

MAINTITLE

Nikolaj Roager Christensen

Student Colloquium in Physics and Astronomy, Aarhus University

March 2021

TITLEIMAGE

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Introduction TIME 3 minutes TIME

Theory and physical background TIME 10 minutes TIME

Solved systems

Eulers Method and the 4th order Runge-Kutta Method TIME 10 minutes TIME

Euler's Method

4th order Runge Kutta

Testing the methods [5 MIN]

Introducing Adaptive step size [5 MIN]

When adaptive step-size fails

Non-analytical systems: Toroidal coils and dipoles [10 MIN]

Conclusion and question

Introduction, what and why

Introduction, what and why

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How: Numeric-ODE solvers

- ▶ When analytical solutions are not practical.

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- ▶ Testing experimental setups.
- ▶ Simulations are not experiments!

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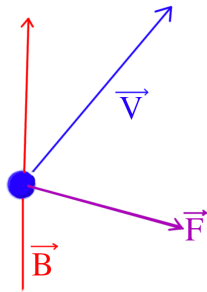
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- ▶ Only 1 particle! so pre-programmed depending on the setup.
- ▶ Could use potentials $\phi(\vec{r}, t)$ $\vec{A}(\vec{r}, t)$ and Hamiltonian.

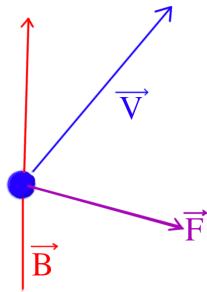
Known results, cyclotron motion \vec{B} fields



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$$dW_{\vec{B}} = \vec{F}_B \cdot d\vec{r} \propto (\vec{v} \times \vec{B}) \cdot \vec{v} = 0.$$



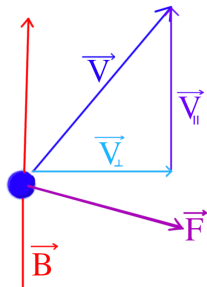
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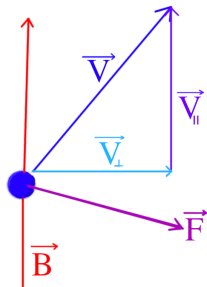
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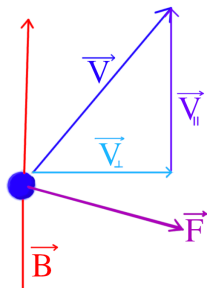
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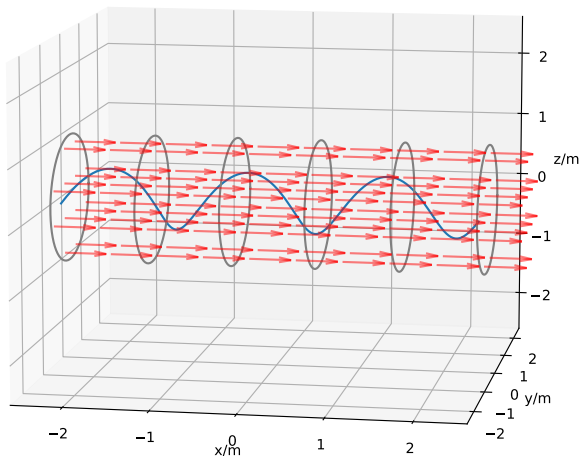
$$|\vec{F}_B| = |q(\vec{v} \times \vec{B})| = |qv_{\perp}B|.$$

- Same as Centripetal force:
Cyclotron motion
- Cyclotron radius and
frequency:

$$R = \frac{v_{\perp} m}{|q|B} \quad \omega_c = \frac{|q|B}{m}.$$

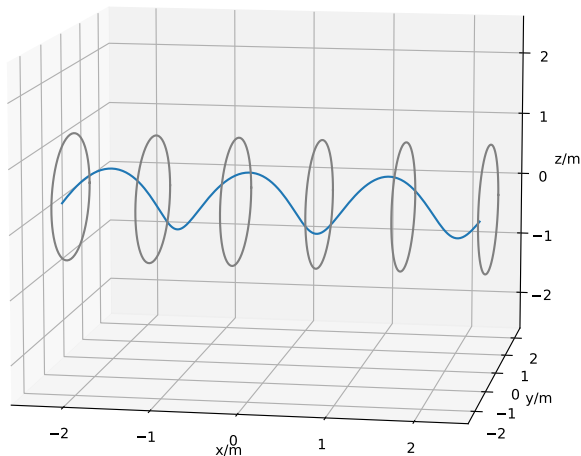


Analytical solution: Protons in a Solenoid



Solenoid with $N = 1000$ turns per m , $I = 5$ A, $r = 1$ m, $|\vec{B}| \approx 6$ mT.
Proton with $E_{kin} = 1$ MeV/ c^2 ($|v| \approx 3.195 \times 10^5$ m/s)

