Physically-based simulation

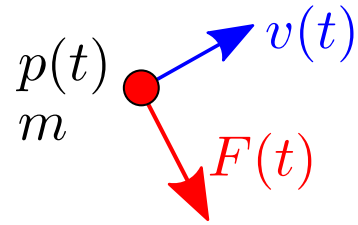
Particle based systems

Reminder - Physically-based particle system

1. Description

Particle is fully described by: Position p, Speed v, Mass m

fundamental quantities: position and linear momentum $P = m\,v$
Momentum preserved through time when no external forces are applied



2. Evolution

- Fundamental principle of the dynamics

Force applied on particle $F(p, v, t)$

$$\begin{cases} p'(t) = v(t) \\ P'(t) = m\,v'(t) = F(p, v, t) \end{cases}$$

- Conservation of energy (ex. kinetic energy $(1/2\,m\,v^2)$+potential energy = const, etc.)

- Lagragian, or Hamiltonian

Reminder - Physically-based particle system

3. Numerical Solution

ODE (Ordinary Differential Equation) formulated as an **Initial Value Problem**

$$\text{ex. } \begin{cases} p'(t) = v(t) \\ m v'(t) = F(p, v, t) \end{cases}, \quad \text{with } v(0) = v_0,\ p(0) = p_0$$

- Discretize in time $t^k = k\,h, \quad h = \Delta t =$ time step.

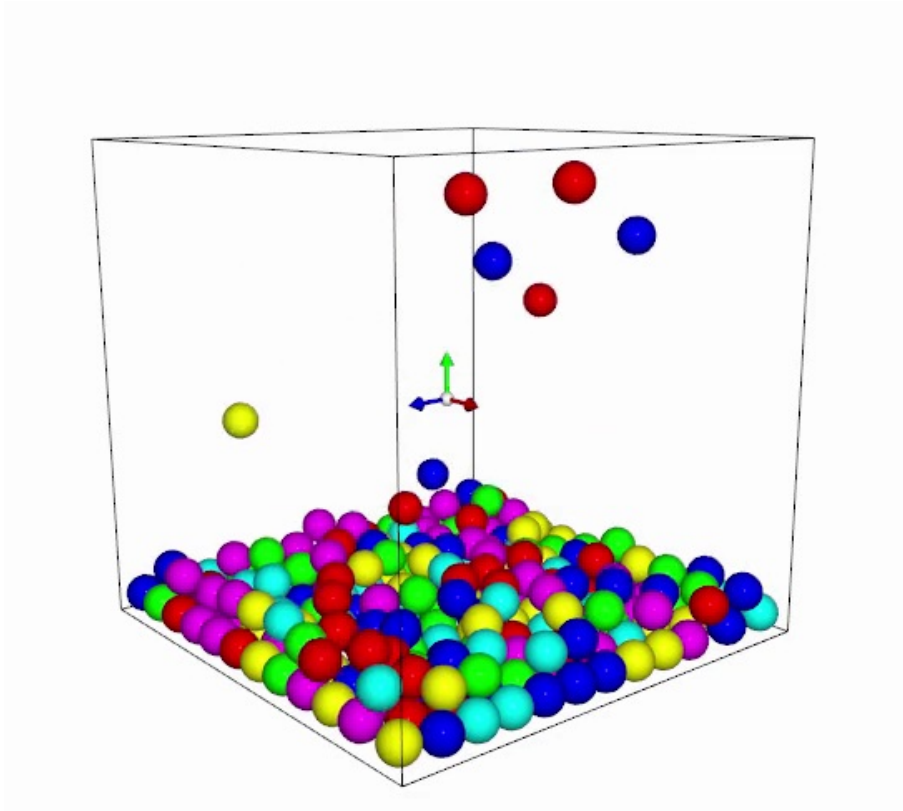
  $\Rightarrow$ Build a discrete numerical solution $p^k = p(t^k), v^k = v(t^k)$.

- We can consider initially the following iterative scheme

$$\begin{cases} v^{k+1} = v^k + h\,F(p^k, v^k, t^k)/m \\ p^{k+1} = p^k + h\,v^{k+1} \end{cases}$$

Simple to implement, reasonably OK for simple examples (more details later).

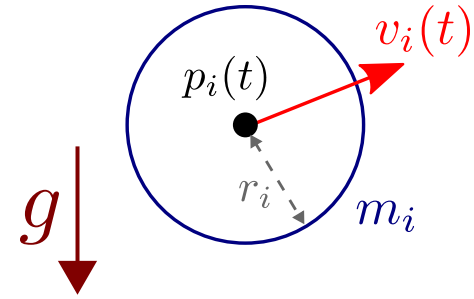
Example : Rigid spheres



System modeling

Particles modeling the center of hard spheres.

- Spheres can collide with surrounding obstacles
- Spheres can collide with each others



- *System*: N particles with position p_i, speed v_i, mass m_i, modeling a sphere of radius r_i.
  - Initial conditions $p_i(0) = p_i^0$, $v_i(0) = v_i^0$

- *Forces*: Single gravity forces $F_i = m_i\, g$. Collisions handled by *impulses*.

- *Temporal evolution*: Fundamental principle of dynamics $v_i(t) = p_i'(t)$, $v_i'(t) = g$

- *Numerical solution*

$$\begin{cases} v^{k+1} = v^k + h\, g \\ p^{k+1} = p^k + h\, v^{k+1} \end{cases}$$

Collision with a plane

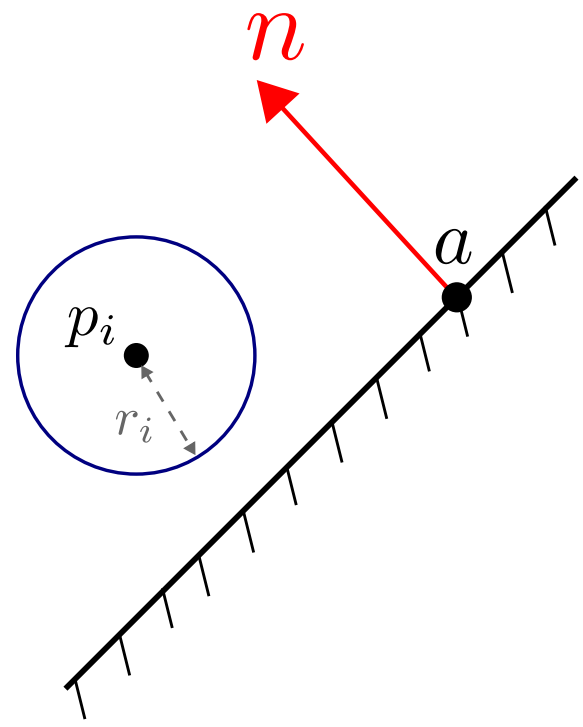
Plane $\mathcal{P}$: parameterized using a point a and its normal n.

$$\{p \in \mathbb{R}^3 \in \mathcal{P} \Rightarrow (p - a) \cdot n = 0\}$$

- Sphere above plane : $(p_i - a) \cdot n > r_i$
- Sphere in collision: $(p_i - a) \cdot n \leq r_i$

- Collision detection algorithm

```
for(int i=0; i<N; ++i)
{
    float detection = dot(p[i]-a, n);
    if (detection <= r[i])
    {
        // ... collision response
    }
}
```



What should we do when a collision is detected

Collision response with plane

Suppose exact contact: $(p_i - a) \cdot n_i = r_i$

Collision response = **Update speed**

Split $v = v_{//} + v_{\perp}$

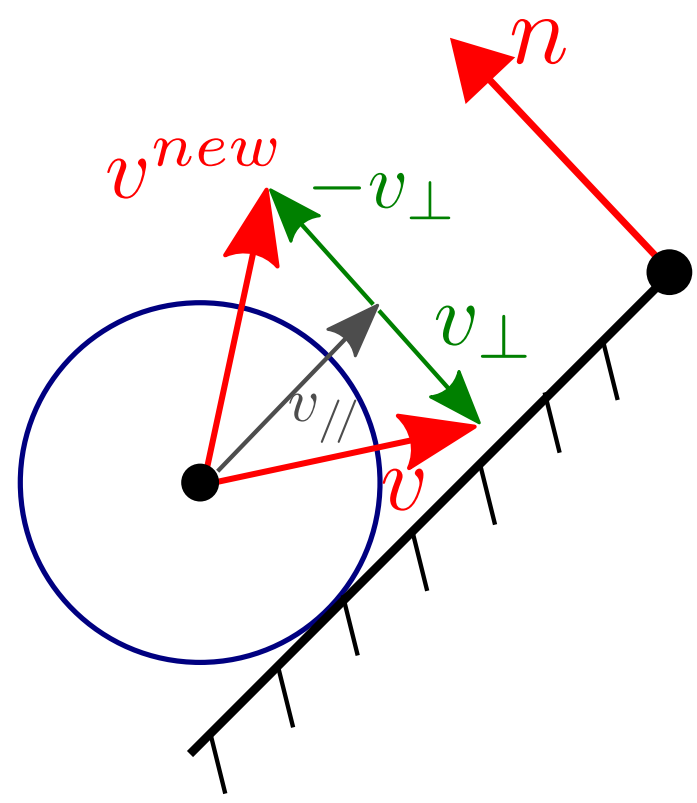
- $v_{\perp} = (v \cdot n)\, n$
- $v_{//} = v - (v \cdot n) n$

New speed

$v^{new} = \alpha\, v_{//} - \beta\, v_{\perp} = \alpha\, v - (\beta + \alpha)\, (v \cdot n) n$

