MAINTITLE

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Student Colloquium in Physics and Astronomy, Aarhus University

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TITLEIMAGE

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Introduction [3 MIN]

Theory and physical background [10 MIN]
- Solved systems

Eulers Method and the 4th order Runge-Kutta Method [10 MIN]
- 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

Introduction, what and why

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How: Numeric-ODE solvers

- When analytical solutions are not practical.

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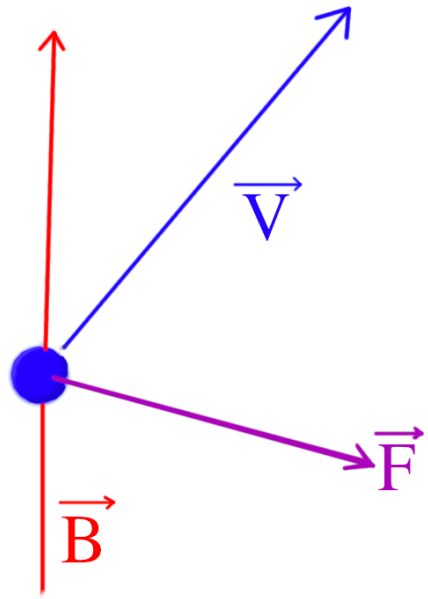
- Only 1 particle! so pre-programmed depending on the setup.
- Could use potentials $\phi(\vec{r}, t)$ $\vec{A}(\vec{r}, t)$ and Hamiltonian.

Known results, cyclotron motion $\vec{B}$ fields



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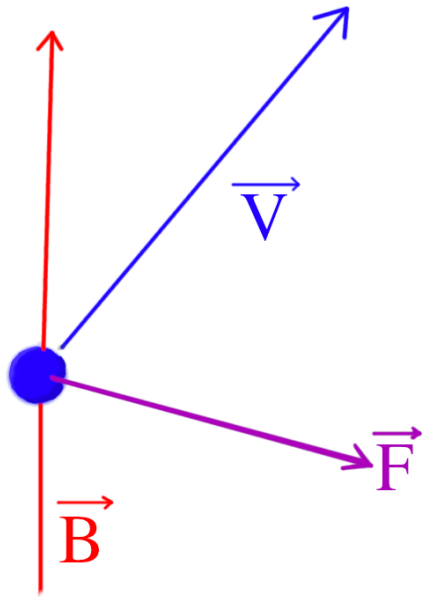

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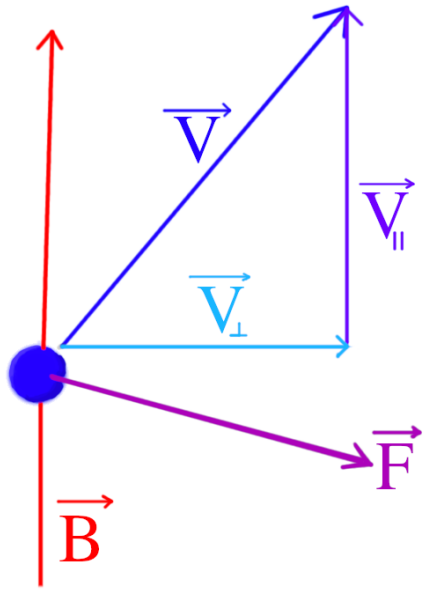

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- Same as Centripetal force:
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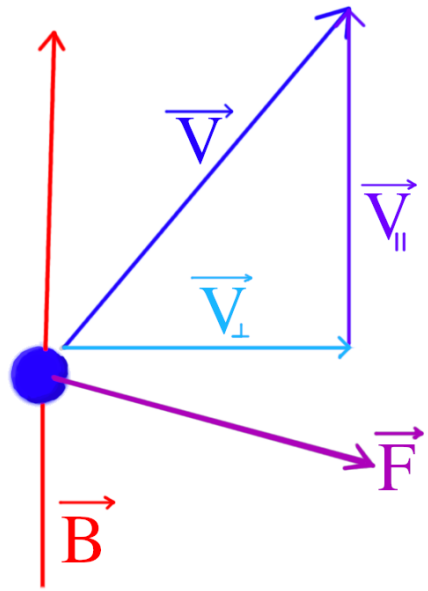

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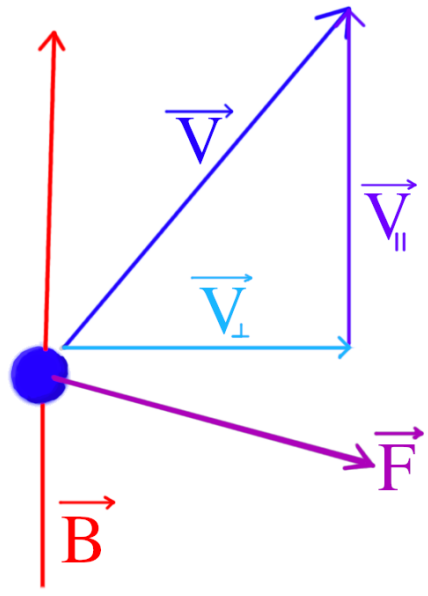
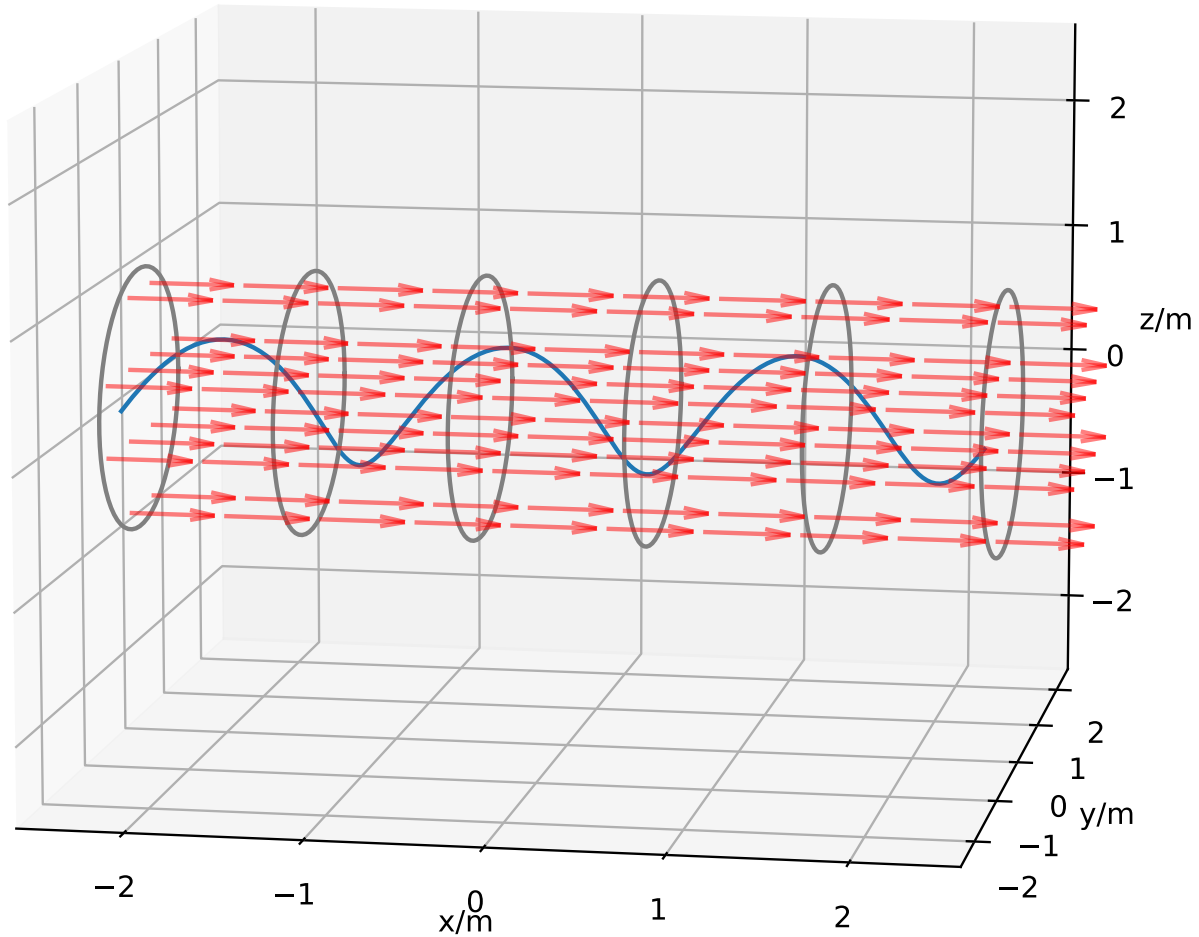
- Same as Centripetal force: Cyclotron motion
- Cyclotron radius and frequency:

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



Analytical solution: Protons in a Solenoid



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

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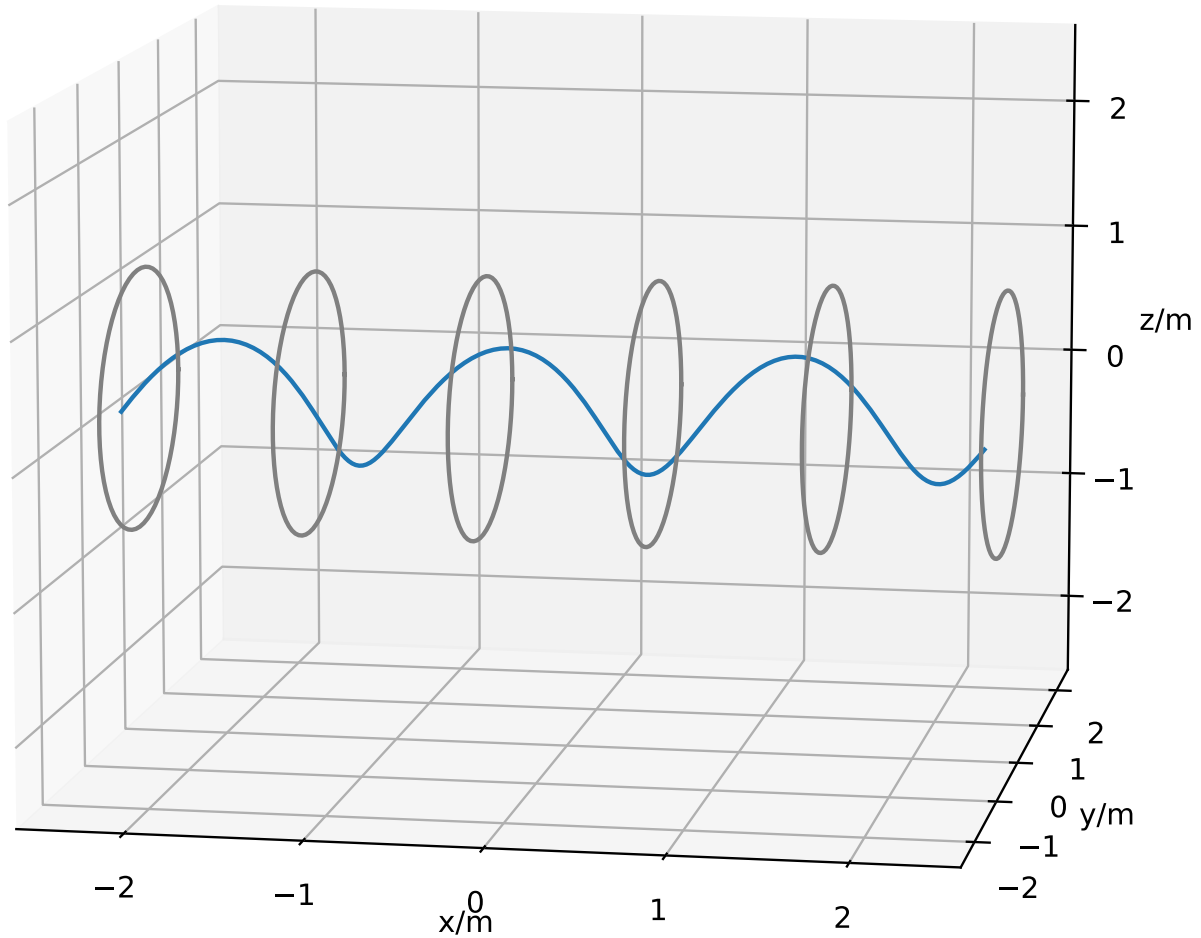

$$R \approx 0.5\,\mathrm{m}\,\sin(\theta) \quad T = \frac{2\pi}{\omega_c} \approx 10\,\mu\mathrm{s}$$

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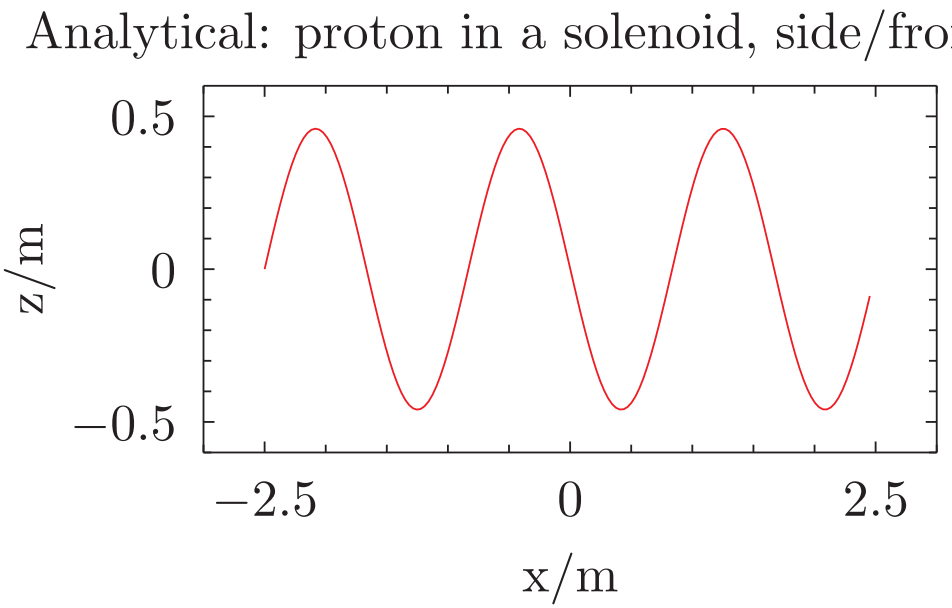

