Moser-Veselov Integrators for a Geometrically Exact Rod Model

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Geometric Integrators for Continuum Dynamics, Ph.D. thesis, Department of Mathematics, Imperial College, 2007. Advisors: D.D. Holm and S. Reich

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Talk Outline

I A brief description of the geometrically exact elastic rod model

II A review of Moser-Veselov integrators for the body and spatial representations of the free rigid body

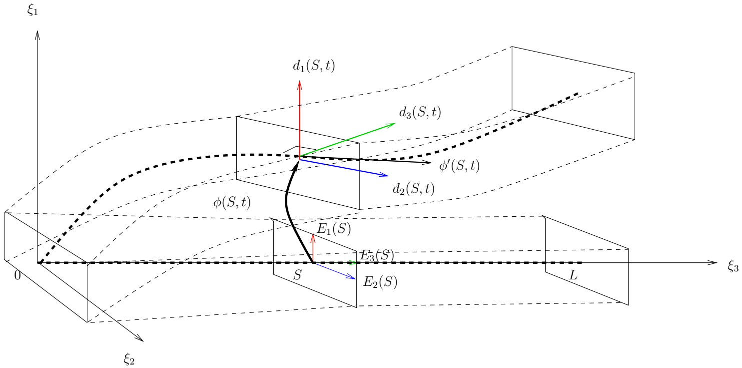
III Derivation of an adaptive discrete Moser-Veselov (DMV) algorithm

IV Application to the discrete geometrically exact elastic rod model

Background

- Holm, D.D. , Marsden, J.E. and Ratiu, T.S. [1986], *The Hamiltonian Structure of Continuum Mechanics in the Material, Inverse Material, Spatial and convected Representations*, Montreal university lectures notes.
- Simo, J.C., Krishnaprasad, P.S. and Marsden, J.E. [1988], *The Hamiltonian Structure of Nonlinear Elasticity: The convected Representation. of Solids, Rods, and Plates*, Arch. Rat. Mech.
- J. Moser and A.P. Veselov [1991], *Discrete Version of Some Classical Integrable Systems and Factorization of Matrix Polynomials*, Comm. Math. Phys.
- Lewis, D. and Simo J.C. [1994], *Conserving algorithms for the dynamics of Hamiltonian systems on Lie groups*, J. Nonlinear Sci.
- West, M. [2004], *Variational Integrators*, Ph.D. thesis, Caltech.
- Cotter, C.J. and Holm D.D. [2007], *Continuous and discrete Clebsch variational principles*, Found. Comp. Math.

The Geometrically Exact Elastic Rod [SKM88]



animate MV Integrator

The Configuration Space

- There exists a unique orthogonal transformation

$$\Lambda_t : [0, L] \to SO(3) \quad : d_i(S,t) = \Lambda_t(S) E_i(S,t), \; i := 1 \to 3,$$

  from the inertial frame $\{E_i\}_{i:=1\to 3}$ to the set of directors.
- The configuration space is

$$\mathcal{C} := \{\Psi := \{\phi, \Lambda\} \mid [0, L] \to \mathbf{R}^3 \times SO(3)\}$$

Notational overview

	Material axial	Convected angular
Velocity	$\mathcal{V}(S,t) := \Lambda^T(S,t)\dot{\phi}(S,t)$	$\Omega(S,t) := \Lambda^T(S,t)\dot{\Lambda}(S,t)$
Strain	$\Gamma(S,t) := \Lambda^T(S,t)(\phi'(S,t) - d_3(S,t))$	$\hat{\Omega}(S,t) := \Lambda^T(S,t)\Lambda'(S,t)$
Momentum	$\mathfrak{m}(S,t) := \rho_0 A\mathcal{V}(S,t)$	$M(S,t) := I_0\Omega(S,t)$
Dual of strain	$\mathfrak{n}(S,t) := C_0\Gamma(S,t)$	$N(S,T) := C_0\hat{\Omega}(S,t)$

The Geometrically Exact Elastic Rod Model

In the convected representation, the Lagrangian $L : SO(3)/T\mathcal{C} \to \mathbf{R}$ takes the form

$$\mathsf{L}\Big((\phi,\Lambda),(\mathcal{V},\Omega);(\Gamma,\hat{\Omega})\Big) = \frac{1}{2}\int_0^L \langle \mathfrak{m},\mathcal{V}\rangle + \langle M,\Omega\rangle dS - \frac{1}{2}\int_0^L \langle \mathfrak{n},\Gamma\rangle + \langle N,\hat{\Omega}\rangle dS$$