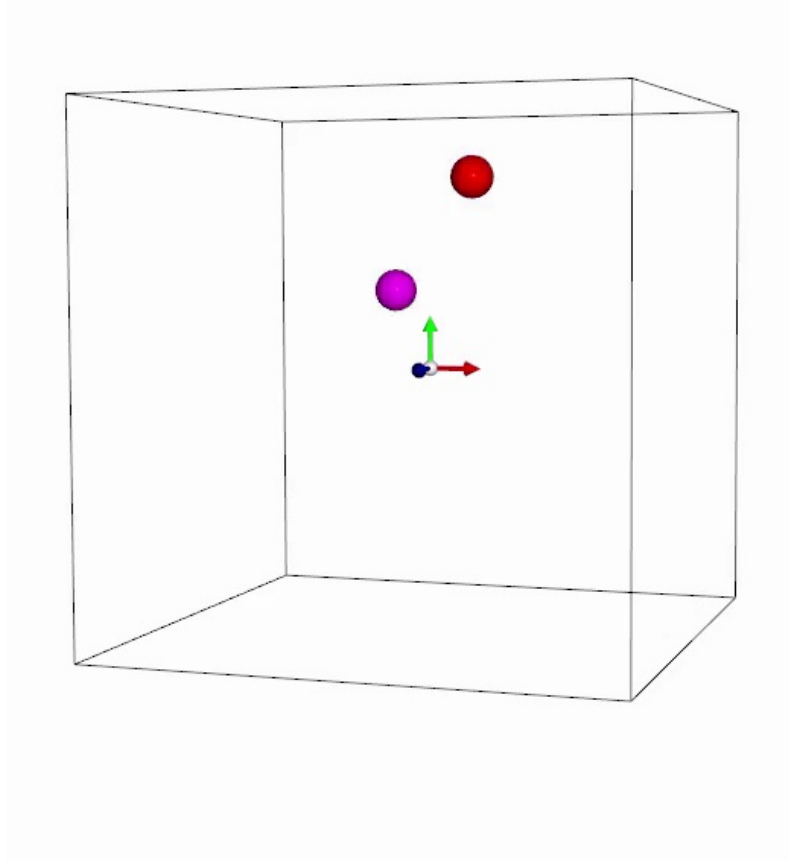
$1 - \alpha \in [0, 1]$ Speed loss in $//$ direction (friction)

$1 - \beta \in [0, 1]$ Speed loss in $\perp$ direction (impact)



Result: Collision response

Applying collision response on speed only



Collision response with plane : position

In real case (discrete time) no exact contact, but penetration $(p_i - a) \cdot n_i < r_i$

$\Rightarrow$ Need to compute collision response at contact point.

Three possibilities

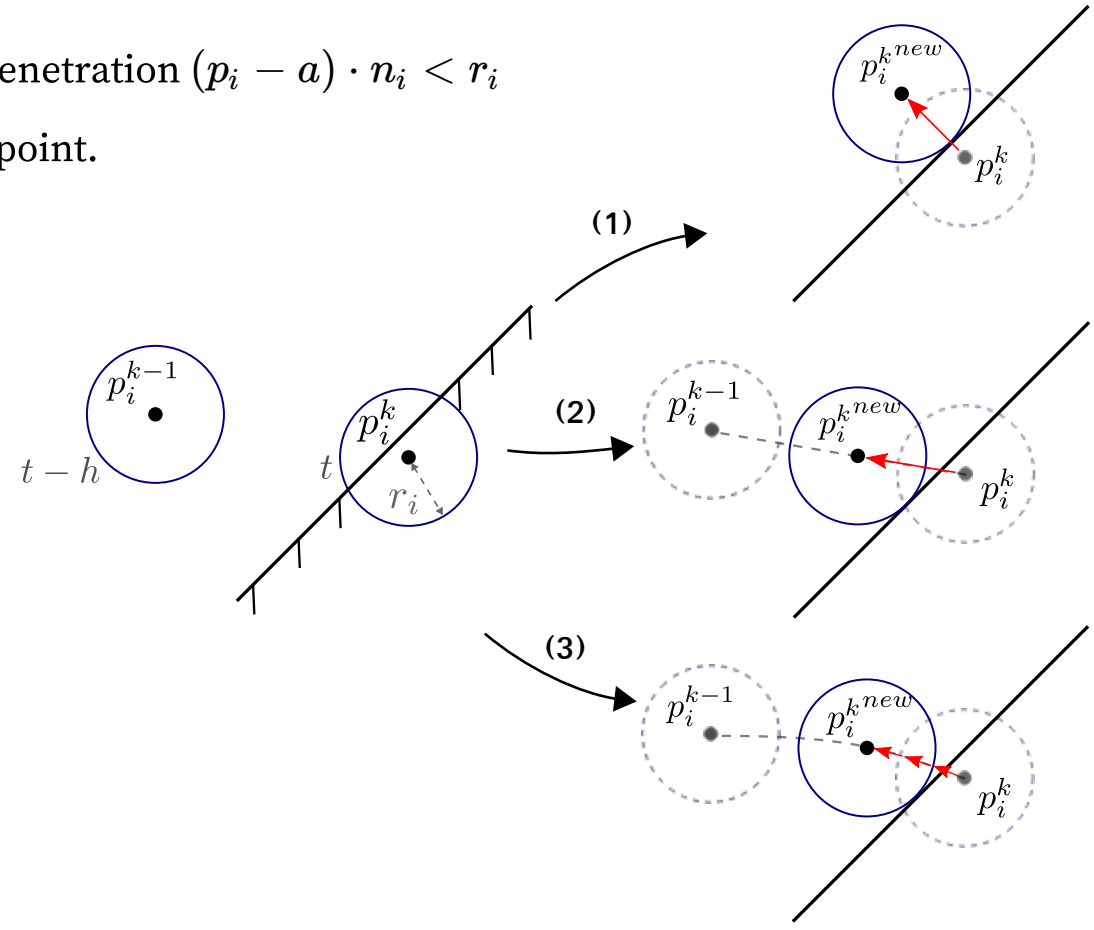
(1) Correct position in projecting on the constaint

(+) Simple to implement
(-) Physically incorrect position

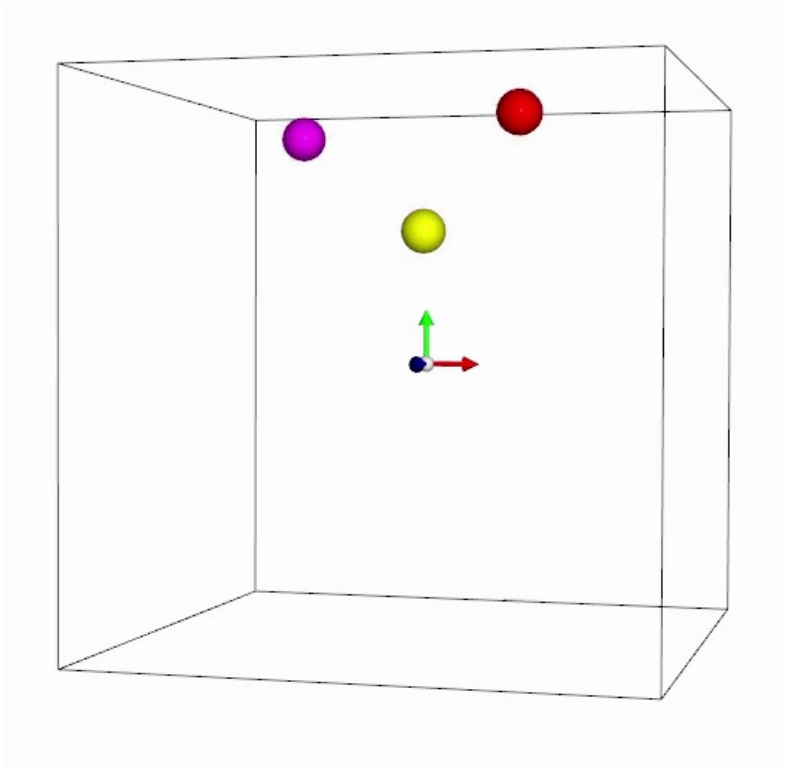
(2) Approximate the correct position

(3) Go backward in to find exact instant of collision

(+) Physically correct
(-) Computationally heavy (binary search, etc.)



Result: Projecting position on plane



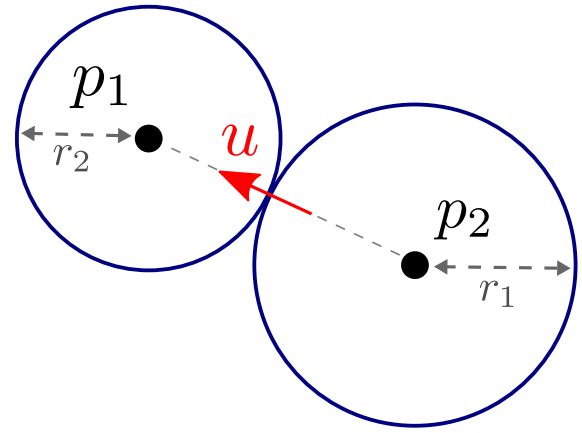
$p_i^{new} = p_i + d\,n$

$d = r_i - (p_i - a) \cdot n_i$: distance of penetration

Collision between sphere

Given 2 spheres (p_1, v_1, r_1, m_1), (p_2, v_2, r_2, m_2).

Collision when $\|p_1 - p_2\| \leq r_1 + r_2$



Response to collision in speed

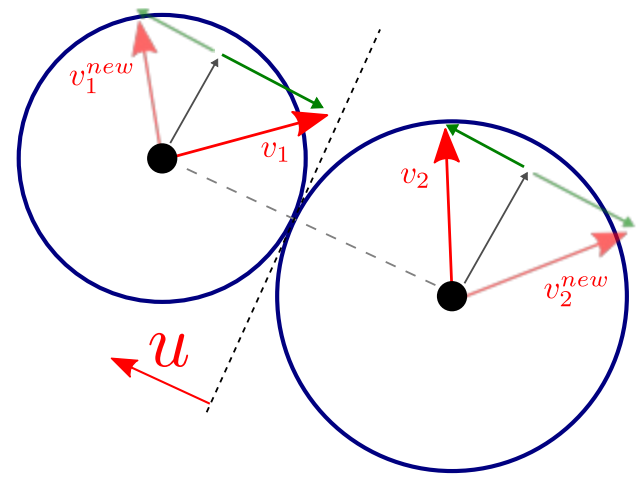
$$\begin{cases} v_1^{new} = v_1 - \dfrac{j}{m_1} u \\ v_2^{new} = v_2 + \dfrac{j}{m_2} u \end{cases}$$

j: impulse (sudden change of momentum)

$$j = 2 \frac{(v_1 - v_2) \cdot u}{\frac{1}{m_1} + \frac{1}{m_2}}$$

$$u = \frac{p_1 - p_2}{\|p_1 - p_2\|}$$

Rem. If $m_1 = m_2$, spheres switch between their $\perp$ speed



Collision response with sphere - Derivation

- Conservation of momentum of the center of mass (COM)

$m_1 v_1 + m_2 v_2 = m_1 v_1^{new} + m_2 v_2^{new}$

$\Rightarrow m_2(v_2^{new} - v_2) = -m_1(v_1^{new} - v_1) = J$, J: the impulse

The impulse is orthogonal to the separating plane between the two surfaces

$J = j\,u,\ u = (p_1 - p_2)/\|p_1 - p_2\|$

- Conservation of the kinetic energy (elastic collision)

