Geometric RATTLE

Geometric Generalisation of SHAKE and RATTLE

Olivier Verdier[1]

(with R. McLachlan[2], K. Modin[2], M. Wilkins[2])

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R. McLachlan, K. Modin, O. Verdier, M. Wilkins
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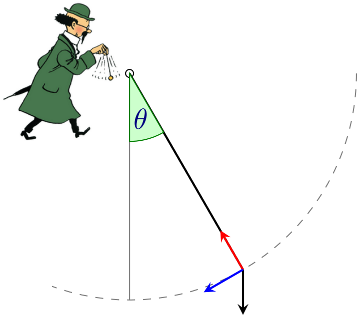
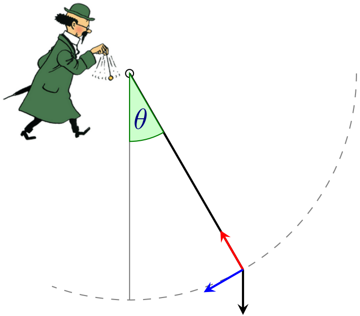
Pendulum: Phase Space



$$\ddot{\theta} = -\frac{g}{\ell}\sin(\theta)$$

Pendulum: Phase Space



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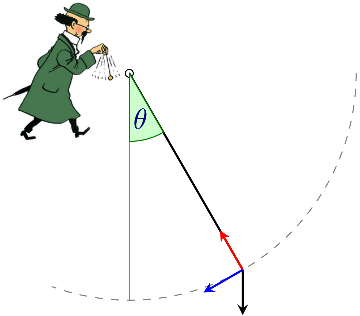

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The phase space is a two dimensional cylinder.

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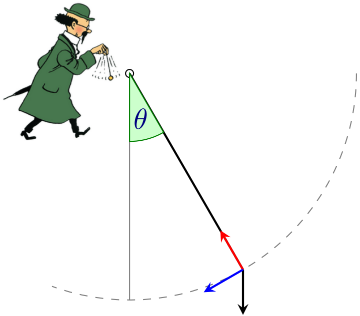

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The phase space is a two dimensional cylinder.

Often: parametrisation is impossible!

Pendulum: Constrained

$$z = (q_1, q_2, p_1, p_2) \equiv (\mathbf{q}, \mathbf{p}) \subset \mathbf{R}^4$$

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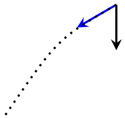

$$H = \frac{\|\mathbf{p}\|^2}{2} - \mathbf{g} \cdot \mathbf{q}$$

$$\begin{cases} \dot{\mathbf{q}} = \mathbf{p} \\ \dot{\mathbf{p}} = \mathbf{g} \end{cases}$$

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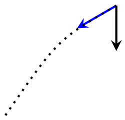

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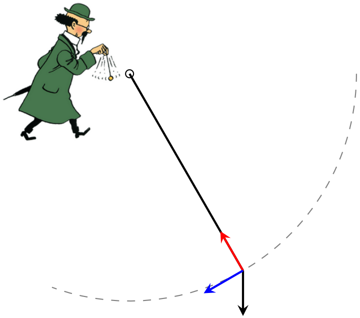

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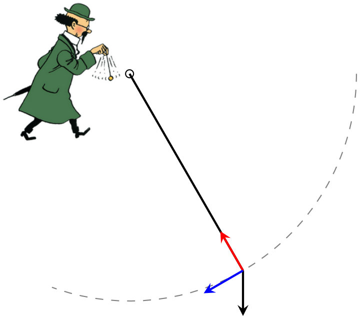

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Hidden constraint:

$$\mathbf{q} \cdot \frac{\partial H}{\partial \mathbf{p}} = 0$$

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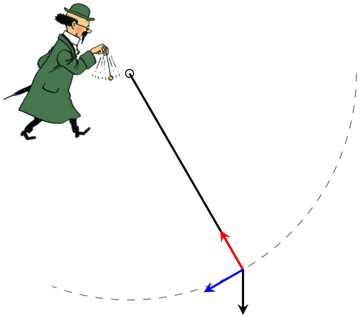
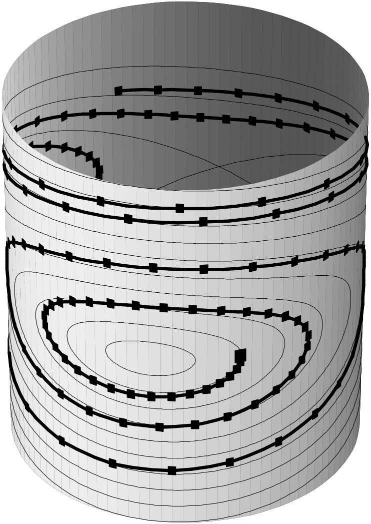


$$\begin{cases} \dot{\mathbf{q}} = \dfrac{\partial H}{\partial \mathbf{p}} + \lambda \dfrac{\partial g}{\partial \mathbf{p}} \\ \dot{\mathbf{p}} = -\dfrac{\partial H}{\partial \mathbf{q}} - \lambda \dfrac{\partial g}{\partial \mathbf{q}} \\ \underbrace{g(q,p) = 0}_{\text{constraint}} \end{cases}$$

Hidden constraint:

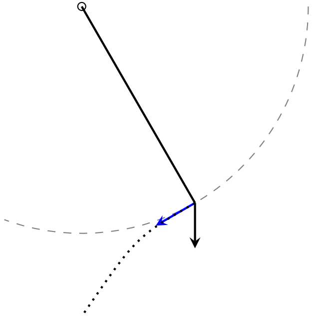
$$\frac{\partial g}{\partial \mathbf{q}} \cdot \frac{\partial H}{\partial \mathbf{p}} - \frac{\partial g}{\partial \mathbf{p}} \cdot \frac{\partial H}{\partial \mathbf{q}} = 0$$