The equations of motion

$\dot{\mathfrak{m}}$	$= \mathfrak{n}' + \hat{\Omega}\times\mathfrak{n} - \Omega\times\mathfrak{m}$	axial momentum
$\dot{M}$	$= M' + \hat{\Omega}\times M + \Gamma\times N - \Omega\times M$	convected angular momentum
$\dot{\Gamma}$	$= \mathcal{V}' + \hat{\Omega}\times\mathcal{V} - \Omega\times\Gamma$	axial strain
$\dot{\hat{\Omega}}$	$= \Omega' + \hat{\Omega}\times\Omega$	convected angular strain

Preliminaries of Continuum Dynamics

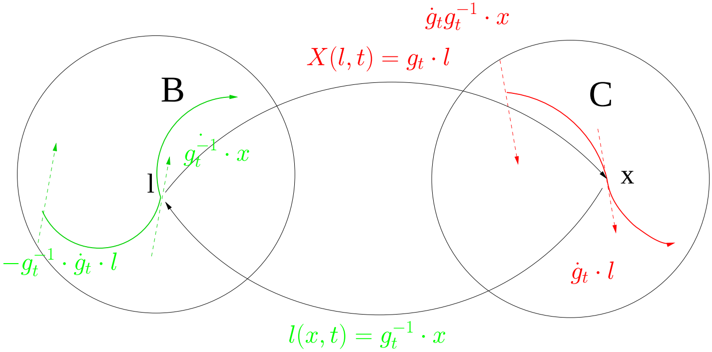
- The *motion* of a material point $\ell \in \mathbb{B}$ is a time dependent curve $g_t \in \text{Diff}(\mathbb{B})$ defining a trajectory of the material point in the container $\mathcal{C}$

$$\text{Forward Map:} \qquad \mathbf{x}(t, \ell) = g_t \cdot \ell, \quad \ell \in \mathbb{B}$$

- The motion of a (fixed) spatial point $\mathbf{x} \in \mathcal{C}$, is a time dependent curve $g_t^{-1} \in \text{Diff}(\mathcal{C})$ defining a trajectory of the spatial point in the reference space

$$\text{Inverse Map:} \qquad \ell(t) = g_t^{-1} \cdot \mathbf{x}, \quad \mathbf{x} \in \mathcal{C}$$

The Forward and Inverse Maps



Spatial and convected Velocities

- The *spatial velocity* is the time derivative of the motion evaluated at a fixed spatial point and takes the right invariant form

$$\mathbf{u}(\mathbf{x}, t) = \dot{g}_t g_t^{-1} \cdot \mathbf{x}$$

- The *convected velocity* is the time derivative of the motion of a spatial point, evaluated at a fixed material coordinate and takes the left invariant form

$$V(\ell, t) = -g_t^{-1}\dot{g}_t \cdot \ell$$

- Holm, Marsden and Ratiu [1986] show that the convected and spatial representations of Hamiltonian dynamics correspond to the body and spatial representations of free rigid body dynamics.

Discrete Motion of the Rigid Body [MR99]

- The configuration of a body $\mathcal{B}$ may be identified with the matrix $SO(3)$ and the $k \in \mathbb{Z}^+$ parameterised sequence of spatial points in $\mathbb{R}^3$ is given by

$$\mathbf{x}_k = \Lambda_k \ell, \quad \Lambda_k := \Lambda(t_k) \in SO(3).$$

  where Λ_k is the *attitude* of the body at time t_k.
- Spatial coordinates are the components of the spatial points relative to the fixed Eulerian frame $(\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3)$
- *Body* coordinates are the components of the material points relative to the frame attached to the body $(\xi_1^k, \xi_2^k, \xi_3^k)$ as given by

$$\xi_i^k = \Lambda_k \mathbf{E}_i, \quad i := 1 \to 3.$$

Discrete Body and Spatial Discrete Velocities

- Define the recursive relations

$$\ell_{k+1} = \Omega_{k+1}^T \ell_k,$$

and

$$\mathbf{x}_{k+1} = \omega_{k+1} \mathbf{x}_k.$$

- $\Omega_{k+1} := \Lambda_k^T \Lambda_{k+1}$ is referred to by Moser and Veselov [MV91] as the discrete body angular 'velocity'.
- $\omega_{k+1} := \Lambda_{k+1} \Lambda_k^T$ is the discrete spatial angular 'velocity'. The two discrete velocities are related to each other by

