How numerical simulations work: Simulating particles in electric and magnetic fields

Nikolaj Roager Christensen

Student Colloquium in Physics and Astronomy, Aarhus University

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TITLEIMAGE

How numerical simulations work: Simulating particles in electric and magnetic fields

Introduction [5 MIN]

Theory and physical background [5 MIN]

Euler's Method and the 4th order Runge-Kutta Method [15 MIN]
- Euler's Method
- Higher order Runge-Kutta methods
- Demonstration, particles in a solenoid

Introducing Adaptive step size [10 MIN]
- Demonstration: magnetic dipole
- Dormand Prince 5 (4) method

Conclusion [2 MIN]
- Extra, the cyclotron
- Extra, toroidal fields

Introduction, what and why

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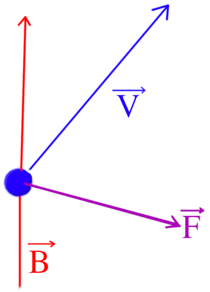
- Only 1 particle! so pre-programmed depending on the setup.
- Could use potentials $\phi(\vec{r}, t)$ $\vec{A}(\vec{r}, t)$ and Hamiltonian.

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



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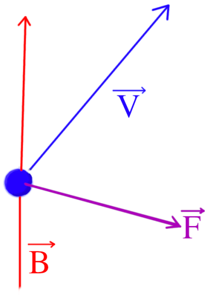

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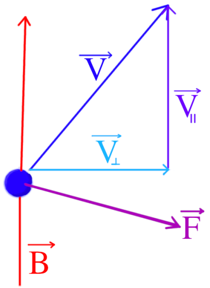

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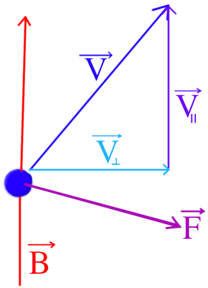
- Same as Centripetal force: Cyclotron motion



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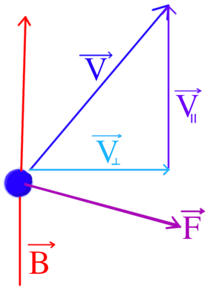
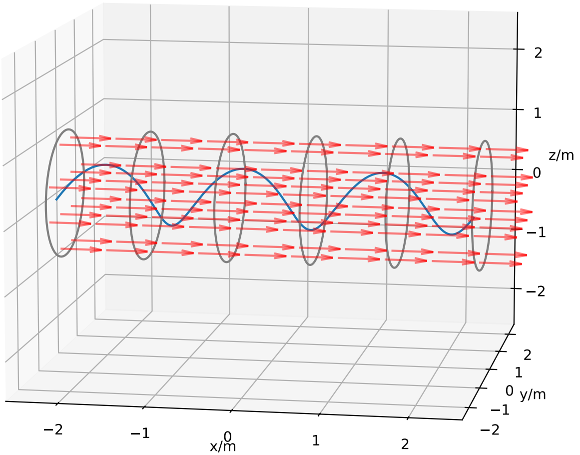
$$|\vec{F}_B| = |q(\vec{v} \times \vec{B})| = |q v_\perp B|.$$

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

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



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

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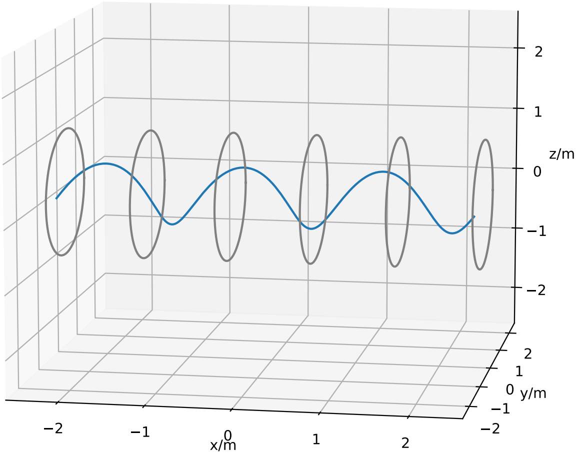

$$R \approx 0.5\,\mathrm{m}\sin(\theta) \qquad T = \frac{2\pi}{\omega_c} \approx 10\,\mu\mathrm{s}$$

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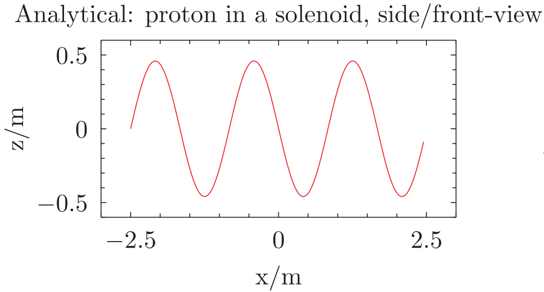

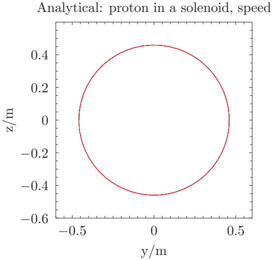

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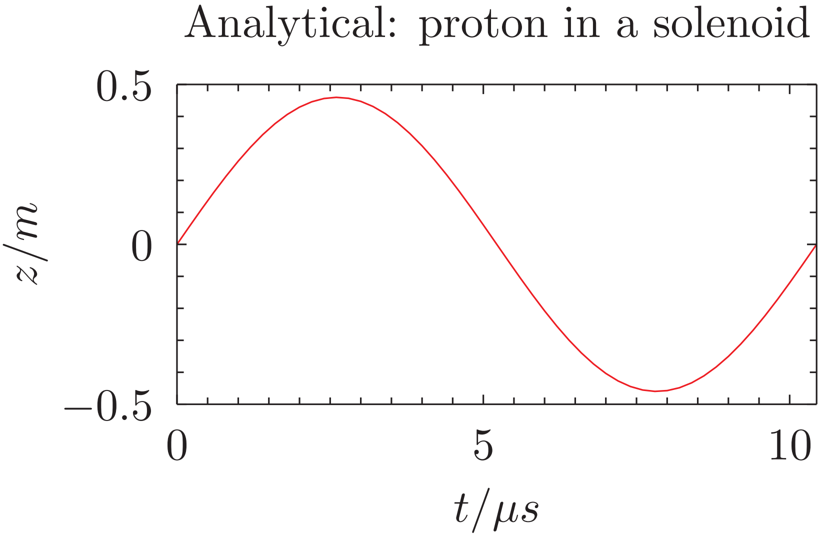