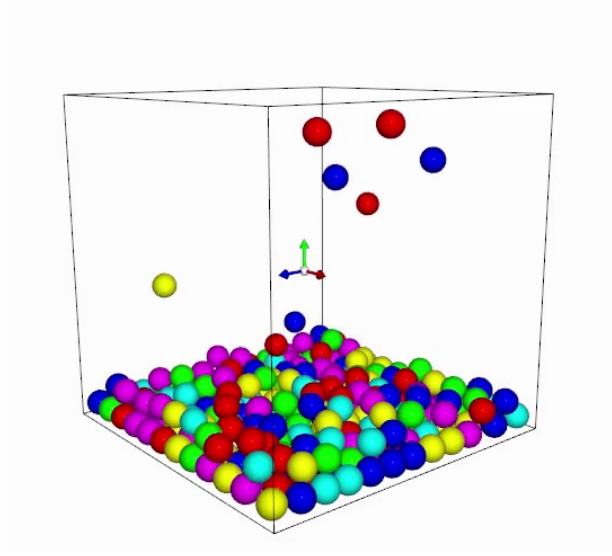
$1/2\,m_1\,v_1^2 + 1/2\,m_2\,v_2^2 = 1/2\,m_1\,(v_1^{new})^2 + 1/2\,m_2\,(v_2^{new})^2$

$\Rightarrow m_1 v_1^2 + m_2 v_2^2 = m_1\left(v_1 - \frac{j}{m_1}u\right)^2 + m_2\left(v_2 + \frac{j}{m_2}u\right)^2$

$\Rightarrow 0 = -2\,j\,v_1 \cdot u + \frac{j^2}{m_1} + 2\,j\,v_2 \cdot u + \frac{j^2}{m_2}$

$\Rightarrow j = 2\frac{v_1 - v_2}{1/m_1 + 1/m_2} \cdot u$

Final result



Reprojection on the contact surface

$$p_1^{new} = p_1 + \frac{m_2}{m_1+m_2} d\,u$$

$$p_2^{new} = p_2 - \frac{m_1}{m_1+m_2} d\,u$$

$$d = r_1 + r_2 - \|p_1 - p_2\|$$

Numerical solution of ODE

General formulation

Consider relation given a system of **first order** differential equation

Mechanical systems are often expressed as

- *scalar equation of second order in* p

- *system of first order in* (p, v)

In general, we can write

$$u'(t) = \mathcal{F}(u(t), t)$$

If $\mathcal{F}$ is an affine function in u

$$u'(t) = \mathrm{A}(t)\, u(t) + b(t)$$

When A is constant through time

$$u'(t) = \mathrm{A}\, u(t) + b(t)$$

Examples of formulation

- Free fall
- Free fall with linear drag
- Pendulum
- 1D spring / Harmonic oscillator
- 1D coupled spring
- 3D mass spring

Spring: usefull to model deformable elastic shapes

Example: Free fall under gravity

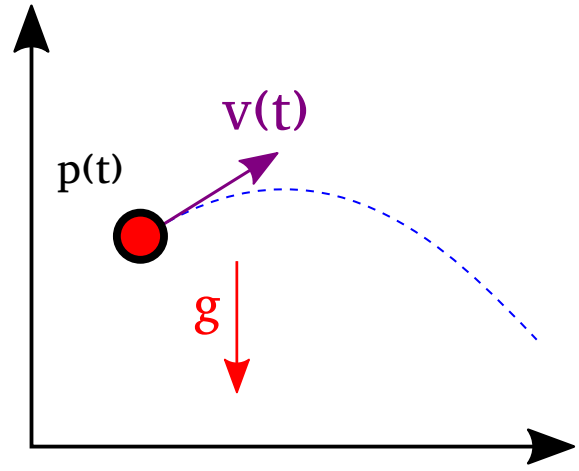
- Force $F(t) = m\,g$

- Second order differential equation: $p''(t) = g$

- First order system $\underbrace{\begin{pmatrix} p \\ v \end{pmatrix}'(t)}_{u'(t)} = \underbrace{\begin{pmatrix} v(t) \\ g \end{pmatrix}}_{\mathcal{F}(u,t)}$

- Linear system $\underbrace{\begin{pmatrix} p \\ v \end{pmatrix}'(t)}_{u'(t)} = \underbrace{\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}}_{\mathrm{A}} \underbrace{\begin{pmatrix} p \\ v \end{pmatrix}(t)}_{u(t)} + \underbrace{\begin{pmatrix} 0 \\ g \end{pmatrix}}_{b(t)}$

- Exact solution known: $p(t) = \frac{1}{2} g\,t^2 + v_0\,t + p_0$



Note: variables are vectors - matrix can be expressed by block, or per components.

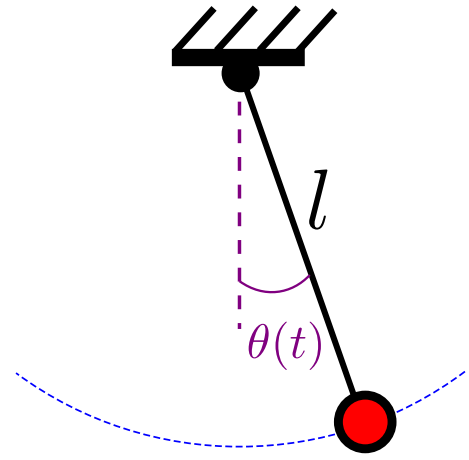
Example: Free fall with linear drag

- Force $F(t) = g - \mu\, v(t)$
- Second order differential equation: $m\, p''(t) + \mu\, p'(t) = m\, g$
- First order system $\underbrace{\begin{pmatrix} p \\ v \end{pmatrix}'(t)}_{u'(t)} = \underbrace{\begin{pmatrix} v(t) \\ g - \mu/m\, v(t) \end{pmatrix}}_{\mathcal{F}(u,t)}$
- Linear system $\underbrace{\begin{pmatrix} p \\ v \end{pmatrix}'(t)}_{u'(t)} = \underbrace{\begin{pmatrix} 0 & 1 \\ 0 & -\mu/m \end{pmatrix}}_{\mathrm{A}} \underbrace{\begin{pmatrix} p \\ v \end{pmatrix}(t)}_{u(t)} + \underbrace{\begin{pmatrix} 0 \\ g \end{pmatrix}}_{b(t)}$

- Exact solution known: $p(t) = p_0 + v_\infty\, t + \frac{v_\infty^2}{g}\left(1 - \frac{v_0}{v_\infty}\right) e^{\left(-\frac{g}{v_\infty} t\right)}$, $v_\infty = \frac{m\, g}{\mu}$

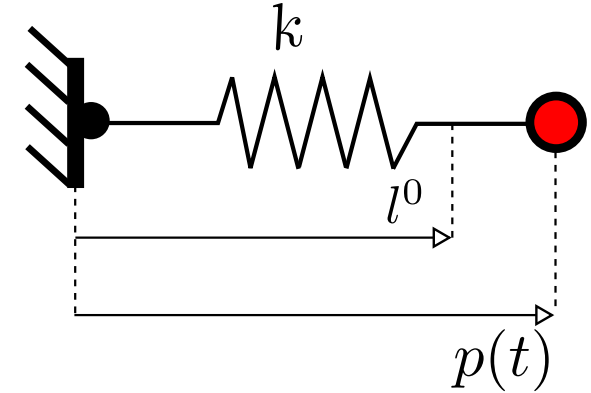
Example: Pendulum

- Scalar equation in θ, derived from Lagrangian
- Second order differential equation: $\theta''(t) = -g/l \ \sin(\theta(t))$
- First order system $\underbrace{\begin{pmatrix} \theta \\ \omega \end{pmatrix}'(t)}_{u'(t)} = \underbrace{\begin{pmatrix} \omega(t) \\ -g/l \ \sin(\theta(t)) \end{pmatrix}}_{\mathcal{F}(u,t)}$
- Not linear (unless $\theta \ll 1$)
- No simple explicit solution



Example: 1D spring (/Harmonic oscillator)

- Force $F(t) = -k\,(p(t) - l^0)$, k spring stiffness, l^0 rest length



- Second order differential equation: $m\,p''(t) + k\,p(t) = k\,l^0$

- First order system $\underbrace{\begin{pmatrix} p \\ v \end{pmatrix}'(t)}_{u'(t)} = \underbrace{\begin{pmatrix} v(t) \\ -k/m\,\left(p(t) - l^0\right) \end{pmatrix}}_{\mathcal{F}(u,t)}$

- Linear system $\underbrace{\begin{pmatrix} p \\ v \end{pmatrix}'(t)}_{u'(t)} = \underbrace{\begin{pmatrix} 0 & 1 \\ -k/m & 0 \end{pmatrix}}_{\mathrm{A}} \underbrace{\begin{pmatrix} p \\ v \end{pmatrix}(t)}_{u(t)} + \underbrace{\begin{pmatrix} 0 \\ k/m\; l^0 \end{pmatrix}}_{b}$

- Exact solution known: $p(t) = A\,\sin(\omega\,t + \varphi) + l^0$

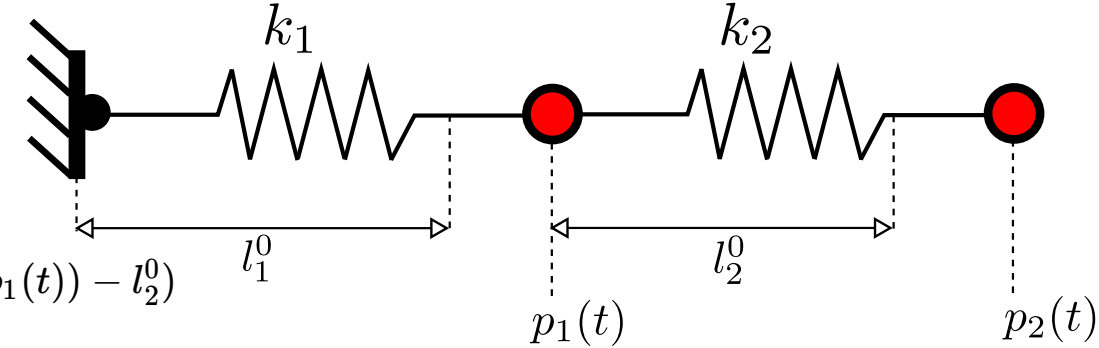
$$\omega = \sqrt{k/m},\; A^2 = (p^0 - l^0)^2 + \left(\frac{v_0}{\omega}\right)^2,\; \tan(\varphi) = \frac{p^0 - l^0}{v^0/\omega}$$