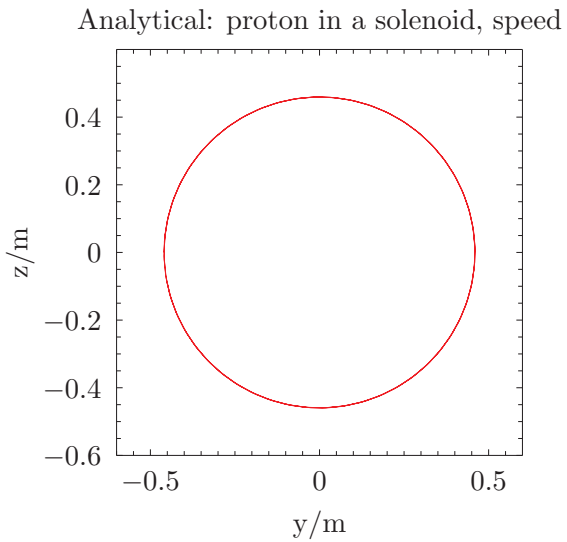

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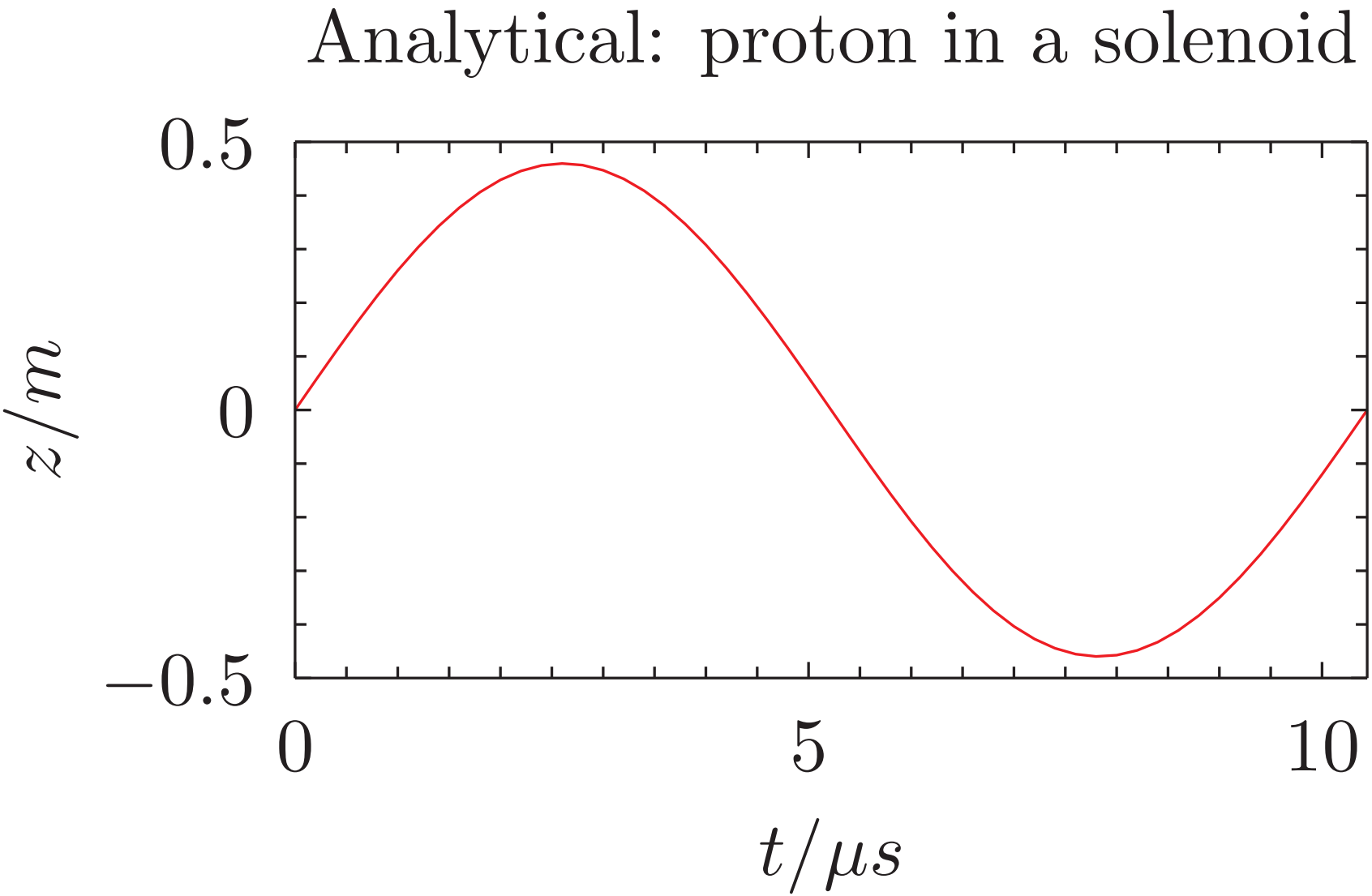

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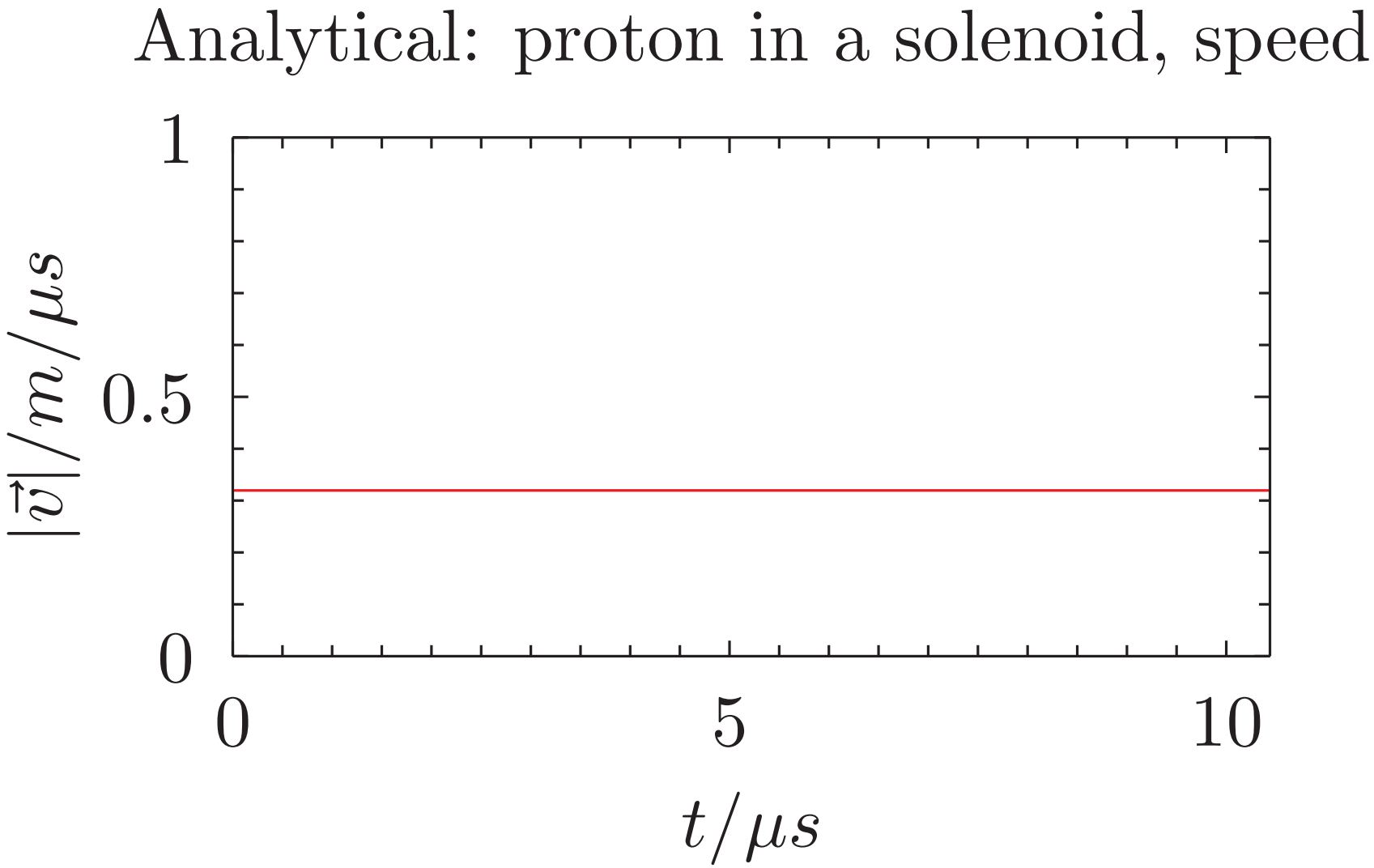

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Cyclotron accelerator

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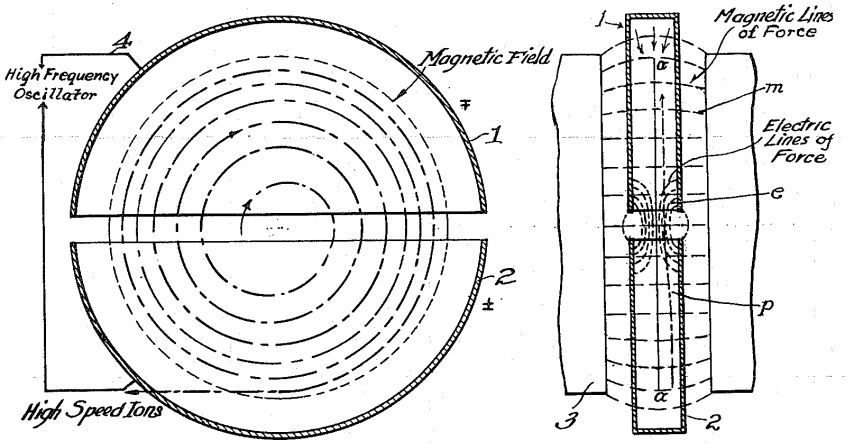

Ernest O. Lawrence, 1934, U.S. Patent 1,948,384; image in Public Domain.

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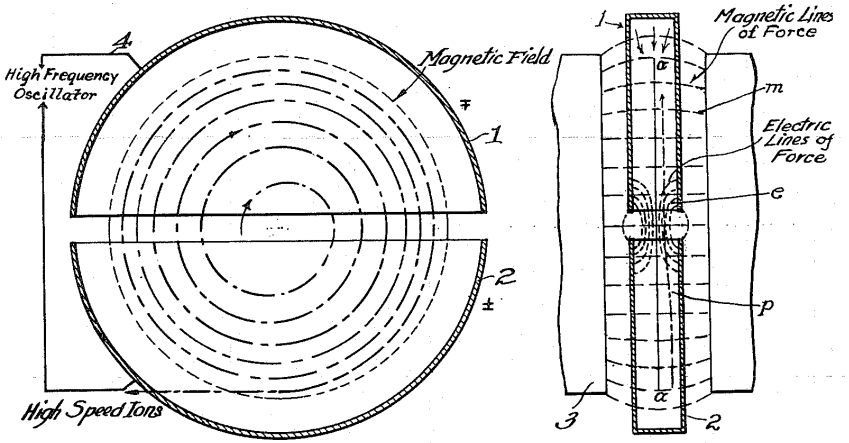

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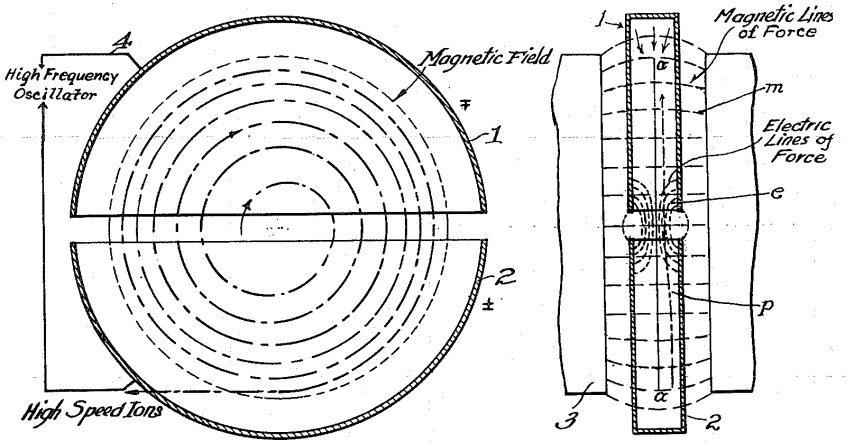

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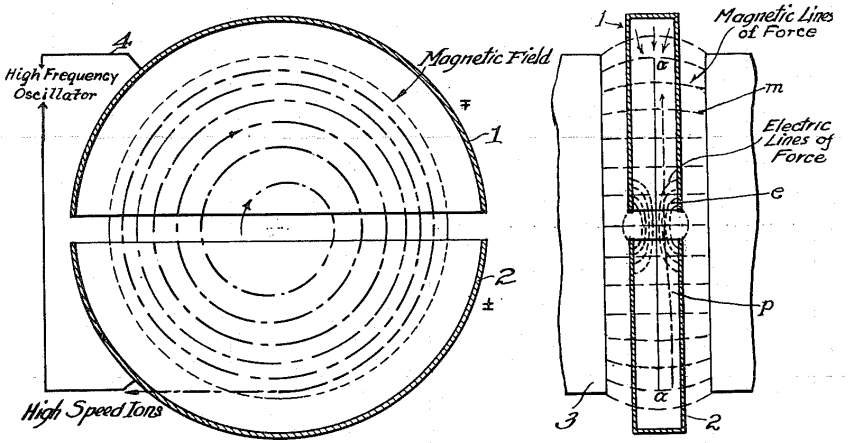
- Final speed:

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



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Ordinary differential equation*s.

- Sources: Zeigler et al. Theory of Modeling and Simulation (Third edition) chapter 3
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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

