MAINTITLE

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Student Colloquium in Physics and Astronomy, Aarhus University

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TITLEIMAGE

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Introduction, what and why

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How: Numeric-ODE solvers

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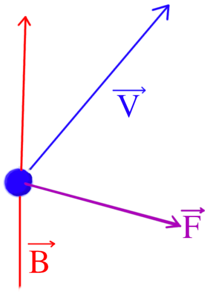
- Only 1 particle! so pre-programmed depending on the setup.
- Could use potentials $\phi(\vec{r}, t)$ $\vec{A}(\vec{r}, t)$ and Hamiltonian.

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



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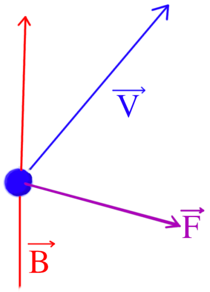
$$dW_{\vec{B}} = \vec{F}_B \cdot d\vec{r} \propto (\vec{v} \times \vec{B}) \cdot \vec{v} = 0.$$



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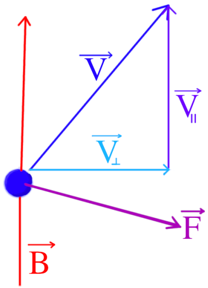

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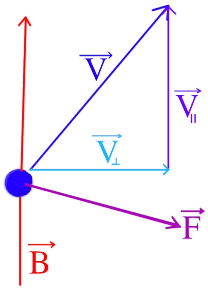
- Same as Centripetal force: Cyclotron motion



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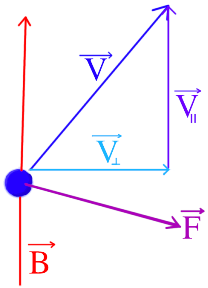
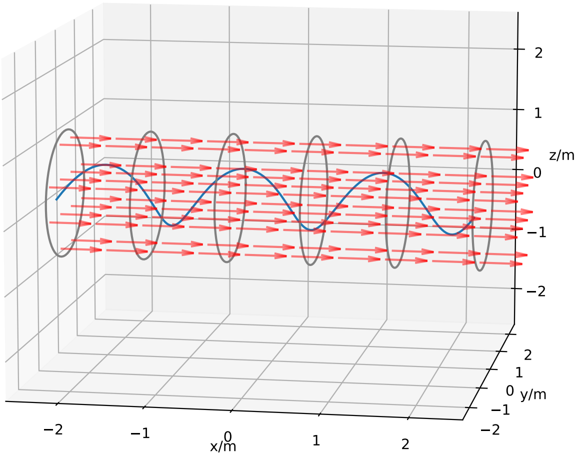
- Same as Centripetal force: Cyclotron motion
- Cyclotron radius and frequency:

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

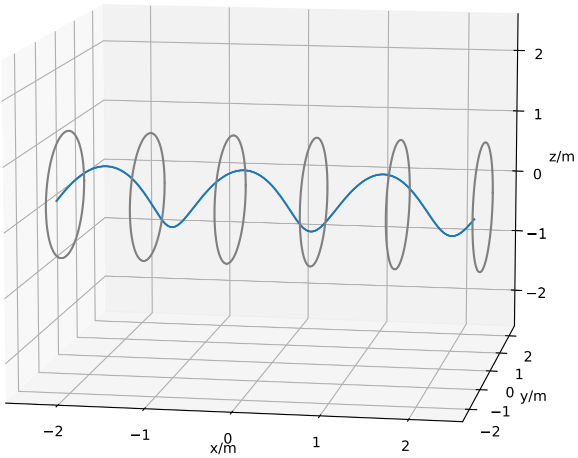


Analytical solution: Protons in a Solenoid



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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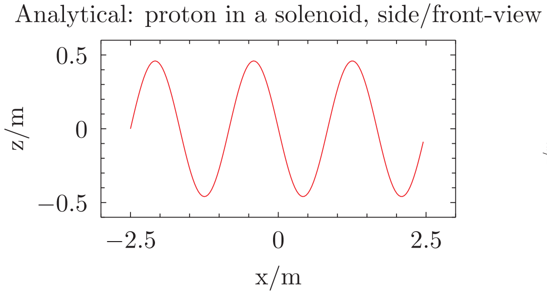

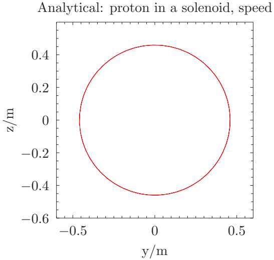

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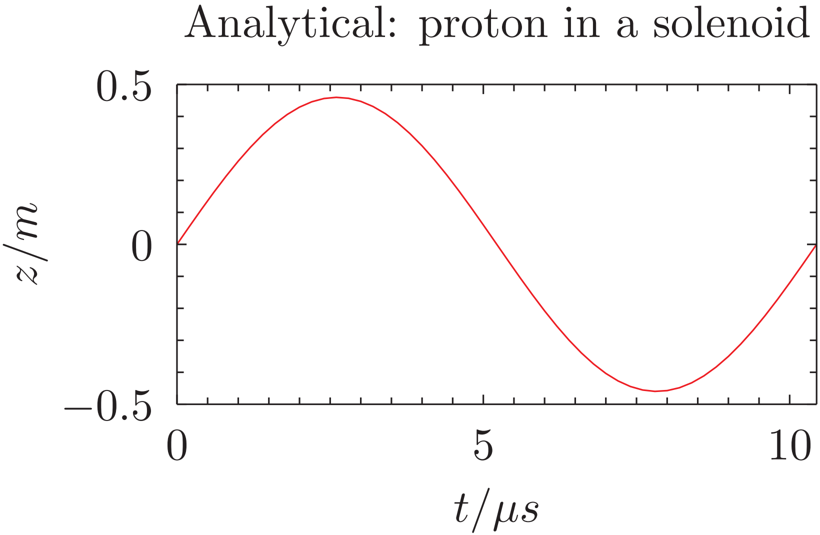

