 0.2xy \qquad y = Ce^{0.1x^2}$$





Direction fields can help in selecting a class of analytical solutions

Methods to solve Differential Equations

- Trial and error
  - Try a class of functions, see if it works
    - Boundary conditions reduce the set of possible solutions
- Look up
  - Reduce the equation to a previously solved case
- Numerical integration

Example: Analytical Solution

- An analytical solution to a differential equation is a function that satisfies the equation
- Example
  - $\frac{dx}{dt} + x(t) = 0$
- Solution
  - $x(t) = e^{-t}$
- Proof
  - $\frac{dx(t)}{dt} = -e^{-t}$
  - $\Rightarrow \frac{dx}{dt} + x(t) = -e^{-t} + e^{-t} = 0$

Stability and Chaos

- Solution of an ODE can be
  - Stable
    - Solutions resulting from perturbations of the initial value remain close to the original solution
  - Asymptotically stable
    - Solutions resulting from the perturbations converge back to the original solution
  - Unstable
    - Solutions resulting from perturbations diverge from the original solutions with bounds

Numerical Solutions

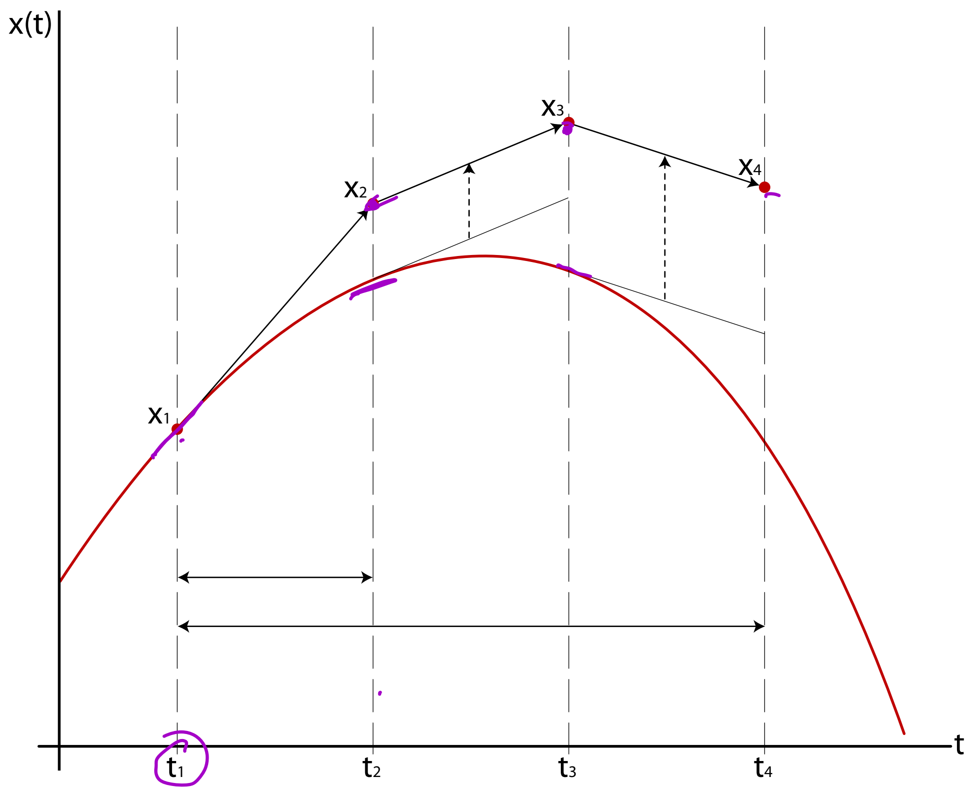
- Approximate solution values are generated step-by-step in increments moving across the interval where the solution is sought
  - i.e. need to solve differential equations in a discrete domain
- In stepping from one discrete point to the next, incur some numerical error
  - Next approximate solution values lie on a different solution from the one we started from
- Stability or instability of solutions determines, in part, whether such errors are magnified or diminished with time

Euler Method

- Example: find the position of a projectile
  - $\cancel{x}^{v}(x, t) = \frac{dx}{dt}$
- Rewrite with partial differences
  - $dx = v(x,t)\,dt$
  - $\Rightarrow \Delta x = v(x,t)\,\Delta t$
- Implementation
  - $\underbrace{x_{i+1} = x_i +}\frac{dx}{dt}\Delta t$
  - $x(0) = x_0$

This is known as the Euler method

Euler Method



A. Ayers, Computational Physics with Python

Euler Method

- Precision limited by step size Δt
  - Decrease Δt to reduce error
- Calculation time scales linearly with the number of steps
  - $N_{\text{steps}} \sim \frac{\tau}{\Delta t}$ where τ is the total time interval to be integrated
- So far limited to first-order ODEs