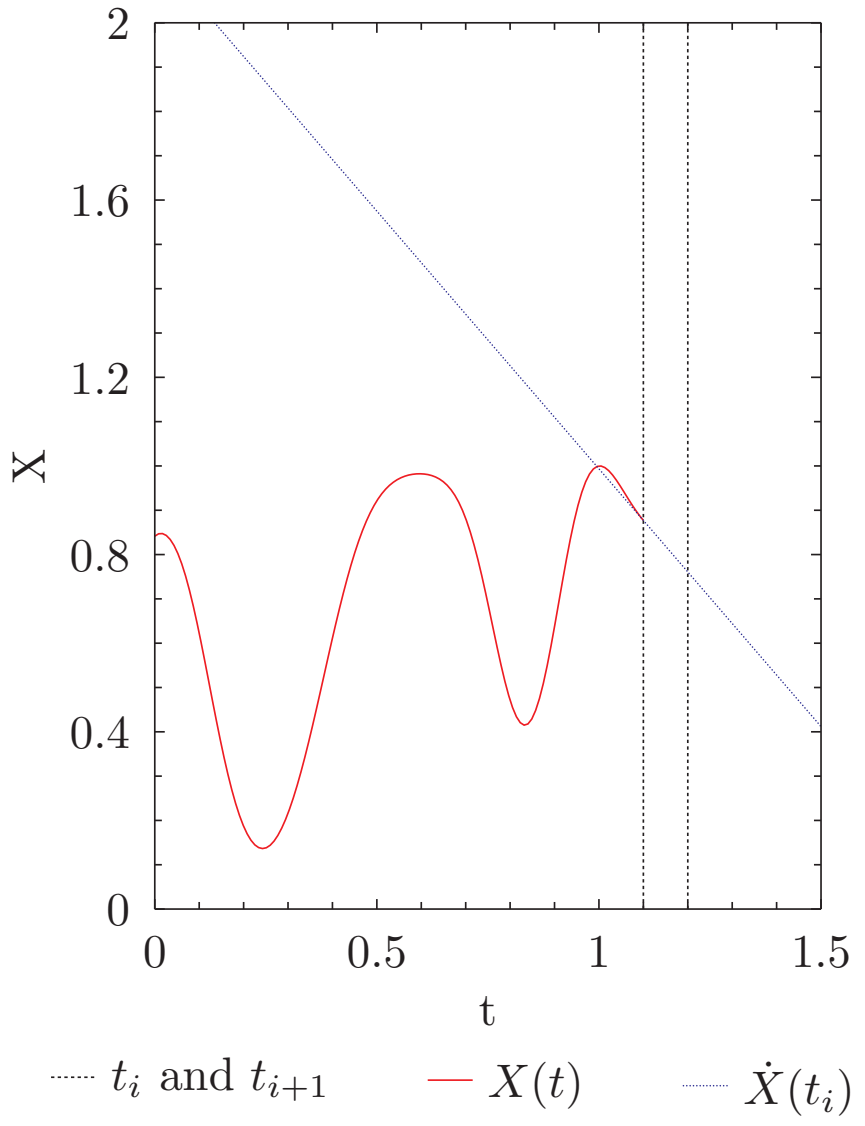
```
auto ODE = [...](const state_type Data, state_type &
    dDatadt, const double t){
    //Extract position and velocity from data
    vec pos = vec(Data[0],Data[1],Data[2]);
    vec velocity = vec(Data[3],Data[4],Data[5]);

    //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.



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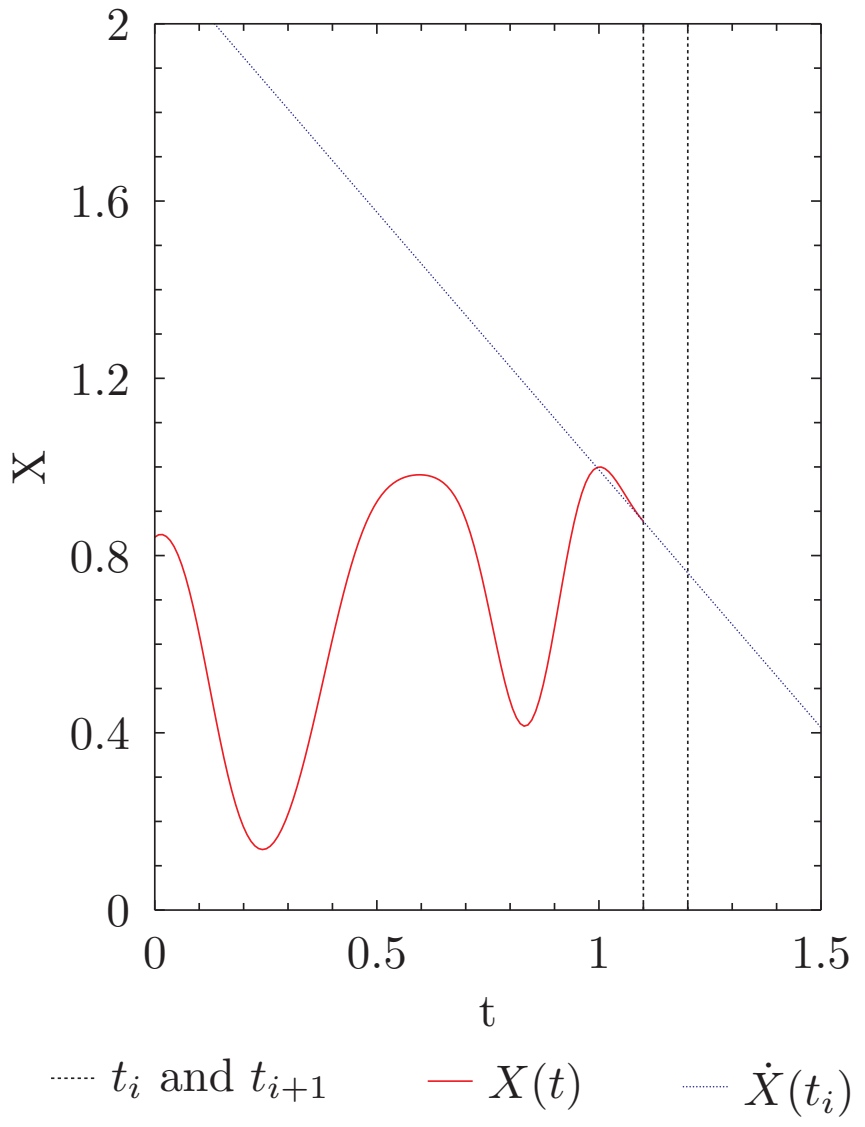
- Let $h = t_{i+1} - t_i > 0$ be constant.
- h, $\mathbf{X}(t)$, t_i and f_{ode} are known.

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



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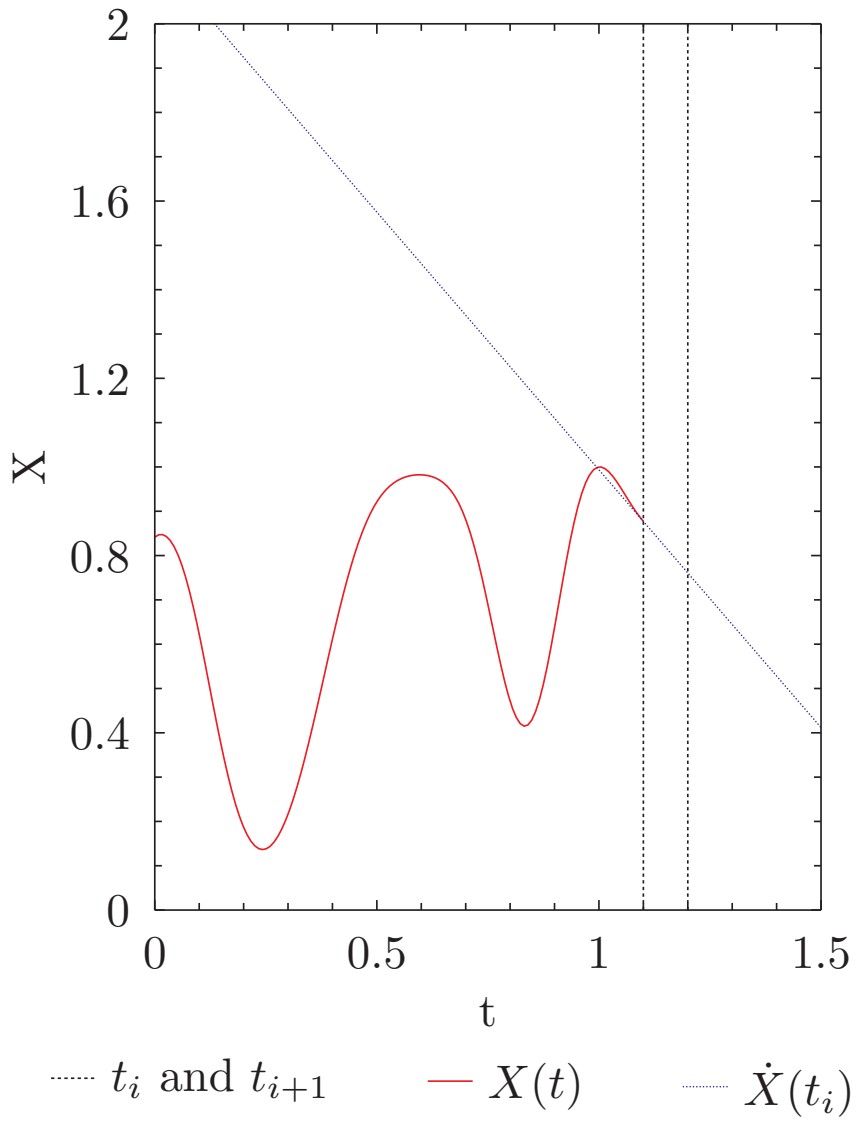

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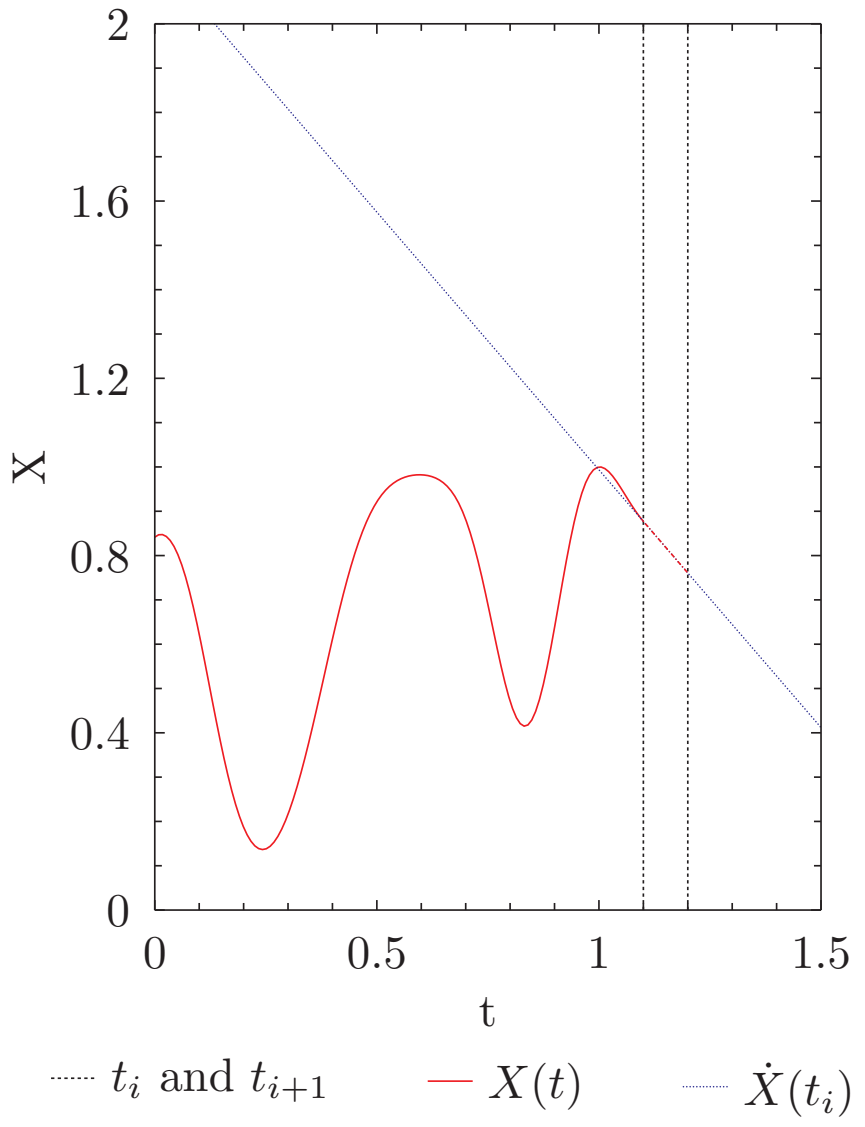

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- How would you find $\mathbf{X}(t_{i+1})$:
- (Explicit) Forward Euler's Method:

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

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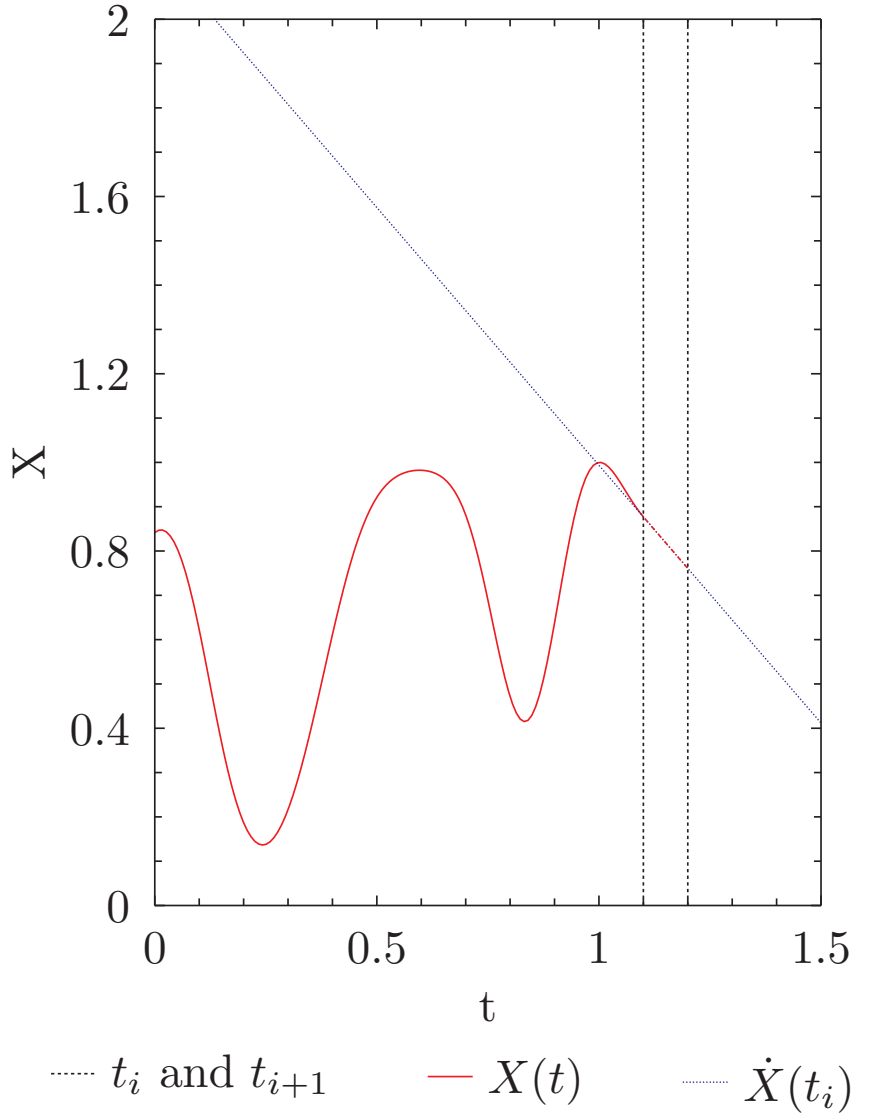

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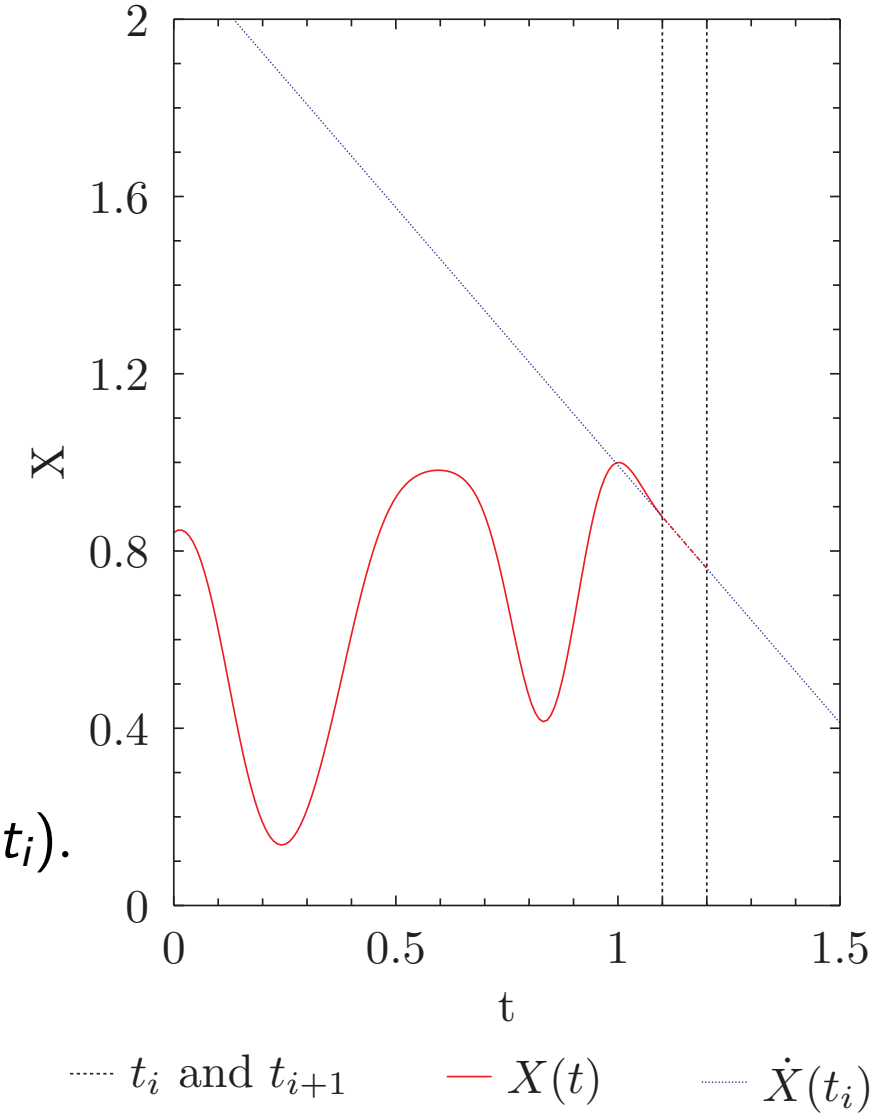

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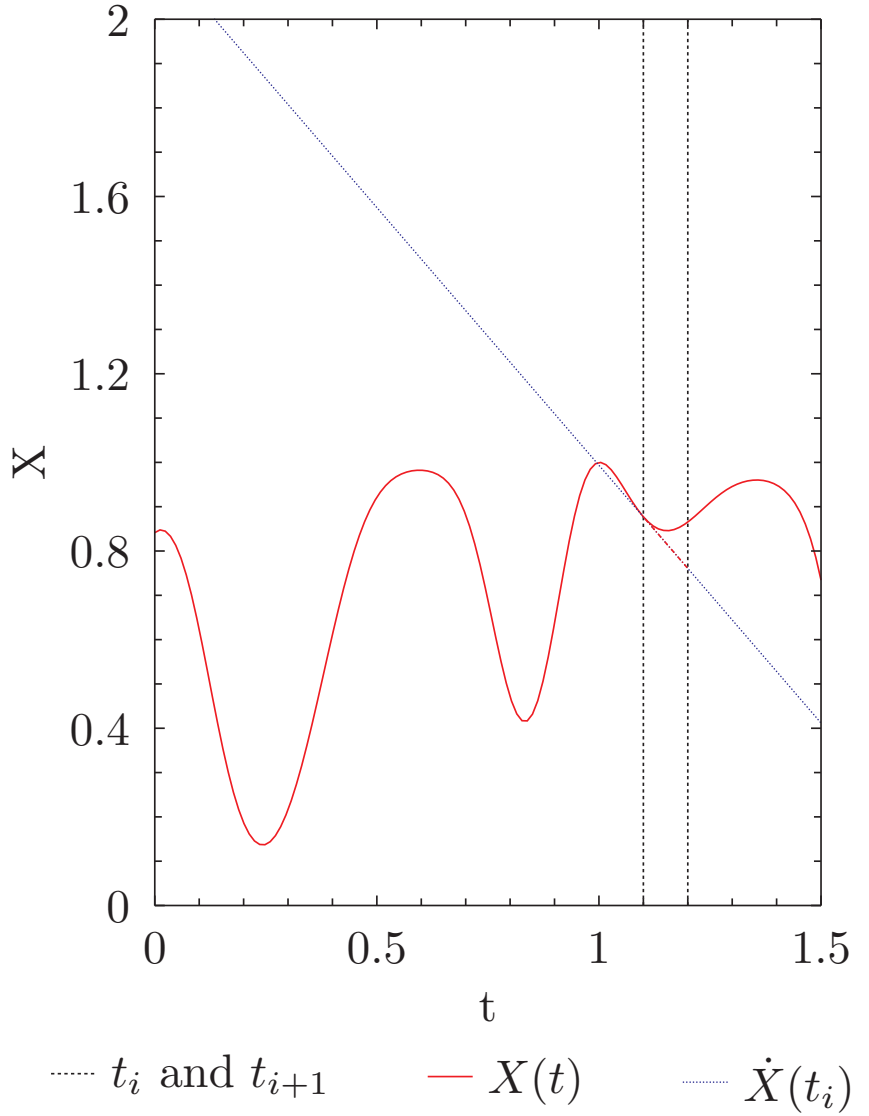

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- Global error $h = h^p$.
- Convergence, but not uniform.

Why does this work? The Runge Kutta family

- In general.

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

- L. Zheng, X. Zhang, Modeling and Analysis of Modern Fluid Problems, 2017, chapter 8:

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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

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

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- Martha L. Abell, James P. Braselton, Differential Equations with Mathematica (Fourth Edition), 2016;

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- Want exact to p'th order. Can be found with taylor expansion of $\mathbf{X}(t_i)$.
- 2nd order (Heun's method):

$$\begin{aligned} \mathbf{X}(t_{i+1}) - \mathbf{X}(t_i) &= \frac{h}{2}(\mathbf{k}_1 + \mathbf{k}_2) \\ \mathbf{k}_1 &= f_{ode}(\mathbf{X}(t_i), t_i) \\ \mathbf{k}_2 &= f_{ode}(\mathbf{X}(t_i) + h\mathbf{k}_1, t_i + h) \end{aligned}$$

- Martha L. Abell, James P. Braselton, Differential Equations with Mathematica (Fourth Edition), 2016:

The 4th order Runge Kutta method

- RK4, often simply called the Runge Kutta method:

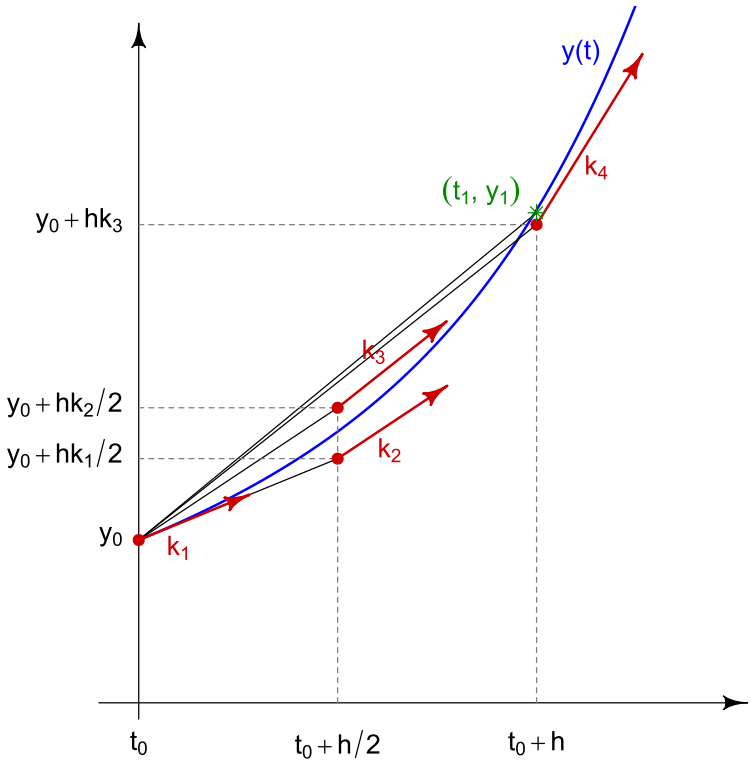
$$\mathbf{X}(t_{i+1}) - \mathbf{X}(t_i) = \frac{h}{6}(\mathbf{k}_1 + 2\mathbf{k}_2 + 2\mathbf{k}_3 + \mathbf{k}_4)$$

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

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

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

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



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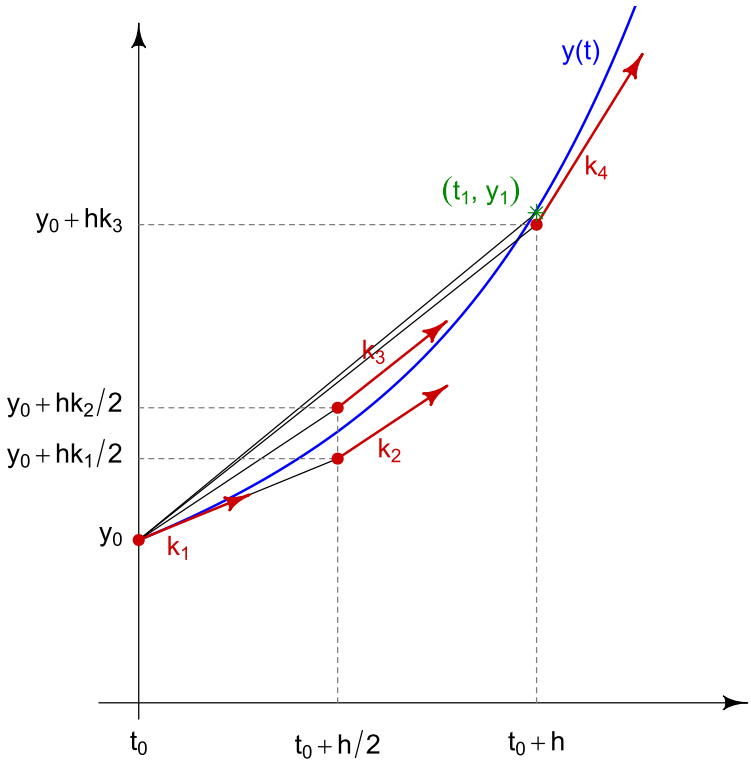

Wikipedia-user HilberTraum, published under creative commins: CC BY-SA 4.0

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

The General explicit Runge Kutta method

- General explicit, single step, fixed size, Runge Kutta method

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

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

$$\mathbf{k}_2 = f_{ode}(\mathbf{X}(t_i) + h a_{21} \mathbf{k}_1, t_i + c_2 h)$$

$$\mathbf{k}_3 = f_{ode}(\mathbf{X}(t_i) + h a_{31} \mathbf{k}_1 + h a_{32} \mathbf{k}_2, t_i + c_3 h) \quad \vdots$$

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- Expressed in Butcher tableu:

$c_1 = 0$			
c_2	a_{21}		
c_3	a_{31}	a_{32}	
c_n	a_{n1}	a_{n2}	$\dots$
	b_1	b_2	$\dots$

Euler Implementations

