

How physics simulations work: simulating particles in electric and magnetic fields

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Introduction

Theory and physical background 10 min

Euler's Method and the 4th order Runge-Kutta Method 15 min

- Euler's Method

- Higher order Runge-Kutta methods

- Demonstration, particles in a solenoid

Embedded algorithms, and adaptive step size 15 min

- Dormand Prince 5 (4) method

- Demonstration: magnetic dipole

Conclusion

Introduction, what and why

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- ▶ Demonstration, charged particles in electric and magnetic fields.
- ▶ Analytically known and not.
- ▶ Simulations are not experiments!

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- ▶ The Lorentz force+N2:

$$\vec{F} = q(\vec{v} \times \vec{B} + \vec{E}).$$
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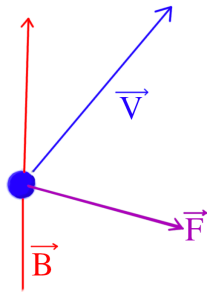
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- ▶ Only 1 particle! so pre-programmed depending on the setup.
- ▶ Could use potentials $\phi(\vec{r}, t)$ $\vec{A}(\vec{r}, t)$ and Hamiltonian, or Lagrangian.
- ▶ Other systems would have other differential equations.

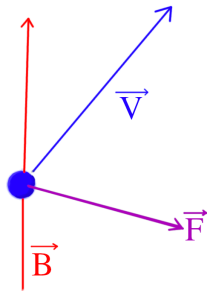
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$$dW_{\vec{B}} = \vec{F}_B \cdot d\vec{r} \propto (\vec{v} \times \vec{B}) \cdot \vec{v} = 0.$$



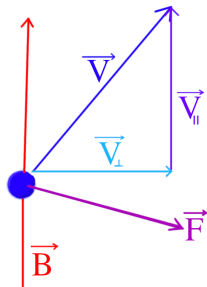
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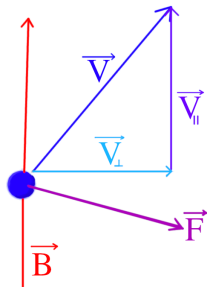
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Cyclotron motion



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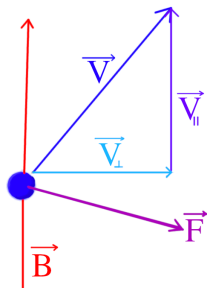
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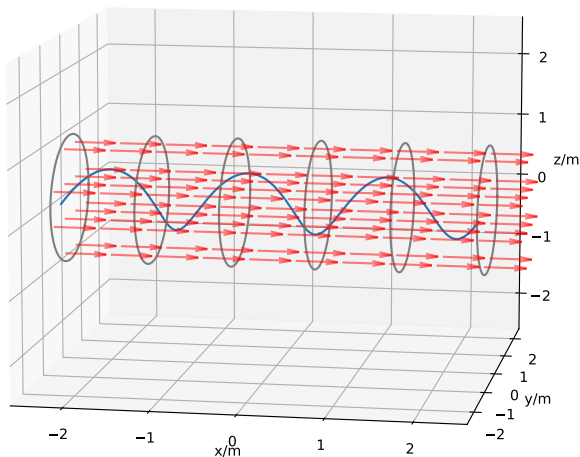
$$|\vec{F}_B| = |q(\vec{v} \times \vec{B})| = |qv_{\perp} B|.$$

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

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



What we expect to see

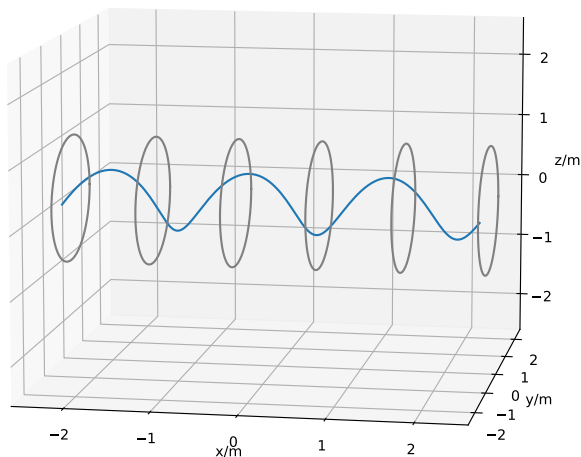


“Cyclotron motion”

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)

What we expect to see

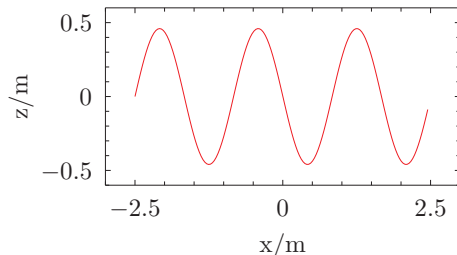


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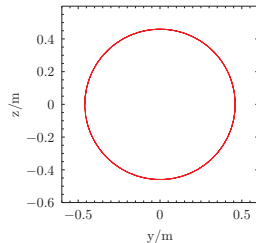
$$R \approx 0.5 \text{ m} \sin(\theta) \quad T = \frac{2\pi}{\omega_c} \approx 10 \mu\text{s}$$