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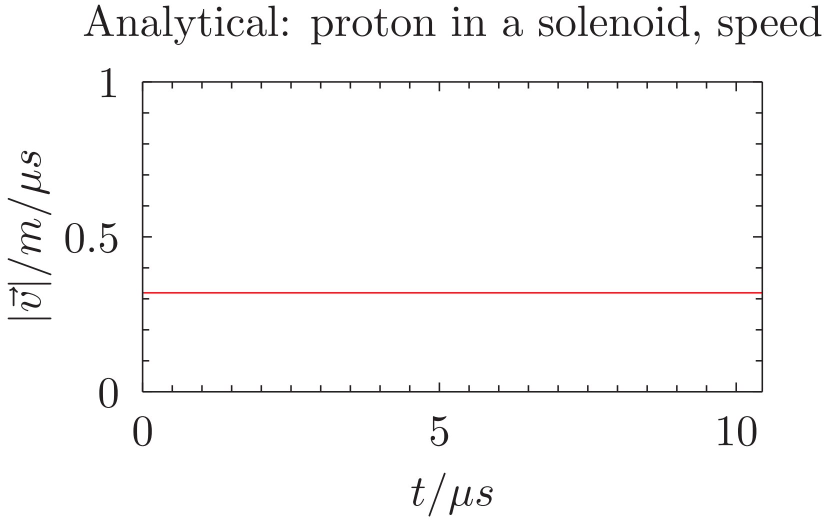

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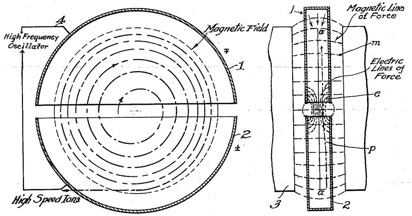
Cyclotron accelerator

- Electric forces do work.



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

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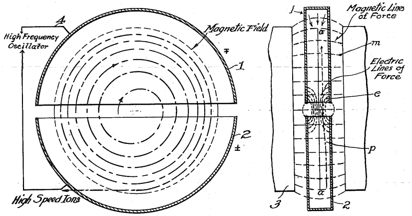

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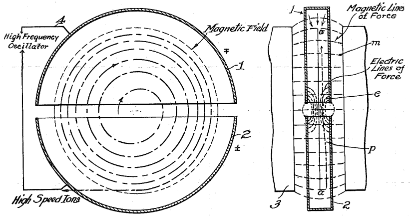

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Cyclotron accelerator

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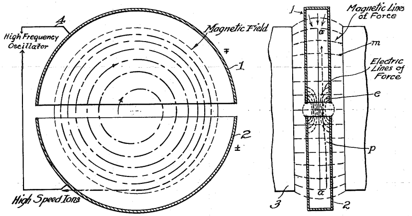
- Practical example, the Cyclotron.
- Single gab, oscillating field.
- Final speed:

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



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Ordinary differential equation*s.

- Sources: Zeigler et al. Theory of Modeling and Simulation (Third edition) chapter 3
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$$\dot{\mathbf{X}} = f_{ode}(\mathbf{X}(t), t).$$

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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

