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

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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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- Simulations are not experiments!

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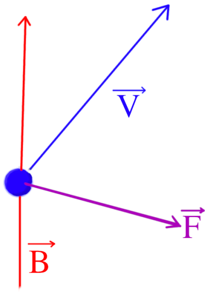
- Only 1 particle! so pre-programmed depending on the setup.
- Could use potentials $\phi(\vec{r}, t)$ $\vec{A}(\vec{r}, t)$ and Hamiltonian, or Lagrangian.
- Other systems would have other differential equations.

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



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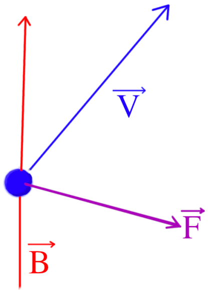
$$dW_{\vec{B}} = \vec{F}_B \cdot d\vec{r} \propto (\vec{v} \times \vec{B}) \cdot \vec{v} = 0.$$



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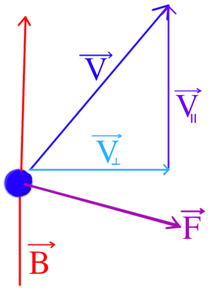

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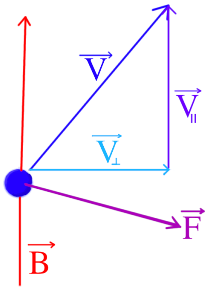

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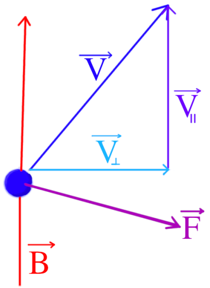
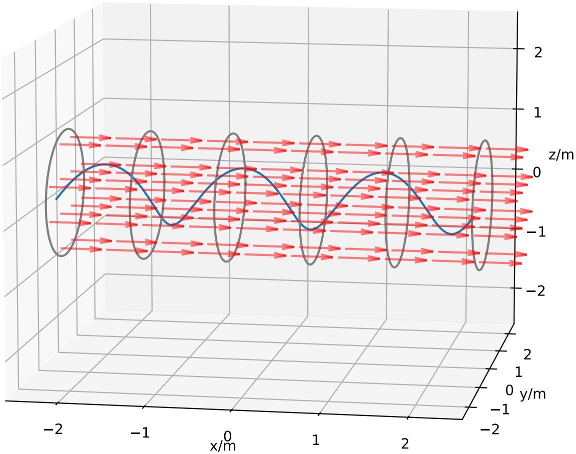
- Cyclotron radius and frequency:

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



What we expect to see

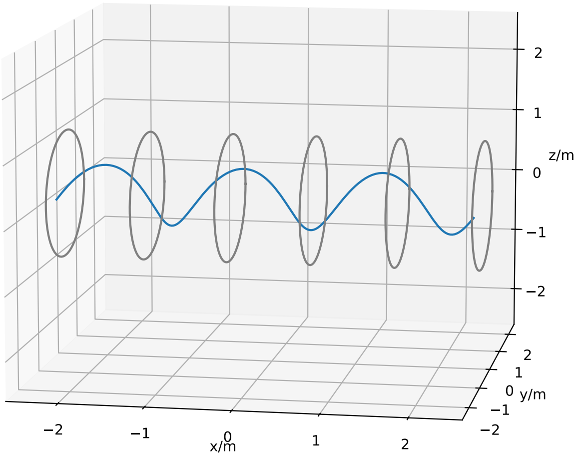


“Cyclotron motion”

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

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

What we expect to see



"Cyclotron motion"

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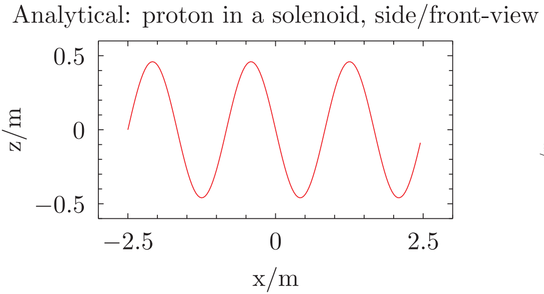

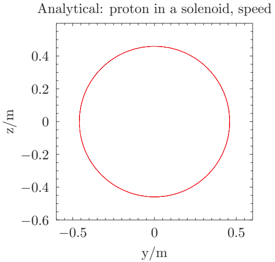

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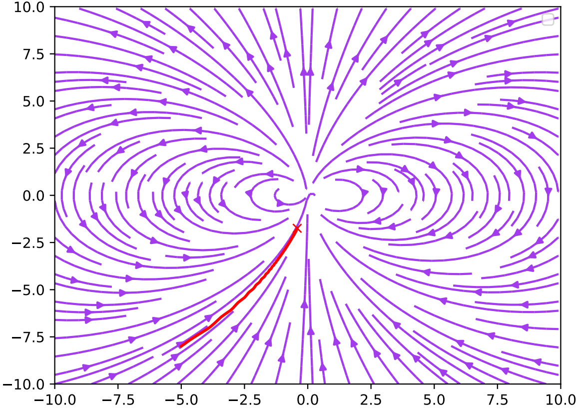

(Actually from my simulation)

Ordinary differential equation's.

