Simulation in Computer Graphics

Particles

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Outline

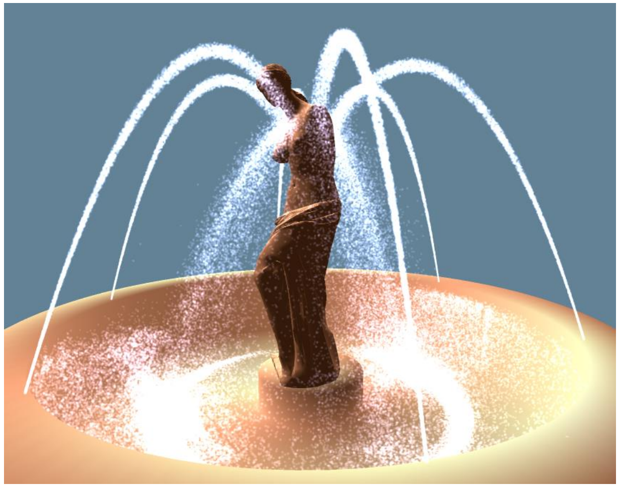
- introduction
- particle motion
- finite differences
- system of first order ODEs
- second order ODE

Motivation

- sets of particles (particle systems) are used to model time-dependent phenomena such as snow, fire, smoke

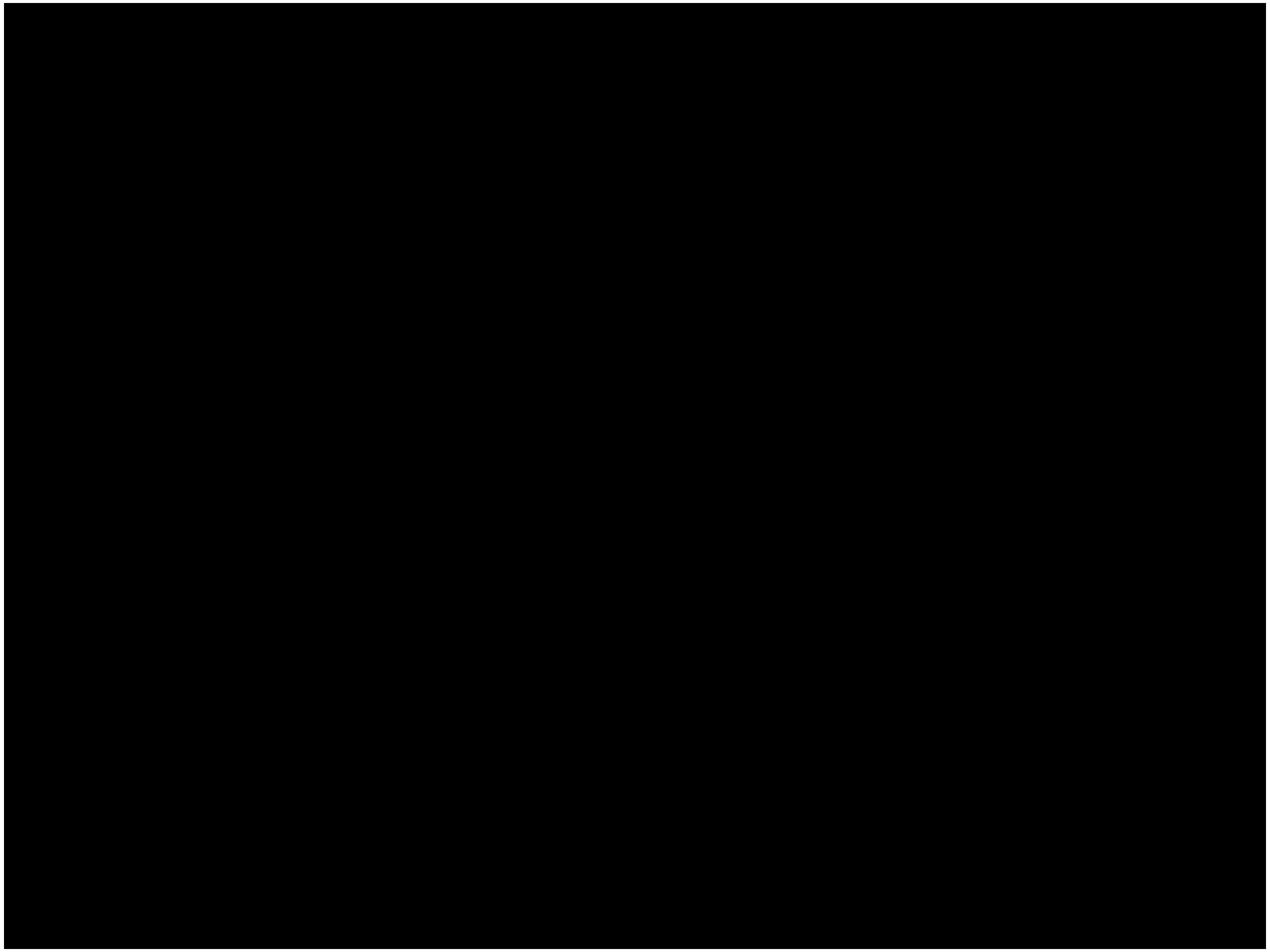
Motivation

- particles are characterized by mass, position and velocity
- forces determine the dynamic behavior
- inter-particle forces are neglected
- particles can carry arbitrary attributes for rendering purposes, e.g., shape, color, transparency, life time



Kolb, Latta, Rezk-Salama

Demo



750,000 particles in XNA,
http://www.youtube.com/watch?v=CyAZ2Y7nOTw

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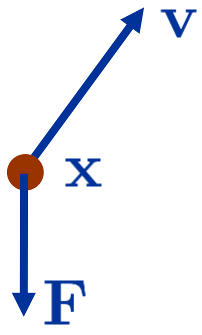
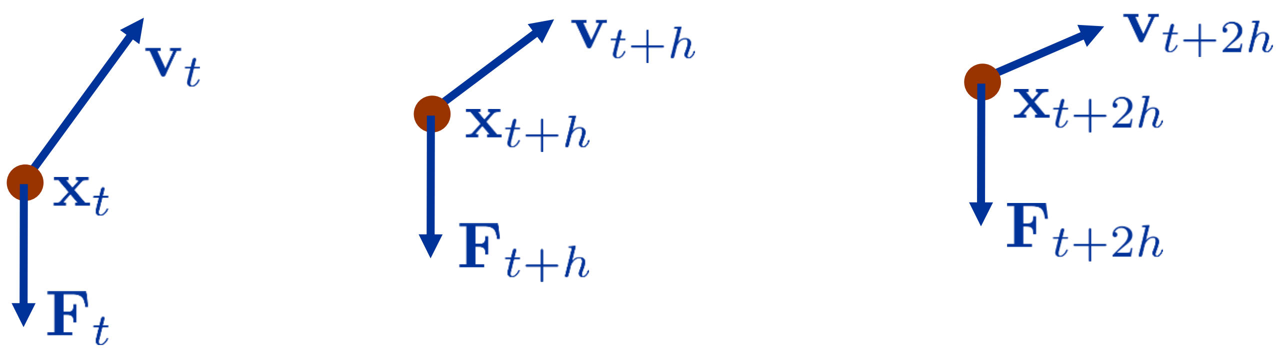
Particle Quantities