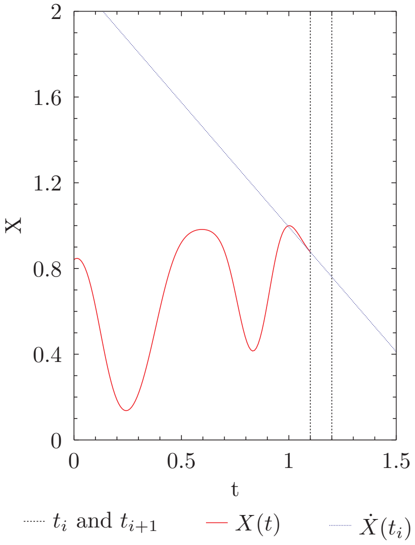
```
auto ODE = [...](const state_type Data, state_type &
    dDatadt, const double t){
     //Extract position and velocity from data
     vec pos = vec(Data[0],Data[1],Data[2]);
     vec velocity = vec(Data[3],Data[4],Data[5]);

     //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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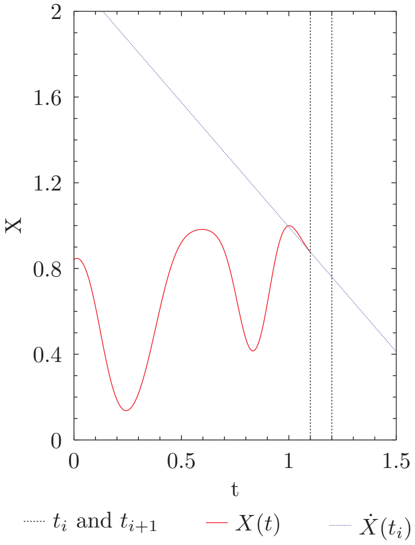

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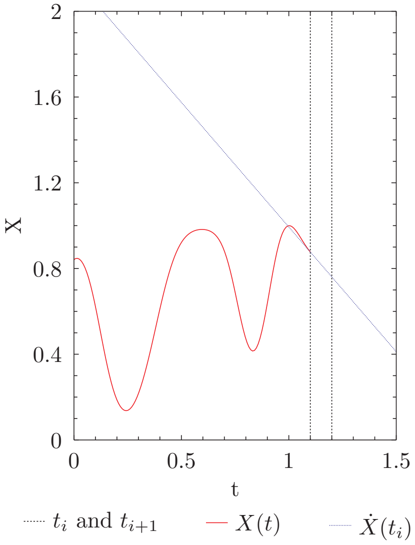

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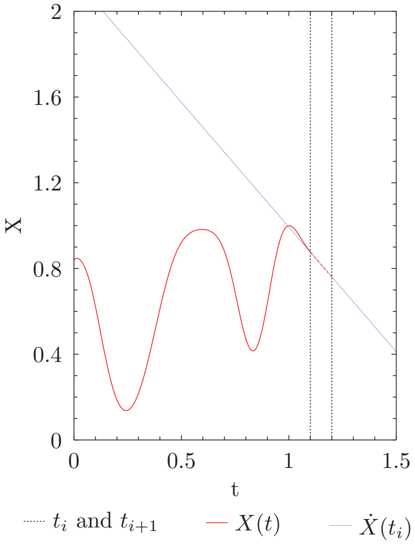

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- How would you find $\mathbf{X}(t_{i+1})$:
- (Explicit) Forward Euler's Method:

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

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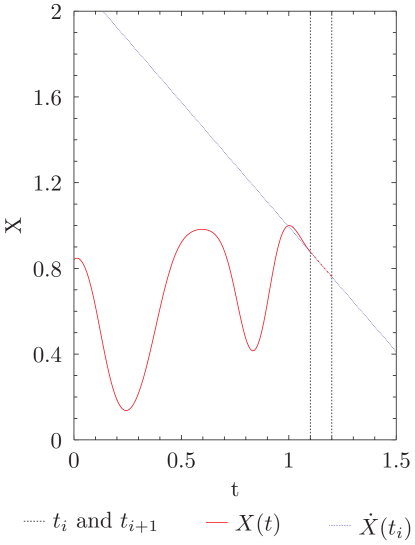

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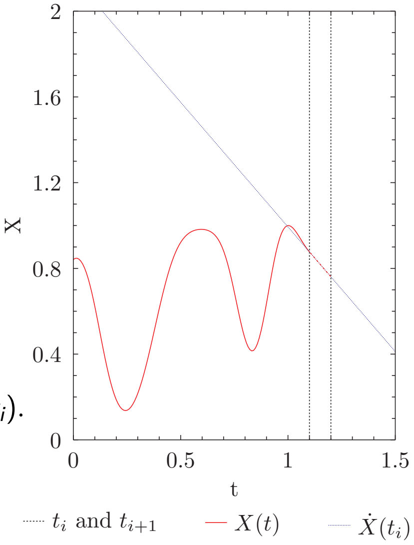

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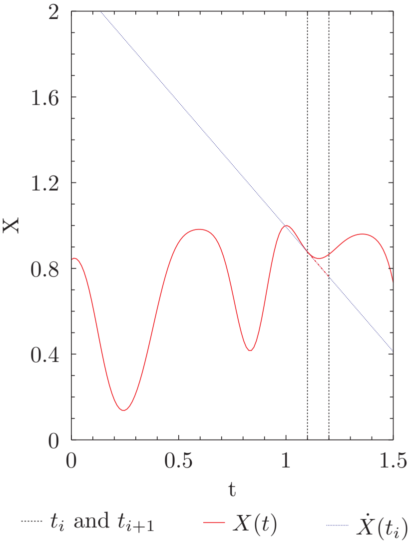

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- "Local truncation error" $h^2 = h^{p+1}$.
- Global error $h = h^p$.
- Convergence, but not uniform.

Why does this work? The Runge Kutta family

- In general.

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

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