What we expect to see

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



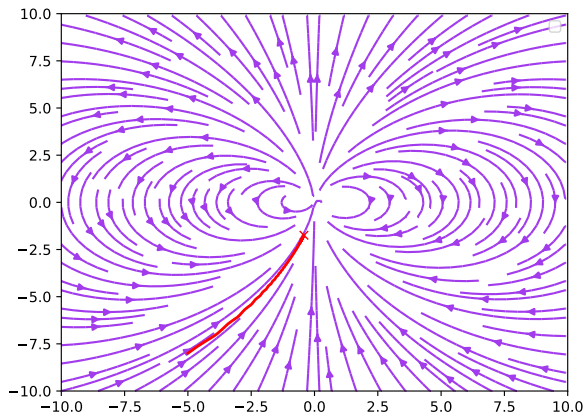
Analytical: proton in a solenoid, speed



“Cyclotron motion”

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What we expect to see



(Actually from my simulation)

Ordinary differential equation's.

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

$$\ddot{\vec{r}}(t) = \frac{q}{m}(\dot{\vec{r}}(t) \times \vec{B}(\vec{r}, t) + \vec{E}(\vec{r}, t)).$$

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- Here:

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

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 V = vec(Data[3],Data[4],Data[5]);
    //Lorentz+Newtons 2nd law
    vec F = Charge*(Fields.get_Efield(pos,t)+
        cross(V,Fields.get_Bfield(pos,t)));
    vec dVdt = F*Inv_mass;
    //Save derivative of data
    dDatadt[0]=V.x;dDatadt[1]=V.y;dDatadt[2]=V.z;
    dDatadt[3]=dVdt.x;Datadt[4]=dVdt.y;dDatadt[5]=
    dVdt.z;
};
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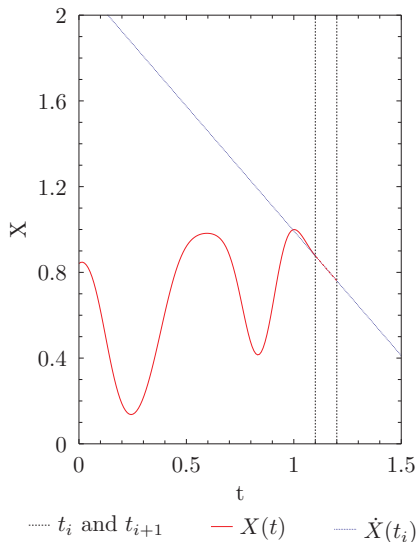
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Solving differential equations

- We know only $\mathbf{X}(t_0)$ and t_0 and f_{ode} .

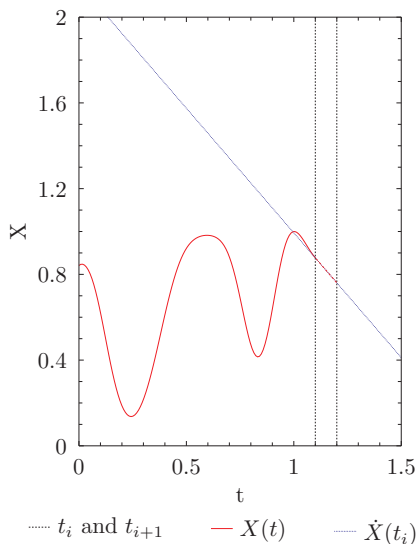
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Solving differential equations

- ▶ We know only $\mathbf{X}(t_0)$ and t_0 and f_{ode} .
- ▶ Can we find $\mathbf{X}(t_0 + h)$ for $h > 0$?

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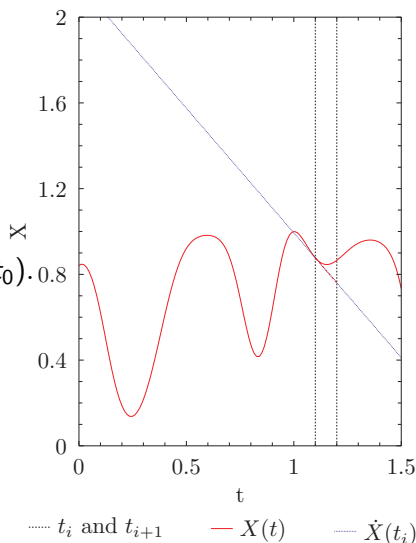


Solving differential equations

- ▶ We know only $\mathbf{X}(t_0)$ and t_0 and f_{ode} .
- ▶ Can we find $\mathbf{X}(t_0 + h)$ for $h > 0$?
- ▶ Euler's Method:

$$\mathbf{X}(t_0+h) = \mathbf{X}(t_0) + hf_{ode}(\mathbf{X}(t_0), t_0).$$

- ▶ Multiple steps
 $t_0, t_1 = t_0 + h, \dots t_i, \dots$
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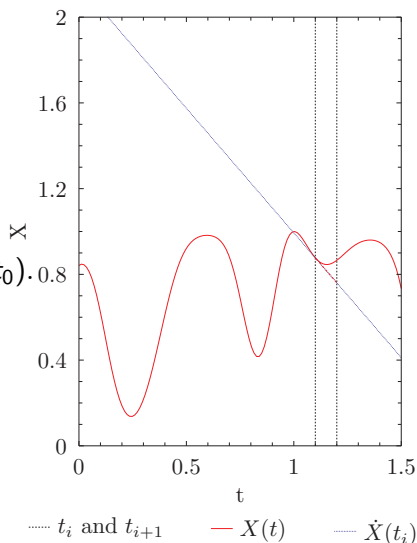


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- ▶ Can this be justified?
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- ▶ Argument suggests we need $\dot{f}_{ode}, \ddot{f}_{ode}, \dots$, we don't!

