Slow Manifold Preserving Integration of the Pauli Particle

Integrating Guiding Centre Dynamics with Canonical Variational Integrators

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Based on Jianyuan Xiao[3], Hong Qin[4], *Slow manifolds of classical Pauli particle enable structure-preserving geometric algorithms for guiding center dynamics*, June 2020, arXiv:2006.03818.

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Motivation

- Pauli's Hamiltonian for electrons (charge -1)

$$H_{\text{Pauli}} = \frac{1}{2}(p - A(x))^2 - \frac{\hbar}{2}\sigma \cdot B(x) + \phi(x)$$

- $\sigma = (\sigma_x, \sigma_y, \sigma_z)$ is the vector of 2×2 Pauli matrices used to describe the intrinsic magnetic moment of electrons observed in the Stern-Gerlach experiment
- in most regimes of classical physics, the intrinsic magnetic moment of charged particles is negligible
- surprisingly, the introduction of a formal magnetic moment term $\mu\,|B|$ in the Hamiltonian for classical particles allows for the construction of structure-preserving integrators for guiding centre dynamics

$$H_{\text{cpp}} = \frac{1}{2}(p - A(x))^2 + \mu\,|B(x)| + \phi(x)$$

- the corresponding Lagrangian reads

$$L_{\text{cpp}} = \frac{1}{2}\,|\dot{x}|^2 + A(x) \cdot \dot{x} - \mu\,|B(x)| - \phi(x)$$

Lagrangians

- charged particle

$$L_{\mathsf{cp}} = \frac{1}{2}|\dot{x}|^2 + A(x)\cdot\dot{x} - \phi(x)$$

- classical Pauli particle

$$L_{\mathsf{cpp}} = \frac{1}{2}|\dot{x}|^2 + A(x)\cdot\dot{x} - \mu\,|B(x)| - \phi(x)$$

- guiding centre

$$L_{\mathsf{gc}} = (A(x) + ub(x))\cdot\dot{x} - \frac{1}{2}u^2 - \mu\,|B(x)| - \phi(x), \qquad u = \dot{x}\cdot b(x)$$

- Pauli guiding centre

$$L_{\mathsf{cpp\text{-}gc}} = (A(x) + ub(x))\cdot\dot{x} - \frac{1}{2}u^2 - \mu'\,|B(x)| - \mu\,|B(x)| - \phi(x), \qquad \mu' = \frac{|\dot{x}\times b(x)|^2}{2\,|B(x)|}$$

Slow Manifolds

- the solutions of classical Pauli particles with (almost) no gyration, $\dot{x} \times b(x) \approx 0$, can be viewed as slow manifolds of the classical Pauli dynamics
- if $\mu = \left|\dot{x} \times b(x)\right|^2 / 2\left|B(x)\right| \approx 0$, the location of the classical Pauli particle should be nearly identical to its guiding centre since the gyro radius is close to zero
- from this perspective, guiding centre dynamics can be identified with the slow manifolds of the classical Pauli particle
- see also Joshua W. Burby, *Guiding center dynamics as motion on a formal slow manifold in loop space*, Journal of Mathematical Physics 61, 012703, 2020 (doi:10.1063/1.5119801)

Symplectic Runge–Kutta Integrator

- symplectic partitioned Runge–Kutta methods

$$\dot{Q}_{n,i} = \frac{\partial H}{\partial p}(Q_{n,i}, P_{n,i}), \qquad \dot{P}_{n,i} = -\frac{\partial H}{\partial q}(Q_{n,i}, P_{n,i}),$$

$$Q_{n,i} = q_n + h \sum_{j=1}^{s} a_{ij} \, \dot{Q}_{n,j}, \qquad P_{n,i} = p_n + h \sum_{j=1}^{s} \bar{a}_{ij} \, \dot{P}_{n,j},$$

$$q_{n+1} = q_n + h \sum_{i=1}^{s} b_i \, \dot{Q}_{n,i}, \qquad p_{n+1} = p_n + h \sum_{i=1}^{s} \bar{b}_i \, \dot{P}_{n,i},$$

with coefficients satisfying the symplecticity conditions

$$b_i \bar{a}_{ij} + \bar{b}_j a_{ji} = b_i \bar{b}_j \qquad \text{and} \qquad \bar{b}_i = b_i$$

