Partial connections and geometric integration

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Choosing group components

Connections, moving frames, etc can be used to decompose vector or curves into group and 'rigid' components.

A judicious choice of decomposition can aid in the analysis and understanding of systems with symmetry.

Example: A particle in a constant magnetic field: $\ddot{q} = \mu \times \dot{q}$.
(Assume unit mass for convenience.)

'Standard' approach: Introduce the velocity $v = \dot{q}$.

$$\begin{aligned} \dot{q} &= v \\ \dot{v} &= \mu \times v \end{aligned} \quad \Longrightarrow \quad \begin{aligned} v(t) &= \exp(t\,\hat{\mu})v_0 \\ q(t) &= q_0 + \textstyle\int_0^t v(\tau)d\tau = q_0 + F(t)v_0, \end{aligned}$$

where $\hat{\mu}u = \mu \times u$ and $F(t) := \int_0^t \exp(\tau\,\hat{\mu})d\tau$.

Qualitative description of motion?

Use a rotating frame:

Let $q(t)$ be a solution curve and set $x(t) := \exp\left(-\frac{t}{2}\,\hat{\mu}\right) q(t)$.

$$\ddot{x} = \exp\left(-\tfrac{t}{2}\,\hat{\mu}\right)\Big(\ddot{q} - \mu \times \dot{q} + \tfrac{1}{4}\mu \times (\mu \times q)\Big) = -\frac{|\mu|^2}{4}\mathbb{P}x,$$

where $\mathbb{P}$ denotes projection onto the plane perpendicular to μ.

$$\mathbb{P}\left(\ddot{x} + \frac{|\mu|^2}{4}x\right) = 0 \qquad \text{and} \qquad (\mathbf{1} - \mathbb{P})\ddot{x} = 0$$

$\Longrightarrow$ solutions of $\ddot{q} = \mu \times \dot{q}$ are combinations of

- steady rotation with generator $\frac{1}{2}\,\mu$
- harmonic motion in the plane perpendicular to μ
- steady translation parallel to μ.

Hamiltonian structure:

The 'standard' Hamiltonian system associated to $\ddot{q} = \mu \times \dot{q}$ is

$$\dot{q} = p \qquad \text{and} \qquad \dot{p} = \mu \times p$$

with Hamiltonian $H(q,p) = \frac{1}{2}|p|^2$ and *noncanonical* symplectic structure with matrix

$$\mathbb{J}_\mu = \begin{pmatrix} \hat{\mu} & \mathbb{I} \\ \text{-}\mathbb{I} & \mathbb{O} \end{pmatrix}.$$

The Hamiltonian system associated to $\ddot{x} + \frac{|\mu|^2}{4}\mathbb{P}x = 0$ is *canonical*, with Hamiltonian

$$H(x,y) = \frac{1}{2}|y|^2 + V_\mu(q),$$

where $V_\mu(q) := \frac{1}{8}|\mu \times x|^2$.

Add a (nonsymmetric) potential V:

The rotating frame approach is too restrictive for this setting —it would lead to a time–dependent system.

A velocity/momentum shift can be used instead: Set

$$w := \dot{q} - \tfrac{1}{2}\,\mu \times q.$$

The resulting system is

$$\dot{q} = w + \tfrac{1}{2}\,\mu \times q \qquad \text{and} \qquad \dot{w} = -\nabla(V + V_\mu)(q) + \tfrac{1}{2}\,\mu \times w,$$

a canonical Hamiltonian system with

$$H(x, w) = \tfrac{1}{2}|w|^2 + \tfrac{1}{2}\,\mu \cdot q \times w + (V + V_\mu)(q).$$

Numerical solutions?

'Standard' version can be integrated using a symplectic Störmer-Verlet–type method due to Scovel.
This is a product formula approach utilizing the exact solution of the potential-free case.

Shifted version can be integrated using the standard Störmer-Verlet update with the potential

$$\tilde{V}_{(\mu,t)}(q) := V\left(\exp\left(t/4\,\hat{\mu}\right)q\right) + V_{\mu}(q),$$

followed by rotation by $\exp\left(t/2\,\hat{\mu}\right)$.

Advantages/disadvatages?

On to connections....

Notation

Assume a Lie group G acts continuously on a manifold M.