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

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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

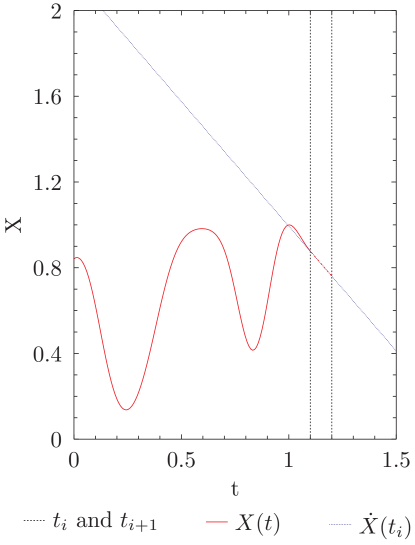
```
auto ODE = [...](const state_type Data, state_type &
    dDatadt, const double t){
     //Extract position and velocity from data
     vec pos = vec(Data[0],Data[1],Data[2]);
     vec velocity = vec(Data[3],Data[4],Data[5]);

     //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;
     ...
};
```

Solving differential equations

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



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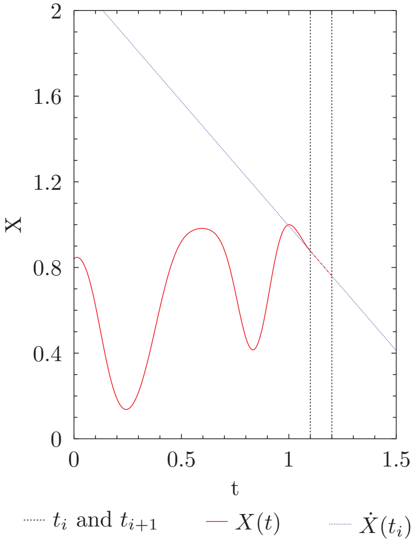
- Can we find $\mathbf{X}(t_0 + h)$ for $h > 0$?.



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- (Explicit Forward) 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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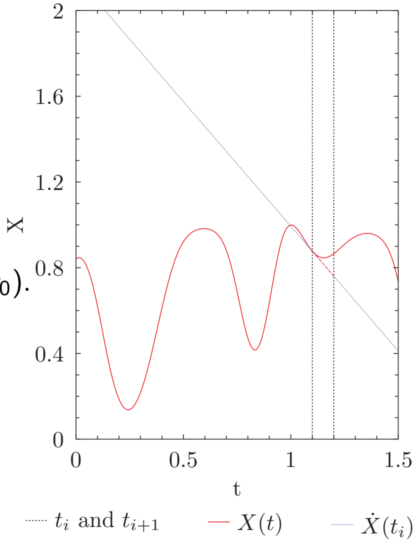

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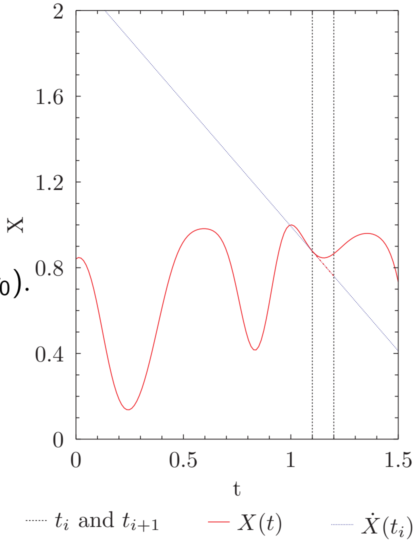
- Can this be justified?
- Bernard P. Zeigler et al. Theory of Modeling and Simulation (Third edition), chapter 3



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- Argument suggests we need $\dot{f}_{ode}, \ddot{f}_{ode}, \ldots$

The Runge Kutta steppers

- In general:

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

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

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

- More commonly written:

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

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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) \\
\mathbf{K}_3 &= f_{ode}(\mathbf{X}(t_i) + ha_{31}\mathbf{K}_1 + ha_{32}\mathbf{K}_2, t_i + c_3 h) \\
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- Taylor series analogy: error h^p.
- Martha L. Abell, James P. Braselton, Differential Equations with Mathematica (Fourth Edition), 2016:

Higher order methods

- 2nd order (Heun's method):