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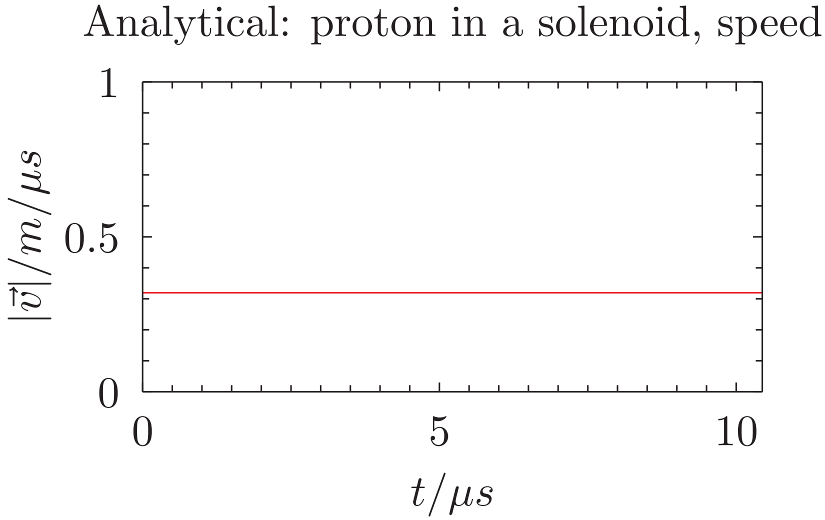

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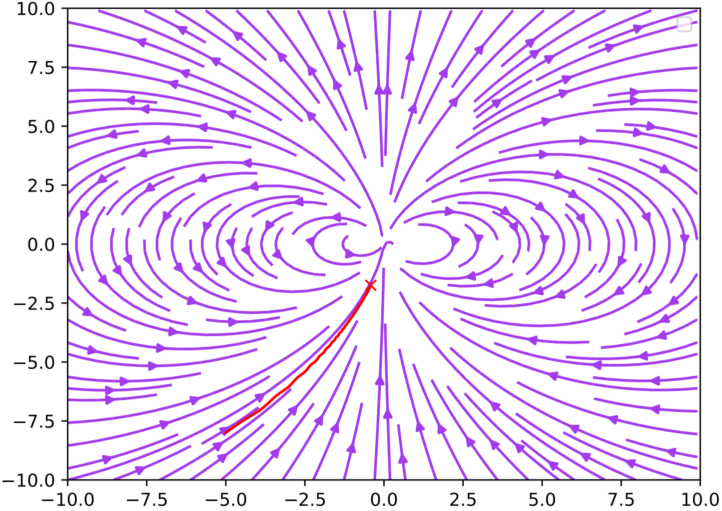

Ordinary differential equation's.

- 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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- 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