Example: 1D coupled springs

- Forces:

$$F_2(t) = -k_2/m_2((p_2(t) - p_1(t)) - l_2^0)$$

$$F_1(t) = -k_1/m_1(p_1(t) - l_1^0) + k_2/m_2((p_2(t) - p_1(t)) - l_2^0)$$



- First order system

$$\underbrace{\begin{pmatrix} p_1 \\ p_2 \\ v_1 \\ v_2 \end{pmatrix}'(t)}_{u'(t)} = \underbrace{\begin{pmatrix} v_1(t) \\ v_2(t) \\ -k_1/m_1(p_1(t) - l_1^0) + k_2/m_2((p_2(t) - p_1(t)) - l_2^0) \\ -k_2/m_2((p_2(t) - p_1(t)) - l_2^0) \end{pmatrix}}_{\mathcal{F}(u,t)}$$

- Linear system

$$\underbrace{\begin{pmatrix} p_1 \\ p_2 \\ v_1 \\ v_2 \end{pmatrix}'(t)}_{u'(t)} = \underbrace{\begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ -k_1/m_1 & k_2/m_2 & 0 & 0 \\ 0 & -k_2/m_2 & 0 & 0 \end{pmatrix}}_{\mathrm{A}} \underbrace{\begin{pmatrix} p_1 \\ p_2 \\ v_1 \\ v_2 \end{pmatrix}(t)}_{u(t)} + \underbrace{\begin{pmatrix} 0 \\ 0 \\ k_1/m_1\ l_1^0 - k_2/m_2\ l_2^0 \\ K_2/m_2\ l_2^0 \end{pmatrix}}_{b}$$

Example: 3D mass spring

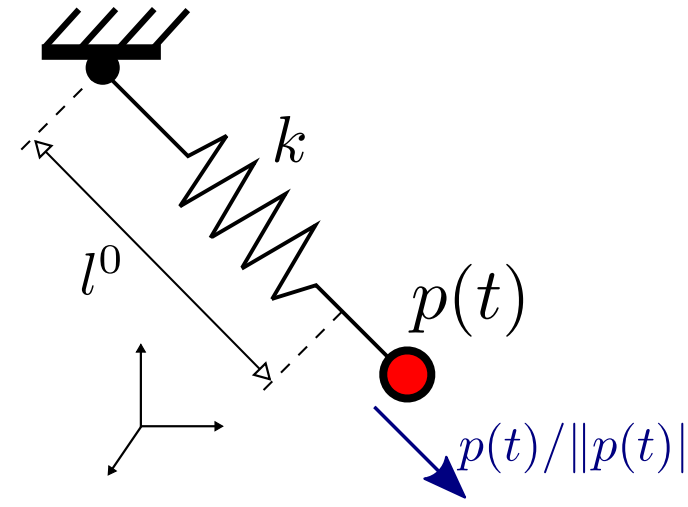
- Force $F(t) = m\,g - k\,(\|p(t)\| - l^0)\,\frac{p(t)}{\|p(t)\|}$, k spring stiffness, l^0 rest length

- Second order differential equation: $m\,p''(t) = mg - k\,(\|p(t)\| - l^0)\,\frac{p(t)}{\|p(t)\|}$

- First order system $\underbrace{\begin{pmatrix} p \\ v \end{pmatrix}'(t)}_{u'(t)} = \underbrace{\begin{pmatrix} v(t) \\ g - k/m\,(\|p(t)\| - l^0)\,\frac{p(t)}{\|p(t)\|} \end{pmatrix}}_{\mathcal{F}(u,t)}$

- Not linear

- No simple explicit solution



Existence of solution

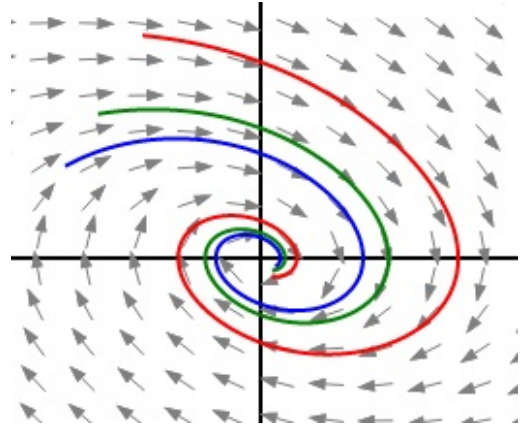
Solving the physical system = Solving the **Initial Value Problem** (IVP)

- Find the solution of $u'(t) = \mathcal{F}(u, t), t \geq 0$
- With initial condition $u(t = 0) = u_0$

Cauchy-Lipschitz (/Picard-Lindelof) theorem states that

If $\mathcal{F}$ is Lipschitz with respect to u and continuous with respect to t

Then there exists a unique solution $u(t)$.



The solution is called the **integral curve** of the IVP.

- $\mathcal{F}$ can be seen as a vector field

  (Vector field in 6D for $p(t) \in \mathbb{R}^3, v(t) \in \mathbb{R}^3$)
- Solution is a path along this vector field passing by u_0

Solving the ODE exactly

Equation is linear

Homogeneous, constant coefficients

$u'(t) = \mathrm{A}u(t), u(0) = u_0$

$\Rightarrow u(t) = u_0 \ \exp(\mathrm{A}\, t)$

Non-Homogeneous, constant coefficients

$u'(t) = \mathrm{A}u(t) + b(t), u(0) = u_0$

$$\Rightarrow u(t) = u_0 \ \exp(\mathrm{A}\, t) + \exp(\mathrm{A}\, t) \int_{t'=0}^{t} b(t') \exp(-\mathrm{A}\, t')\, \mathrm{d}t'$$

Homogeneous, variable coefficients

$u'(t) = \mathrm{A}(t)\, u(t), u(0) = u_0$

$\Rightarrow$ No closed-form solution in the general case

- *Rem.* Unfortunately, in general, $u(t)$ is **not** $u_0 \ \exp\left(\int_0^t \mathrm{A}(t')\, \mathrm{d}t'\right)$

Equation is non linear

No general method

$\Rightarrow$ Numerical approaches are required most of the time

Numerical solution

1st order Explicit Euler

Naive numerical scheme: Approximation of the derivative

$$\frac{u^{k+1} - u^k}{h} = \mathcal{F}(u^k, t^k)$$

$$\Rightarrow u^{k+1} = u^k + h\,\mathcal{F}(u^k, t^k)$$

In the linear case

$$u^{k+1} = (\mathrm{I} + h\,\mathrm{A})\; u^k + h\,b^k$$

Pro : very easy to implement

Is u^k a good approximation of the true solution $\tilde{u}(t^k)$?

Explicit Euler - study case

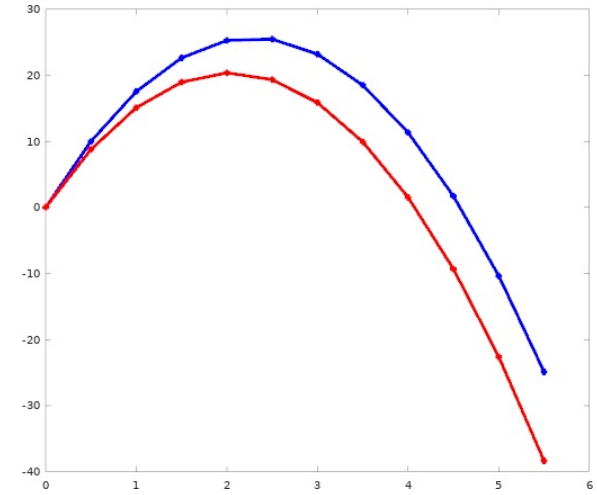
Free fall under gravity

- True solution $\tilde{u}(k\,h) = p_0 + (k\,h)v_0 + \frac{(k\,h)^2}{2}\,g$

- Numerical scheme: $\begin{pmatrix} p \\ v \end{pmatrix}^{k+1} = \begin{pmatrix} 1 & h \\ 0 & 1 \end{pmatrix} \begin{pmatrix} p \\ v \end{pmatrix}^{k} + \begin{pmatrix} 0 \\ h\,g \end{pmatrix}$

- Numerical solution: $p^k = p_0 + k\,h\,v_0 + \frac{k(k-1)}{2}\,h^2\,g$

$\Rightarrow$ **Not exact** : Error $e^k = |u^k - \tilde{u}(k\,h)| = \frac{g}{2}k\,h^2$



red: true solution

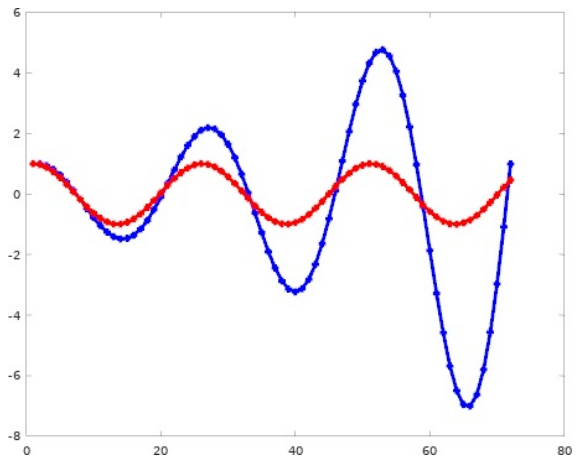
blue: numerical solution

Explicit Euler - study case

1D spring

- True solution: permanent oscillation

- Numerical scheme: $\begin{pmatrix} p \\ v \end{pmatrix}^{k+1} = \begin{pmatrix} 1 & h \\ -K/m\,h & 1 \end{pmatrix} \begin{pmatrix} p \\ v \end{pmatrix}^{k} + \begin{pmatrix} 0 \\ K/m\,h\,l^0 \end{pmatrix}$



red: true solution
red: numerical solution

- Numerical solution diverge to ∞
- Worse than bad accuracy for Graphics

Explicit Euler - study case

1D spring: Analysis of the system energy

- Energy $E = \frac{1}{2}mv^2 + \frac{K}{2}(p - l^0)^2$

$$E^{k+1} = \frac{1}{2}m\left(-\frac{K}{m}\Delta t\left(p^k - l^0\right) + v^k\right)^2 + \frac{1}{2}K\left(p^k + \Delta t\, v^k - l^0\right)^2$$

$$E^{k+1} = \underbrace{\frac{1}{2}m\left(v^k\right)^2 + \frac{1}{2}K(p^k - l^0)^2}_{E^k} + \frac{1}{2}\left[\underbrace{\frac{K^2}{m}(\Delta t)^2(p^k - l^0)^2}_{>0} - \underbrace{2\,K\Delta t\left(p^k - l^0\right)\,v^k + 2K\Delta t\left(p^k - l^0\right)v^k}_{=0} + \underbrace{K(\Delta t)^2\left(v^k\right)^2}_{>0}\right]$$

$$E^{k+1} = E^k + \epsilon\,(\Delta t)^2, \epsilon > 0$$

$\Rightarrow$ gain of energy

$\Rightarrow$ divergence

Accuracy of a numerical method - general definition

- Define the **local truncation error** τ:

  Error accumulated during one step, assuming perfect knowledge of the true solution

  $\tau_k = \|\tilde{u}(t^k) - u^k\|$, assuming $u^{k-1} = \tilde{u}(t^{k-1})$

- A numerical scheme is said to be accurate of order k, if its local truncation error is in $\mathcal{O}(h^{k+1})$.

