MAINTITLE

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TITLEIMAGE

Introduction, what and why

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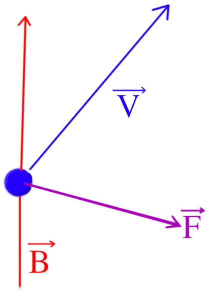
- Only 1 particle! so pre-programmed depending on the setup.
- Could use potentials $\phi(\vec{r}, t)$ $\vec{A}(\vec{r}, t)$ and Hamiltonian.

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



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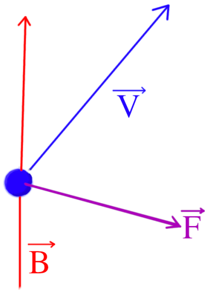

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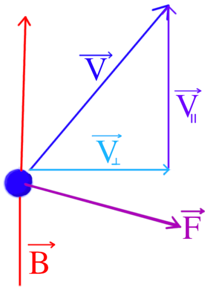

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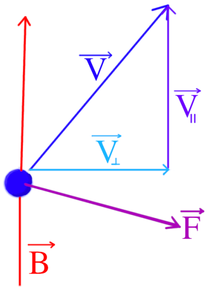
- Same as Centripetal force: Cyclotron motion



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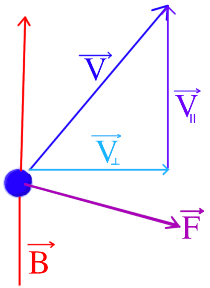
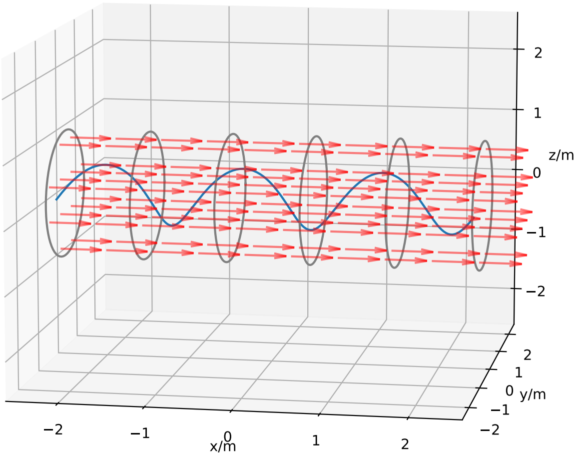
- Same as Centripetal force: Cyclotron motion
- Cyclotron radius and frequency:

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

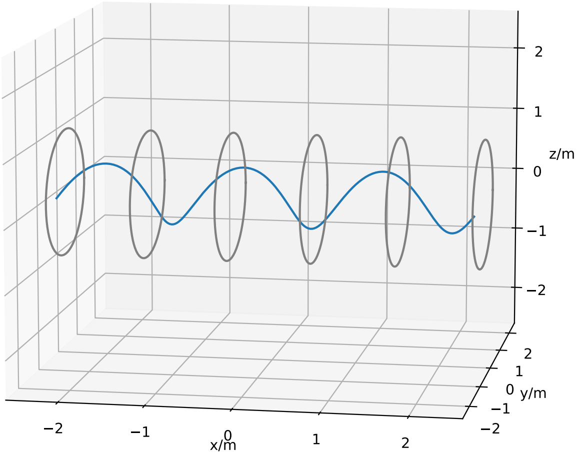


Analytical solution: Protons in a Solenoid



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

Analytical solution: Protons in a Solenoid



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

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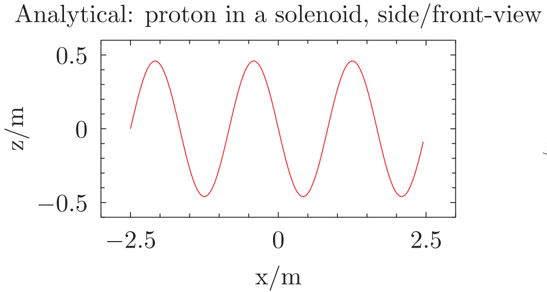

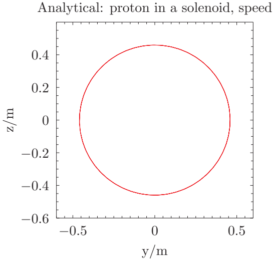

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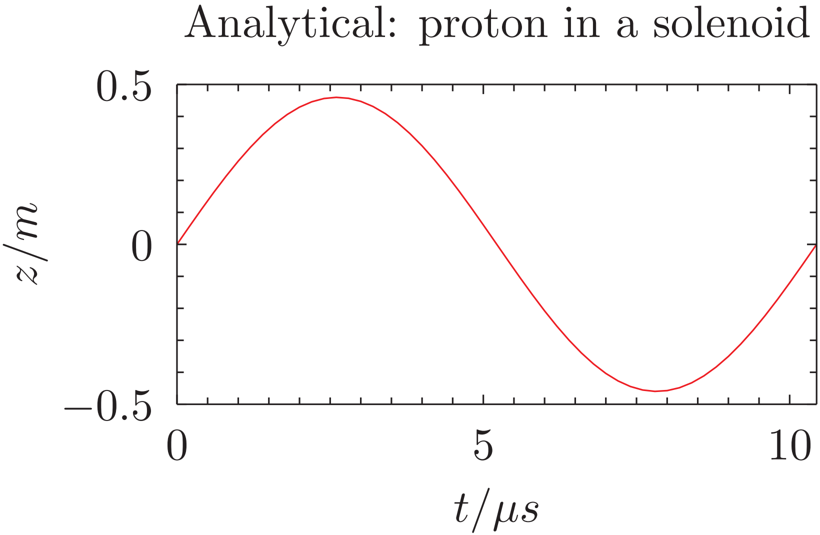