- quantities relevant for the motion of a particle:
  - mass $m \in \mathbb{R}$
  - position $\mathbf{x} \in \mathbb{R}^3$
  - velocity $\mathbf{v} \in \mathbb{R}^3$
  - force $\mathbf{F} \in \mathbb{R}^3$ acting on the particle
  - force $\mathbf{F}$ generally depends on position and velocity



Particle Motion

- quantities are considered at discrete time points



- particle simulations are concerned with the computation of unknown future particle quantities $\mathbf{x}_{t+h}, \mathbf{v}_{t+h}$ using known current information $\mathbf{x}_t, \mathbf{v}_t, \mathbf{F}_t$

Governing Equation

- Newton’s Second Law, Newton's motion equation, motion equation of a particle
- the force acting on an object is equal to the rate of change of its momentum

$$\mathbf{F}_t = \frac{d}{dt}(m\mathbf{v}_t) = \frac{dm}{dt}\mathbf{v}_t + m\frac{d\mathbf{v}_t}{dt}$$

- constant mass

$$\mathbf{F}_t = m\frac{d\mathbf{v}_t}{dt} = m\frac{d^2\mathbf{x}_t}{dt^2}$$

Governing Equation

- $\mathbf{F}_t = m \frac{d^2 \mathbf{x}_t}{dt^2}$ is an ordinary differential equation ODE
- describes the behavior of $\mathbf{x}_t$ in terms of its derivatives with respect to time
- numerical integration can be employed to numerically solve the ODE, i.e. to approximate the unknown function $\mathbf{x}_t$

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Governing Equation

- initial value problem of second order

$$\frac{d^2\mathbf{x}_t}{dt^2} = \frac{1}{m}\mathbf{F}_t \qquad \mathbf{x}_{t_0} = \mathbf{x}_0 \quad \frac{d\mathbf{x}_{t_0}}{dt} = \mathbf{v}_0$$

- second-order ODEs can be rewritten as a system of two coupled equations of first order
- initial value problem of first order

$$\frac{d\mathbf{x}_t}{dt} = \mathbf{v}_t \qquad \mathbf{x}_{t_0} = \mathbf{x}_0$$

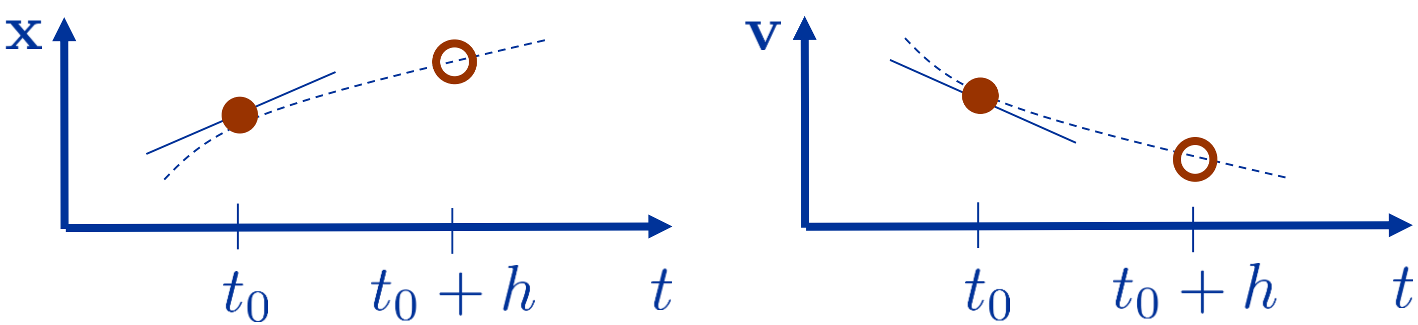
$$\frac{d\mathbf{v}_t}{dt} = \frac{1}{m}\mathbf{F}_t \qquad \mathbf{v}_{t_0} = \mathbf{v}_0$$

Initial Value Problem of First Order

- functions $\mathbf{x}_t, \mathbf{v}_t$ represent the particle motion
- initial values are given $\mathbf{x}_{t_0}, \mathbf{v}_{t_0}$
- first-order differential equations are given

$$\frac{d\mathbf{x}_t}{dt} = \mathbf{v}_t \qquad \frac{d\mathbf{v}_t}{dt} = \frac{1}{m}\mathbf{F}_t$$

- the functions and their first derivatives are known at t_0
- how to compute $\mathbf{x}_{t_0+h}, \mathbf{v}_{t_0+h}$



Forces

- generally depend on positions and velocities
  - friction / fluid viscosity depend on velocities
  - spring forces, shear, stretch depend on positions
  - contact handling forces depend
    on positions and velocities
- can be arbitrarily expensive to compute
  - consider one particle (particle system) or
    sets of particles (deformables, fluids)
  - require additional effort, e.g., contact handling forces
    - detect collisions of particles with obstacles
    - compute penalty force from penetration depth

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Finite Differences

- Taylor-series approximation

$$\mathbf{x}_{t+h} = \mathbf{x}_t + \frac{d\mathbf{x}_t}{dt} h + O(h^2)$$

$O(h^2)$ – truncation or discretization error

$$\frac{d\mathbf{x}_t}{dt} = \frac{\mathbf{x}_{t+h} - \mathbf{x}_t}{h} + O(h)$$

$O(h)$ – error order of, e.g., a scheme that employs such approximation

- continuous ODEs are replaced with discrete finite-difference equations FDEs

$$\frac{d\mathbf{x}_t}{dt} = \mathbf{v}_t \quad \Rightarrow \quad \frac{\mathbf{x}_{t+h} - \mathbf{x}_t}{h} = \mathbf{v}_t$$

$$\frac{d\mathbf{v}_t}{dt} = \frac{1}{m}\mathbf{F}_t \quad \Rightarrow \quad \frac{\mathbf{v}_{t+h} - \mathbf{v}_t}{h} = \frac{1}{m}\mathbf{F}_t$$

Finite Differences

- polynomial fitting (line fitting in case of one sample)

$$\mathbf{x}_t = \mathbf{a}t + \mathbf{b}$$

$$\Rightarrow \frac{d\mathbf{x}_t}{dt} = \mathbf{a} \qquad \Rightarrow \mathbf{b} = \mathbf{x}_t - \frac{d\mathbf{x}_t}{dt}t$$

$$\mathbf{x}_{t+h} = \frac{d\mathbf{x}_t}{dt}(t+h) + \mathbf{x}_t - \frac{d\mathbf{x}_t}{dt}t$$

which results in

$$\frac{d\mathbf{x}_t}{dt} = \frac{\mathbf{x}_{t+h} - \mathbf{x}_t}{h} + O(h)$$

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Euler Method

$$\frac{d\mathbf{x}_t}{dt} = \dot{\mathbf{x}} = \mathbf{v}_t \qquad \frac{d\mathbf{v}_t}{dt} = \dot{\mathbf{v}} = \frac{1}{m}\mathbf{F}_t$$

