5. Numerics: particle motion and drift kinetics (discussion and correction: 7.1.2014)

A) Integrate numerically the equation of motion of a hydrogen ion in a magnetic field $B = (0, 0, B_z)$ with the initial velocity $v = (v_x, 0, v_z)$. ($B_z = 1T, v_x = v_z = 1 \cdot 10^7 m/s$) Use the explicit/implicit Euler and the Runge Kutta 4th order scheme. In order to diagnose the energy drift, calculate the total energy E at each time step and compare it to the initial energy. Normalise times to the cyclotron frequency $\Omega_c = eB/m$ and lengths to the the Larmor radius and integrate 100 cyclotron periods. Write out (ASCII) and plot the trajectory $(t, x, y, z, vx, vy, vz, E)$. Compare the limit on the time step!

B) Add an external E-field $E_{ext} = (E_{ext,x}, 0, 0)$ to the equations of motion ($E_{ext} = 10000V/m$) and calculate how much the particle drifted after 1000 cyclotron times.

C) Use the guiding centre (=drift kinetic) formulation to numerically solve the problem B! How much cheaper is this?

D)* Use a simple harmonic oszillator problem to demonstrate the energy conserving properties of the explicit, implicit and partitioned Euler method!

Solution

A/B) The normalised force equation is:

$$\frac{d\mathbf{v}}{v_0 dt} = \Omega_{c,h}(\frac{\mathbf{E}}{Bv_0} + \mathbf{v}/v_0 \times \mathbf{b})$$

In dimensionless units $E_{ext} = 0.001$.
Explizit Euler:
Calculate the new position and the new velocities via the force equation above and $dx = vdt$:

$$x_{n+1} = x_n + v_{x,n}dt; \quad y_{n+1} = y_n + v_{y,n}dt; \quad z_{n+1} = z_n + v_{z,n}dt;$$

$$v_{x,n+1} = (E_x + v_{y,n} \cdot b_z)dt + v_{x,n}$$

$$v_{y,n+1} = (E_y - v_{x.n} \cdot b_z) + v_{y,n}dt$$

$$v_{z,n+1} = E_z dt + v_{z,n}$$

b_Z is 1 by definition.

Implicit Euler:
One has to solve:

$$y_{n+1} = y_n + dtf(t_{n+1}, y_{n+1})$$

or writing down the forces:

$$\begin{pmatrix} x \\ y \\ z \\ v_x \\ v_y \\ v_z \end{pmatrix}_{n+1} = \begin{pmatrix} x \\ y \\ z \\ v_x \\ v_y \\ v_z \end{pmatrix}_n + dt \begin{pmatrix} v_x \\ v_y \\ v_z \\ v_y \\ -v_x \\ v_z \end{pmatrix}_{n+1}$$

Now we solve for the vector $(x, y, z, v_x, v_y, v_z)_{n+1}$ (matrix inversion) and obtain:

$$\begin{pmatrix} x \\ y \\ z \\ v_x \\ v_y \\ v_z \end{pmatrix}_{n+1} = \begin{pmatrix} 1 & 0 & 0 & Ndt & Ndt^2 & 0 \\ 0 & 1 & 0 & -Ndt^2 & Ndt & 0 \\ 0 & 0 & 1 & 0 & 0 & dt \\ 0 & 0 & 0 & N & Ndt & 0 \\ 0 & 0 & 0 & -Ndt & N & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \\ v_x \\ v_y \\ v_z \end{pmatrix}_n$$

with $N = \frac{1}{1+dt^2}$. This can be coded up as before (explicit). In more complicated cases, the solution for the $n+1$-th state vector has to be found numerically, e.g. Newton method.

Runge-Kutta 4th order:

$$y_{n+1} = y_n + \frac{1}{6}\left(k_1 + 2k_2 + 2k_3 + k_4\right) \qquad t_{n+1} = t_n + h$$

for $n = 0, 1, 2, 3, ...$, using:

$$k_1 = hf(t_n, y_n), \quad k_2 = hf(t_n+\frac{1}{2}h, \quad y_n+\frac{1}{2}k_1), \quad k_3 = hf(t_n+\frac{1}{2}h, y_n+\frac{1}{2}k_2), \quad k_4 = hf(t_n+h, y_n+k_3)$$

If we want the error in energy to be less than 2% after 100 gyrations, it is sufficient to use 2000 steps ($dt = 100 * 2\pi/2000$). The same condition on the final error requires 10 000 000 time steps for the Euler methods. If we take into accout that we need $2000 * 4$ calls for the force vector, RK4 is roughly 10000 times faster!
B) RK4: The particle drifts by one gyro-radius in the negative y-direction.

C) The equation of motion for the guiding-centre is:

$$v_y = -E_{ext}/B$$

which is a linear relationship with no explixit forces. Therefore, one step (any method) with $y = v_y dt$ gives the correct result.