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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.

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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:

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

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

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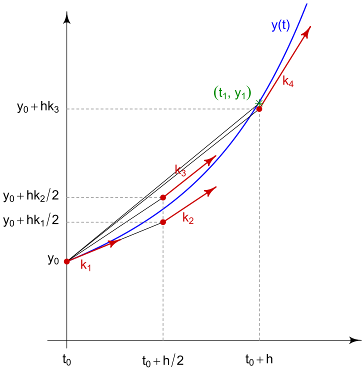

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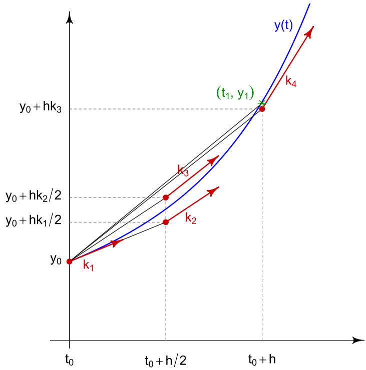

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- Almost default in `scipy.integrate.solve_ivp` and matlab ode45.

The General explicit Runge Kutta method

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

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

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

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

- Expressed in Butcher tableu:

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

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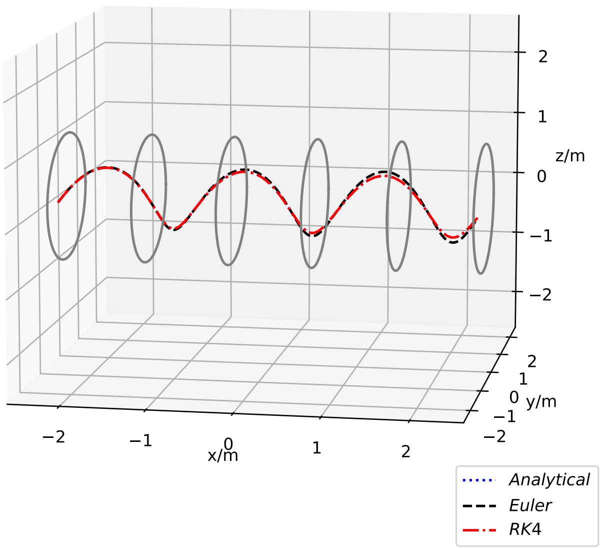
- Consider $\theta = 60^\circ$, $h = 0.01\,\mu\mathrm{s}$, $h = 0.1\,\mu\mathrm{s}$ and $h = 0.1\,\mu\mathrm{s}$.
- Check error on $|\vec{v}|$, $R = \sqrt{y^2 + z^2}$ and $x(t)$.

At a glance, 3D view

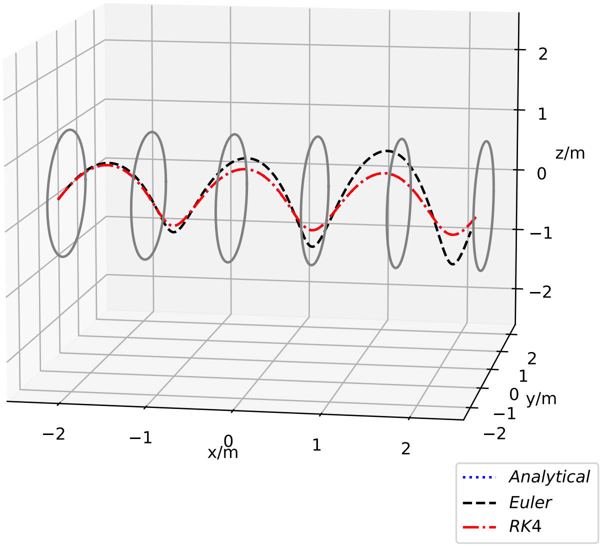
$h = t_{i+1} - t_i = 0.01\,\mu s$



3129 steps

