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

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Motivation and introductions.

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- Demonstration, charged particles in electric and magnetic fields.
- Simulations are not experiments!

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$$\vec{F} = q(\vec{v} \times \vec{B} + \vec{E}).$$

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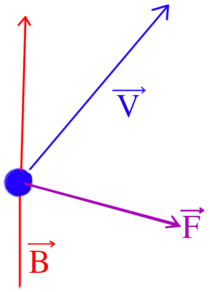
- Could use potentials $\phi(\vec{r}, t)$ $\vec{A}(\vec{r}, t)$ and Hamiltonian, or Lagrangian.
- Other systems would have other differential equations.

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



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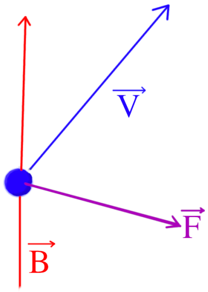

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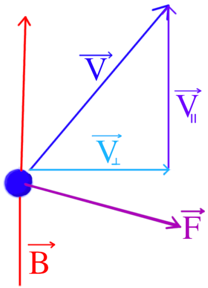

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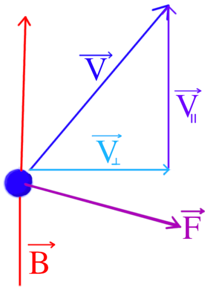

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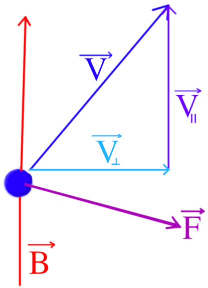
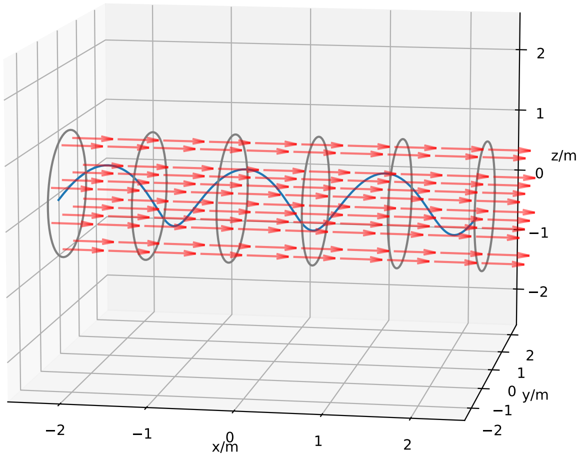
- Cyclotron radius and frequency:

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



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 $|v| \approx 3.195 \times 10^5\,\mathrm{m/s}$

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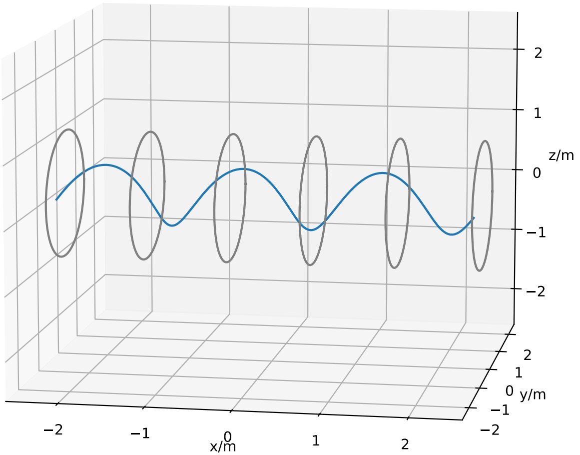

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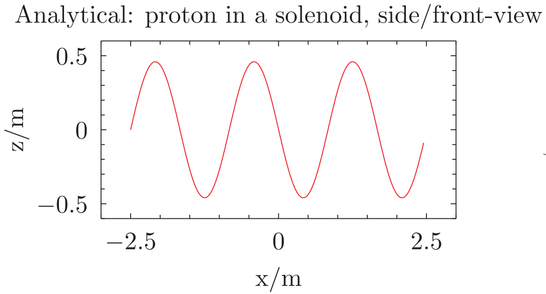

