

A system of first-order ODEs can be solved by any of the methods

· Care must be taking to ensure the proper copying all the solutions.

· When predictor - corrector or Runge-Kutta methods are used, each

step must be applied to all the equations before proceeding to the

5+1

n+>

X(4)

X (+)

· The step-size must be the same for all of the equations.

Ś

n-1

A system of first-order ODEs

developed for solving single ODEs.

next step.

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## **Higher-order ODEs**

- In the first part we considered solutions of first-order ordinary differential equations by finite difference methods.
- Many problems in physics are governed by higher-order ODEs. The second-order ODEs are most common ODEs.
- In general, a higher-order ODE can be replaced by a system of firstorder ODEs.

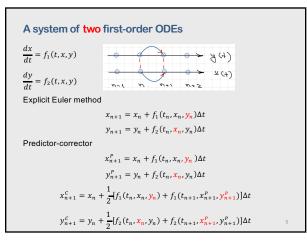
Example: Newton's second law provides us with equation of motion

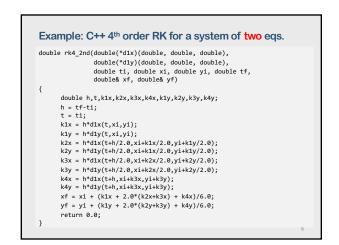
$$\frac{d^2x}{dt^2} = f\left(t, x, \frac{dx}{dt}\right)$$

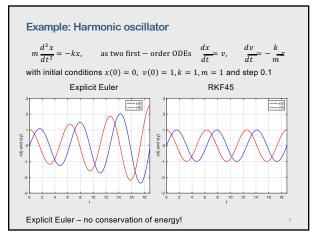
Introducing dx/dt = v, we get a system of two first-order ODEs

$$\frac{dx}{dt} = v, \qquad \frac{dv}{dt} = f(t, x, v)$$

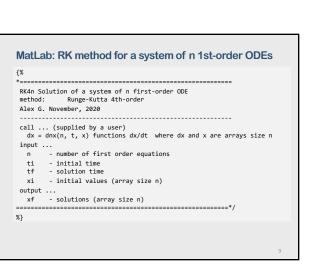
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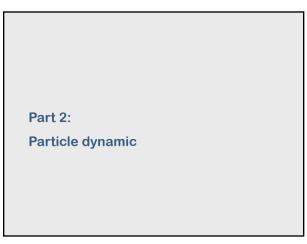


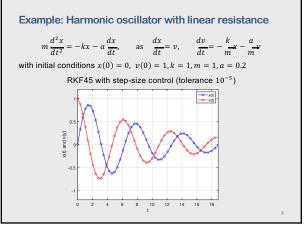


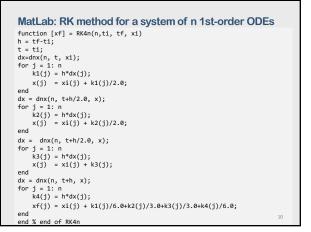




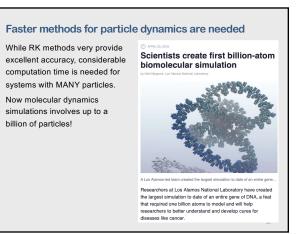


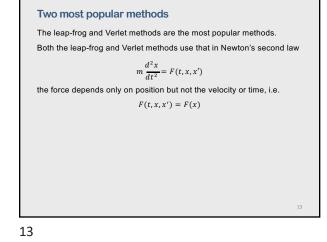


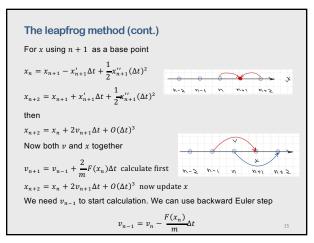


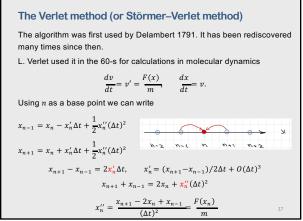


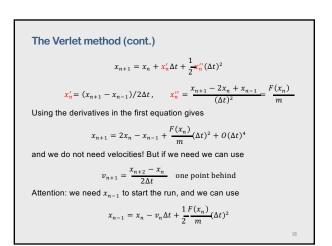












# The leapfrog method - summary

The leapfrog method

Consider Newton's second law

Using n as a base point we can write

then taking the difference  $v_{n+1} - v_{n-1}$  gives

- The leapfrog method is a second-order method
- It is conditionally stable, as long as the time-step  $\Delta t$  is constant

