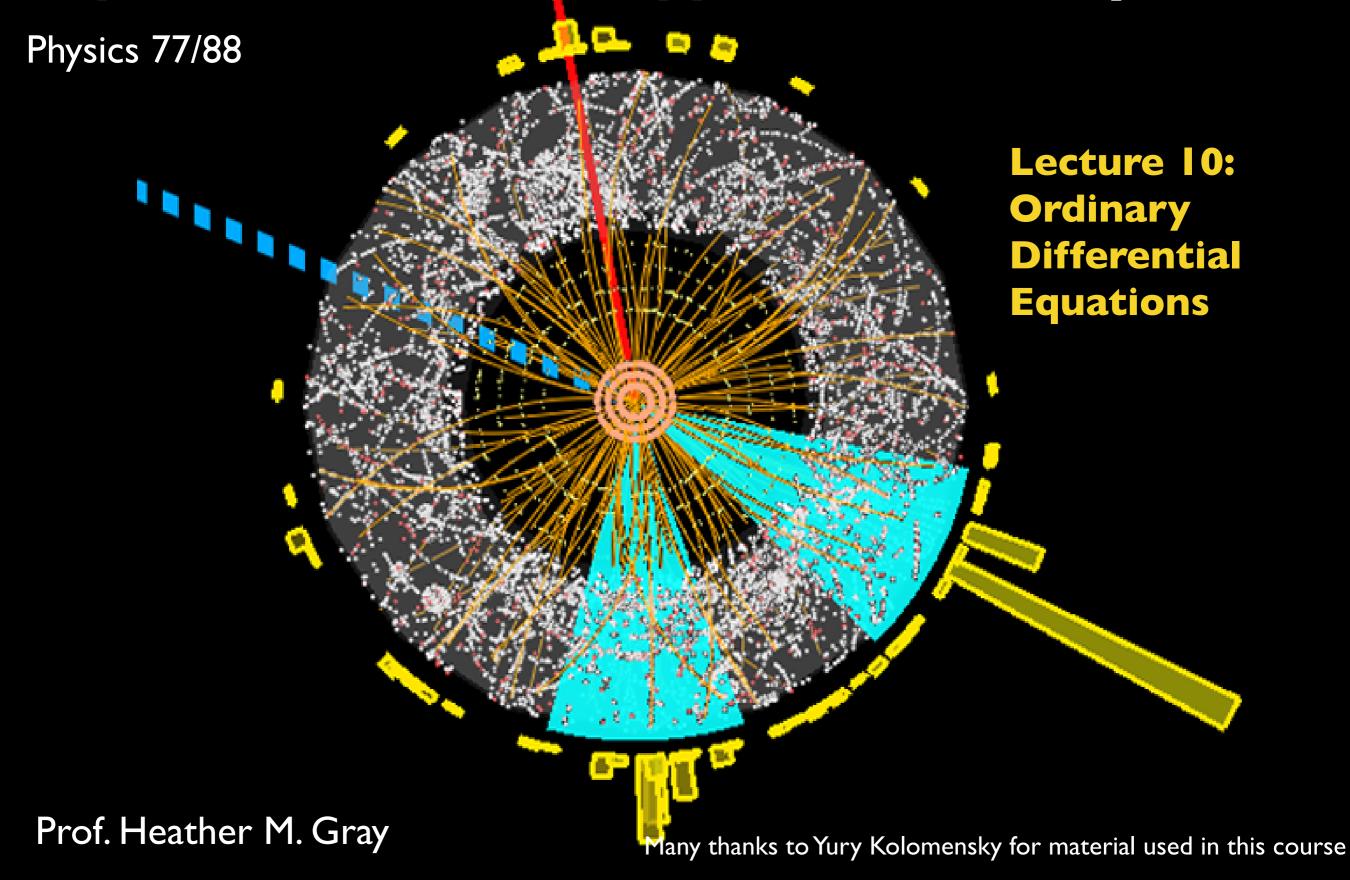
Introduction to Computational Techniques in Physics/Data Science Applications in Physics