```
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:

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

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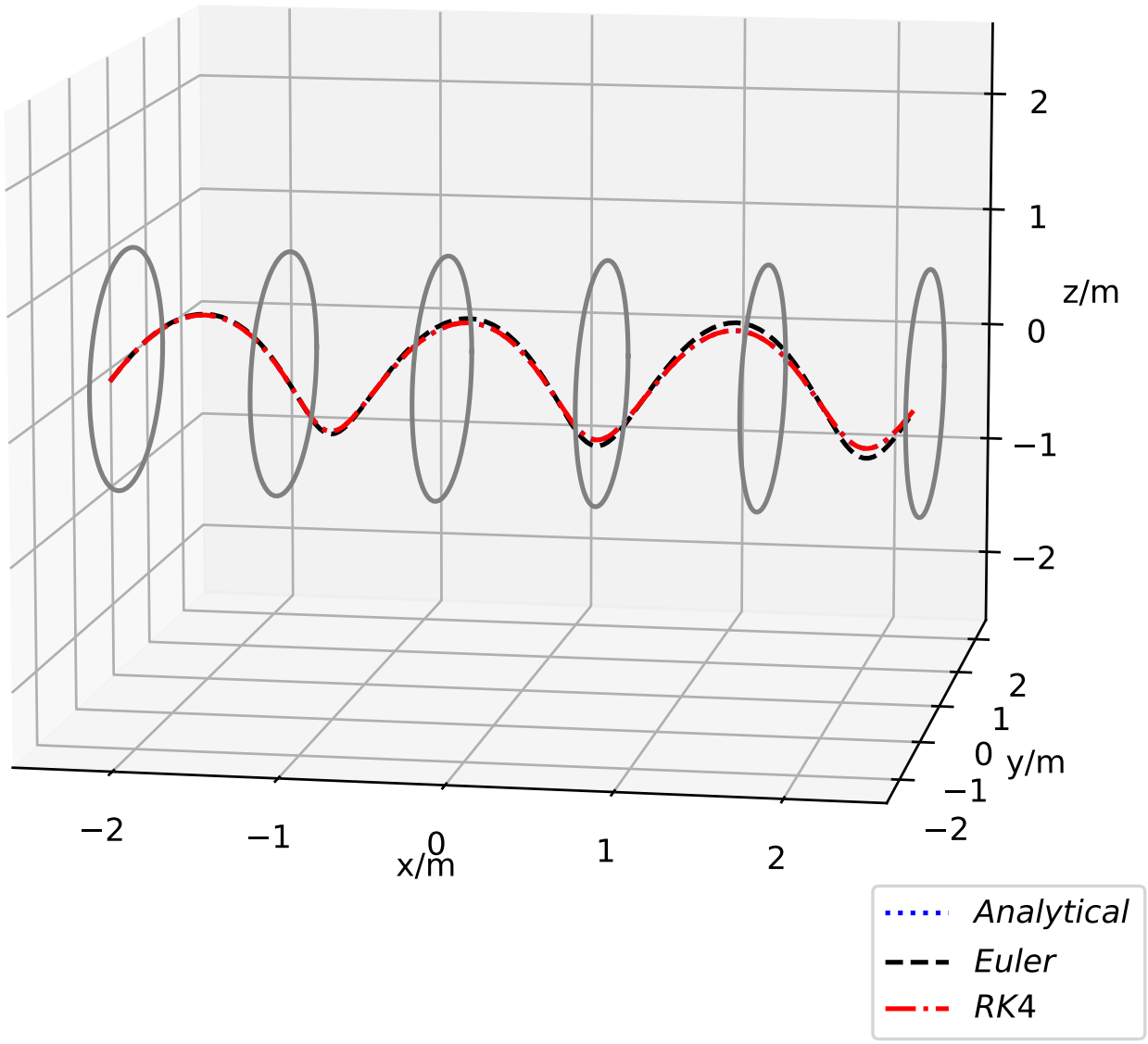
- Consider $\theta = 60^\circ$, $h = 0.01\,\mu\text{s}$, $h = 0.1\,\mu\text{s}$ and $h = 0.1\,\mu\text{s}$.
- Check error on $|\vec{v}|$, $R = \sqrt{y^2 + z^2}$ and $x(t)$.

