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

Nikolaj Roager Christensen

Student Colloquium in Physics and Astronomy, Aarhus University

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Numerical integration of ordinary differential equations: motion of charged particles in electromagnetic fields

Introduction, what and why

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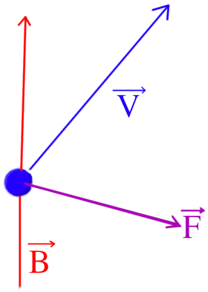
- Only 1 particle! so pre-programmed depending on the setup.
- Could use potentials $\phi(\vec{r}, t)$ $\vec{A}(\vec{r}, t)$ and Hamiltonian, or Lagrangian.
- Other systems would have other differential equations.

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



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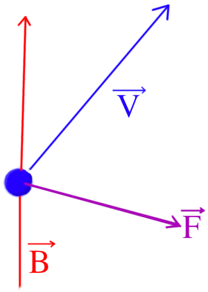

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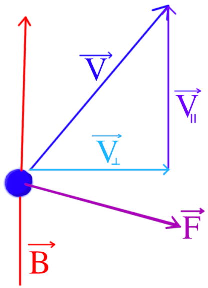

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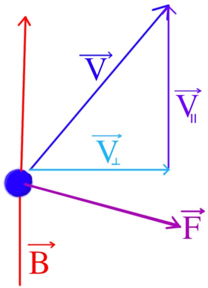
- Same as Centripetal force: Cyclotron motion



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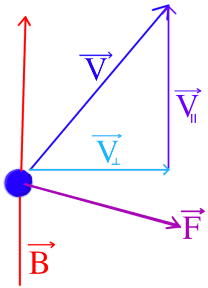
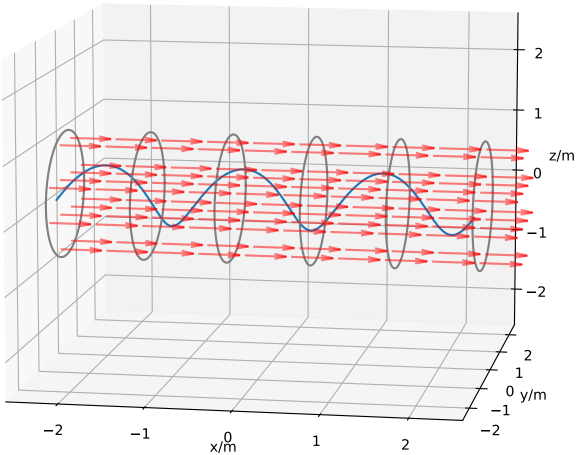
- Cyclotron radius and frequency:

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



What we expect to see



"Cyclotron motion"

Solenoid with $N = 1000$ turns per m, $I = 5\,\mathrm{A}$, $r = 1\,\mathrm{m}$, $|\vec{B}| \approx 6\,\mathrm{mT}$.

Proton with $E_{kin} = 1\,\mathrm{MeV/c^2}$ ($|v| \approx 3.195 \times 10^5\,\mathrm{m/s}$)

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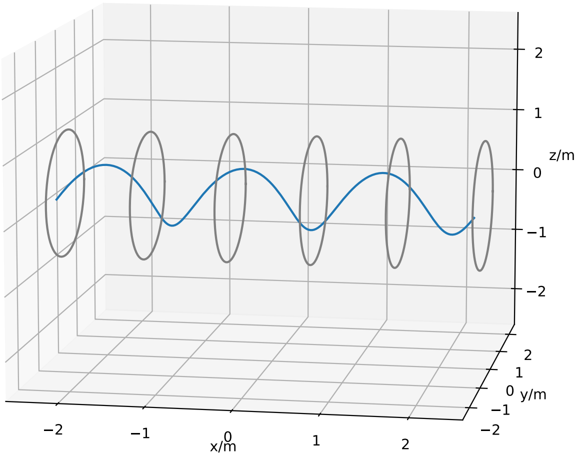

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$$R \approx 0.5\,\mathrm{m}\sin(\theta) \qquad T = \frac{2\pi}{\omega_c} \approx 10\,\mu\mathrm{s}$$

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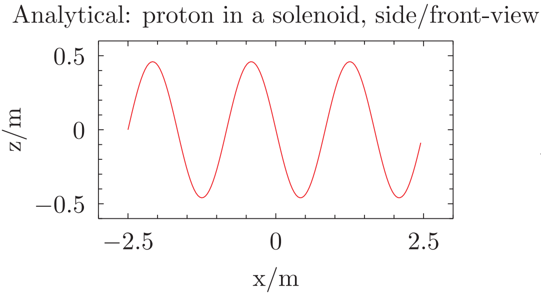