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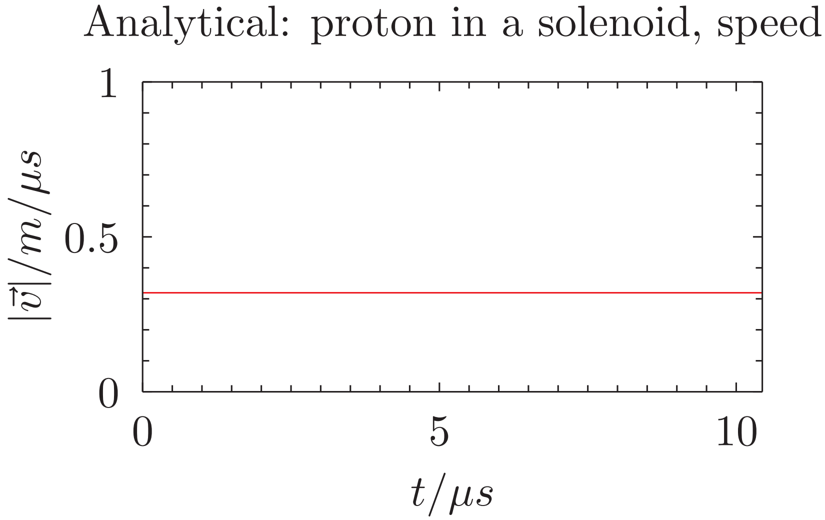

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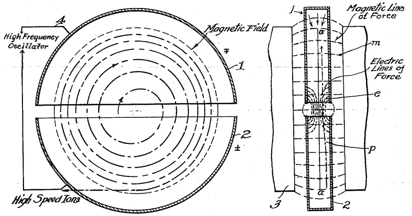
Cyclotron accelerator

- Electric forces do work.



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

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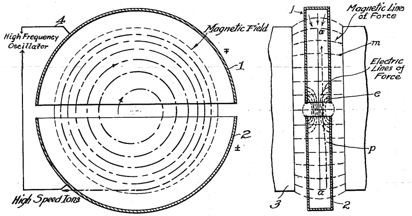

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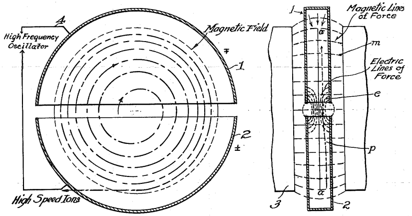

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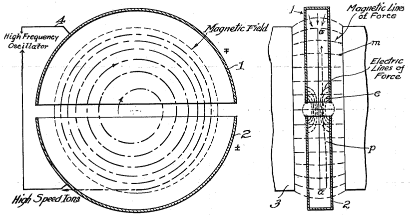
- Practical example, the Cyclotron.
- Single gab, oscillating field.
- Final speed:

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



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Ordinary differential equation*s.

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

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

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

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- Here:

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

The ODE to solve

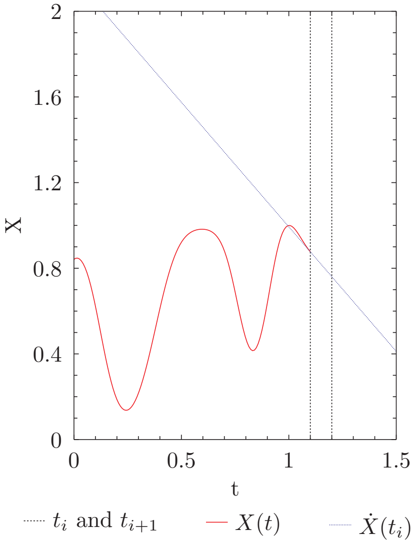
```
auto ODE = [...](const state_type Data, state_type &
    dDatadt, const double t){
     //Extract position and velocity from data
     vec pos = vec(Data[0],Data[1],Data[2]);
     vec velocity = vec(Data[3],Data[4],Data[5]);

     //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.
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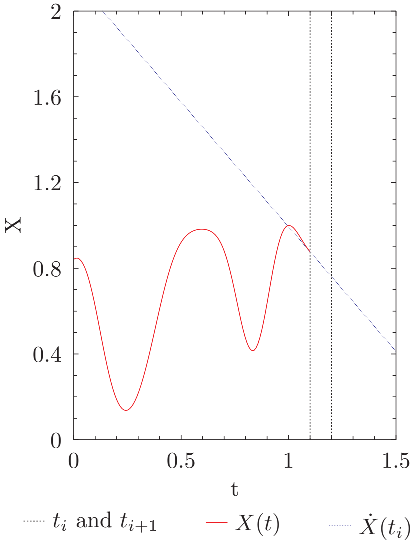

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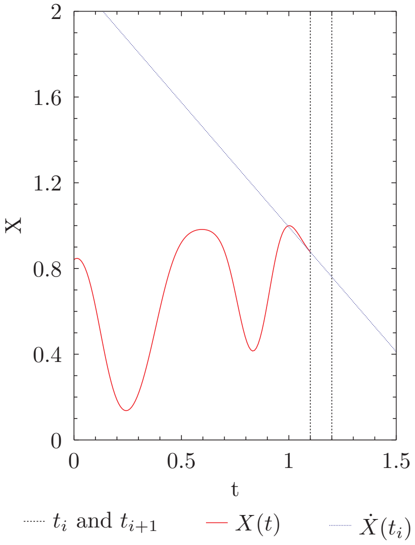

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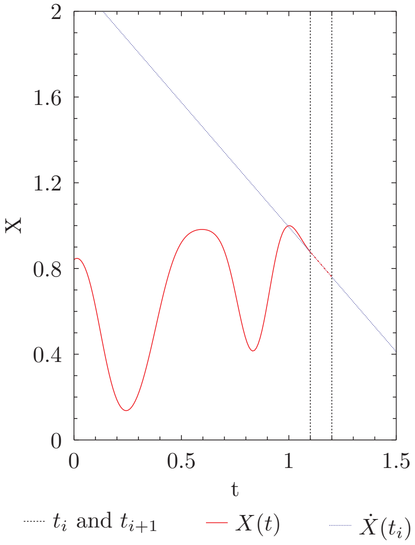

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- How would you find $\mathbf{X}(t_{i+1})$:
- (Explicit) Forward Euler's Method:

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

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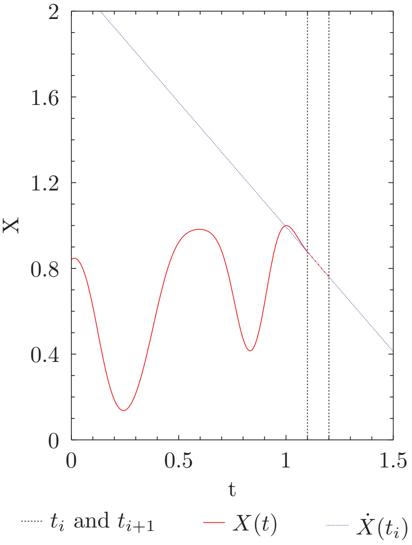

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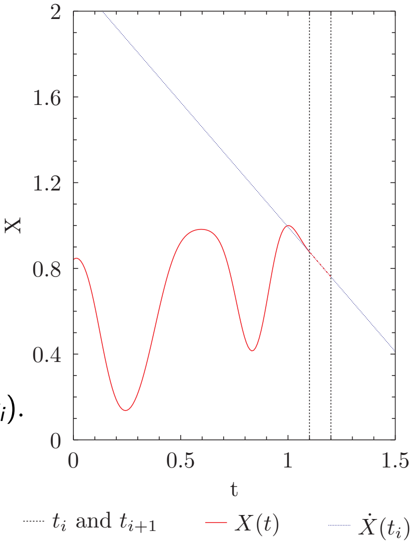

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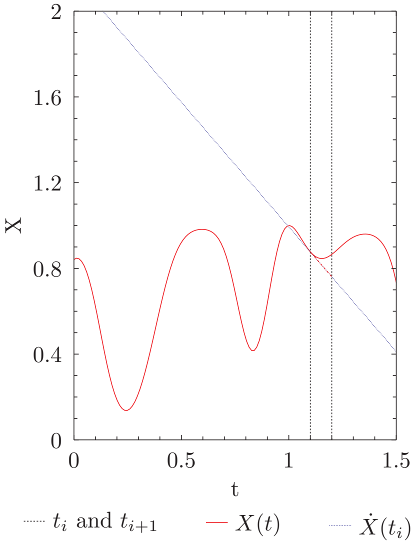

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- Global error $h = h^p$.
- Convergence, but not uniform.

Why does this work? The Runge Kutta family

- In general.

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

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

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