At a glance, 3D view

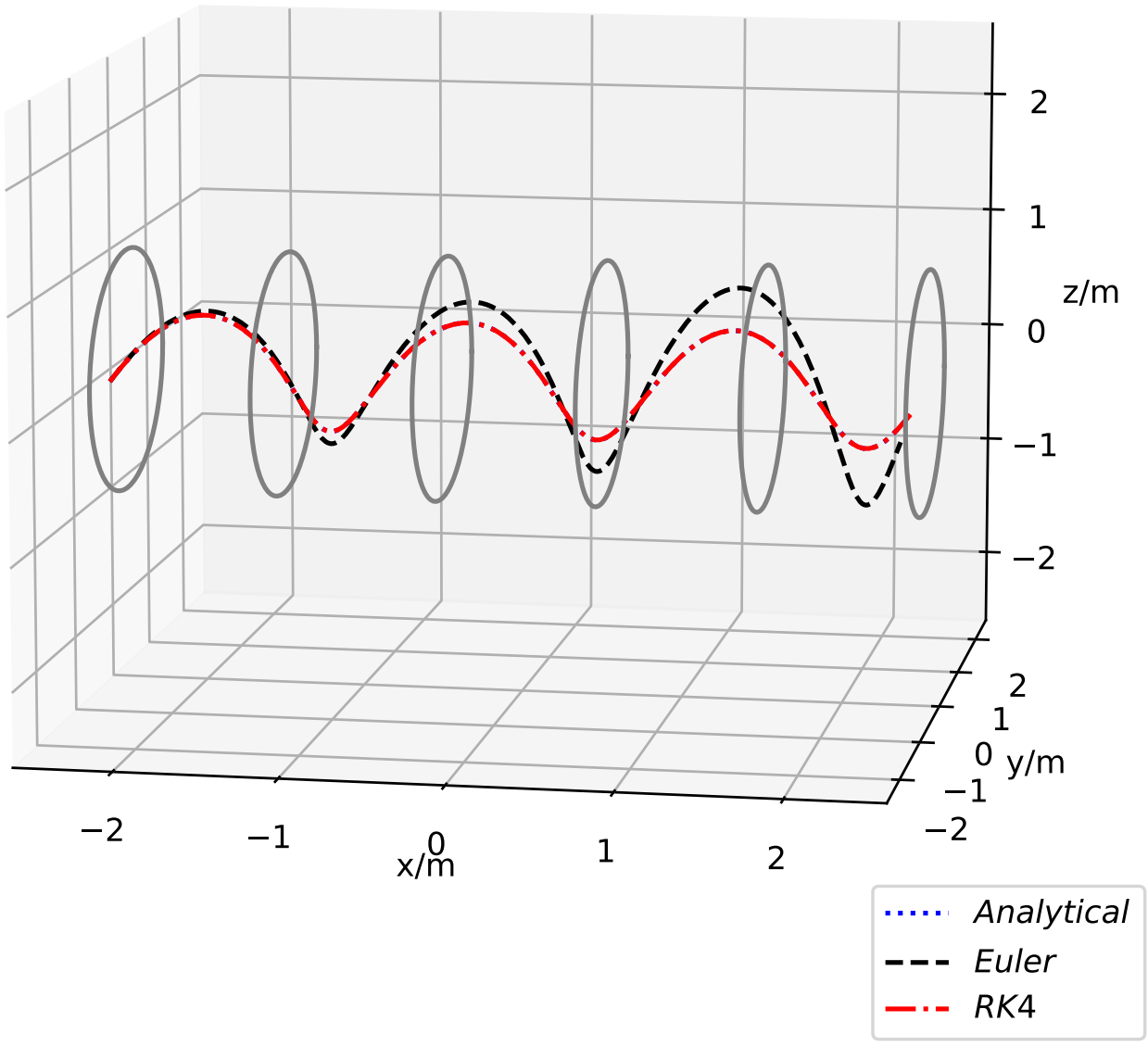
$$h = t_{i+1} - t_i = 0.01\,\mu s$$



3129 steps

At a glance, 3D view

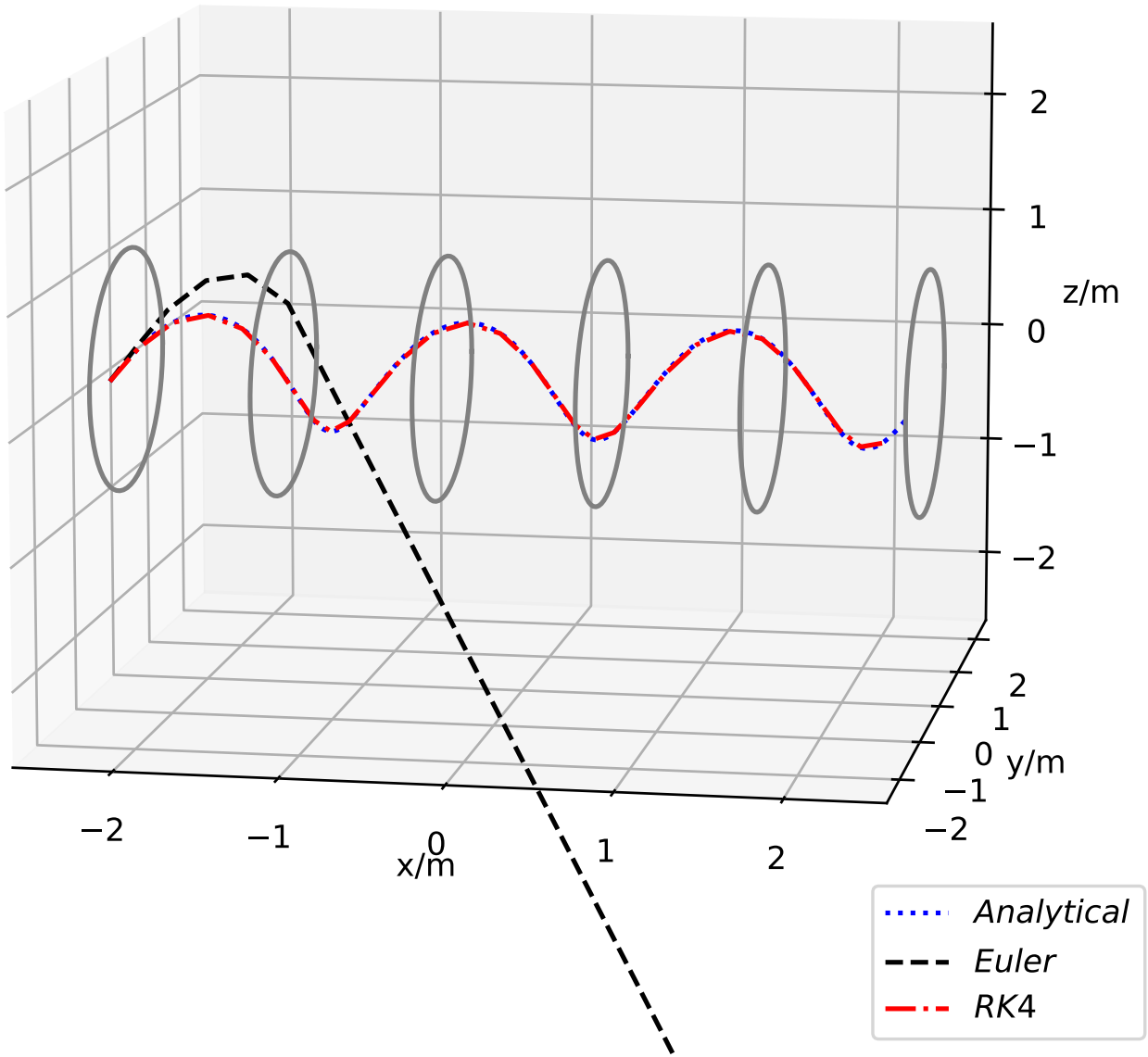
$$h = t_{i+1} - t_i = 0.1\,\mu s$$



312 steps

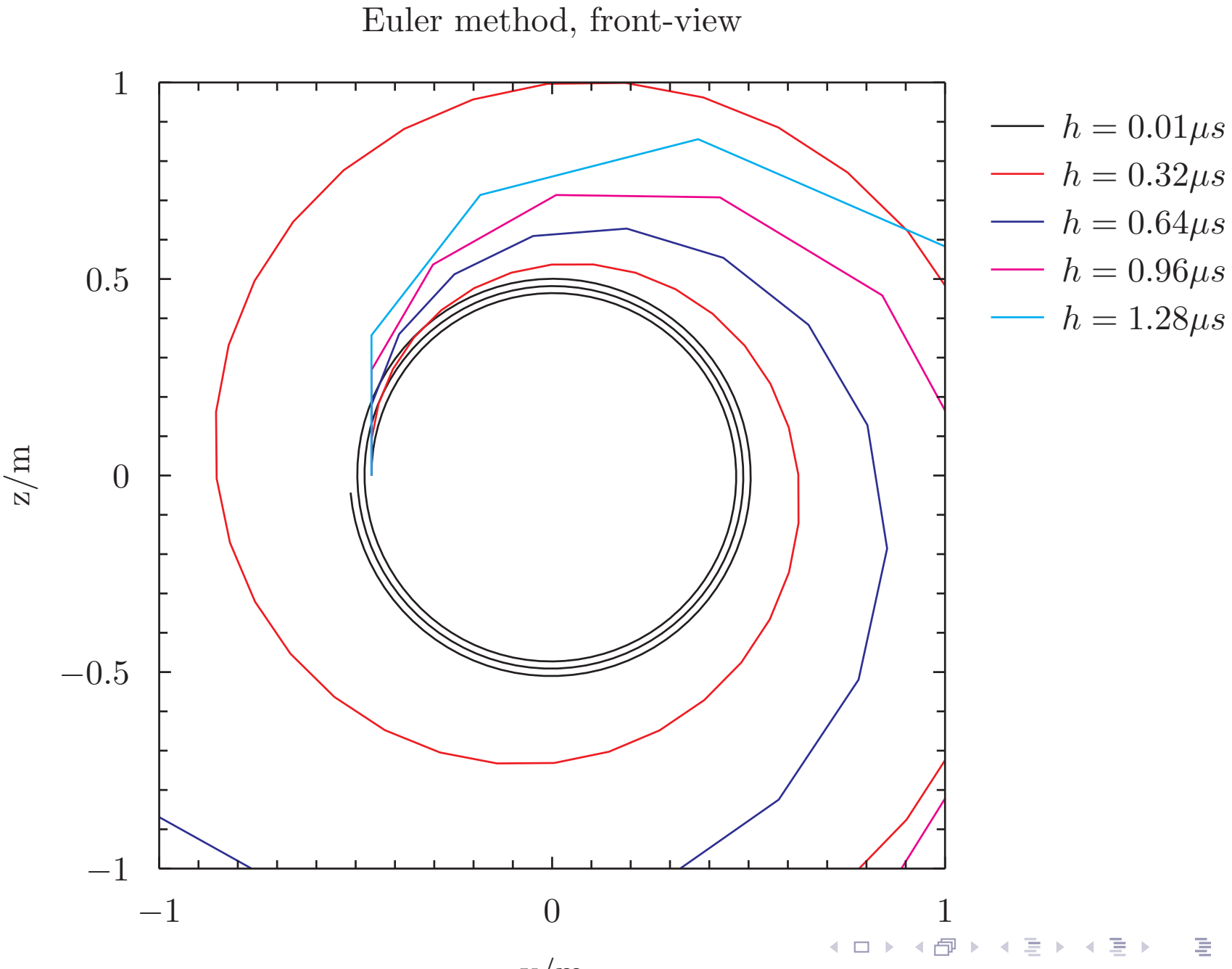
At a glance, 3D view

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

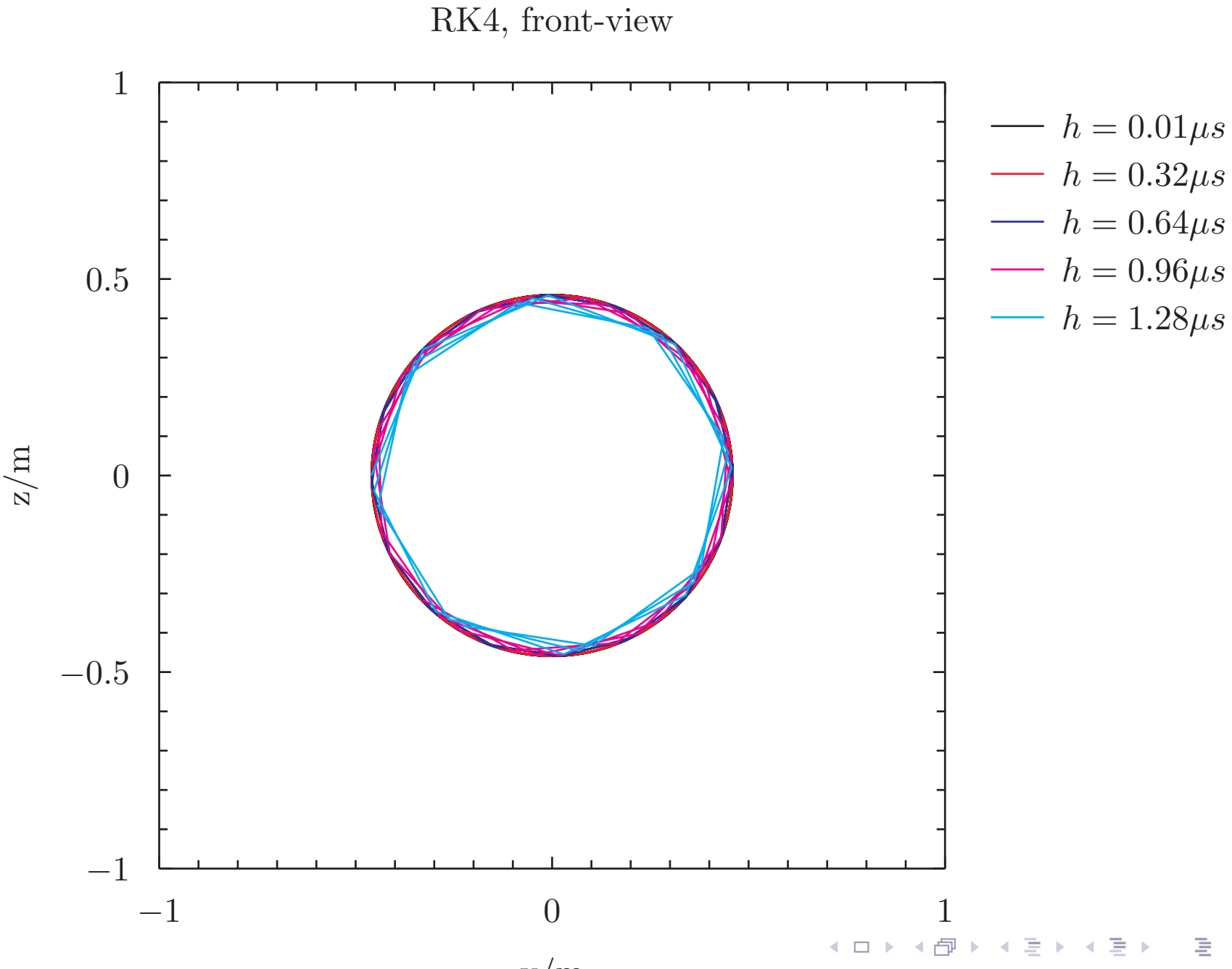


31 steps.