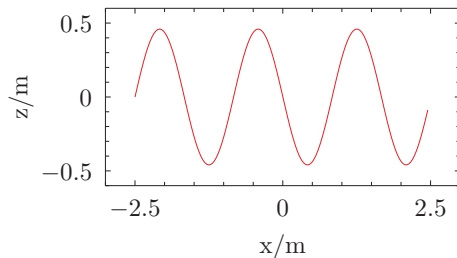
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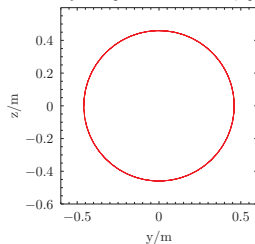
$$R \approx 0.5 \text{ m} \sin(\theta) \quad T = \frac{2\pi}{\omega_c} \approx 10 \mu\text{s}$$

Analytical solution: Protons in a Solenoid

Analytical: proton in a solenoid, side/front-view



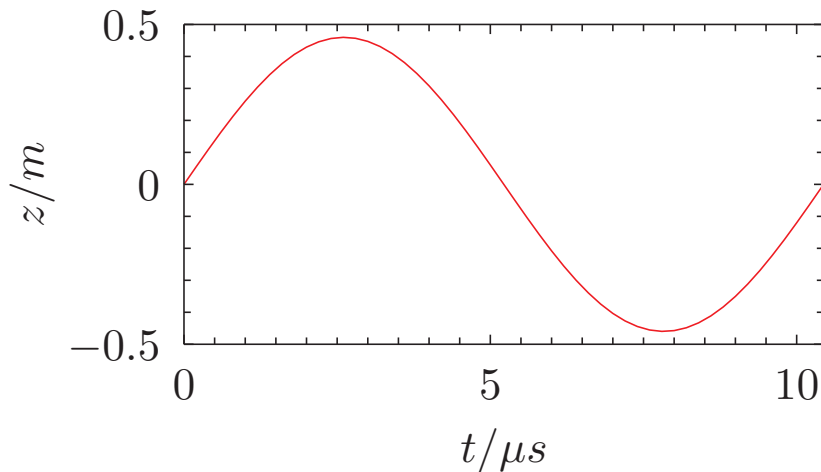
Analytical: proton in a solenoid, speed



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Analytical solution: Protons in a Solenoid

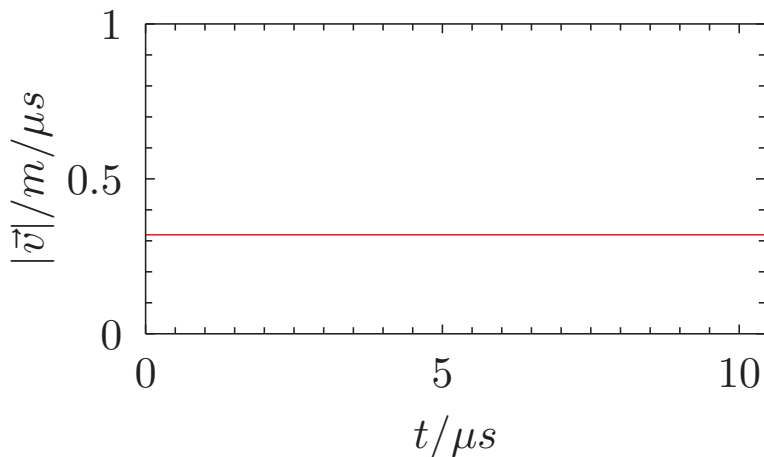
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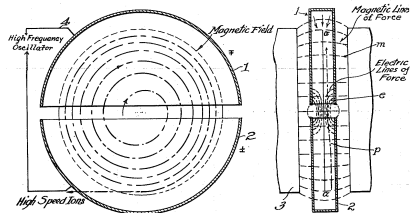
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Cyclotron accelerator

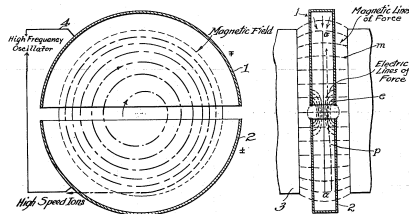
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Ernest O. Lawrence, 1934, U.S.
Patent 1,948,384; image in
Public Domain.

Cyclotron accelerator

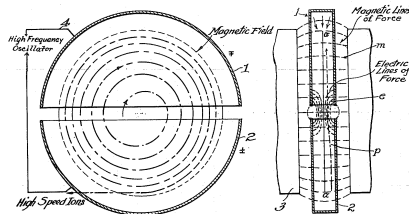
- ▶ Electric forces do work.
- ▶ Practical example, the Cyclotron.



