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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

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

Introducing $d x / d t=v$, we get a system of two first-order ODEs
$\frac{d x}{d t}=v, \quad \frac{d v}{d t}=f(t, x, v)$

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## A system of two first-order ODEs

$$
\begin{aligned}
& \begin{array}{l}
\frac{d x}{d t}=f_{1}(t, x, y) \\
\frac{d y}{d t}=f_{2}(t, x, y) \\
\text { Explicit Euler method } \\
\\
\qquad \begin{array}{l}
x_{n+1}=x_{n}+f_{1}\left(t_{n}, x_{n}, y_{n}\right) \Delta t \\
y_{n+1}=y_{n}+f_{2}\left(t_{n}, x_{n}, y_{n}\right) \Delta t
\end{array} \\
\text { Predictor-corrector } \\
\qquad x_{n+1}^{P}=x_{n}+f_{1}\left(t_{n}, x_{n}, y_{n}\right) \Delta t
\end{array} \\
& \qquad y_{n+1}^{P}=y_{n}+f_{2}\left(t_{n}, x_{n}, y_{n}\right) \Delta t
\end{aligned}
$$

## Part 1:

## Second-order ODEs

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## A system of first-order ODEs

A system of first-order ODEs can be solved by any of the methods developed for solving single ODEs.

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


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## Example: C++ $4^{\text {th }}$ order RK for a system of two eqs.

```
double rk4_2nd(double(*d1x)(double, double, double),
        double(*d1y)(double, double, double),
        double ti, double xi, double yi, double tf,
        double& xf, double& yf)
{
    double h,t,k1x,k2x,k3x,k4x,k1y,k2y,k3y,k4y;
    h = tf-ti;
    t = ti;
    k1x = h*d1x(t,xi,yi);
    k1y = h*d1y(t,xi,yi);
    k2x = h*d1x(t+h/2.0,xi+k1x/2.0,yi+k1y/2.0);
    k2y = h*d1y(t+h/2.0,xi+k1x/2.0,yi+k1y/2.0);
    k3x = h*d1x(t+h/2.0,xi+k2x/2.0,yi+k2y/2.0);
    k3y = h*d1y(t+h/2.0,xi+k2x/2.0,yi+k2y/2.0);
    k4x = h*d1x(t+h,xi+k3x,yi+k3y);
    k4y = h*d1y(t+h,xi+k3x,yi+k3y);
    xf = xi + (k1x + 2.0*(k2x+k3x) + k4x)/6.0;
    yf=yi + (k1y + 2.0*(k2y+k3y) + k4y)/6.0;
    return 0.0;
}
```

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| Example: Harmonic oscillator <br> $m \frac{d^{2} x}{d t^{2}}=-k x, \quad$ as two first - order ODEs $\quad \frac{d x}{d t}=v, \quad \frac{d v}{d t}=-\frac{k}{m} x$ with initial conditions $x(0)=0, v(0)=1, k=1, m=1$ and step 0.1 <br> Explicit Euler <br> RKF45 |  |  |  |  |  |  |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  |  |  |  |  |  |  |  |  |  |  |  |  |
|  |  |  |  |  |  |  |  |  |  |  |  |  |
|   <br> Explicit Euler - no conservation of energy! |  |  |  |  |  |  |  |  |  |  |  |  |
|  |  |  |  |  |  |  |  |  |  |  |  |  |
|  |  |  |  |  |  |  |  |  |  |  |  |  |
|  |  |  |  |  |  |  |  |  |  |  |  |  |

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MatLab: RK method for a system of n 1 1st-order ODEs
个\%
RK4n Solution of a system of $n$ first-order ODE
method: Runge-Kutta 4th-order
Alex G. November, 2020
call ... (supplied by a user)
$d x=d n x(n, t, x)$ functions $d x / d t$ where $d x$ and $x$ are arrays size $n$ input ...
n - number of first order equations
ti - initial time

- solution time
- initial values (array size n)
output ..
xf - solutions (array size $n$ )
\%==