Differential Equations

 Equations that are composed of and their are called differential equations

- *v*: variable
- t: variable
- importance in physics:
 - problems: naturally in terms of of some
 - Equations of motion: relate to
 - Thermodynamics: gradient to
 - E&M: to

Ordinary Differential Equations (ODEs)

Most

are described by a (set of)

- e.g. $F(x, t) = m\ddot{x}$
- Solutions are not always
 - Only for the

you find in a textbook

- e.g.
- We will consider the
 - solutions

Classification of ODEs

- ODE can be classified in different ways
 - lacktriangle
- •
- •

- conditions
 - value problems
 - value problems

Order of ODE

- The of an ordinary differential equation is the order of the
 - Examples
 - $\frac{dy}{dx} y = e^x$: order ODE

 - $(\frac{d^2y}{dx^2})^3 \frac{dy}{dx} + 2y^4 = 1$: order ODE

Linear vs Nonlinear ODEs

- An ODE is if the and its appear to power
 - And there is of the unknown function and/ or its derivatives

Examples

•
$$(\frac{d^2y}{dx^2})^3 - \frac{dy}{dx} + \sqrt{y} = 1$$
 ODE

Initial Conditions

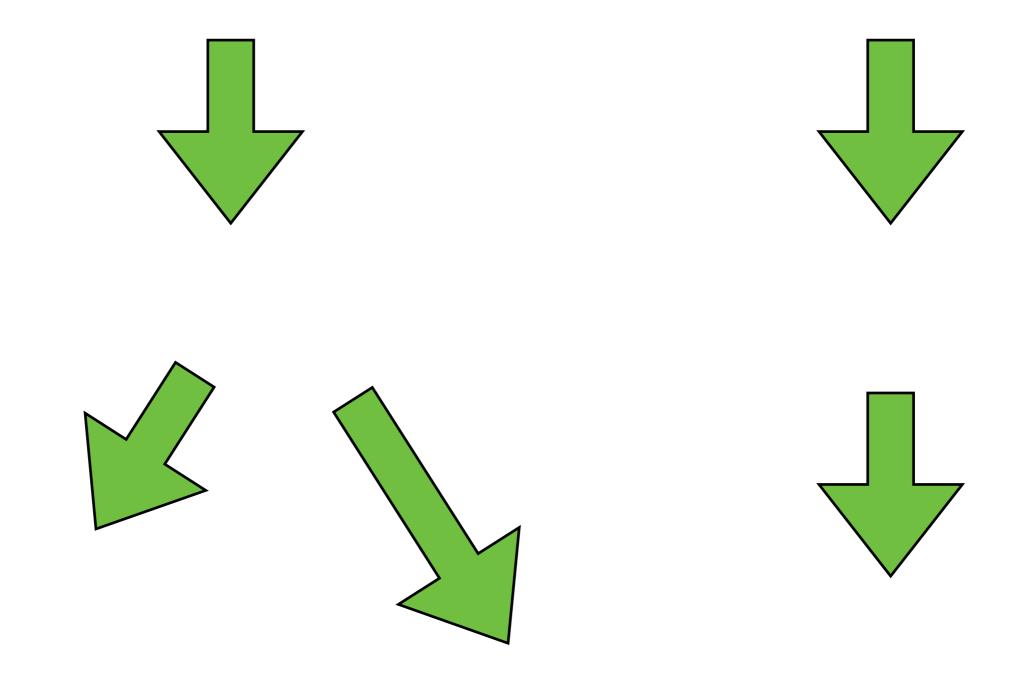
- problems
 - The are at of the

• e.g.
$$y'' + 2y' + y = e^{-2x}$$

- problems
 - The are at one point of the independent variable

• e.g.
$$y'' + 2y' + y = e^{-2x}$$

Analytical vs Numerical Solutions



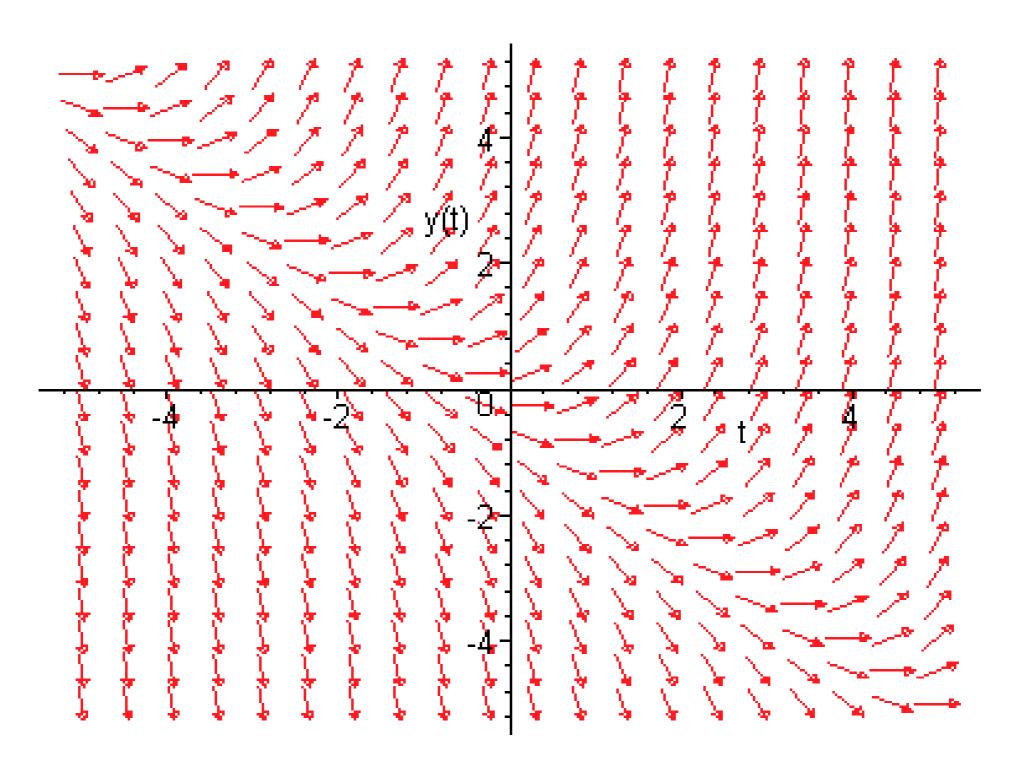
Visualization: Direction Fields

Consider the differential equation

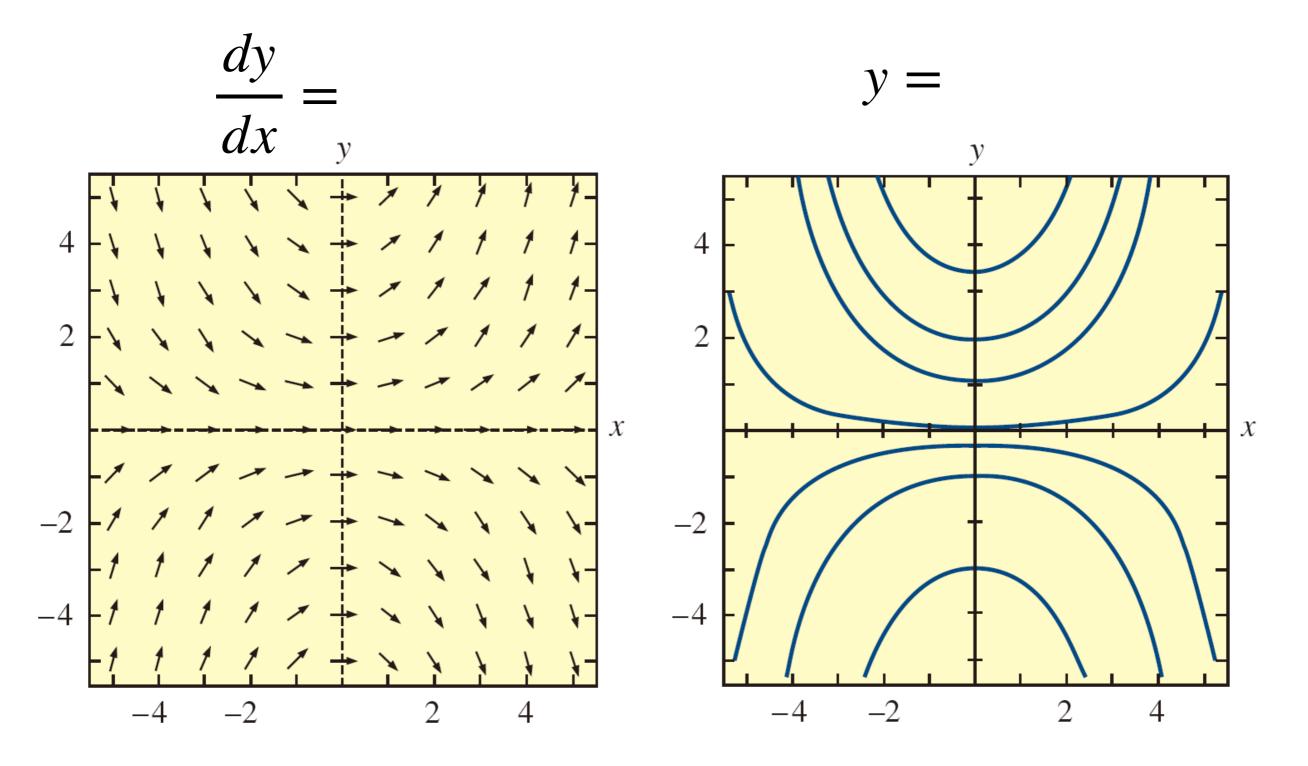
- Equation specifies at each in the
- Gives the that a to the must have at
- A plot of drawn at in the x-y plane showing the of the s
 - field
 - field gives the

Example

$$f(t, y) =$$



Example



Direction fields can help in selecting a class of

Methods to solve Differential Equations

• Try a

, see if it

solutions

reduce the set of possible

• Reduce the equation to a

Example: Analytical Solution

- An to a differential equation is a that satisfies the equation
- Example

$$\cdot \frac{dx}{dt} + x(t) = 0$$

Solution

•
$$x(t) =$$

Proof

$$\cdot \frac{dx(t)}{dt} =$$

$$\Rightarrow$$

Stability and Chaos

Solution of an ODE can be

Solutions resulting from of the remain to the original solution

 Solutions resulting from the perturbations to the original solution

 Solutions resulting from perturbations the original solutions

Numerical Solutions

- solution values are
 in moving across the where the
 is sought
 - i.e. need to solve differential equations in a
- In stepping from to the , incur some
 - Next approximate lie on a from the one we started from
- or of solutions determines, in part,
 whether such are or with
 time