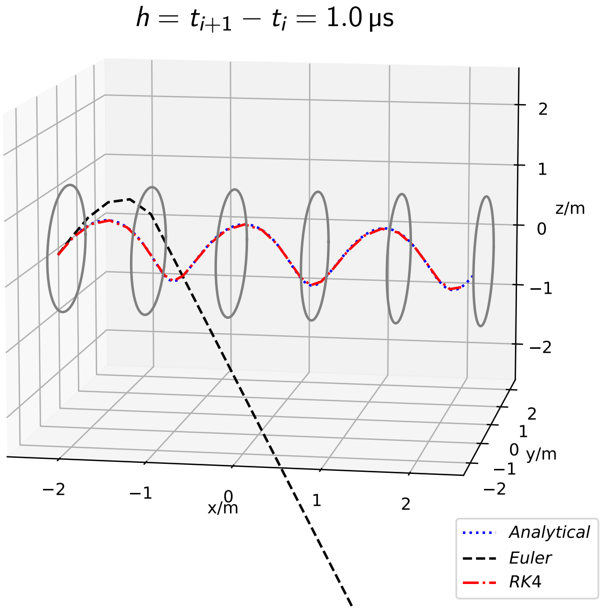
At a glance, 3D view

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



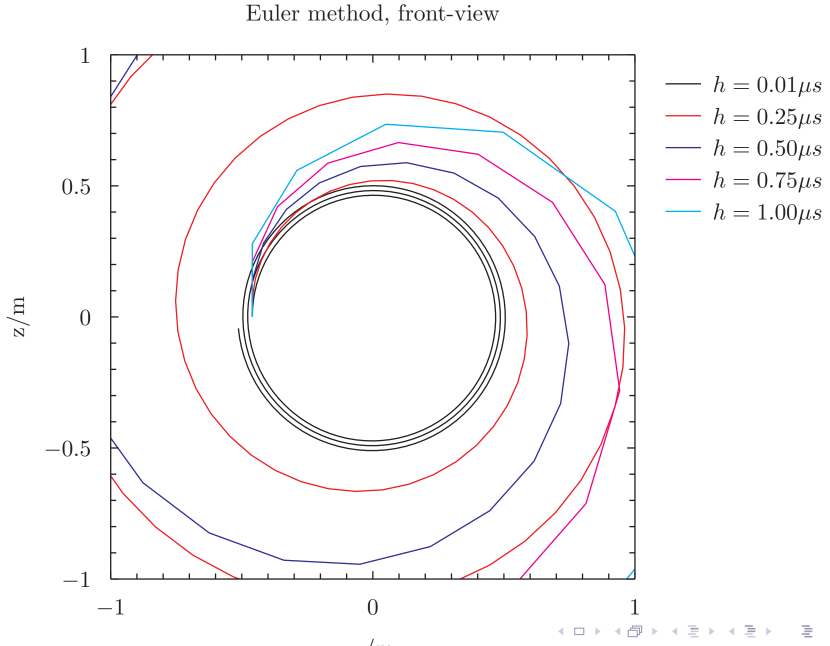
312 steps

At a glance, 3D view

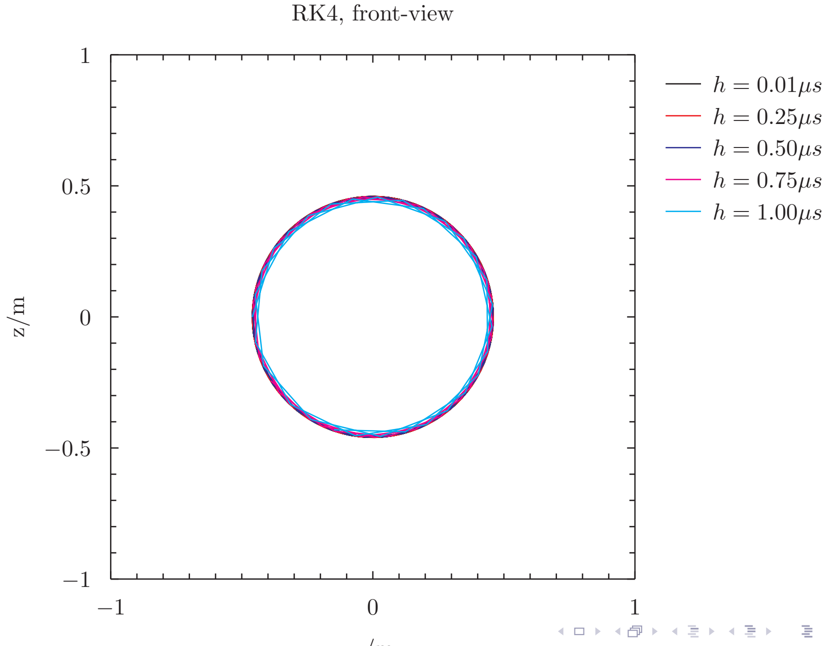


31 steps.

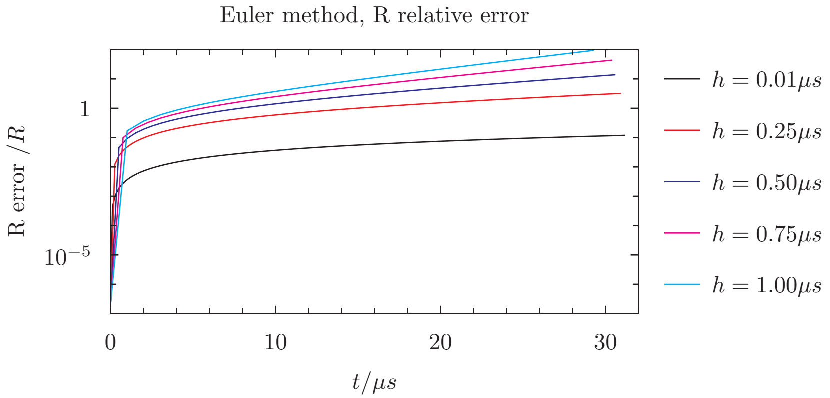
At a glance, front view, no border



At a glance, front view, no border



Constant radius?



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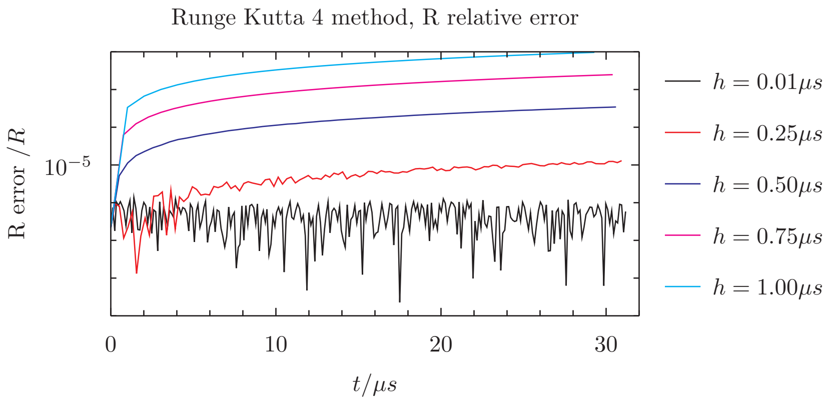
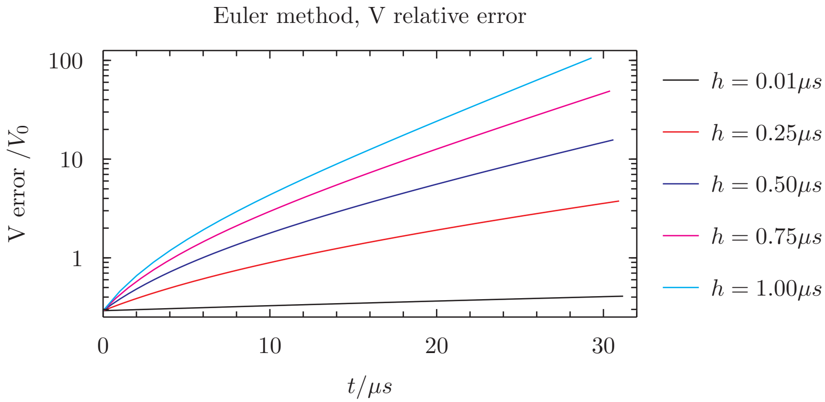
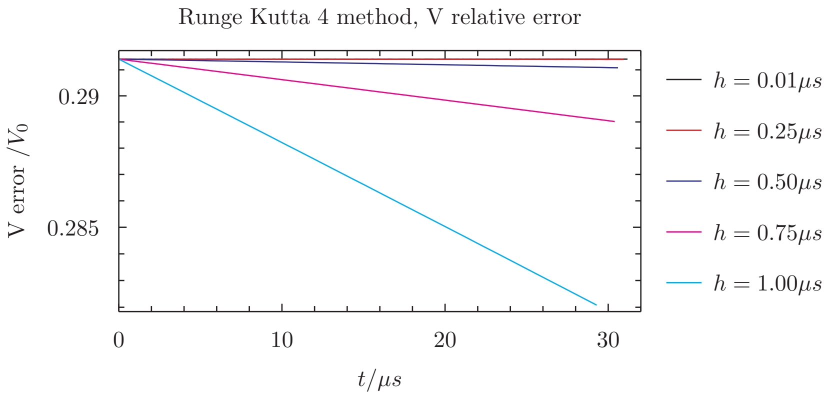


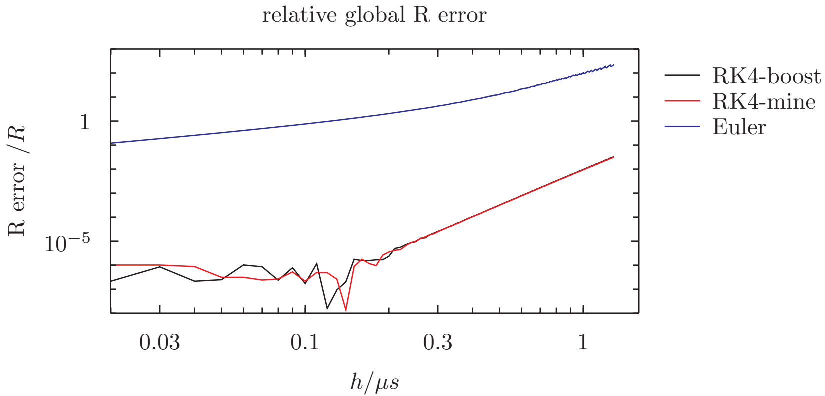
Constant speed?



Constant speed?



Error as function of h



Adaptive step size, why

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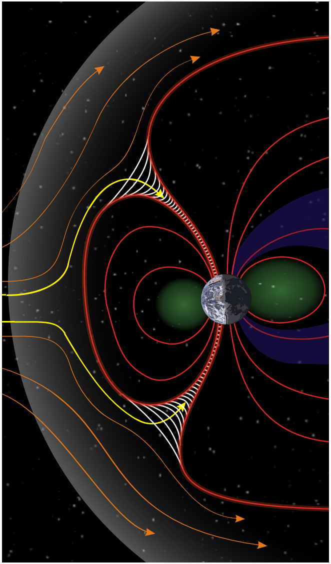

Illustration originally from Nasa. Published on wikipedia, in Public

Adaptive step size, why

- h must be small "enough"
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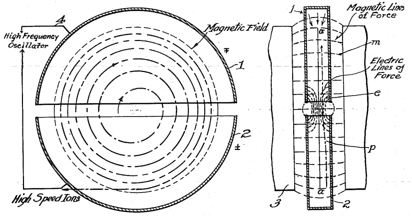
- time dependent fields (here the cyclotron, bad example)



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

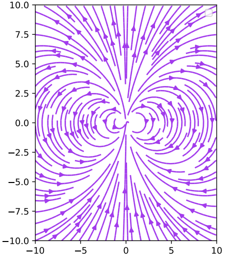
Adaptive step size, why

- 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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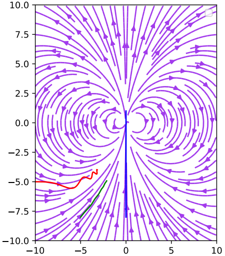

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- Weak field, little change, long steps.