 $\frac{dv}{dt} = v' = \frac{F(x)}{m}, \qquad \frac{dx}{dt} = v.$ 

 $v_{n+1} = v_n + v'_n \Delta t + \frac{1}{2} v''_n (\Delta t)^2$   $v_{n+1} = v_n + v'_n \Delta t + \frac{1}{2} v''_n (\Delta t)^2$   $v_{n+1} = v_n + v'_n \Delta t + \frac{1}{2} v''_n (\Delta t)^2$   $v_{n+1} = v_n + v'_n \Delta t + \frac{1}{2} v''_n (\Delta t)^2$ 

 $v_{n+1} = v_{n-1} + 2v'_n \Delta t + O(\Delta t)^3$  $v_{n+1} = v_{n-1} + \frac{2}{m} F(x_n) \Delta t$ 

- It conserves (mostly) the energy of dynamical systems in a long run. This is especially useful when computing orbital dynamics, as many other integration schemes, such as 4<sup>th</sup> order Runge-Kutta method, do not conserve energy and allow the system to drift substantially over time.
- The method is time-reversible, i.e. one can integrate forward n steps, and then reverse the direction of integration and integrate backwards n steps to arrive at the same starting position.
- · There are a couple variations of the method.

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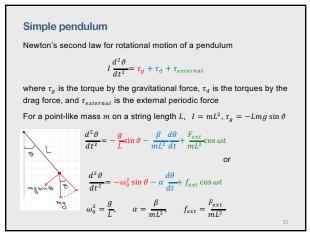
# The Verlet method- summary

- Global errors: for  $x \sim O(\Delta t)^3$ , for  $v \sim O(\Delta t)^2$
- The method is very popular in computing trajectories in molecular dynamics simulations
- · The Verlet method provides good numerical stability
- · The method is time-reversible
- There is a velocity Verlet version similar to the leapfrog method.



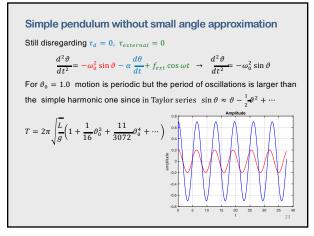
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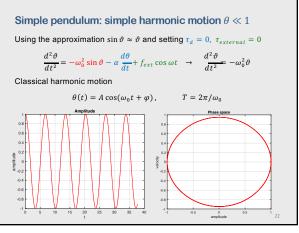
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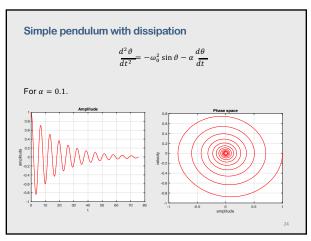


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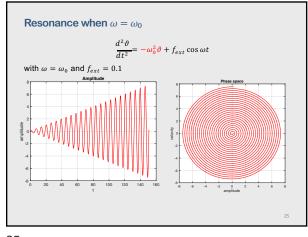
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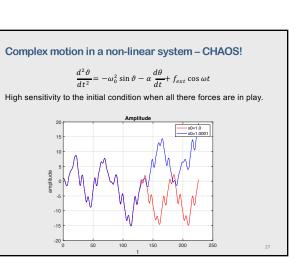








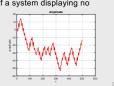


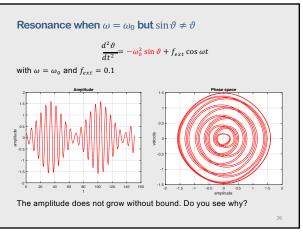




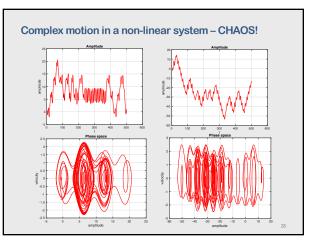
- A chaotic system is one with an extremely high sensitivity to parameters or initial conditions
- The sensitivity to even miniscule changes is so high that, in practice, it is impossible to predict the long range behavior unless the parameters are known to infinite precision (which they never are in practice)
- Chaotic motion is not random
- Chaos is the deterministic behavior of a system displaying no
  discernable regularity