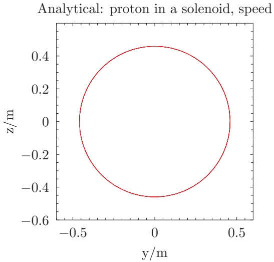

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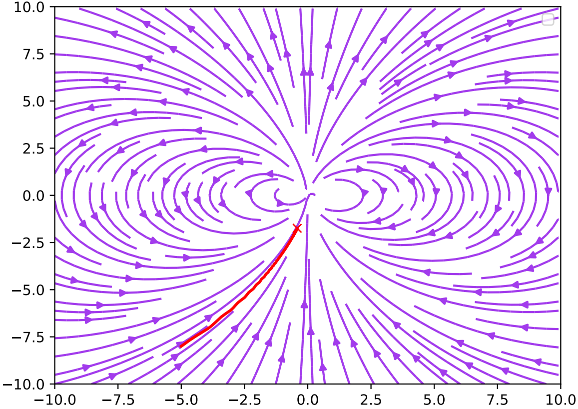

(Actually from my simulation)

Ordinary differential equation's.

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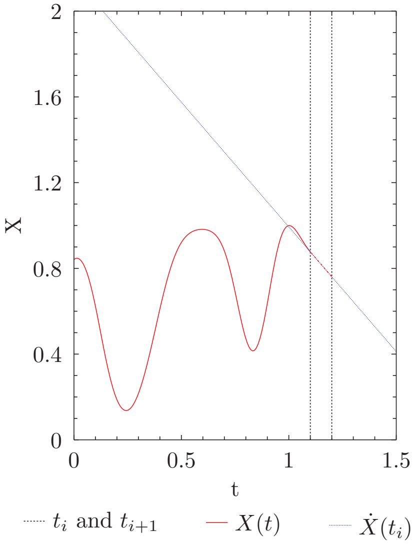
Solving differential equations

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



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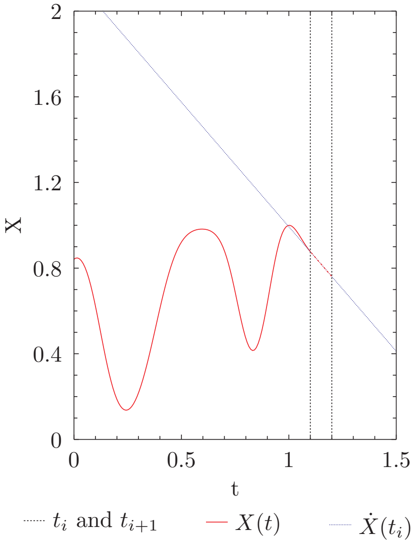
- Can we find $\mathbf{X}(t_0 + h)$ for $h > 0$?.



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- Euler's Method:

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

- Multiple steps $t_0, t_1 = t_0 + h, \ldots t_i, \ldots$.
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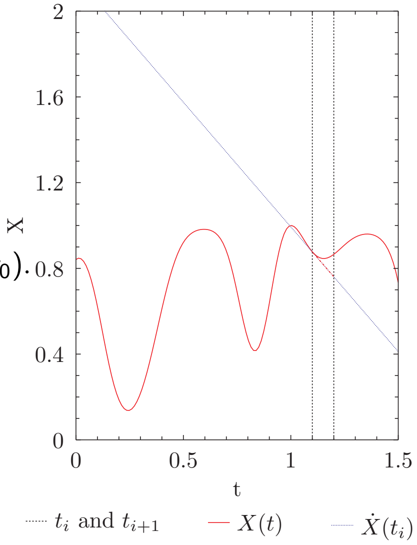

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- Can this be justified?
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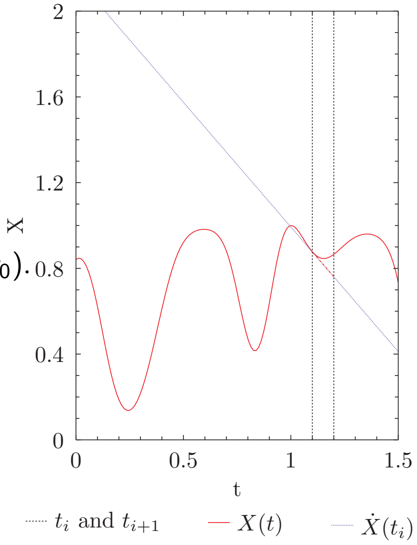

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- Argument suggests we need $\dot{f}_{ode}, \ddot{f}_{ode}, \ldots$, we don't!