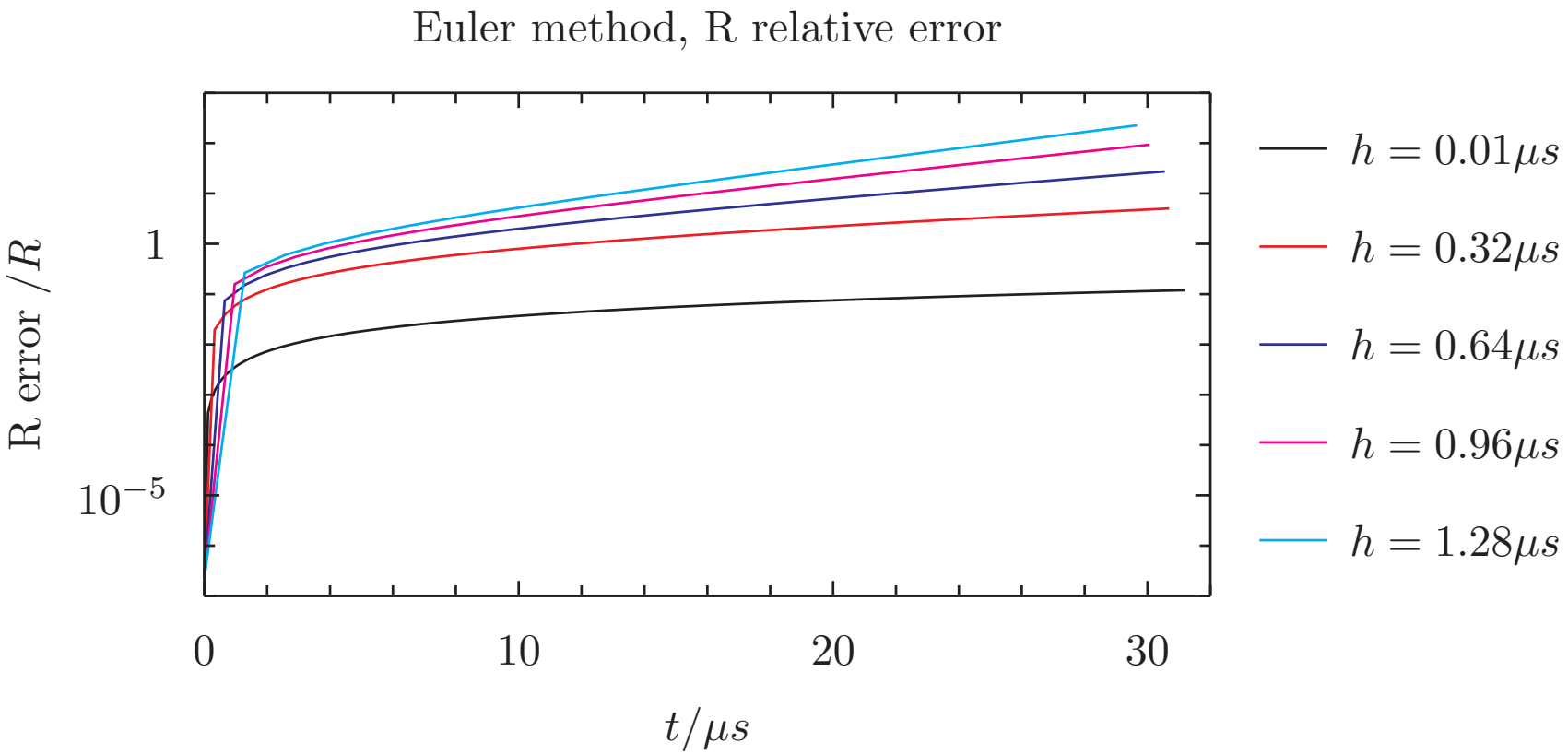
At a glance, front view, no border



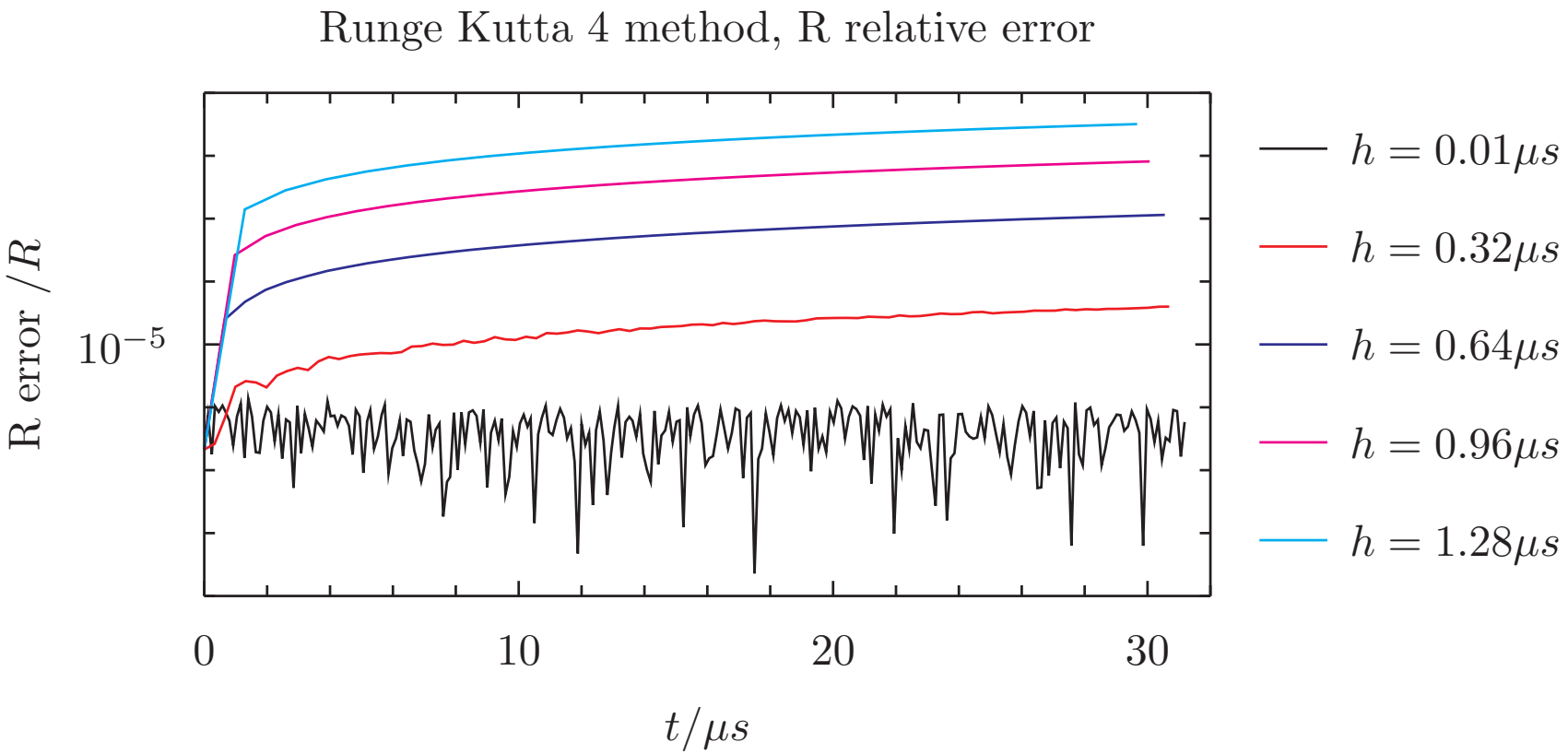
At a glance, front view, no border



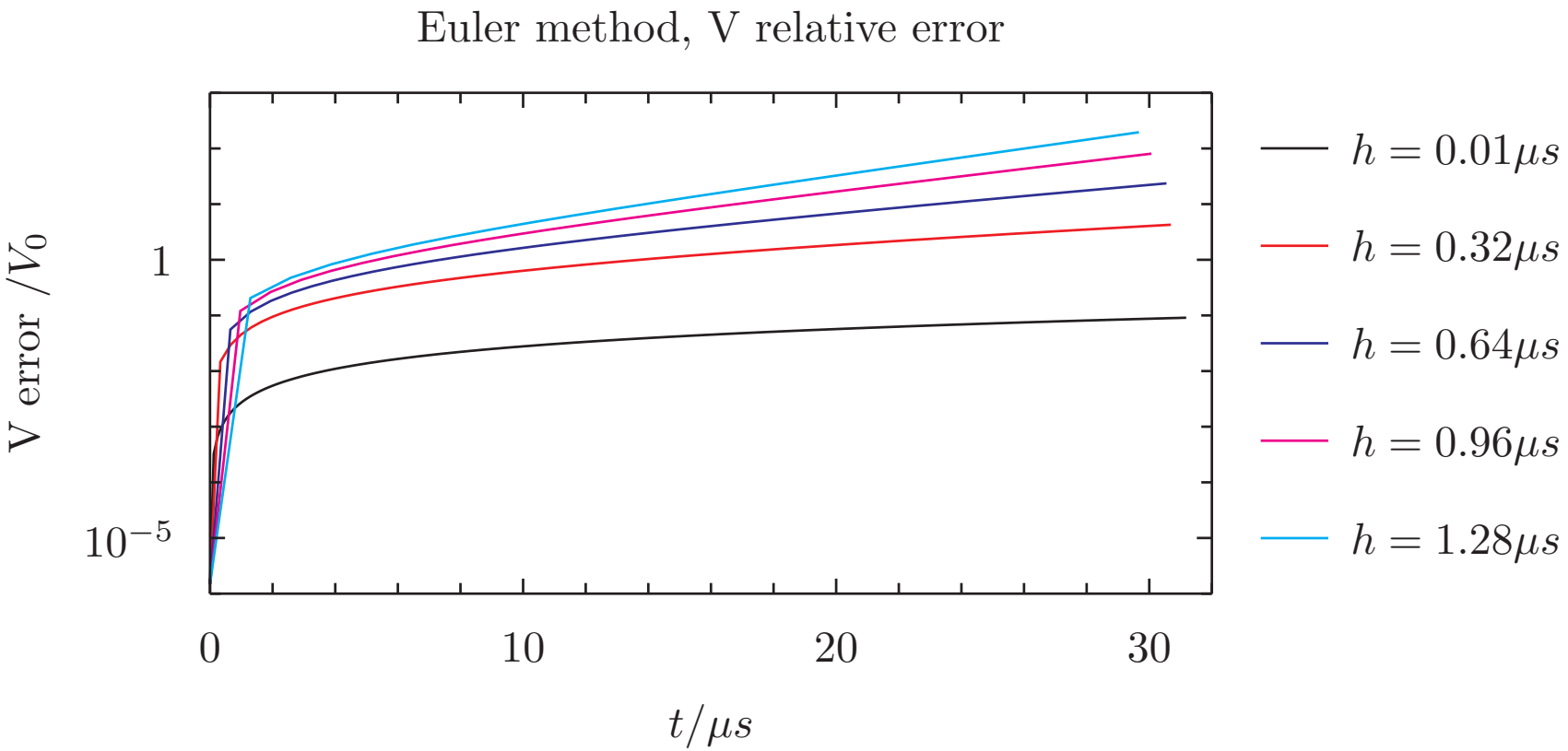
Constant radius?



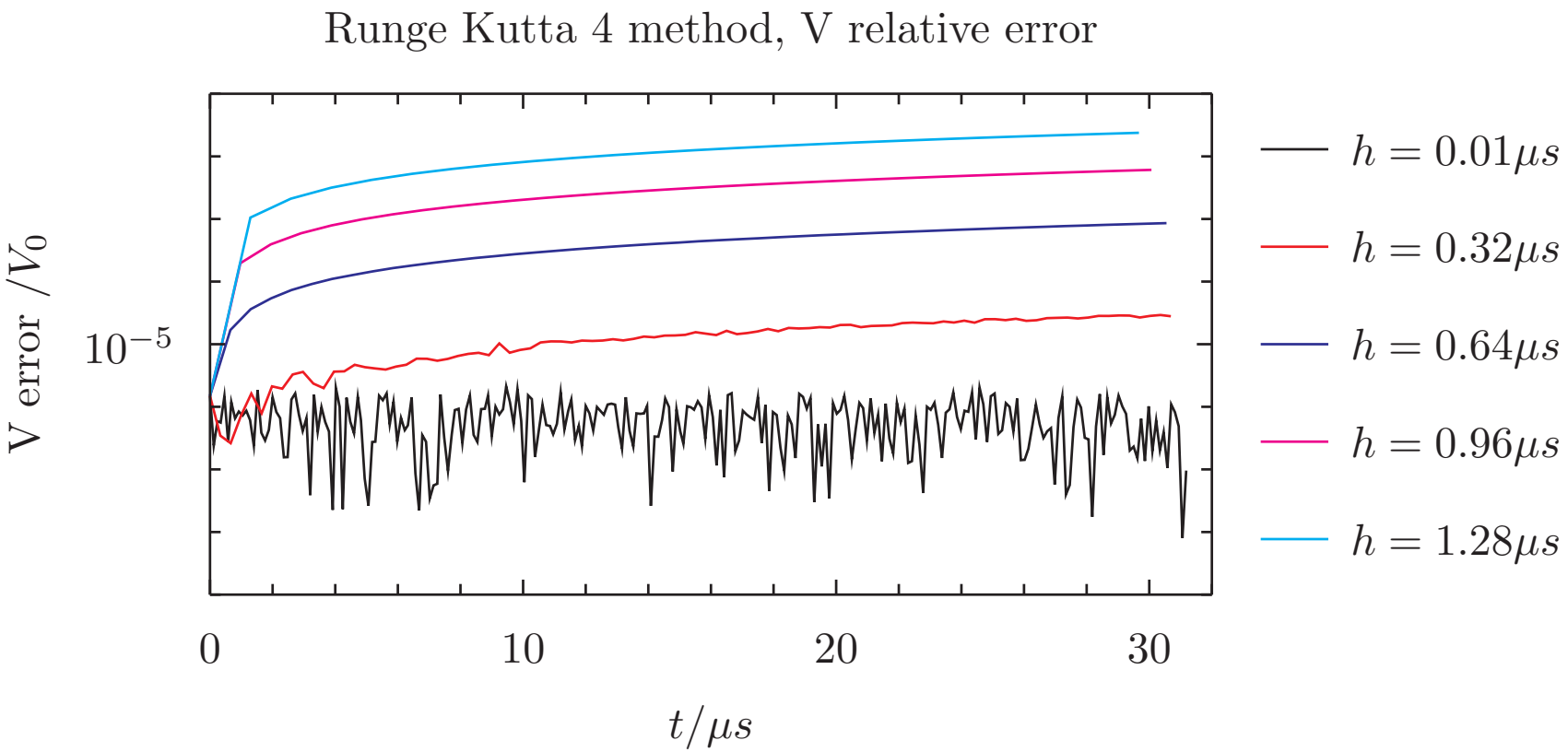
Constant radius?



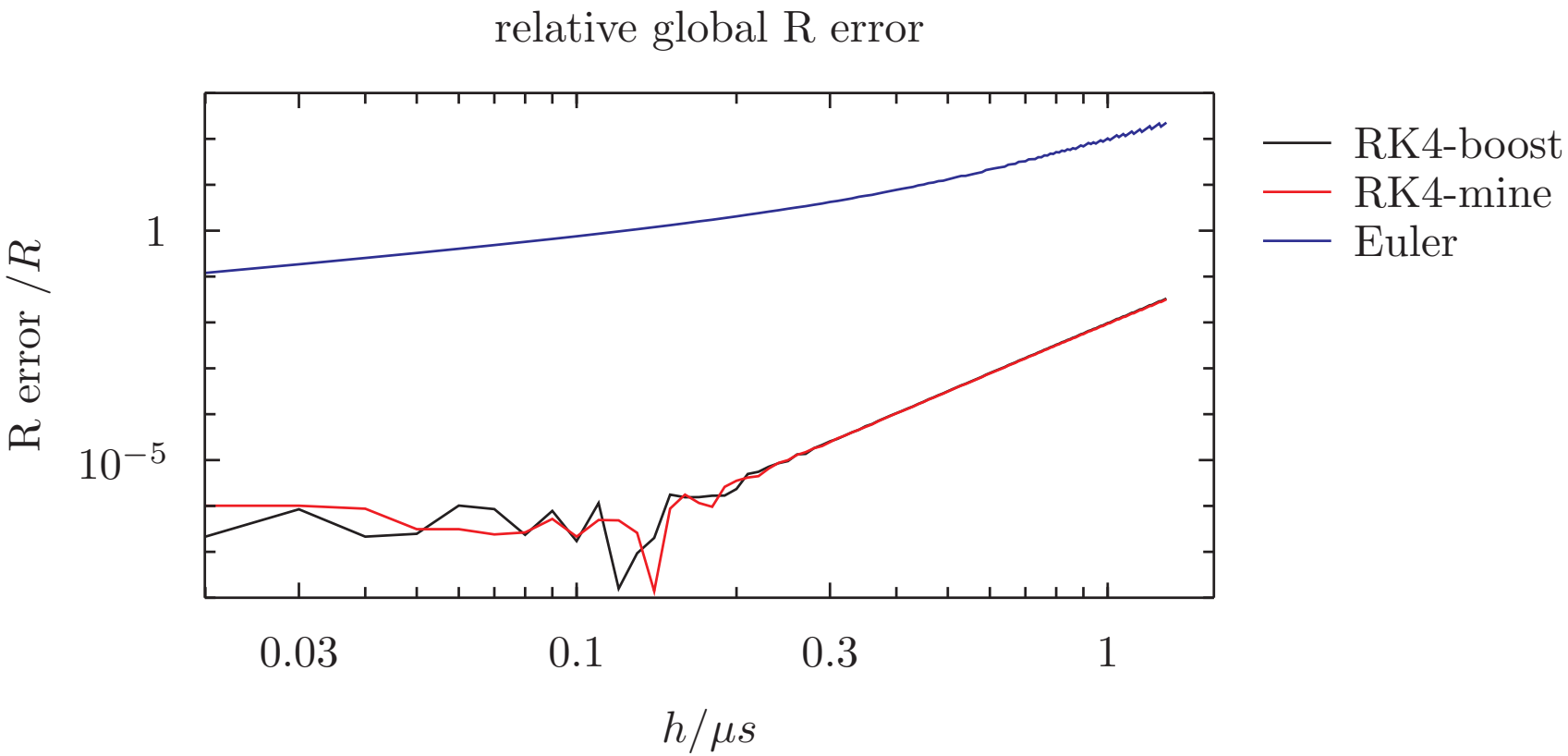
Constant speed?



Constant speed?



Error as function of h



Adaptive step size, why

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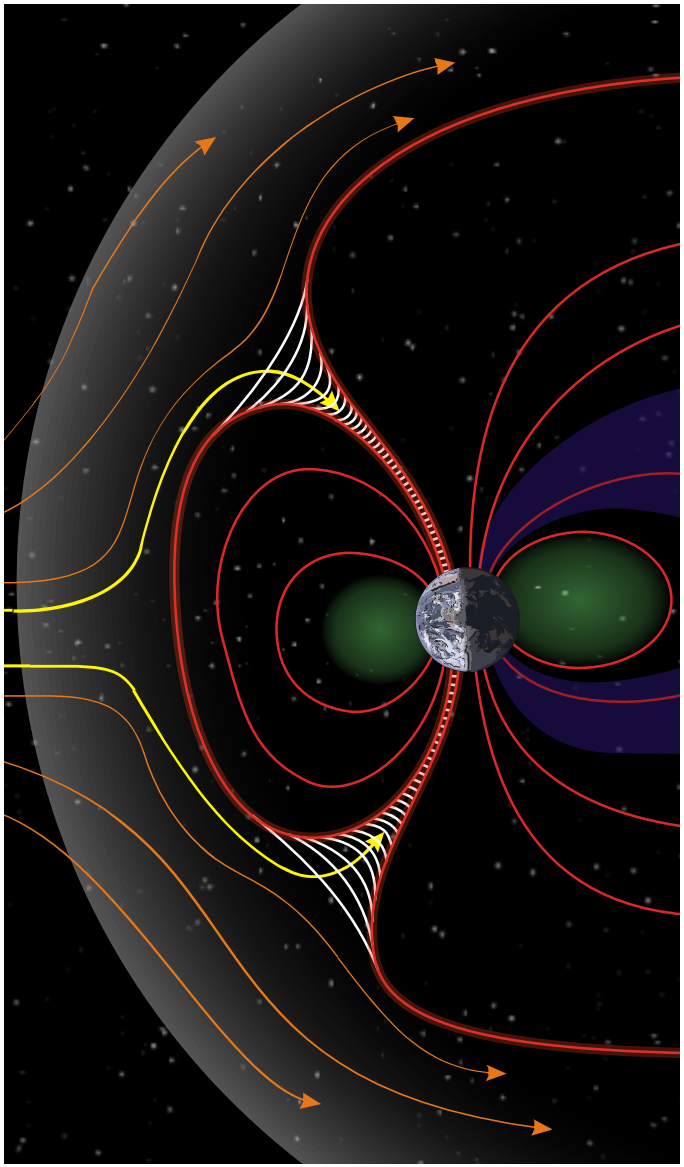
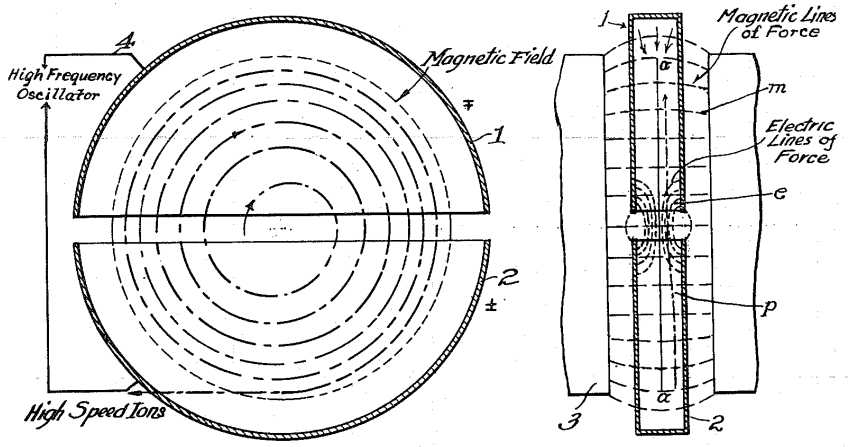


Illustration originally from Nasa. Published on wikipedia, in Public

Adaptive step size, why

- h must be small "enough"
- Hard to pick, and may change:
- Inhomogeneous fields (here Earth magnetic field)
- time dependent fields (here the cyclotron)



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

Adaptive step size, why

- h must be small "enough"
- Hard to pick, and may change:
- Inhomogeneous fields (here Earth magnetic field)
- time dependent fields (here the cyclotron)
- Let the computer pick h.

Runge-Kutta Adaptive step size, how

- Reduce h until the "error" is small enough

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- Approximate "Error" as $|\mathbf{x}(t_{i+1}) - \mathbf{x}'(t_{i+1})|$.
- Most often order 4 and 5 with same $\mathbf{k}_i$.

Runge-Kutta Dormund Prince 4-5,

- ode45 in Matlab , RungeKutta_dopri5 in boost::odeint.