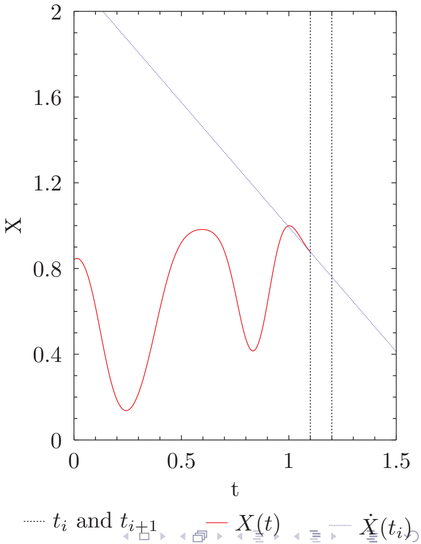
```
auto ODE = [...](const state_type Data, state_type &
    dDatadt, const double t){
     //Extract position and velocity from data
     vec pos = vec(Data[0],Data[1],Data[2]);
     vec velocity = vec(Data[3],Data[4],Data[5]);

     //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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The Forward Euler's Method

- Let $h = t_{i+1} - t_i > 0$ be constant.
- h, $\mathbf{X}(t)$, t_i and f_{ode} are known.

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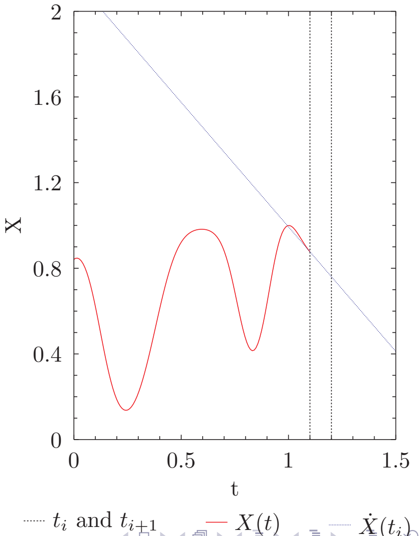

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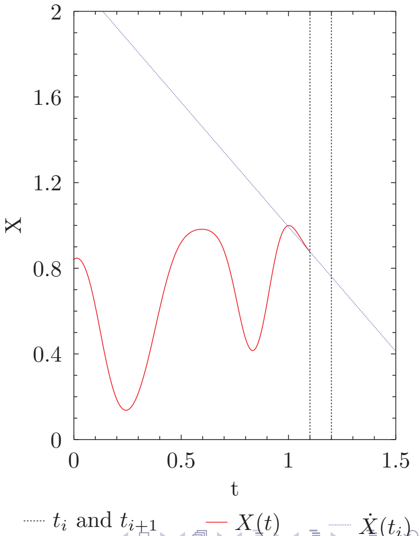

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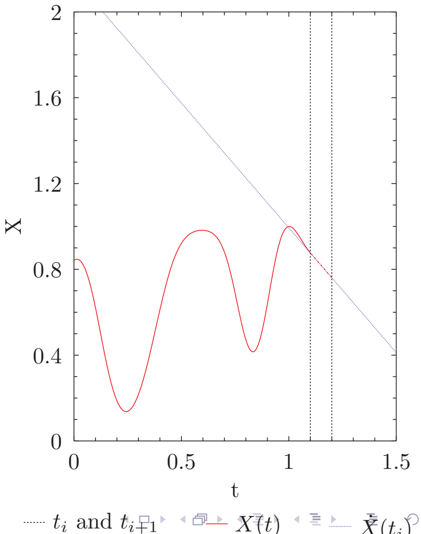
- How would you find $\mathbf{X}(t_{i+1})$:
- (Explicit) Forward Euler's Method:

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



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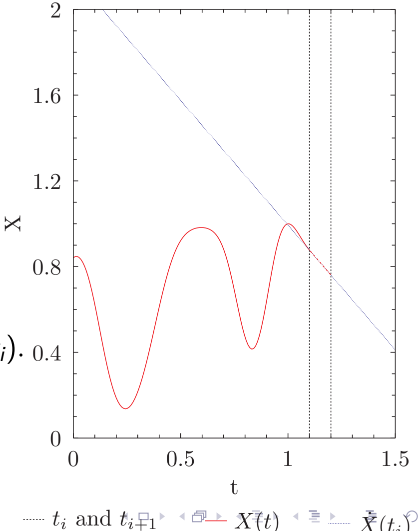

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- Chain together multiple steps from t_0...with step size h.
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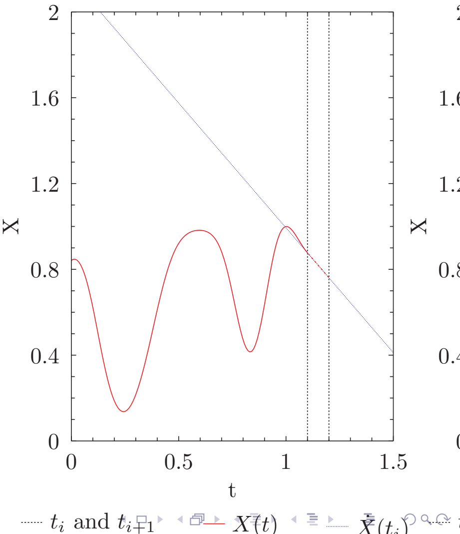

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- "Local truncation error" h^2.