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

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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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$$\begin{aligned}
\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_2 h) \\
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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 tableu:

$$
\begin{array}{c|cccc}
c_1 = 0 & & & \\
c_2 & a_{21} & & \\
c_3 & a_{31} & a_{32} & \\
c_n & a_{n1} & a_{n2} & \dots \\
\hline
 & b_1 & b_2 & \dots
\end{array}
$$

Higher order methods

- 2nd order (Heun's method):

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

Higher order methods

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

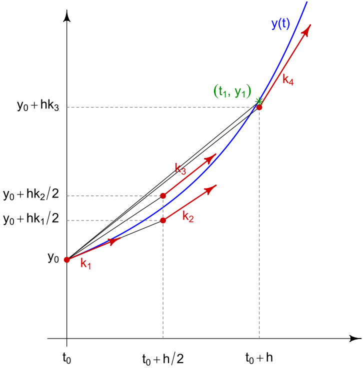
$$\mathbf{X}(t_{i+1}) - \mathbf{X}(t_i) = \frac{h}{6}(\mathbf{k}_1 + 2\mathbf{k}_2 + 2\mathbf{k}_3 + \mathbf{k}_4)$$

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

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

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

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



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:

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

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- Compare Analytic, Euler, Runge-Kutta 4.

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- Compare Analytic, Euler, Runge-Kutta 4.
- Consider $\theta = 60^\circ$ at different h.

Does it work

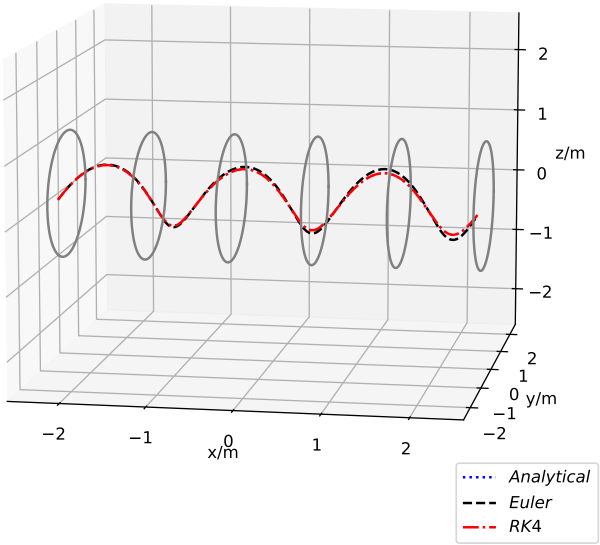
- Test, same proton in a solenoid use $\theta = 60^\circ$ reference, had:

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

- 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

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



3129 steps

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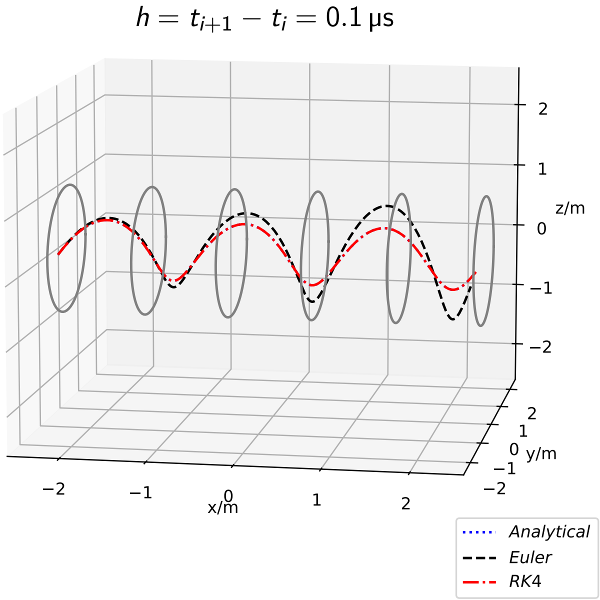
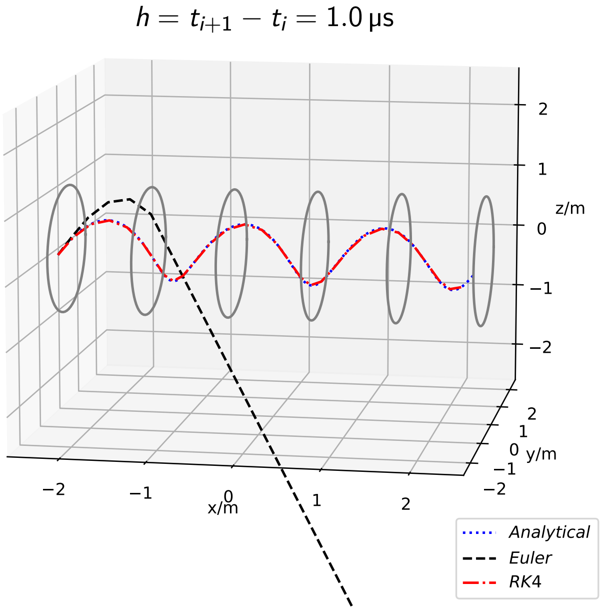


