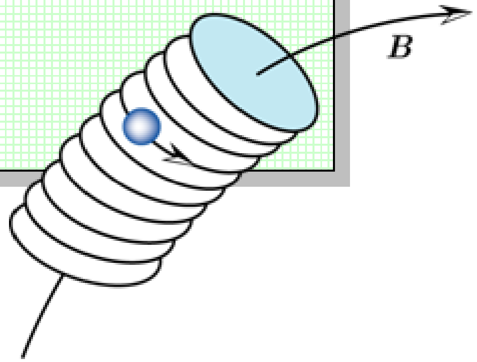
Variational Symplectic Integrator of the Guiding Center Motion



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DOE OFES Theory Seminar

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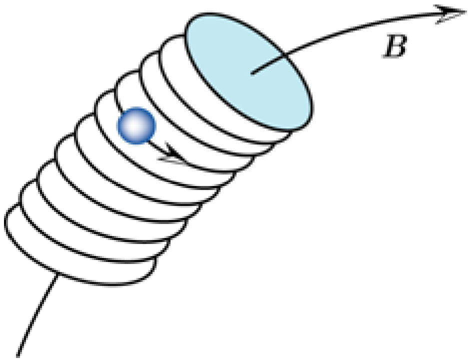
www.pppl.gov/~hongqin/Gyrokinetics.php

Gyrocenter dynamics and algorithms

$$\frac{d\boldsymbol{X}}{dt} = u\boldsymbol{b} + \frac{\mu\,\boldsymbol{\nabla} B\times\boldsymbol{b}}{B} + \frac{\boldsymbol{E}\times\boldsymbol{b}}{B} + \frac{u^2\boldsymbol{b}\times(\boldsymbol{b}\cdot\boldsymbol{\nabla} b)}{B}$$
$$\frac{du}{dt} = -\frac{\mu\boldsymbol{b}\cdot\boldsymbol{\nabla} B}{B} + \boldsymbol{b}\cdot\boldsymbol{E}$$

Carl Runge
(1856-1927)

Martin Kutta
(1867-1944)