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

- We want:

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

- With: $\mathbf{K}_1 = f_{ode}(\mathbf{X}(t_i), t_i)$, $\mathbf{K}_2 = f_{ode}(\mathbf{X}(t_i) + ha_{21}\mathbf{K}_1, t_i + c_2 h)$ etc.

- 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):

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

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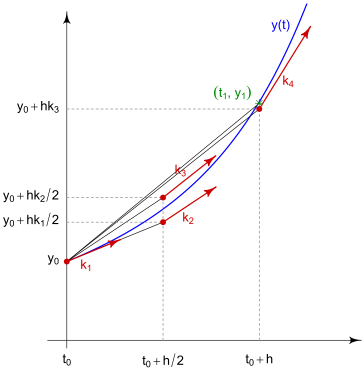
The 4th order Runge Kutta method

- RK4, often simply called the Runge Kutta method:

$$
\begin{aligned}
\mathbf{X}(t_{i+1}) - \mathbf{X}(t_i) &= \frac{h}{6}(\mathbf{k}_1 + 2\mathbf{k}_2 + 2\mathbf{k}_3 + \mathbf{k}_4) \\
\mathbf{k}_1 &= f_{ode}(\mathbf{X}(t_i), t_i) \\
\mathbf{k}_2 &= f_{ode}(\mathbf{X}(t_i) + \frac{h}{2}\mathbf{k}_1, t_i + \frac{h}{2}) \\
\mathbf{k}_3 &= f_{ode}(\mathbf{X}(t_i) + \frac{h}{2}\mathbf{k}_2, t_i + \frac{h}{2}) \\
\mathbf{k}_4 &= f_{ode}(\mathbf{X}(t_i) + h\mathbf{k}_3, t_i + h)
\end{aligned}
$$



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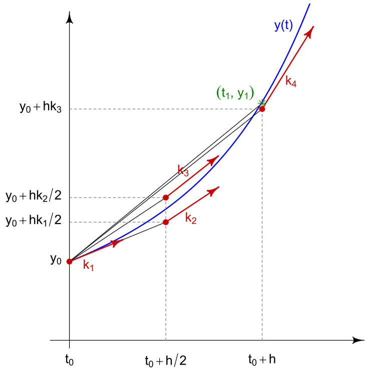
$$\mathbf{k}_1 = f_{ode}(\mathbf{X}(t_i), t_i)$$

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

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

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



- 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

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

$$\begin{aligned}
\mathbf{k}_1 &= f_{ode}(\mathbf{X}(t_i), t_i) \\