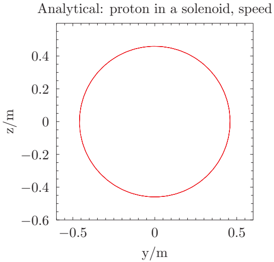

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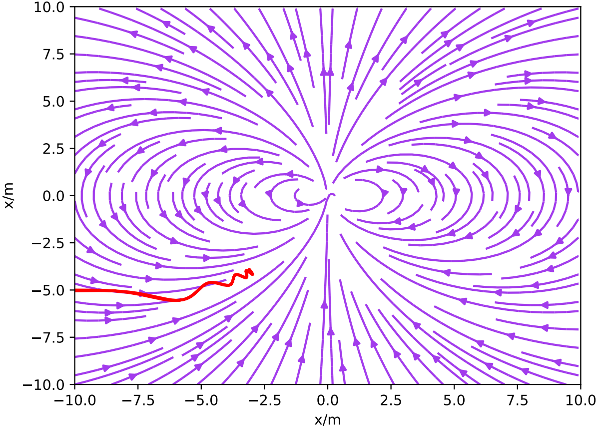

(Actually from my simulation)

Ordinary differential equation's.

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Solving differential equations.

- We know only $\mathbf{X}(t_i)$ and $t_i = t_0 + i\Delta t$ and $\mathbf{f}_{ode}$.

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

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- We want "better" (larger Δt (fewer steps, fewer calls), same error).
- Argument suggests we need $\dot{\mathbf{f}}_{ode}, \ddot{\mathbf{f}}_{ode}, \ldots$, we don't!

The Runge Kutta steppers.

- In general:

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

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- Cant guess anything ... unless $\mathbf{X}(t)$ is polynomial.
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Runge Kutta methods.

- More commonly written:

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\mathbf{K}_1 &= \mathbf{f}_{ode}(\mathbf{X}(t_i), t_i) \\
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\mathbf{K}_3 &= \mathbf{f}_{ode}(\mathbf{X}(t_i) + \Delta t a_{31}\mathbf{K}_1 + \Delta t a_{32}\mathbf{K}_2, t_i + c_3 \Delta t) \\
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The General explicit Runge Kutta method.

- Expressed in Butcher tableu:

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

Higher order methods.

- 2nd order (Heun's method):

$$\begin{aligned}
\mathbf{X}(t_{i+1}) - \mathbf{X}(t_i) &= \frac{\Delta t}{2}(\mathbf{K}_1 + \mathbf{K}_2), \\
\mathbf{K}_1 &= \mathbf{f}_{ode}(\mathbf{X}(t_i), t_i), \\
\mathbf{K}_2 &= \mathbf{f}_{ode}(\mathbf{X}(t_i) + \Delta t\mathbf{K}_1, t_i + \Delta t).
\end{aligned}$$

Higher order methods.

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

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

$$\mathbf{K}_1 = \mathbf{f}_{ode}(\mathbf{X}(t_i), t_i)$$

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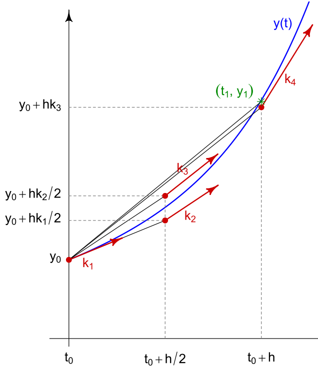

Does it work.

- Test, same proton in a solenoid use same starting conditions with:

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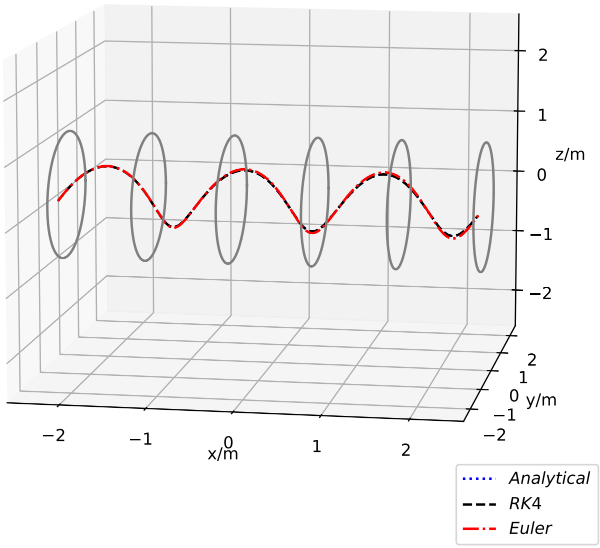
- Compare Analytic, Euler, Runge-Kutta 4. At different Δt_{equiv}.
- $\Delta t_{equiv} = 4\Delta t$ for 4th order method.
- Check error on $|\vec{v}|$, $R = \sqrt{y^2 + z^2}$.