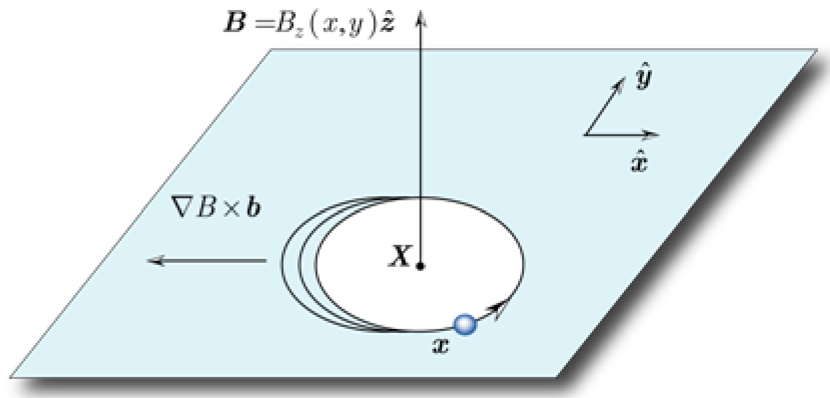


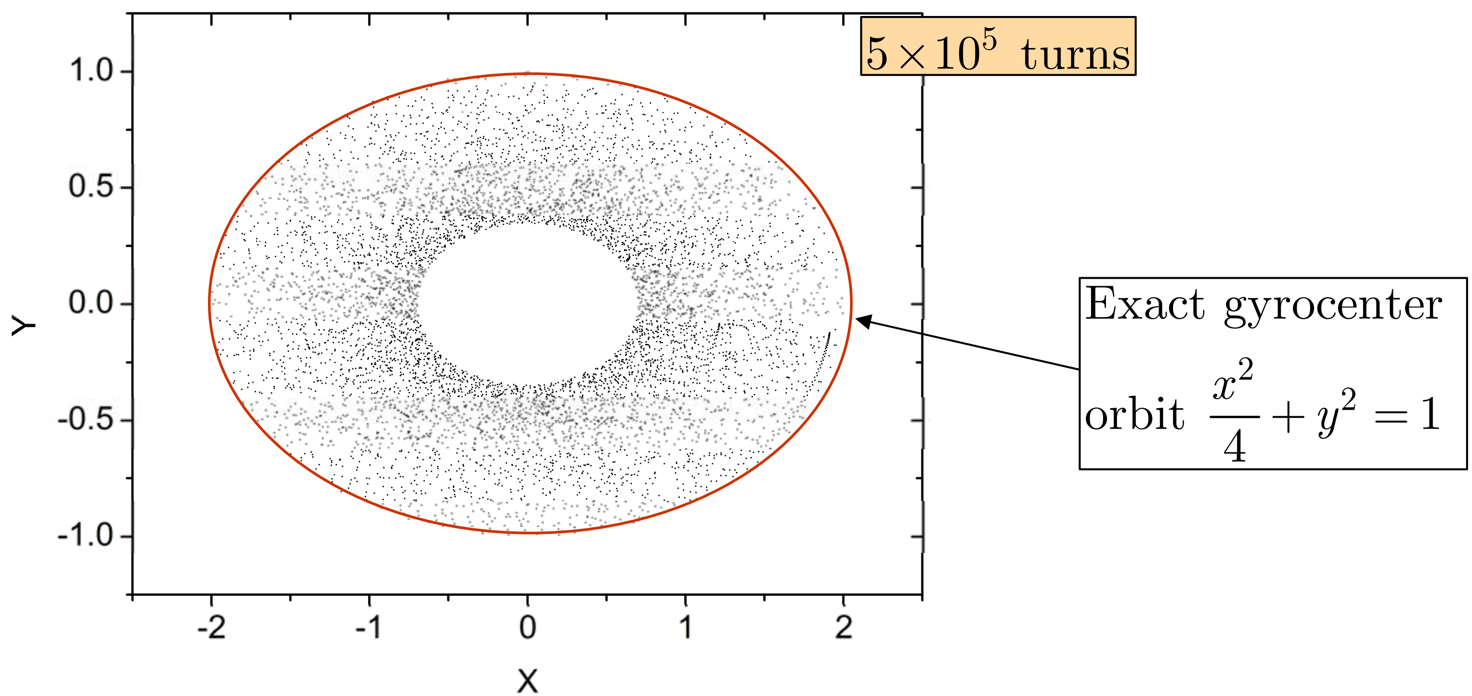
nth (4^{th}) order Runge-Kutta methods

- Long time non-conservation.
- Errors add up coherently.

Example – gradient drift

$$B_z(x,y) = 1 + 0.05\left(\frac{x^2}{4} + y^2\right)$$





Can we do better than RK4? -- symplectic integrator

Feng (1983)

Ruth (1984)

Conserves symplectic structure;
Bound energy error globally

Symplectic integrator ?

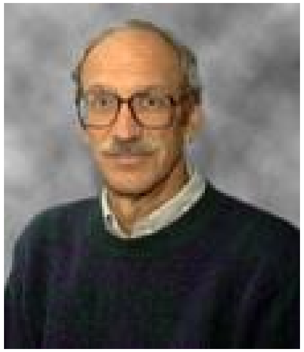
Requires canonical
Hamiltonian structure

$$\begin{pmatrix} \dot{q} \\ \dot{p} \end{pmatrix} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} H_{,q} \\ H_{,p} \end{pmatrix}$$

Application areas:

- Accelerator physics (everybody)
- Planetary dynamics (S. Tremaine)
- Nonlinear dynamics (everybody)

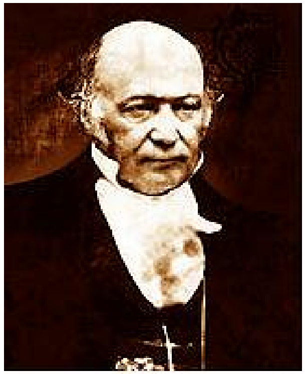
What is the canonical structure for gyrocenter dynamics?



R. White

Gyrocenter dynamics does not have a global canonical structure

Geometry of gyrocenter



Hamilton

Exterior derivative

Inner product

$$i_{\mathcal{T}} d\gamma = 0$$

Worldline

$$\gamma = \omega - \left(\tfrac{1}{2}u^2 + \mu B + \phi\right)dt$$
$$\omega = (A + u\boldsymbol{b}) \cdot d\boldsymbol{X}$$