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- ▶ Practical example, the Cyclotron.
- ▶ Single gap, oscillating field.

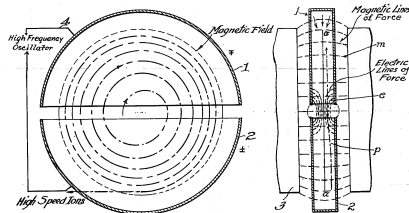


Ernest O. Lawrence, 1934, U.S. Patent 1,948,384; image in Public Domain.

Cyclotron accelerator

- ▶ Electric forces do work.
- ▶ Practical example, the Cyclotron.
- ▶ Single gap, oscillating field.
- ▶ Final speed:

$$\frac{R|q|B}{m} = v_{\perp}$$



Ernest O. Lawrence, 1934, U.S. Patent 1,948,384; image in Public Domain.

Ordinary differential equation*s.

- ▶ Sources: Zeigler et al. Theory of Modeling and Simulation (Third edition) chapter 3
- ▶ Algorithms exists for ODEs:

$$\dot{\mathbf{X}} = f_{ode}(\mathbf{X}(t), t).$$

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- Here:

$$\mathbf{X} = \begin{pmatrix} \vec{r} \\ \dot{\vec{r}} \end{pmatrix} \quad f_{ode}(\vec{r}, t) = \begin{pmatrix} \dot{\vec{r}} \\ \frac{q}{m}(\dot{\vec{r}} \times \vec{B}(\vec{r}, t) + \vec{E}(\vec{r}, t)) \end{pmatrix}.$$

The ODE to solve

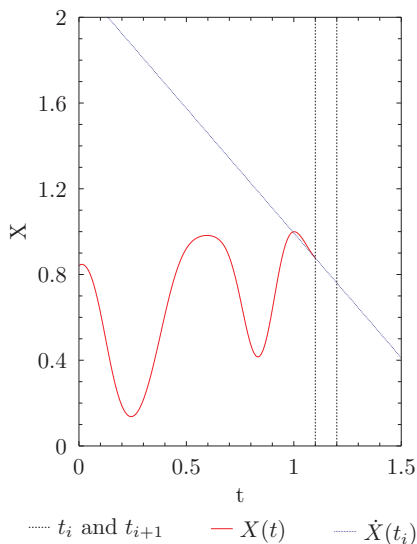
```
auto ODE = [...](const state_type Data, state_type &
    dDatadt, const double t){
    //Extract position and velocity from data
    vec pos = vec(Data[0],Data[1],Data[2]);
    vec velocity = vec(Data[3],Data[4],Data[5]);

    //Lorentz+Newtons 2nd law
    vec F = Charge*(Fields.get_Efield(pos,t)+
        cross(velocity,Fields.get_Bfield(pos,t)));
    vec dVdt = F*Inv_mass;

    //Save derivative of data
    dDatadt[0]=velocity.x;
    ...
};
```


The Forward Euler's Method

- ▶ Let $h = t_{i+1} - t_i > 0$ be constant.
- ▶ Bernard P. Zeigler et al.
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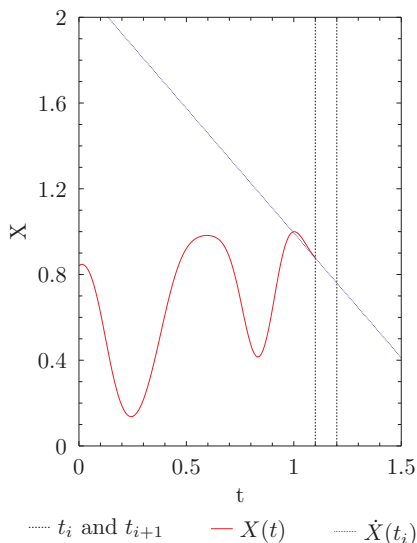