Naive Simulation Fail



Essential Idea on Pendulum

Idea: use the *unconstrained* flow (we have integrators for that)



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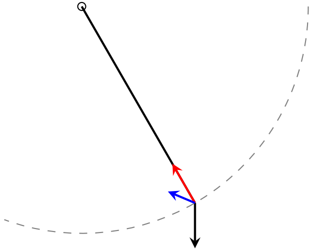

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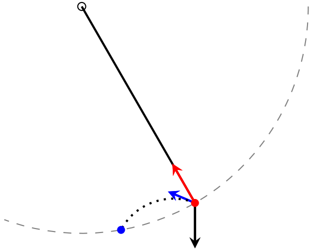


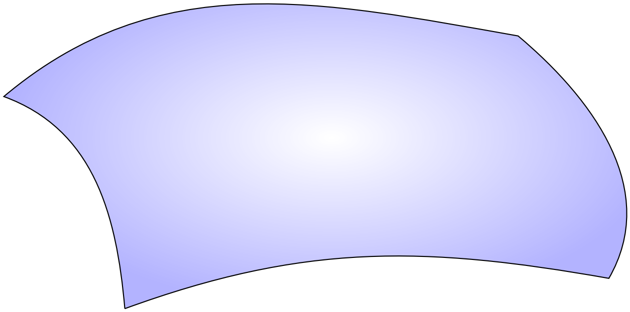
1. “kick” with the reaction force...
2. ...so that after free fall (no constraint) during Δt, one lands on the constraint manifold.

The Essential Ideas

Pendulum

Ambient space: $\mathbf{R}^4$

The Essential Ideas

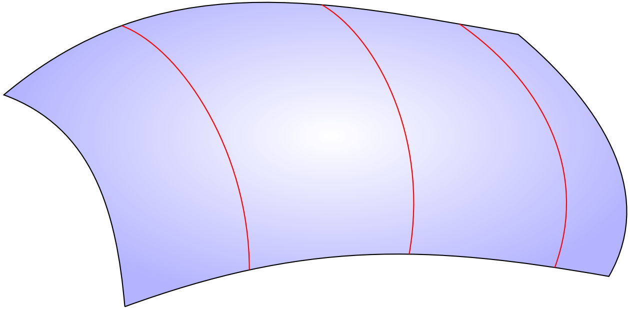


Pendulum

Constraints

$$\|\mathbf{q}\|^2 = 1$$

The Essential Ideas

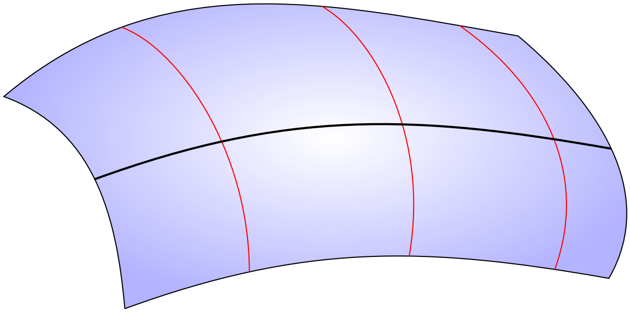


Pendulum

Fibres

$$(\mathbf{q}, \mathbf{p} + \lambda\mathbf{q}) \quad \lambda \in \mathbf{R}$$

The Essential Ideas

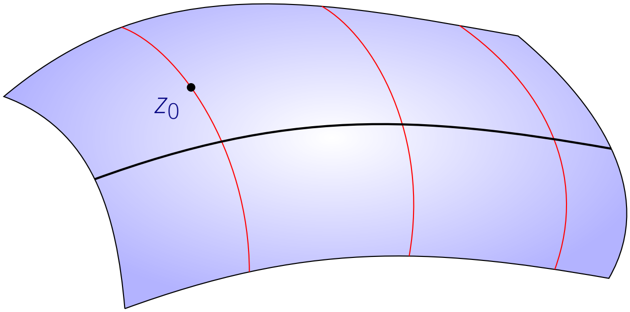


Pendulum

Hidden Constraints $\longrightarrow$ Phase Space

$$\mathbf{q} \cdot \mathbf{p} = 0$$

The Essential Ideas



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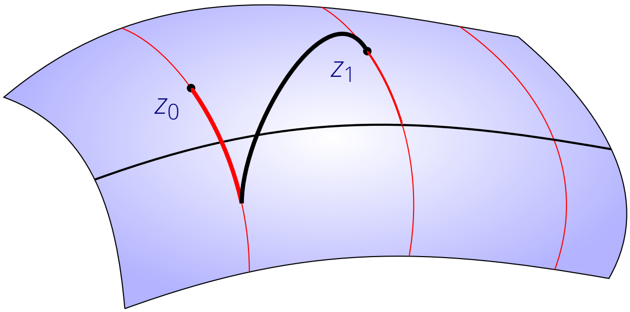


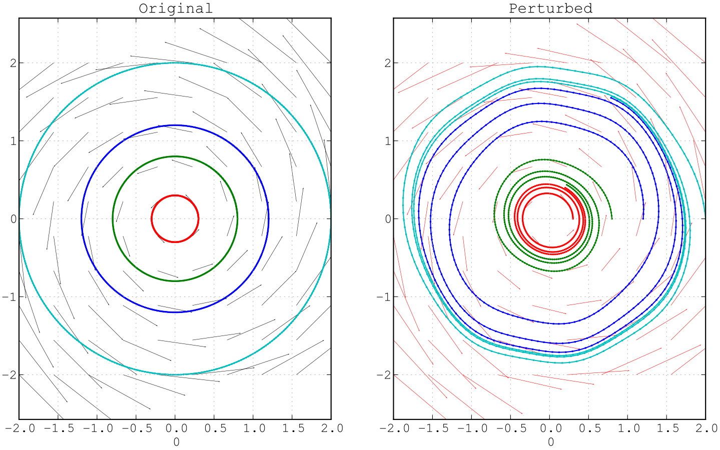
Pendulum

Kick + free fall

Questions

- Are there conditions on the constraints? on H, for this to work?
- Why is it a good idea?