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

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

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$$\mathbf{k}_i = f_{ode}(\mathbf{X}(t_i) + h \sum_{j}^{i-1} a_{ki} \mathbf{k}_i + h a_{32}, t_i + c_3 h) \quad \vdots$$

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$$\mathbf{k}_i = f_{ode}(\mathbf{X}(t_i) + h \sum_{j}^{i-1} a_{ki} \mathbf{k}_i + h a_{32}, t_i + c_3 h) \quad \vdots$$

- 4th and 5th order, hence ode 45. Keeps 5th order term if error less than absolute and relative threshold.
  Dormand, J. R.; Prince, P. J. (1980), "A family of embedded Runge-Kutta formulae", Journal of Computational and

Butcher Tableu of Dormund Prince 4/5

c_i	a_{ij}	...						
0								
$\frac{1}{5}$	$\frac{1}{5}$							
$\frac{3}{10}$	$\frac{3}{40}$	$\frac{9}{40}$						
$\frac{4}{5}$	$\frac{40}{45}$	$-\frac{56}{15}$	$-\frac{32}{9}$					
$\frac{8}{9}$	$\frac{19372}{6561}$	$\frac{25360}{2187}$	$\frac{64448}{6561}$	$\frac{212}{729}$				
1	$\frac{9017}{3168}$	$-\frac{355}{33}$	$\frac{46732}{5247}$	$\frac{49}{176}$	$-\frac{5103}{18656}$			
1	$\frac{35}{384}$	0	$\frac{500}{1113}$	$\frac{125}{192}$	$-\frac{2187}{6784}$	$\frac{11}{84}$		
$/b$	$\frac{35}{384}$	0	$\frac{500}{1113}$	$\frac{125}{192}$	$-\frac{2187}{6784}$	$\frac{11}{84}$	0	
$/b'$	$\frac{5179}{57600}$	0	$\frac{7571}{16695}$		$\frac{393}{640}$	$-\frac{92097}{339200}$	$\frac{187}{2100}$	$\frac{1}{40}$

Testing adaptive step-size

```
#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_adaptive(
    runge_kutta_dopri5< state_type >(),
    ODE,   //Lorentz-force
    Data0 ,//{pos0,v0}
    0.0 ,  //t0=0
    T ,    //max time
    timestep ,//length of each step (initial)
    save_step //User defined save data function
);
```

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...
size_t steps = integrate_adaptive(
    make_controled( absErr, relErr ,
    runge_kutta_dopri5< state_type >() ),
    ODE,   //Lorentz-force
    Data0 ,//{pos0,v0}
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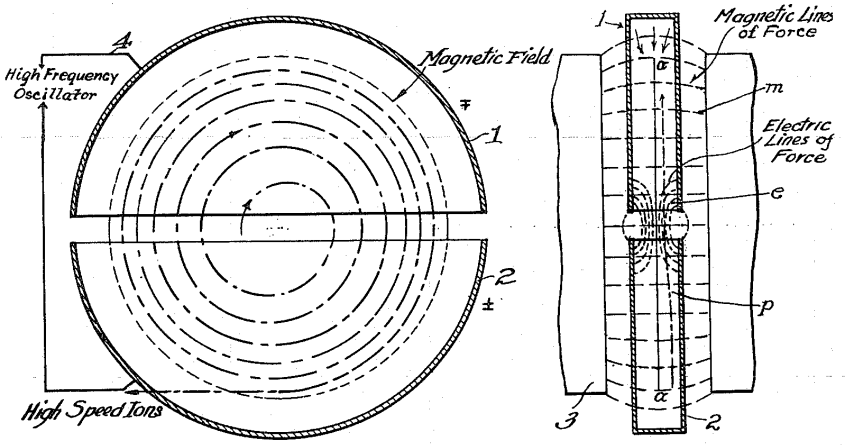
);
```

Example, cyclotron

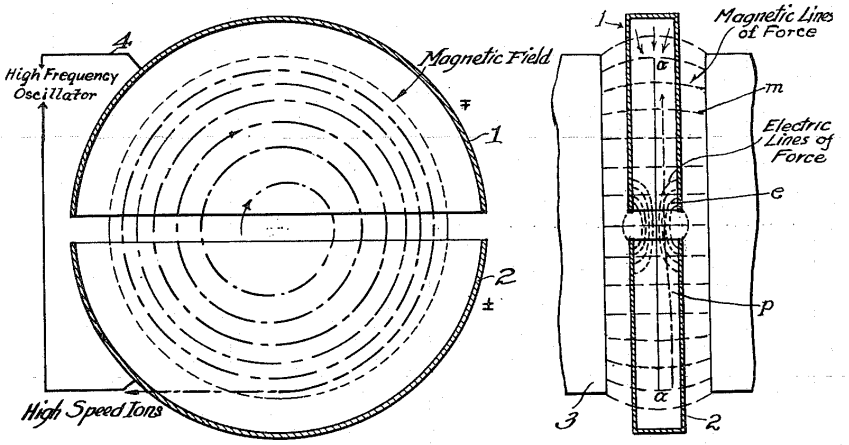
- Electric field accelerates, magnetic contains.



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

Example, cyclotron

- Electric field accelerates, magnetic contains.
- Single gab, oscillating field.



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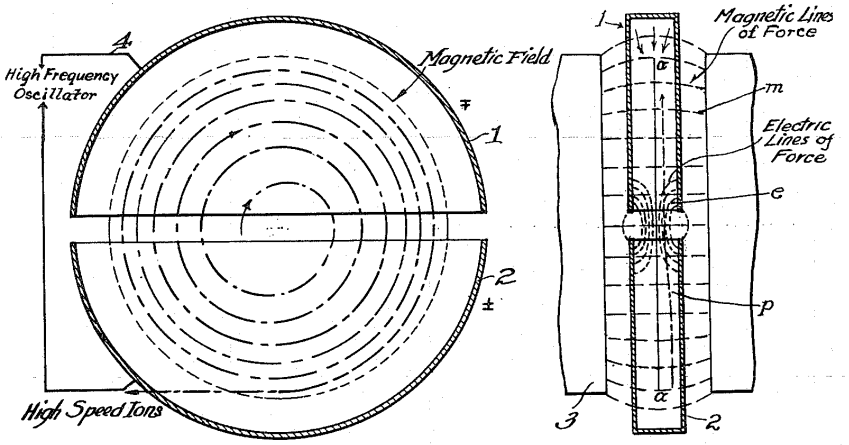
Example, cyclotron

- Electric field accelerates, magnetic contains.
- Single gab, oscillating field.
- Uses Cyclotron frequency

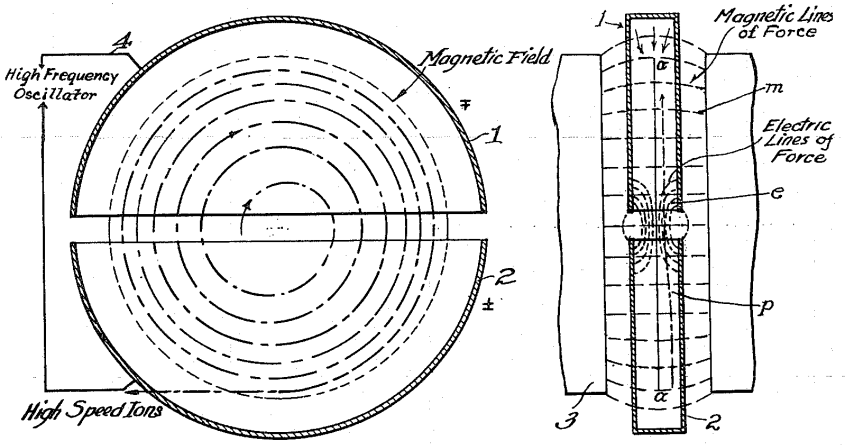


Ernest O. Lawrence, 1934, U.S. Patent 1,948,384; image in Public Domain.

Example, cyclotron

- Electric field accelerates, magnetic contains.
- Single gab, oscillating field.
- Uses Cyclotron frequency
- Analytical final speed, in principle path.

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



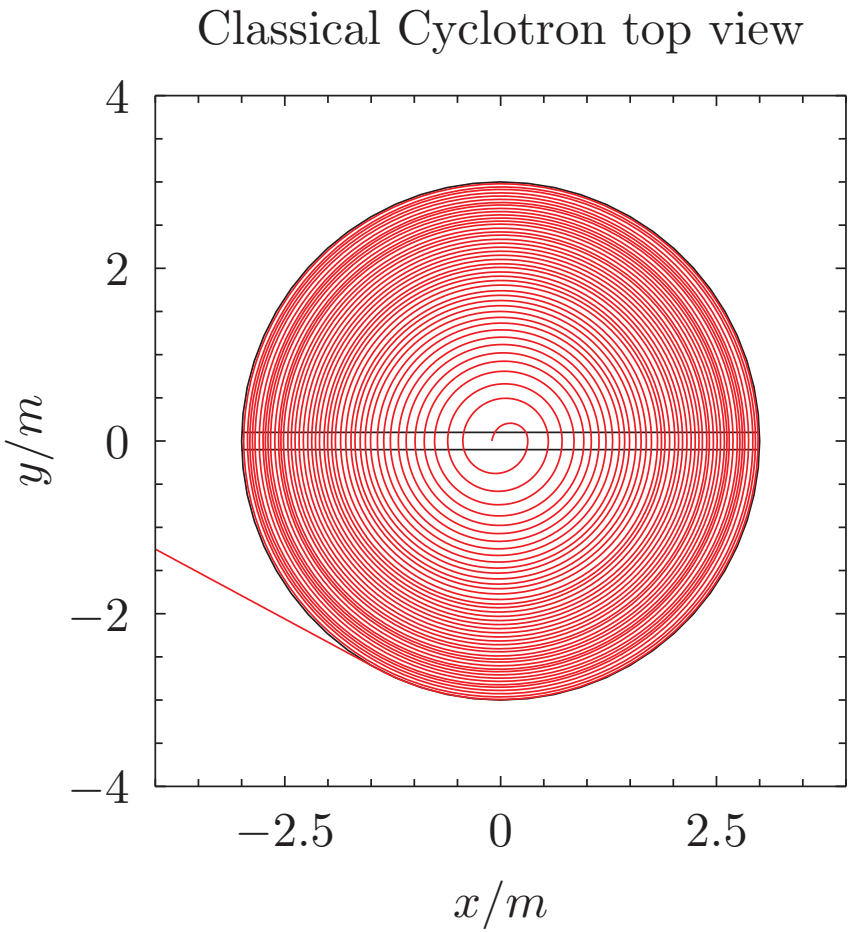
Ernest O. Lawrence, 1934, U.S. Patent 1,948,384; image in Public Domain.

Naive setup