- strong field, large change, short steps.
- No analytical solution (afaik.)
- Arbitrarily set $\frac{\mu_0}{4\pi}|\vec{m}| = 0.155\,\mathrm{T/m^3}$.
- Protons with speed

Runge-Kutta Adaptive step size, how

- Reduce h until the "error" is small enough

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Runge-Kutta Adaptive step size, how

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- Use 2 different methods, $\mathbf{x}(t_{i+1})$, $\mathbf{x}'(t_{i+1})$.
- Approximate “Error” as $|\mathbf{x}(t_{i+1}) - \mathbf{x}'(t_{i+1})|$.
- Most often order 4 and 5 with same $\mathbf{k}_i$.

Runge-Kutta Dormand Prince 4-5

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

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

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

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

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

Runge-Kutta Dormand Prince 4-5

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

- 4th and 5th order, hence ode 45. Keeps 5th order term if error less than absolute and relative threshold.
- Should also decide to increase step size.

Dormand, J. R.; Prince, P. J. (1980), "A family of embedded

Butcher Tableu of Dormand Prince 4/5

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

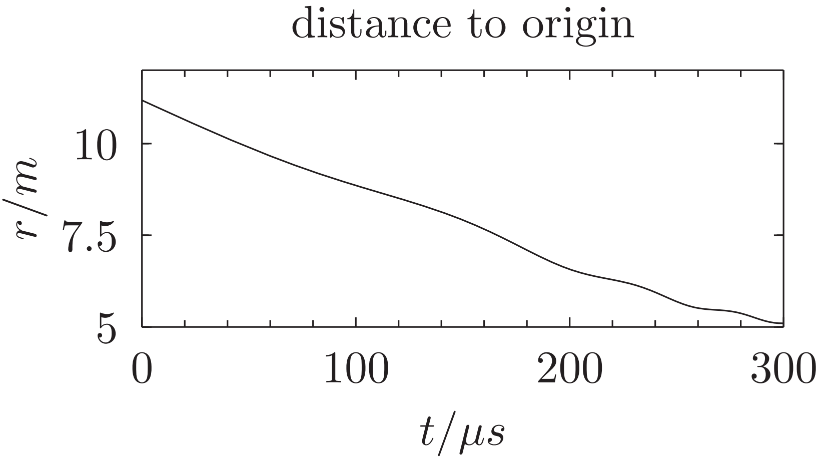
Adaptive step-size