Variational Runge–Kutta Integrator

- discrete action principle

$$\mathcal{A}_d = \sum_{n=0}^{N-1} \left(h \sum_{i=1}^{s} b_i \left[L\big(Q_{n,i}, \dot{Q}_{n,i} \big) + \dot{P}_{n,i} \cdot \left(Q_{n,i} - q_n - h \sum_{j=1}^{s} a_{ij} \, \dot{Q}_{n,j} \right) \right] - p_{n+1} \cdot \left(q_{n+1} - q_n - h \sum_{i=1}^{s} b_i \, \dot{Q}_{n,i} \right) \right)$$

- variational partitioned Runge–Kutta methods

$$P_{n,i} = \frac{\partial L}{\partial \dot{q}} (Q_{n,i}, \dot{Q}_{n,i}), \qquad \dot{P}_{n,i} = \frac{\partial L}{\partial q} (Q_{n,i}, \dot{Q}_{n,i}),$$

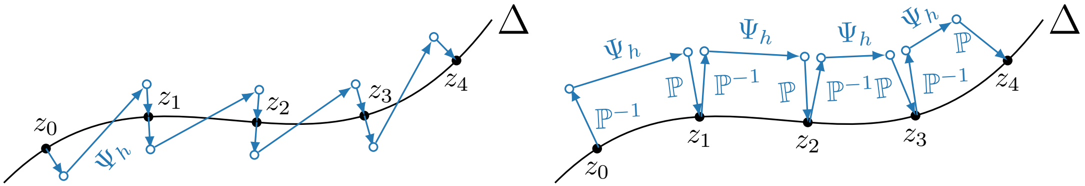
$$Q_{n,i} = q_n + h \sum_{j=1}^{s} a_{ij} \, \dot{Q}_{n,j}, \qquad P_{n,i} = p_n + h \sum_{j=1}^{s} \bar{a}_{ij} \, \dot{P}_{n,j},$$

$$q_{n+1} = q_n + h \sum_{i=1}^{s} b_i \, \dot{Q}_{n,i}, \qquad p_{n+1} = p_n + h \sum_{i=1}^{s} \bar{b}_i \, \dot{P}_{n,i},$$

with coefficients satisfying the symplecticity conditions

$$b_i \bar{a}_{ij} + \bar{b}_j a_{ji} = b_i \bar{b}_j \qquad \text{and} \qquad \bar{b}_i = b_i$$

Variational Integrator with Projection



- symmetric projection $z = (q, p)$

$$
\begin{aligned}
\tilde{z}_n &= z_n + h\,\Omega^{-1}\nabla\phi^T(z_n)\,\lambda_{n+1/2}, \\
\tilde{z}_{n+1} &= \Psi_h(\tilde{z}_n), \\
z_{n+1} &= \tilde{z}_{n+1} + h\,R(\infty)\,\Omega^{-1}\nabla\phi^T(z_{n+1})\lambda_{n+1/2}, \\
0 &= \phi(z_{n+1})
\end{aligned}
$$

- $\phi(q, p) = p - \vartheta(q)$ is the Dirac constraint of the degenerate Lagrangian $L(q, \dot{q}) = \vartheta(q) \cdot \dot{q} - H(q)$
- Ψ_h is a variational partitioned Runge–Kutta method with stability function $R(\infty)$

Initial Conditions

- magnetic potential in (R, Z, ϕ) coordinates

$$A(R, Z, \phi) = \frac{B_0 R_0}{2} \frac{Z}{R} \, \mathrm{d}R - \frac{B_0 R_0}{2} \ln\left(\frac{R}{R_0}\right) \mathrm{d}Z - \frac{B_0 r^2}{2 q_0} \, \mathrm{d}\phi, \qquad B_0 = 1, \; R_0 = 1, \; q = 2$$