Let $\Phi_g : M \to M$ and $\widehat{\Phi}_m : G \to M$ denote the maps

$$\widehat{\Phi}_m(g) := \Phi_g(m) := g \cdot m.$$

Given $\xi \in \mathfrak{g} = T_e G$, define the *infinitesimal generator* ξ_M by

$$\xi_M(m) := d\widehat{\Phi}_m \xi.$$

$\widetilde{\mathfrak{g}}$ denotes the bundle of infinitesimal groups motions, i.e.

$$\widetilde{\mathfrak{g}}|_m := T_m(G \cdot m) = \operatorname{range} d_e\widehat{\Phi}.$$

Connections on principal bundles

A *connection* on a principal bundle P is a differential system Γ satisfying

$$TP = \widetilde{\mathfrak{g}} \oplus \Gamma \qquad \text{and} \qquad d\Phi_g \cdot \Gamma_m = \Gamma_{g \cdot m}$$

$\forall\, m \in P$ and $g \in G$.

A connection Γ determines an equivariant, $\mathfrak{g}$–valued one–form α — called the *connection form* — satisfying

$$\ker \alpha = \Gamma \qquad \text{and} \qquad \alpha \circ \xi_P \equiv \xi \quad \forall \xi \in \mathfrak{g}.$$

The connection specifies a decomposition of each tangent vector:

$$\begin{array}{rcccl} v_m = & d\widehat{\Phi}_m(\alpha(v)) & + & w_m \\ & \text{‘rigid’} \in \widetilde{\mathfrak{g}}|_m & & \text{‘internal’} \in \Gamma|_m \end{array}$$

Isotropy

The subgroup

$$G_m = \{g \in G : g \cdot m = m\}$$

is the *isotropy subgroup* of the point m, with algebra $\mathfrak{g}_m := \ker[d_e\widehat{\Phi}_m]$.

If $\mathfrak{g}_m$ is nontrivial, the Lie algebra $\mathfrak{g}$ and the tangent space $\widetilde{\mathfrak{g}}_m := \mathrm{range}[d_e\widehat{\Phi}_m]$ to the group orbit through m are *not* isomorphic.

Generators of infinitesimal group motions are not uniquely determined; hence generalizations of connection forms to nonfree actions will not be uniquely determined by the connection.

The design of numerical methods on homogeneous manifolds — with trivial horizontal spaces—motivated the development of generalizations of connection forms.

Isotropically distinct generators yield identical *exact* continuous time trajectories, but typically yield distinct *approximate* discrete time trajectories.

Example: The reduced free rigid body

The free rigid body is a canonical Hamiltonian system on $T^*SO(3) \approx SO(3) \times \mathbb{R}^3$:

$$\dot{\Lambda} = \Lambda\widehat{\Omega} \qquad \dot{\Pi} = \Pi \times \Omega, \qquad \text{where} \quad \Omega = \mathbb{I}^{-1}\Pi.$$

Here $\mathbb{I}$ denotes the inertia tensor of the body.

This system is equivariant with respect to the left action of $SO(3)$ (material frame invariance).

Energy and spatial angular momentum

$$H(\Lambda, \Pi) = \tfrac{1}{2}\Pi \cdot \mathbb{I}^{-1}\Pi \qquad \text{and} \qquad J(\Lambda, \Pi) = \Lambda\Pi$$

are conserved. Hence the momentum component of a trajectory $(\Lambda(t), \Pi(t))$ lies on the intersection of an ellipsoid and a sphere.

Symplectic reduction to S^2 yields the vector field

$$X(m) = m \times \mathbb{I}^{-1} m.$$

A family of geometric 'Euler's methods' for this system is

$$\Upsilon^{\sigma}(m, \Delta t) = \mathrm{Exp}(\Delta \mathrm{t}\ (-\mathbb{I}^{-1}\mathrm{m} + \sigma(\mathrm{m})\,\mathrm{m})) \cdot \mathrm{m}$$