$$\Omega_{k+1} = \Lambda_k^T \omega_{k+1} \Lambda_k.$$

Discrete Action Principle for the Rigid Body

- [MV91] consider a discrete action principle

$$S_d = \sum_k \mathcal{L}(\Lambda_k, \Lambda_{k+1}),$$

- The discrete time Lagrangian $\mathcal{L} : SO(3) \times SO(3) \to \mathbb{R}$ is a smooth function defined as

$$\mathcal{L}(\Lambda_k, \Lambda_{k+1}) = Tr(\Lambda_k I_0 \Lambda_{k+1}^T),$$

- I_0 is a positive definite, symmetric and constant matrix and

Symmetry Reduction to the Body Representation

Definition

The (left) ***diagonal action*** *of G on G × G is defined as*
$\Psi_f : G \times (G \times G) \to G \times G \mid \Psi(f, (g, h)) = f \cdot (g, h) = (fg, fh).$

- The discrete time Lagrangian $\mathcal{L}$ is invariant under the (left) action of Ψ.
- Reduce the Lagrangian on $SO(3) \times SO(3)$ by Ψ to obtain the reduced Lagrangian $\mathbf{l} : SO(3) \to \mathbb{R}$ given in body variables by

$$\mathbf{l}(\Omega_{k+1}) = Tr(\Omega_{k+1} I_0), \qquad \Omega_{k+1} := \Lambda_k^T \Lambda_{k+1}.$$

- The principal G-Bundle $(G \times G, G, \pi)$ and natural projection $\pi : G \times G \to G \times G/G$ furnish the description of discrete symmetry reduction to the body representation.

Constrained Lagrangian Dynamics in Vector Spaces

- Marsden and Wendlandt (1997) embed $SO(3)$ in the linear space $\mathcal{V}$ of real 3×3 matrices, the symmetric part of which is denoted V.
- Define the reduced discrete Lagrangian $l : \mathcal{V} \to \mathbb{R}$ (in body variables) which takes the form

$$l^c(\Omega_{k+1}) = Tr(\Omega_{k+1} I_0) - Tr\left(\Theta_{k+1}(\Omega_{k+1}\Omega_{k+1}^T - I_d)\right)$$

- The matrix Lagrange multipliers $\Theta_{k+1} \in V^*$ constrain the family of curves extremising $\delta S_d = \sum_k \delta l^c(\Omega_{k+1})$ to $SO(3)$.

Clebsch Potentials and Momentum Maps

- (Cotter and Holm 2007) Clebsch potentials are added to l^c

$$\tilde{l}^{k+1} = l^c(\Omega_{k+1}) + Tr\left(P_{k+1}^T(\Lambda_{k+1} - \Lambda_k \Omega_{k+1})\right)$$

- Extremising $\delta S_d = \sum_k \delta \tilde{l}^{k+1}$ gives the discrete symplectic flow

$$\mathbf{z}_{k+1} = \Phi'_{\Omega_{k+1}}(\mathbf{z}_k), \; \mathbf{z}_k := [\Lambda_k, \; P_k]$$

- The right momentum map $J_{k+1}^R : T^*G \to \mathfrak{g}^*$ for cotangent lifted actions of G on T^*G is

$$J_{k+1}^R(z_k) = P_k \diamond \Lambda_k$$

where $\diamond : \mathcal{V}^* \times \mathcal{V} \to \mathfrak{g}^*$ is defined by the pairing

$$\langle P_k \diamond \Lambda_k, \zeta \rangle = \langle P_k, \zeta \Lambda_k \rangle.$$

Clebsch Potentials and Momentum Maps

- Under the symplectic flow, the pre-image of the momentum map is updated by

$$\Lambda_k^T P_k = \Omega_k^T \Lambda_{k-1}^T P_{k-1} \Omega_k .$$

- J_{k+1}^R projects the skew-symmetric component of this equation onto $\mathfrak{so}(3)^*$ to give the Moser-Veselov integrator

$$\boxed{M_{k+1} = Ad^*_{\Omega_k} M_k, \quad M_{k+1} = I_0 \Omega_{k+1}^T - \Omega_{k+1} I_0,}$$

where the body angular momentum $M_{k+1} \in \mathfrak{so}(3)^*$ is defined as

$$M_{k+1} := 2skew(\nabla_{\Omega_{k+1}} l^k \Omega_{k+1}^T).$$

The Body Representation in Continuous and Discrete Time

Property	Continuous	Discrete
Body attitude	$\Lambda(t) \in SO(N)$	$\Lambda_k \in SO(N)$
Angular velocity	$\Omega = \Lambda^T \dot{\Lambda} = -\Omega^T$	$\Omega_{k+1} = \Lambda_k^T \Lambda_{k+1}$
Angular momentum	$M = I_0 \Omega - \Omega^T I_0$	$M_k = I_0 \Omega_k^T - \Omega_k I_0$
Equations of motion	$\dot{M} = ad^*_{\Omega} M$	$M_{k+1} = Ad^*_{\Omega_k} M_k$
Right momentum map	$J_R = P \diamond \Lambda$	$J_R^{k+1} = P_k \diamond \Lambda_k$