Only has a non-canonical symplectic structure $\Omega \equiv d\omega$

Gyrocenter dynamics

R. Littlejohn (1983)

$$\boxed{i_\tau d\gamma = 0} \quad \approx \quad \boxed{\begin{aligned} A &= \int_0^{t_1} L\,dt \\ L &= (\boldsymbol{A} + u\boldsymbol{b})\cdot\dot{\boldsymbol{X}} - \left(\tfrac{1}{2}u^2 + \mu B + \phi\right) \end{aligned}}$$

$$\frac{d\boldsymbol{X}}{dt} = \frac{\boldsymbol{B}^\dagger}{B_\parallel^\dagger}\left(u + \frac{\mu}{2}\boldsymbol{b}\cdot\boldsymbol{\nabla}\times\boldsymbol{b}\right) - \frac{\boldsymbol{b}\times\boldsymbol{E}^\dagger}{B_\parallel^\dagger}$$

$$\frac{du}{dt} = \frac{\boldsymbol{B}^\dagger\cdot\boldsymbol{E}^\dagger}{B_\parallel^\dagger}$$

$$\boldsymbol{B}^\dagger \equiv \boldsymbol{\nabla}\times\boldsymbol{A}^\dagger, \quad \boldsymbol{A}^\dagger \equiv \boldsymbol{A} + u\boldsymbol{b}$$

$$B_\parallel^\dagger = \boldsymbol{B}^\dagger\cdot\boldsymbol{b}, \quad \boldsymbol{E}^\dagger \equiv \boldsymbol{E} - \mu\boldsymbol{\nabla}B$$

Darboux Theorem

Jean Gaston Darboux
(1842-1917)

Darboux Theorem (1882):

Every symplectic structure is **locally** canonical.

↓

Gyrocenter dynamics can be canonical **locally**.

↓

No symplectic integrator for gyrocenter?

Variational symplectic integrator

J. Marsden (2001)

$i_\tau d\gamma = 0$ $\approx$

$$A = \int_0^{t_1} L\,dt$$

$$L = (\boldsymbol{A} + u\boldsymbol{b}) \cdot \dot{\boldsymbol{X}} - \left(\tfrac{1}{2}u^2 + \mu B + \phi\right)$$

discretize on

$t = [0, h, 2h, ..., (N-1)h]$

$$A \approx A_d = \sum_{k=0}^{N-1} h L_d(k, k+1)$$

$$L_d(k, k+1) \equiv L_d(\boldsymbol{x}_k, u_k, \boldsymbol{x}_{k+1}, u_{k+1})$$

minimize w.r.t. $(\mathbf{x}_k, u_k)$

$$\frac{\partial}{\partial x_k^j}[L_d(k-1, k) + L_d(k, k+1)] = 0, (j = 1, 2, 3)$$

$$\frac{\partial}{\partial u_k}[L_d(k-1, k) + L_d(k, k+1)] = 0$$

discretized Euler-Lagrangian Eq.

$\left[(\mathbf{x}_{k-1}, u_{k-1}), (\mathbf{x}_k, u_k)\right]$

$\rightarrow (\mathbf{x}_{k+1}, u_{k+1})$

Conserved symplectic structure

$$\theta^{+}(k,k+1) \equiv \frac{\partial}{\partial \boldsymbol{x}_{k+1}} L_d(k,k+1) \cdot d\boldsymbol{x}_{k+1} + \frac{\partial}{\partial u_{k+1}} L_d(k,k+1) du_{k+1}$$

$$\theta^{-}(k,k+1) \equiv -\frac{\partial}{\partial \boldsymbol{x}_{k}} L_d(k,k+1) \cdot d\boldsymbol{x}_{k} - \frac{\partial}{\partial u_{k}} L_d(k,k+1) du_{k}$$

$$dL_d(k,k+1) = \theta^{+}(k,k+1) - \theta^{-}(k,k+1)$$

minimize w.r.t. $(\mathbf{x}_k, u_k)$

$$\Omega_d(k,k+1) \equiv d\theta^{+} = d\theta^{-}$$

$$dA_d = \theta^{+}(0,1) - \theta^{-}(N-1,N)$$

$$\Omega_d(0,1) = \Omega_d(N-1,N)$$

1^{st} order variational symplectic integrator

$$\boxed{L_d(k,k+1) \equiv \frac{\left[\boldsymbol{A}^{\dagger}(k+1)+\boldsymbol{A}^{\dagger}(k)\right]}{2}\cdot\frac{\left[\boldsymbol{x}_{k+1}-\boldsymbol{x}_k\right]}{h}-\frac{u_k u_{k+1}}{2}-\mu B(k)-\varphi(k)}$$