- initialize $\mathbf{x}_{t_0} = \mathbf{x}_0,\ \mathbf{v}_{t_0} = \mathbf{v}_0,\ \mathbf{F}_{t_0},\ m,\ h$
- numerical integration of position and velocity

$$\mathbf{x}_{t_0+h} = \mathbf{x}_{t_0} + h\dot{\mathbf{x}}_{t_0} = \mathbf{x}_{t_0} + h\mathbf{v}_{t_0}$$

$$\mathbf{v}_{t_0+h} = \mathbf{v}_{t_0} + h\dot{\mathbf{v}}_{t_0} = \mathbf{v}_{t_0} + h\frac{1}{m}\mathbf{F}_{t_0}$$

Coupled Equations

- Euler step from t_0 to $t_0 + h$

$$\mathbf{x}_{t_0+h} = \mathbf{x}_{t_0} + h\mathbf{v}_{t_0}$$

$$\mathbf{v}_{t_0+h} = \mathbf{v}_{t_0} + h\frac{1}{m}\mathbf{F}_{t_0}(\mathbf{x}_{t_0}, \mathbf{v}_{t_0})$$

- Euler step from $t_0 + h$ to $t_0 + 2h$

$$\mathbf{x}_{t_0+2h} = \mathbf{x}_{t_0+h} + h\mathbf{v}_{t_0+h}$$

$$\mathbf{v}_{t_0+2h} = \mathbf{v}_{t_0+h} + h\frac{1}{m}\mathbf{F}_{t_0+h}(\mathbf{x}_{t_0+h}, \mathbf{v}_{t_0+h})$$

- the position update depends on velocity
- the velocity update depends on position and velocity

Accuracy and Stability

- discretization error is defined as the difference between the solution of the ODE and the solution of the FDE
- the FDE is consistent, if the discretization error vanishes if the time step h approaches zero
- the FDE is stable, if previously introduced errors (discretization, round-off) do not grow within a simulation step
- the FDE is convergent, if the solution of the FDE approaches the solution of the ODE

Accuracy and Stability

- although the discretization error is diminished by smaller time steps in consistent schemes, the discretization error is introduced in each step of the FD scheme
- if previously introduced discretization errors are not amplified by the FD scheme, then it is stable
- consistent and stable schemes are convergent

Stability

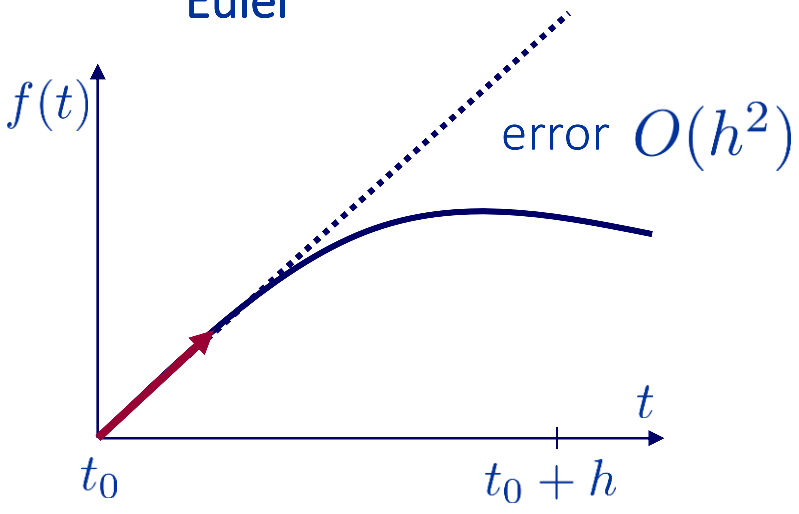
- if stability is influenced by the time step, the FD scheme is conditionally stable
- if the FD scheme is stable or unstable for arbitrary time steps, it is unconditionally stable or unstable
- ODE, FDE and the parameters influence the stability of a system
- schemes with improved stability work with larger time steps

Time Step

- larger time steps typically speed up a simulation
- smaller time steps can improve the stability
- arbitrarily small time steps are not feasible due to round-off errors
  - for larger time steps, the error is dominated by the discretization error
  - for smaller time steps, the error is dominated by round-off errors
- performance of an FD scheme is trade-off between error order in terms of the time step and computing complexity

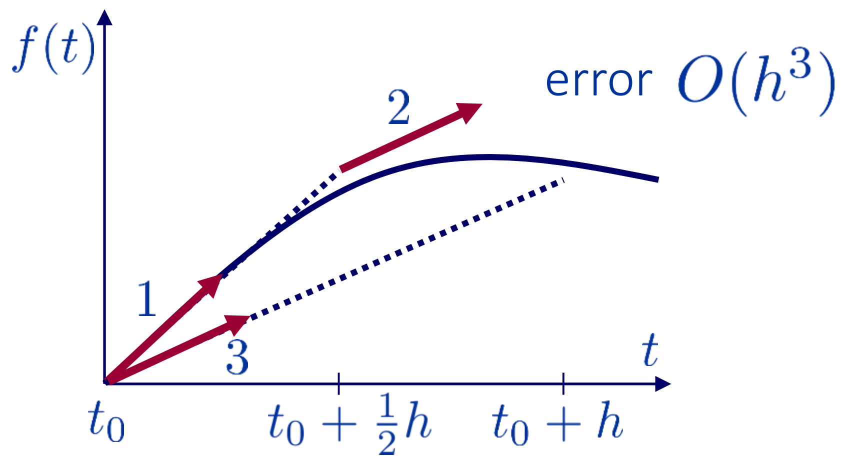
Second-Order Runge-Kutta
Midpoint Method

Euler



- compute the derivative at t_0
- **approximate $f(t_0 + h)$ using the derivative at t_0**

Midpoint Method



- compute the derivative at t_0
- compute $f(t_0 + h/2)$
- compute the derivative at $t_0 + h/2$
- **approximate $f(t_0 + h)$ using the derivative at $t_0 + h/2$**

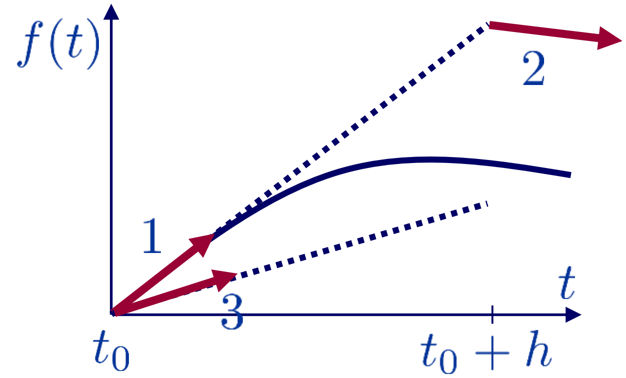
Second-Order Runge-Kutta Midpoint Method

$$\dot{\mathbf{x}} = \mathbf{v}_t \qquad \dot{\mathbf{v}}_{\mathbf{x}_t,\mathbf{v}_t} = \frac{1}{m}\mathbf{F}_{\mathbf{x}_t,\mathbf{v}_t}$$