Structural Stability



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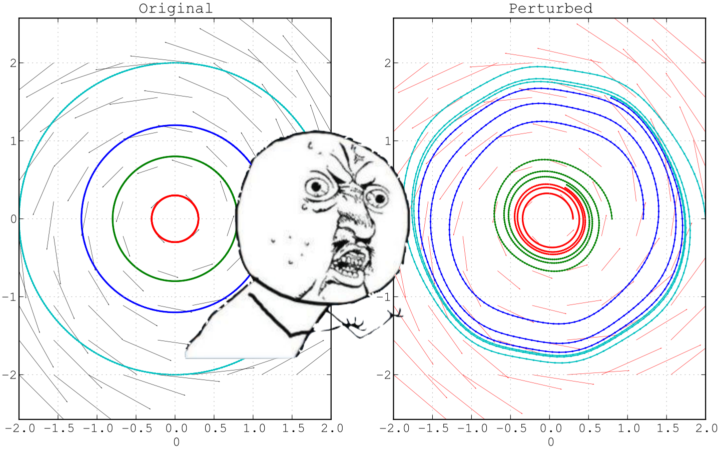
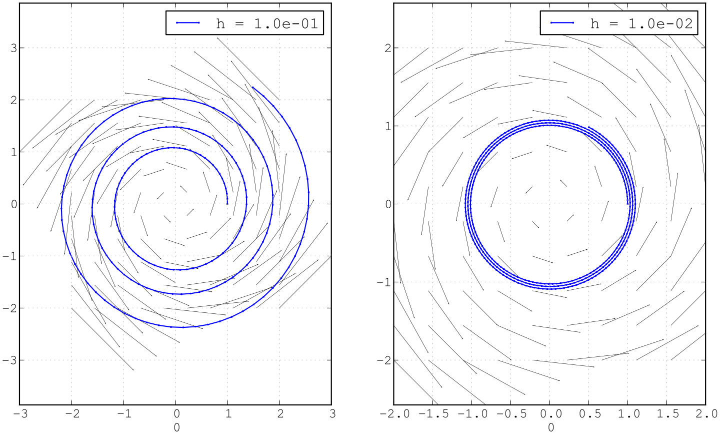


Invariants are destroyed by arbitrary perturbation of the vector field

Backward Error Analysis

A numerical method is an exact solution of a modified vector field



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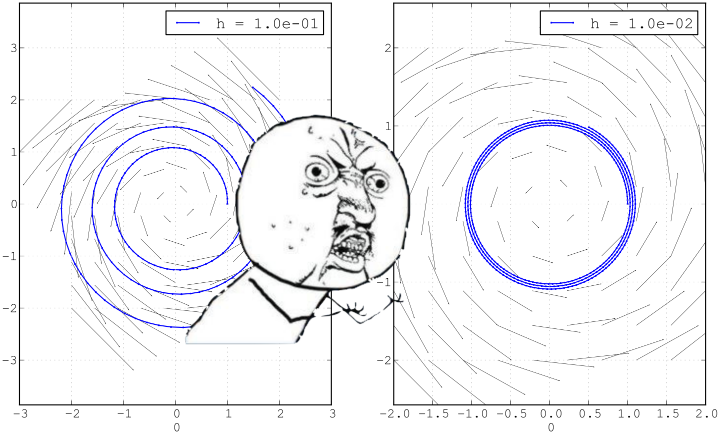
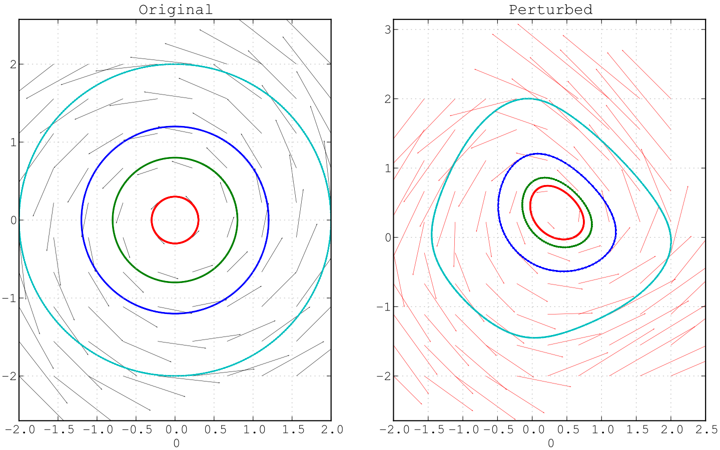


In general, numerical methods destroy the invariants

Symplectic Perturbation



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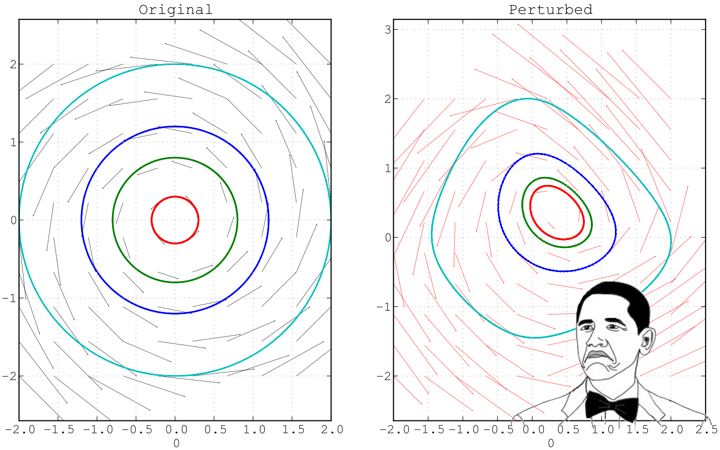

Symplectic perturbations do not destroy all invariants!