Explicit Euler is of order 1*, at every step we add an error in* $\mathcal{O}(h^2)$.

Stability of a numerical method - general definition

- Classical stability of a method studied on $u'(t) = \lambda\, u(t)$, $\lambda \in \mathbb{C}$.
  - The true solution $\tilde{u}(t) = \exp(\lambda\, t)$ converge if $\mathbb{R}_e(\lambda) \leq 0$.
  - For linear system, λ refers to eigenvalues of $\mathbf{A}$.
  - For non linear system, λ refers to eigenvalues of the Jacobian of $\mathcal{F}$

- A numerical method is *unconditionnaly stable* if $\mathbb{R}_e(\lambda) \leq 0 \Rightarrow$ stable discrete solution.

- Otherwise, it is conditionnally stable/unstable.

- Region of stability: Set of conditions on λ such that the discrete solution doesn't diverge.

Rem.

- A numerical solution can diverge even when the true ODE solution converge when using unstable numerical method.
- Converseley, a numerical solution can converge even when the true ODE solution diverge when using stable numerical method.
- Stability ! $=$ Accuracy.

Stability analysis of explicit Euler

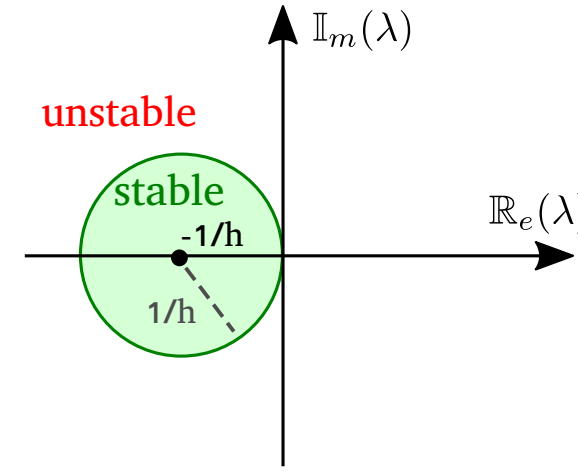
$u'(t) = \lambda\, u(t)$

$\Rightarrow u^{k+1} = u^k + \lambda\, u^k$ using explicit Euler

$\Rightarrow u^{k+1} = (1 + \lambda\, h)\, u^k$

$\Rightarrow$ Stable if $|1 + \lambda\, h| \leq 1$ (conditionnal stability)

$|1/h + \lambda| \leq 1/h$: Interior of a disc centered on $(-1/h, 0)$ with radius $1/h$



Rem. For 1D elastic spring

$\lambda = \pm i\sqrt{K/m}$

$\Rightarrow |1 + i\sqrt{K/m}h| = \sqrt{1 + K/m\, h^2} > 1$

$\Rightarrow$ Explicit euler is always unstable on the elastic spring problem.

Other approach: Implicit method

Other approach: Implicit Euler

Explicit Euler

$u^{k+1} = u^k + h\,\mathcal{F}(u^k, t^k)$

u^k is known to compute u^{k+1}

- In the linear case

$u^{k+1} = (\mathrm{I} + h\,\mathrm{A})\,u^k + h\,b(t^k)$

Implicit Euler

$u^{k+1} = u^k + h\,\mathcal{F}(u^{k+1}, t^{k+1})$

u^{k+1} appears in RHS

$\Rightarrow$ Need to solve $u^{k+1} - h\,\mathcal{F}(u^{k+1}, t^{k+1}) = u^k$

- In the linear case : solve a linear system

$u^{k+1} = u^k + h\,\left(\mathrm{A}u^{k+1} + b(t^{k+1})\right)$

$\Rightarrow u^{k+1} = (\mathrm{I} - h\,\mathrm{A})^{-1}\,\left(u^k + h\,b(t^{k+1})\right)$

Implicit Euler - study case

Free fall under gravity

- True solution $\tilde{u}(k\,\Delta t) = p_0 + (k\,\Delta t)v_0 + \frac{(k\,\Delta t)^2}{2}\,g$

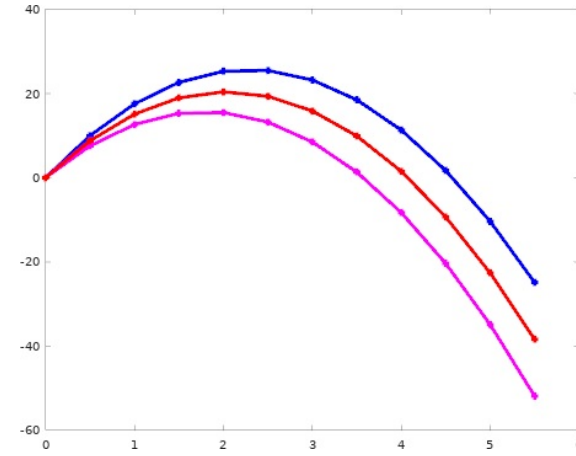
- Numerical scheme: $\begin{pmatrix} p \\ v \end{pmatrix}^{k+1} = \begin{pmatrix} 1 & -h \\ 0 & 1 \end{pmatrix}^{-1} \left(\begin{pmatrix} p \\ v \end{pmatrix}^{k} + \begin{pmatrix} 0 \\ g \end{pmatrix} \right)$

$$\Rightarrow \begin{pmatrix} p \\ v \end{pmatrix}^{k+1} = \begin{pmatrix} 1 & h \\ 0 & 1 \end{pmatrix} \begin{pmatrix} p \\ v \end{pmatrix}^{k} + \begin{pmatrix} h^2\,g \\ h\,g \end{pmatrix}$$

- Numerical solution: $p^k = p_0 + (k\,\Delta t)v_0 + \frac{k(k+1)}{2}\,(\Delta t)^2\,g$

$\Rightarrow$ Not exact : Error $e^k = |u^k - \tilde{u}(k\,\Delta t)| = \frac{k}{2}(\Delta t)^2 g$

Same error magnitude than explicit Euler



- *red: True solution*
- *magenta: Implicit Euler*
- *blue: Explicit Euler*

Implicit Euler - study case

1D spring

- True solution: permanent oscillations

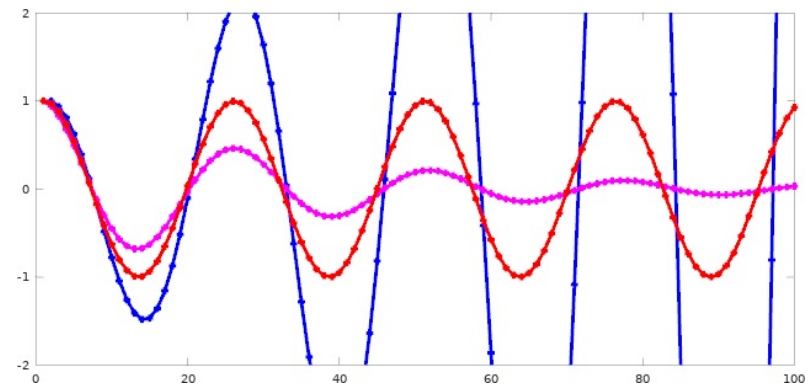
- Numerical scheme: $\begin{pmatrix} p \\ v \end{pmatrix}^{k+1} = \begin{pmatrix} 1 & -h \\ K/m\,h & 1 \end{pmatrix}^{-1} \left(\begin{pmatrix} p \\ v \end{pmatrix}^{k} + \begin{pmatrix} 0 \\ K/m\,h\,l^0 \end{pmatrix} \right)$

$$\Rightarrow \begin{pmatrix} p \\ v \end{pmatrix}^{k+1} = \frac{1}{1+h^2\,K/m} \left(\begin{pmatrix} 1 & h \\ -K/m\,h & 1 \end{pmatrix} \begin{pmatrix} p \\ v \end{pmatrix}^{k} + \begin{pmatrix} K/m\,h^2\,l^0 \\ K/m\,h\,l^0 \end{pmatrix} \right)$$

Eigenvalues of $(\mathrm{I} - \mathrm{A}h)^{-1}$ are $\frac{1 \pm i\sqrt{\frac{K}{m}}h}{1+\frac{K}{m}h^2}$

$$\Rightarrow \left| \frac{1 \pm i\sqrt{\frac{K}{m}}h}{1+\frac{K}{m}h^2} \right| = \frac{1}{\sqrt{1+\frac{K}{m}h^2}} < 1 \Rightarrow \text{always converge}$$

Even if the true solution oscillates



Stability analysis of Implicit Euler

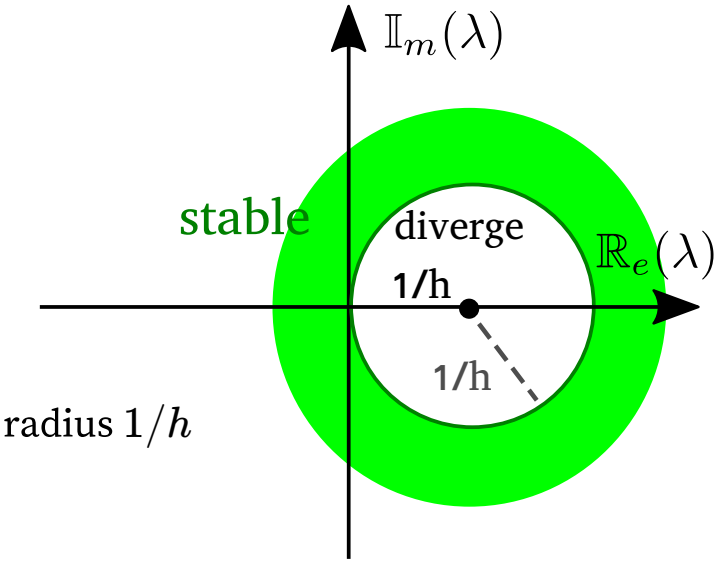
What are the general conditions for which $u'(t) = \lambda\, u(t)$ converge using Implicit Euler ?