The Runge Kutta steppers

- In general:

$$\mathbf{X}(t_{i+1}) - \mathbf{X}(t_i) = \int_{t_i}^{t_{i+1}} \dot{\mathbf{X}}(t) dt.$$

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- More generally, (*Explicit and single step*), Runge-Kutta family:

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

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- Guess $\tau_1 = t_i$ use $f_{ode}(\mathbf{X}(t_i), t_i)$ to approximate $\mathbf{X}(\tau_2)$ to approximate $\mathbf{X}(\tau_3)$ etc.
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Runge Kutta methods

- More commonly written:

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

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- Taylor series analogy: Local error h^{p+1} , global h^p .
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The General explicit Runge Kutta method

- Expressed in Butcher tableau:

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

Higher order methods

- 2nd order (Heun's method):

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

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

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

Higher order methods

- 4th order, often simply called the Runge Kutta method:

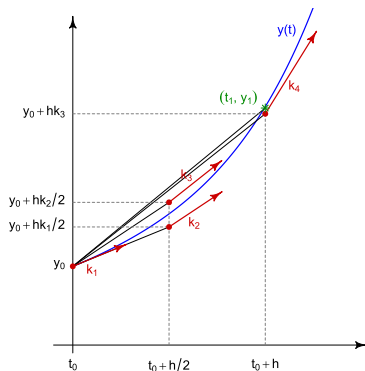
$$\mathbf{X}(t_{i+1}) - \mathbf{X}(t_i) = \frac{h}{6}(\mathbf{k}_1 + 2\mathbf{k}_2 + 2\mathbf{k}_3 + \mathbf{k}_4)$$

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

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

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

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



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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;

    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);

    //substep 2
    temp=Data+timestep*K1/2;
    ODE(temp,K2,t+timestep/2);
```

RK4 Implementations (2/2)