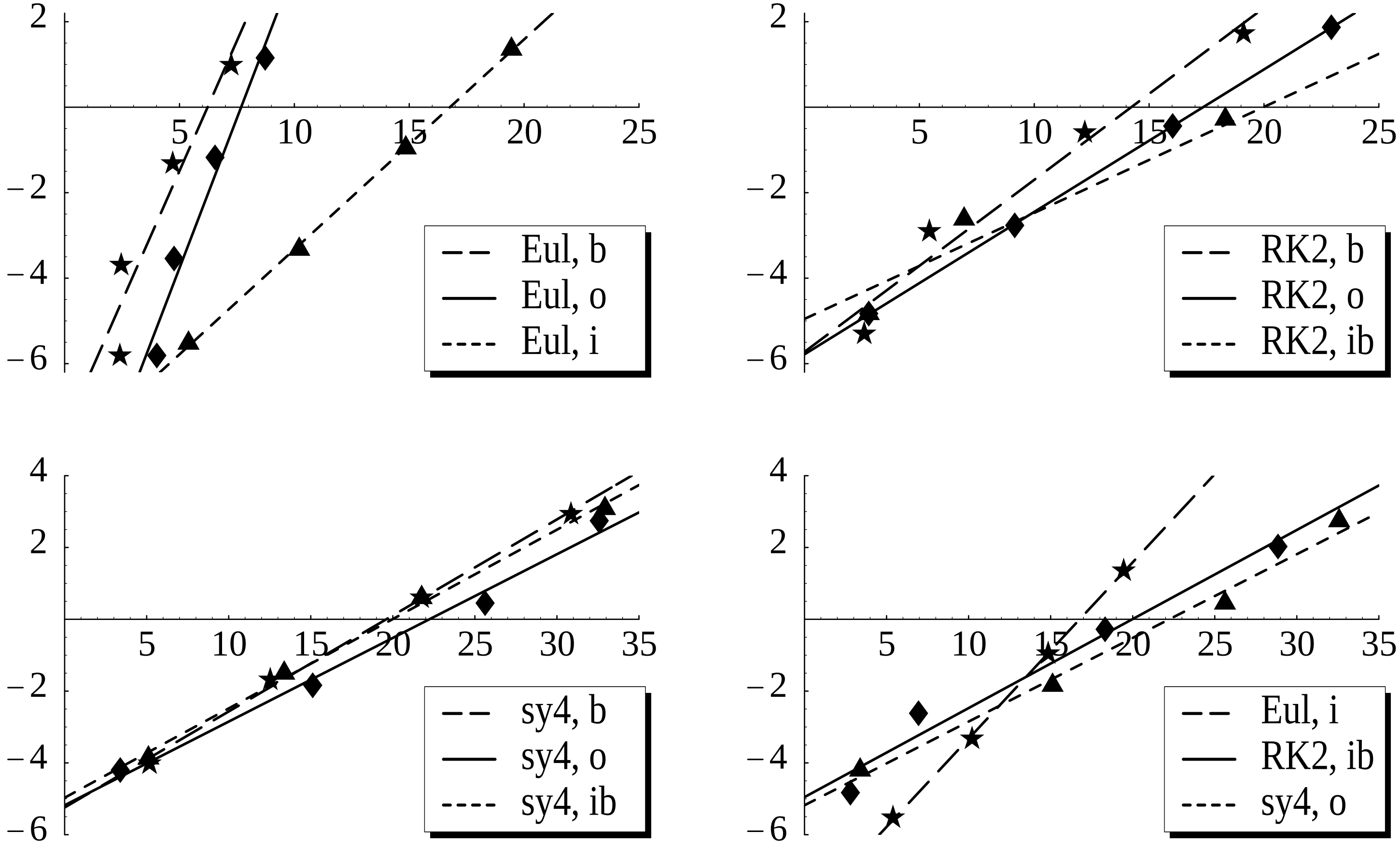
for some function $\sigma : S^2 \to \mathbb{R}$ and 'algorithmic exponential' $\mathrm{Exp} : \mathbb{R}^3 \to \mathrm{SO}(3)$ (e.g. matrix exponential or Cayley transform).

Any such update method yields discrete trajectories on the sphere.

Three sample generators:

- ‘basic’ the negative of angular velocity
  the generator suggested by the unreduced dynamics
- ‘orthogonal’ perpendicular to point m
  move along the great circle tangent to the true solution at m
- ‘improved’ best circular match to the true trajectory
  move along the circle tangent to the true solution at m with the same geodesic curvature as the true solution

The following figure shows CPU time as a function of the energy error (ln/(-ln) plots) for some first, second, and fourth order methods for the reduced rigid body.


Eul, b
Eul, o
Eul, i
RK2, b
RK2, o
RK2, ib
sy4, b
sy4, o
sy4, ib
Eul, i
RK2, ib
sy4, o

Conserving algorithms

The ‘correction’ σ_{i} can be derived from energy conservation considerations:

If Exp is the Cayley transform, then

$$H(\Upsilon^{\sigma}(m,\Delta t)) - H(m) = \frac{P_{m,\Delta t}(\sigma)}{(Q_{m,\Delta t}(\sigma))^2}$$

for some cubic polynomial $P_{m,\Delta t}$ and quadratic polynomial $Q_{m,\Delta t}$.