$$\downarrow$$

$$\frac{1}{2h}A^{\dagger i}_{,j}(k)\left(x^i_{k+1}-x^i_{k-1}\right)-\frac{1}{2h}\left[A^{\dagger j}(k+1)-A^{\dagger j}(k-1)\right]=\mu B_{,j}(k)+\varphi_{,j}(k)$$

$$\frac{1}{2h}b^i(k)\left(x^i_{k+1}-x^i_{k-1}\right)=\frac{u_{k+1}+u_{k-1}}{2}$$

$$\left[\left(\mathbf{x}_{k-1},u_{k-1}\right),\left(\mathbf{x}_k,u_k\right)\right]$$
$$\rightarrow\left(\mathbf{x}_{k+1},u_{k+1}\right)$$

implicit

Semi-explicit Newton's method

$$\Big[\, A^{\dagger j}(k+1) - A^{\dagger j}(k-1) \Big] \approx A^{\dagger j}_{,i}(k)\Big(x^i_{k+1} - x^i_{k-1} \Big) + b^j\,(\,k\,)\Big(\,u_{k+1} - u_{k-1}\,\Big)$$

$$\frac{1}{2h}\Big[\, A^{\dagger i}_{,j}(k) - A^{\dagger j}_{,i}(k) \Big]\Big(x^i_{k+1} - x^i_{k-1} \Big) - \frac{b^j\,(\,k\,)}{2h}\left[2u_{k-1} - \frac{b^i\,(\,k\,)}{h}\Big(x^i_{k+1} - x^i_{k-1} \Big) \right]$$

$$= \mu B_{,j}\,(\,k\,) + \varphi_{,j}\,(\,k\,)$$

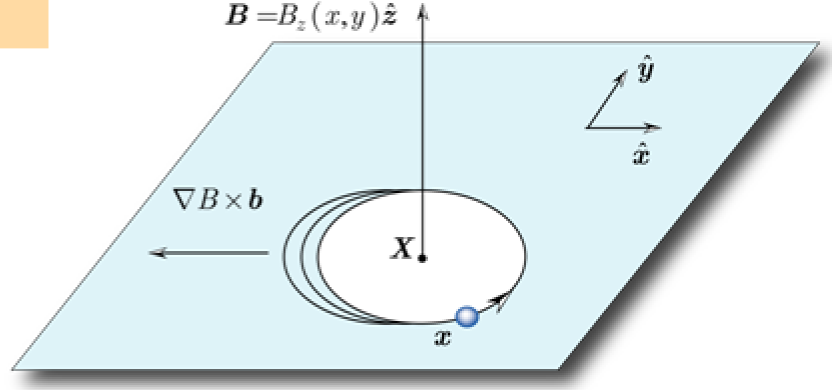
$$\frac{1}{2h} b^i\,(\,k\,)\Big(x^i_{k+1} - x^i_{k-1} \Big) = \frac{u_{k+1} + u_{k-1}}{2}$$