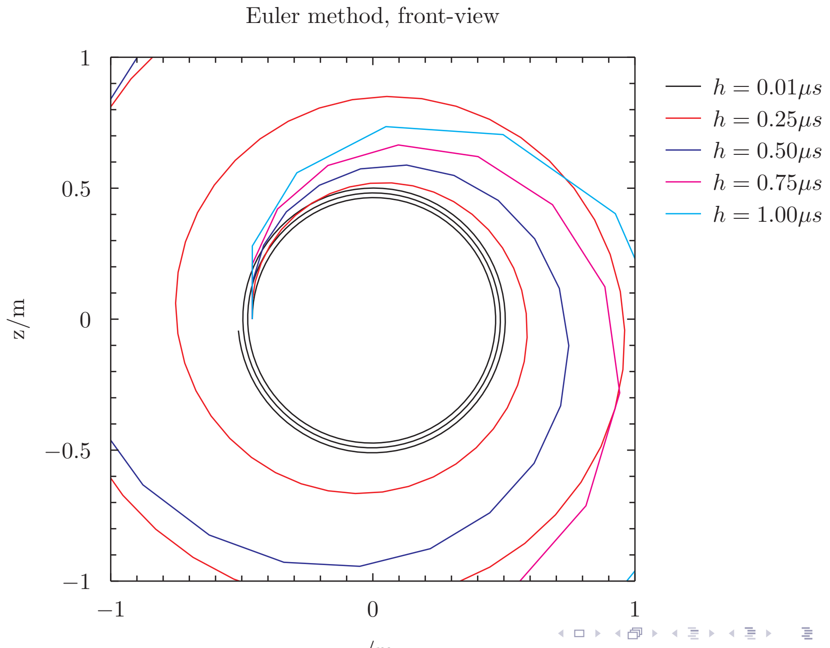
312 steps

At a glance, 3D view



31 steps.

At a glance, front view, no border



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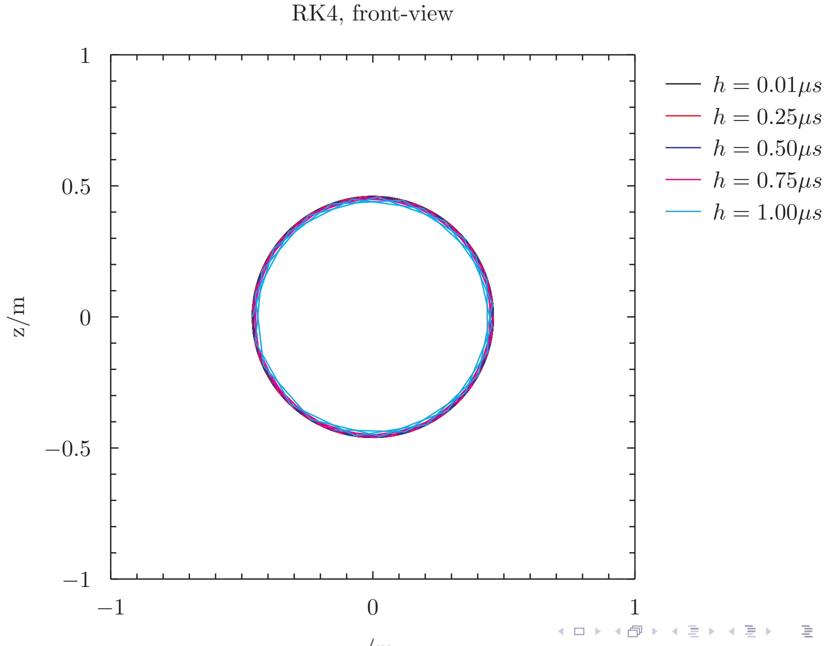
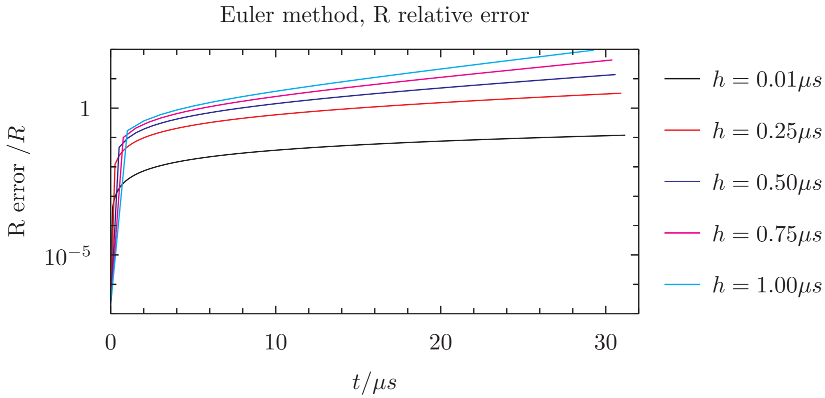


Constant radius?