Solving $P_{m,\Delta t}(\sigma) = 0$ to the desired order yields arbitrarily accurate energy capture.

The lowest order ‘correction’, σ_{i}, captures energy to second order.

Challenge: Develop machinery to facilitate selection of ‘optimal’ generators for much more complicated systems.

Partial connections and singular points

At singular points, where the dimensions of the isotropy algebras jump, any complementary distribution must be singular.

How to specify that complements to $\widetilde{\mathfrak{g}}_m$ vary as smoothly as possible with m?

Want to use smooth forms to carve out subspaces, but 'connection forms' aren't continuous at points with nontrivial isotropy.

A $\mathfrak{g}$–valued one–form α determines a map

$$\mathbb{P}_\alpha := d\widehat{\Phi} \circ \alpha : TM \to \widetilde{\mathfrak{g}} := \cup_{m \in M} \widetilde{\mathfrak{g}}_m.$$

$\mathbb{P}_\alpha$ is an equivariant projection onto $\widetilde{\mathfrak{g}} \Longleftrightarrow \alpha$ is equivariant (modulo isotropy) and satisfies the normalization condition

$$\operatorname{range}(\mathbb{1} - \alpha \circ d_e \widehat{\Phi}_m) \subseteq \mathfrak{g}_m \qquad \forall\, m \in M.$$

The normalization condition forces discontinuity at singular points.

Drop normalization, replacing $\mathfrak{g}$–valued forms with smooth $\mathfrak{g}^*$–valued forms:

An *equivariant partial connection* is a (singular) equivariant differential system Γ satisfying

$$TM = \widetilde{\mathfrak{g}} \oplus \Gamma$$

and

Γ is smooth and/or

$\Gamma = \ker \mu$ for some smooth $\mathfrak{g}^*$–valued one–form μ.

Dual connection forms

An *equivariant dual connection form* μ is a smooth equivariant $\mathfrak{g}^*$–valued one–form satisfying

$$T_m M = \widetilde{\mathfrak{g}} \oplus \ker \mu_m \qquad \forall\, m \in M.$$

Let λ_m denote the left handed inverse of μ_m, so that

$$\lambda_m \circ \mu_m|_{\widetilde{\mathfrak{g}}_m} = \mathrm{id}.$$

$\mathbb{P}_\mu := \lambda \circ \mu : TM \to \widetilde{\mathfrak{g}}$ a equivariant projection.

An *equivariant inertia factor* is an equivariant map $\chi : M \to \mathfrak{L}(\mathfrak{g}, \mathfrak{g}^*)$ satisfying

$$\ker \chi(m) = \mathfrak{g}_m \qquad \forall\, m \in M.$$

An equivariant $\mathfrak{g}^*$–valued one–form μ is a dual connection form

$\iff$

$\chi(m) := \mu \circ d_e\widehat{\Phi}_m$ is an inertia factor satisfying

$$\operatorname{range}\chi(m) = \operatorname{range}\mu_m.$$

An *equivariant partial connection form* α is a $\mathfrak{g}$–valued one–form such that

$\mathbb{P}_\alpha = d\widehat{\Phi} \circ \alpha$ is an equivariant projection onto $\widetilde{\mathfrak{g}}$ and

$\ker \mathbb{P}_\alpha$ is an equivariant partial connection.

A *partial connection pair* (α, χ) consists of a partial connection form α and an inertia factor χ such that $\mu := \chi\,\alpha$ is a dual connection form.

Partial connection pairs allow us to move between the familiar $\mathfrak{g}$-valued forms and smooth $\mathfrak{g}^*$ valued forms.

We will use partial connection pairs to develop our notion of curvature…

Motivating example: $SO(3)$ acting on $\mathbb{R}^3$

The Euclidean orthogonal complements to $\widetilde{\mathfrak{g}}$ satisfy

$$\widetilde{\mathfrak{g}}^{\perp}|_m = \begin{cases} \text{span}[m] & m \neq 0 \\ \mathbb{R}^3 & m = 0 \end{cases} .$$

Any $f : \mathbb{R}^3 \backslash \{0\} \to \mathbb{R}$ determines a $\mathbb{R}^3$–valued one–form

$$\alpha(v) = \begin{cases} ||m||^{-2} m \times v + f(m) \langle m, v \rangle m & v \in T_m\mathbb{R}^3, \ m \neq 0 \\ 0 & v \in T_0\mathbb{R}^3 \end{cases} .$$

Angular *velocity* isn't well–defined at the origin, but angular *momentum* is.