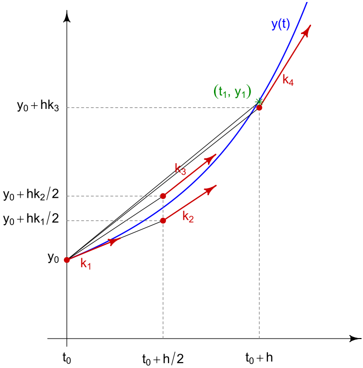
$$
\begin{aligned}
\mathbf{X}(t_{i+1}) - \mathbf{X}(t_i) &= \frac{h}{2}(\mathbf{k}_1 + \mathbf{k}_2) \\
\mathbf{k}_1 &= f_{ode}(\mathbf{X}(t_i), t_i) \\
\mathbf{k}_2 &= f_{ode}(\mathbf{X}(t_i) + h\mathbf{k}_1, t_i + h)
\end{aligned}
$$

Higher order methods

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

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

$$\begin{aligned}
\mathbf{k}_1 &= f_{ode}(\mathbf{X}(t_i), t_i) \\
\mathbf{k}_2 &= f_{ode}(\mathbf{X}(t_i) + \frac{h}{2}\mathbf{k}_1, t_i + \frac{h}{2}) \\
\mathbf{k}_3 &= f_{ode}(\mathbf{X}(t_i) + \frac{h}{2}\mathbf{k}_2, t_i + \frac{h}{2}) \\
\mathbf{k}_4 &= f_{ode}(\mathbf{X}(t_i) + h\mathbf{k}_3, t_i + h)
\end{aligned}$$



The General explicit Runge Kutta method

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- Expressed in Butcher tableu:

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

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 );
}
```

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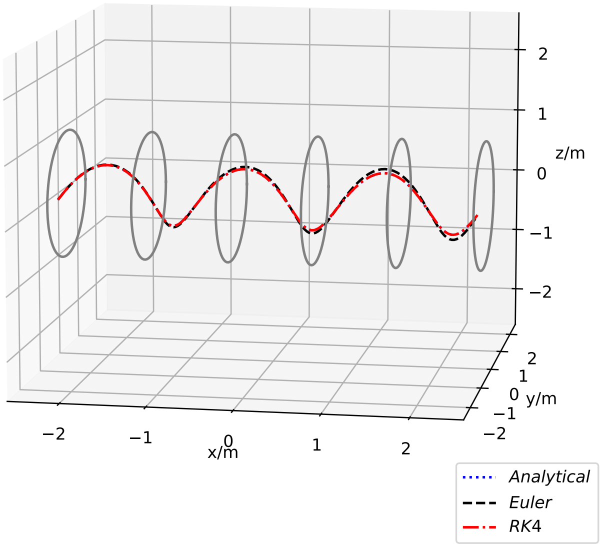
- Compare Analytic, Euler, Runge-Kutta 4.
- Consider $\theta = 60^\circ$ at different h.
- Check error on $|\vec{v}|$, $R = \sqrt{y^2 + z^2}$ and $x(t)$.

At a glance, 3D view

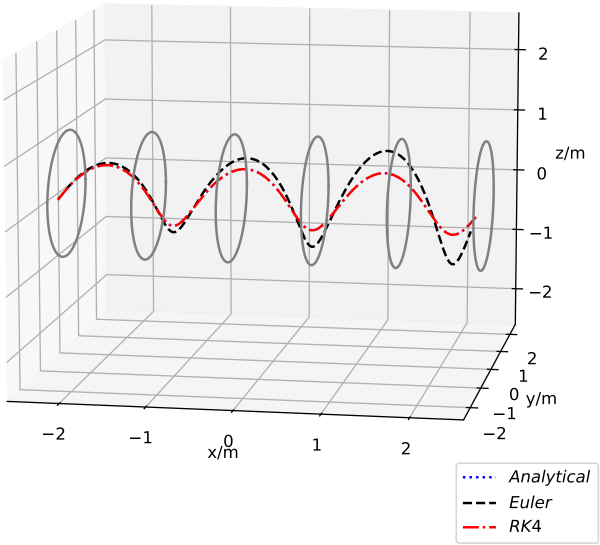
$$h = t_{i+1} - t_i = 0.01\,\mu\text{s}$$



3129 steps

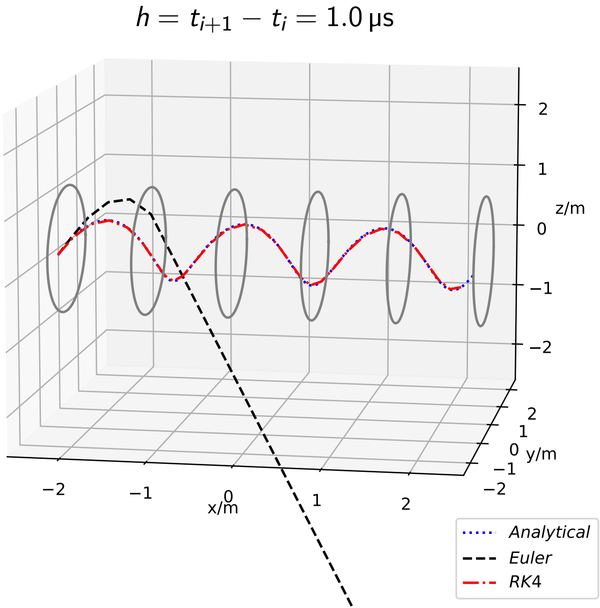
At a glance, 3D view

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



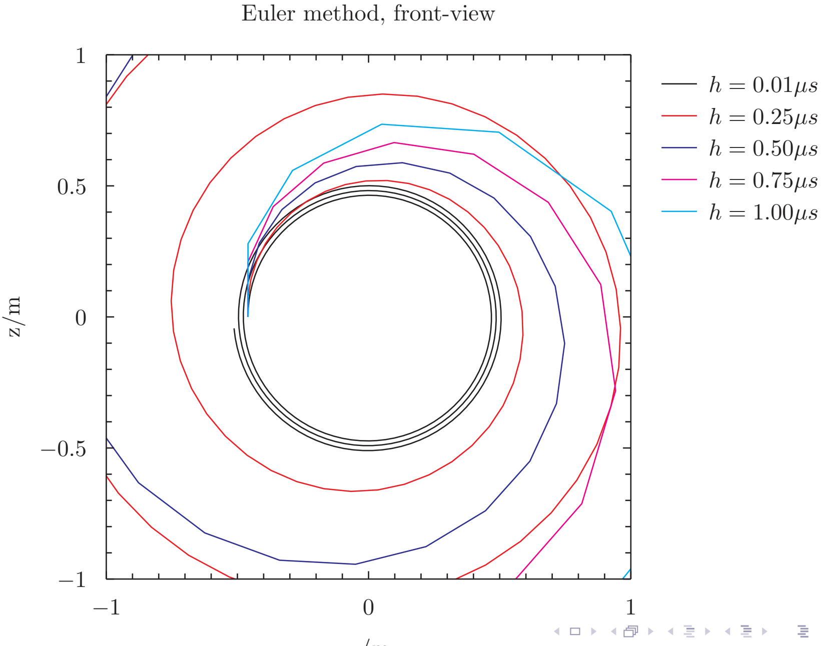
312 steps

At a glance, 3D view



31 steps.

At a glance, front view, no border



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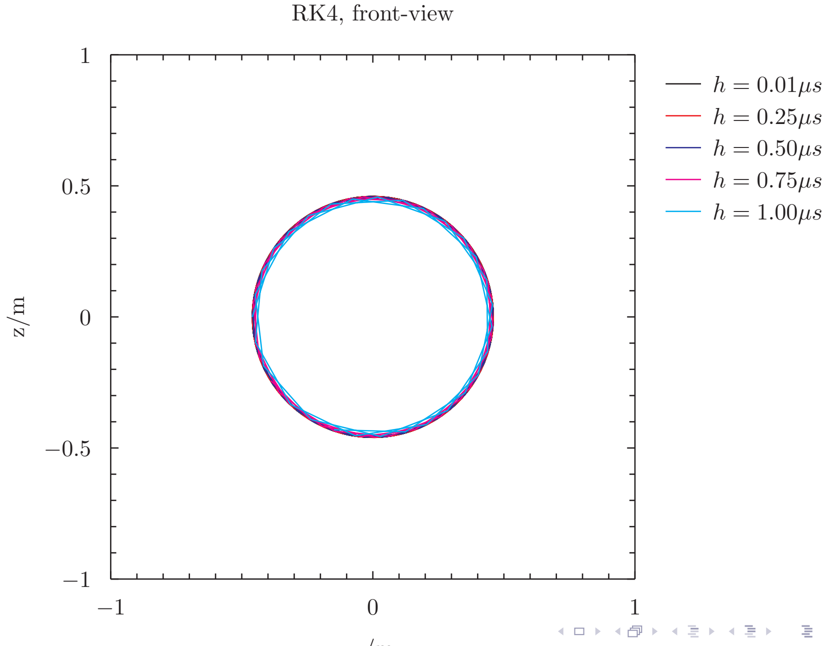
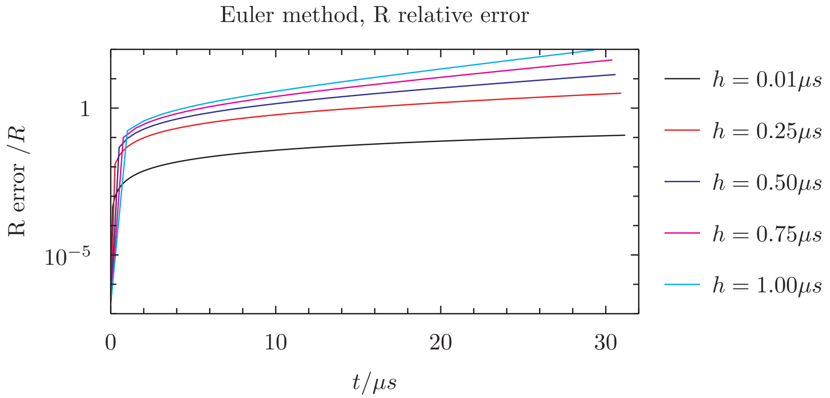


Constant radius?



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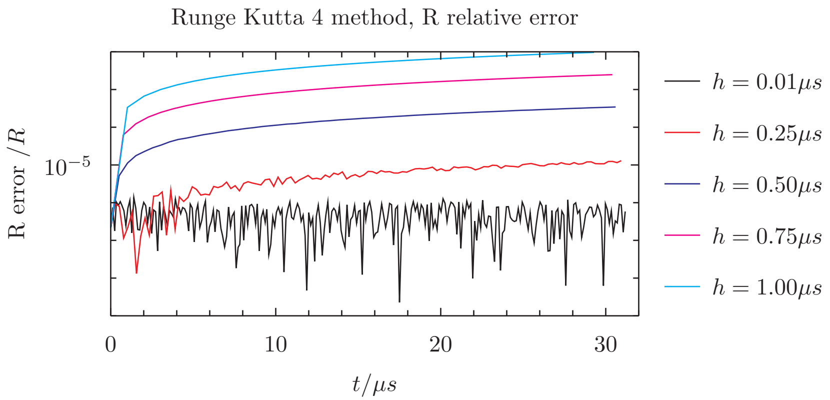
