Variational Symplectic Integrator of the Guiding Center Motion

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US-Japan Workshop on Progress of Multi-Scale Simulation Models
Nov. 20, 2008, Dallas, USA

www.pppl.gov/~hongqin/Gyrokinetics.php
How to Calculate the Guiding Center Motion?

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You Don’t How to Calculate the Guiding Center Motion!

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Gyrocenter dynamics and algorithms

\[
\begin{align*}
\frac{dX}{dt} &= ub + \frac{\mu \nabla B \times b}{B} + \frac{E \times b}{B} + \frac{u^2 b \times (b \cdot \nabla b)}{B} \\
\frac{du}{dt} &= -\frac{\mu b \cdot \nabla b}{B} + b \cdot E
\end{align*}
\]

nth (4th) order Runge-Kutta methods

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

Carl Runge (1856-1927)

Martin Kutta (1867-1944)
Example – banana orbit go bananas

\[ \Delta t = \frac{T}{100} \]

Numerical result by RK4

Exact banana orbit

ITER: \( T_{\text{burn}} \approx 3 \times 10^6 T_{\text{banana}} \)
EAST: \( T_{\text{run}} \approx 10 \times 10^6 T_{\text{banana}} \)

H. Qin and X. Guan, PRL 100, 035006 (2008).
X. Xiao and S. Wang, submitted to PoP.
Example – passing orbit go bananas too

\[ \Delta t = T / 33 \]

Numerical result by RK4

Numerical banana

Exact passing orbit

ITER: \( T_{\text{burn}} \sim 3 \times 10^6 T_{\text{banana}} \)

EAST: \( T_{\text{run}} \sim 10 \times 10^6 T_{\text{banana}} \)
60 million years ago …..
Can we do better than RK4? -- symplectic integrator


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)
- Plasma physics (J. Cary 89')
What is the canonical structure for gyrocenter dynamics?

R. White
Gyrocenter dynamics does not have a global canonical structure

Geometry of gyrocenter

Inner product

Worldline

Exterior derivative

\[ i_{\tau} d\gamma = 0 \]

\[ \gamma = \omega - \left( \frac{1}{2}u^2 + \mu B + \phi \right) dt \]

\[ \omega = (A + ub) \cdot dX \]

Only has a non-canonical symplectic structure \( \Omega \equiv d\omega \)
**Gyrocenter dynamics**

\( \gamma = (A + ub) \cdot dX + \mu d\theta - \left( \frac{1}{2}u^2 + \mu B + \phi \right) dt \)

\( i_r d\gamma = 0 \)

\( L = (A + ub) \cdot \dot{X} + \mu \dot{\theta} - \left( \frac{1}{2}u^2 + \mu B + \phi \right) \)

\(~\)

**E-L Eq.**

\[ \frac{dX}{dt} = \frac{B^\dagger}{B_{\parallel}} (u + \frac{\mu}{2} b \cdot \nabla \times b) - \frac{b \times E^\dagger}{B^\dagger} \]

\[ \frac{du}{dt} = \frac{B^\dagger \cdot E^\dagger}{B^\dagger} \]

\[ \frac{d\theta}{dt} = B, \quad \frac{d\mu}{dt} = 0 \]

\[ B^\dagger \equiv \nabla \times A^\dagger, \quad A^\dagger \equiv A + ub \]

\[ B^\parallel = B^\dagger \cdot b, \quad E^\dagger \equiv E - \mu \nabla B \]
Darboux Theorem (1882):
Every symplectic structure is \textit{locally} canonical.

Gyrocenter dynamics can be canonical \textit{locally}.

No symplectic integrator for gyrocenter?
Variational symplectic integrator

\[ i \cdot d \gamma = 0 \approx A = \int_0^{t_1} L dt \]

\[ L = (A + u b) \cdot \dot{X} - \left( \frac{1}{2} u^2 + \mu B + \phi \right) \]

Discretize on

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

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

\[ L_d(k, k+1) \equiv L_d(x_k, x_{k+1}, u_k, u_{k+1}) \]

Minimize w.r.t. \( (x_k, u_k) \)

\[ \frac{\partial}{\partial x^j_k} \left[ L_d(k-1, k) + L_d(k, k+1) \right] = 0, (j = 1, 2, 3) \]

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

Discretized Euler-Lagrangian Eq.

\[ \left[ (x_{k-1}, u_{k-1}), (x_k, u_k) \right] \rightarrow (x_{k+1}, u_{k+1}) \]