Euler Method

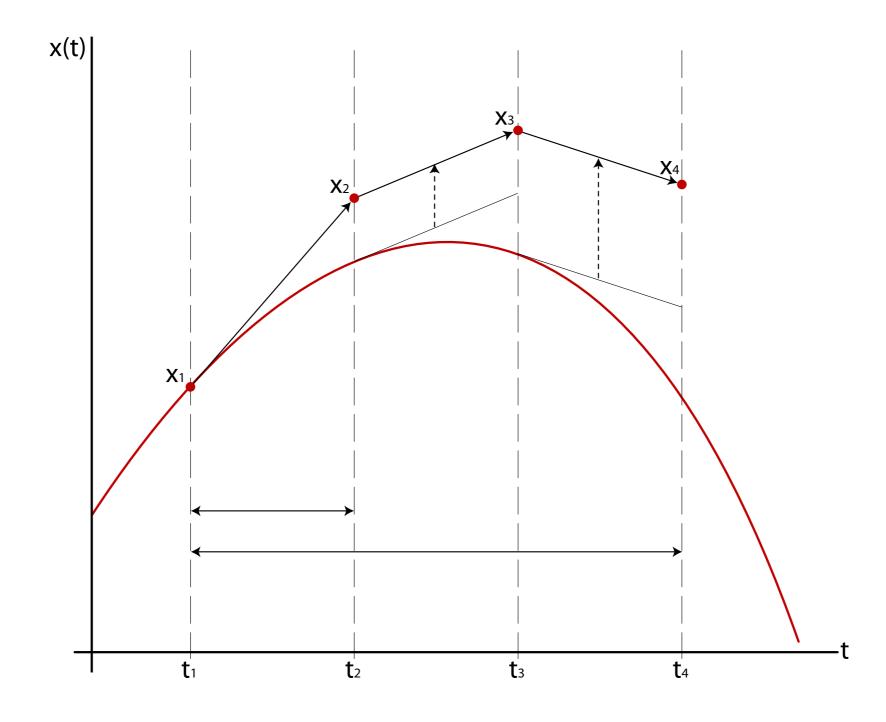
• Example: find the of a

$$\bullet x(x,t) =$$

- Rewrite with partial differences
 - $\bullet dx =$
 - $\Rightarrow \Delta x = 1$
- Implementation

This is known as the Euler method

Euler Method



A. Ayers, Computational Physics with Python

Euler Method

- Precision limited by
 - Δt to reduce
- Calculation time scales with the
 - ${\bf N}_{\rm steps} \sim {\bf Where} \; \tau \; {\rm is \; the} \; {\bf to \; be}$ integrated
- So far limited to

order ODE into

Euler Method for 2nd Order ODE

- Standard trick: convert a
 a of order ODEs
 - Example:
 - •
 - Define
 - •
 - Solutions can be obtained by applying the Euler method