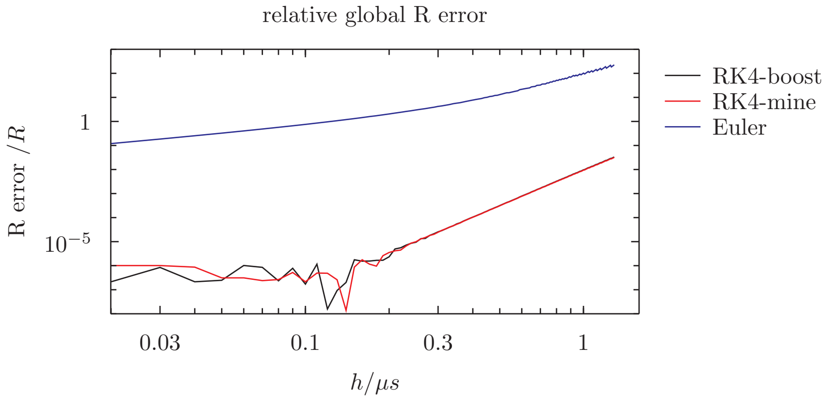


Error as function of h



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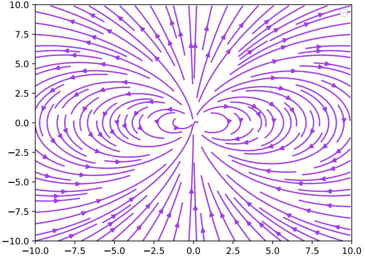

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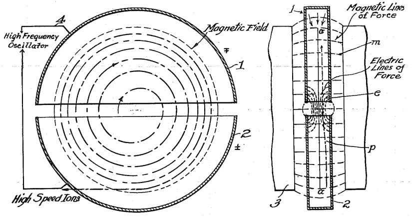

Ernest O. Lawrence, 1934, U.S. Patent 1,948,384; image in Public Domain.

Adaptive step size, why

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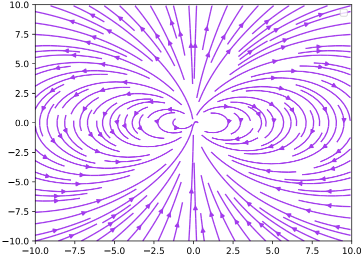
- Let the computer pick h.



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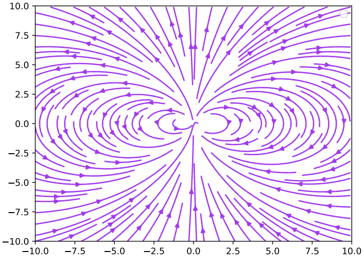

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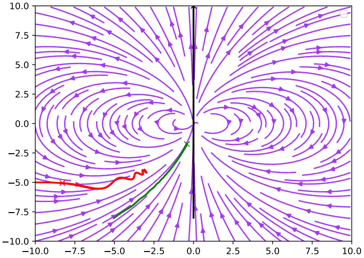

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Protons with speed around $10\,000\,\mathrm{m/s}$

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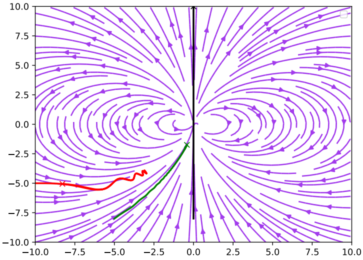

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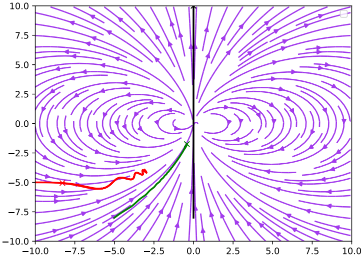