```
//substep 3
```

```
temp=Data+timestep*K2/2;  
ODE(temp,K3,t+timestep/2);
```

```
//substep 4
```

```
temp=Data+timestep*K3;  
ODE(temp,K4,t+timestep);
```

```
//Read data
```

```
Data+=timestep*(K1+2.0*K2+2.0*K3+K4)/6.0;  
save_step( Data , i*timestep );}
```

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 $\theta = 60^\circ$ at different h .

Does it work

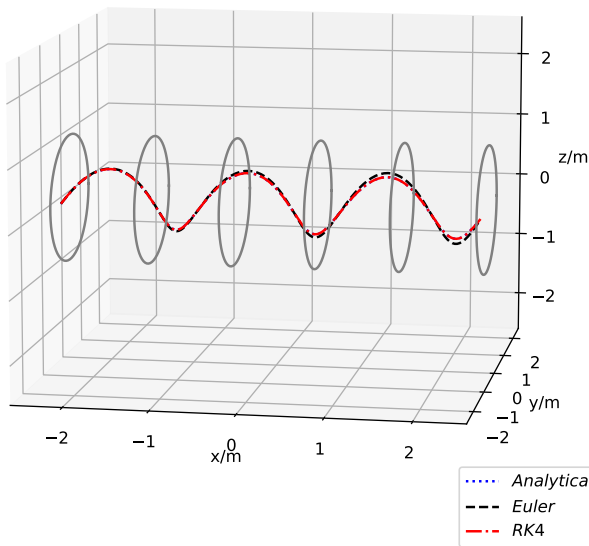
- ▶ Test, same proton in a solenoid use $\theta = 60^\circ$ reference, had:

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

- ▶ Compare Analytic, Euler, Runge-Kutta 4.
- ▶ Consider $\theta = 60^\circ$ at different h .
- ▶ Check error on $|\vec{v}|$, $R = \sqrt{y^2 + z^2}$.

At a glance, 3D view

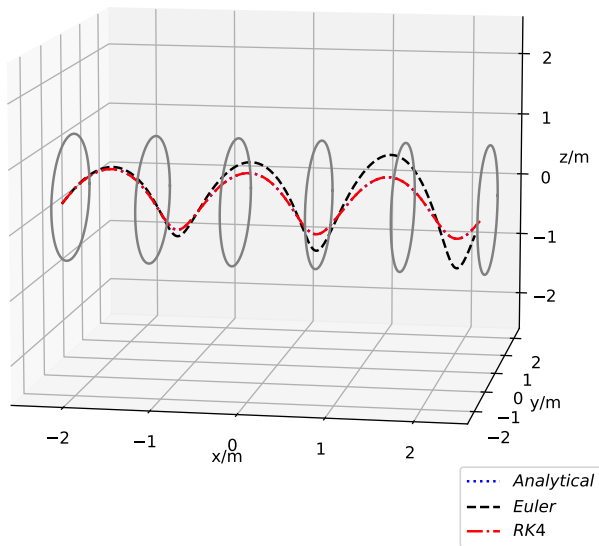
$$h = t_{i+1} - t_i = 0.01 \mu\text{s}$$



3129 steps

At a glance, 3D view

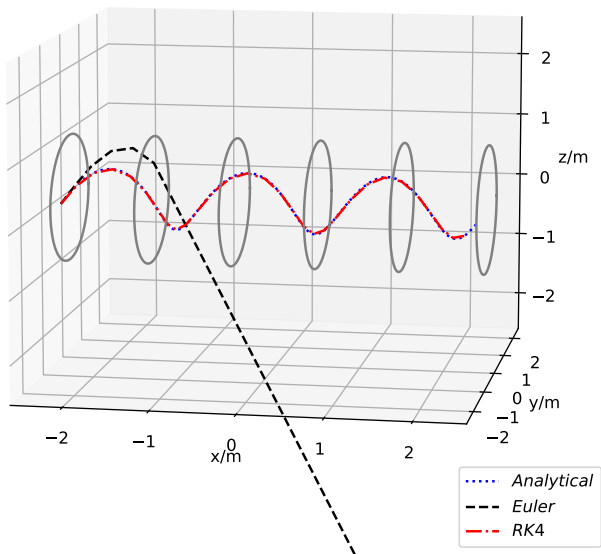
$$h = t_{i+1} - t_i = 0.1 \mu\text{s}$$



312 steps

At a glance, 3D view

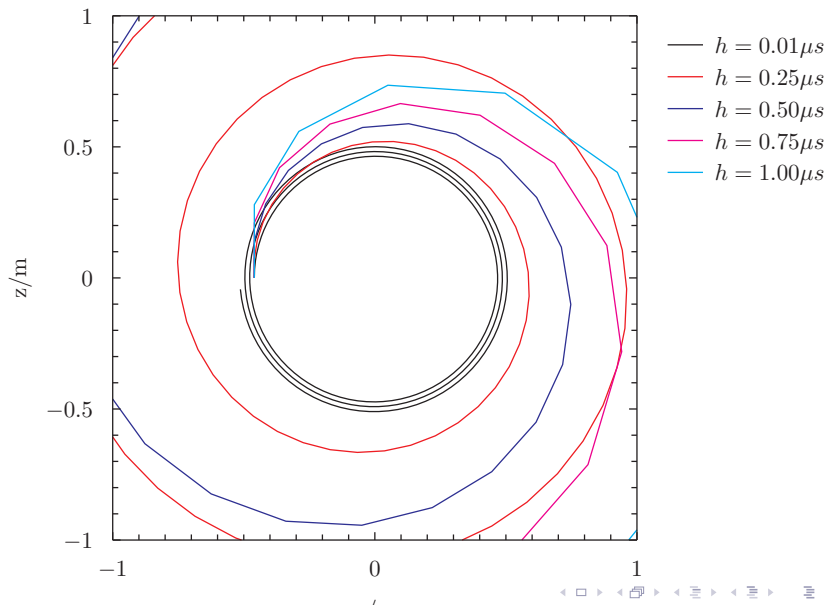
$$h = t_{i+1} - t_i = 1.0 \mu\text{s}$$



31 steps.

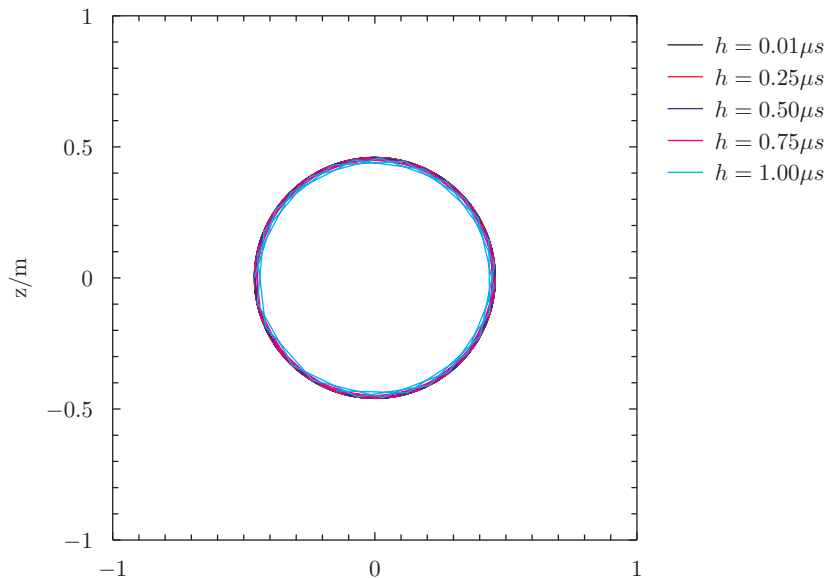
At a glance, front view, no border

Euler method, front-view

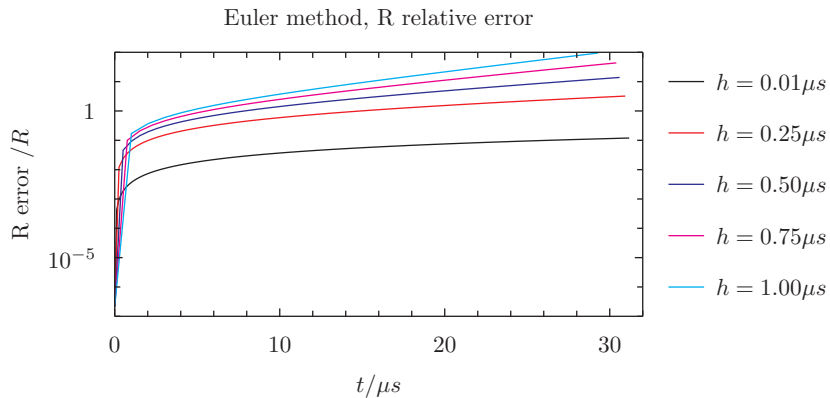


At a glance, front view, no border

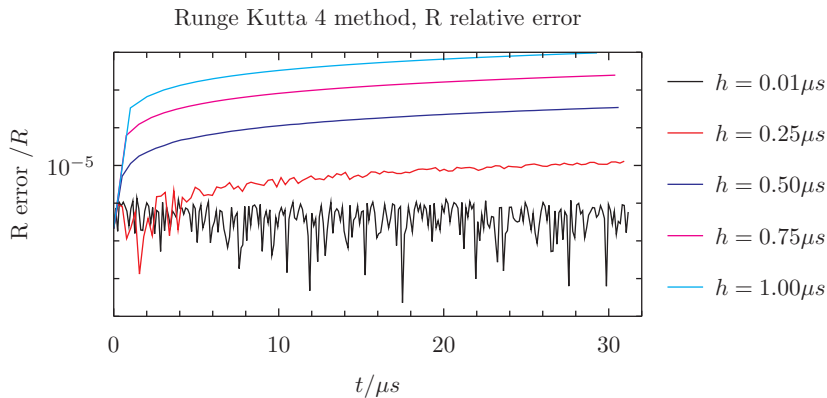