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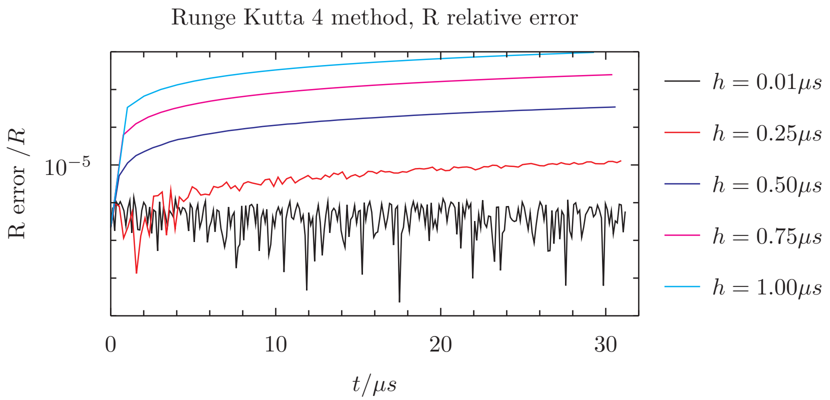
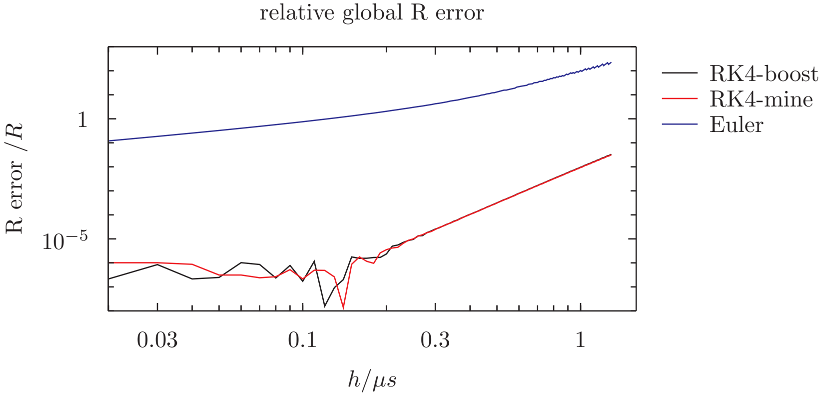


Error as function of h



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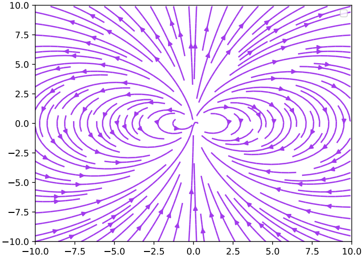

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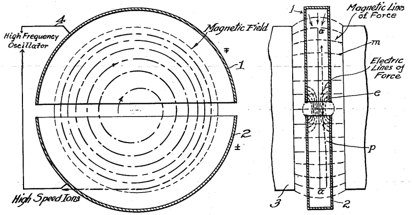

Ernest O. Lawrence, 1934, U.S. Patent 1,948,384; image in Public Domain.

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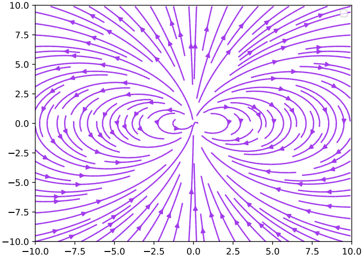
- Let the computer pick h for error.



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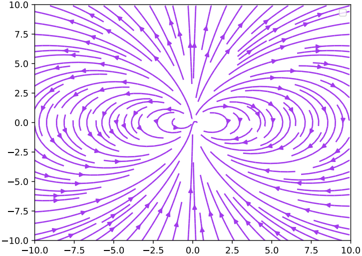
$$\vec{B} = \frac{\mu_0}{4\pi r^3}\left[3\hat{\vec{r}}(\vec{m}\cdot\hat{\vec{r}} - \vec{m})\right].$$



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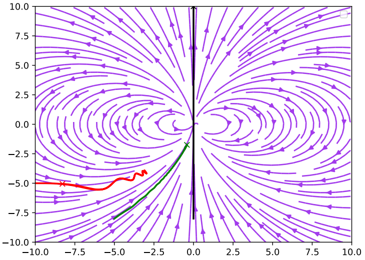

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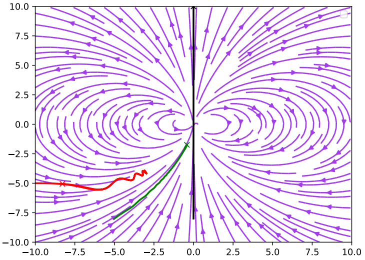

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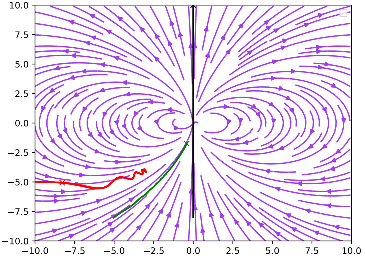
- No analytical solution.