```
#include <boost/array.hpp>
#include <boost/numeric/odeint.hpp>
using namespace boost::numeric::odeint;
typedef boost::array< double, 6 > state_type;
...
size_t steps = integrate_adaptive(
     make_controled( absErr, relErr ,
    runge_kutta_dopri5< state_type >() ),
     ODE,    //Lorentz-force
     Data0 ,//{pos0,v0}
     0.0 ,   //t0=0
     T ,     //max time
     timestep ,//length of each step (initial)
     save_step //User defined save data function
);
```

Adaptive step-size

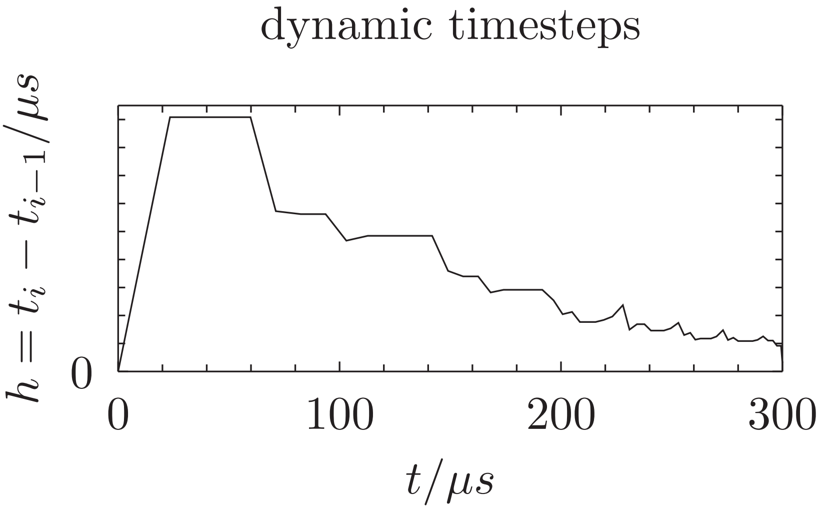
```cpp
#include <boost/array.hpp>
#include <boost/numeric/odeint.hpp>
using namespace boost::numeric::odeint;
typedef boost::array< double, 6 > state_type;
...
size_t steps = integrate(
    ODE,   //Lorentz-force
    Data0 ,//{pos0,v0}
    0.0 ,  //t0=0
    T ,    //max time
    timestep ,//length of each step (initial)
    save_step //User defined save data function
);
```

Does it work?



Boost Odeint Dormand-Prince, relative and absolute error 10^{-6}.

Does it work?

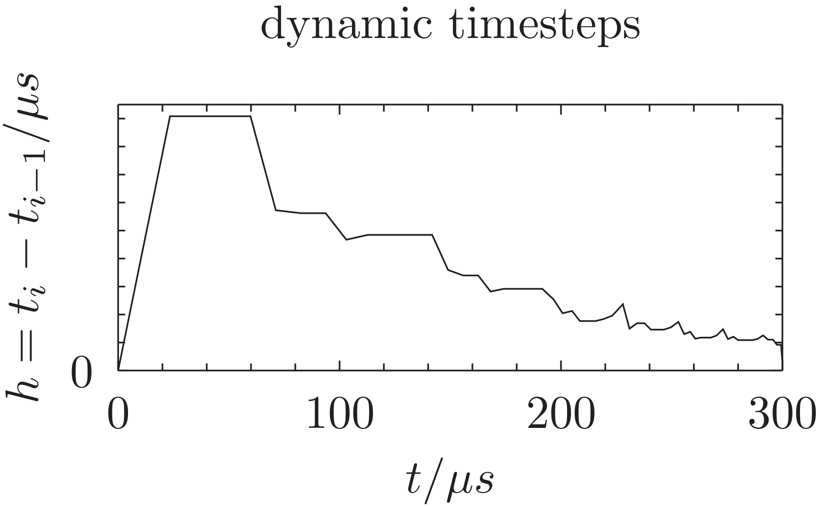


Boost Odeint Dormand-Prince, relative and absolute error 10^{-6}.

Does it work? Another curious result

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

Does it work? Another curious result



Magnetic "mirror" or "bottle"

Extra examples-“if time permits”

- The cyclotron

Extra examples-“if time permits”

- The cyclotron
- Toroidal fields

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- The cyclotron
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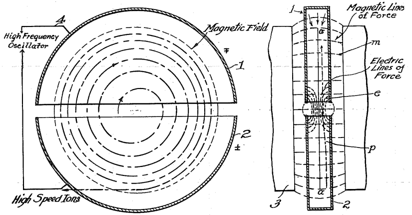
Example, cyclotron

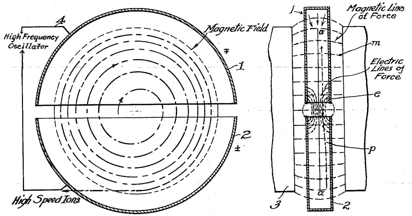
- Electric field accelerates, magnetic contains.



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

Example, cyclotron

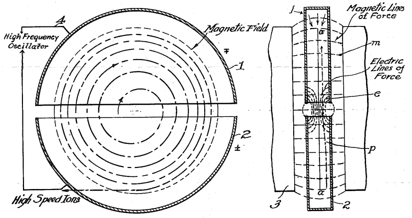
- Electric field accelerates, magnetic contains.
- Single gab, oscillating field.