- compute **x**’*(t)*
- compute **v**’*(t)*
- compute **x**’*(t+h/2)*
- compute **v**’*(t+h/2)* with **x***(t+h/2)* and **v***(t+h/2)*
- compute **x***(t+h)* with **x**’*(t+h/2)*
- compute **v***(t+h)* with **v**’*(t+h/2)*

$$\begin{aligned}
\mathbf{k}_1 &= \dot{\mathbf{x}}_t \\
\mathbf{l}_1 &= \dot{\mathbf{v}}_{\mathbf{x}_t,\mathbf{v}_t} \\
\mathbf{k}_2 &= \dot{\mathbf{x}}_t + \mathbf{l}_1 \frac{h}{2} \\
\mathbf{l}_2 &= \dot{\mathbf{v}}_{\mathbf{x}_t+\mathbf{k}_1\frac{h}{2},\mathbf{k}_2} \\
\mathbf{x}_{t+h} &= \mathbf{x}_t + h\mathbf{k}_2 \\
\mathbf{v}_{t+h} &= \mathbf{v}_t + h\mathbf{l}_2
\end{aligned}$$

Second-Order Runge-Kutta Heun

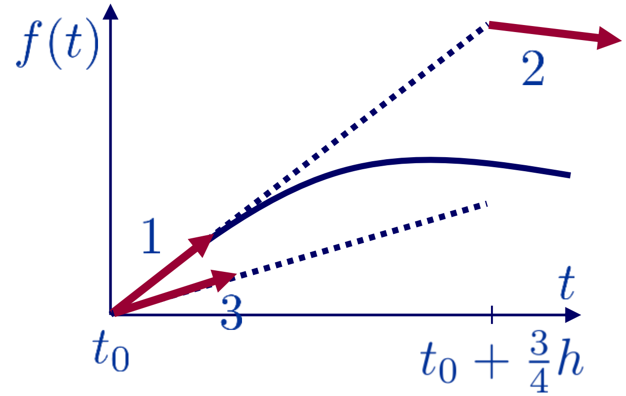


$$\dot{\mathbf{x}} = \mathbf{v}_t \qquad \dot{\mathbf{v}}_{\mathbf{x}_t,\mathbf{v}_t} = \frac{1}{m}\mathbf{F}_{\mathbf{x}_t,\mathbf{v}_t}$$

- compute **x**' *(t)*
- compute **v**' *(t)*
- compute **x**' *(t+h)*
- compute **v**' *(t+h)*
- c. **x** *(t+h)* with **x**' *(t)* and **x**' *(t+h)*
- c. **v** *(t+h)* with **v**' *(t)* and **v**' *(t+h)*

$$\begin{aligned}
\mathbf{k}_1 &= \dot{\mathbf{x}}_t \\
\mathbf{l}_1 &= \dot{\mathbf{v}}_{\mathbf{x}_t,\mathbf{v}_t} \\
\mathbf{k}_2 &= \dot{\mathbf{x}}_t + \mathbf{l}_1 h \\
\mathbf{l}_2 &= \dot{\mathbf{v}}_{\mathbf{x}_t+\mathbf{k}_1 h,\mathbf{k}_2} \\
\mathbf{x}_{t+h} &= \mathbf{x}_t + h(\frac{1}{2}\mathbf{k}_1 + \frac{1}{2}\mathbf{k}_2) \\
\mathbf{v}_{t+h} &= \mathbf{v}_t + h(\frac{1}{2}\mathbf{l}_1 + \frac{1}{2}\mathbf{l}_2)
\end{aligned}$$

Second-Order Runge-Kutta Ralston Method



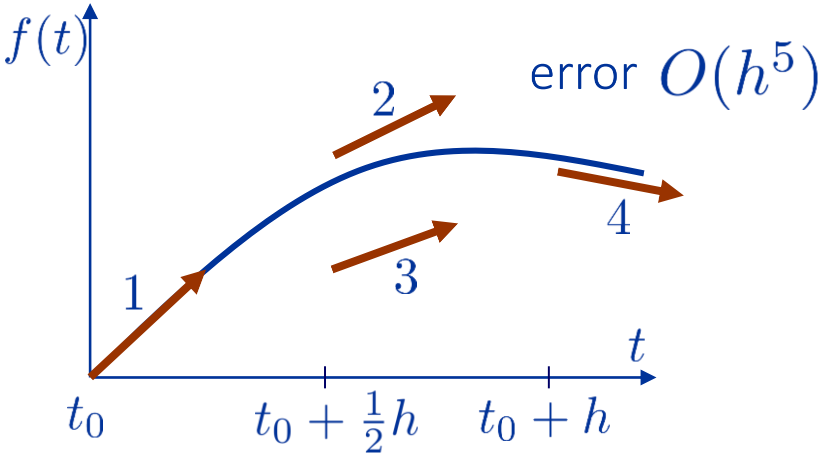
$$\dot{\mathbf{x}} = \mathbf{v}_t \qquad \dot{\mathbf{v}}_{\mathbf{x}_t,\mathbf{v}_t} = \frac{1}{m}\mathbf{F}_{\mathbf{x}_t,\mathbf{v}_t}$$

- compute **x**'*(t)*
- compute **v**'*(t)*
- compute **x**'*(t+3h/4)*
- compute **v**'*(t+3h/4)* with **x***(t+3h/4)* and **v***(t+3h/4)*
- c. **x***(t+h)* with **x**'*(t)* and **x**'*(t+3h/4)*
- c. **v***(t+h)* with **v**'*(t)* and **v**'*(t+3h/4)*

$$\begin{aligned}
\mathbf{k}_1 &= \dot{\mathbf{x}}_t \\
\mathbf{l}_1 &= \dot{\mathbf{v}}_{\mathbf{x}_t,\mathbf{v}_t} \\
\mathbf{k}_2 &= \dot{\mathbf{x}}_t + \mathbf{l}_1 \frac{3}{4} h \\
\mathbf{l}_2 &= \dot{\mathbf{v}}_{\mathbf{x}_t + \mathbf{k}_1 \frac{3}{4} h, \mathbf{k}_2} \\
\mathbf{x}_{t+h} &= \mathbf{x}_t + h\left(\frac{1}{3}\mathbf{k}_1 + \frac{2}{3}\mathbf{k}_2\right) \\
\mathbf{v}_{t+h} &= \mathbf{v}_t + h\left(\frac{1}{3}\mathbf{l}_1 + \frac{2}{3}\mathbf{l}_2\right)
\end{aligned}$$

Fourth-Order Runge-Kutta
Runge

- compute $f'(t_0)$ (1)
- compute $f(t_0+h/2)$
  with $f(t_0)$ and $f'(t_0)$
- compute $f'(t_0+h/2)$ (2)
- compute $f(t_0+h/2)$
  with $f(t_0)$ and $f'(t_0+h/2)$
- compute $f'(t_0+h/2)$ (3)
- compute $f(t_0+h)$
  with $f(t_0)$ and $f'(t_0+h/2)$
- compute $f'(t_0+h)$ (4)
- compute $f(t_0+h)$ with $f(t_0)$ and a
  weighted average of all derivatives (1) – (4)