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Embedded Runge-Kutta algorithms

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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 AppliMathematics

(1)

Runge-Kutta Dormand Prince 5 (4)

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

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- 7 $\mathbf{k}_j$'s (actually 6 by clever re-usage).
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Butcher Tableu of Dormand Prince (5) 4

c_i	a_{ij}	$\dots$						
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	$\frac{500}{1113}$	$\frac{125}{192}$	$-\frac{2187}{6784}$	$\frac{11}{84}$		
$/\, b^{(5)}$	$\frac{35}{384}$	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):

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

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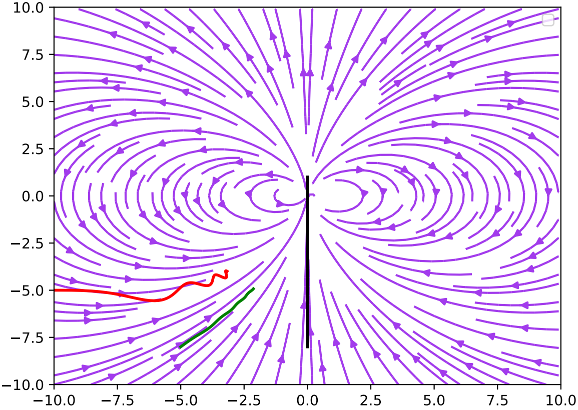
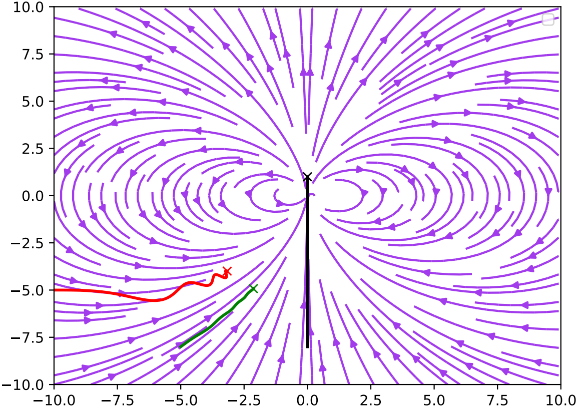
- Scale by step size $\frac{h_{old}}{T}$, "Fail safe" $\sqrt{\ldots}$.
  Dormand, J. R.; Prince, P. J. (1980), "A family of embedded Runge-Kutta formulae", Journal of Computational and Applied Mathematics

Does it work?



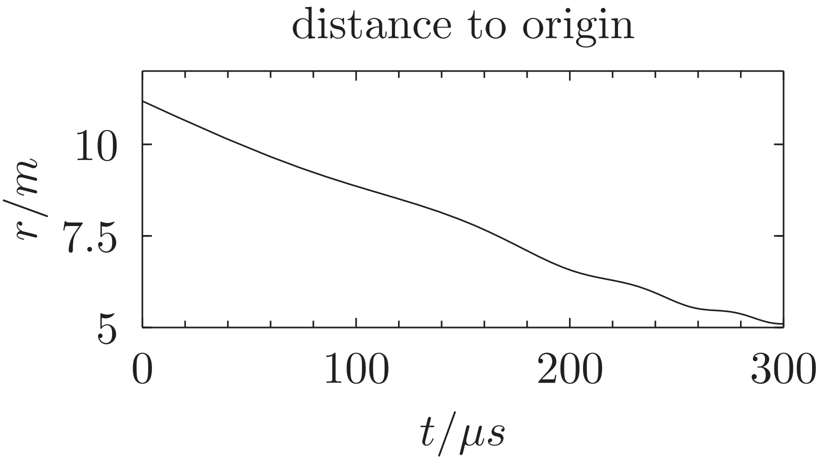
My version relative and absolute error 10^{-6}. 94 steps (+ 14 rejected).

Does it work?



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

Does it work?