Equivariant MV integrators for body and spatial representations of the rigid body

$$\dot{M} = ad^*_\Omega M \quad \underset{Ad^*_\Lambda(M, I_0)}{\overset{Ad^*_{\Lambda^{-1}}(m, I)}{\rightleftarrows}} \quad \dot{m} = ad^*_\omega m + \nabla_I l_I \diamond I, \quad \dot{I} = [\omega, I]$$

$$\downarrow \Omega \approx \frac{\Lambda_k^T}{h}(\Lambda_{k+1} - \Lambda_k) \qquad \omega \approx (\Lambda_{k+1} - \Lambda_k)\frac{\Lambda_k^T}{h} \downarrow$$

$$M_{k+1} = Ad^*_{\Omega_k} M_k \quad \underset{Ad^*_{(\Lambda_k)}(M_k, I_0)}{\overset{Ad^*_{(\Lambda_k)^{-1}}(m_k, I_k)}{\rightleftarrows}} \quad m_{k+1} = Ad^*_{\omega^T_{k+1}}(m_k + 2\nabla_{I_k} l_{I_k} \diamond I_k)$$

$$I_{k+1} = \omega_{k+1} I_k \omega^T_{k+1}$$

Body

▸ Spatial

Homogeneous Elasticity: Ellipsoidal Motion

- Consider the Lagrangian of the continuous time ellipsoidal motion

$$L = \frac{1}{2}\int_{\mathcal{B}} \rho(\ell)\langle \dot{Q}\cdot\ell, C_0\dot{Q}\cdot\ell\rangle d^n\ell = \frac{1}{2} Tr\left(C_0\dot{Q}I_0\dot{Q}^T\right),$$

- where $C_0 \in V$ is the *Cauchy-Green* metric defining the shape of the container, $I_0 \in V^* : (I_0)_{ab} = \int_{\mathcal{B}} \rho(\ell)\ell^a\ell^b d^n\ell$ is the *shape matrix* of the body.
- The *deformation gradient* $\partial x^i/\partial \ell_j = Q_{ij}(t) \in GL^+(n)$ is spatially invariant.

The Isotropic Pseudo-Rigid Body

- As a special case, consider the continuous time Lagrangian defined on $TGL(3)^+$ of the form

$$L = \frac{Tr}{2}(\dot{Q}\dot{Q}^T), \quad Q \in GL(3)^+$$

- Polar decompose $Q = R^T DS$ where $R, S \in SO(3)$ and D is a diagonal matrix with positive determinant.
- Rewrite the Lagrangian in terms of the angular velocities $\Omega := \dot{R}R^T$ and $\mathfrak{s} = \dot{S}S^T$ to give

$$l = \frac{Tr}{2}\left(-\Omega^2 D^2 - \mathfrak{s}^2 D^2 + 2\Omega D \mathfrak{s} D + \dot{D}^2\right), \quad \Omega = \dot{R}R^T, \quad \mathfrak{s} = \dot{S}S^T$$

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The discrete Isotropic Pseudo-Rigid Body

- The discrete action principle for the isotropic pseudo-rigid body

$$\begin{aligned} S_d = \sum_k Tr\left(\Omega_{k+1}^T \mathfrak{s}_{k+1}\right) - \frac{Tr}{2}\left(P_{k+1}^T (Q_{k+1} - \mathfrak{u}_{k+1} Q_k)\right) \\ - Tr\left(\Theta_{k+1}^R (\Omega_{k+1}\Omega_{k+1}^T - I_d)\right) - Tr\left(\Theta_{k+1}^S (\mathfrak{s}_{k+1}\mathfrak{s}_{k+1}^T - I_d)\right) \end{aligned}$$

$\Omega_{k+1} := R_{k+1} R_k^T$, $\mathfrak{s}_{k+1} := S_{k+1} S_k^T$ and $\mathfrak{u}_{k+1} := Q_{k+1} Q_k^T$