- No analytical solution (afaik.)



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Runge-Kutta Adaptive step size, how

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

$$\mathbf{X}^{(4)}(t_{i+1}) - \mathbf{X}(t_i) = h \sum_{j=1}^{m} b_j^{(4)} \mathbf{k}_j.$$

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

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

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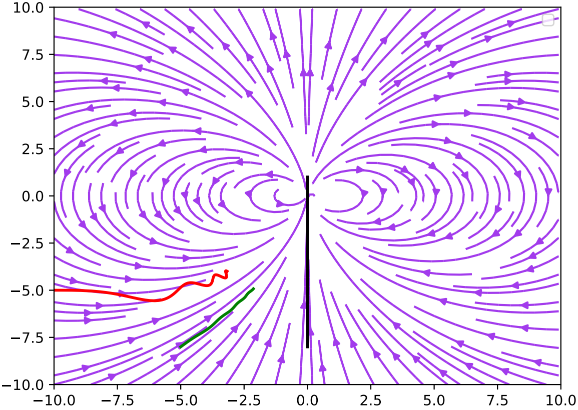
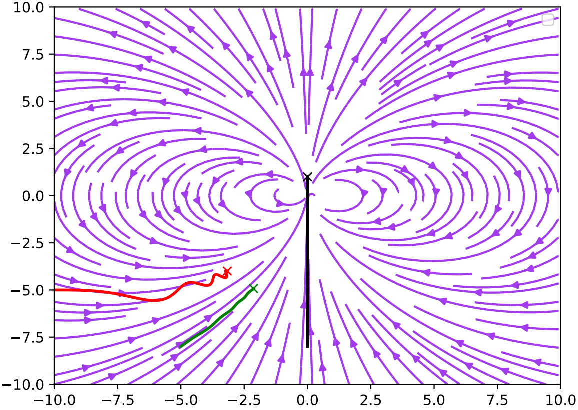
- Scale by step size $\frac{h_{old}}{T}$, "Fail safe" $\sqrt{\ldots}$.
Dormand, J. R.; Prince, P. J. (1980), "A family of embedded Runge-Kutta formulae", Journal of Computational and Applied Mathematics

Does it work?



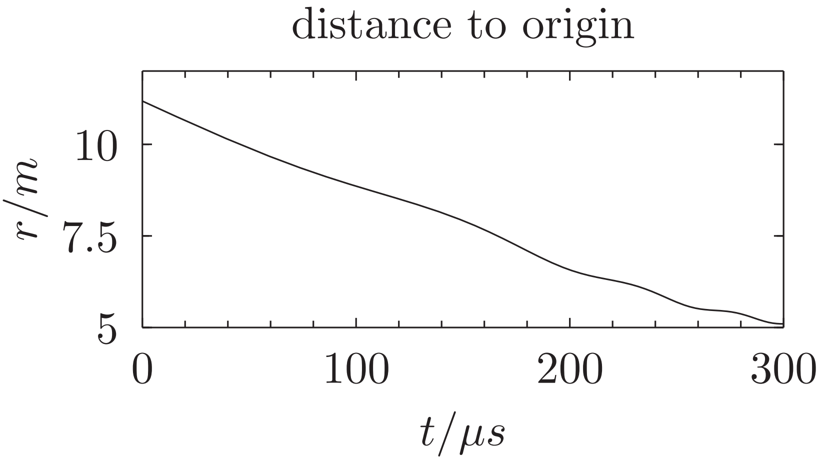
My version relative and absolute error 10^{-6}. 94 steps (+ 14 rejected).

Does it work?



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

Does it work?