 Note: a double pendulum is a good system to study chaos





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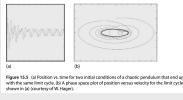
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# Chaotic structure in phase space

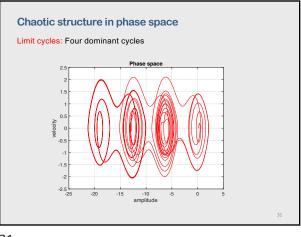
# Limit cycles

When a chaotic pendulum is driven by a not-too-large driving torque, it is possible to pick the magnitude for this torque such that after the initial transients die off, the average energy put into the system during one period exactly balances the average energy dissipated by friction during that period.

This leads to *limit cycles* that appear as closed ellipse-like figures. (Yet unstable solutions may make sporadic jumps between limit cycles.)



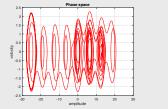
\* from Landau et al. Computational Physics (2015)



#### Chaotic structure in phase space

### Strange attractors

Well-defined, yet complicated, semi-periodic behaviors that appear to be uncorrelated with the motion at an earlier time. They are distinguished from predictable attractors by being fractal chaotic, and highly sensitive to the initial conditions. Even after millions of oscillations, the motion remains attracted to them.

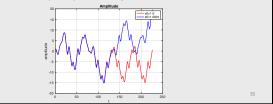


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### **Butterfly effect**

One of the classic remarks about the hypersensitivity of chaotic systems to the initial conditions is that the weather pattern in North America is hard to predict well because it is sensitive to the flapping of butterfly wings in South America.

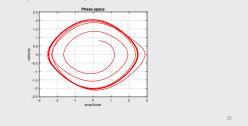
Although this appears to be counterintuitive because we know that systems with essentially identical initial conditions should behave the same, eventually the systems diverge.



# Chaotic structure in phase space

#### Predictable attractors

There are orbits, such as fixed points and limit cycles, into which the system settles or returns to often, and that are not particularly sensitive to initial conditions. If your location in phase space is near a predictable attractor, ensuing times will bring you to it.



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#### Chaotic structure in phase space

#### Chaotic paths

Regions of phase space that appear as filled-in bands rather than lines. Continuity within the bands implies complicated behaviors, yet still with simple underlying structure.

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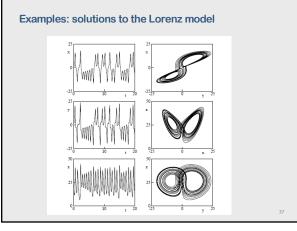
#### The Lorenz model

In 1962 Lorenz was looking for a simple model for weather predictions and simplified the heat-transport equations to the three equations.

 $\frac{dx}{dt} = 10(y - x)$  $\frac{dy}{dt} = -xz + 28x - y$ 

$$\frac{dz}{dt} = xy - \frac{8}{3}z$$

The solution of these simple nonlinear equations gave the complicated behavior that has led to the modern interest in chaos!





How can we quantify this lack of predictably?

This divergence of the trajectories can be described by the Lyapunov exponent  $\lambda,$  which is defined by the relation

 $|\Delta x_n| = |\Delta x_0| e^{\lambda_n}$ 

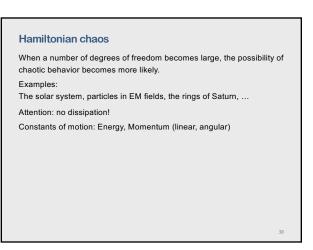
where  $\Delta x_n$  is the difference between the trajectories at time n. If the Lyapunov exponent  $\lambda$  is positive, then nearby trajectories diverge exponentially.

Chaotic behavior is characterized by the exponential divergence of nearby trajectories.