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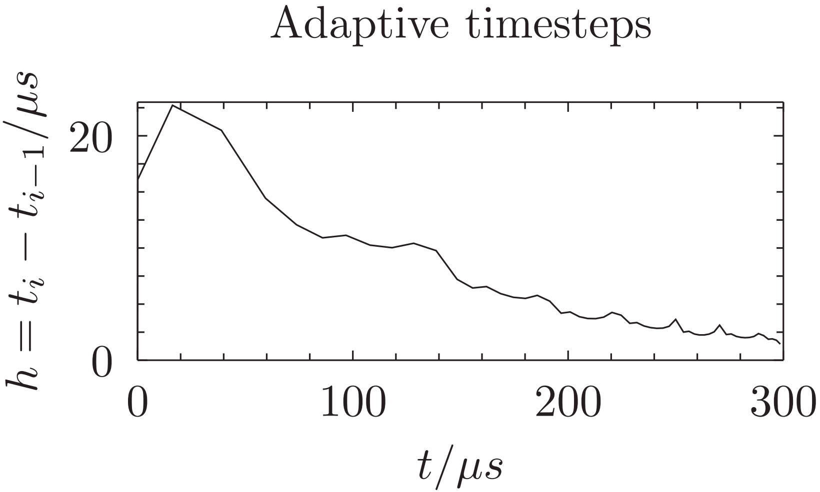
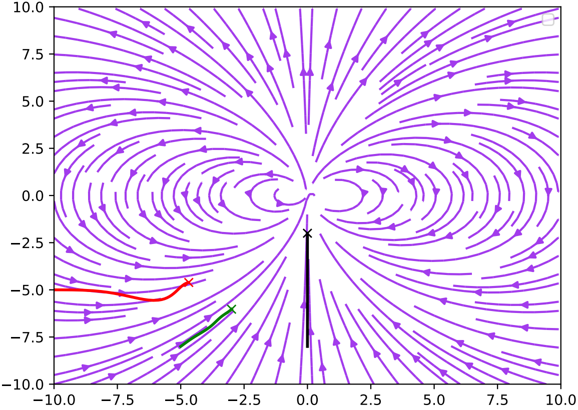


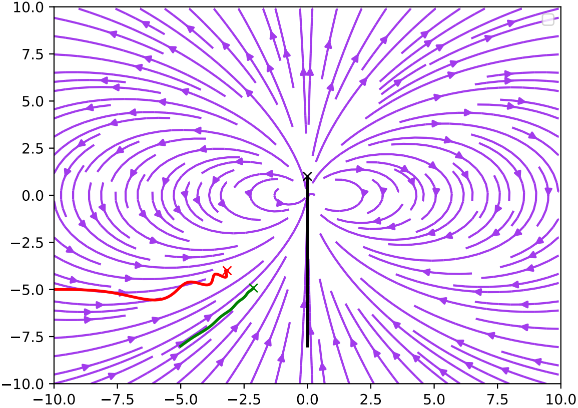
My version, adaptive step size.

Another curious result



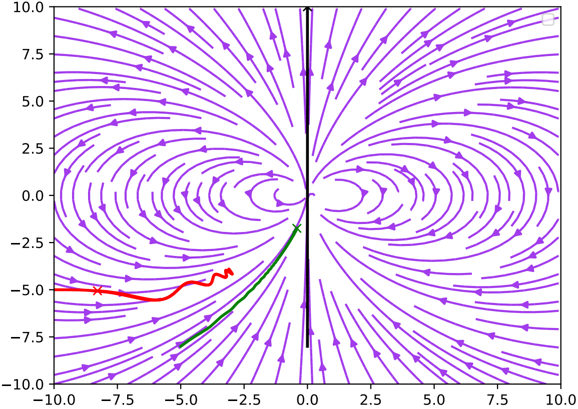
$T = 0.2\,\mathrm{ms}$

Another curious result



$T = 0.3\,\mathrm{ms}$

Another curious result



$T = 0.6\,\mathrm{ms}$

Magnetic “mirror” or “bottle”.

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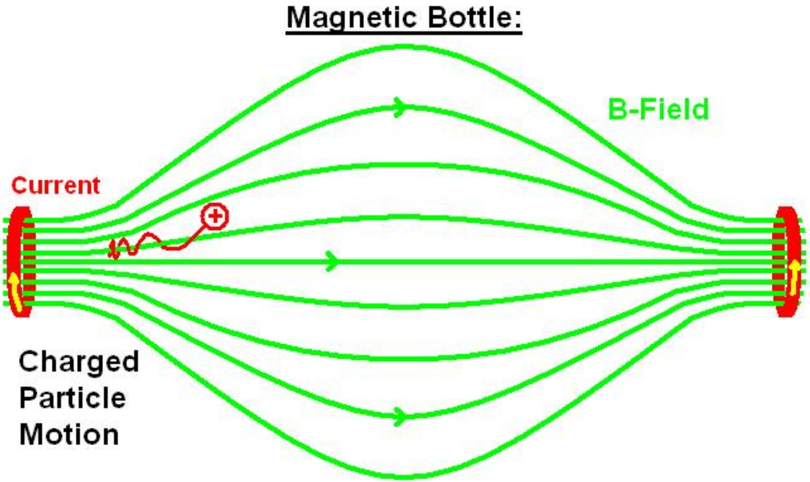

Wikipedia user WikiHelper2134 , Public Domain.