RK4, front-view



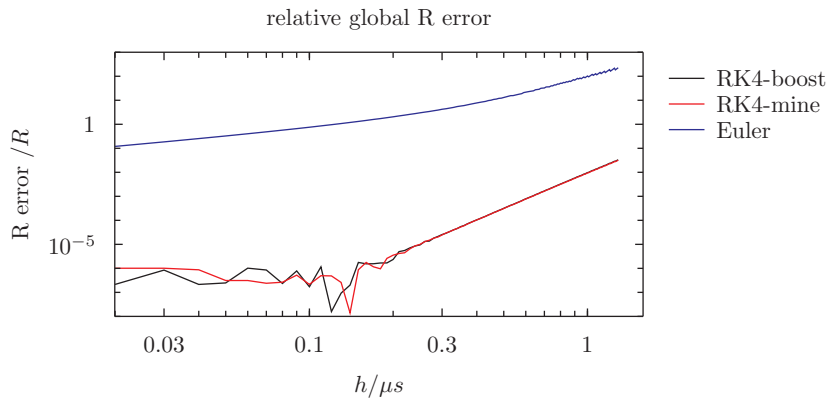
Constant radius?



Constant radius?



Error as function of h



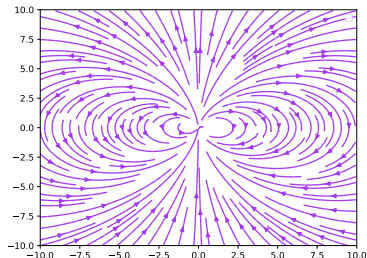
What is not to like?

What is not to like?

- ▶ Usually don't know error.
- ▶ Hard to pick h , and may change:

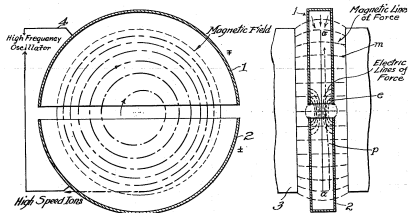
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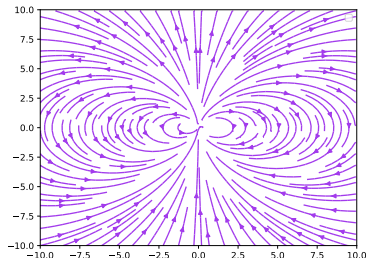
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Ernest O. Lawrence, 1934, U.S. Patent 1,948,384; image in Public Domain.

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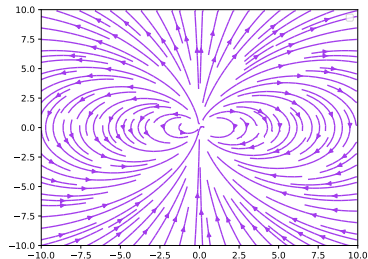
- ▶ Usually don't know error.
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- ▶ Let the computer pick h for error.



Example, magnetic dipole

- True dipole:

$$\vec{B} = \frac{\mu_0}{4\pi r^3} \left[3\hat{r}(\vec{m} \cdot \hat{r}) - \vec{m} \right].$$

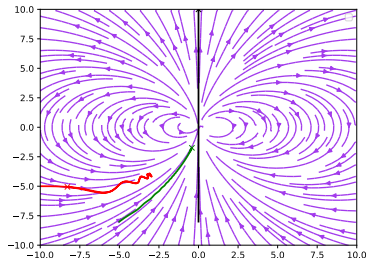


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Arbitrarily set

$$\frac{\mu_0}{4\pi} |\vec{m}| = 0.155 \text{ T/m}^3.$$

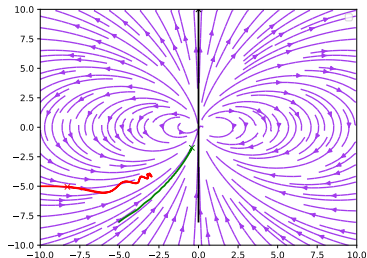
Protons with speed around
10 000 m/s

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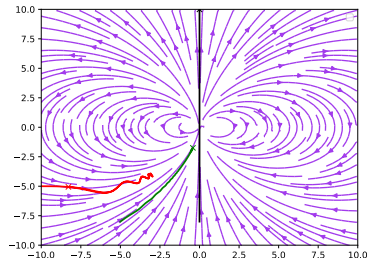
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- ▶ No analytical solution.