At a glance, 3D view.

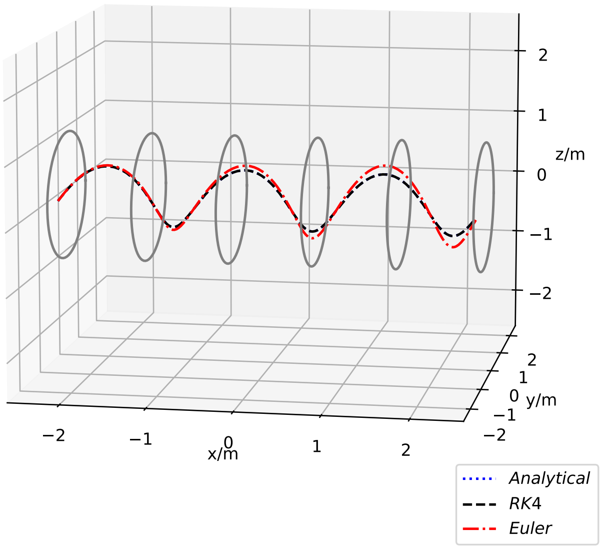
$\Delta t_{equiv} \approx 1/1000\, T_c$



3129 steps

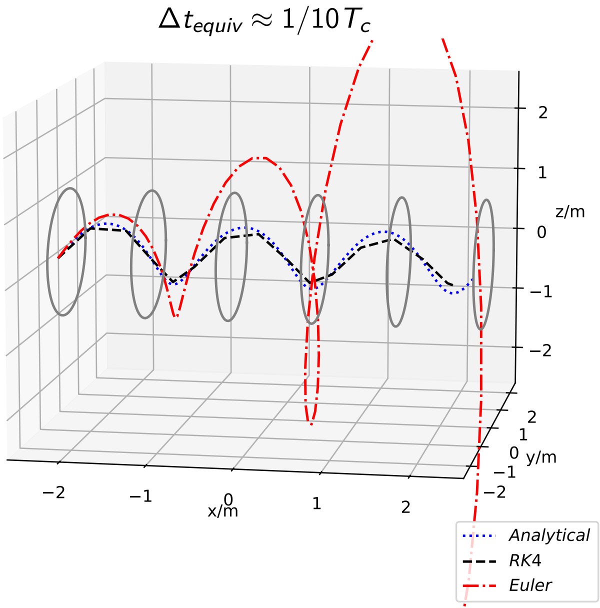
At a glance, 3D view.

$$\Delta t_{equiv} \approx 1/100\, T_c$$



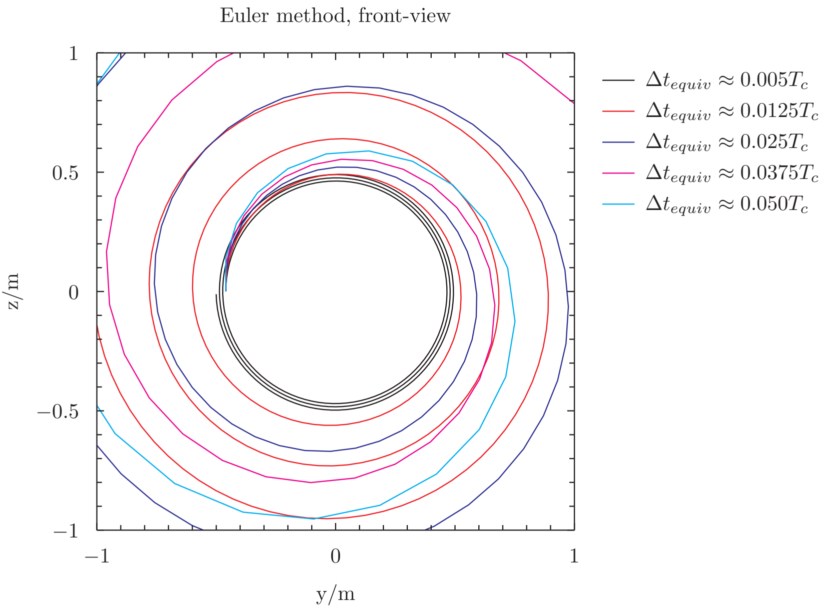
312 steps

At a glance, 3D view.