- charged particle

$$x_0 = \left[1.05, \, 0, \, 0\right], \qquad v_0 = \left[2.1 \times 10^{-3}, \, 0, \, -4.3 \times 10^{-4}\right]$$

- Pauli particle

$$x_0 = \left[1.05, \, 0, \, 0\right], \qquad v_\parallel = v_0 \cdot b(x_0) \, b(x_0) \approx \left[0, \, -1.128 \times 10^{-5}, \, -4.297 \times 10^{-4}\right],$$

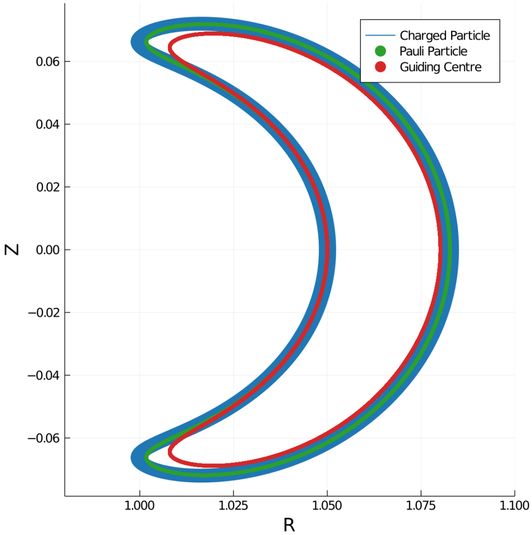
$$\mu = \frac{|v_\perp|^2}{2 \, |B(x_0)|} \approx 2.315 \times 10^{-6}, \qquad v_\perp = v_0 - v_\parallel \approx \left[2.1 \times 10^{-3}, \, -1.128 \times 10^{-5}, \, -2.699 \times 10^{-7}\right]$$

- guiding centre

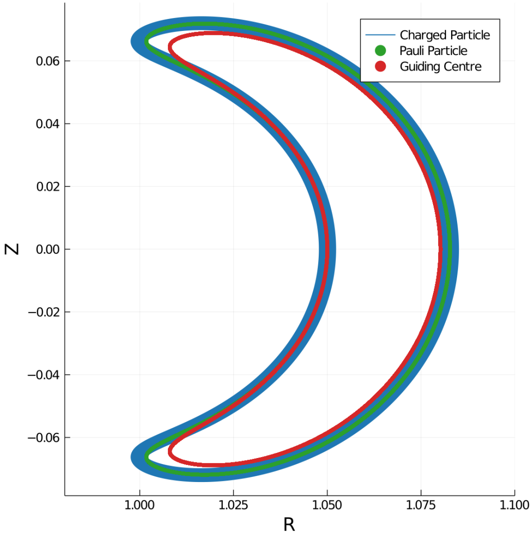
$$q_0 = [x_0, u_0], \qquad u_0 = \left|v_\parallel\right| \approx 4.299 \times 10^{-4}, \qquad \mu \approx 2.315 \times 10^{-6}$$

Numerical Experiments: Small Time Steps ($\Delta t = 0.1$)