Generalize

Rewrite in vector form

Vector of derivatives is

$$\cdot \dot{y} =$$

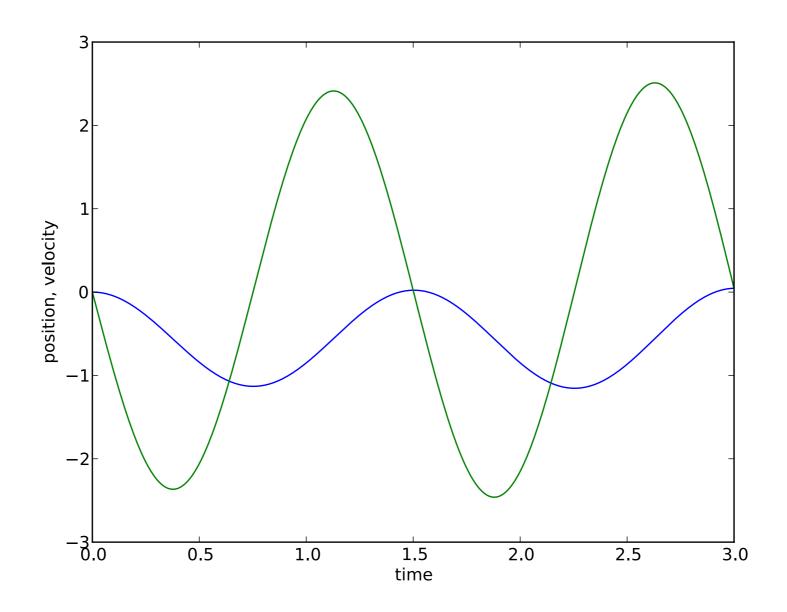
Euler solution

•
$$y_{i+1} =$$

See notebok for implementation

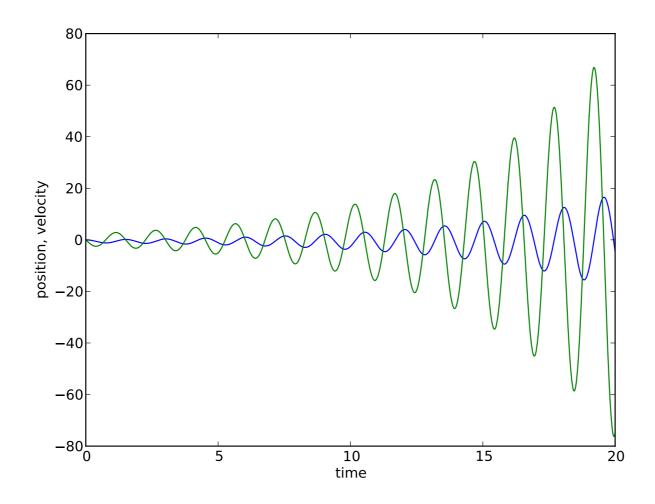
Solutions

- Example:
 - Mass on a vertical spring
 - *F* =



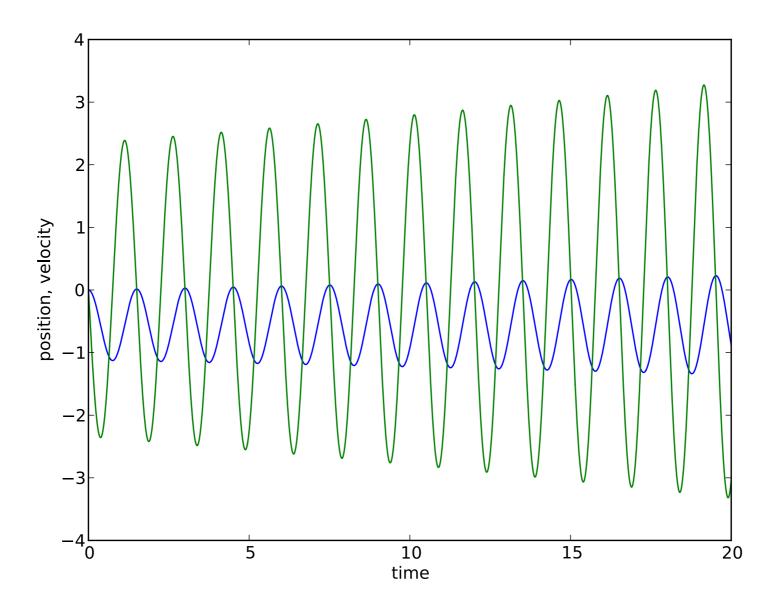
Problems

- Euler method
 - Energy is



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

Problems



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

Euler-Cromer Method

- Trick that works for (SHO)
 - Replace derivative with derivative

$$\bullet y_{i+1} = y_i + \dot{y}_{i+1} \Delta t$$

• Not a , so we need to do better

 $g_a \equiv$

Runge-Kutta Methods

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

Apply the chain rule

$$\ddot{y} =$$

$$g_{ab} \equiv$$

Runge-Kutta Methods

- Similarly,
 - ÿ =
 - 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:

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

+

Compare to an alternative polynomial expansion:

•
$$y(t + \Delta t) =$$

Runge-Kutta Methods

- Polynomials:
 - $k_1 =$
 - $k_2 =$
 - $k_3 =$
 - •
 - $k_n =$
- Coefficients and are determined by against Taylor expansion
 - Determined by
 - i.e. order RK, order RK, etc

2nd order RK

$$y(t + \Delta t) =$$

•

$$k_2 =$$

• =

• Follows:

•
$$y(t + \Delta t) =$$

•
$$\alpha_1 + \alpha_2 =$$

•
$$\alpha_1 v_{21} =$$

2nd order RK

- Standard solution:
 - $v_{21} =$
 - $\alpha_1 = \alpha_2 =$
 - $y(t + \Delta t) =$
 - $k_1 =$
 - $k_2 =$

4th Order RK

•
$$y(t + \Delta t) =$$

$$+ O(\Delta t^4)$$

•
$$k_1 =$$

$$\bullet k_2 =$$

•
$$k_3 =$$

•
$$k_4 =$$

- 4th order RK is a
 - good trade off between

and

Runge-Kutta Illustration