Euler Method for 2nd Order ODE

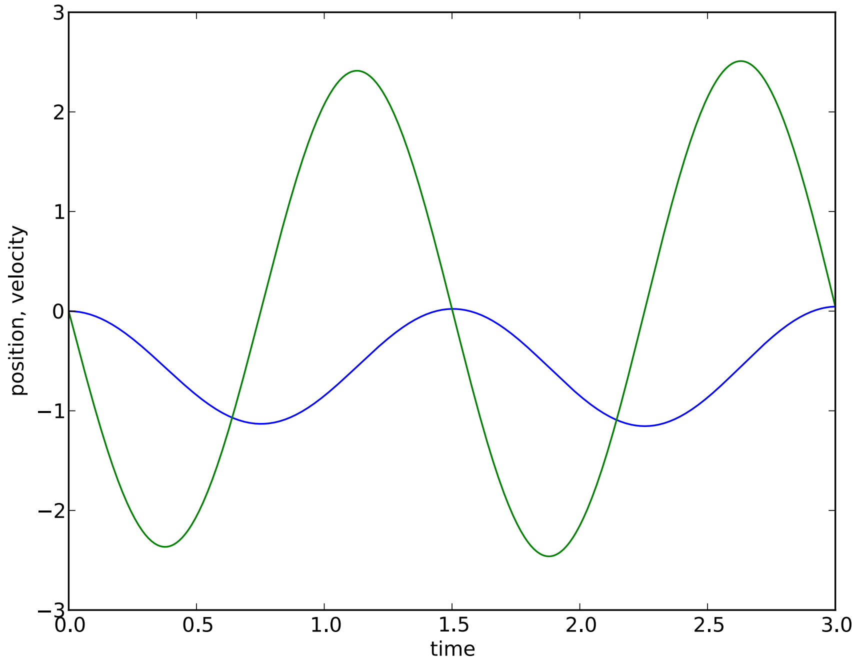
- Standard trick: convert a 2nd (or higher) order ODE into a system of 1st order ODEs
  - Example: free fall
    - $\ddot{x} = -g$
    - Define
      - $\dot{x} = v$
      - $\dot{v} = -g$
  - Solutions can be obtained by applying the Euler method
    - $x_{i+1} = x_i + \dot{x}\Delta t$
    - $v_{i+1} = v_i + \dot{v}\Delta t$

Generalize

- Rewrite in vector form
  - $y = \begin{bmatrix} x \\ v \end{bmatrix}$
- Vector of derivatives is
  - $\dot{y} = \begin{bmatrix} v \\ -g \end{bmatrix}$
- Euler solution
  - $y_{i+1} = y_i + \dot{y}_i \Delta t$
- See notebok for implementation

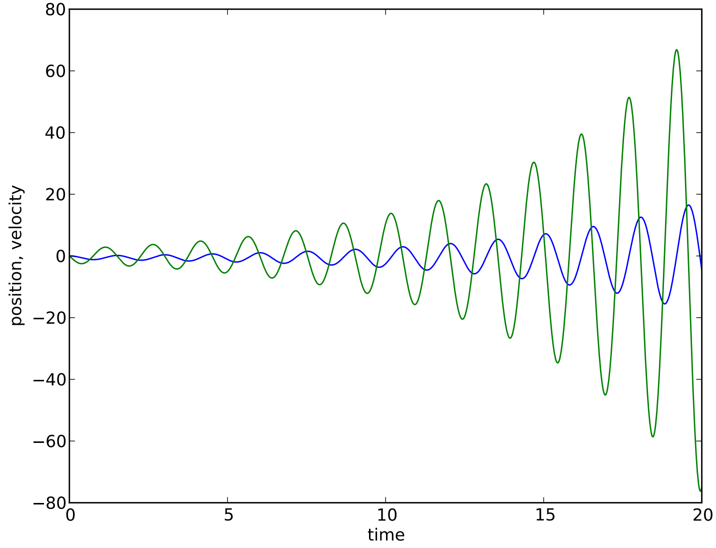
Solutions

- Example: simple harmonic motion
  - Mass on a vertical spring
    - $F =$ $-mg + kx$