31 steps.

At a glance, front view, no border.



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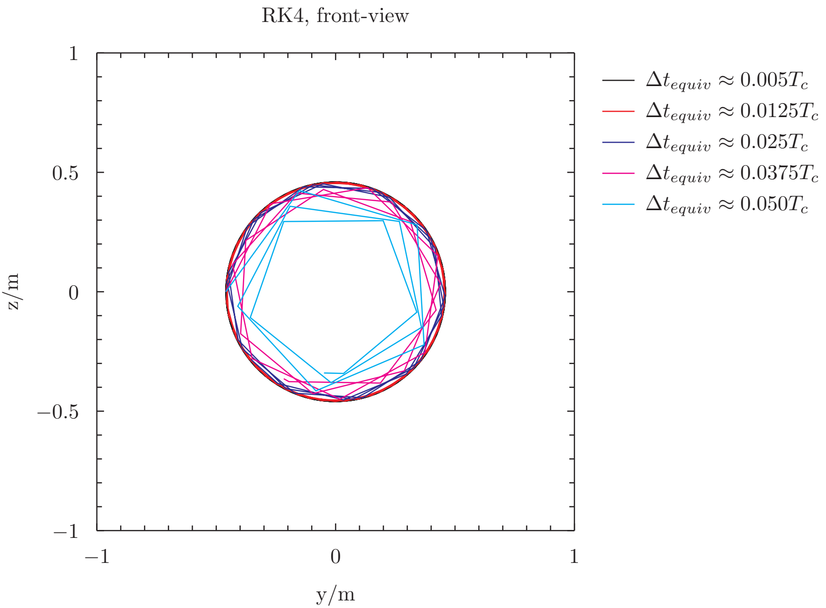
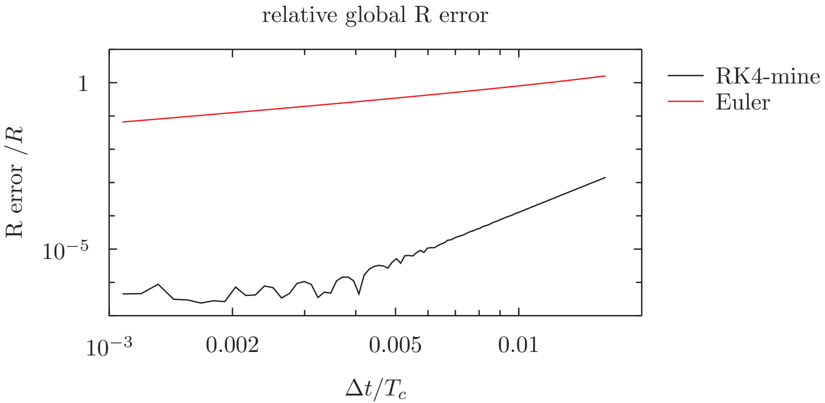


Error as function of Δt_{equiv}.



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- Usually don't know error.
- Hard to pick Δt , and may change:

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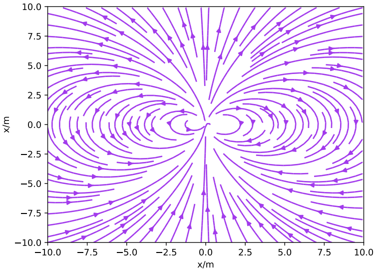
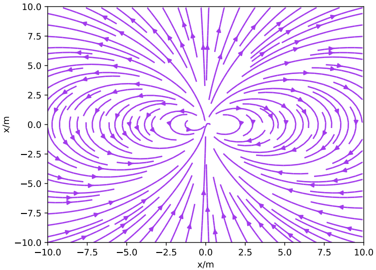
- Inhomogeneous or time dependent fields (here, a true dipole).



What is not to like?

- Usually don't know error.
- Hard to pick Δt , and may change:
- Inhomogeneous or time dependent fields (here, a true dipole).
- Let the computer pick Δt for error.



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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.

Runge-Kutta Dormand Prince 5 (4).