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Embedded Runge-Kutta algorithms

- ▶ Need estimate for error.

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- ▶ Adjust step size to keep the error(s) small (Implementations differ!).

Dormand, J. R.; Prince, P. J. (1980), "A family of embedded Runge-Kutta formulae", Journal of Computational and Applied Mathematics

(1)

Runge-Kutta Dormand Prince 5 (4)

- ode45 in Matlab, `scipy.solve_ivp` in Python ,
`RungeKutta_dopri5` in `boost::odeint`.

$$\mathbf{X}^{(5)}(t_{i+1}) - \mathbf{X}(t_i) = h \sum_{j=1}^m b_j^{(5)} \mathbf{k}_j$$

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- ▶ 7 \mathbf{k}_j 's (actually 6 by clever re-usage).
Dormand, J. R.; Prince, P. J. (1980), "A family of embedded Runge-Kutta formulae", Journal of Computational and Applied Mathematics

Butcher Tableau of Dormand Prince (5) 4

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

Runge-Kutta Dormand Prince 5 (4)

- Step size correction (Dormand Prince):

$$h_{new} = 0.9h_{old} \left[\frac{\delta}{||E||} \right]^{\frac{1}{p+1}}$$

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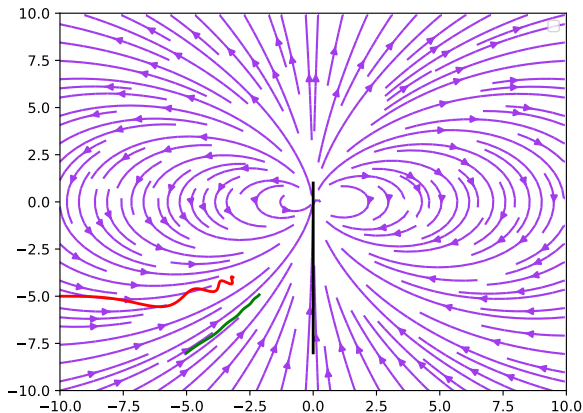
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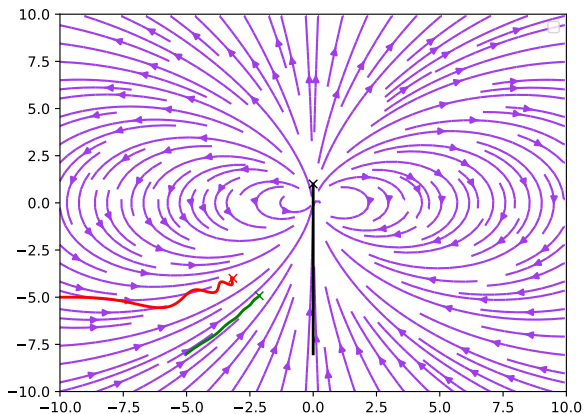