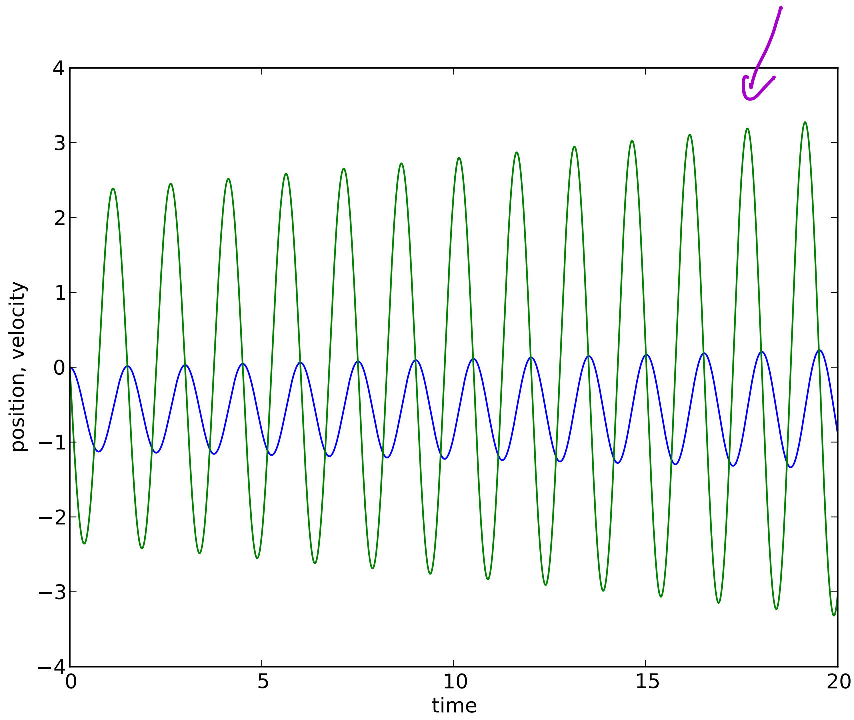
Problems

- Euler method underestimates curvature
  - Energy is not conserved



Example with a total time of 20 seconds and N =1000

Problems



Example with a total time of 20 seconds and N = 10000
Better, but the energy is still increasing with time

Euler-Cromer Method

- Trick that works for simple harmonic oscillator (SHO)
  - Replace derivative with derivative evaluated at the next step
    - $y_{i+1} = y_i + \dot{y}_{i+1} \Delta t$
- Not a general solution , so we need to do better

Runge-Kutta Methods

- General case:
  - Find a function $y(t)$ with its time derivative

$$g(y,t) = \dot{y} = \frac{dy}{dt}$$

  - Apply the chain rule

$$\ddot{y} = \frac{d}{dt}\left[\dot{y}\right]$$

$$= \frac{d}{dt}\left[g(y,t)\right]$$

- $$= \frac{\partial g}{\partial t} + \frac{\partial g}{\partial y}\frac{\partial y}{\partial t}$$

$$= g_t + g_y \, g$$

$$g_a \equiv \frac{\partial y}{\partial a}$$

$$g_{ab} \equiv \frac{\partial^2 y}{\partial a \partial b}$$

Runge-Kutta Methods

- Similarly,
  - $\dddot{y} = \quad g_{tt} + 2g\,g_{ty} + g^2 g_{yy} + g\,g_y^2 + g_t\,g_y$
  - Reminder

$$g_a \equiv \frac{\partial y}{\partial a}$$

- $$g_{ab} \equiv \frac{\partial^2 y}{\partial a \partial b}$$

Runge-Kutta Methods

- Taylor expansion:

$$y(t+\Delta t) = y(t)$$
$$+ \; g \Delta t$$
$$+ \; \frac{\Delta t^2}{2!} (g_t + g_y g)$$
$$+ \; \frac{\Delta t^3}{3!} (g_{tt} + 2 g g_{ty} + g^2 g_{yy} + g g_y^2 + g_t g_y)$$
$$+ \; O(\Delta t^4)$$

- Compare to an alternative polynomial expansion:
  - $y(t+\Delta t) =$ $y(t) + \alpha_1 k_1 + \alpha_2 k_2 + \cdots + \alpha_n k_n$

Runge-Kutta Methods

- Polynomials:
  - $k_1 = \Delta t\, g(y, t)$
  - $k_2 = \Delta t\, g(y + v_{21} k_1,\ t + v_{21} \Delta t)$
  - $k_3 = \Delta t\, g(y + v_{31} k_1 + v_{32} k_2,\ t + v_{31} \Delta t + v_{32} \Delta t)$
  - $\vdots$
  - $k_n = \Delta t\, g\left(y + \sum_{l=1}^{n-1} v_{nl} k_l,\ t + \Delta t \sum_{l=1}^{n-1} v_{nl}\right)$
- Coefficients α_i and v_{nl} are determined by matching coefficients against Taylor expansion
  - Determined by expansion order
  - i.e. 2nd order RK, 4th order RK, etc