- Global error h^1.
- Convergence, but not uniform.

Why does this work? The Runge Kutta family

- In general.

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

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

Explicit Runge Kutta methods

- We want:

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

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- Want exact to p'th order. Can be found with Taylor expansion of $\mathbf{X}(t_i)$.
- Local/global error h^{p+1}, Global error h^p.
- 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:

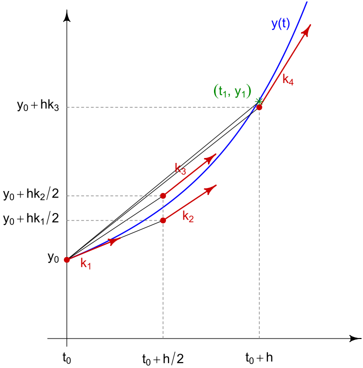
$$\mathbf{X}(t_{i+1}) - \mathbf{X}(t_i) = \frac{h}{6}(\mathbf{k}_1 + 2\mathbf{k}_2 + 2\mathbf{k}_3 + \mathbf{k}_4)$$

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

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

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

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



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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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\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;

    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

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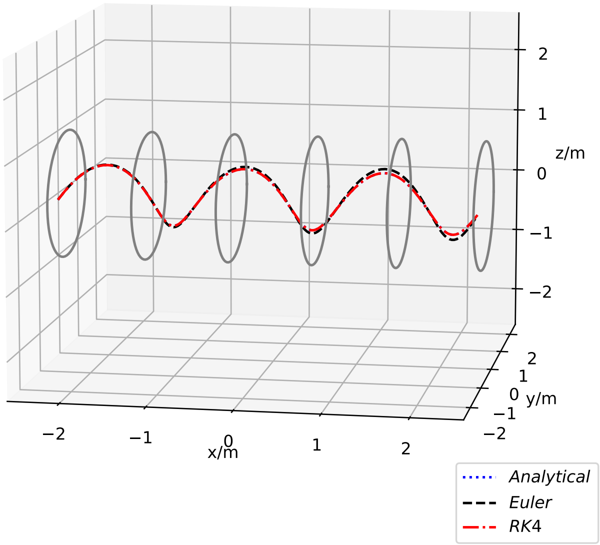
At a glance, 3D view

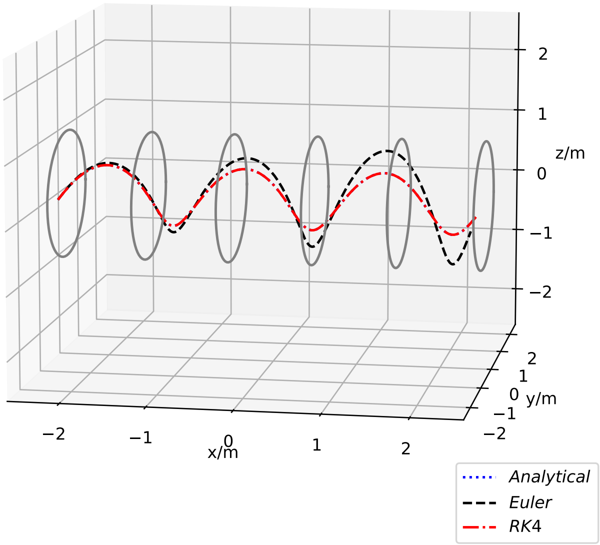
$h = t_{i+1} - t_i = 0.01\,\mu s$



3129 steps

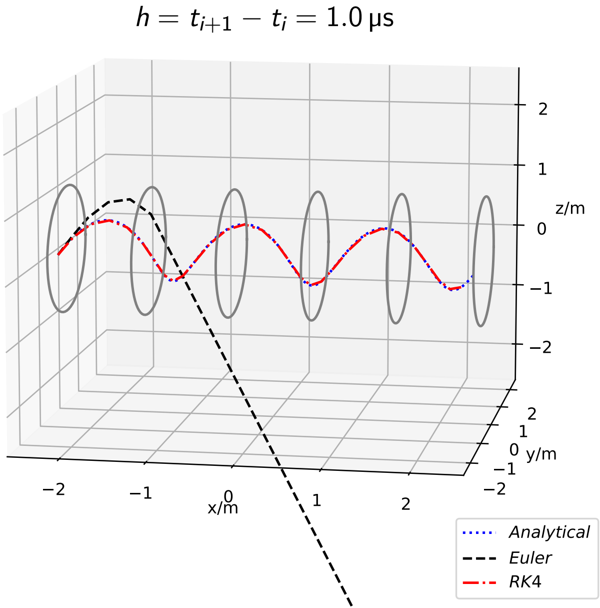
At a glance, 3D view

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



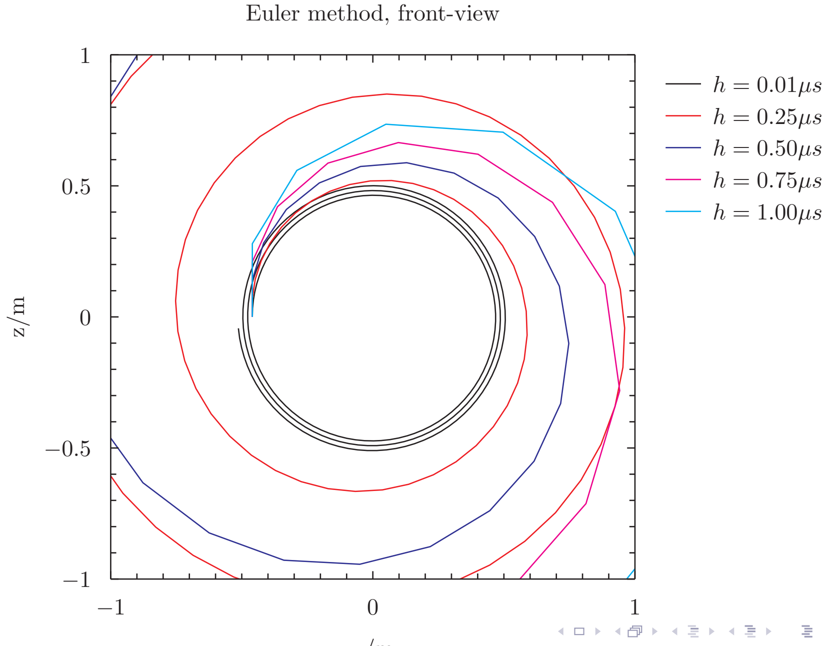
312 steps

At a glance, 3D view

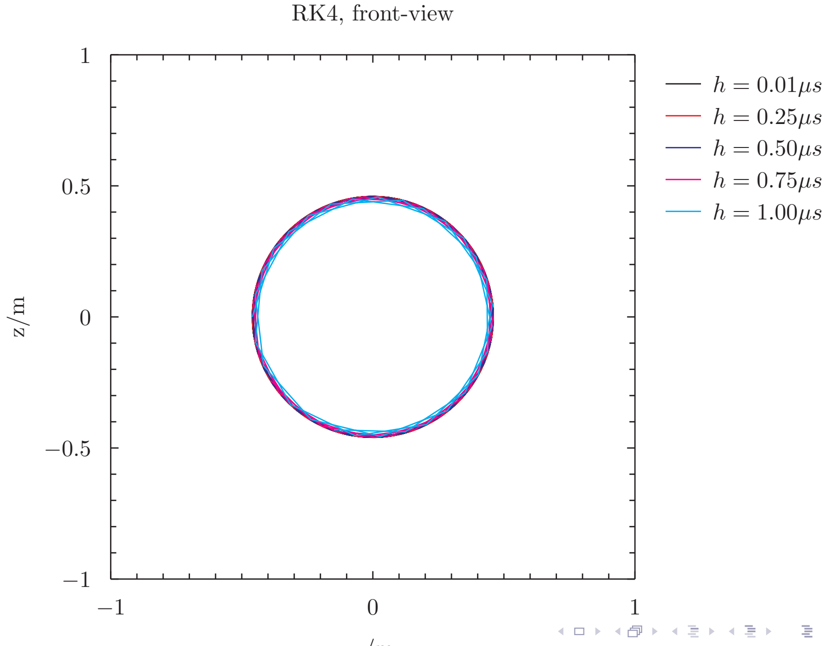


31 steps.

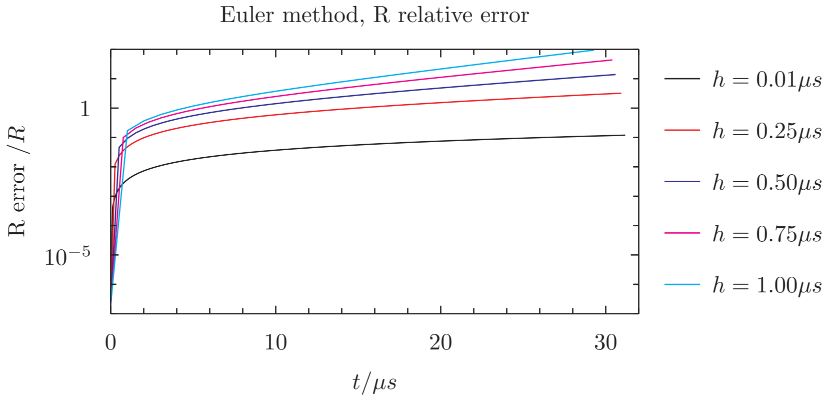
At a glance, front view, no border



At a glance, front view, no border



Constant radius?



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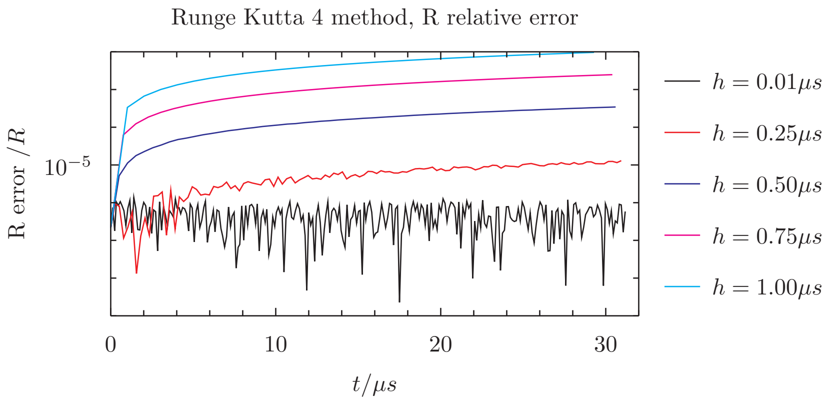
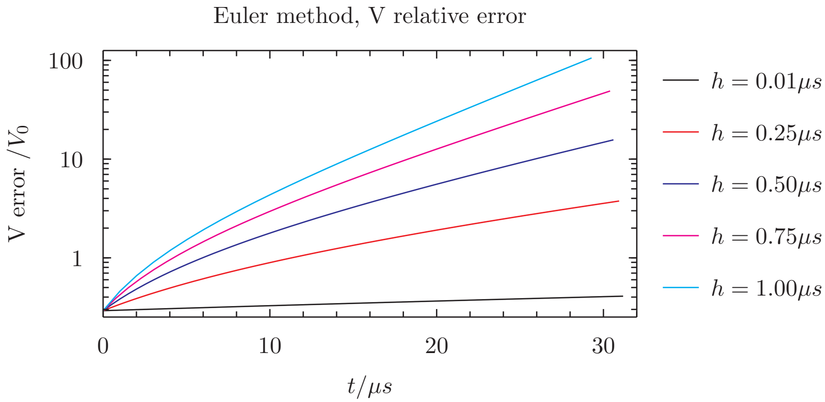


Constant speed?



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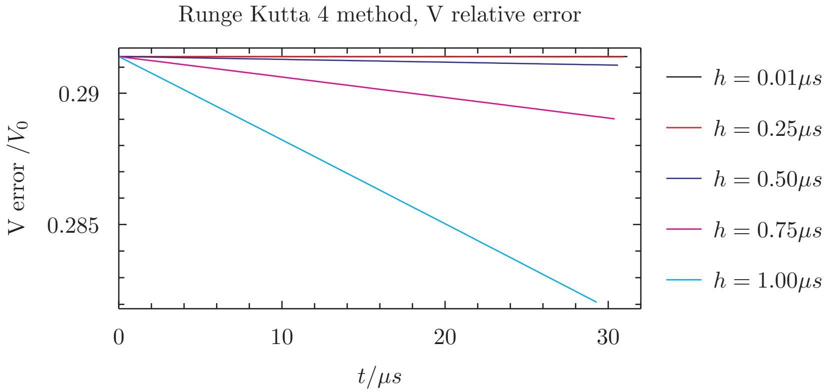
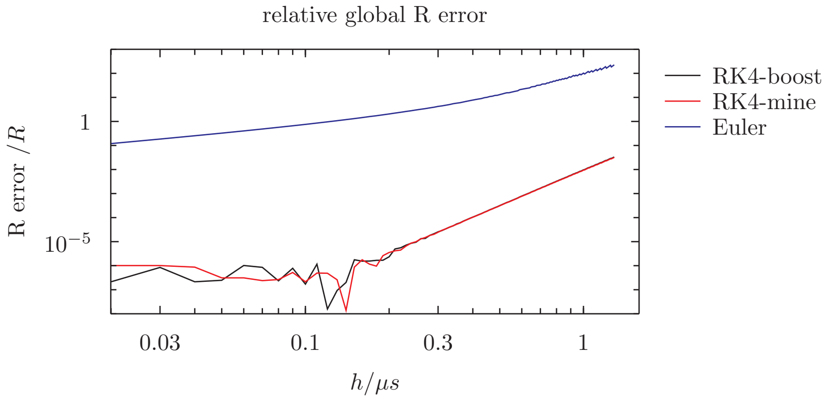


Error as function of h



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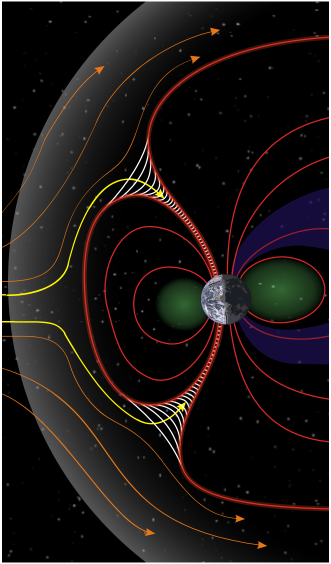

Illustration originally from Nasa. Published on wikipedia, in Public

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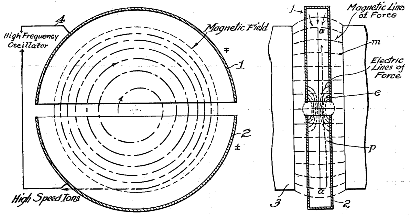


Ernest O. Lawrence, 1934, U.S. Patent 1,948,384; image in Public Domain.

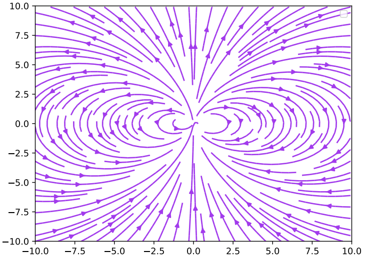
Adaptive step size, why