\mathbf{k}_2 &= f_{ode}(\mathbf{X}(t_i) + ha_{21}\mathbf{k}_1, t_i + c_2 h) \\
\mathbf{k}_3 &= f_{ode}(\mathbf{X}(t_i) + ha_{31}\mathbf{k}_1 + ha_{32}\mathbf{k}_2, t_i + c_3 h) \quad \vdots
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\end{aligned}$$

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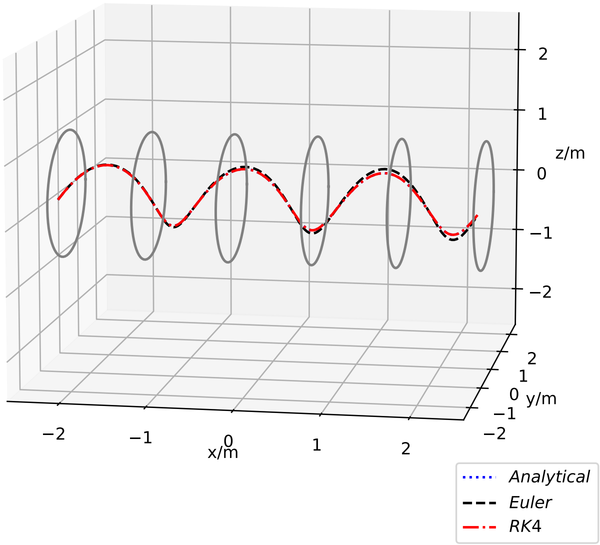
- Consider $\theta = 60°$, $h = 0.01\,\mu\mathrm{s}$, $h = 0.1\,\mu\mathrm{s}$ and $h = 0.1\,\mu\mathrm{s}$.
- Check error on $|\vec{v}|$, $R = \sqrt{y^2 + z^2}$ and $x(t)$.

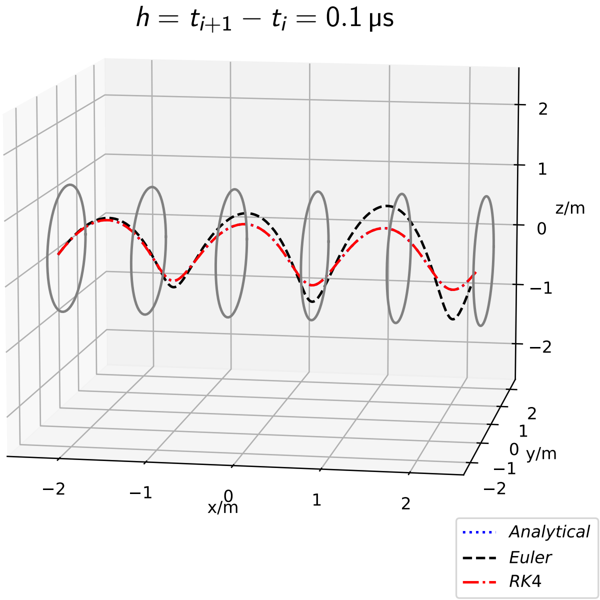
At a glance, 3D view

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



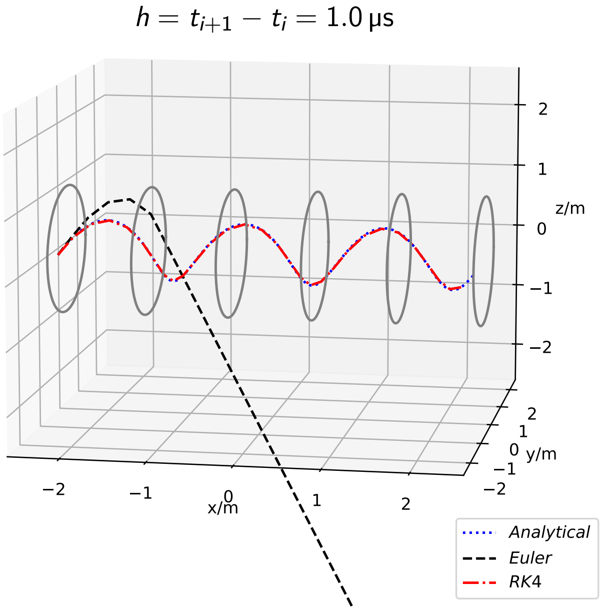
3129 steps

At a glance, 3D view



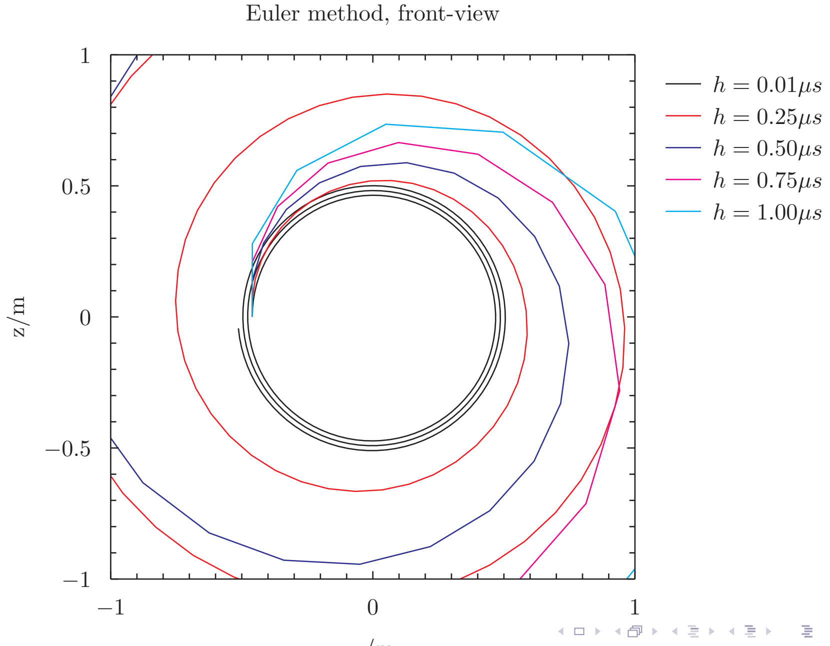
312 steps

At a glance, 3D view



31 steps.

At a glance, front view, no border



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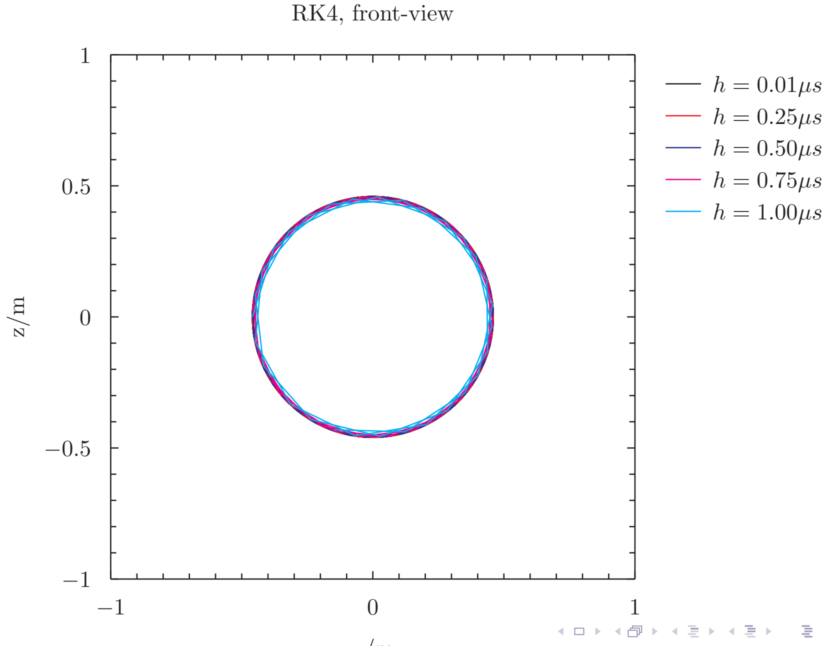
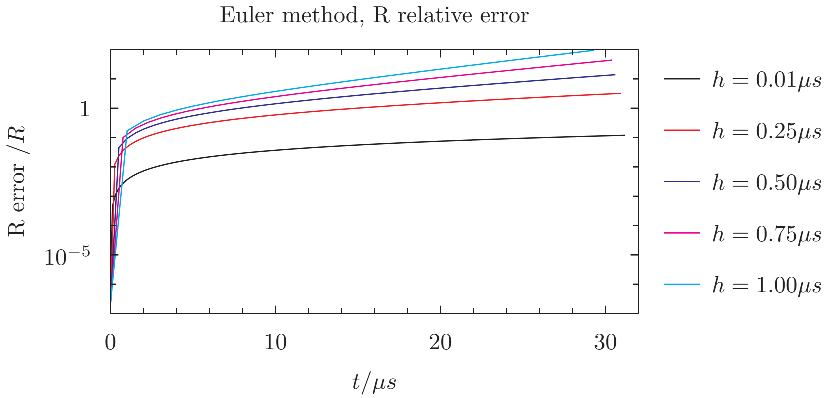


Constant radius?



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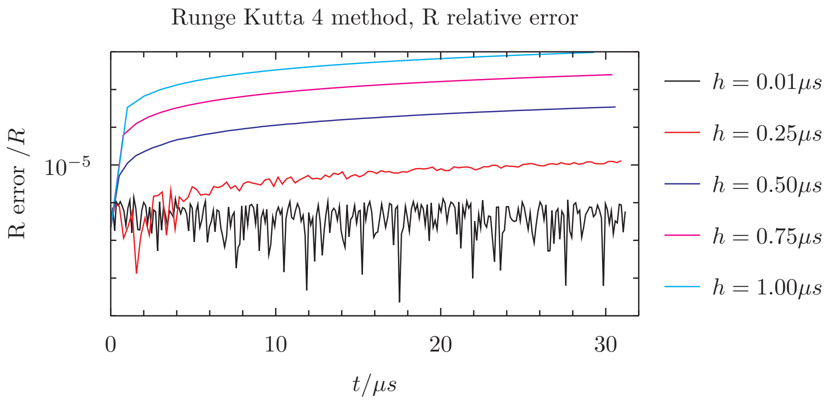
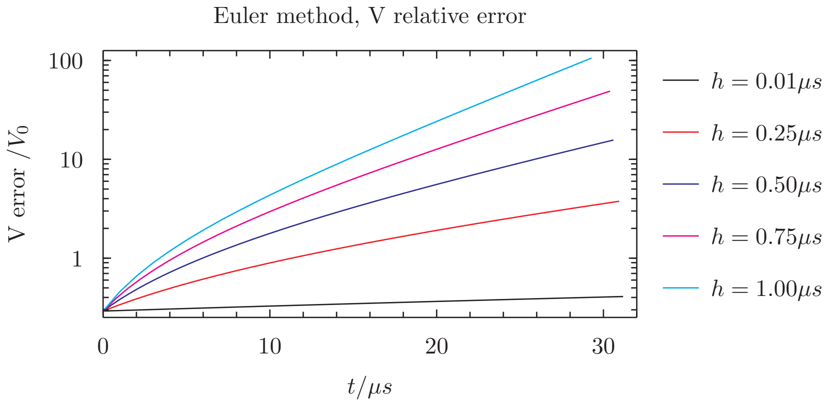


Constant speed?



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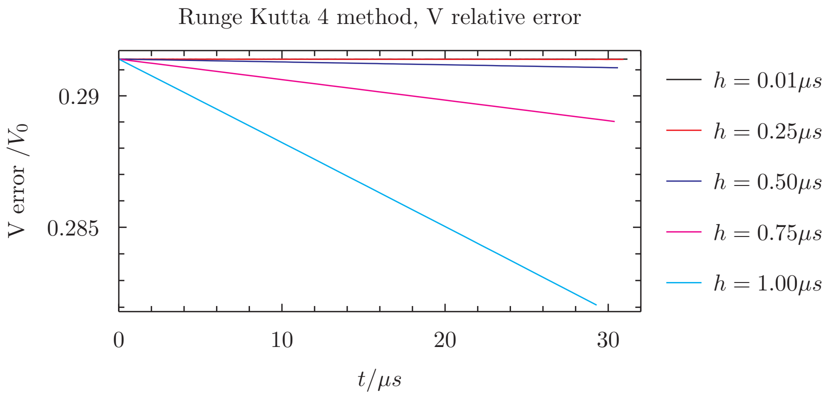
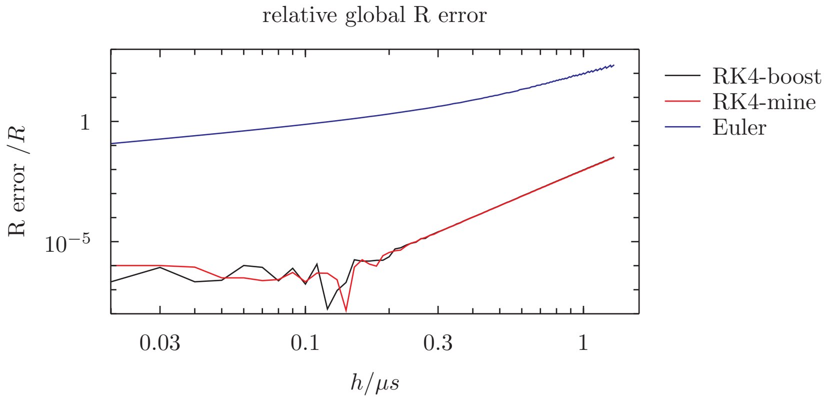


Error as function of h



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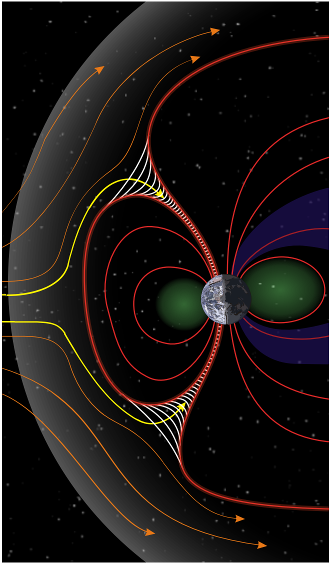

Illustration originally from Nasa. Published on wikipedia, in Public

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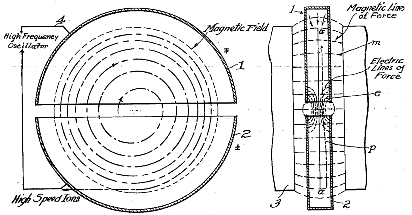