$u^{k+1} = u^k + h\,\lambda\, u^{k+1}$

$\Rightarrow (1 - h\,\lambda)\, u^{k+1} = u^k$

$\Rightarrow u^{k+1} = \frac{1}{1-h\,\lambda}\, u^k$

Stability condition: $\left|\frac{1}{1-h\lambda}\right| \leq 1 \Rightarrow |1 - h\lambda| \geq 1$



$|1/h - \lambda| \geq 1/h$: exterior of a disc centered on $(1/h, 0)$ with radius $1/h$

$\Rightarrow$ Fully enclose $\mathbb{R}_e(\lambda) \leq 0$

$\Rightarrow$ Implicit euler is unconditionally stable

Rem. May converges even when the true solution does not.

Comparison Explicit Euler / Implicit Euler

Explicit Euler

- $u^k = u^k + h\,\mathcal{F}(u^k, t^k)$
- $u^k = (\mathrm{I} + h\,\mathrm{A})\,u^k + h\,b(t^k)$
- Accuracy: 1st Order
- Stability:

  Conditional $|1 + h\lambda| \geq 1$

  Solution to spring model diverges

Implicit Euler

- $u^{k+1} = u^k + h\,\mathcal{F}(u^{k+1}, t^{k+1})$
- $u^k = (\mathrm{I} - h\,\mathrm{A})^{-1}\left(u^k + h\,b(t^{k+1})\right)$
- Accuracy: 1st Order
- Stability:

  Unconditionnaly stable

  Solution to spring model converge to l^0

Higher order accurate methods : Runge-Kutta

Higher order method

Higher accuracy can be achived using Taylor expansion.

ex. $u^{k+1} = u^k + h\,\mathcal{F}(u^k, t^k) + \dfrac{h^2}{2}\dfrac{\mathrm{d}\mathcal{F}}{\mathrm{d}t}(u^k, t^k)$

- Second order accurate: **2nd order explicit Euler**

- Can achieve arbitrary accuracy.

- In practice: computing derivatives of $\mathcal{F}$ is complex.

$\Rightarrow$ Not often used

Runge-Kutta methods

Runge-Kutta numerical methods allow to

- Reach higher order accuracy
- Only involve knowledge of $\mathcal{F}$, without its derivatives
- Involves several evaluation of $\mathcal{F}$ at various points

2nd order Runge-Kutta: RK2

$$u^{k+1} = u^k + \frac{1}{2}(k_1 + k_2)$$
$$k_1 = h\,\mathcal{F}(u^k, t^k)$$
$$k_2 = h\,\mathcal{F}(u^k + k_1, t^k + h)$$

Accuracy, stability ?

Computing Accuracy

Reminder: Local truncation error

$\tau_k = \|\tilde{u}(t^k + h) - u(t^k + h)\|$

Assuming true solution at time t_k: $\tilde{u}(t^k) = u(t^k)$ (and all its derivatives).

General methodology to compute accuracy

(1) Compute Taylor expansion of the numerical scheme

- Express $u(t^k + h)$ at position (u^k, t^k)

(2) Compute Taylor expansion of the exact differential equation

- Express $\tilde{u}(t^k + h)$ at position (u^k, t^k), given $\tilde{u}'(t^k) = \mathcal{F}(u^k, t^k)$

(3) Compare both expressions

RK2 - Accuracy

(1) Compute Taylor expansion of the numerical scheme

RK2 definition: $u(t^k + h) = u^k + \frac{1}{2}(k_1 + k_2)$

$k_1 = h\,\mathcal{F}(u^k, t^k)$

$k_2 = h\,\mathcal{F}(u^k + k_1, t^k + h)$

$$\Rightarrow k_2 = h\left(\mathcal{F}(u^k, t^k) + k_1\,\frac{\partial \mathcal{F}}{\partial u}(u^k, t^k) + h\,\frac{\partial \mathcal{F}}{\partial t}(u^k, t^k) + \mathcal{O}(h^2)\right) \quad \text{(differential on } k_1 \text{ and on } h\text{)}$$

$$\Rightarrow k_2 = h\mathcal{F} + h^2\,\mathcal{F}\frac{\partial F}{\partial u} + h^2\frac{\partial \mathcal{F}}{\partial t} + \mathcal{O}(h^3) \qquad \textit{(dropping parameters } (u^k, t^k)\textit{)}$$

$$u(t^k + h) = u^k + \frac{1}{2}\left[h\mathcal{F} + \left(h\,\mathcal{F} + h^2\,\frac{\partial \mathcal{F}}{\partial u}\,\mathcal{F} + h^2\,\frac{\partial \mathcal{F}}{\partial t} + \mathcal{O}(h^3)\right)\right]$$

$$\Rightarrow u(t^k + h) = u^k + h\,\mathcal{F} + \frac{h^2}{2}\left(\frac{\partial \mathcal{F}}{\partial u}\,\mathcal{F} + \frac{\partial F}{\partial t}\right) + \mathcal{O}(h^3)$$

RK2 - Accuracy

(2) Compute Taylor expansion of the exact differential equation

$$\tilde{u}(t^k + h) = \tilde{u}(t^k) + h\,\tilde{u}'(t^k) + \frac{h^2}{2}\tilde{u}''(t^k) + \mathcal{O}(h^3)$$

Assuming exact solution at t^k: $\tilde{u}^{(n)}(t^k) = u^{(n)}(t^k)$ + Injecting the ODE relation $u'(t^k) = \mathcal{F}(u^k, t^k)$

$$\Rightarrow \tilde{u}(t^k + h) = u(t^k) + h\,\mathcal{F}(u^k, t^k) + \frac{h^2}{2}\frac{\mathrm{d}\mathcal{F}}{\mathrm{d}t}(u^k, t^k) + \mathcal{O}(h^3)$$

$$\Rightarrow \tilde{u}(t^k + h) = u(t^k) + h\,\mathcal{F}(u^k, t^k) + \frac{h^2}{2}\left(\frac{\partial \mathcal{F}}{\partial u}(u^k, t^k)\,u'(t^k) + \frac{\partial \mathcal{F}}{\partial t}(u^k, t^k)\right) + \mathcal{O}(h^3)$$

Drop parameter $(u^k, t^k) \Rightarrow \tilde{u}(t^k + h) = u^k + h\,\mathcal{F} + \frac{h^2}{2}\left(\frac{\partial \mathcal{F}}{\partial u}\,\mathcal{F} + \frac{\partial F}{\partial t}\right) + \mathcal{O}(h^3)$

(3) Compare both epxressions

$$\tau_k = \|\tilde{u}(t^k + h) - u(t^k + h)\| = \mathcal{O}(h^3)$$

$\Rightarrow$ **RK2 is 2nd order accurate**

RK2 - Stability

Study $u'(t) = \lambda\, u(t) \Rightarrow \mathcal{F}(u,t) = \lambda\, u(t)$

- $k_1 = h\,\mathcal{F}(u^k, t^k) = h\,\lambda\,u^k$
- $k_2 = h\,\mathcal{F}(u^k + k_1, t^k + h) = h\,\lambda\,(u^k + h\lambda\,u^k) = (h\lambda + h^2\lambda^2)\,u^k$

$\Rightarrow u^{k+1} = u^k + \frac{1}{2}(k_1 + k_2)$

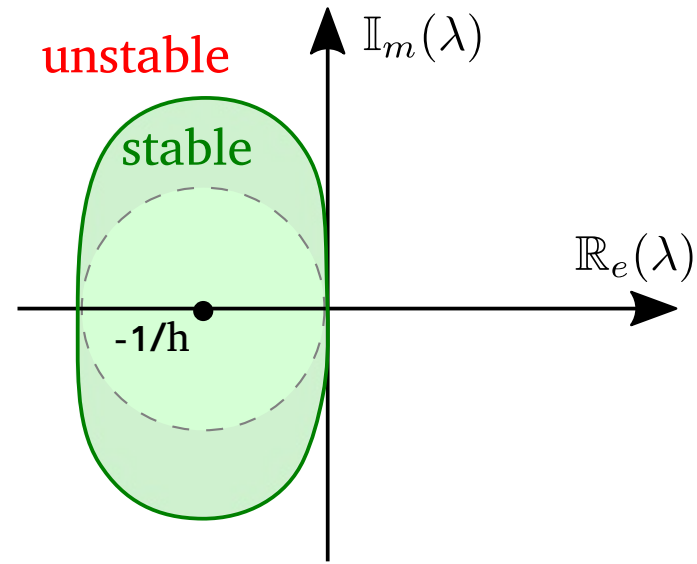
$\Rightarrow u^{k+1} = (1 + h\lambda + \frac{h^2}{2}\lambda^2)\,u^k$

Stability condition $\left|1 + h\lambda + \frac{h^2}{2}\lambda^2\right| \leq 1$

$\Rightarrow$ RK2 is conditionnaly stable (explicit method)

More stable than explicit Euler

(Still unstable for oscillatory 1D spring)



Other Runge-Kutta methods

Midpoint method (2nd order accuracy)

$$
\begin{aligned}
k_1 &= h\,\mathcal{F}(u^k, t^k) \\
k_2 &= h\,\mathcal{F}(u^k + k_1/2, t^k + h/2) \\
u^{k+1} &= u^k + h\,k_2
\end{aligned}
$$

RK4 (Classical Runge-Kutta)

$$
\begin{aligned}
k_1 &= h\,\mathcal{F}(u^k, t^k) \\
k_2 &= h\,\mathcal{F}\left(u^k + \frac{k_1}{2}, t^k + \frac{h}{2}\right) \\
k_3 &= h\,\mathcal{F}\left(u^k + \frac{k_2}{2}, t^k + \frac{h}{2}\right) \\
k_4 &= h\,\mathcal{F}\left(u^k + k_3, t^k + h\right) \\
u^{k+1} &= u^k + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4)
\end{aligned}
$$