- Variations in Q_k and P_k give the symplectic equations

$$\begin{aligned} P_{k+1} &= \mathfrak{u}_{k+1} P_k \,, \\ Q_{k+1} &= \mathfrak{u}_{k+1} Q_k \,, \end{aligned}$$

The Discrete Lagrangian for a Mooney-Rivlin Pseudo-Rigid Body

- Adding a Mooney-Rivlin potential $W(D_k)$,

$$\begin{aligned} l_k^c = & \frac{Tr}{2}\{(4(\Omega_{k+1} + \mathfrak{s}_{k+1}) - 6I_d)D_k^2 \\ & - 2\Omega_{k+1}D_k\mathfrak{s}_{k+1}D_k - (D_{k+1} - D_k)^2\} \\ & - \frac{Tr}{2}\left(\Theta_{k+1}^S(\mathfrak{s}_{k+1}\mathfrak{s}_{k+1}^T - I_d)\right) \\ & - \frac{Tr}{2}\left(\Theta_{k+1}^R(\Omega_{k+1}\Omega_{k+1}^T - I_d)\right) - h^2 W(D_k) \end{aligned}$$

where

$$W(D_k) = aI_1(D_k^2) + bI_2(D_k^2) + c|D_k|^2 - dLog(|D_k|), \;\; a, b, c, d > 0.$$

Elastic Motion of a Mooney-Rivlin Pseudo-Rigid Body

- The two momentum maps take the form

$$M_{k+1} := J(\mathfrak{s}_{k+1})\Omega_{k+1}^T - \Omega_{k+1}J^T(\mathfrak{s}_{k+1}) = P_{k+1}^R R_{k+1}^T,$$
$$N_{k+1} := J(\Omega_{k+1})\mathfrak{s}_{k+1}^T - \mathfrak{s}_{k+1}J^T(\Omega_{k+1}) = P_{k+1}^S S_{k+1}^T.$$

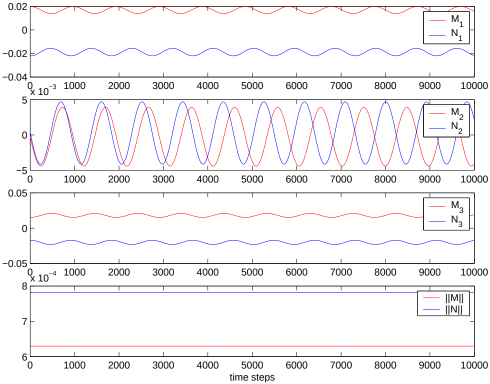
- Momentum updates of the rotational components

$$Ad^*_{\Omega_{k+1}} M_{k+1} = M_k,$$
$$Ad^*_{\mathfrak{s}_{k+1}} N_{k+1} = N_k.$$

- Additive update of the stretching component

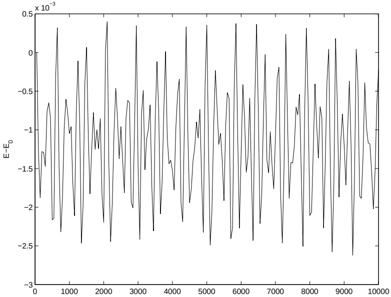
$$D_{k+1} = -4\pi_D(-\Omega_{k+1} + 2I_d - \mathfrak{s}_{k+1})D_k$$
$$+ \pi_D(\Omega_{k+1}D_k\mathfrak{s}_{k+1} + \mathfrak{s}_{k+1}D_k\Omega_{k+1}) - D_{k-1} + h^2\nabla_{D_k}W(D_k).$$

A Mooney-Rivlin Pseudo-Rigid Body: angular momentum and vorticity

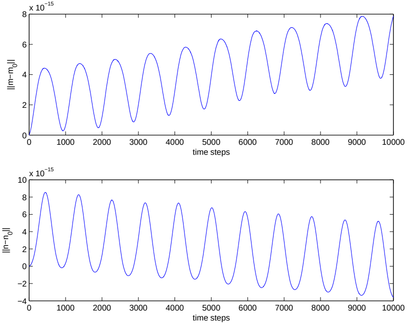


$\Delta t = 0.05$, $(d_1 = 1,\ d_2 = 0.8,\ d_3 = 1/0.8)$ and the Mooney-Rivlin parameters are $a = 0.1, b = 10, c = 10, d = 50.$