The Forward Euler's Method

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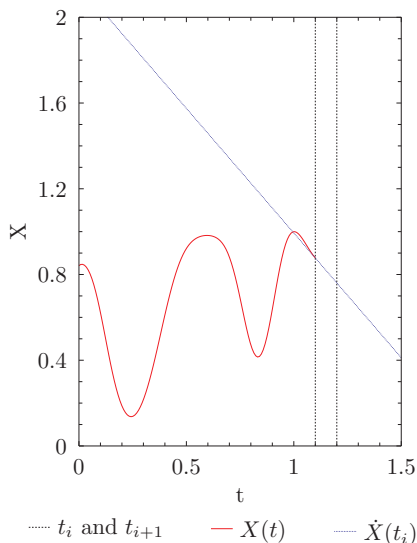
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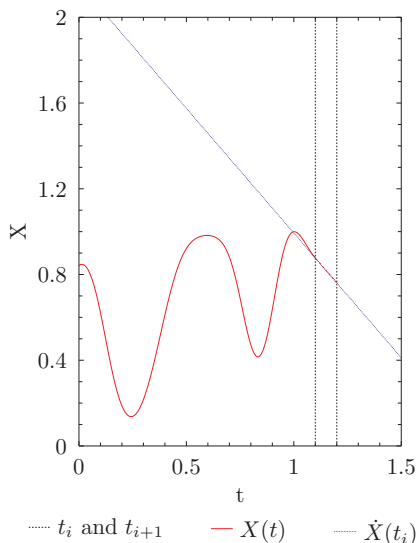
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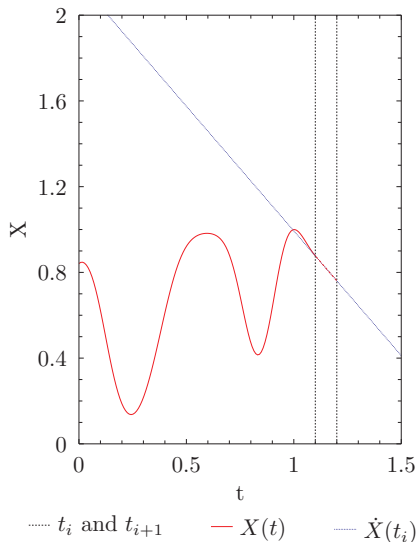
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- ▶ How would you find $\mathbf{X}(t_{i+1})$:
- ▶ (Explicit) Forward Euler's Method:

$$\mathbf{X}(t_{i+1}) = \mathbf{X}(t_i) + hf_{ode}(\mathbf{X}(t_i), t_i).$$

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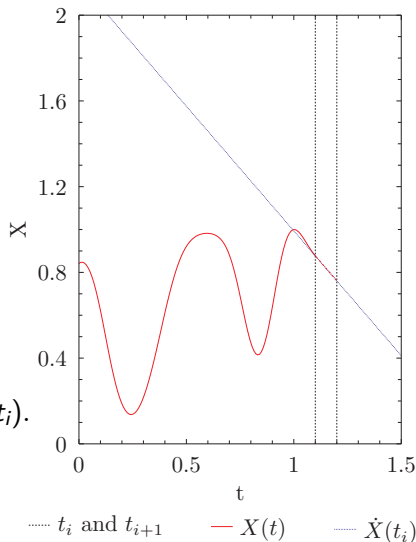
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The Forward Euler's Method

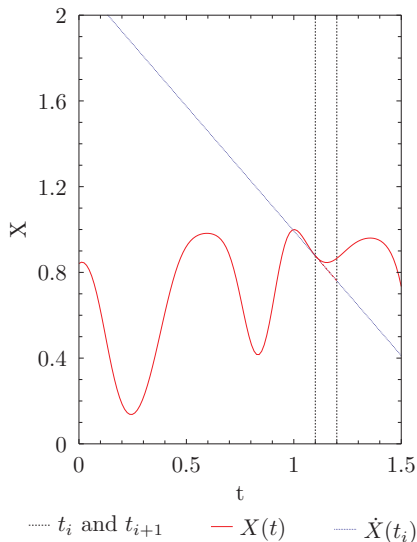
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- ▶ “Local truncation error” $h^2 = h^{p+1}$.
- ▶ Global error $h = h^p$.
- ▶ Convergence, but not uniform.

Why does this work? The Runge Kutta family

- In general.

$$\mathbf{X}(t_{i+1}) - \mathbf{X}(t_i) = \int_{t_i}^{t_{i+1}} f_{ode}(\mathbf{X}(t), t) dt$$

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$$\mathbf{X}(t_{i+1}) - \mathbf{X}(t_i) = \int_{t_i}^{t'} f_{ode}(\mathbf{X}(t), t) dt + \dots \int_{t^{(m)}}^{t_{i+1}} f_{ode}(\mathbf{X}(t), t) dt$$

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- Use $f_{ode}(\mathbf{X}(t_i), t_i)$ to approximate $\mathbf{X}(\tau_1)$ etc.
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Explicit Runge Kutta methods