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

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

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

$$\mathbf{K}_j = \mathbf{f}_{ode}(\mathbf{X}(t_i) + \Delta t \sum_{k}^{j-1} a_{kj} \mathbf{K}_j, t_i + c_3 \Delta t).$$

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- 7 $\mathbf{K}_j$'s (actually 6 by clever re-usage) (First same as last principle).
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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):

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

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- Scale by step size $\frac{\Delta t_{old}}{T}$, "Fail safe" $\sqrt{\ldots}$.
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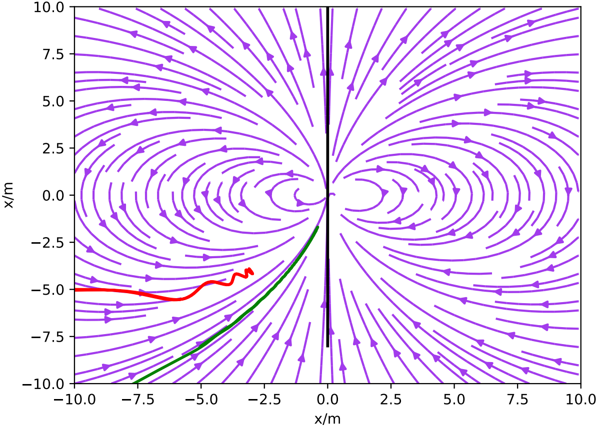
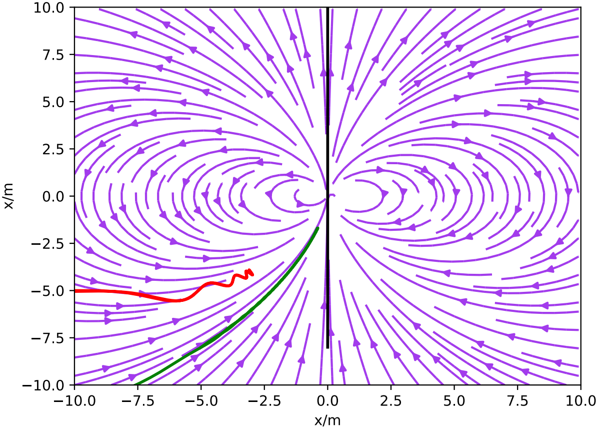
Does it work?



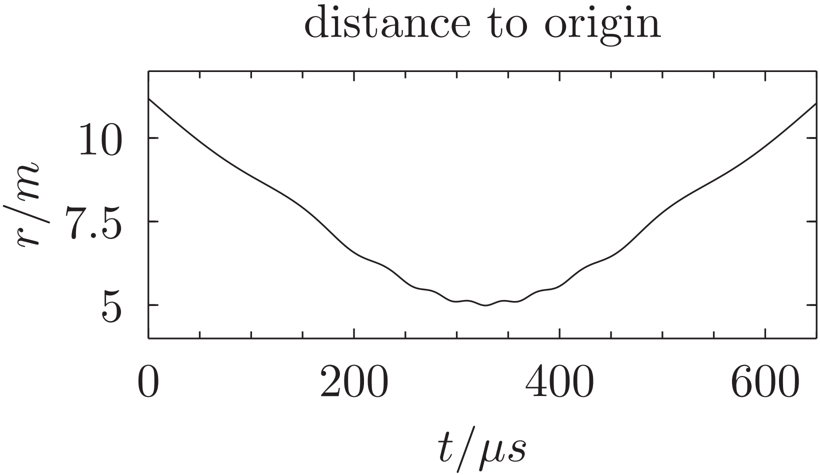
My version relative and absolute error 10^{-6}. 313 steps (+ 25 rejected).

Does it work?



Odeint library relative and absolute error 10^{-7}. 249 steps.

Does it work?