Fourth-Order Runge-Kutta
Runge

- four derivative computations per time step
- error $O(h^5)$

$$\begin{aligned}\mathbf{k}_1 &= \dot{\mathbf{x}}_t \\ \mathbf{l}_1 &= \dot{\mathbf{v}}_{\mathbf{x}_t,\mathbf{v}_t} \\ \mathbf{k}_2 &= \dot{\mathbf{x}}_t + \mathbf{l}_1 \frac{1}{2} h \\ \mathbf{l}_2 &= \dot{\mathbf{v}}_{\mathbf{x}_t + \mathbf{k}_1 \frac{1}{2} h, \mathbf{k}_2}\end{aligned}$$

$$\begin{aligned}\mathbf{k}_3 &= \dot{\mathbf{x}}_t + \mathbf{l}_2 \frac{1}{2} h \\ \mathbf{l}_3 &= \dot{\mathbf{v}}_{\mathbf{x}_t + \mathbf{k}_2 \frac{1}{2} h, \mathbf{k}_3} \\ \mathbf{k}_4 &= \dot{\mathbf{x}}_t + \mathbf{l}_3 h \\ \mathbf{l}_4 &= \dot{\mathbf{v}}_{\mathbf{x}_t + \mathbf{k}_3 h, \mathbf{k}_4}\end{aligned}$$

$$\begin{aligned}\mathbf{x}_{t+h} &= \mathbf{x}_t + h \frac{1}{6} (\mathbf{k}_1 + 2\mathbf{k}_2 + 2\mathbf{k}_3 + \mathbf{k}_4) \\ \mathbf{v}_{t+h} &= \mathbf{v}_t + h \frac{1}{6} (\mathbf{l}_1 + 2\mathbf{l}_2 + 2\mathbf{l}_3 + \mathbf{l}_4)\end{aligned}$$

Fourth-Order Runge-Kutta

Kutta

- four derivative computations per time step
- error $O(h^5)$

$$\mathbf{k}_1 = \dot{\mathbf{x}}_t$$

$$\mathbf{l}_1 = \dot{\mathbf{v}}_{\mathbf{x}_t,\mathbf{v}_t}$$

$$\mathbf{k}_2 = \dot{\mathbf{x}}_t + \mathbf{l}_1 \frac{1}{3} h$$

$$\mathbf{l}_2 = \dot{\mathbf{v}}_{\mathbf{x}_t + \mathbf{k}_1 \frac{1}{3} h, \mathbf{k}_2}$$

$$\mathbf{k}_3 = \dot{\mathbf{x}}_t + (-\frac{1}{2}\mathbf{l}_1 + \frac{3}{2}\mathbf{l}_2)\frac{2}{3} h$$

$$\mathbf{l}_3 = \dot{\mathbf{v}}_{\mathbf{x}_t + (-\frac{1}{2}\mathbf{k}_1 + \frac{3}{2}\mathbf{k}_2)\frac{2}{3} h, \mathbf{k}_3}$$

$$\mathbf{k}_4 = \dot{\mathbf{x}}_t + (\mathbf{l}_1 - \mathbf{l}_2 + \mathbf{l}_3) h$$

$$\mathbf{l}_4 = \dot{\mathbf{v}}_{\mathbf{x}_t + (\mathbf{k}_1 - \mathbf{k}_2 + \mathbf{k}_3) h, \mathbf{k}_4}$$

$$\mathbf{x}_{t+h} = \mathbf{x}_t + h\frac{1}{8}(\mathbf{k}_1 + 3\mathbf{k}_2 + 3\mathbf{k}_3 + \mathbf{k}_4)$$

$$\mathbf{v}_{t+h} = \mathbf{v}_t + h\frac{1}{8}(\mathbf{l}_1 + 3\mathbf{l}_2 + 3\mathbf{l}_3 + \mathbf{l}_4)$$

Performance

Euler	Runge-Kutta
• **one** computation of the derivative per time step • error $O(h^2)$	• **two (four)** computations of the derivative per time step • error $O(h^3), O(h^5)$ • allows larger time steps

- similar performance if the time step for RK 2 is twice the time step for Euler
- Does RK allow for faster simulations than Euler?

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Implementation

- Euler
  - one function evaluation
  - force computation
  - position and velocity update
- Runge-Kutta
  - multiple function evaluations
  - computation of auxiliary forces, positions, velocities
    - once for second order
    - three times for fourth order
  - position and velocity update

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Predictor-Corrector Methods

- predict a value from current (and previous) derivatives
- correct the predicted value with its derivative
- second-order Adams-Bashforth predictor

$$f_{t+h} = f_t + h\tfrac{1}{2}(3\dot{f}_t - \dot{f}_{t-h}) + O(h^3)$$

- second-order Adams-Moulton corrector

$$f_{t+h} = f_t + h\tfrac{1}{2}(3\dot{f}_{t+h} - \dot{f}_t) + O(h^3)$$

- based on Lagrange polynomials or Taylor approximations
- can be efficiently implemented with
  two derivative computations per simulation step
- requires values at previous time steps,
  not self-starting

Adams-Bashforth Predictors

$$
\begin{aligned}
f_{t+h} &= f_t + h\dot{f}_t + O(h^2) \\
f_{t+h} &= f_t + h\frac{1}{2}(3\dot{f}_t - \dot{f}_{t-h}) + O(h^3) \\
f_{t+h} &= f_t + h\frac{1}{12}(23\dot{f}_t - 16\dot{f}_{t-h} + 5\dot{f}_{t-2h}) + O(h^4) \\
f_{t+h} &= f_t + h\frac{1}{24}(55\dot{f}_t - 59\dot{f}_{t-h} + 37\dot{f}_{t-2h} - 9\dot{f}_{t-3h}) + O(h^5) \\
f_{t+h} &= f_t + h\frac{1}{720}(1901\dot{f}_t - 2774\dot{f}_{t-h} + 2616\dot{f}_{t-2h} - 1274\dot{f}_{t-3h} + 251\dot{f}_{t-4h}) \\
&\quad + O(h^6) \\
&\ldots
\end{aligned}
$$

Adams-Moulton Correctors

$$
\begin{aligned}
f_{t+h} &= f_t + h\dot{f}_{t+h} + O(h^2) \\
f_{t+h} &= f_t + h\frac{1}{2}(\dot{f}_{t+h} + \dot{f}_t) + O(h^3) \\
f_{t+h} &= f_t + h\frac{1}{12}(5\dot{f}_{t+h} + 8\dot{f}_t - \dot{f}_{t-h}) + O(h^4) \\
f_{t+h} &= f_t + h\frac{1}{24}(9\dot{f}_{t+h} + 19\dot{f}_t - 5\dot{f}_{t-h} + \dot{f}_{t-2h}) + O(h^5) \\
f_{t+h} &= f_t + h\frac{1}{720}(251\dot{f}_{t+h} + 646\dot{f}_t - 264\dot{f}_{t-h} + 106\dot{f}_{t-2h} - 19\dot{f}_{t-3h}) \\
&\quad + O(h^6) \\
&\quad \ldots
\end{aligned}
$$

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Explicit and Implicit Integration

explicit Euler

$$\mathbf{x}_{t+h} = \mathbf{x}_t + h\mathbf{v}_t$$

$$\mathbf{v}_{t+h} = \mathbf{v}_t + h\frac{1}{m}\mathbf{F}_t$$

- one unknown per equation
- direct calculation of **x**_(t+h)_ and **v**_(t+h)_
- non-linear equations have no effect on the approach
- can handle non-analytical, procedural forces

implicit Euler

$$\mathbf{x}_{t+h} = \mathbf{x}_t + h\mathbf{v}_{t+h}$$

$$\mathbf{v}_{t+h} = \mathbf{v}_t + h\frac{1}{m}\mathbf{F}_{t+h}$$

- system of algebraic equations with many unknowns
- simultaneous computation of **x**_(t+h)_ and **v**_(t+h)_
- solution of a system of equations
- non-linear equations are commonly linearized to get a system of linear equations