Angular momentum $\mu(v) = m \times v$ is a $so(3)^*$–one–form with $\ker \mu = \widetilde{\mathfrak{g}}^{\perp}$.

The inertia tensor $\chi(m) := \mu \circ d_e\widehat{\Phi}_m \in \mathbb{R}^{3\times 3}$ satisfies

$$\chi(m) = \begin{cases} ||m||^2\mathbb{P}_\perp & m \neq 0 \\ 0 & m = 0 \end{cases}$$

Simple mechanical systems

Let M be Riemannian and G be a subgroup of (local) isometries of M.

The orthogonal complement to $\widetilde{\mathfrak{g}}$ is the prototype of a *partial connection.*

Define a equivariant $\mathfrak{g}^*$–valued one–form μ by

$$\mu(v) \cdot \xi := \langle v, \xi_M(m) \rangle_m$$

and the *locked inertia tensor* $\chi : M \to \mathfrak{L}(\mathfrak{g}, \mathfrak{g}^*)$ by

$$(\chi(m)\xi) \cdot \eta = \langle \xi_M(m), \eta_M(m) \rangle_m \,.$$

If G acts freely and properly, $\ker \mu$ is the *simple mechanical connection* and

$$\alpha(v) := \chi(m)^{-1} \mu(v) \qquad \forall\, v \in T_m M,\ m \in M$$

is the associated connection form.

Connection forms and moving frames

A *moving frame* is a G–equivariant map $\rho : M \to G$ on a manifold M with a (locally) free G action.

The trivialized derivative $d^\natural\rho : M \to \mathfrak{g}$ of a moving frame ρ, given by

$$d^\natural_m\rho := d_m(\rho(m)^{-1}\rho),$$

is a connection.

A (left) *partial moving frame* is a map $\phi : M \to G$ satisfying

$$\phi(g \cdot m)\phi(m)^{-1} = g \qquad \mod \quad G_m.$$

A partial moving frame determines a global cross section as the image of the map $\pi_\phi : M \to M$ given by

$$\pi_\phi(m) := \phi(m)^{-1} \cdot m.$$

The trivialized deriviative $d^\natural\phi : M \to \mathfrak{g}$ of a partial moving frame ϕ is a partial connection form with respect to a relaxed standard of equivariance.

Curvature

The curvature Ω of a connection Γ on a principal bundle is the covariant derivative of the unique associated connection form α

$$\Omega = \nabla\alpha = \mathbb{P}_\Gamma^* \mathrm{d}\alpha,$$

where $\mathbb{P}_\Gamma$ denotes projection onto the connection.

Two key difficulties in extending this notion to partial connections:

the nonuniqueness of the partial connection form,

the singularity of partial connection forms at singular points.

A partial connection form *is* smooth at regular points.

Define the *curvature* Ω of a partial connection form α at a regular point m as

$$\Omega_m := d\widehat{\Phi}_m \circ \nabla\alpha : (T_m M)^2 \to \widetilde{\mathfrak{g}}|_m,$$

where $\nabla\alpha = \mathbb{P}_\Gamma^* \mathrm{d}\alpha$ as usual.

Curvature at singular points

If (α, χ) is a partial connection pair,

$$\nabla(\chi\,\alpha) = \nabla(\chi\,\alpha) - \nabla\chi \wedge (\alpha \circ \mathbb{P}_\Gamma) = \chi\,\nabla\alpha \qquad (*)$$

at regular points, since range $\nabla\chi(m) \subseteq \mathrm{Ann}\ \mathfrak{g}_m$.

The left hand side of $(*)$ is well-defined even at singular points. Can it be used to develop a reasonable extension of $\nabla\alpha$ to singular points?

Complication: the covariant derivative of a dual connection form at m need not take values in the range of the form at m.

A dual connection form μ is *docile* at m if range $\nabla_m\mu \subseteq$ range μ_m.

If μ is docile at m, then define the *curvature* Ω_m of μ at m as

$$\Omega_m := \lambda_\mu(m)^{-1} \circ \nabla \mu_m.$$

The curvature of a partial connection pair (α, χ) satisfies

$\chi(\alpha \circ \Omega + \alpha \wedge \alpha) = \mathrm{d}(\chi\, \alpha) - \mathrm{d}\chi \wedge \alpha$ 'structure equations'

Is this ever interesting? At least nonzero?

Example: Let G be a Lie group with an Ad–invariant inner product on $\mathfrak{g}$ and let H be a subgroup of G.