explict, initial guess for the Newton's method

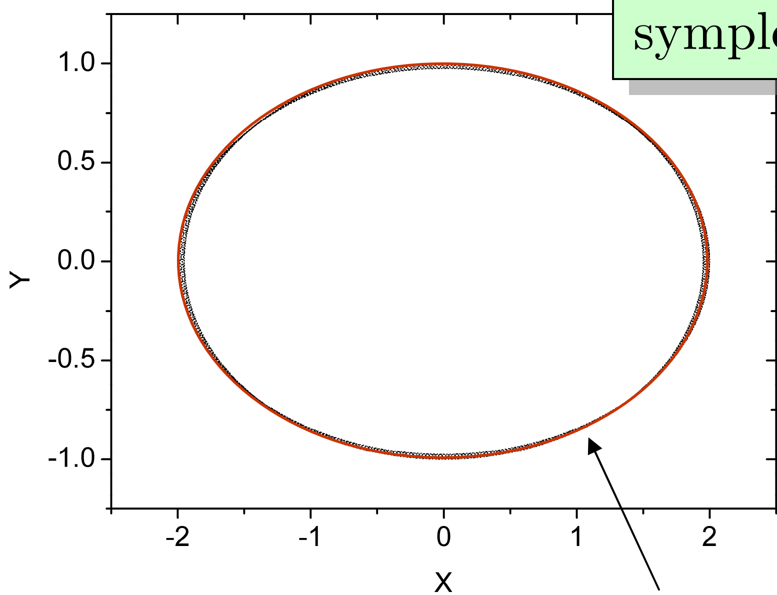
Example – gradient drift

$$\boldsymbol{B} = B(x,y)\hat{\boldsymbol{z}}$$

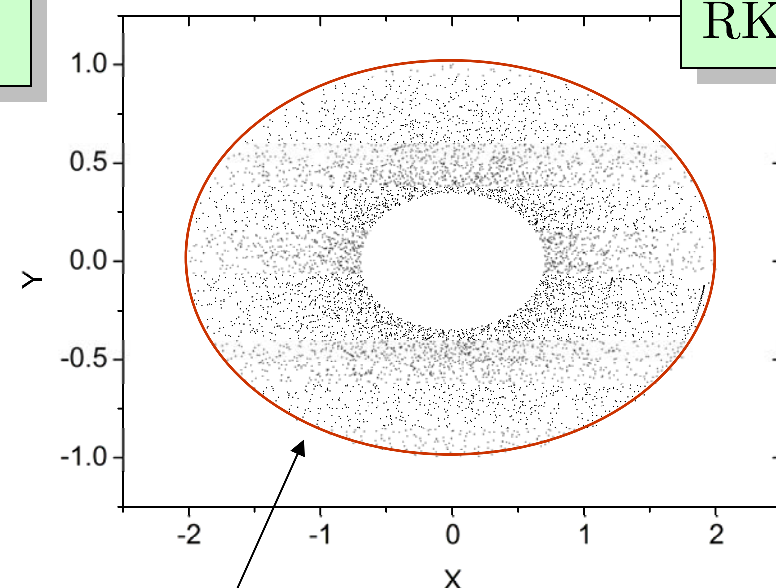
$$B(x,y) = 1 + 0.05\left(\frac{x^2}{4} + y^2\right)$$



Variational symplectic



RK4

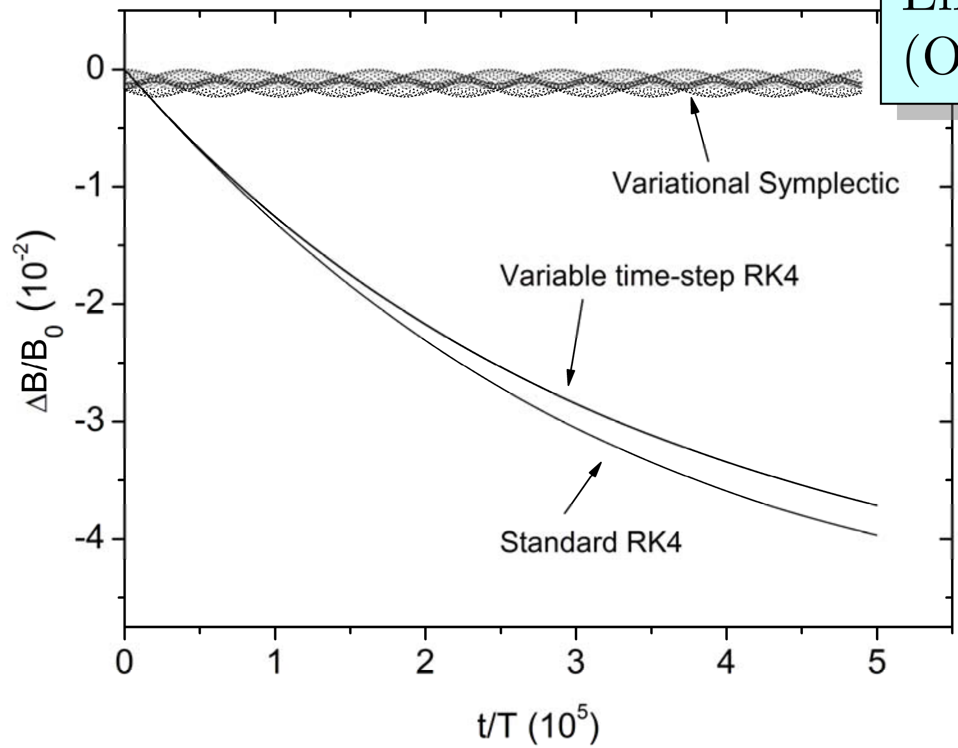


Exact gyrocenter orbit $\dfrac{x^2}{4} + y^2 = 1$

5×10^5 turns

Variational symplectic globally bounds energy error

Energy error
(Orbit deviation)



Conclusions

Physics is geometry. So is algorithm.

Symplectic bounds error **globally**, others do not.