A Mooney-Rivlin Pseudo-Rigid Body: energy, angular momentum and vorticity error



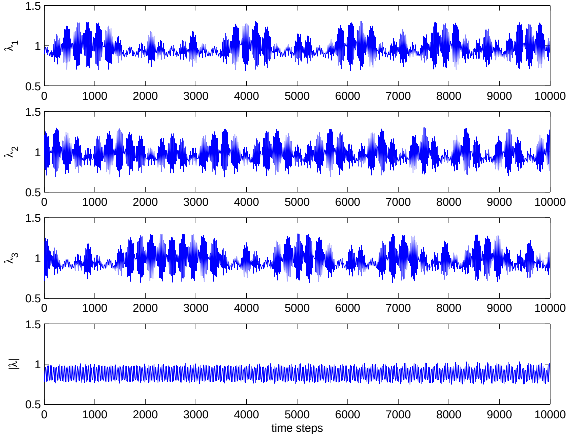
(a) Energy error



(b) momentum/vorticity error

$\Delta t = 0.05$, $(d_1 = 1,\ d_2 = 0.8,\ d_3 = 1/0.8)$ and the Mooney-Rivlin parameters are $a = 0.1, b = 10, c = 10, d = 50$.

The Eigenvalues of a Mooney-Rivlin Pseudo-Rigid Body



$\Delta t = 0.05$, $(d_1 = 1,\ d_2 = 0.8,\ d_3 = 1/0.8)$ and the Mooney-Rivlin parameters are $a = 0.1, b = 10, c = 10, d = 50.$

Uniqueness of Orthogonal Solutions

- Solve for $\Omega \in SO(3)$

$$M = I_0 \Omega^T - \Omega I_0$$

- Quadratic in $W = I_0 \Omega^T$

$$W^2 - WM - I_0^2 = 0, \qquad WW^T = I_0^2$$

- For any eigenvalue λ of W

$$det(\lambda^2 I - \lambda M - I_0^2) = 0,$$

- or in matrix form $det(A - \lambda I) = 0$,

$$\text{A=}\begin{bmatrix} 0 & \text{I} \\ \text{I}_0^2 & \text{M} \end{bmatrix}$$

- [MV91] showed that a unique solution W exists if the real part of any root does not vanish.

Reduction to an Algebraic Riccati Equation

Theorem (Cardoso and Leite, 2001)

Ω is an orthogonal solution if and only if $S = sym(I_0\Omega^T)$ is a symmetric solution of the a.r.e.

$$S^2 + S(M/2) + (M/2)^T S - (M^2/4 + I_0^2) = 0.$$

Hamiltonian matrix

$$\mathrm{H}= \begin{bmatrix} \mathrm{M/2} & \mathrm{I} \\ \mathrm{M/2} + \mathrm{I}_0^2 & \mathrm{M} \end{bmatrix}$$

S is found by orthogonalizing the eigenspace of H (Schur form)

Solution of the Algebraic Riccati Equation

1. Find the eigenvectors $v \in V$ of $\mathcal{H}$

$$\mathcal{H}v = \lambda v$$

2. decompose $V = QR$
3. Q= $\begin{bmatrix} Q_{11} & Q_{12} \\ Q_{21} & Q_{22} \end{bmatrix}$
4. $S = Q_{21}Q_{12}^{-1}$
5. $\Omega = (S + M/2)I_0^{-1}$

The DMV algorithm [McLachlan and Zanna]

Algorithm

- Set $M_0^h = M_0 \Delta t$
- For $k := 0 \to N-1$
  1. $\Omega_k^h = (S_k^h + M_k^h/2) I_0^{-1}$
  2. $M_{k+1}^h = \Omega_k^h M_k^h \Omega_k^{h^T}$
- $\Omega_N^h = (S_N^h + M_N^h/2) I_0^{-1}$
- $M_N = M_N^h / \Delta t$.

- Ω_k^h is the unique orthogonal solution of

$$M_k^h = I_0 \Omega_k^{h^T} - \Omega_k^h I_0 = M(t_k) \Delta t$$

- $\Delta t < \Delta t_k^s$

Unique Solution Time-step Constraint

- The characteristic polynomial of A

$$P(\lambda) = det(\lambda^2 I - \lambda M \Delta t_s - I_0^2) = 0$$

- Since $P(\lambda) = P(-\lambda)$, set $z = \lambda^2$ to give the cubic equation[a]

$$z^3 + a_2 z^2 + a_1 z + a_0 = 0.$$

- When $q^3 + r^2 = 0$ the real components of z are zero,

$$\begin{aligned} q &= \tfrac{1}{3} a_1(\Delta t_s) - \tfrac{1}{9} a_2^2(\Delta t_s), \\ r &= \tfrac{1}{6}(a_1(\Delta t_s) a_2(\Delta t_s) - 3a_0) - \tfrac{1}{27} a_2^3(\Delta t_s) \end{aligned}$$

- Solve for Δt_s as a function of $|\mathbf{M}(t)|$ and $H(t)$

[a] $a_2(\Delta t_s) = \Delta t_s^2 |\mathbf{M}|^2 - Tr(I_0^2)$, $a_1(\Delta t_s) = (I_1^2 I_2^2 + I_2^2 I_3^2 + I_3^2 I_1^2 - 2H\Delta t_s^2)$ and $a_0 = -det|I_0^2|$.