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MatLab: RK method for a system of $\mathbf{n}$ 1st-order ODEs
function $[x f]=\operatorname{RK} 4 n(n, t i, t f, x i)$
$\mathrm{h}=\mathrm{tf}-\mathrm{ti} ;$
$\mathrm{t}=\mathrm{ti} ;$
$t=\operatorname{tn} ;(n, t, x i)$
$d x=\ln$
for $\mathrm{j}=1$ : $n$
$\mathrm{k} 1(\mathrm{j})=h^{*} \mathrm{dx}(\mathrm{j})$;
$x(j)=x i(j)+k 1(j) / 2.0 ;$
end
$\mathrm{dx}=\mathrm{dnx}(\mathrm{n}, \mathrm{t}+\mathrm{h} / 2.0, \mathrm{x})$;
for $\mathrm{j}=1$ : n
$x(j)=x i(j)+k 2(j) / 2.0 ;$
end
$d x=d n x(n, t+h / 2.0, x)$
$d x=\operatorname{dnx}(n, n$
for $j=1$ : $n$
$\mathrm{k} 3(\mathrm{j})=\mathrm{h} * \mathrm{dx}(\mathrm{j})$;
$x(j)=x i(j)+k 3(j) ;$
end
$\mathrm{dx}=$
$d x=\operatorname{dnx}(n, t+h, x)$;
or $j=1$ : n
$x f(j)=x i(j)+k 1(j) / 6.0+k 2(j) / 3.0+k 3(j) / 3.0+k 4(j) / 6.0 ;$
end
end \% end of RK4n
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## Part 2:

## Particle dynamic

Faster methods for particle dynamics are needed
While RK methods very provide excellent accuracy, considerable computation time is needed for systems with MANY particles
Now molecular dynamics simulations involves up to a billion of particles!

Scientists create first billion-atom biomolecular simulation


A Los Alamos leod team created the largess simulation to dotato of an entire geno. Researchers at Los Alamos National Laboratory have created
the largest simulation to date of an entire gene of DNA, a feat that required one billion atoms to model and will help researchers to better understand and develop cures for diseases like cancer.

## Two most popular methods

The leap-frog and Verlet methods are the most popular methods. Both the leap-frog and Verlet methods use that in Newton's second law

$$
m \frac{d^{2} x}{d t^{2}}=F\left(t, x, x^{\prime}\right)
$$

the force depends only on position but not the velocity or time, i.e.

$$
F\left(t, x, x^{\prime}\right)=F(x)
$$

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## The leapfrog method (cont.)

For $x$ using $n+1$ as a base point
$x_{n}=x_{n+1}-x_{n+1}^{\prime} \Delta t+\frac{1}{2} x_{n+1}^{\prime \prime}(\Delta t)^{2}$
$x_{n+2}=x_{n+1}+x_{n+1}^{\prime} \Delta t+\frac{1}{2} x_{n+1}^{\prime \prime}(\Delta t)^{2}$
then
$x_{n+2}=x_{n}+2 v_{n+1} \Delta t+O(\Delta t)^{3}$
Now both $v$ and $x$ together
$v_{n+1}=v_{n-1}+\frac{2}{m} F\left(x_{n}\right) \Delta t$ calculate first
$x_{n+2}=x_{n}+2 v_{n+1} \Delta t+O(\Delta t)^{3}$ now update $x$
We need $v_{n-1}$ to start calculation. We can use backward Euler step

$$
v_{n-1}=v_{n}-\frac{F\left(x_{n}\right)}{m} \Delta t
$$

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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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## Simple pendulum

Newton's second law for rotational motion of a pendulum

$$
I \frac{d^{2} \vartheta}{d t^{2}}=\tau_{g}+\tau_{d}+\tau_{\text {external }}
$$

where $\tau_{g}$ is the torque by the gravitational force, $\tau_{d}$ is the torques by the drag force, and $\tau_{\text {external }}$ is the external periodic force
For a point-like mass $m$ on a string length $L, I=m L^{2}, \tau_{g}=-L m g \sin \vartheta$


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Simple pendulum without small angle approximation
Still disregarding $\tau_{d}=0, \tau_{\text {external }}=0$

$$
\frac{d^{2} \vartheta}{d t^{2}}=-\omega_{0}^{2} \sin \vartheta-\alpha \frac{d \theta}{d t}+f_{\text {ext }} \cos \omega t \rightarrow \frac{d^{2} \vartheta}{d t^{2}}=-\omega_{0}^{2} \sin \vartheta
$$

For $\vartheta_{0}=1.0$ motion is periodic but the period of oscillations is larger than

$$
\text { the simple harmonic one since in Taylor series } \sin \vartheta \approx \vartheta-\frac{1}{2} \boldsymbol{q}^{2}+\cdots
$$

$$
T=2 \pi \sqrt{\frac{L}{g}}\left(1+\frac{1}{16} \vartheta_{0}^{2}+\frac{11}{3072} \vartheta_{0}^{4}+\cdots\right)
$$