- We want:

$$\mathbf{X}(t_{i+1}) - \mathbf{X}(t_i) = h \sum_{j=1}^m b_j \mathbf{K}_j$$

- With: $\mathbf{K}_1 = f_{ode}(\mathbf{X}(t_i), t_i)$, $\mathbf{K}_2 = f_{ode}(\mathbf{X}(t_i) + ha_{21}\mathbf{K}_1, t_i + c_2h)$
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- Can be found with taylor expansion of $\mathbf{X}(t_i)$.
- 2nd order (Heun's method):

$$\mathbf{X}(t_{i+1}) - \mathbf{X}(t_i) = \frac{h}{2}(\mathbf{k}_1 + \mathbf{k}_2)$$

$$\mathbf{k}_1 = f_{ode}(\mathbf{X}(t_i), t_i)$$

$$\mathbf{k}_2 = f_{ode}(\mathbf{X}(t_i) + h\mathbf{k}_1, t_i + h)$$

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The 4th order Runge Kutta method

- RK4, often simply called the Runge Kutta method:

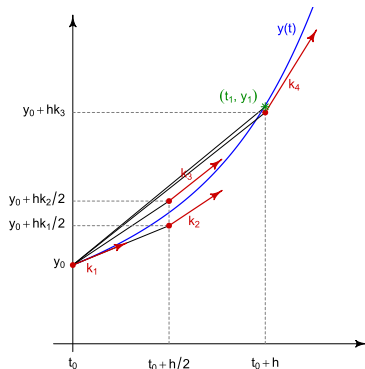
$$\mathbf{X}(t_{i+1}) - \mathbf{X}(t_i) = \frac{h}{6}(\mathbf{k}_1 + 2\mathbf{k}_2 + 2\mathbf{k}_3 + \mathbf{k}_4)$$

$$\mathbf{k}_1 = f_{ode}(\mathbf{X}(t_i), t_i)$$

$$\mathbf{k}_2 = f_{ode}\left(\mathbf{X}(t_i) + \frac{h}{2}\mathbf{k}_1, t_i + \frac{h}{2}\right)$$

$$\mathbf{k}_3 = f_{ode}\left(\mathbf{X}(t_i) + \frac{h}{2}\mathbf{k}_2, t_i + \frac{h}{2}\right)$$

$$\mathbf{k}_4 = f_{ode}(\mathbf{X}(t_i) + h\mathbf{k}_3, t_i + h)$$



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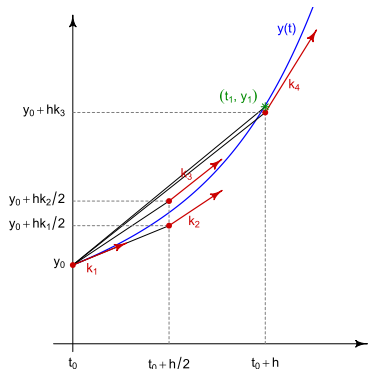
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$$\mathbf{k}_2 = f_{ode}\left(\mathbf{X}(t_i) + \frac{h}{2}\mathbf{k}_1, t_i + \frac{h}{2}\right)$$

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$$\mathbf{k}_4 = f_{ode}(\mathbf{X}(t_i) + h\mathbf{k}_3, t_i + h)$$



- Almost default in scipy.
`integrate.solve_ivp` and
`matlab ode45`.

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Euler Implementations

[fragile]

```
state_type Data = Data0;
state_type dDatadt;
size_t time_res = T/timestep;
for (size_t i = 1; i < time_res; ++i)
{
    double t=i*dt;
    ODE(Data,dDatadt,t);
    //Euler time evolution
    //Data +=timestep*dDatadt; 1 variable
    for (uint i = 0; i<Data.size(); ++i)
        Data[i]+=timestep*dDatadt[i];
    save_step( Data , i*timestep );
};
```

RK4 Implementations (1/2)

```
state_type Data = Data0;
state_type temp=Data0;
state_type K1,K2,K3,K4;
size_t time_res = T/timestep;
for (size_t i = 1; i < time_res; ++i)
{
    double t=i*timestep;
    //substep 1
    ODE(Data,K1,t);
    for (uint i = 0; i<Data.size(); ++i)
        temp[i]=Data[i]+timestep*K1[i]/2;
    //substep 2
    ODE(Data,K2,t+timestep/2);
    for (uint i = 0; i<Data.size(); ++i)
        temp[i]=Data[i]+timestep*K2[i]/2;
```

RK4 Implementations (2/2)

```
//substep 3
ODE(Data,K3,t+timestep/2);
for (uint i = 0; i<Data.size(); ++i)
    temp[i]=Data[i]+timestep*K3[i];
//substep 4
ODE(temp,K4,t+timestep);
//Read data
for (uint i = 0; i<Data.size(); ++i)
    Data[i]+=timestep*(K1[i]+2.0*K2[i]+2.0*K3[i]+
K4[i])/6.0;
    save_step( Data , i*timestep );
}
```