Roots of the Characteristic Equation $I_1 = I_2 < I_3$

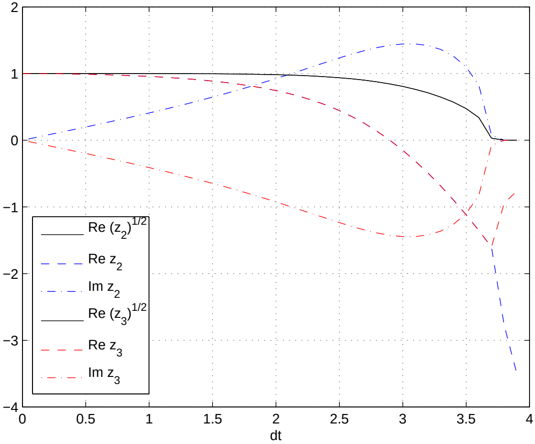


Figure: $I_1 = 1,\ I_2 = 1,\ I_3 = 2,\ M_1(0) = 0.1,\ M_2(0) = 0,\ M_3(0) = 1.$

Roots of the Characteristic Equation $I_1 = I_3 > I_2$

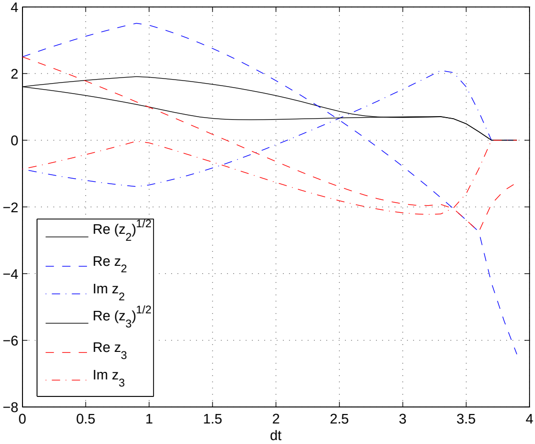


Figure: $I_1 = 2,\ I_2 = 1,\ I_3 = 2,\ M_1(0) = 0.1,\ M_2(0) = 0,\ M_3(0) = 1.$

Roots of the Characteristic Equation $I_1 < I_2 < I_3$

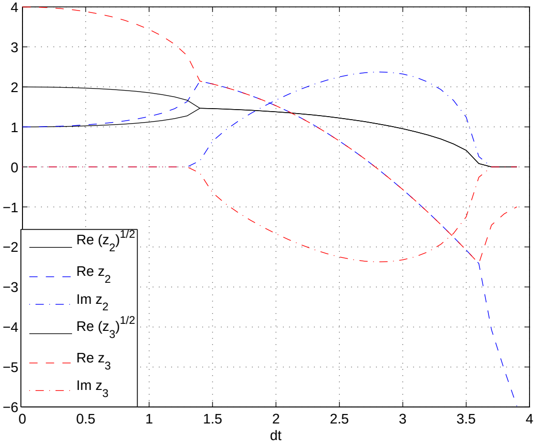


Figure: $I_1 = 1,\ I_2 = 2,\ I_3 = 2,\ M_1(0) = 0.1,\ M_2(0) = 0,\ M_3(0) = 1.$

An Adaptive DMV Algorithm

Algorithm

For $k := 0 \rightarrow N - 1$

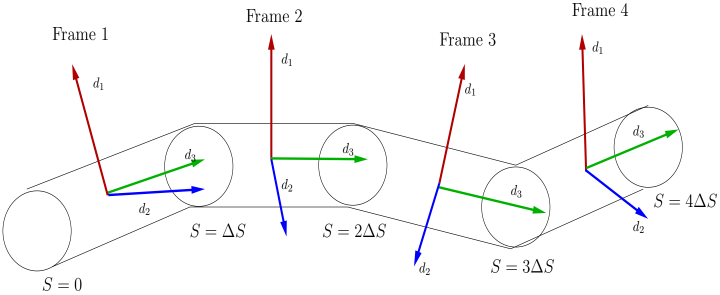
1. $\Omega_k = (S_k + M_k/2)I_0^{-1}$
2. Determine $\Delta t_k^s = f(||\Omega_k M_k {\Omega_k}^T||, H_{k+1})$
3. Set $\Delta t = min(\Delta t, \Delta t_k^s)$
4. $\Omega_k^h = (S_k^h + \frac{M_k}{2\Delta t_k})I_0^{-1}$
5. $M_{k+1} = \Omega_k^h M_k \Omega_k^{h^T}$