2nd order RK

- $y(t + \Delta t) =$ $y = \alpha_1 k_1 + \alpha_2 k_2$

  $= y + \alpha_1 [\Delta t\, g(y,t)] + \alpha_2 [\Delta t\, g(y + v_{21} k_1, t + v_{21} \Delta t)]$

- $k_2 =$ $\Delta t [g + v_{21} k_1 g_y + v_{21} \Delta t\, g_t + O(\Delta t^2)]$

  $=$ $\Delta t\, g + v_{21} \Delta t^2 g g_y + v_{21} \Delta t^2 g_t + O(\Delta t^3)$

- Follows:
  - $y(t + \Delta t) =$ $y + [(\alpha_1 + \alpha_2) g] \Delta t + [\alpha_2 v_{21} (g g_y + g_t)] \Delta t^2$
    - $\alpha_1 + \alpha_2 =$ 1
    - $\alpha_1 v_{21} =$ $\frac{1}{2}$

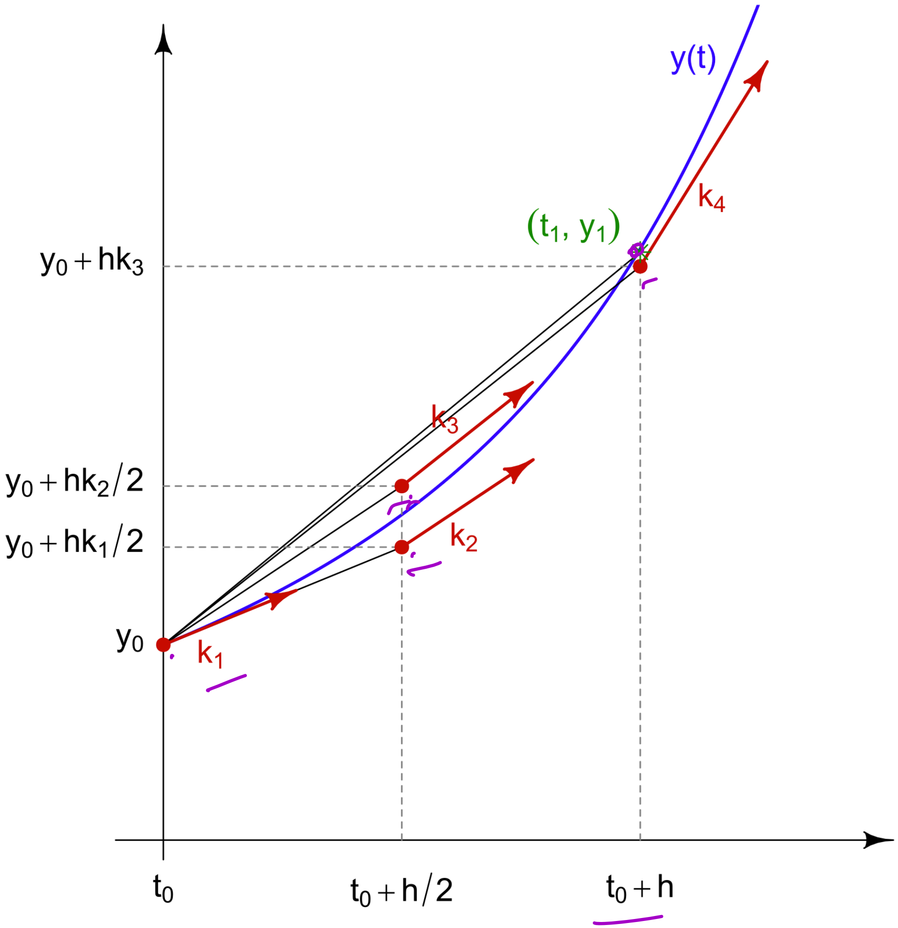
2nd order RK

- Standard solution:
  - $v_{21} =$ 1
  - $\alpha_1 = \alpha_2 =$ 0.5
    - $y(t + \Delta t) =$ $y + \frac{1}{2}k_1 + \frac{1}{2}k_2 + O(\Delta t^3)$
    - $k_1 =$ $\Delta t\, g(y, t)$
    - $k_2 =$ $\Delta t\, g(y + k, t + \Delta t)$

4th Order RK

- $y(t+\Delta t) = y(t) + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4) + O(\Delta t^4)$
  - $k_1 = g(y, t)\,\Delta t$
  - $k_2 = g(y + \frac{1}{2}k_1,\ t + \frac{1}{2}\Delta t)\,\Delta t$
  - $k_3 = g(y + \frac{1}{2}k_2,\ t + \frac{1}{2}\Delta t)\,\Delta t$
  - $k_4 = g(y + k_3,\ t + \Delta t)\,\Delta t$
- 4th order RK is a standard tool
  - good trade off between precision and speed

Runge-Kutta Illustration



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