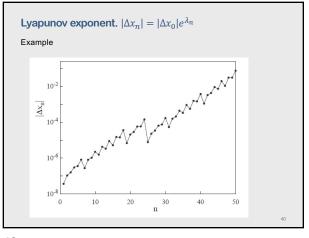
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# "Control your chaos" from the movie - The Witcher

- The dream of classical physics was that if the initial conditions and all the forces acting on a system were known, then we could predict the future with as much precision as we desire.
- · The existence of chaos has shattered that dream.
- However, if a system is chaotic, we can still control its behavior with small, but carefully chosen, perturbations of the system.
- Good illustration can be found in Gould et all, Computer simulation methods. Application to physical systems (2007)



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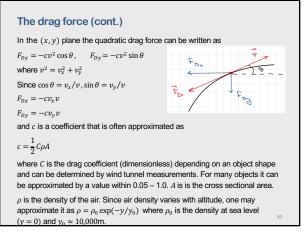
Part 3a: Projectile motion

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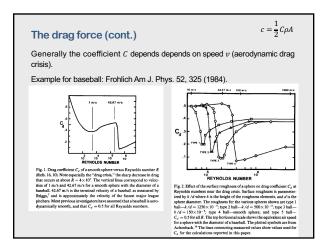
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# **2D** (2-dimensional) projectile motion Forces: gravity, drag force and potentially magnus force (spin related) $m \frac{d^2x}{dt^2} = F_{Dx}$ or $\frac{dx}{dt} = v_x$ , $m \frac{dv_x}{dt} = F_{Dx}(v_x, v_y)$ $m \frac{d^2y}{dt^2} = -mg + F_{Dy}$ or $\frac{dy}{dt} = v_y$ , $m \frac{dv_y}{dt} = -mg + F_{Dy}(v_x, v_y)$ Initial value problem: $x(0) = x_0$ , $x'(0) = v_x(0) = v_{x0}$ $y(0) = y_0$ , $y'(0) = v_y(0) = v_{y0}$ The system of two second-order ODEs can be rewritten as a system of four first-order ODEs. All the methods studied before for solving first-order ODEs can be used here.

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# The drag force

The drag force  $\vec{F}_D$  and the velocity  $\vec{v}$  point in opposite directions

 $\vec{F}_D = -f(v)\hat{v},$ 

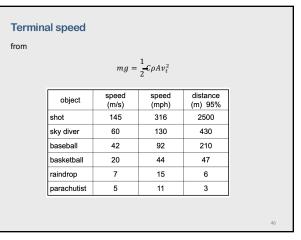
where  $\hat{v}$  is the unit vector in the direction of velocity, and f(v) is the magnitude of the drug force.

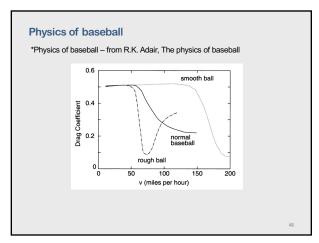
The function f(v) that give the magnitude of the air resistance varies with v in a complicated way, however often it can be well approximated as<sup>\*</sup>

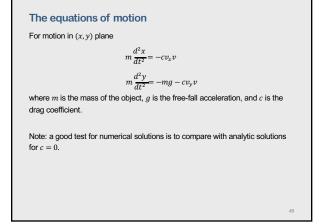
$$f(v) = bc + cv^2 = f_{lin} + f_{quad}$$

In many practical cases we will work with the quadratic drag component The physical origin of the terms: The linear term corresponds to the viscosity drag of the medium. The quadratic term describes the acceleration of the mass of air pushed by the projectile. \*for more details see Classical mechanics by J.R Taylor (Chapter 2)

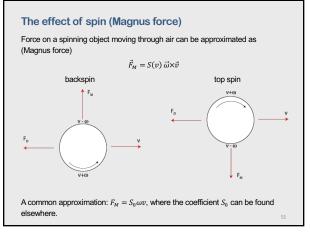
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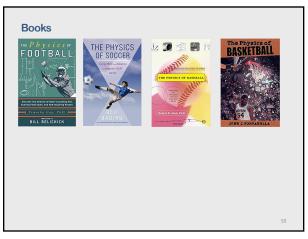