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Linearization of Scalar Functions

- one-dimensional scalar field

$$f_{x+h} = f_x + h\dot{f}_x + O(h^2)$$

- multi-dimensional scalar field

$$f_{\mathbf{x}+\mathbf{h}} = f_{\mathbf{x}} + \mathbf{h} \cdot \operatorname{grad} f_{\mathbf{x}} + O(\|\mathbf{h}\|^2)$$

- gradient

$$\operatorname{grad} f_{\mathbf{x}} = \nabla f_{\mathbf{x}} = \left(\frac{\partial f_{\mathbf{x}}}{\partial x_1}, \frac{\partial f_{\mathbf{x}}}{\partial x_2}, \ldots, \frac{\partial f_{\mathbf{x}}}{\partial x_n} \right)^{\mathrm{T}}$$

- nabla, del

$$\nabla = \left(\frac{\partial}{\partial x_1}, \frac{\partial}{\partial x_2}, \ldots, \frac{\partial}{\partial x_n} \right)^{\mathrm{T}}$$

Linearization of Vector Fields

- multi-dimensional vector field

$$\mathbf{F}_{\mathbf{x}+\mathbf{h}} = \mathbf{F}_{\mathbf{x}} + \mathbf{J}_{\mathbf{F}_{\mathbf{x}}}\mathbf{h} + O(\|\mathbf{h}\|^2)$$

- Jacobi matrix

$$\mathbf{J}_{\mathbf{F}_{vx}} = \frac{\partial \mathbf{F}_{\mathbf{x}}}{\partial \mathbf{x}} = \begin{pmatrix} \text{grad}^{\mathrm{T}}\ F_{1,\mathbf{x}} \\ \cdots \\ \text{grad}^{\mathrm{T}}\ F_{m,\mathbf{x}} \end{pmatrix} = \begin{pmatrix} \frac{\partial F_{1,\mathbf{x}}}{\partial x_1} & \cdots & \frac{\partial F_{1,\mathbf{x}}}{\partial x_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial F_{m,\mathbf{x}}}{\partial x_1} & \cdots & \frac{\partial F_{m,\mathbf{x}}}{\partial x_n} \end{pmatrix}$$

Implicit Integration
Theta Scheme

- general form

$$\mathbf{x}_{t+h} = \mathbf{x}_t + h((1-\theta)\mathbf{v}_t + \theta \mathbf{v}_{t+h})$$

$$\mathbf{v}_{t+h} = \mathbf{v}_t + h((1-\theta)\frac{\mathbf{F}_t}{m} + \theta \frac{\mathbf{F}_{t+h}}{m})$$

- explicit Euler $\theta = 0$
- implicit Euler $\theta = 1$
- Crank Nicolson $\theta = 0.5$

Theta Scheme
Example Implementation

- rewriting the problem for $\theta = 0.5$

$$m\mathbf{v}_{t+h} = m\mathbf{v}_t + \frac{h}{2}(\mathbf{F}_{\mathbf{x}_t} + \mathbf{F}_{\mathbf{x}_{t+h}})$$

In this example, force **F** depends on **x**, not on **v**.

- force linearization

$$\mathbf{F}_{\mathbf{x}_{t+h}} = \mathbf{F}_{\mathbf{x}_t + \frac{h}{2}(\mathbf{v}_t + \mathbf{v}_{t+h})} \approx \mathbf{F}_{\mathbf{x}_t} + \frac{\partial \mathbf{F}_{\mathbf{x}_t}}{\partial \mathbf{x}} \cdot \frac{h}{2} \cdot (\mathbf{v}_t + \mathbf{v}_{t+h})$$

- solving a linear system for $\mathbf{v}_{t+h}$

$$\left[m\mathbf{I} - \frac{h^2}{4} \cdot \frac{\partial \mathbf{F}_{\mathbf{x}_t}}{\partial \mathbf{x}}\right] \cdot \mathbf{v}_{t+h} \approx m \cdot \mathbf{v}_t + h \cdot \mathbf{F}_{\mathbf{x}_t} + \frac{\partial \mathbf{F}_{\mathbf{x}_t}}{\partial \mathbf{x}} \cdot \frac{h^2}{4}\mathbf{v}_t$$

Theta Scheme
Conjugate Gradient

- linear system $\mathbf{A} \cdot \mathbf{v} = \mathbf{b}$

- gradient of a function $\nabla \mathbf{f}(\mathbf{v}) = \mathbf{A} \cdot \mathbf{v} - \mathbf{b}$

  with $\nabla \mathbf{f}(\mathbf{v}) = \mathbf{0}$

- iterative solution for $\mathbf{v}$ with initial value $\mathbf{v}_0$

$$\mathbf{v}_{i+1} = \mathbf{v}_i + \alpha \cdot \mathbf{w}(\nabla \mathbf{f}(\mathbf{v}_i))$$

Conjugate Gradient Method

- $\mathbf{v}_0 = \mathbf{v}(t)$
- direction $\mathbf{d}$
- residual $\mathbf{r}$
- step size α
- $\mathbf{v}(t+h) = \mathbf{v}_i$

- $\mathbf{A}$ is symmetric, positive-definite
- $-\mathbf{r}_0$, $-\mathbf{d}_0$ gradient of function $\mathbf{f}$
- $\mathbf{d}_i$, $\mathbf{d}_j$ are conjugate, i.e. $\mathbf{d}_i^T \mathbf{A}\, \mathbf{d}_j = 0$
- $\mathbf{r}_i = 0$ in maximal n steps, if $\mathbf{v}$ has n components

$$\mathbf{d}_0 = \mathbf{r}_0 = \mathbf{b} - \mathbf{A} \cdot \mathbf{v}_0$$

$$\alpha = \frac{\mathbf{r}_i^{\mathrm{T}} \mathbf{r}_i}{\mathbf{d}_i^{\mathrm{T}} \mathbf{A} \mathbf{d}_i}$$

$$\mathbf{v}_{i+1} = \mathbf{v}_i + \alpha \mathbf{d}_i$$

$$\mathbf{r}_{i+1} = \mathbf{r}_i - \alpha \mathbf{A} \mathbf{d}_i$$

$$\mathbf{d}_{i+1} = \mathbf{r}_{i+1} + \frac{\mathbf{r}_{i+1}^{\mathrm{T}} \mathbf{r}_{i+1}}{\mathbf{r}_i^{\mathrm{T}} \mathbf{r}_i} \mathbf{d}_i$$

Euler-Cromer (semi-implicit)

$$\mathbf{v}_{t+h} = \mathbf{v}_t + h\frac{1}{m}\mathbf{F}_t$$

$$\mathbf{x}_{t+h} = \mathbf{x}_t + h\mathbf{v}_{t+h}$$

Euler	Euler-Cromer

...
computeForces(); //F(t)
positionEuler(h); //x=x(t+h)=x(t)+**hv(t)**
velocityEuler(h); //v=v(t+h)=v(t)+ha(t)
...
	...
	computeForces(); //F(t)
	velocityEuler(h); //v=v(t+h)=v(t)+ha(t)
	positionEuler(h); //x=x(t+h)=x(t)+**hv(t+h)**
	...