- Scale by step size $\frac{h_{old}}{T}$, "Fail safe" $\sqrt{\dots}$.
Dormand, J. R.; Prince, P. J. (1980), "A family of embedded Runge-Kutta formulae", Journal of Computational and Applied Mathematics

Does it work?



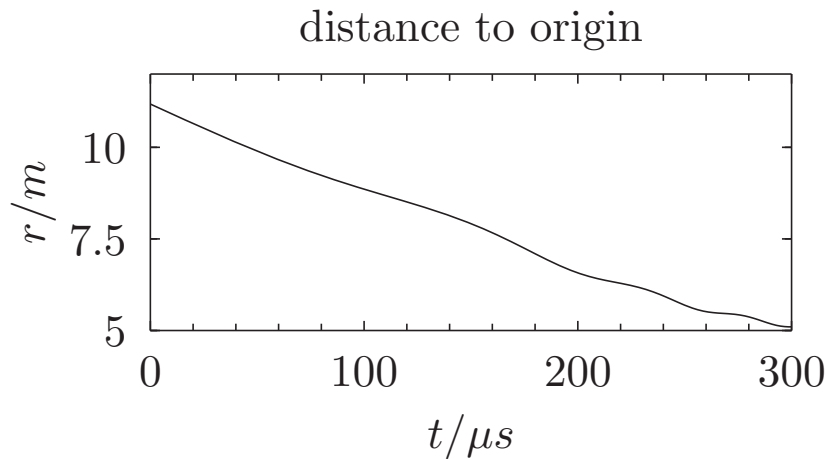
My version relative and absolute error 10^{-6} . 94 steps (+ 14 rejected).

Does it work?



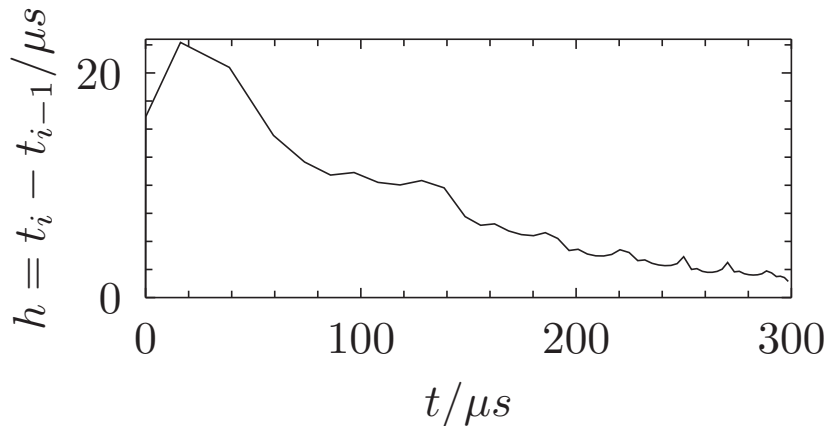
Odeint library relative and absolute error 10^{-7} . 92 steps.

Does it work?



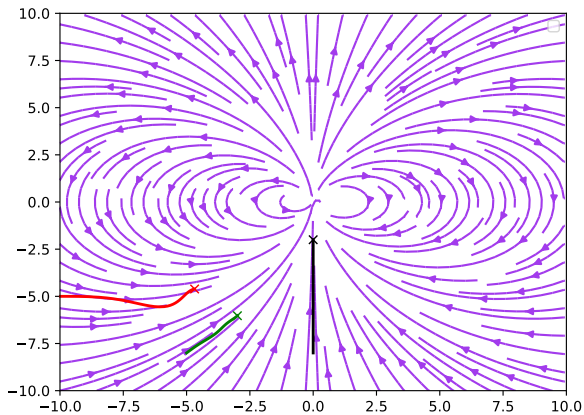
Does it work?

Adaptive timesteps



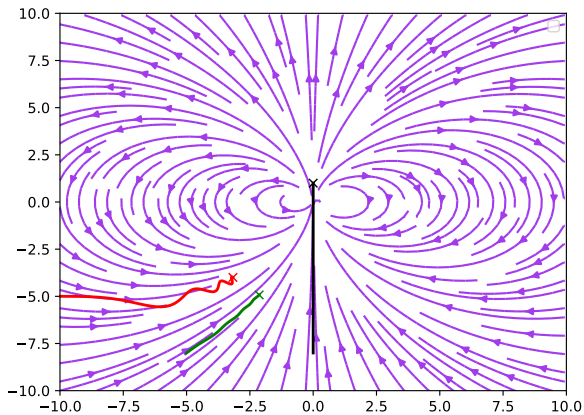
My version, adaptive step size.

Another curious result



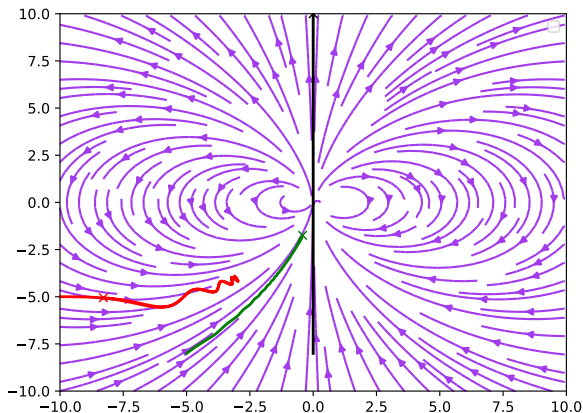
$T = 0.2 \text{ ms}$

Another curious result



$T = 0.3 \text{ ms}$

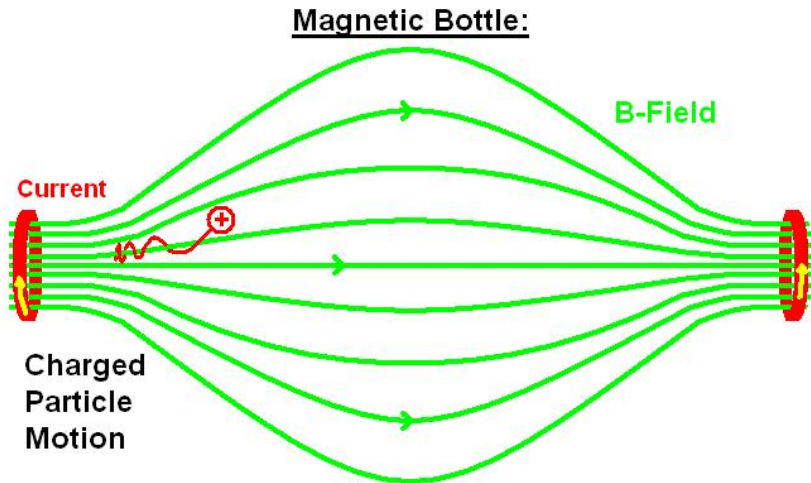
Another curious result



$$T = 0.6 \text{ ms}$$

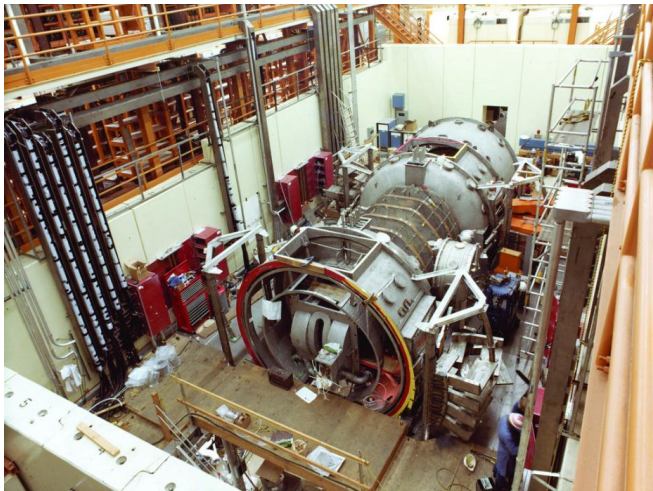
Magnetic “mirror” or “bottle”.

Another curious result



Wikipedia user WikiHelper2134 , Public Domain.

Another curious result



Tandem Mirror Experiment, The Lawrence Livermore National Laboratory, 1978.

Conclusion

- ▶ Simulating particles in electric and magnetic fields.

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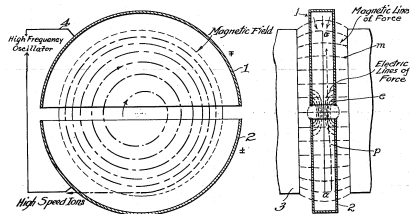