```
size_t steps = integrate(
//Default to adaptive- Dopri5, this is fine
    ODE       , //Lorentz-force
    Data0     , //{pos0,v0}
    0.0       , //t0=0
    T         , //Here 500 micro second
    timestep , //Here 0.1 (intentionally too large)
    save_step);//User defined save data function
```

Does it help/work

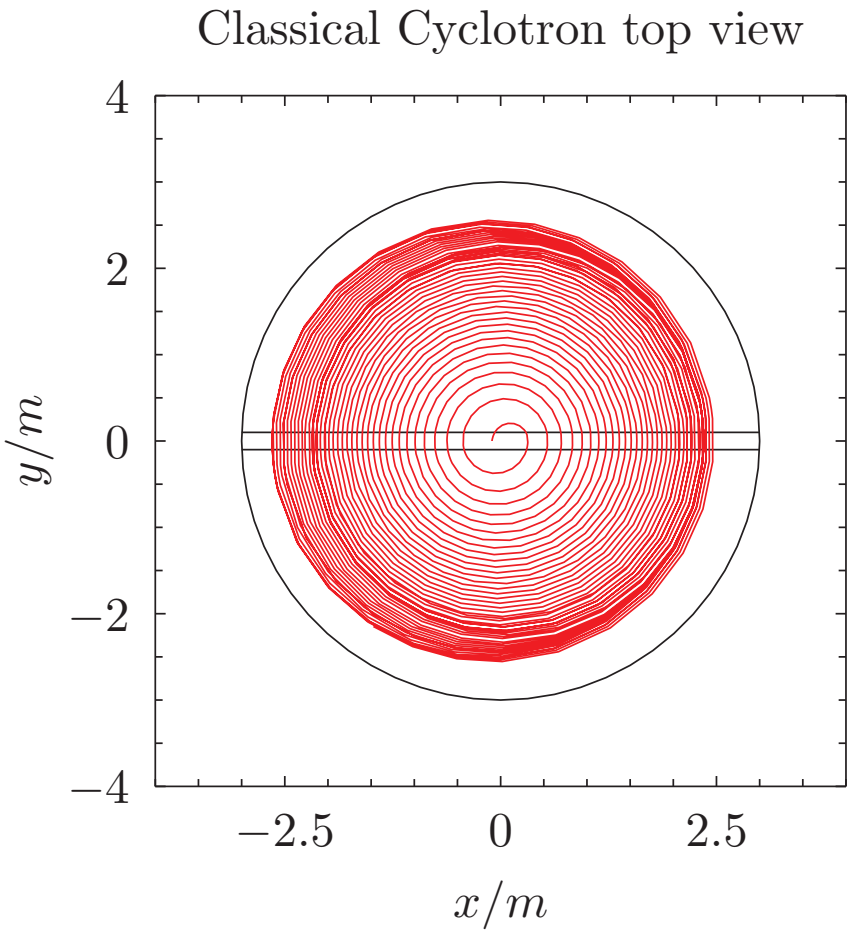
- With fixed step size (Same method, accept all) 4999 points



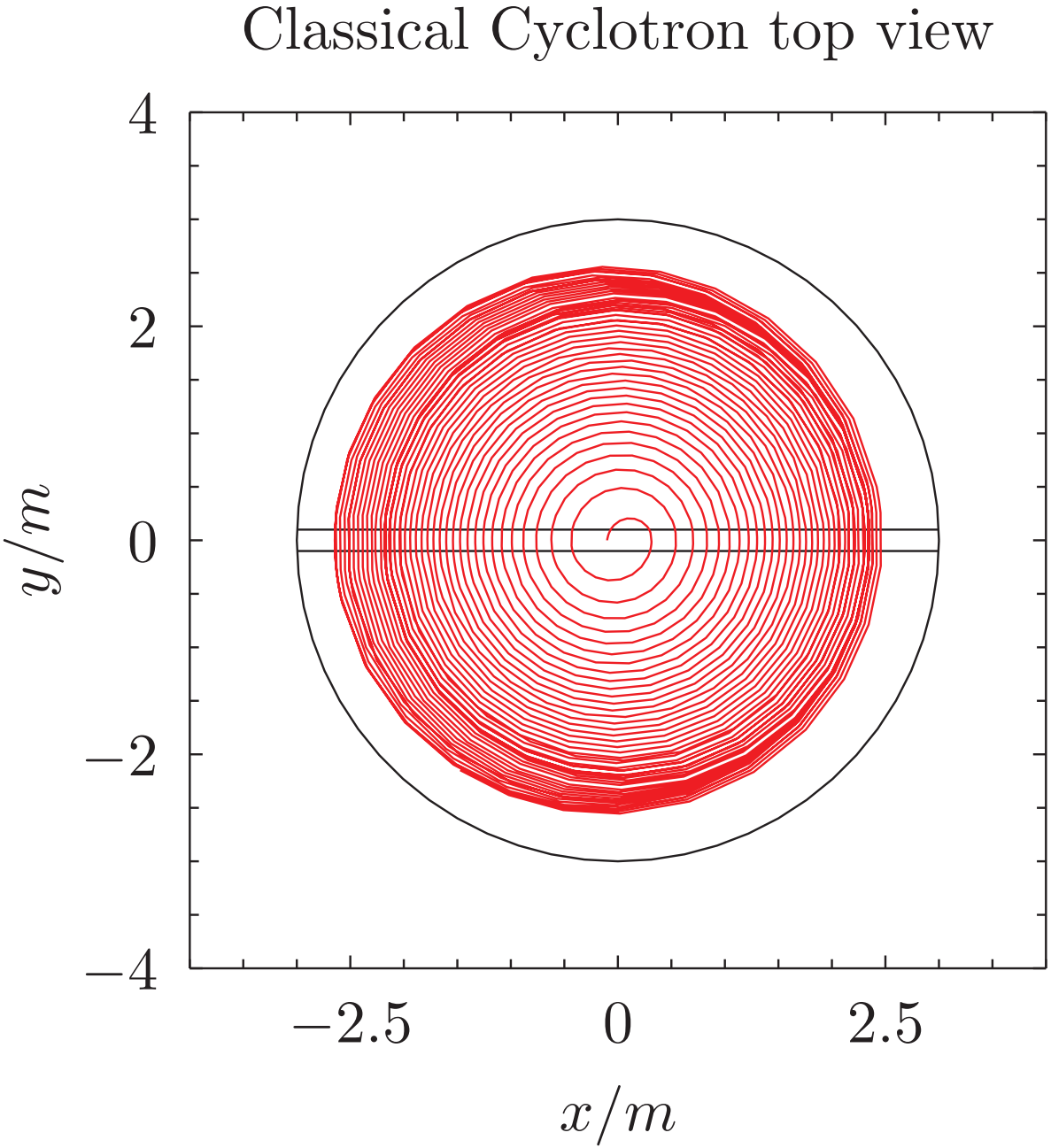
4999 points!

Does it help/work

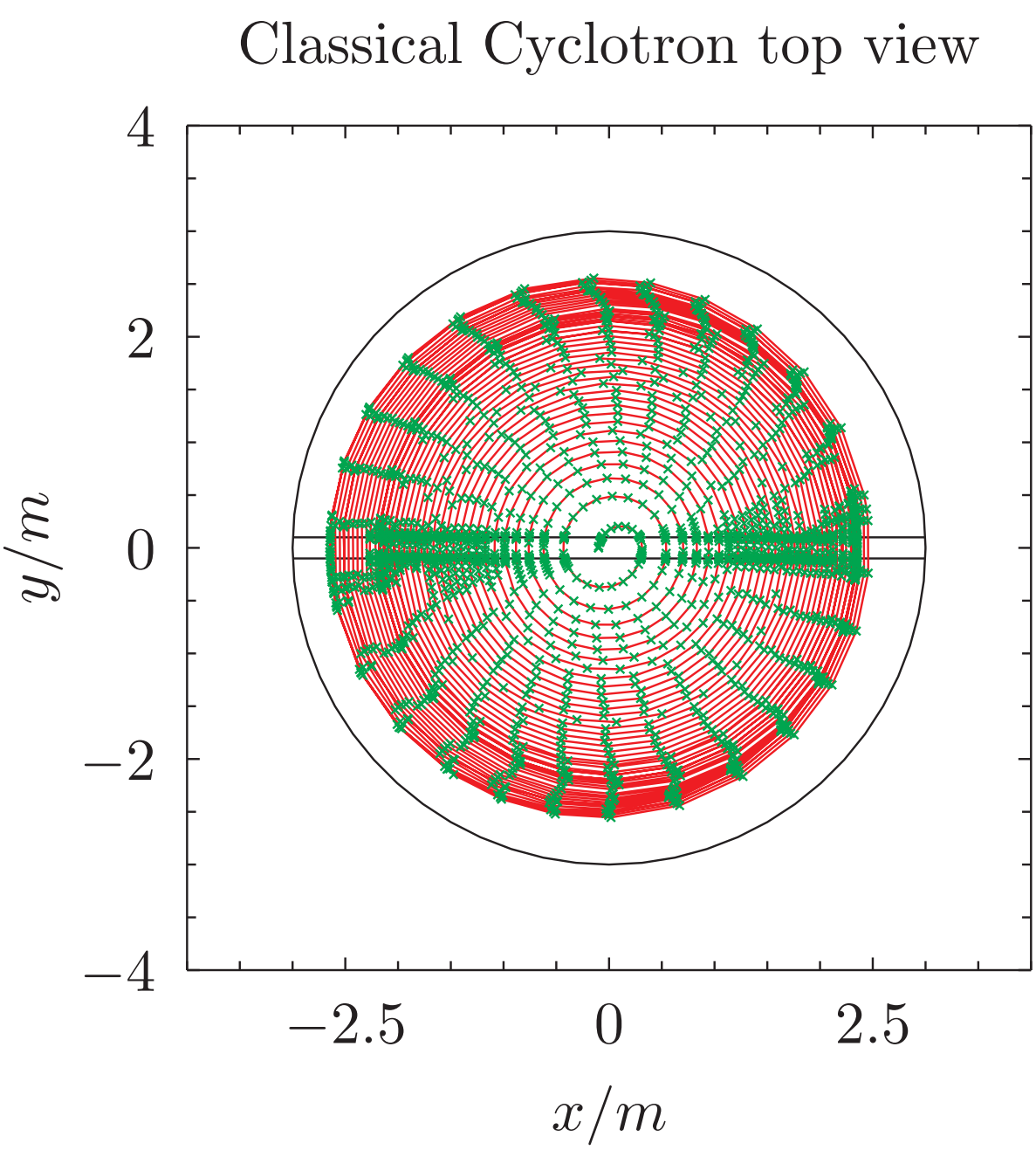
- With fixed step size (Same method, accept all) 4999 points
- Trust default setup:
- Epic fail Why?



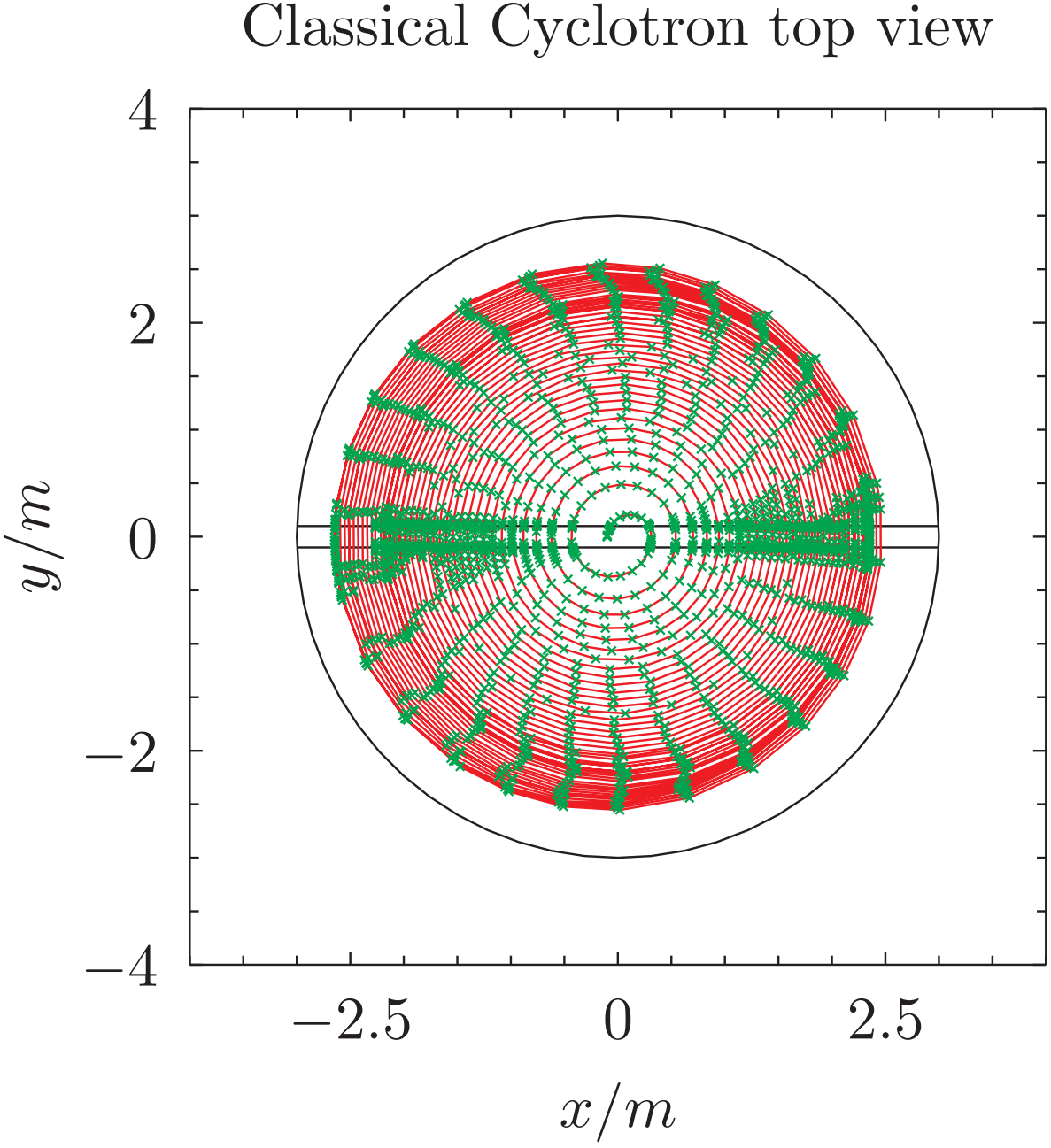
2070 points



Default choice, 2070 points.

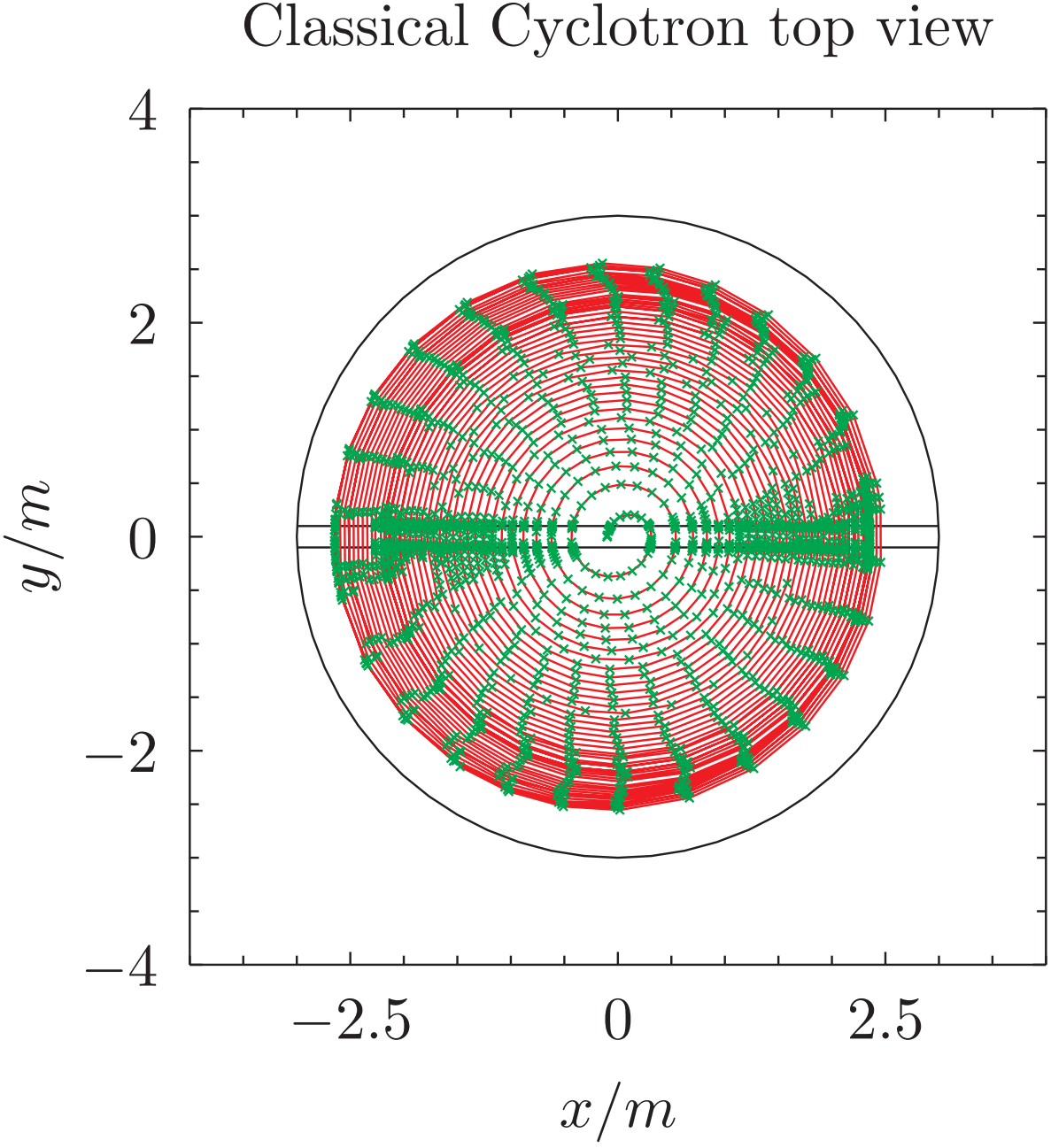


Default choice, 2070 points.



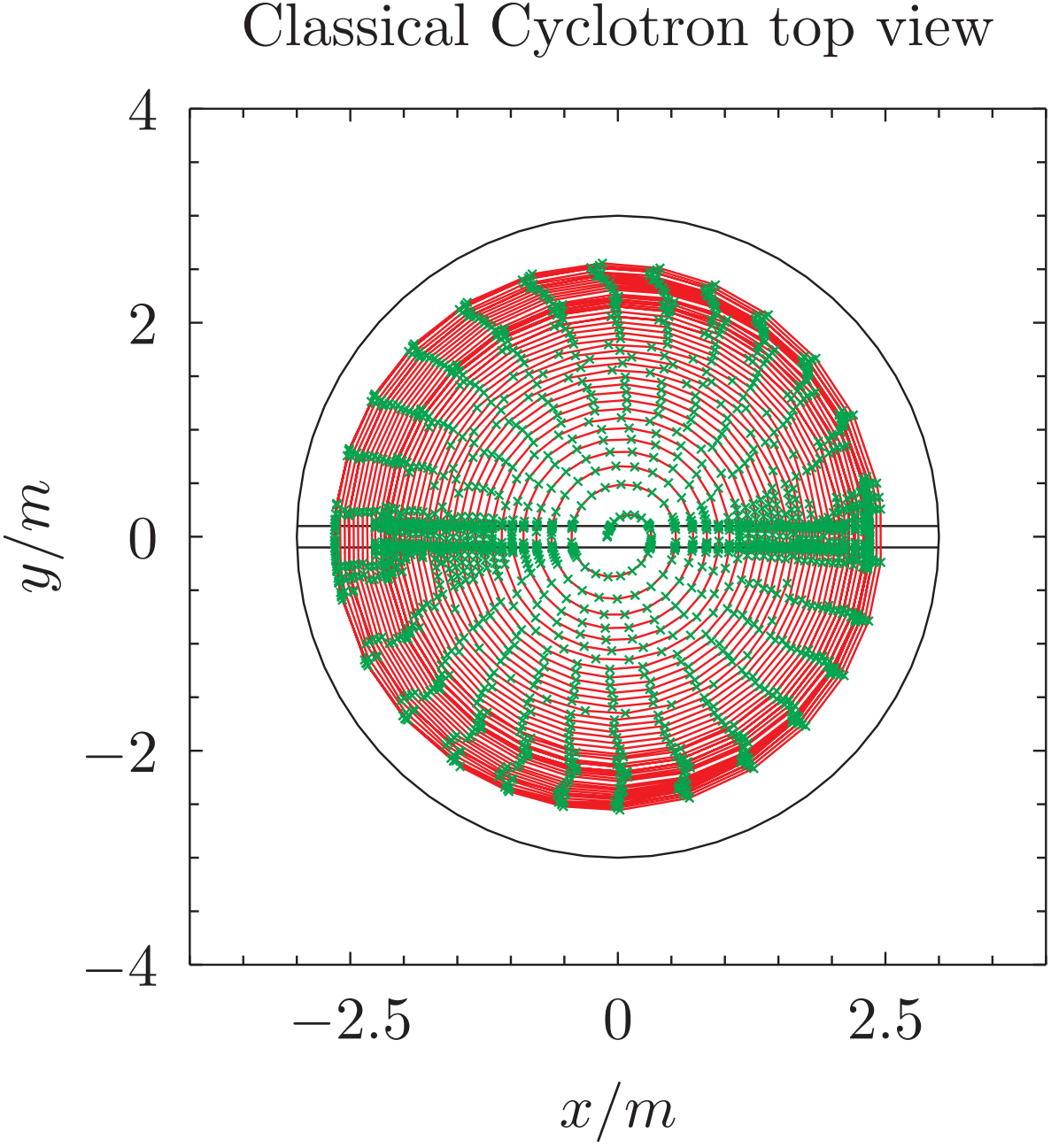
Default choice, 2070 points.

Classical Cyclotron top view



Default choice, 2070 points.

Classical Cyclotron top view



Default choice, 2070 points.

Classical Cyclotron top view

Non-analytic systems

Questions