Symplectic Vector Field

Maps a vector field to a "gradient".

In $\mathbf{R}^4$

$$\omega = \begin{bmatrix} & -I_2 \\ I_2 & \end{bmatrix}$$

$$z = (\mathbf{q}, \mathbf{p}) \qquad \mathrm{d}H = \left(\frac{\partial H}{\partial \mathbf{q}}, \frac{\partial H}{\partial \mathbf{p}}\right)$$

$$\omega(\dot{z}) = \mathrm{d}H \iff \begin{cases} \dot{\mathbf{q}} = \dfrac{\partial H}{\partial \mathbf{p}} \\ \dot{\mathbf{p}} = -\dfrac{\partial H}{\partial \mathbf{q}} \end{cases}$$

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Goal: symplectic integrator on the phase space.

Submanifold Fibration

Submanifold $\mathcal{M}$ of a symplectic manifold $\mathcal{P}$.

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$\ker \omega|_{\mathcal{M}}$ is defined by:

$$X \in \ker \omega|_{\mathcal{M}} \iff \begin{cases} X \in \mathrm{T}_z\mathcal{M} \\ \langle \omega(X), Y \rangle = 0 \qquad \forall Y \in \mathrm{T}_z\mathcal{M} \end{cases}$$

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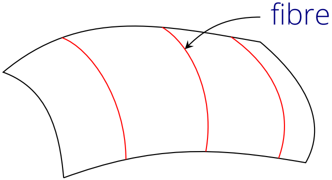
These directions are integrable.



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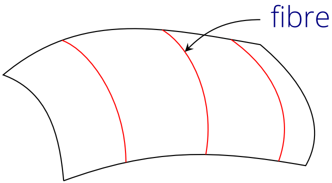

$\mathrm{Tfibre} = \ker \omega|_{\mathcal{M}}$

Pendulum

$$\mathrm{fibre} = \left\{ (\mathbf{q}, \mathbf{p} + \lambda \mathbf{q}) : \lambda \in \mathbf{R} \qquad \|q\|^2 = 1 \right\}$$

Coisotropy Assumption

We assume that dim fibre is “as big as possible”

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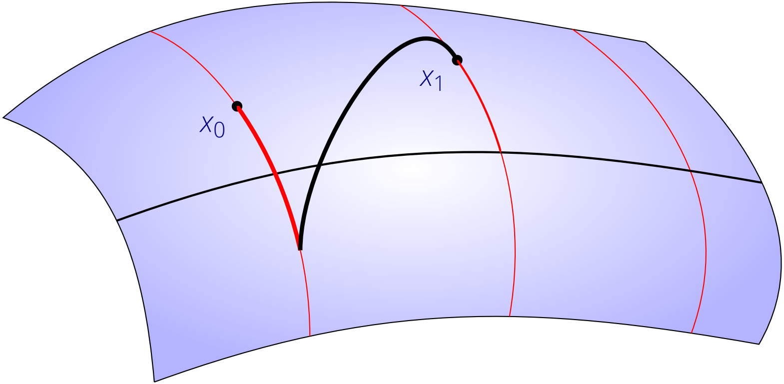
Pendulum

$$g = \|q\|^2 - 1$$

$$\Big[\text{Fibre dimension} = 1 = \text{nb constraints}\Big] \implies \text{coisotropy}$$

Why Coisotropy?



Constrained Problem

Use a *weak formulation*:

$$\omega \quad (\dot{z}(t)) = \mathrm{d}H$$

$$\iff$$

$$\langle \omega(\dot{z}(t)), Y \rangle = \langle \mathrm{d}H, Y \rangle$$
$$\forall Y$$

Constrained Problem

On a Constraint Manifold $\mathcal{M}$

Use a *weak formulation*:

$$\omega|_{\mathcal{M}}(\dot{z}(t)) = \mathrm{d}H|_{\mathcal{M}}$$

$$\Longleftrightarrow \quad \begin{aligned} \langle \omega(\dot{z}(t)), Y \rangle &= \langle \mathrm{d}H, Y \rangle \\ \forall Y &\in \mathrm{T}\mathcal{M} \\ z(t) &\in \mathcal{M} \end{aligned}$$

Lagrange Multipliers

Equivalently, if $\mathcal{M} = \{ g_i = 0 \}$:

$$\omega(\dot{z}(t)) - \mathrm{d}H \in \mathsf{T}\mathcal{M}^{\perp} = \mathrm{span}\{\mathrm{d}g_1, \ldots, \mathrm{d}g_k\}$$