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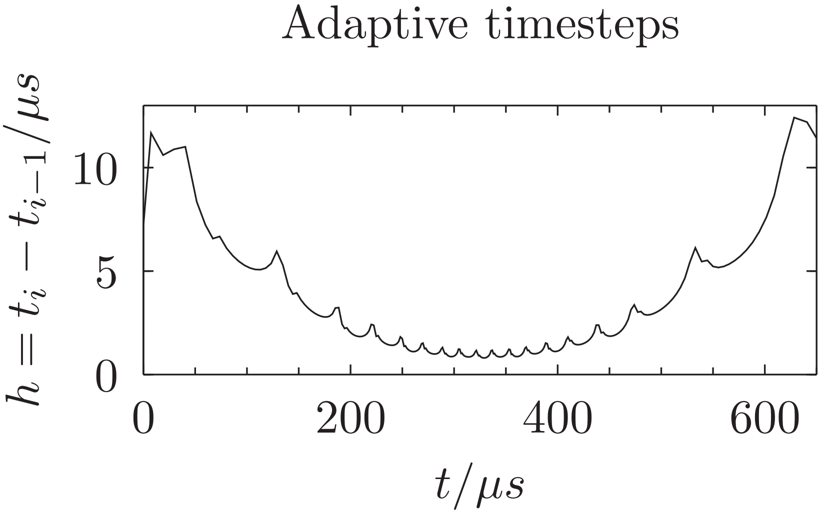

My version, adaptive step size.

Conclusion.

- Simulating particles in electric and magnetic fields.

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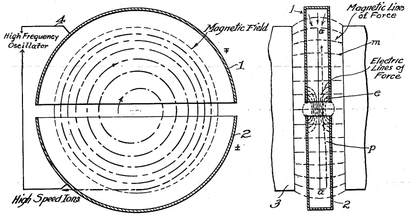
- Numerically solving ordinary differential equations.
- Can easily be generalized to other systems.

Example, cyclotron.

- Electric field accelerates, magnetic contains.



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

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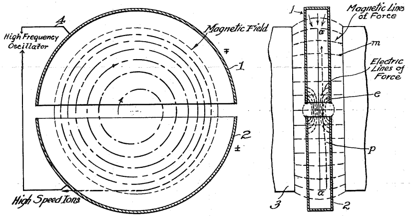

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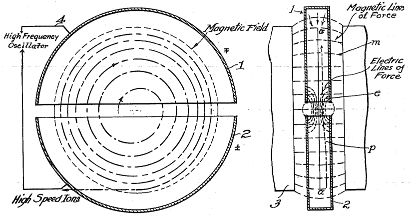

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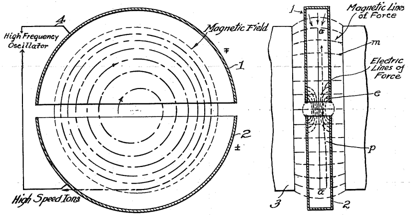
Example, cyclotron.

- 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.

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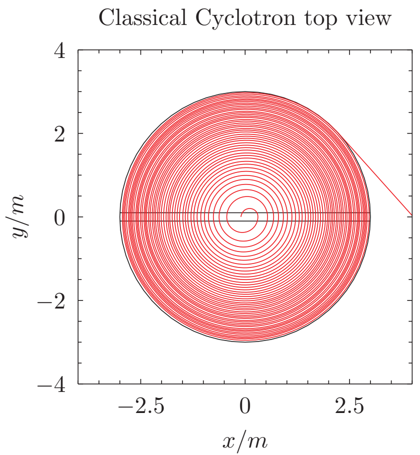

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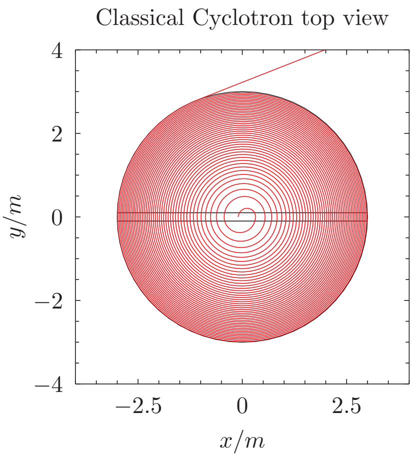

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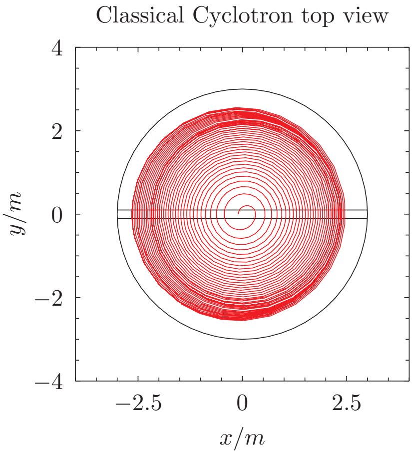

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