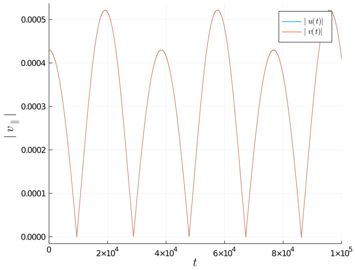
Symplectic Midpoint

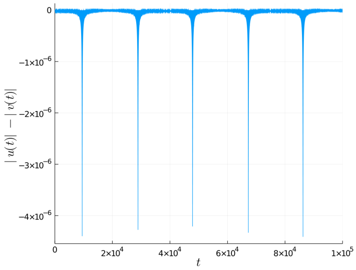


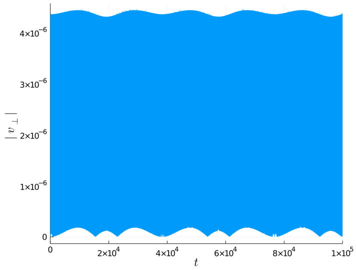
Variational Midpoint



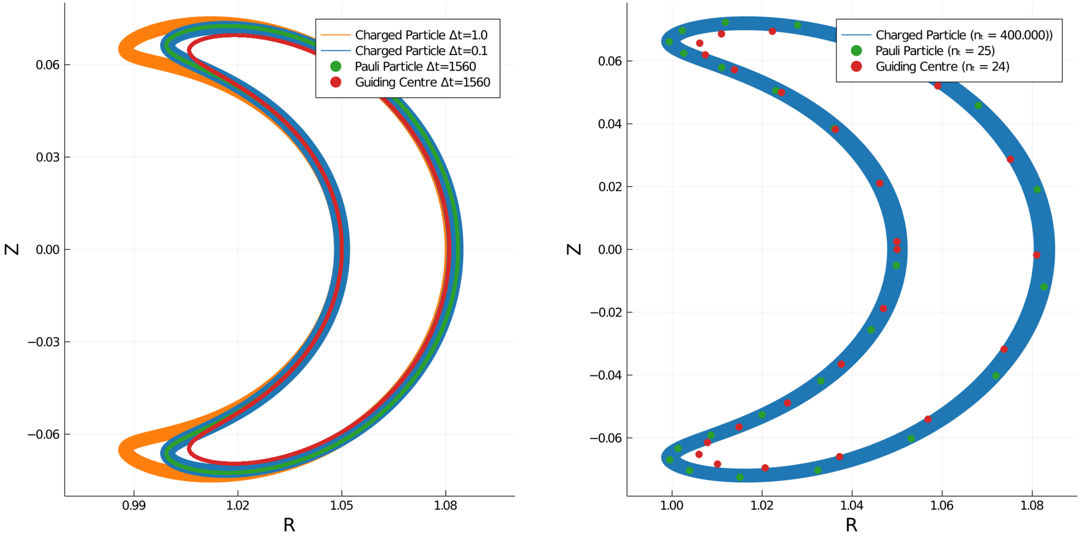
Numerical Experiments: Parallel and Perpendicular Velocity



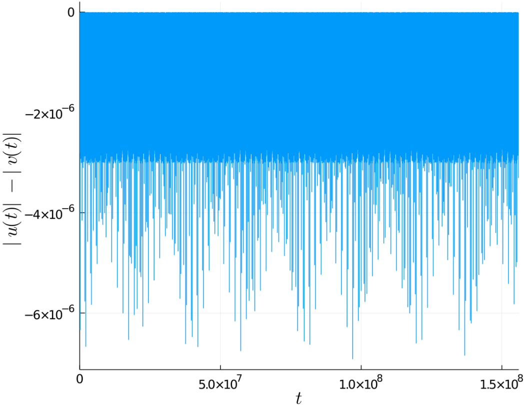


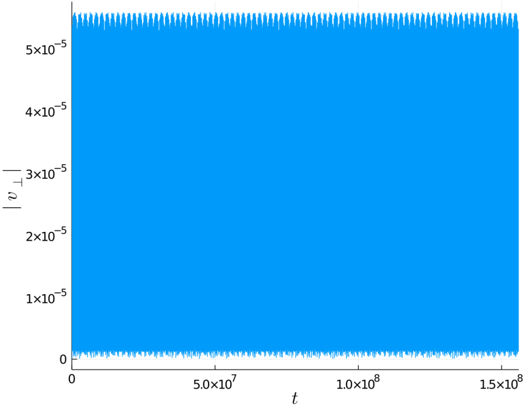


Numerical Experiments: Variational Integrators with Large Time Steps



Numerical Experiments: Parallel and Perpendicular Velocity





Particle-in-cell Action Principle

- action

$$\mathcal{A} = \sum_a \int w_a \, L_a\big(q_a(t), \dot{q}_a(t)\big) \, dt + \int L_f\big(\phi, A\big) \, dt$$