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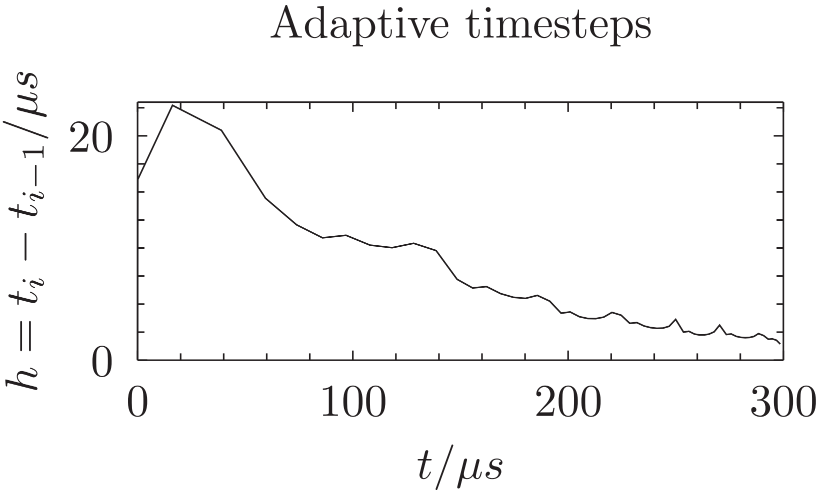
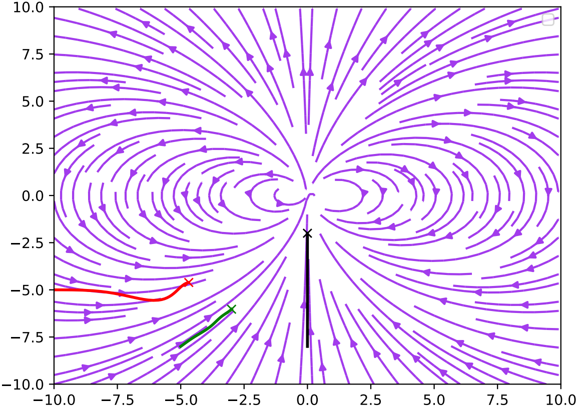


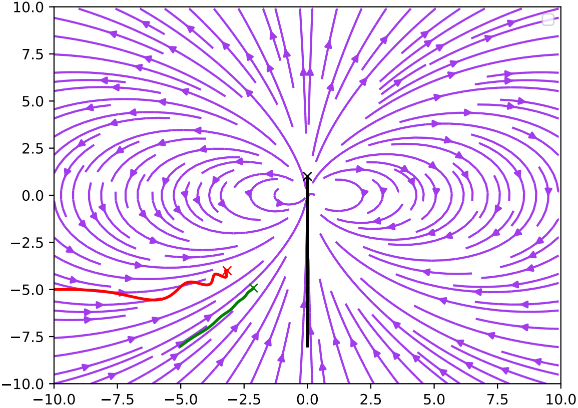
My version, adaptive step size.

Another curious result



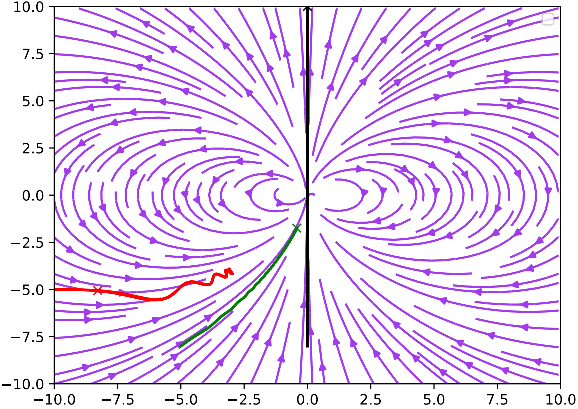
$T = 0.2\,\mathrm{ms}$

Another curious result



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

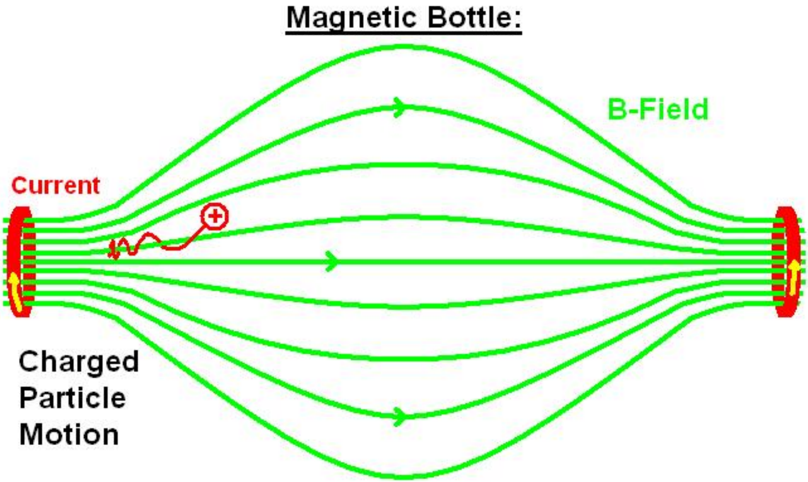
Another curious result



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

Magnetic "mirror" or "bottle".

Another curious result



Wikipedia user WikiHelper2134 , Public Domain.

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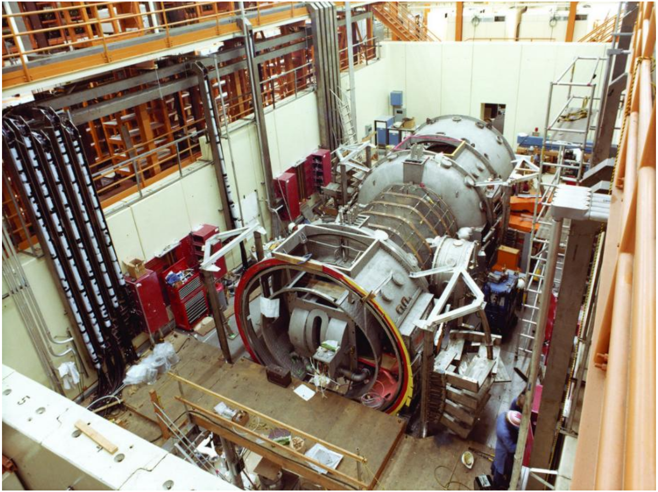

Tandem Mirror Experiment, The Lawrence Livermore National Laboratory, 1978.

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- Limitation, simulations are not experiments.

Example, cyclotron

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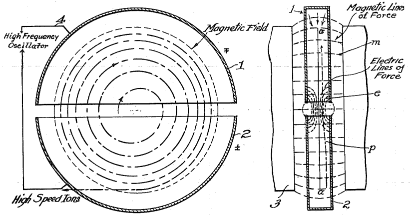