- 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

- 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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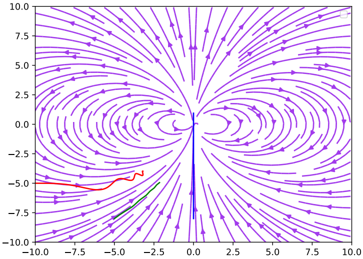

Arbitrarily set $\frac{\mu_0}{4\pi}|\vec{m}| = 0.155\,\mathrm{T/m^3}$. Protons with speed around $10\,000\,\mathrm{m/s}$

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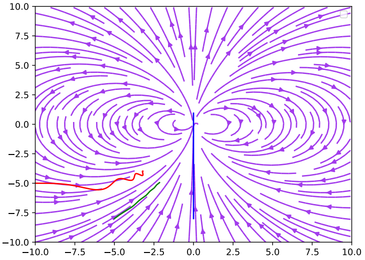

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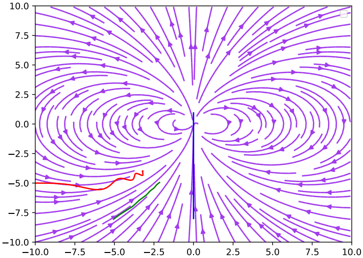
- No analytical solution (afaik.)



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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 Applied Mathematics

(1)

Runge-Kutta Dormand Prince 5 (4)

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

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

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

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

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

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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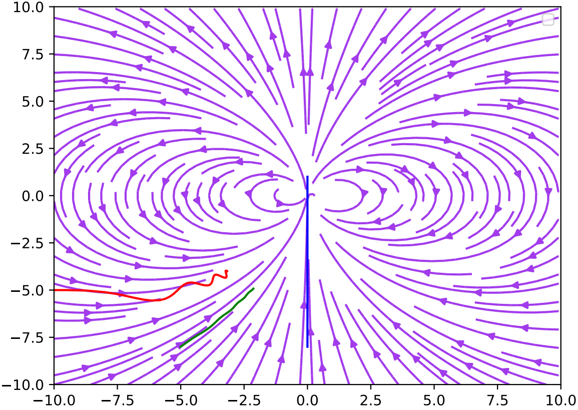
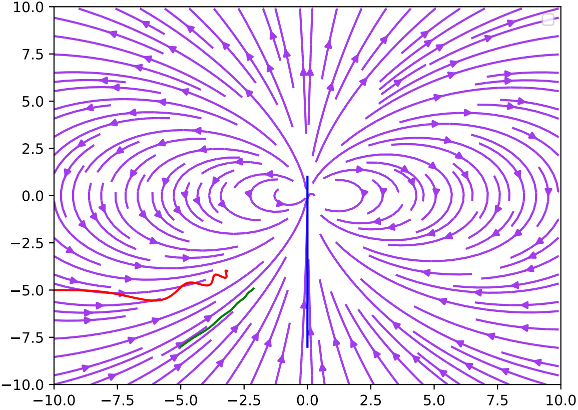
- Relative and absolute error at end. "Fail safe" $\sqrt{\ldots}$.