RK4 - Case study

- Rk4 conditionally stable for oscillating spring

  Not permanent oscillations: Slight decrease of magnitude through time

- Large improvement of accuracy compared to implicit Euler

Stability region: $\left|1 + h\lambda + \frac{h^2}{2}\lambda + \frac{h^3}{6}\lambda^3 + \frac{1}{24}h^4\lambda^4\right| \leq 1$

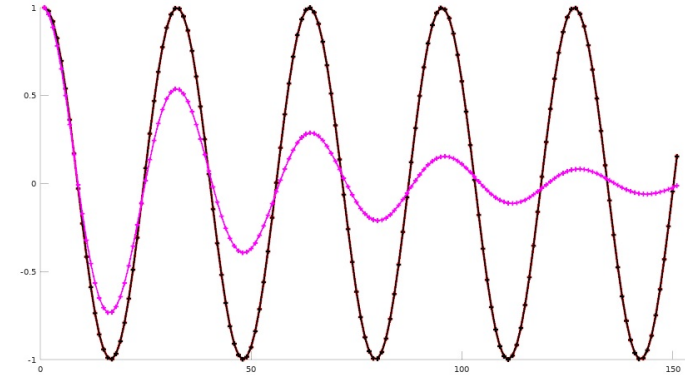
In the case of oscillating spring: $\lambda = i\sqrt{K/m} = i\omega$

Stable if $\left|1 + ih\omega - \frac{h^2}{2}\omega^2 - i\frac{h^3}{6}\omega^3 + \frac{h^4}{24}\omega^4\right| \leq 1$

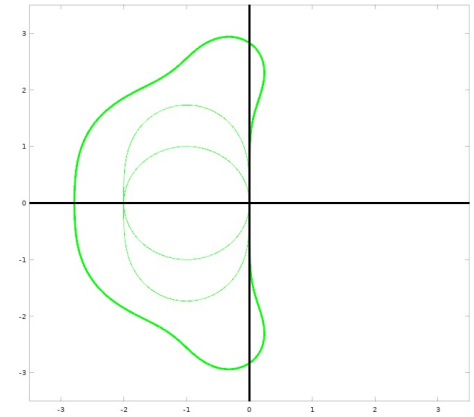
$\Rightarrow 1 - \frac{h^6\omega^6}{72} + \frac{h^8\omega^8}{576} \leq 1$

$\Rightarrow h^6\,\omega^6\,(h^2\omega^2 - 8)/576 \leq 0$

$\Rightarrow h \leq \frac{2^{3/2}}{\omega} = \frac{2^{3/2}}{\sqrt{K/m}} \simeq \frac{2.8}{\sqrt{K/m}}$



$h = 0.2$, error rk4 $\simeq 10^{-4}$
- *red: true solution*
- *black: rk4*
- *magenta: implicit Euler*



Dormand Prince (ode45)

$$
\begin{aligned}
k_1 &= h\,\mathcal{F}(u^k, t^k) \\
k_2 &= h\,\mathcal{F}\left(u^k + \frac{1}{5}k_1, t^k + \frac{1}{5}h\right) \\
k_3 &= h\,\mathcal{F}\left(u^k + \frac{3}{40}k_1 + \frac{9}{40}k_2, t^k + \frac{3}{10}h\right) \\
k_4 &= h\,\mathcal{F}\left(u^k + \frac{44}{45}k_1 - \frac{56}{15}k_2 + \frac{32}{9}k_3, t^k + \frac{4}{5}h\right) \\
k_5 &= h\,\mathcal{F}\left(u^k + \frac{19372}{6561}k_1 - \frac{25360}{2187}k_2 + \frac{64448}{6561}k_3 - \frac{212}{729}k_4, t^k + \frac{8}{9}h\right) \\
k_6 &= h\,\mathcal{F}\left(u^k + \frac{9017}{3168}k_1 - \frac{355}{33}k_2 + \frac{46732}{5247}k_3 + \frac{49}{176}k_4 - \frac{5103}{18656}k_5, t^k + h\right) \\
k_7 &= h\,\mathcal{F}\left(u^k + \frac{35}{384}k_1 + \frac{500}{1113}k_3 + \frac{125}{192}k_4 - \frac{2187}{6784}k_5 + \frac{11}{84}k_6, t^k + h\right)
\end{aligned}
$$

$$
u_5^{k+1} = u^k + h\left(\frac{35}{384}k_1 + \frac{500}{1113}k_3 + \frac{125}{192}k_4 - \frac{2187}{6784}k_5 + \frac{11}{84}k_6\right)
$$

$$
u_4^{k+1} = u^k + h\left(\frac{5179}{57600}k_1 + \frac{7571}{16695}k_3 + \frac{393}{640}k_4 - \frac{92097}{339200}k_5 + \frac{187}{2100}k_6 + \frac{1}{40}k_7\right)
$$

u_5^{k+1} is 5th order, u_4^{k+1} is 4th order $\Rightarrow$ Automatic error estimation for adaptive time steps.

Embedded method

[J. Dormand, P. Prince. A family of embedded Runge-Kutta formulae. J. of Computation and Applied Mathematics, 1980].

Symplectic methods / semi-implicit

Introduction to symplectic methods

Standard approaches trade-off

- Explicit methods: (+) Simple to compute, (-) limited stability
- Implicit methods: (-) Hard to compute (especially on non linear functions), (+) very stable
- Oscillatory systems are not easy to model
  (-) Numerical solution either diverge or converge.

Symplectic approach

- *Remark*: Mechanical systems have position and speed variables
  - Derivative of position is linear w/r speed
  - Derivative of speed is more complex (forces - non linear)

$\Rightarrow$ *General idea*: separate treatment of speed and position

Semi-implicit:

- Implicit scheme for position p^{k+1} (linear part)
- Explicit scheme for speed v^{k+1} (non linear part)

$\Rightarrow$ In practice: use speed v^{k+1} to evaluate p^{k+1}.

Pro

(+) As simple as explicit method to implement
(+) Improved stability
(+) Well adapted to oscillatory systems

Semi implicit method

Simplest semi-implicit method: **Semi-implicit Euler** / **Verlet**

General case

$$v^{k+1} = v^k + h\,\mathcal{F}_v(p^k, v^k, t^k)$$

$$p^{k+1} = p^k + h\,\mathcal{F}_p(p^k, v^{k+1}, t^k)$$

Application to classical mechanical cases

$p'(t) = v(t), m\,v'(t) = F(p, v, t)$

$$\Rightarrow \begin{cases} v^{k+1} = v^k + h\,F(p^k, v^k, t^k)/m \\ p^{k+1} = p^k + h\,v^{k+1} \end{cases}$$

(+) Trivially easy to convert explicit Euler to semi-implicit Euler

Expressed using positions only

$$p^{k+1} = p^k + h(v^k + h\,F(p^k, v^k, t^k))$$

$$p^{k+1} = p^k + h\left(\tfrac{p^k - p^{k-1}}{h} + h\,F(p^k, v^k, t^k)/m\right)$$

$$\Rightarrow p^{k+1} = 2\,p^k - p^{k-1} + h^2\,F(p, v, t)/m$$

1st order accurate (like explicit/implicit Euler) in position and speed.

Stability on oscillatory system

1D spring system: $F(p^k, v^k, t^k) = -K\,p^k$

$p^{k+1} = 2\,p^k - p^{k-1} - h^2\,K/m\,p^k$

$\Rightarrow p^{k+1} = (2 - h^2\,K/m)\,p^k - p^{k-1}$

Stable and permanent oscillation when $h < \frac{2}{\sqrt{K/m}}$

Demonstration

- Study the roots of the associated caracteristic equation
- $x^2 + (y-2)x + 1 = 0$, with $y = h^2\,K/m$
- Discriminant $\Delta = y(y-4)$, with roots $r = \frac{(2-y) \pm \sqrt{y(y-4)}}{2}$

- Two cases:

  $\Delta < 0 \Rightarrow y \in]0,4[: r = \frac{(2-y) \pm i\sqrt{y(4-y)}}{2} \Rightarrow |r| = 1/2\,\sqrt{(2-y)^2 + y(4-y)} = 1 \Rightarrow$ Permanent oscillations (stable)

  $\Delta \geq 0 \Rightarrow y \leq 0,$ or $y \geq 4 : |r| > 1$ Unstable solution

- Finally, stable for $y \in]0,4[\Rightarrow h^2 K/m < 4 \Rightarrow h < \frac{2}{\sqrt{K/m}}$, and system oscillate permanently

Higher order symplectic

2nd order Velocity Verlet

$$\begin{cases} v^{k+1/2} &= v^k + \frac{h}{2} F(p^k, v^k, t^k)/m \\ p^{k+1} &= p^k + h\, v^{k+1/2} \\ v^{k+1} &= v^{k+1/2} + \frac{h}{2} F(p^{k+1}, v^{k+1/2}, t^{k+1})/m \end{cases}$$

- Remains stable with permanent oscillation for $h \leq \frac{2}{\sqrt{K/m}}$

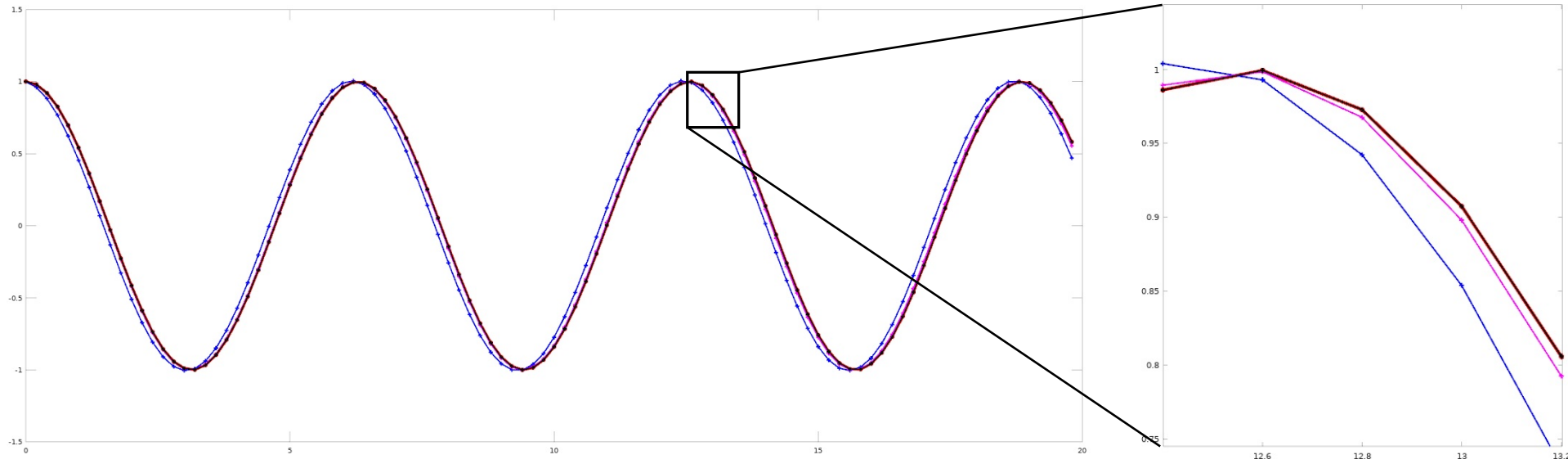
- Still simple to implement

Example for 1D elastic spring

```
for(int k=0; k<N; ++k) {
    v = v + h/2 * (-K/m*p);
    p = p + h*v;
    v = v + h/2 * (-K/m*p);
}
```