Ernest O. Lawrence, 1934, U.S. Patent 1,948,384; image in Public Domain.

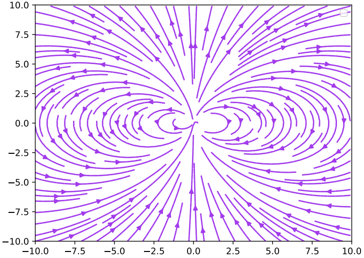
Adaptive step size, why

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

Example, magnetic dipole

- Not good approximation of the Earth magnetic field.
- True dipole:

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



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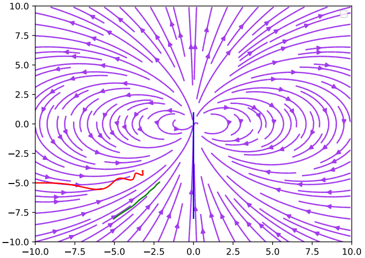

Arbitrarily set $\frac{\mu_0}{4\pi}|\vec{m}| = 0.155\,\mathrm{T/m^3}$.
Protons with speed around $10\,000\,\mathrm{m/s}$

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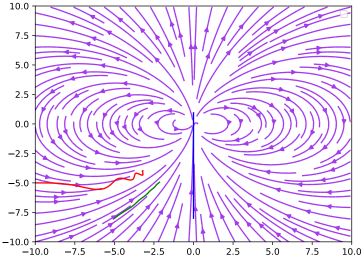

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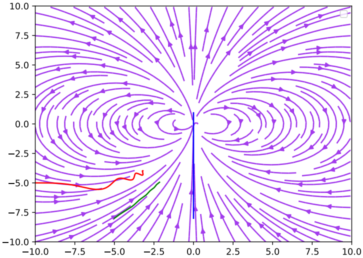
- strong field, large change, short steps.
- No analytical solution (afaik.)



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- Approximate "Error" as $\mathbf{E} = |\mathbf{x}^{(p+1)}(t_{i+1}) - \mathbf{x}^{(p)}(t_{i+1})|$.
- 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)

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

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):

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

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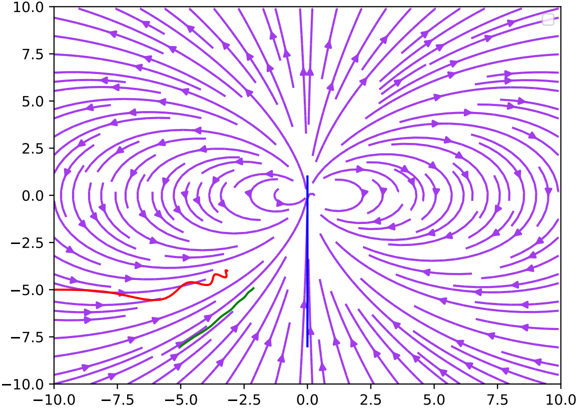
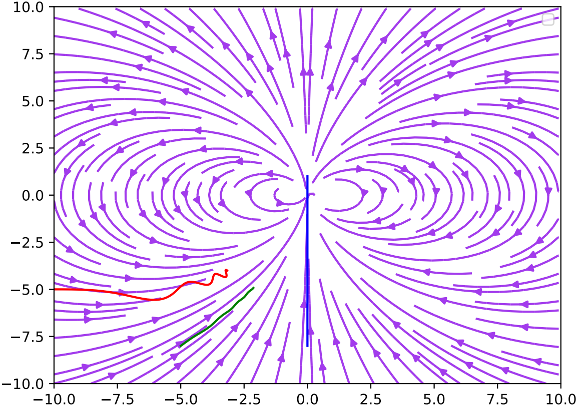
- Worst case correction. Relative and absolute error.
- “Fail safe” $\sqrt{h_{old}}$.