## Part 3a:

Oscillatory motion and chaos

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Simple pendulum: simple harmonic motion $\theta \ll 1$
Using the approximation $\sin \vartheta \approx \vartheta$ and setting $\tau_{d}=0, \tau_{\text {external }}=0$

$$
\frac{d^{2} \vartheta}{d t^{2}}=-\omega_{0}^{2} \sin \vartheta-\alpha \frac{d \theta}{d t}+f_{\text {ext }} \cos \omega t \rightarrow \frac{d^{2} \vartheta}{d t^{2}}=-\omega_{0}^{2} \vartheta
$$

Classical harmonic motion


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## Simple pendulum with dissipation

$$
\frac{d^{2} \vartheta}{d t^{2}}=-\omega_{0}^{2} \sin \vartheta-\alpha \frac{d \theta}{d t}
$$





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Complex motion in a non-linear system - CHAOS!

$$
\frac{d^{2} \vartheta}{d t^{2}}=-\omega_{0}^{2} \sin \vartheta-\alpha \frac{d \theta}{d t}+f_{\text {ext }} \cos \omega t
$$

High sensitivity to the initial condition when all there forces are in play.


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## Complex motion in a non-linear system - CHAOS!

- 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



## 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.)



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## 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.

## 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.


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## 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.

## 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.

$$
\begin{gathered}
\frac{d x}{d t}=10(y-x) \\
\frac{d y}{d t}=-x z+28 x-y \\
\frac{d z}{d t}=x y-\frac{8}{3} z
\end{gathered}
$$

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


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## Lyapunov exponent

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

$$
\left|\Delta x_{n}\right|=\left|\Delta x_{0}\right| e^{\lambda_{n}}
$$

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)


## Hamiltonian chaos

When a number of degrees of freedom becomes large, the possibility of chaotic behavior becomes more likely.
Examples:
The solar system, particles in EM fields, the rings of Saturn, ...
Attention: no dissipation
Constants of motion: Energy, Momentum (linear, angular)

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Part 3a:
Projectile motion

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## 2D (2-dimensional) projectile motion

Forces: gravity, drag force and potentially magnus force (spin related)

$$
\begin{array}{llll}
m \frac{d^{2} x}{d t^{2}}=F_{D x} & \text { or } & \frac{d x}{d t}=v_{x}, & m \frac{d v_{x}}{d t}=F_{D x}\left(v_{x}, v_{y}\right) \\
m \frac{d^{2} y}{d t^{2}}=-m g+F_{D y} & \text { or } & \frac{d y}{d t}=v_{y}, & m \frac{d v_{y}}{d t}=-m g+F_{D y}\left(v_{x}, v_{y}\right)
\end{array}
$$

Initial value problem:

$$
\begin{array}{ll}
x(0)=x_{0}, & x^{\prime}(0)=v_{x}(0)=v_{x 0} \\
y(0)=y_{0}, & y^{\prime}(0)=v_{y}(0)=v_{y 0}
\end{array}
$$

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 (cont.)

In the $(x, y)$ plane the quadratic drag force can be written as
$F_{D x}=-c v^{2} \cos \theta, \quad F_{D y}=-c v^{2} \sin \theta$
where $v^{2}=v_{x}^{2}+v_{y}^{2}$
Since $\cos \theta=v_{x} / v, \sin \theta=v_{y} / v$
$F_{D x}=-c v_{x} v$
$F_{D y}=-c v_{y} v$
and $c$ is a coefficient that is often approximated as
$c=\frac{1}{2} C \rho A$
where $C$ is the drag coefficient (dimensionless) depending on an object shape and can be determined by wind tunnel measurements. For many objects it can be approximated by a value within $0.05-1.0$. $A$ is is the cross sectional area.
$\rho$ is the density of the air. Since air density varies with altitude, one may approximate it as $\rho=\rho_{0} \exp \left(-y / y_{0}\right)$ where $\rho_{0}$ is the density at sea level $(y=0)$ and $y_{0} \approx 10,000 \mathrm{~m}$.