Comparison between approaches

Small $h = 0.2/\omega$

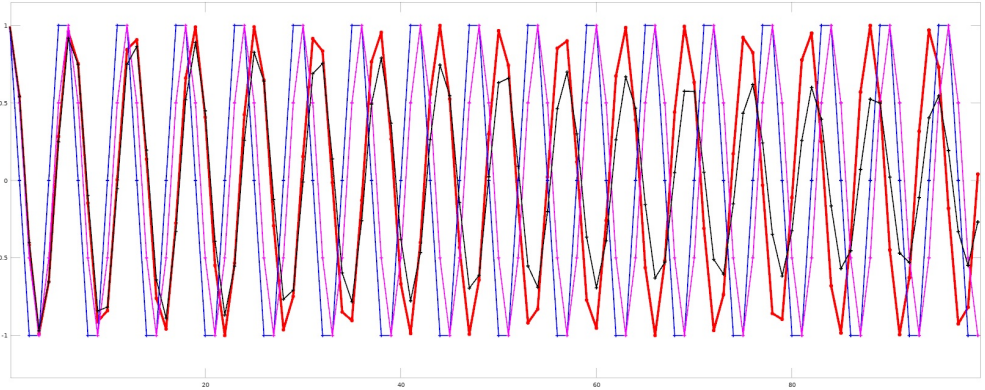


True solution , *Semi-implicit Euler* , *Velocity Verlet* , *Runge-Kutta RK4*

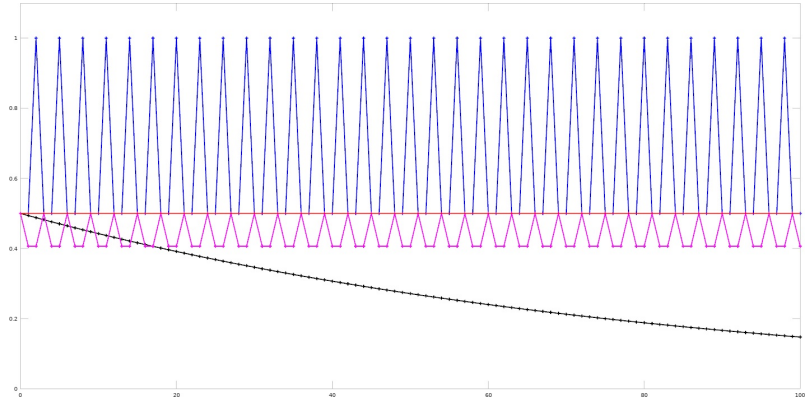
- RK4 - best behavior (undistinguishable from true solution)

Comparison between approaches

Larger $h = 1.0/\omega$



Temporal evolution of p^k



Temporal evolution of energy

$$E = 1/2m\,(v^k)^2 + 1/2K(p^k)^2$$

True solution , *Semi-implicit Euler* , *Velocity Verlet* , *Runge-Kutta RK4*

- RK4 loose energy and p^k converge toward l^0

- Symplectic integrator keep oscillating

Summary and extensions

Summary of numerical schemes

Implicit methods

(+) Good to deal with **stiff problem** - very stable

(-) Add numerical damping (converge even if solution oscillates)

(-) Hard/computationally costly to apply on non linear problem

Explicit Runge-Kutta

(+) Good **accuracy**

(+) Efficient to apply

(+/-) Stability OK for non-stiff problem, diverge on stiff problem

(-) Artificial damping for constant energy system

Symplectic integrator

(+) Handle well constant energy system, preserves energy (Hamiltonian systems)

(+) Simple and efficient to implement

(-) Less accurate than RK

(-) Diverge on stiff problem

Explicit Euler should be avoided - worst in all situations

Extension - Automatic time steping

Ajust h to limit errors at each step

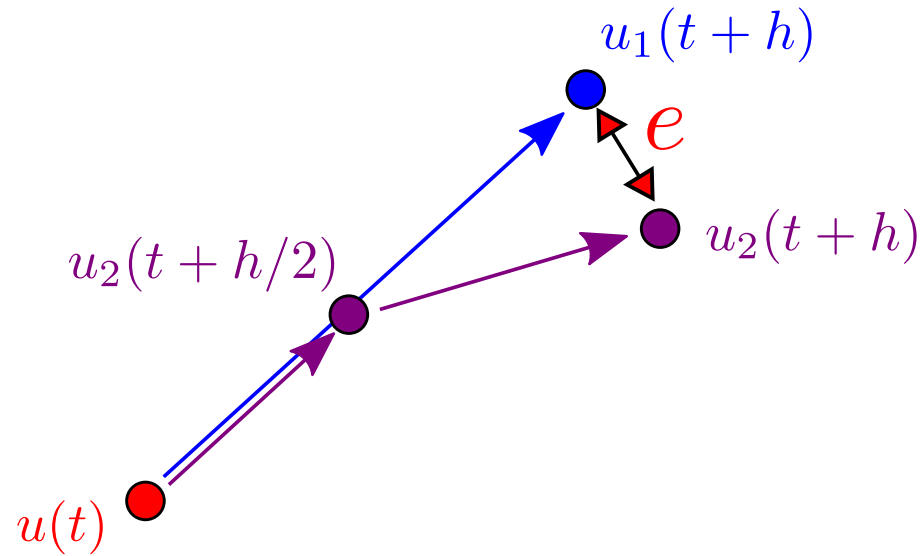
(1) Evaluate error in comparing:

- u_1^k computed using one step h
- u_2^k computed using two steps $h/2$.
- $e^k = \|u_1^k - u_2^k\|$

(2) Using embedded method $e^k = \|u_1^k - u_2^k\|$

Update

- $h^{new} = A\ h$ when $e^k < C_1$, $(A > 1)$
- $h^{new} = h/A$ when $e^k > C_2$



Implicit Euler on non-linear problem

$u^{k+1} = u^k + h\,\mathcal{F}(u^{k+1}, t^{k+1})$

- For high dimensional $\mathcal{F}$ - no explicit known inverse function

- Idea: Linearize $\mathcal{F}$ at u^k, assuming $\|u^{k+1} - u^k\|$ small.

$$u^{k+1} = u^k + h\left(\mathcal{F}(u^k, t^{k+1}) + (u^{k+1} - u^k)\frac{\partial \mathcal{F}}{\partial u}(u^k, t^{k+1})\right)$$

$$\Rightarrow \left(\mathrm{I} - h\,\tfrac{\partial \mathcal{F}}{\partial u}(u^k, t^{k+1})\right) u^{k+1} = \left(\mathrm{I} - h\,\tfrac{\partial \mathcal{F}}{\partial u}(u^k, t^{k+1})\right) u^k + h\,\mathcal{F}(u^k, t^{k+1})$$

$$u^{k+1} = u^k + \left(\mathrm{I} - h\,\frac{\partial \mathcal{F}}{\partial u}(u^k, t^{k+1})\right)^{-1} \mathcal{F}(u^k, t^{k+1})$$

- In theory only conditionally stable; In practice: very stable

- Requires the expression of Jacobian matrix $\frac{\partial \mathcal{F}}{\partial u}$ - large sparse matrix
- Requires inversion of a linear system at every steps

$\Rightarrow$ Used for stable simulation with large time step

Implicit Euler on non-linear problem - particle system

For standard particles systems

- $p^{k+1} = p^k + h\, v^k$
- $v^{k+1} = v^k + h\, \mathrm{M}^{-1}\, F(p^{k+1}, v^{k+1})$

With M the diagonal matrix of particles masses, assuming force F doesn't depends on t.

Linear approximation on force F

$$\mathrm{M}\, v^{k+1} = \mathrm{M}\, v^k + h\Big(F(p^k, v^k) + \underbrace{(p^{k+1} - p^k)}_{h\, v^{k+1}} \frac{\partial F}{\partial p}(p^k, v^k) + (v^{k+1} - v^k) \frac{\partial F}{\partial v}(p^k, v^k)\Big)$$

$$\Rightarrow \left(\mathrm{M} - h\frac{\partial F}{\partial v} - h^2 \frac{\partial F}{\partial p}\right) v^{k+1} = \left(\mathrm{M} - h\, \frac{\partial F}{\partial v}\right) + h\, F$$

[D. Baraff, A. Witkin. Large steps in Cloth Simulation. ACM SIGGRAPH 98]

Position based dynamics (PBD)

Non-linear constraints (non penetration, constant length, etc)

- can make explicit integration diverging (arbitrary gain of energy)
- are hard to integrate within implicit integrators

PBD - Use symplectic integrator expressed using position only

- Speed is computed implicitly as $(p^{k+1} - p^k)/h$
- Handle constraints using explicit projection of positions.

```
PBD algorithm
For all k
    Integrate position (without constraints) p[k+1]=integrator(p[k],p[k-1],t}
    For all constraints
        Project p[k+1] on constraints
    Compute new speed if needed v[k+1]=(p[k+1]-p[k])/h
```

(+) Unconditionnaly stable even for stiff constraints

(+) Simple to implement

(-) Low accuracy, no energy preserving

Popular in Computer Graphics

[M. Muller et al. Position Based Dynamics. VRIPHYS 2006]

Extensions: XPBD, Projective dynamics, ...