  Dormand, J. R.; Prince, P. J. (1980), "A family of embedded Runge-Kutta formulae", Journal of Computational and Applied Mathematics

Does it work?



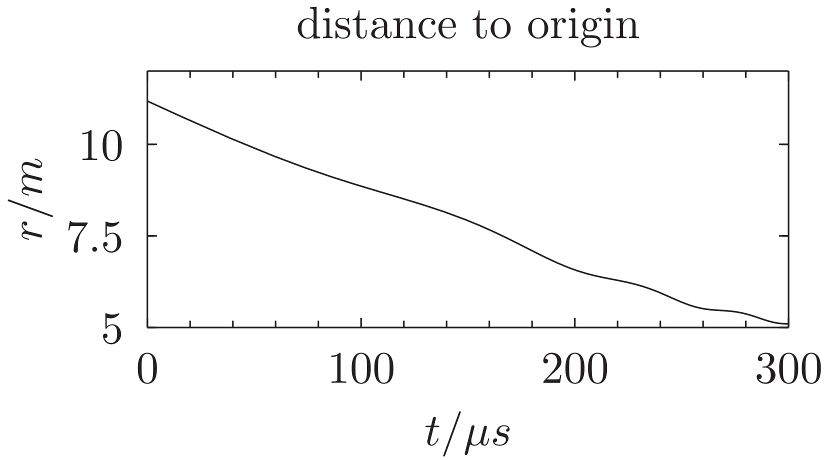
My version relative and absolute error 10^{-6}. 94 steps (+ 14 rejected).

Does it work?



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

Does it work?



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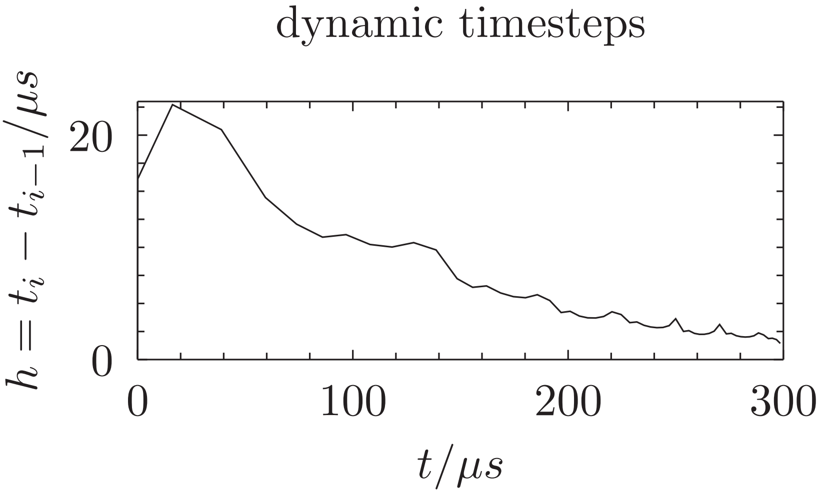
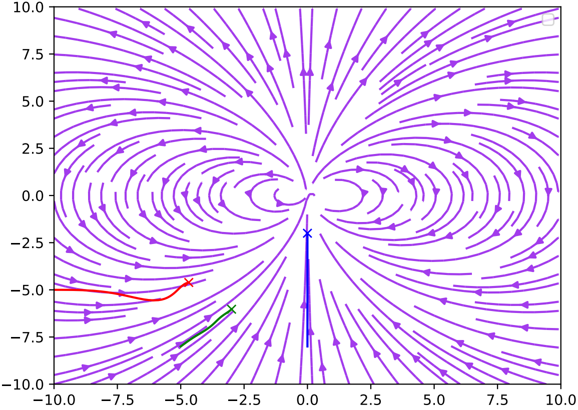
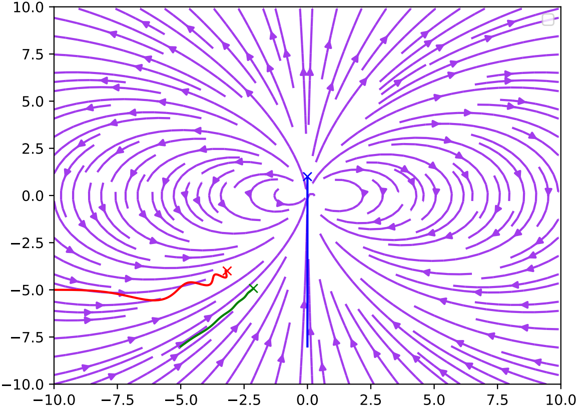


Another curious result



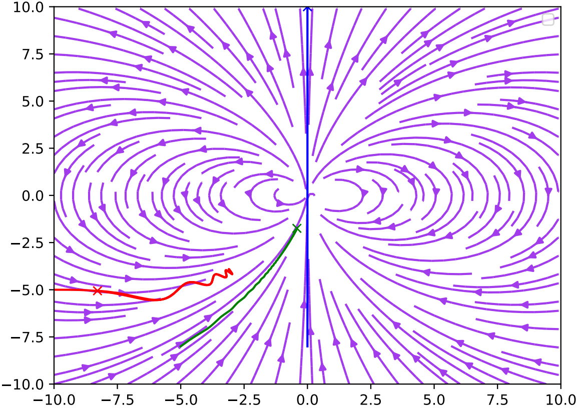
$T = 0.2\,\mathrm{ms}$

Another curious result



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

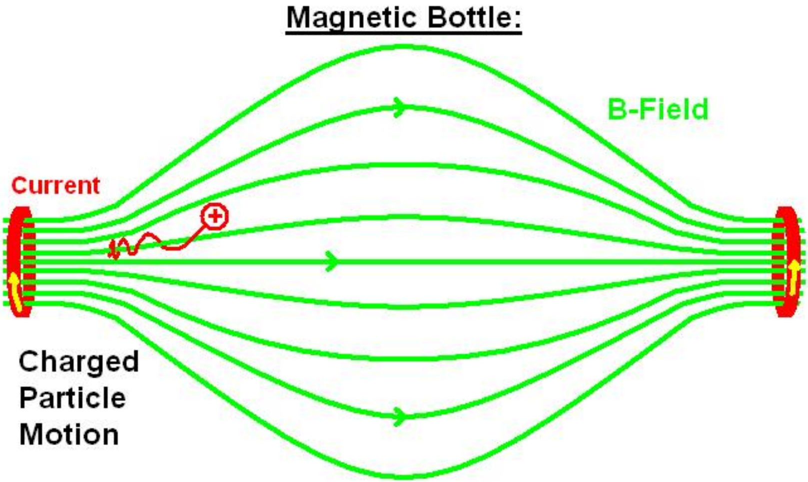
Another curious result



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

Magnetic "mirror" or "bottle".

Another curious result



Wikipedia user WikiHelper2134 , Public Domain.

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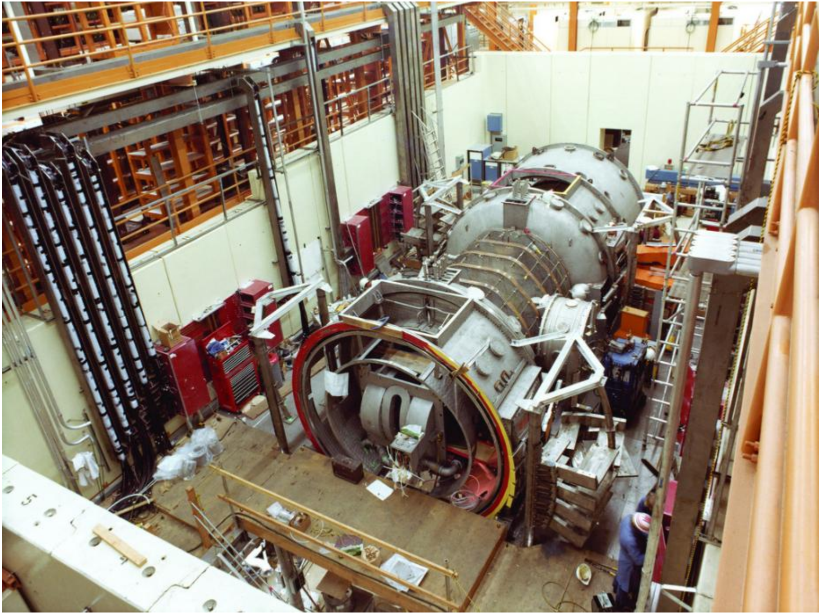

Tandem Mirror Experiment. The Lawrence Livermore National

Extra examples-"if time permits"

- The cyclotron
  - When the Dormand Prince method fails

Extra examples-“if time permits”

- The cyclotron
  - When the Dormand Prince method fails
- Toroidal fields [TBD]
  - Another non-analytic setup.