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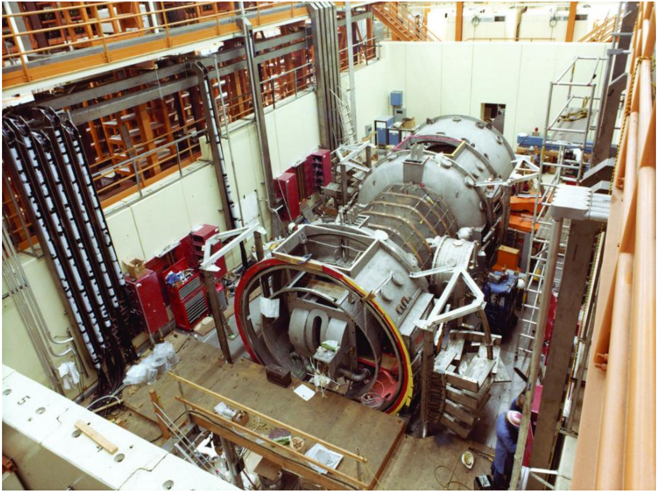

Tandem Mirror Experiment, The Lawrence Livermore National Laboratory, 1978.

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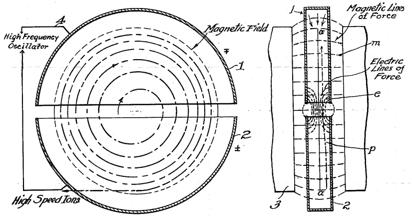
- Limitation, simulations are not experiments.

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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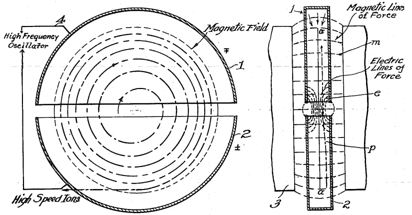

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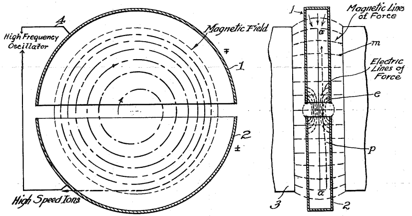

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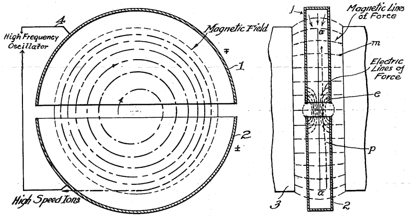
- Analytical final speed, in principle path.

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



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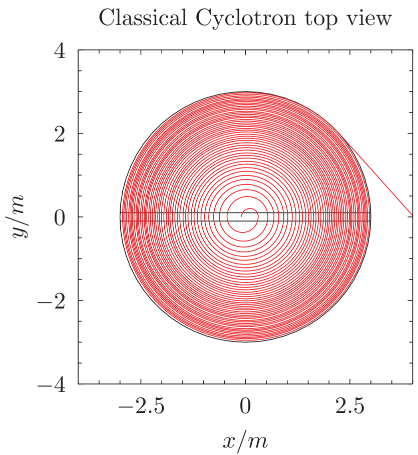

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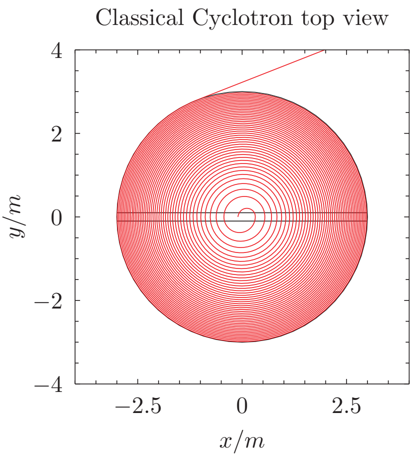

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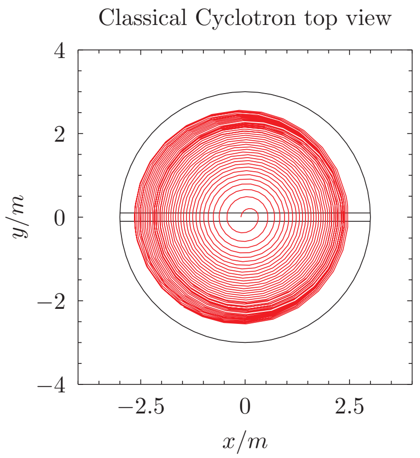

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