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$$g(\mathbf{q}) = \|\mathbf{q}\|^2 - 1$$

$$-\dot{\mathbf{p}} - \frac{\partial H}{\partial \mathbf{q}} = \lambda \mathbf{q}$$

$$\dot{\mathbf{q}} - \frac{\partial H}{\partial \mathbf{p}} = 0$$

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$$z = (q_1, q_2, p_1, p_2) \qquad g(\mathbf{q}) = \|\mathbf{q}\|^2 - 1$$

$$\begin{aligned} -\dot{\mathbf{p}} + \mathbf{g} &= \lambda \mathbf{q} \\ \dot{\mathbf{q}} - \mathbf{p} &= 0 \end{aligned} \qquad H = \frac{\|\mathbf{p}\|^2}{2} - \mathbf{g} \cdot \mathbf{q}$$

Differential Algebraic Equation

Recall the weak form

$$\left\langle \omega\big(\dot{z}(t)\big), Y \right\rangle = \langle \mathrm{d}H, Y \rangle \qquad Y \in \mathrm{T}\mathcal{M}$$
$$z(t) \in \mathcal{M}$$

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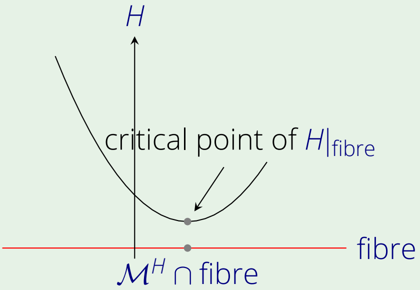
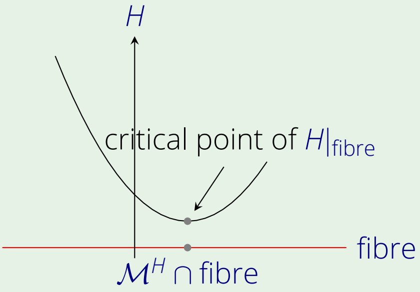
"Hidden" Constraint:

$$\mathcal{M}^H = \{\, z \in \mathcal{M} : \mathrm{d}H = 0 \quad \text{in the fibre direction} \,\}$$

Pendulum



Pendulum



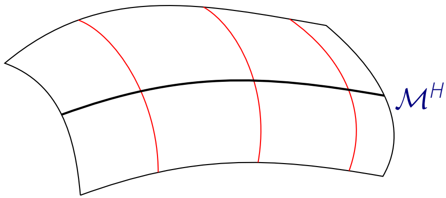
$$\mathcal{H}(\lambda) := H|_{\text{fibre}}(\lambda) = \frac{\|\mathbf{p} + \lambda \mathbf{q}\|^2}{2} - \mathbf{g} \cdot \mathbf{q}$$

$$\mathcal{H}'(\lambda) = 0 \iff \mathbf{p} \cdot \mathbf{q} = 0$$

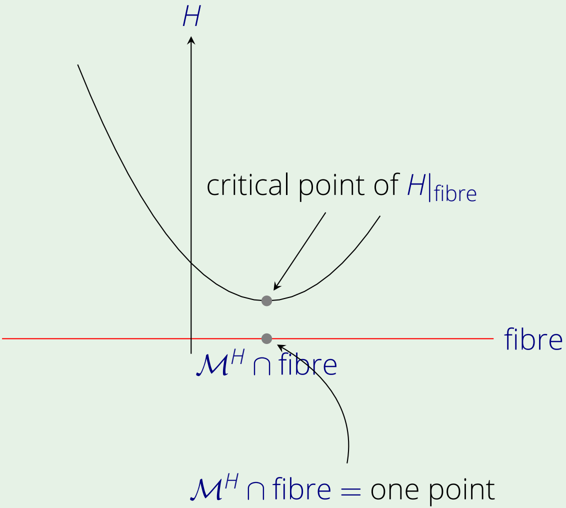
Nondegeneracy Assumption

$$\mathcal{M}^H = \{\, z \in \mathcal{M} : \mathrm{d}H = 0 \quad \text{in the fibre direction} \,\}$$

The assumption is
Hidden constraint $\mathcal{M}^H$ has no fibres (zero-dimensional)

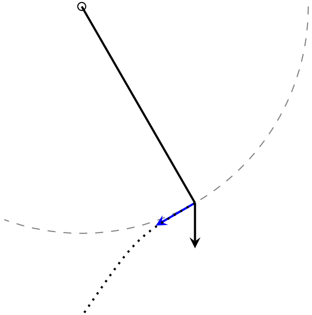


Pendulum


H
critical point of $H|_{\text{fibre}}$
fibre
$\mathcal{M}^H \cap$ fibre
$\mathcal{M}^H \cap$ fibre = one point

Essential Idea on Pendulum

Idea: use the *unconstrained* flow (we have integrators for that)



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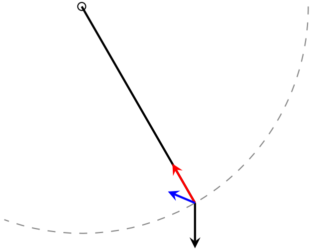

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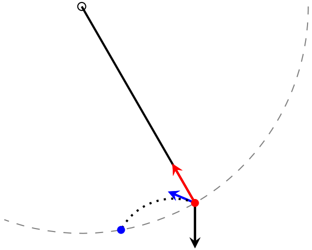

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2. ...so that after free fall (no constraint) during Δt, one lands on the constraint manifold.