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- Limitation, simulations are not experiments.

Example, cyclotron

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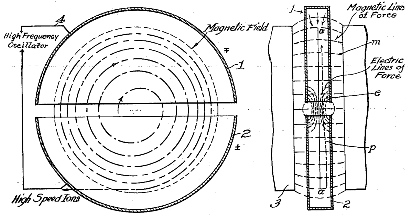

Ernest O. Lawrence, 1934, U.S. Patent 1,948,384; image in Public Domain.

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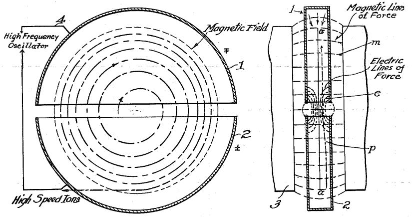

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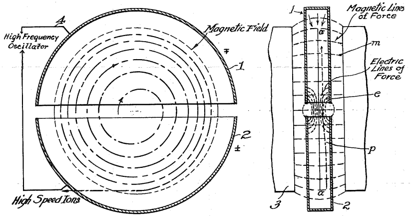
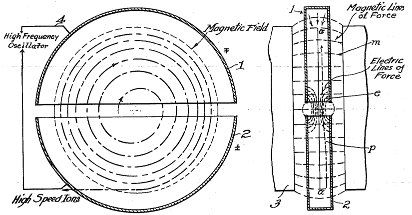


Ernest O. Lawrence, 1934, U.S. Patent 1,948,384; image in Public Domain.

Example, cyclotron

- Electric field accelerates, magnetic contains.
- 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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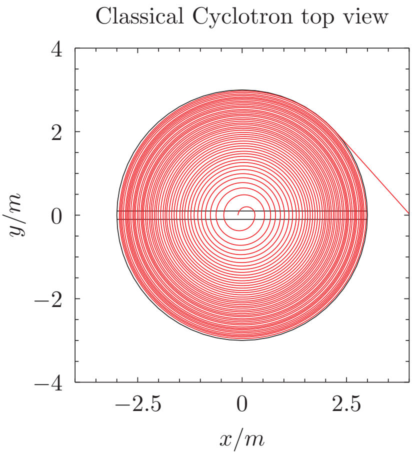
can it be simulated

- with fixed step size, looks bad 4999 points



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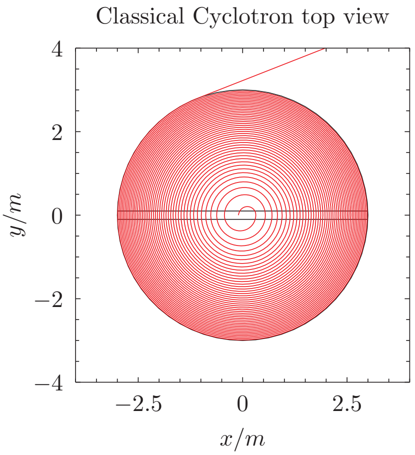

500000 points.

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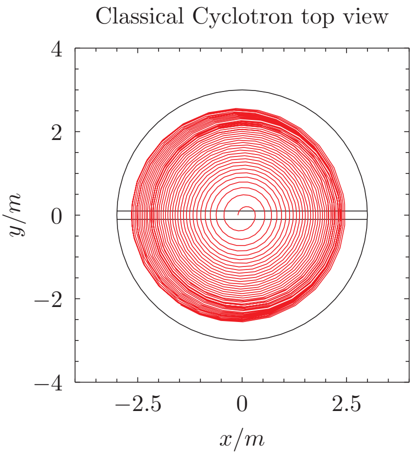
- odeint library



2070 points.

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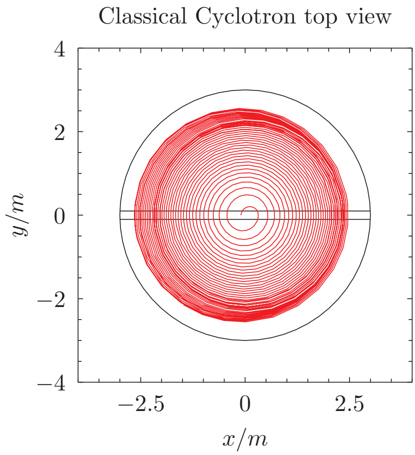
- odeint library
- non-continuous ode are bad.



2070 points.

TBD