  Dormand, J. R.; Prince, P. J. (1980), ”A family of embedded Runge-Kutta formulae”, Journal of Computational and Applied Mathematics

Does it work?



My version relative and absolute error 10^{-7}. 49 steps (or 62).

Does it work?



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

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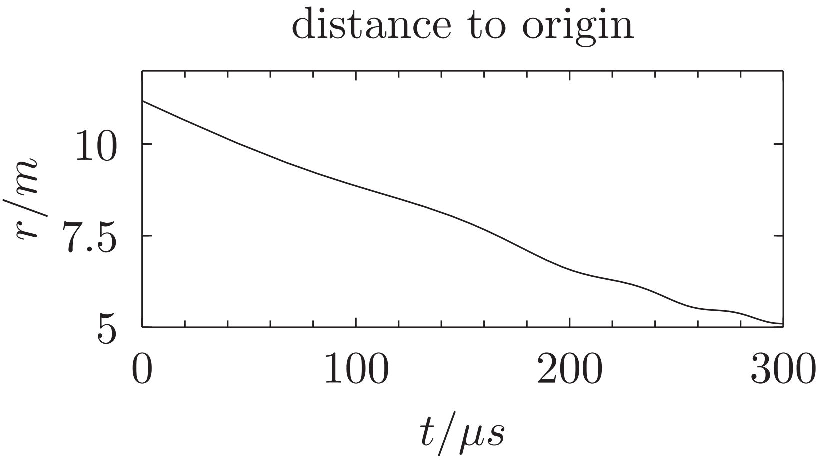

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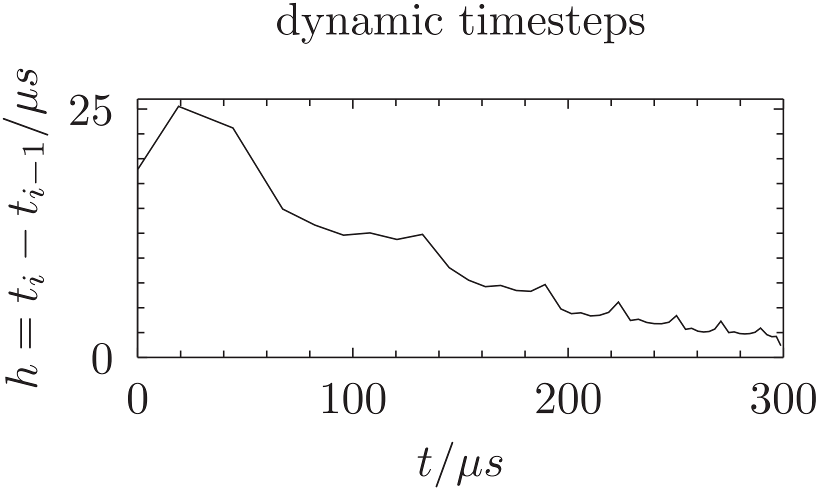
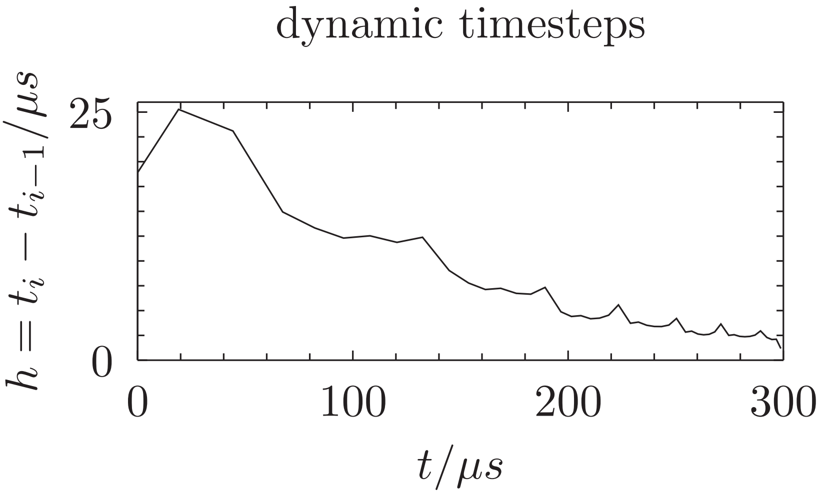


Another curious result

At most 62 points from $t = 0\,\mu s$ to $t = 600\,\mu s$, adaptive.

Another curious result



Magnetic “mirror” or “bottle”

Extra examples-"if time permits"

- The cyclotron

Extra examples-“if time permits”

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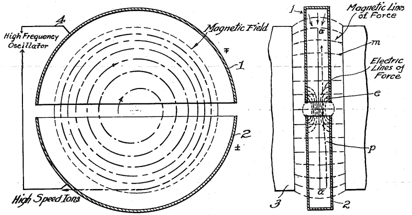
- Electric field accelerates, magnetic contains.



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

Example, cyclotron

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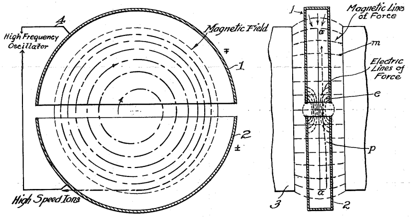

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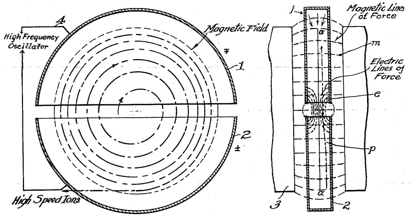

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Example, cyclotron

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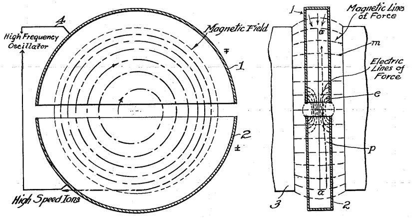
- Analytical final speed, in principle path.

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



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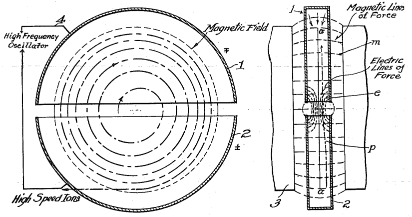