Let $H \times H$ act on G by $(h, k) \cdot g = hgk^{-1}$.

A 'tamed' version of the momentum map associated to the action of $H \times H$ on G has curvature

$$\Omega_g(\xi, \eta) = (\mathbb{P}_{\mathfrak{h}} - \mathbb{P}_{\mathrm{Ad}_g \mathfrak{h}})[\mathbb{P}_{\Gamma_g} \xi, \mathbb{P}_{\Gamma_g} \eta],$$

where $\mathbb{P}_V : \mathfrak{g} \to V$ denotes projection onto a subspace V.

Note that $\Omega_g = 0$ if $g \in N(H)$.

Take $G = SU(3)$ and H the two–torus of diagonal matrices in $SU(3)$.

For g corresponding to a rotation through θ about the vertical axis, $\theta \neq \frac{n\,\pi}{2}$, then g has a one dimensional isotropy algebra and Ω_g has rank two.

Curvature and involutivity

A *horizontal* vector field takes values only in a (partial) connection.

If vector fields X and Y are horizontal, the vector field $\Omega(X, Y) + [X, Y]$ is horizontal.

Hence if Ω is identically zero on some open set containing only regular points, then Γ is involutive on that set.

If m_0 is singular, then $\dim \Gamma|_m > \dim \Gamma|_m$ at nearby points m.

Hence we can't find local horizontal vector fields spanning $\Gamma|_{m_0}$ if m_0 is singular, or invoke the identity relating exterior derivatives and commutators of vector fields.

We locally enlarge the partial connection by including a copy of the tangent space to the G_{m_0} orbit at each point 'rotated' so as to yield a smooth differential system containing Γ.

Almost horizontal vector fields

An *adaptor* ϕ for m_0 is a smooth local G_{m_0}–equivariant map $\phi : \mathcal{U} \to G$ satisfying

$$\mathrm{Ad}_{\phi(m)}\mathfrak{g}_{m_0} \supseteq \mathfrak{g}_m \qquad\qquad \forall\ m \in \mathcal{U},\ \ \phi(m_0) \in G_{m_0}.$$

A partial connection Γ and an adaptor ϕ determine the local *almost horizontal* differential system

$$\Xi := \Gamma \oplus \mathrm{Ad}_\phi \mathfrak{g}_{m_0}.$$

If G acts properly, then there exists an adaptor for any point in M and the curvature at a singular point m_0 is determined by the equation

$$\Omega(X, Y)(m_0) = (\mathbb{P}_\Gamma - \mathbb{1})[X, Y](m_0)$$

for almost horizontal vector fields X and Y.

A special case: slices

A *slice* generalizes the notion of a local cross section, allowing some overlap of the slice and the group orbits near singular points.

Specifically, a slice at m_0 is a submanifold S through m_0 satisfying

$T_{m_0}M = T_{m_0}S \oplus \widetilde{\mathfrak{g}}|_{m_0}$ and

$T_mM = T_mS + \widetilde{\mathfrak{g}}|_m$ for all $m \in S$

if $m \in S$ and $g \in G$, then $g \cdot m \in S$ if and only if $g \in G_{m_0}$.

If

G acts properly,

$G_{m_0} \subseteq G$ is a normal subgroup,

$G_m \subseteq G_{m_0}$ for all m in a neighborhood of m_0, and

$$\operatorname{range}\Omega \subseteq \widetilde{\mathfrak{g}_{m_0}} \text{ on that neighborhood,}$$

then some neighborhood of m_0 in the integral submanifold of Ξ containing m_0 is a slice.

Geometric integration: The LLG equation

The Landau–Lifschitz–Ginzburg equation for a micromagnetic field μ is

$$\dot{\mu} = \omega(\mu) \times \mu,$$

where

$$\omega(\mu) = \frac{1}{1+\lambda^2}\left(H_{\text{eff}}(\mu) + \lambda\mu \times H_{\text{eff}}(\mu)\right)$$

and

$$H_{\text{eff}}(\mu) = A\Delta\mu + \psi_0\left(-\nabla\phi + H_{\text{app}}\right) + K(\mu \cdot \mathbf{e})\mathbf{e}.$$

Renormalizing μ to correct for drift introduces significant changes in the demagnetizing field $\nabla\phi$.

Use geometric methods, with:

(i) Freedom to use existing sophisticated codes for computing the demagnetization field.

(ii) Cheap evaluation of updated points given an infinitesimal update.

(iii) Cheap, 'natural', and/or 'improving' choices of σ.