Pendulum

First, “move in the fibre”, or “kick”…

$$\widetilde{\mathbf{q}_0} = \mathbf{q}_0$$
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Pendulum

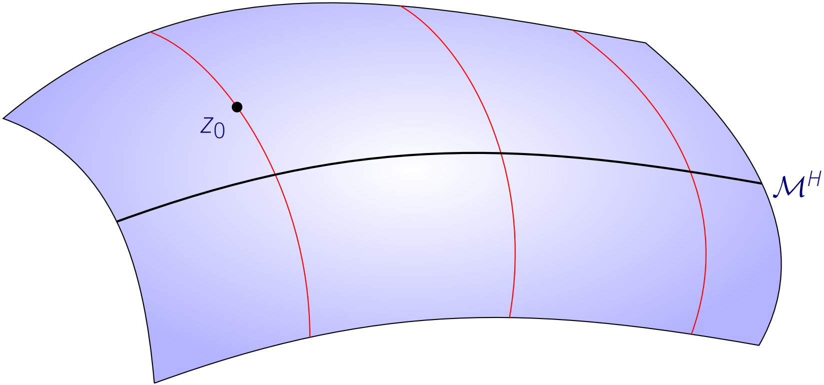
First, "move in the fibre", or "kick"...

$$\widetilde{\mathbf{q}_0} = \mathbf{q}_0$$
$$\widetilde{\mathbf{p}_0} = \mathbf{p}_0 + \lambda \mathbf{q}_0$$

...and find λ such that with the unconstrained problem with symplectic Euler

$$\mathbf{q}_1 = \widetilde{\mathbf{q}_0} + hH_p(\mathbf{q}_0, \mathbf{p}_1)$$
$$\mathbf{p}_1 = \widetilde{\mathbf{p}_0} - hH_q(\mathbf{q}_0, \mathbf{p}_1)$$
$$0 = g(\mathbf{q}_1, \mathbf{p}_1)$$

How SHAKE Works



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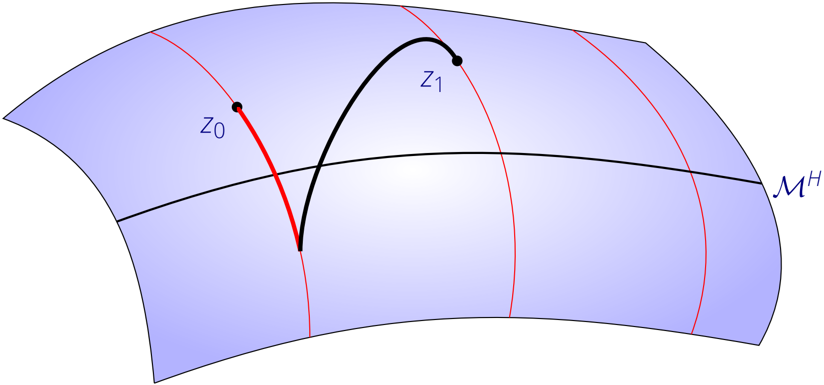

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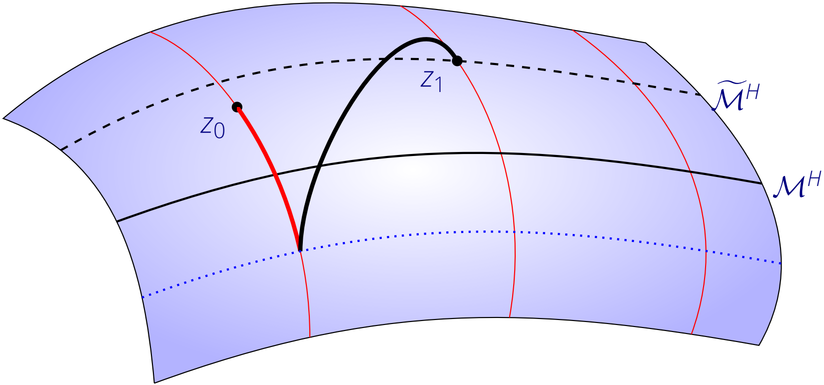

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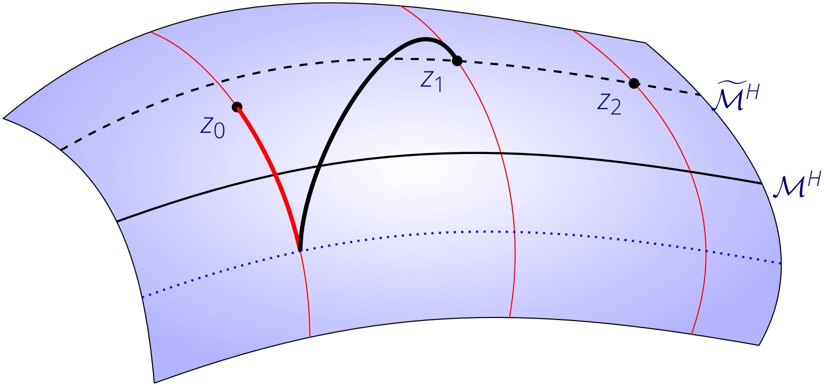

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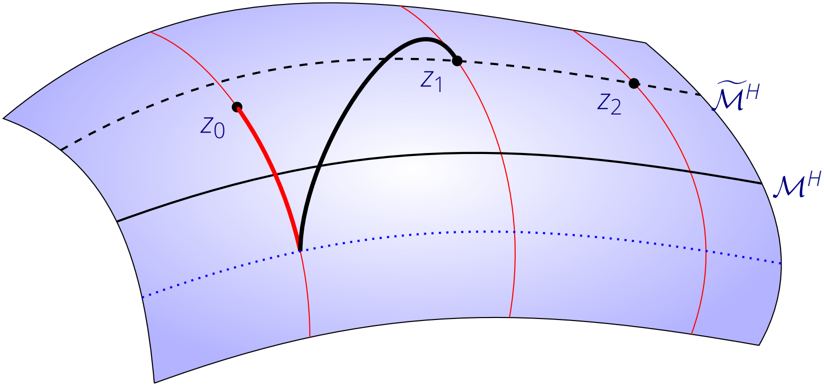