- single-particle Lagrangian L_a

$$L_a = \Big(m_a \dot{x}_a(t) + e_a A_{\text{ext}}(x_a(t)) + e_a A(t, x_a(t)) \Big) \cdot \dot{x}_a(t) \\ - \Big(\tfrac{1}{2} \, m_a \, |\dot{x}_a(t)|^2 + e_a \phi(t, x_a(t)) + \mu_a \underbrace{|B_{\text{ext}}(x_a(t)) + B(t, x_a(t))|}_{\approx b_{\text{ext}}(x_a(t)) \cdot (B(t, x_a(t)) + B_{\text{ext}}(x_a(t)))\ ?} \Big)$$

- field Lagrangian L_f

$$L_f = \frac{1}{2} \int \left[\varepsilon_0 \left| \nabla\phi(t, x) - \frac{\partial A}{\partial t}(t, x) \right|^2 - \frac{1}{\mu_0} \left| \nabla \times A(t, x) \right|^2 \right] dx$$

Higher-order Drift Kinetic Action Principle

- drift-kinetic particle Lagrangian

$$L_a(x_a, u_a, \dot{x}_a, \dot{u}_a) = \Big(m_a u_a b(x_a) + e_a A_{\mathsf{ext}}(x_a) + e_a A(t, x_a) \Big) \cdot \dot{x}_a - H(x_a,\, u_a)$$

with higher-order terms in the Hamiltonian $H = K_0 + K_1 + K_2$

$$K_0(x,u) = \frac{1}{2} m u^2 + \mu \left| B_{\mathsf{ext}}(x) \right|,$$

$$K_1(x,u) = \mu\, b_{\mathsf{ext}}(x) \cdot B(t,x),$$

$$K_2(x,u) = \left(\mu \left| B_{\mathsf{ext}}(x) \right| - m u^2 \right) \frac{1}{2} \frac{\left| B_\perp(t,x) \right|^2}{\left| B_{\mathsf{ext}}(x) \right|} - \frac{m}{2} \frac{\left| E\perp(t,x) \right|^2}{\left| B_{\mathsf{ext}}(x) \right|} + m u \frac{E(t,x) \times b_{\mathsf{ext}}(x) \cdot B(t,x)}{\left| B_{\mathsf{ext}}(x) \right|^2}$$

- heuristic idea: replace $ub(t,x)$ with $\dot{x}$ assuming $\dot{x}_0 = u_0 b(0, x_0)$

$$L_a(x_a, u_a, \dot{x}_a, \dot{u}_a) = \Big(m_a \dot{x}_a + e_a A_{\mathsf{ext}}(x_a) + e_a A(t, x_a) \Big) \cdot \dot{x}_a - H(x_a,\, u_a)$$

Quasi-neutrality

- take the $\varepsilon \to 0$ limit in the field Lagrangian L_f

$$L_f = -\frac{1}{2\mu_0} \int \left| \nabla \times A(t,x) \right|^2 dx$$

- instead of the Ampere and Poisson equations, we thus obtain

$$\begin{aligned} \nabla \times \nabla \times A(t,x) &= \mu_0 \sum_a w_a e_a \dot{x}_a(t), \\ 0 &= \sum_a w_a e_a \delta(x - x_a) \end{aligned}$$

- ϕ acts as a Lagrange multiplier to enforce quasi-neutrality (similar to the pressure enforcing divergence-freeness of the velocity field in incompressible fluids)
- see Cesare Tronci, Enrico Camporeale, *Neutral Vlasov kinetic theory of magnetized plasmas*, Physics of Plasmas 22, 020704, 2015 (doi:10.1063/1.4907665)

Remarks, Open Questions, Perspectives

Remarks

- Symplectic integrators for the Pauli particle do not seem to support large time steps.
- The Boris algorithms is applicable to the Pauli particle (but only volume-preserving).

Open Questions

- Is the Hamiltonian splitting slow manifold preserving?
- Do explicit, slow manifold preserving symplectic or variational integrators exist?
- Proof of equivalence between guiding centre dynamics and Pauli particle dynamics?
- Proof of slow manifold preservation for variational or symplectic integrators?

Perspectives

- More experiments: initial conditions, integrators, ...
- Extension of GEMPIC. Modified Hamiltonian splitting. Implementation.
- Variational Pauli-PIC scheme, including gauge invariance and variational splitting.