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 classical Cyclotron frequency



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

Example, cyclotron

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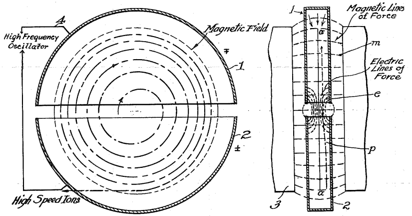
- Uses classical Cyclotron frequency
- Analytical final speed, in principle path.

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



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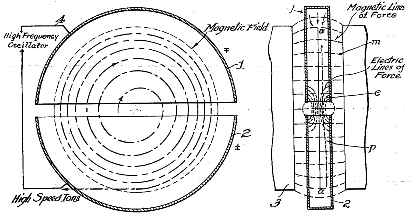

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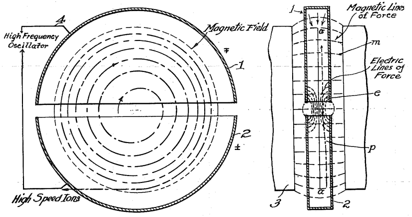

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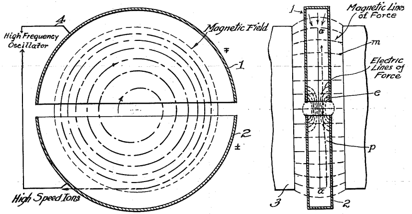

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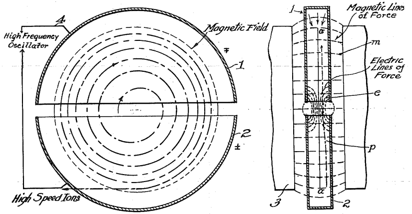


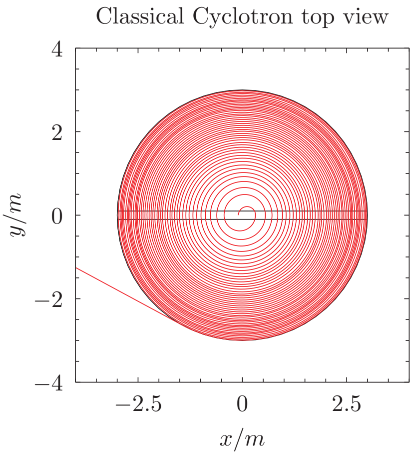
Ernest O. Lawrence, 1934, U.S. Patent 1,948,384; image in Public Domain.

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

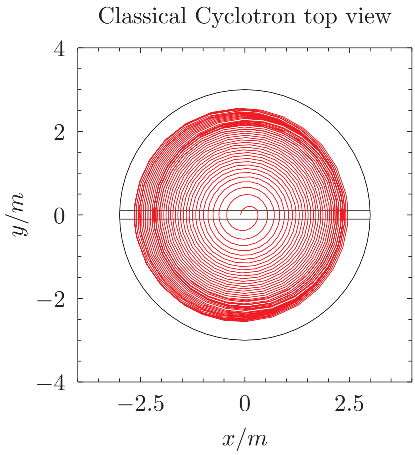
- With fixed step size (Same method, accept all) 4999 points



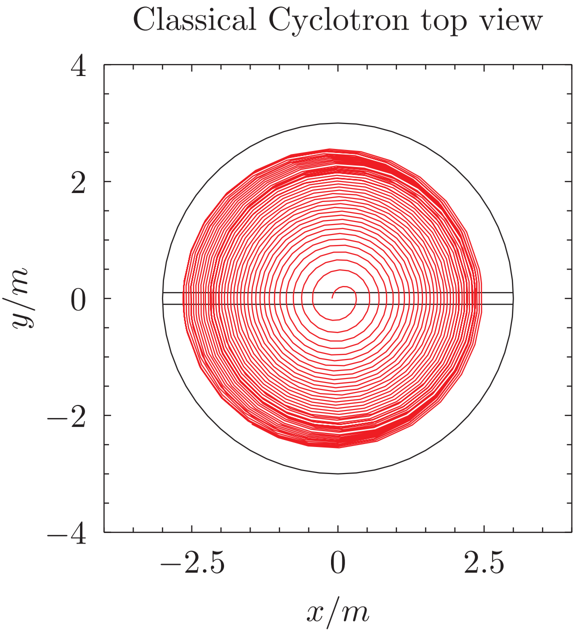
4999 points!

Does it help/work

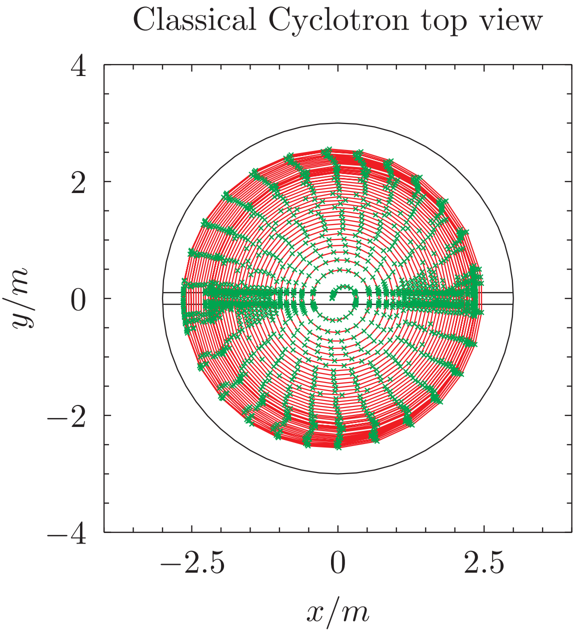
- With fixed step size (Same method, accept all) 4999 points
- Trust default setup:
- Epic fail Why?
- Discontinuous ODE is bad!



2070 points

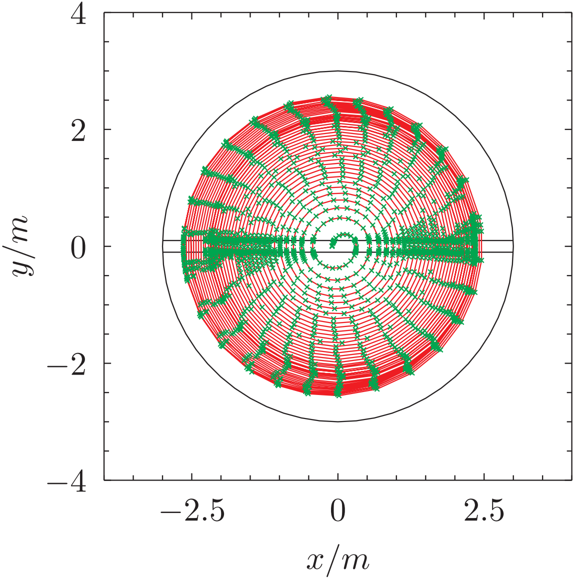


Default choice, 2070 points.



Default choice, 2070 points.

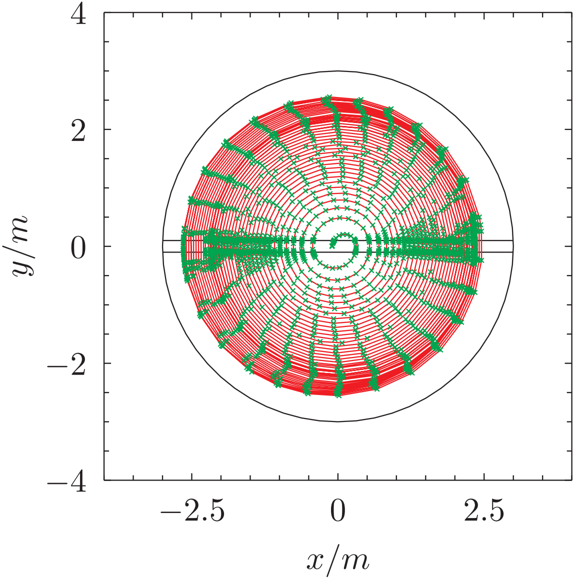
Classical Cyclotron top view



Default choice, 2070 points.

Classical Cyclotron top view

Classical Cyclotron top view



Default choice, 2070 points.

Classical Cyclotron top view

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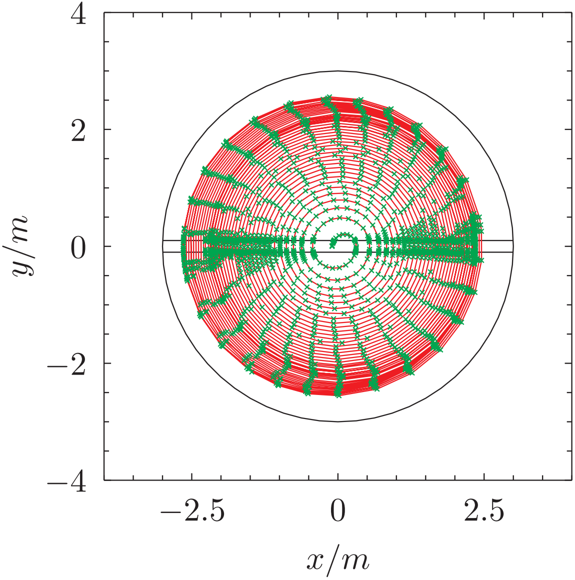

Default choice, 2070 points.

Classical Cyclotron top view

Analytic agreement

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Questions