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## Terminal speed

$$
m g=\frac{1}{2} \epsilon \rho A v_{t}^{2}
$$

| object | speed <br> $(\mathrm{m} / \mathrm{s})$ | speed <br> $(\mathrm{mph})$ | distance <br> $(\mathrm{m}) 95 \%$ |
| :--- | :---: | :---: | :---: |
| shot | 145 | 316 | 2500 |
| sky diver | 60 | 130 | 430 |
| baseball | 42 | 92 | 210 |
| basketball | 20 | 44 | 47 |
| raindrop | 7 | 15 | 6 |
| parachutist | 5 | 11 | 3 |

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*

$$
f(v)=b c+c v^{2}=f_{\text {lin }}+f_{\text {quad }}
$$

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)

## from

## Physics of baseball

*Physics of baseball - from R.K. Adair, The physics of baseball



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The effect of spin (Magnus force)
Force on a spinning object moving through air can be approximated as (Magnus force)


A common approximation: $F_{M}=S_{0} \omega v$, where the coefficient $S_{0}$ can be found elsewhere.

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## Example: the effect of air resistance



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## Example



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## Part 3b:

Classical scattering


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| Rutherford angle (analytical) | $=52.89 \mathrm{deg}$ |
| ---: | :--- |
| Angle projectile (numerical) | $=52.23 \mathrm{deg}$ |



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## Classical scattering on a light target

In case of scattering on a light target (when the target can move) equations of motion are

$$
\begin{aligned}
& m_{1} \frac{d^{2} x_{1}}{d t^{2}}=k \frac{Z_{1} Z_{2}}{r^{3}}\left(x_{1}-x_{2}\right) \\
& m_{1} \frac{d^{2} y_{1}}{d t^{2}}=k \frac{Z_{1} Z_{2}}{r^{3}}\left(y_{1}-y_{2}\right) \\
& m_{2} \frac{d^{2} x_{2}}{d t^{2}}=k \frac{Z_{1} Z_{2}}{r^{3}}\left(x_{2}-x_{1}\right) \\
& m_{2} \frac{d^{2} y_{2}}{d t^{2}}=k \frac{Z_{1} Z_{2}}{r^{3}}\left(y_{1}-y_{2}\right)
\end{aligned}
$$

Where $m_{1}$ and $m_{2}$ are masses of the projectile and target, etc.

$$
r=\left|r_{1,2}\right|=\left[\left(x_{1}-x_{2}\right)^{2}+\left(y_{1}+y_{2}\right)^{2}\right]^{1 / 2}
$$


their perpendicular distance from the projectiles incoming straight line path to parallel axis through the target's center.
The scattering angle $\theta$ is defined as the angle between the incoming and outgoing velocities of the projectile.
The differential cross section can be calculated from

$$
\frac{d \sigma}{d \Omega}=\frac{b}{\sin \theta}\left|\frac{d b}{d \theta}\right|
$$

Calculations can be tested by using the analytic solution (Rutherford scattering)

$$
\theta=2 \operatorname{atan}\left(\frac{k Z_{p} Z_{t}}{b m v_{0}^{2}}\right) \quad \frac{d \sigma}{d \Omega}=\left(\frac{k Z_{p} Z_{t}}{4 K \sin ^{2}(\theta / 2)}\right)^{2} \quad K=\frac{m v_{0}^{2}}{2} \quad 56
$$

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## Scattering on light target (recoil)



$$
\begin{aligned}
& m_{1} \frac{d^{2} x_{1}}{d t^{2}}=k \frac{Z_{1} Z_{2}}{r_{1,2}^{3}}\left(x_{1}-x_{2}\right)+k \frac{Z_{1} Z_{3}}{r_{1,3}^{3}}\left(x_{1}-x_{3}\right) \\
& m_{1} \frac{d^{2} y_{1}}{d t^{2}}=k \frac{Z_{1} Z_{2}}{r_{1,2}^{3}}\left(y_{1}-y_{2}\right)+k \frac{Z_{1} Z_{3}}{r_{1,3}^{3}}\left(y_{1}-y_{3}\right)
\end{aligned}
$$

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## Gravitational force

Newton's universal law of gravitation states that a particle of mass $M$ attracts another particle of mass $m$ with a force given by

$$
\vec{F}=-G \frac{m M}{r^{3}} \hat{r}
$$

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 constant.
$\mu$


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## Equations of motion

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

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

It is convenient to write the forces and equations of motion in Cartesian coordinates with $r^{2}=x^{2}+y^{2}$
$F_{x}=-G \frac{m M}{r^{2}} \cos \vartheta=-G \frac{m M}{r^{3}} x$
$F_{y}=-G \frac{m M}{r^{2}} \sin \vartheta=-G \frac{m M}{r^{3}} y$
$\frac{d^{2} x}{d t^{2}}=-G \frac{M}{r^{3}} x$
$\frac{d^{2} y}{d t^{2}}=-G \frac{M}{r^{3}} y$
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Examples: Apollo 13 (the mission to the Moon)
simulation


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