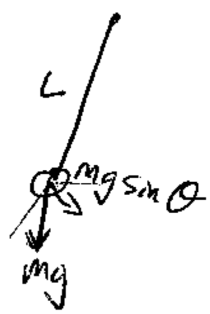
Solving Differential Equations on the Computer
Accuracy, Fidelity, & Stability

Ordinary Differential Equations (ODEs): $y(t)$

$$\boxed{dy/dt = f(y,t)}$$

Exponential decay $\frac{dy}{dt} = -Ay \quad (y = e^{-At})$

Pendulum: $\vec{F} = ma \Rightarrow a = \frac{d^2\theta}{dt^2} = -\frac{g}{L}\sin\theta$



<u>Trick</u>: Split second order $\frac{d^2\theta}{dt^2}$ into two first-order

$$\frac{d\theta}{dt} = v$$

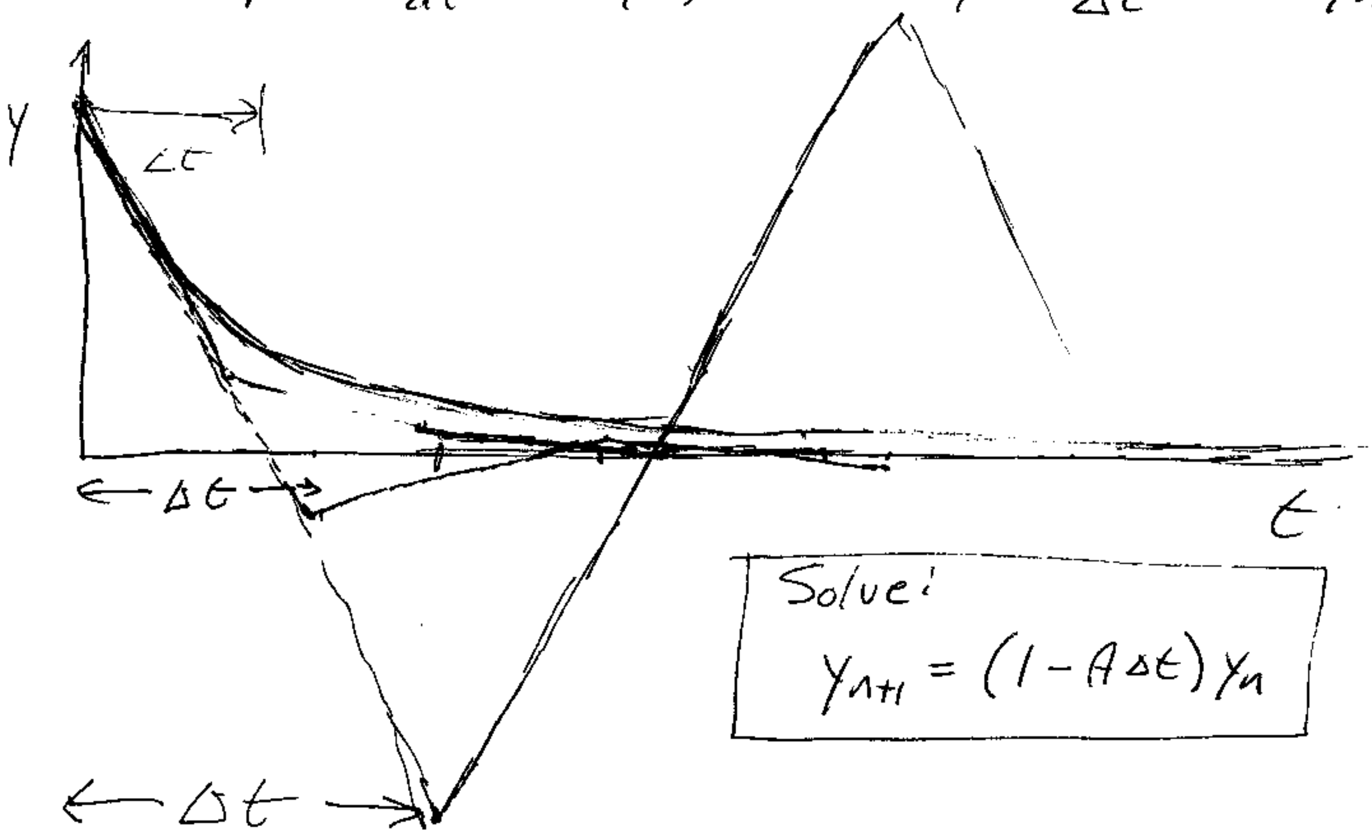
$$\frac{dv}{dt} = -\frac{g}{L}\sin\theta$$

Evolve $\vec{y} = (\theta, v)$

Molecular dynamics $\vec{a} = F/m$ 3-N vectors...
N atoms $\vec{y} = (\vec{x}, \vec{v})$

Must <u>discretize</u>: solve at times $t_n = n\,\Delta t$ for y_n.

Example: $\frac{dy}{dt} = -Ay$, Euler step $\frac{y_{n+1} - y_n}{\Delta t} = -Ay_n$



Solve:

$$\boxed{y_{n+1} = (1 - A\Delta t)\,y_n}$$

<u>Accuracy</u>: $e^{-A\Delta t}y_n \approx (1 - A\Delta t)\,y_n + \underbrace{\frac{(A\Delta t)^2}{2!}y_n}_{\text{Error}} + \ldots$

Error in one time step $= \frac{A\Delta t^2}{2}y_n \sim \mathcal{O}(\Delta t^2)$

Error in interval $T = N\Delta t \sim N\Delta t^2 \sim \left(\frac{T}{\Delta t}\right)\Delta t^2 \sim O(\Delta t)$

<u>Fidelity</u>: If $\Delta t > 1/A$, goes <u>negative</u> (unphysical!)

<u>Stability</u>: If $\Delta t > 2/A$, blows up

Pendulum Module

Accuracy, Fidelity, Stability
for Hamiltonian system
(Conserves energy, no attractors, ...)

- Fidelity $\Leftrightarrow$ Algorithms that conserve an approximate energy (Verlet)

- Goes unstable before accuracy seriously problem
- Illustrates use of ODE solver

Walker module

- ODE solver

- Human locomotion, biomechanics (Walks by itself; thought needed only to steer, minimal energy expenditure)

- Events (Heel strikes)

Molecular Dynamics, Cardiac Dynamics (PDE)

More later