“Correct” way

```
#include <boost/array.hpp>
#include <boost/numeric/odeint.hpp>
using namespace boost::numeric::odeint;
typedef boost::array< double, 6 > state_type;
...
size_t steps = integrate_const(
    runge_kutta4< state_type >(),
    ODE,      //Lorentz-force
    Data0 , //{pos0,v0}
    0.0 ,    //t0=0
    T ,      //max time
    timestep ,//length of each step
    save_step //User defined save data function
);
```

Does it work

- ▶ Test, same proton in a solenoid use $\theta = 60^\circ$ reference, had:

$$R \approx 0.5 \text{ m} \sin(\theta) \approx 0.45 \text{ m} \quad T = \frac{2\pi}{\omega_c} \approx 10 \mu\text{s}$$

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- ▶ Compare Analytic, Euler, Runge-Kutta 4.
- ▶ Consider $\theta = 60^\circ$, $h = 0.01 \mu\text{s}$, $h = 0.1 \mu\text{s}$ and $h = 0.1 \mu\text{s}$.

Does it work

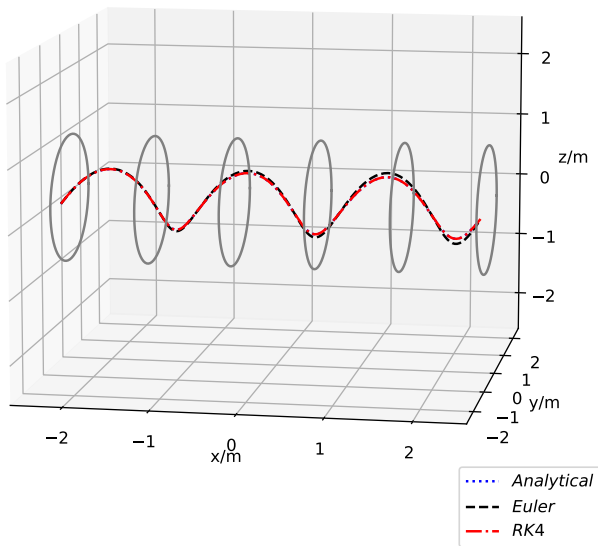
- ▶ Test, same proton in a solenoid use $\theta = 60^\circ$ reference, had:

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- ▶ Compare Analytic, Euler, Runge-Kutta 4.
- ▶ Consider $\theta = 60^\circ$, $h = 0.01 \mu\text{s}$, $h = 0.1 \mu\text{s}$ and $h = 0.1 \mu\text{s}$.
- ▶ Check error on $|\vec{v}|$, $R = \sqrt{y^2 + z^2}$ and $x(t)$.

At a glance, 3D view

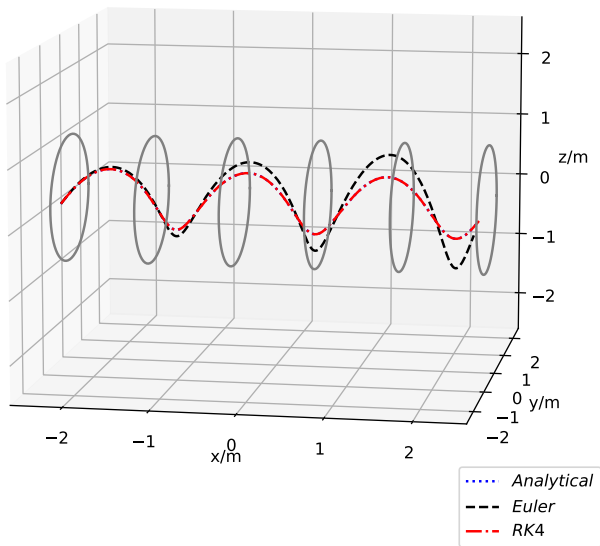
$$h = t_{i+1} - t_i = 0.01 \mu\text{s}$$