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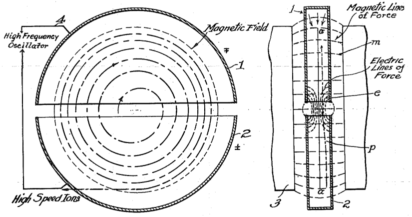

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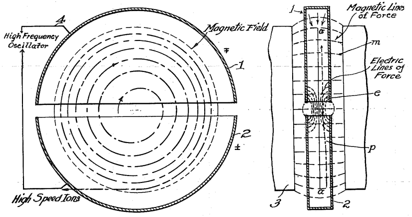
- Single gab, oscillating field.
- Uses Cyclotron frequency

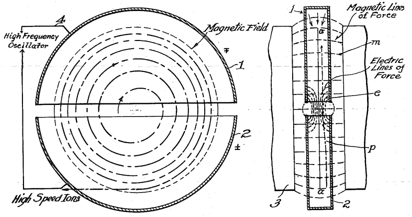


Ernest O. Lawrence, 1934, U.S. Patent 1,948,384; image in Public Domain.

Example, cyclotron

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

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



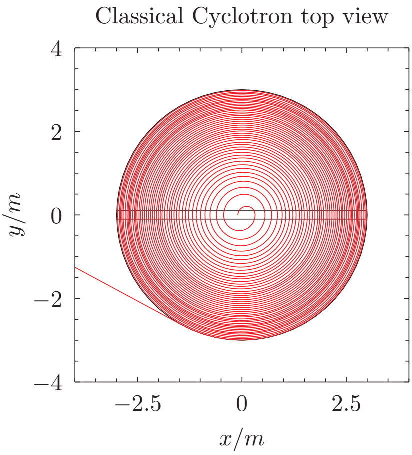
Ernest O. Lawrence, 1934, U.S. Patent 1,948,384; image in Public Domain.

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

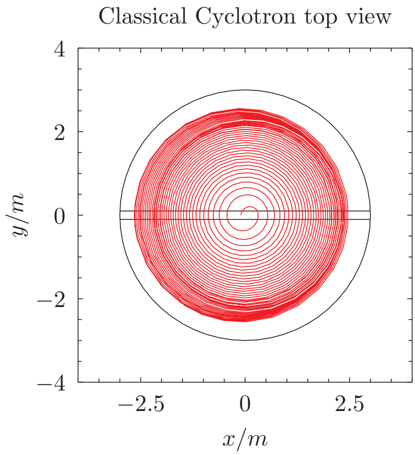
- With fixed step size (Same method, accept all) 4999 points



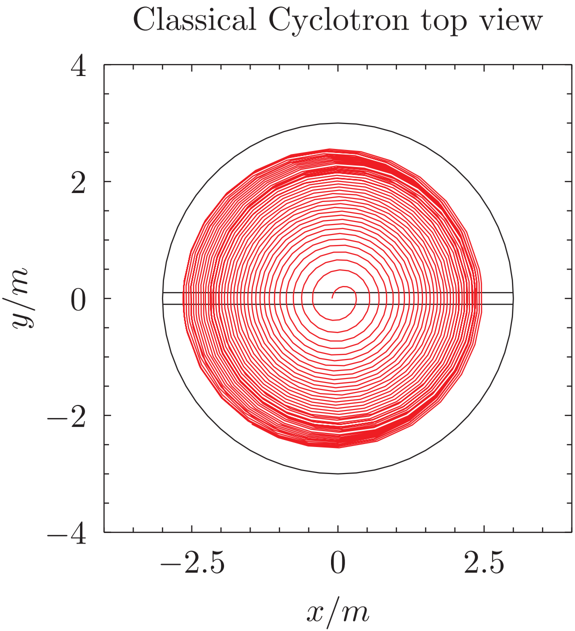
4999 points!

Does it help/work

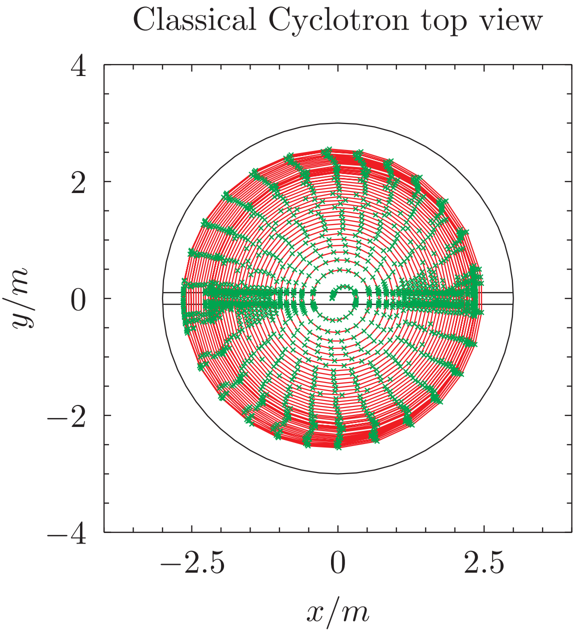
- With fixed step size (Same method, accept all) 4999 points
- Trust default setup:
- Epic fail Why?
- Discontinuous ODE is bad!



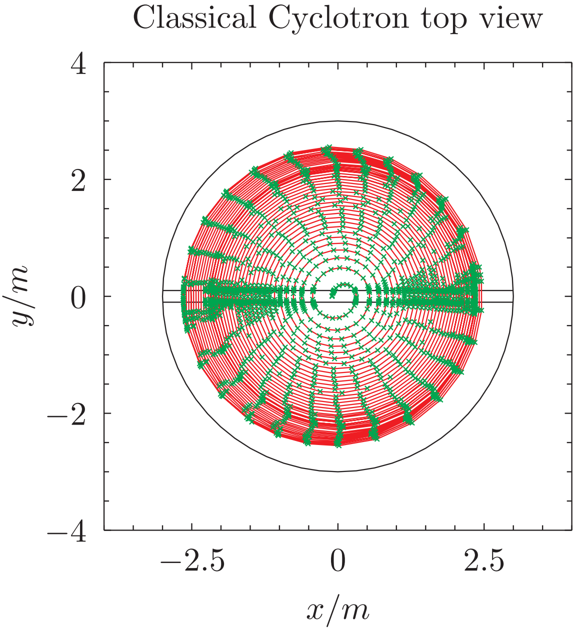
2070 points



Default choice, 2070 points.



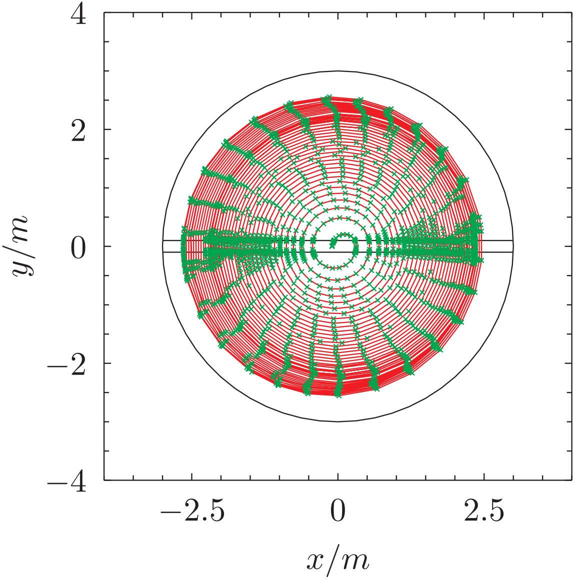
Default choice, 2070 points.



Default choice, 2070 points.

Classical Cyclotron top view

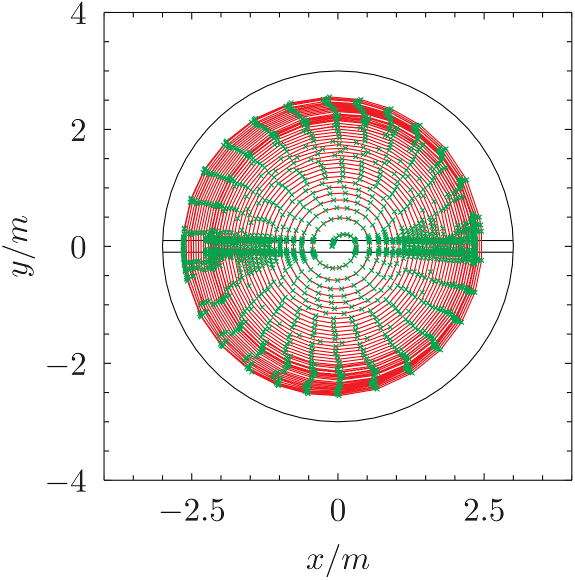
Classical Cyclotron top view



Default choice, 2070 points.

Classical Cyclotron top view

Classical Cyclotron top view



Default choice, 2070 points.

Classical Cyclotron top view

Analytic agreement

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Questions