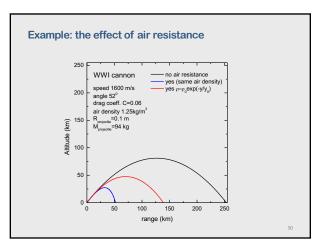


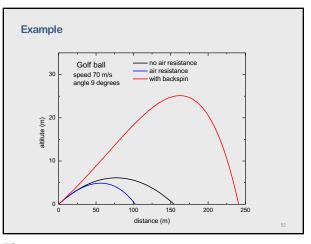




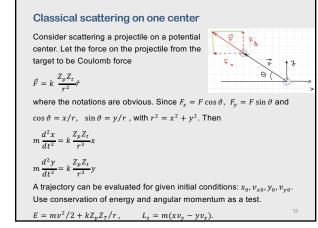




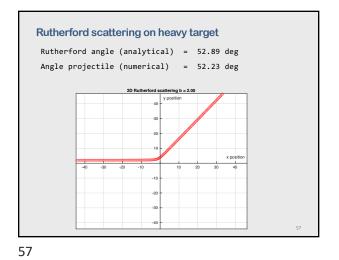


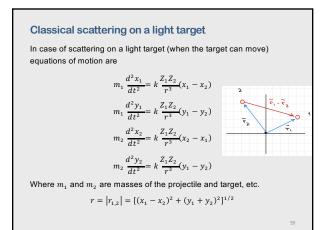


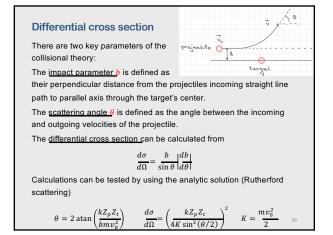
Part 3b: Classical scattering

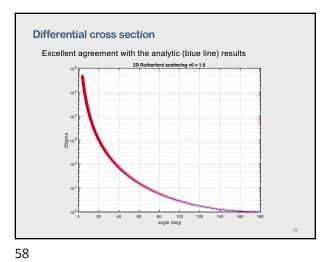








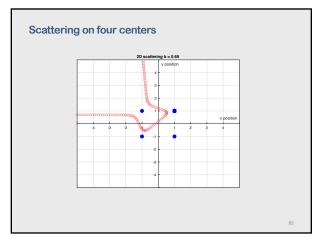




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Scattering on two centers (or more centers) Let a projectile (particle 1) scatters on two centers (2 and 3)  $m_1 \frac{d^2 x_1}{dt^2} = k \frac{Z_1 Z_2}{r_{1,2}^3} (x_1 - x_2) + k \frac{Z_1 Z_3}{r_{1,3}^3} (x_1 - x_3)$   $m_1 \frac{d^2 y_1}{dt^2} = k \frac{Z_1 Z_2}{r_{1,2}^3} (y_1 - y_2) + k \frac{Z_1 Z_3}{r_{1,3}^3} (y_1 - y_3)$ 



Newton's universal law of gravitation states that a particle of mass M

 $\vec{F} = -G \, \frac{mM}{r^3} \hat{r}$  where the vector  $\hat{r}$  is directed from *M* to *m*. The negative sign in implies that the gravitational force is attractive. And *G* is the gravitational

attracts another particle of mass m with a force given by

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# Properties of the gravitational force

1. Central force

The gravitational force has two general properties: its magnitude depends only on the separation of the particles, and its direction is along the line joining the particles. Such a force is called a central force. The assumption of a central force implies that the orbit of the Earth (if *m* is Earth and *M* is the Sun) is restricted to a plane (x, y), and the angular momentum is conserved

 $L_z = m(xy_y - yv_x)$ 

2. Total energy is conserved

$$E = \frac{1}{2}mv^2 - G\frac{mM}{r}$$

# Equations of motion

тM

**Gravitational force** 

constant.

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If we fix the coordinate system at the mass M, the equation of motion of of mass m is

$$m\frac{d^2\vec{r}}{dt^2} = -G\frac{mM}{r^3}\hat{r}$$

It is convenient to write the forces and equations of motion in Cartesian coordinates with  $r^2=x^2+y^2$ 

$$\begin{aligned} & \frac{1}{r_x} = -G \frac{mM}{r^2} \cos \vartheta = -G \frac{mM}{r^3} x \\ & \frac{1}{r_y} = -G \frac{mM}{r^2} \sin \vartheta = -G \frac{mM}{r^3} y \\ & \frac{d^2 x}{dt^2} = -G \frac{M}{r^3} x \\ & \frac{d^2 y}{dt^2} = -G \frac{M}{r^3} y \end{aligned}$$

mM