Leap Frog

$$\mathbf{v}_{t+\frac{h}{2}} = \mathbf{v}_{t-\frac{h}{2}} + h\frac{1}{m}\mathbf{F}_t = \mathbf{v}_{t-\frac{h}{2}} + h\frac{1}{m}\mathbf{F}_{\mathbf{x}_t,\mathbf{v}_t}$$

$$\mathbf{x}_{t+h} = \mathbf{x}_t + h\mathbf{v}_{t+\frac{h}{2}}$$

- error $O(h^3)$
- can generally handle larger time steps *h* compared to Euler

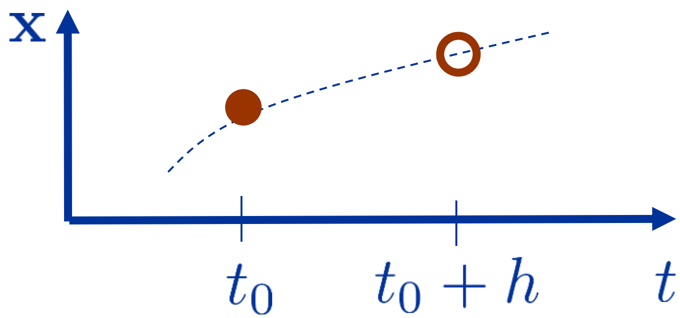
Euler	Leap Frog
	initV() // v(0) = v(0) – (h/2)a(0)
...	...
computeForces(); //F(t)	computeForces(); //F(t)
positionEuler(h); //x=x(t+h)=x(t)+**hv(t)**	velocityEuler(h); //v=v(t+h)=v(t)+ha(t)
velocityEuler(h); //v=v(t+h)=v(t)+ha(t)	positionEuler(h); //x=x(t+h)=x(t)+**hv(t+h)**
...	...

Outline

- introduction
- particle motion
- finite differences
- system of first order ODEs
- second order ODE

Initial Value Problem of Second Order

- function $\mathbf{x}_t$ represents the particle motion
- initial values are given $\mathbf{x}_{t_0}, (\dot{\mathbf{x}}_{t_0})$
- second-order differential equation is given
  $\frac{d^2\mathbf{x}_t}{dt^2} = \ddot{\mathbf{x}}_t = \frac{1}{m}\mathbf{F}_t$
- at time t_0, the function and their derivatives are known
- how to compute $\mathbf{x}_{t_0+h}, (\dot{\mathbf{x}}_{t_0+h})$



Overview of Integration Schemes

integration methods for first-order ODEs	integration methods for second-order ODE (Newton's motion equation)
Euler, Heun, Ralston, Midpoint method, 4^{th} order Runge-Kutta	Verlet, velocity Verlet, Beeman, Gear, Euler-Cromer, Leap-Frog

Verlet

- Taylor approximations of $\mathbf{x}_{t+h}$ and $\mathbf{x}_{t-h}$

$$\mathbf{x}_{t+h} = \mathbf{x}_t + h\mathbf{v}_t + \frac{h^2}{2}\frac{\mathbf{F}_t}{m} + \frac{h^3}{6}\mathbf{x}_t^{(3)} + O(h^4)$$

$$\mathbf{x}_{t-h} = \mathbf{x}_t - h\mathbf{v}_t + \frac{h^2}{2}\frac{\mathbf{F}_t}{m} - \frac{h^3}{6}\mathbf{x}_t^{(3)} + O(h^4)$$

- adding both approximations

$$\mathbf{x}_{t+h} = 2\mathbf{x}_t - \mathbf{x}_{t-h} + h^2\frac{\mathbf{F}_t}{m} + O(h^4)$$

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Verlet

- independent of velocity
- one derivative computation per time step
- efficient to compute, comparatively accurate
- third-order in the position
- if required, velocity can be computed, e.g. using
  $\mathbf{v}_{t+h} = \frac{\mathbf{x}_{t+h} - \mathbf{x}_t}{h} + O(h)$
- velocity is commonly required
  for collision response or damping

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Velocity Verlet

- one force (derivative) computation per time step
- second-order accuracy in position and velocity

$$\mathbf{x}_{t+h} = \mathbf{x}_t + h\mathbf{v}_t + \frac{h^2}{2}\frac{\mathbf{F}_t}{m} + O(h^3)$$

$$\mathbf{v}_{t+h} = \mathbf{v}_t + \frac{h}{2}\left(\frac{\mathbf{F}_t}{m} + \frac{\mathbf{F}_{t+h}}{m}\right) + O(h^3)$$

F_{t+h} is computed using x_{t+h}, v_{t+h}

- equivalent to

$$\begin{aligned} \mathbf{v}_{t+\frac{h}{2}} &= \mathbf{v}_t + \frac{h}{2}\frac{\mathbf{F}_t}{m} \\ \mathbf{x}_{t+h} &= \mathbf{x}_t + h\mathbf{v}_{t+\frac{h}{2}} \\ \mathbf{v}_{t+h} &= \mathbf{v}_{t+\frac{h}{2}} + \frac{h}{2}\frac{\mathbf{F}_{t+h}}{m} \end{aligned}$$

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Beeman

- one force (derivative) computation per time step
- efficient to compute
- third-order accuracy in position and velocity

$$\mathbf{x}_{t+h} = \mathbf{x}_t + h\mathbf{v}_t + h^2 \left(\frac{2}{3} \frac{\mathbf{F}_t}{m} - \frac{1}{6} \frac{\mathbf{F}_{t-h}}{m} \right) + O(h^4)$$

$$\mathbf{v}_{t+h} = \mathbf{v}_t + h \left(\frac{5}{12} \frac{\mathbf{F}_{t+h}}{m} + \frac{2}{3} \frac{\mathbf{F}_t}{m} - \frac{1}{12} \frac{\mathbf{F}_{t-h}}{m} \right) + O(h^4)$$