3129 steps

At a glance, 3D view

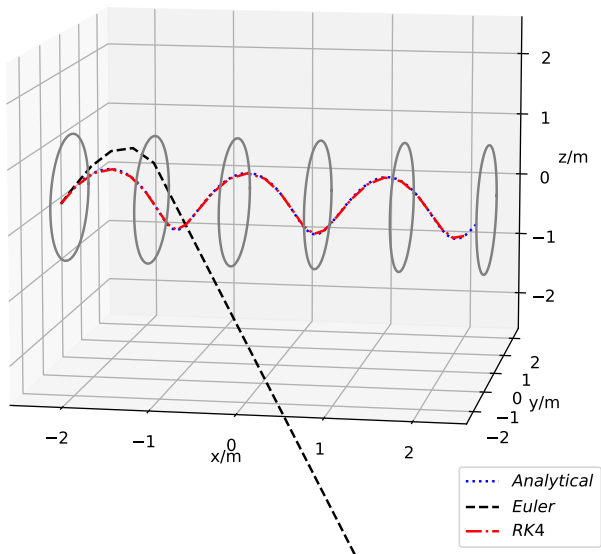
$$h = t_{i+1} - t_i = 0.1 \mu\text{s}$$



312 steps

At a glance, 3D view

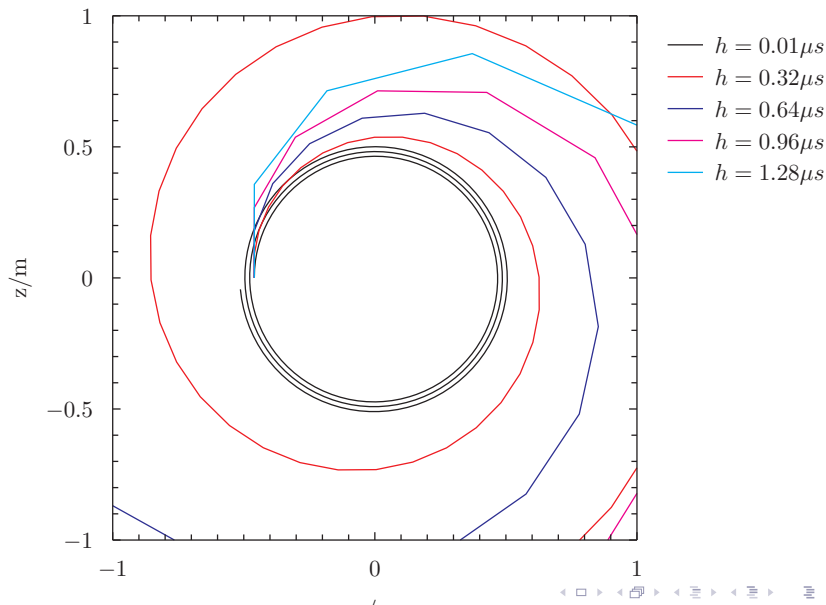
$$h = t_{i+1} - t_i = 1.0 \mu\text{s}$$



31 steps.