Ernest O. Lawrence, 1934, U.S. Patent 1,948,384; image in Public Domain.

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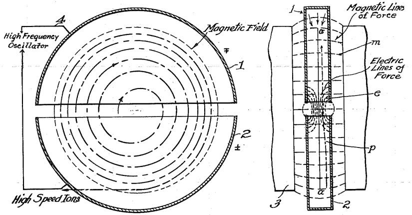

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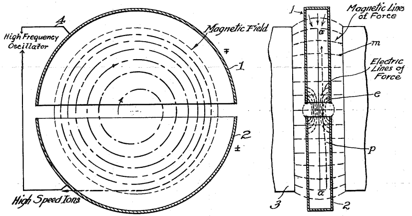

Ernest O. Lawrence, 1934, U.S. Patent 1,948,384; image in Public Domain.

Example, cyclotron

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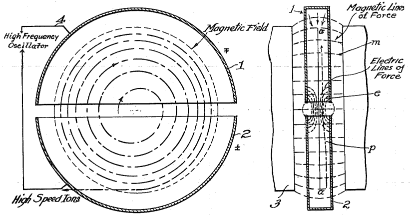
- Single gab, oscillating field.
- Uses classical Cyclotron frequency
- Analytical final speed, in principle path.

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



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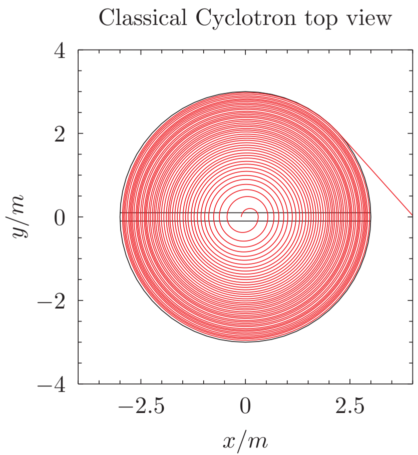

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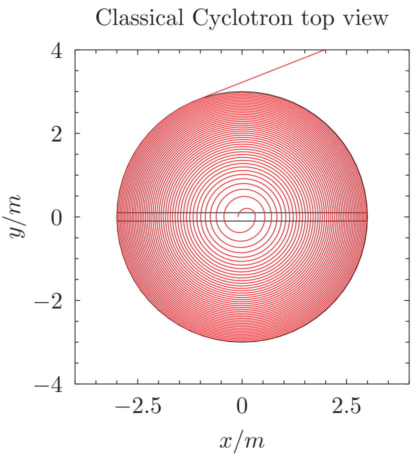

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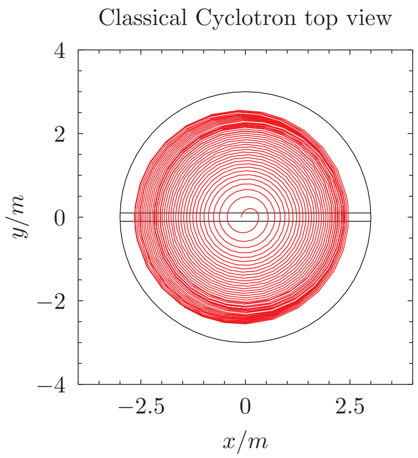

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