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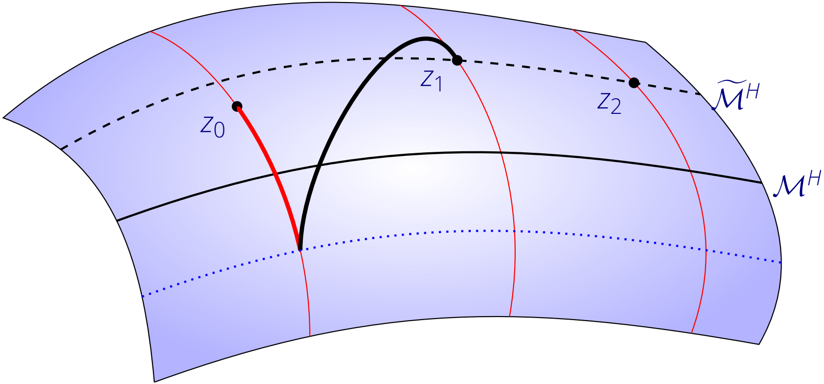

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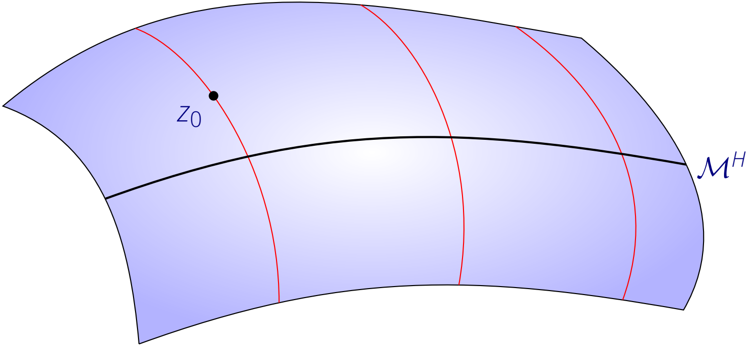
fibre sliding $\implies$ SHAKE is (pre)symplectic on $\mathcal{M}$

How RATTLE Works



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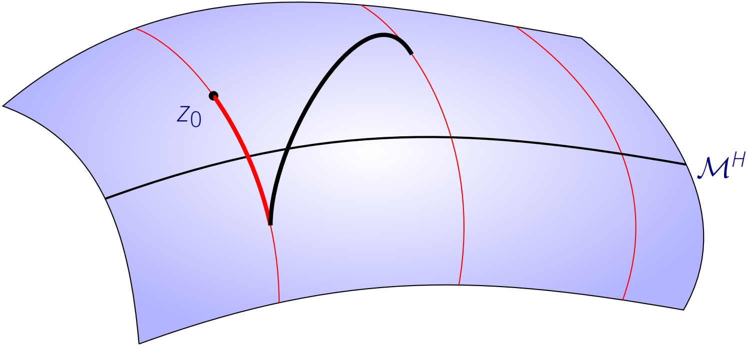

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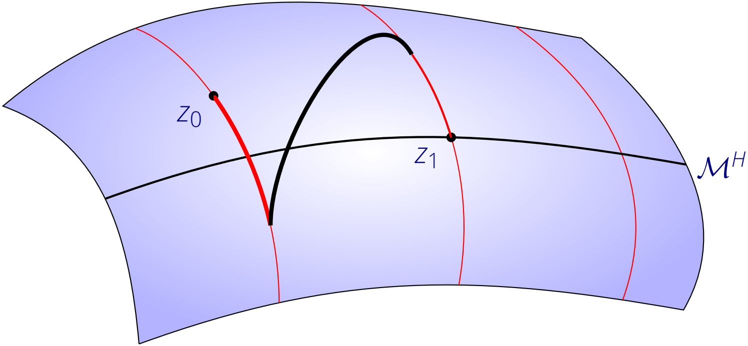

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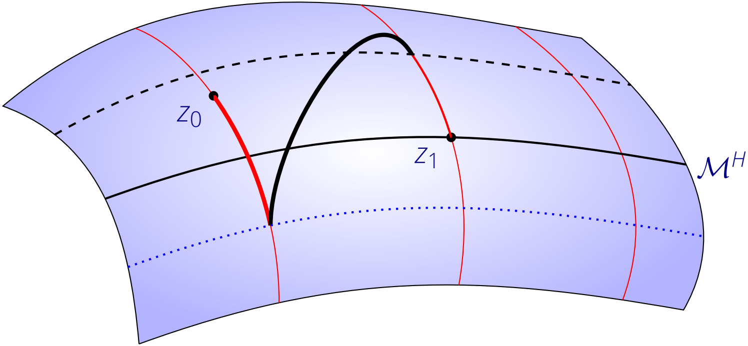

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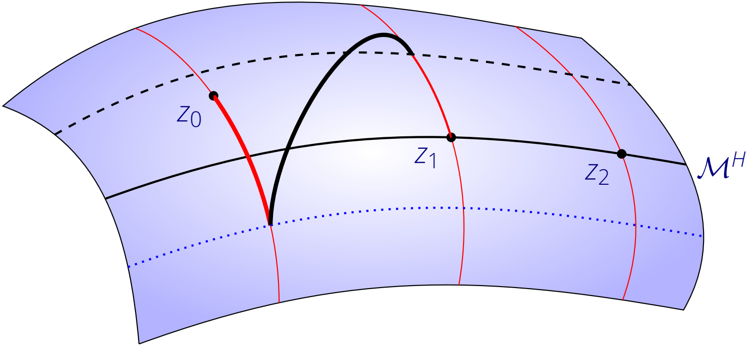