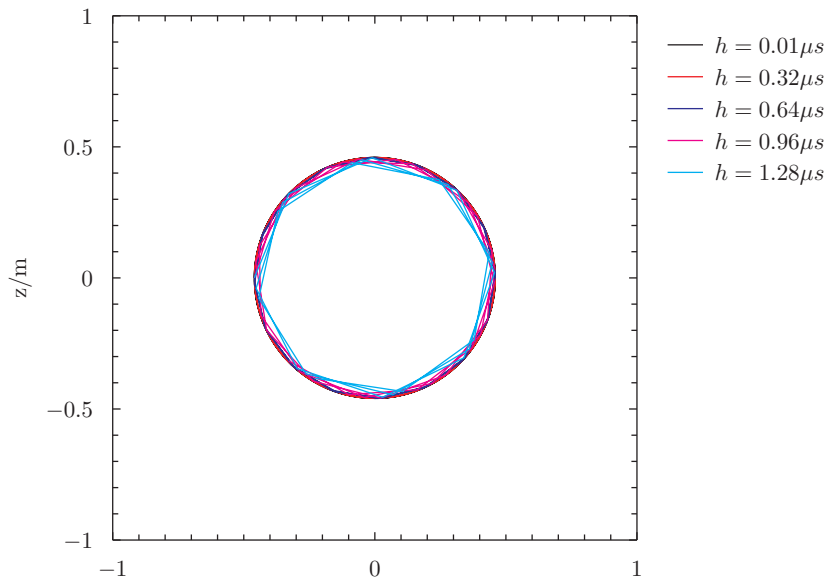
At a glance, front view, no border

Euler method, front-view

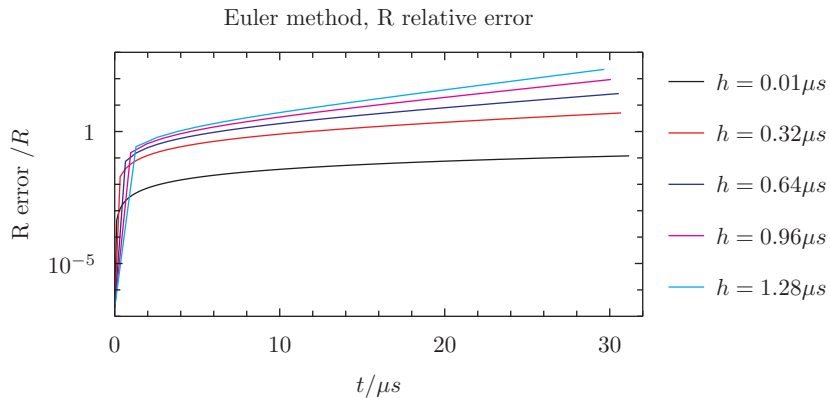


At a glance, front view, no border

RK4, front-view

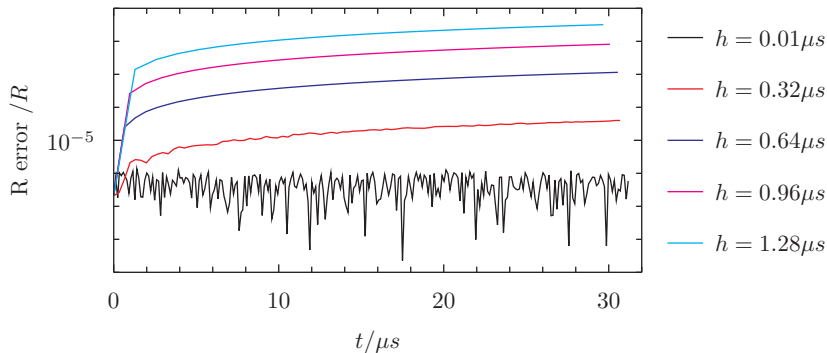


Constant radius?

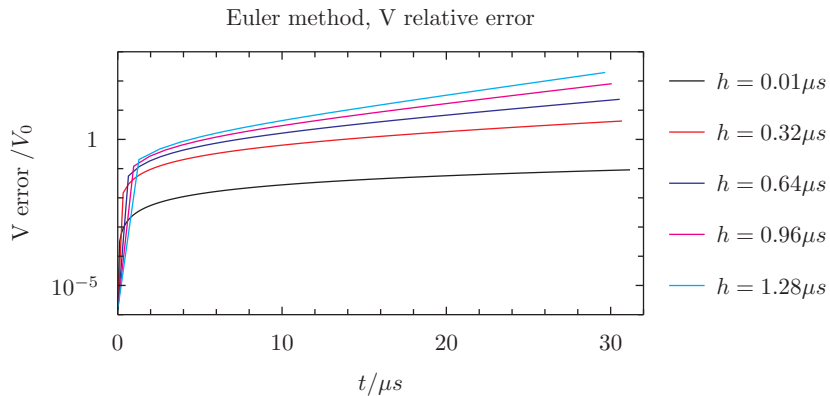


Constant radius?

Runge Kutta 4 method, R relative error

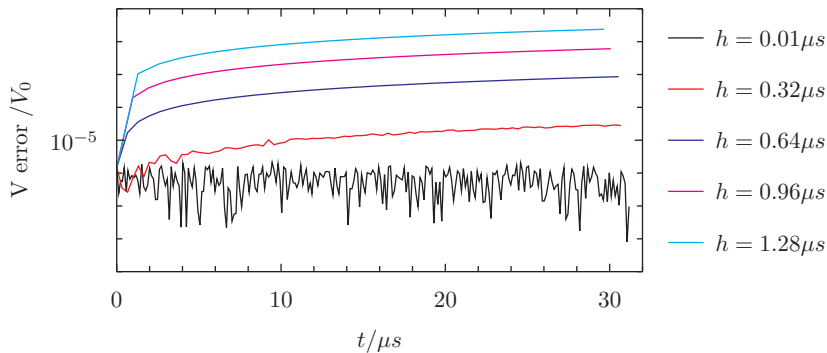


Constant speed?

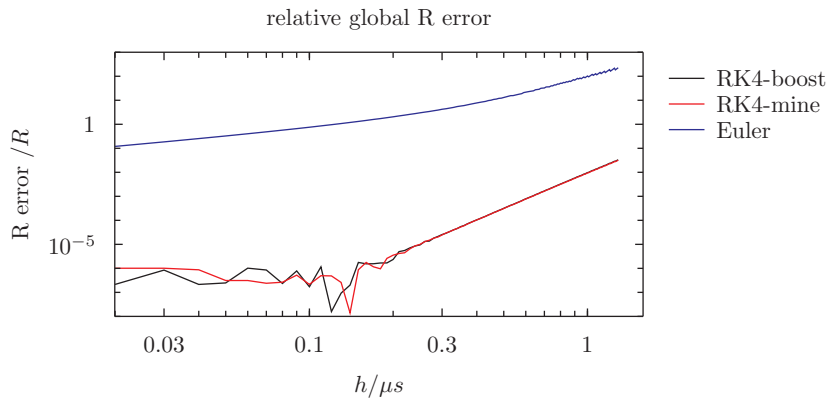


Constant speed?

Runge Kutta 4 method, V relative error



Order of the error



Adaptive step size, introduce it + when it fails

Non-analytic systems

Questions