- $\mathbf{F}_{t+h}$ is computed using $\mathbf{x}_{t+h}, \mathbf{v}_{t+h}$

Gear Integration

position velocity acceleration

$$\mathbf{x}_{t+h} = \mathbf{x}_t + \frac{\mathbf{x}_t^{(1)}}{1!}h + \frac{\mathbf{x}_t^{(2)}}{2!}h^2 + \frac{\mathbf{x}_t^{(3)}}{3!}h^3 + \frac{\mathbf{x}_t^{(4)}}{4!}h^4 + \frac{\mathbf{x}_t^{(5)}}{5!}h^5 + \dots$$

$$\mathbf{r}_{t+h}^0 = \mathbf{r}_t^0 + \mathbf{r}_t^1 + \mathbf{r}_t^2 + \mathbf{r}_t^3 + \mathbf{r}_t^4 + \mathbf{r}_t^5 + \dots$$

$$\mathbf{r}_t^k = \frac{d^k \mathbf{x}_t}{dt^k} \cdot \frac{h^k}{k!}$$

Gear Integration

$$\mathbf{x}_{t+h} = \mathbf{x}_t + \frac{\mathbf{x}_t^{(1)}}{1!}h + \frac{\mathbf{x}_t^{(2)}}{2!}h^2 + \frac{\mathbf{x}_t^{(3)}}{3!}h^3 + \frac{\mathbf{x}_t^{(4)}}{4!}h^4 + \frac{\mathbf{x}_t^{(5)}}{5!}h^5 + \dots$$

$$\mathbf{r}_{t+h}^0 = \mathbf{r}_t^0 + \mathbf{r}_t^1 + \mathbf{r}_t^2 + \mathbf{r}_t^3 + \mathbf{r}_t^4 + \mathbf{r}_t^5 + \dots$$

$$h\mathbf{x}_{t+h}^{(1)} = h\mathbf{x}_t^{(1)} + h\frac{\mathbf{x}_t^{(2)}}{1!}h + h\frac{\mathbf{x}_t^{(3)}}{2!}h^2 + h\frac{\mathbf{x}_t^{(4)}}{3!}h^3 + h\frac{\mathbf{x}_t^{(5)}}{4!}h^4 + \dots$$

$$\mathbf{r}_{t+h}^1 = \mathbf{r}_t^1 + 2\mathbf{r}_t^2 + 3\mathbf{r}_t^3 + 4\mathbf{r}_t^4 + 5\mathbf{r}_t^5 + \dots$$

$$\frac{h^2}{2}\mathbf{x}_{t+h}^{(2)} = \frac{h^2}{2}\mathbf{x}_t^{(2)} + \frac{h^2}{2}\frac{\mathbf{x}_t^{(3)}}{1!}h + \frac{h^2}{2}\frac{\mathbf{x}_t^{(4)}}{2!}h^2 + \frac{h^2}{2}\frac{\mathbf{x}_t^{(5)}}{3!}h^3 + \dots$$

$$\mathbf{r}_{t+h}^2 = \mathbf{r}_t^2 + 3\mathbf{r}_t^3 + 6\mathbf{r}_t^4 + 10\mathbf{r}_t^5 + \dots$$

Gear - Prediction

$$\begin{aligned}
\mathbf{x}_{t+h} = \mathbf{r}^0_{t+h} &= \mathbf{r}^0_t + \mathbf{r}^1_t + \mathbf{r}^2_t + \mathbf{r}^3_t + \mathbf{r}^4_t + \mathbf{r}^5_t \\
h\mathbf{v}_{t+h} = \mathbf{r}^1_{t+h} &= \mathbf{r}^1_t + 2\mathbf{r}^2_t + 3\mathbf{r}^3_t + 4\mathbf{r}^4_t + 5\mathbf{r}^5_t \\
\frac{h^2}{2}\frac{\mathbf{F}_{t+h}}{m} = \mathbf{r}^2_{t+h} &= \mathbf{r}^2_t + 3\mathbf{r}^3_t + 6\mathbf{r}^4_t + 10\mathbf{r}^5_t \\
\mathbf{r}^3_{t+h} &= \mathbf{r}^3_t + 4\mathbf{r}^4_t + 10\mathbf{r}^5_t \\
\mathbf{r}^4_{t+h} &= \mathbf{r}^4_t + 5\mathbf{r}^5_t \\
\mathbf{r}^5_{t+h} &= \mathbf{r}^5_t
\end{aligned}$$

Gear - Correction

- error

$$\text{error}_{t+h} = \mathbf{r}^2_{t+h} - \frac{\mathbf{F}_{t+h}}{m}\frac{h^2}{2!}$$

$$\mathbf{r}^k_{t+h} = \mathbf{r}^k_{t+h} - C_k \text{error}_{t+h}$$

- error correction coefficients C_k

k = 0	k = 1	k = 2	k = 3	k = 4	k = 5
$\frac{3}{20}$	$\frac{251}{360}$	1	$\frac{11}{18}$	$\frac{1}{6}$	$\frac{1}{60}$

Gear - Implementation

- initialization

$$\mathbf{r}_0^0 = \mathbf{x}_0 \qquad \mathbf{r}_0^2 = \frac{\mathbf{F}_0}{m}\frac{h^2}{2}$$

$$\mathbf{r}_0^1 = \mathbf{v}_0 h \qquad \mathbf{r}_0^3 = \mathbf{r}_0^4 = \mathbf{r}_0^5 = 0$$

- integration
  - prediction
  - error estimation
  - correction

$$\mathbf{r}_{t+h}^0 = \mathbf{r}_t^0 + \ldots + \mathbf{r}_t^5$$

$$\mathbf{r}_{t+h}^i = \ldots$$

$$\mathrm{error}_{t+h} = \mathbf{r}_{t+h}^2 - \frac{\mathbf{F}_{t+h}}{m}\frac{h^2}{2!}$$

$$\mathbf{r}_{t+h}^k = \mathbf{r}_{t+h}^k - C_k \mathrm{error}_{t+h}$$

Comparison – Explicit Schemes

method	force comp. per time step	error order position	error order velocity
Euler	1	1	1
RK 2nd order	2	2	2
RK 4th order	4	4	4
Verlet	1	3	1
Velocity Verlet	1	2	2
Beeman	1	3	3

Comparison – Explicit Schemes

- methods for first-order ODEs
  - accuracy corresponds to computing complexity
  - position and velocity have the same error order
- methods for second-order ODEs
  - improved accuracy with minimal computing complexity
  - error order might differ for position and velocity
- implicit methods cannot be compared this way
  - do not only compute forces (derivatives)
  - commonly require to solve a linear system
  - improved stability even for low error orders,
    implicit Euler with error order one can be unconditionally stable, e. g. for harmonic oscillators (springs)

Advantages / Disadvantages

- explicit methods
  - simple to set up and program
  - fast computation per integration step
  - suitable for parallel architectures
  - small time steps required for stability
  - many computing steps required for a given time interval t
- implicit methods
  - stability is maintained for large time steps
  - require less steps for a given interval t
  - large time steps can cause large truncation errors
  - complicate to set up
  - less flexible, problems with non-analytical forces
  - large computing time per integration step

Advantages / Disadvantages

- predictor-corrector methods
  - not self-starting
  - have to be re-initialized in case of discontinuities, e. g. due to collision response
- in general, implicit methods are more robust (stable) compared to explicit methods
  - if an explicit scheme is not conditionally or unconditionally stable it cannot be used regardless of its efficiency
- explicit methods can be computed efficiently which is essential if frequent updates are required
  - if an implicit scheme cannot be computed at interactive rates, it cannot be used in interactive applications regardless of the time step

Summary

- motion equation for a mass point
  - second-order differential equation
  - coupled system of first-order differential equations
- numerical integration
  - initial values $\mathbf{x}_t$ and $\mathbf{v}_t$
  - approximate integration of $\mathbf{v}$ and $\mathbf{x}$ through time with time step h
- integration schemes
  - Euler, Runge-Kutta 2nd , Runge-Kutta 4th
  - Crank-Nicolson, implicit Euler, Euler-Cromer, Leap-Frog
  - Gear, Verlet, velocity Verlet, Beeman
- trade-off between accuracy and computing cost
- goal: maximizing the ratio of time step and computing cost