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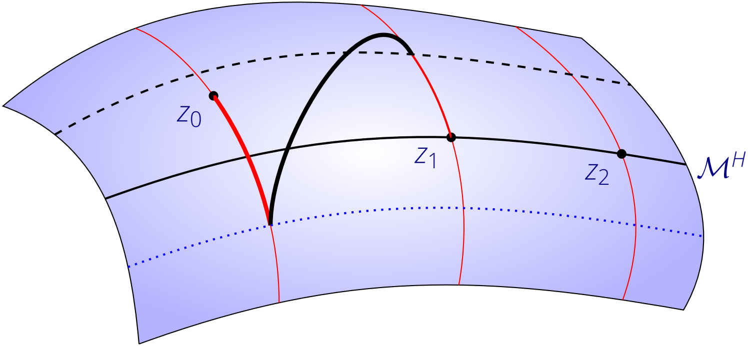

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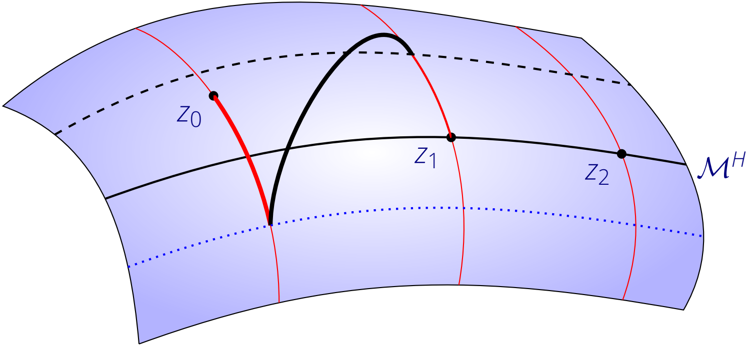

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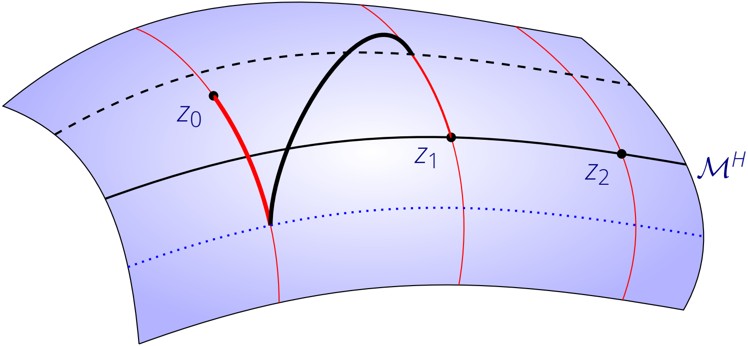

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RATTLE is a cosmetic improvement over SHAKE (in fact SHAKE $=$ RATTLE as fibre mappings)

fibre sliding $\implies$ RATTLE is symplectic on $\mathcal{M}^H$

Fibre Parametrization

To use SHAKE, we need a parametrization of the fibres (which are arbitrary manifolds)

In practice, X_{g_i} is exactly solvable $\implies$ fibres are parametrizable

Pendulum

This is the group action:

$$\lambda \cdot (\mathbf{q}, \mathbf{p}) = (\mathbf{q}, \mathbf{p} + \lambda \mathbf{q})$$

Summary

1. Coisotropy (fibres are as big as possible)
2. Nondegeneracy (hidden constraint has no fibres)
3. Parametrized Fibres

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then

1. $$\mathcal{M}^H = \left\{ z \in \mathcal{M} : \mathrm{d}H = 0 \quad \text{in the fibre direction} \right\}$$
   is the phase space
2. SHAKE/RATTLE methods are symplectic on $\mathcal{M}/\mathcal{M}^H$

Classical SHAKE Revisited

When the constraints functions g_i depend only on position, i.e.,

$$g_i(q, p) = g_i(q)$$

then:

- Coisotropy always holds
- Fibres are vector spaces $\implies$ always parametrizable
- One assumes $g' H_{pp} g'$ invertible $\iff$ nondegeneracy

“Hopf Oscillator”

Example of a new system we can handle

$$z = (q_1, q_2, p_1, p_2) \in \mathbf{R}^4$$

$$g = \|\mathbf{q}\|^2 + \|\mathbf{p}\|^2 - 1$$

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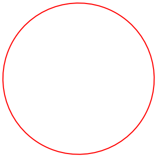

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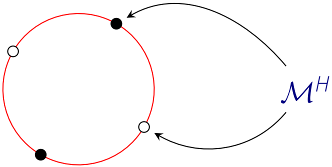

$$H = \frac{\|\mathbf{p}\|^2}{2}$$

“Hopf Pendulum”

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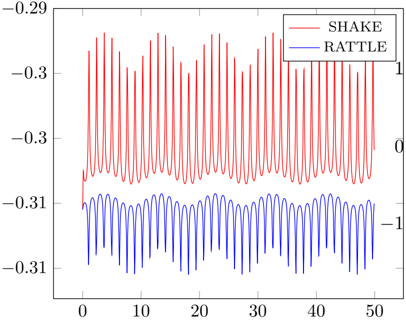

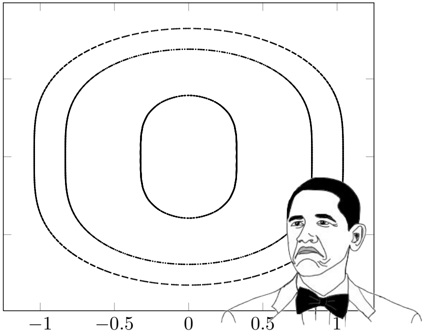

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Thank you for your attention

KUNGL. VETENSKAPS-AKADEMIEN
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