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- ▶ Numerically solving ordinary differential equations
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Conclusion

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- ▶ Numerically solving ordinary differential equations
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- ▶ Can easily be generalized to other systems.
- ▶ Limitation, simulations are not experiments.

Example, cyclotron

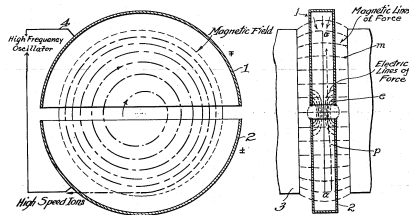
- Electric field accelerates, magnetic contains.



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

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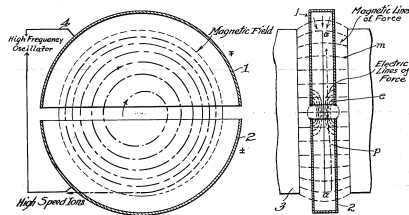
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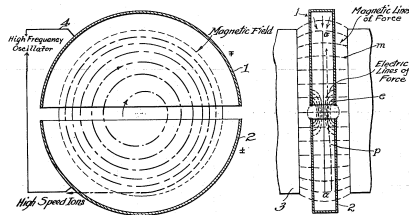


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Example, cyclotron

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

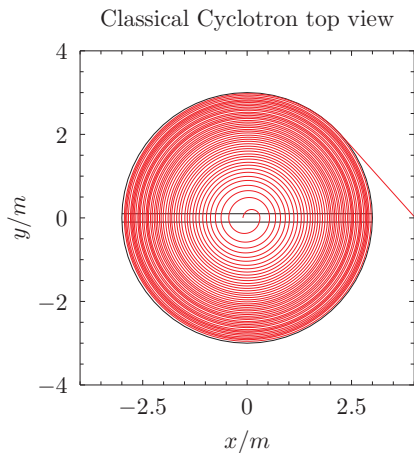
$$\frac{R|q|B}{m} = v_{\perp}$$



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

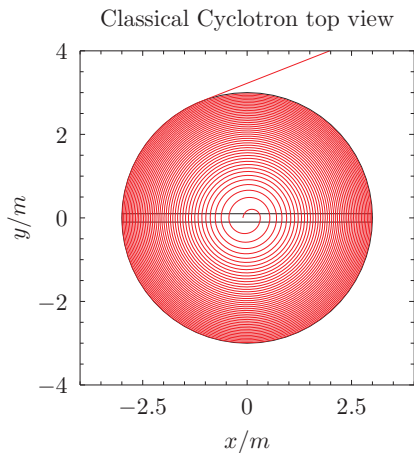
can it be simulated

- ▶ with fixed step size, looks bad 4999 points



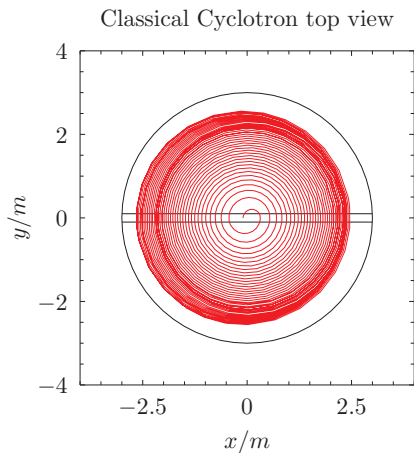
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