J. Marsden (2001)
**Conserved symplectic structure**

\[
\theta^+(k,k+1) \equiv \frac{\partial}{\partial x_{k+1}} L_d(k,k+1) \cdot dx_{k+1} + \frac{\partial}{\partial u_{k+1}} L_d(k,k+1) du_{k+1}
\]

\[
\theta^-(k,k+1) \equiv -\frac{\partial}{\partial x_k} L_d(k,k+1) \cdot dx_k - \frac{\partial}{\partial u_k} L_d(k,k+1) du_k
\]

\[
dL_d(k,k+1) = \theta^+(k,k+1) - \theta^-(k,k+1)
\]

\[
\Omega_d(k,k+1) \equiv d\theta^+ = d\theta^-
\]

minimize w.r.t. \((x_k, u_k)\)

\[
dA_d = \theta^+(0,1) - \theta^-(N-1,N)
\]

\[
\Omega_d(0,1) = \Omega_d(N-1,N)
\]
1st order variational symplectic integrator

\[ L_d(k, k+1) \equiv \frac{[A^\dagger(k+1) + A^\dagger(k)]}{2} \cdot \frac{[x_{k+1} - x_k]}{h} - \frac{u_k u_{k+1}}{2} - \mu B(k) - \varphi(k) \]

\[ \frac{1}{2h} A_{ij}^\dagger(k) (x_{k+1}^i - x_{k-1}^i) - \frac{1}{2h} [A^\dagger j(k+1) - A^\dagger j(k-1)] = \mu B_{j}(k) + \varphi_{j}(k) \]

\[ \frac{1}{2h} b^i(k) (x_{k+1}^i - x_{k-1}^i) = \frac{u_{k+1} + u_{k-1}}{2} \]

\[ \left[ (x_{k-1}, u_{k-1}), (x_k, u_k) \right] \rightarrow \left( x_{k+1}, u_{k+1} \right) \]

H. Qin and X. Guan, PRL 100, 035006 (2008).
Semi-explicit Newton’s method

\[
\left[ A^{t,j}(k+1) - A^{t,j}(k-1) \right] \approx A^{t,j}(k)\left( x^i_{k+1} - x^i_{k-1} \right) + b^j(k)(u_{k+1} - u_{k-1})
\]

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

\[
= \mu B_{i,j}(k) + \varphi_{i,j}(k)
\]

\[
\frac{1}{2h}b^i(k)(x^i_{k+1} - x^i_{k-1}) = \frac{u_{k+1} + u_{k-1}}{2}
\]

explicit, initial guess for the Newton’s method
Variational symplectic integrator, banana orbits

\[ \Delta t = \frac{T}{100} \]

\[ \Delta t = \frac{T}{33} \]

Transport reduction by integration errors

\[ 9 \times 10^4 \text{ turns} \]

H. Qin and X. Guan, PRL 100, 035006 (2008).
Variational symplectic integrator bounds energy error globally
Variational symplectic integrator, no numerical banana

\[ \Delta t = T / 100 \]

\[ \Delta t = T / 33 \]

Transport reduction by integration errors

Numerical banana

9 \times 10^4 \text{ turns}
Variational symplectic integrator bounds energy error globally

Parabolic growth of energy error

$0.03 \ T_{\text{burn}}$
How to calculate guiding center motion?

Physics is geometry. So is algorithm.

Symplectic bounds error **globally**, others do not.
Multi-scale dynamics needs global algorithms

“Can Billy come out and compete in the global economy?”
How about collisions?

Frequent heartburns do not cure stomach cancer.

Collisions do not remove the energy errors of RK4.

Global energy errors of RK4 are numerical noises to collisional physics.
How about implicitness?

Implicit root search does destroy the symplectic structure.

Approximate solution is much better than no solution.
Example – gradient drift

\[ B = B(x, y) \hat{z} \]

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

\[ \nabla B \times b \]

\[ \begin{array}{c}
\dot{x} = B_y(x, y) \\
\dot{y} = B_x(x, y) \\
\dot{z} = -B_x(x, y) y + B_y(x, y) x
\end{array} \]

\[ \text{Exact gyrocenter orbit } \frac{x^2}{4} + y^2 = 1 \]

5 × 10^5 turns

Variational symplectic

RK4
Example 1 – gradient drift

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

Numerical result by RK4

Exact gyrocenter orbit \( \frac{x^2}{4} + y^2 = 1 \)

5 × 10^5 turns
Variational symplectic globally bounds energy error

Parabolic growth of energy error

Energy error (Orbit deviation)