Summary of Moser-Veselov Integrators

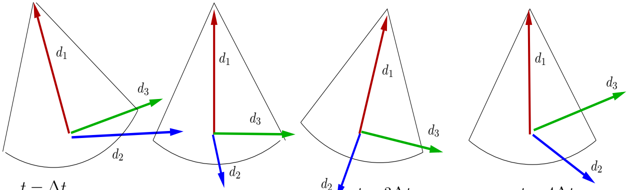
- Discrete Clebsch potentials give momentum maps which encode MV integrators for body and spatial representations of rigid body motions
- A free rigid body DMV algorithm [McLachlan and Zanna] finds the unique symmetric solution to a corresponding algebraic Riccati equation
- An adaptive variant of the DMV algorithm is applicable to coupled rigid body motions

The Discrete Kirchhoff Kinetic Analogy

Kirchhoff rod



Heavy top



Analogy between the Static Elastic Rod and the Lagrange Top

Kirchhoff rod		Lagrange top	
Discrete angular strain at S_α	$\hat{\Omega}_\alpha$	Discrete body angular velocity at time t_k	Ω_k
Stiffness matrix	C_0	Inertia matrix	I_0
Rod tension	$\mathbf{p}_0$	Position of centre of mass	χ_0
Tangent vector at S_α	$\mathbf{t}_\alpha$	Orientation of gravity vector at time t_k	Γ_k

Preliminaries

Definition (Discrete Ribbon)

A discrete ribbon is a space curve $\{\phi(S_\alpha)\}$ parameterised by arc-length $S_\alpha \in \{\alpha\Delta S,\ \alpha := 0 \to N\}$ with three smooth orthonormal unit vectors $\{\mathbf{d}_1, \mathbf{d}_2, \mathbf{d}_3\}(S_\alpha)$.

- The discrete angular strain $\hat{\Omega}_{\alpha+1} := \Lambda_\alpha^T \Lambda_{\alpha+1}$
- $\mathbf{p}_0$ enforces the inextensibility constraint $\phi(S_N) - \phi(S_1) = \sum_\alpha \mathbf{t}(S_\alpha)$.

Preliminaries

Definition (Discrete Elastic Rod)

A discrete elastic rod is an arc-length S_α parameterised ribbon of fixed length L extremizing the functional

$$F_d = \sum_{\alpha=1}^{N} l_c(\hat{\Omega}_\alpha) = \underbrace{\sum_{\alpha=1^N} \langle C_0, \hat{\Omega}_{\alpha+1}\rangle}_{\text{elastic energy}} - \underbrace{\langle \mathbf{p}_0, \mathbf{t}_\alpha \rangle}_{\text{inextensibility constraint}}$$

The Discrete Elastic Rod

- The Moser-Veselov integrator is

$$N_{\alpha+1} = Ad^*_{\hat{\Omega}^T_\alpha} N_\alpha + 2\nabla_{\mathbf{t}_\alpha} l_{\mathbf{t}\alpha} \diamond \mathbf{t}_\alpha,$$
$$\mathbf{t}_{\alpha+1} = \hat{\Omega}_\alpha \mathbf{t}_\alpha.$$

- The dual to the angular strain N is given by $N_\alpha := \frac{2}{h^2} skew\left((\nabla_{\hat{\Omega}_{\alpha+1}} l_c)^T \hat{\Omega}_{\alpha+1} \right)$ and
- $\mathbf{t}_\alpha := \mathbf{t}(S_\alpha)$ is the unit tangent vector to the curve at S_α.
- The map $(N_\alpha, \mathbf{t}_\alpha) \mapsto (N_{\alpha+1}, \mathbf{t}_{\alpha+1}) \in \mathfrak{g}^* \times (\mathbb{R}^3)$, is Poisson w.r.t. to the $(\pm)$ Lie-Poisson brackets on $\mathfrak{s}^* = \mathfrak{g}^* Ⓢ \mathbb{R}^3$.

The Dynamic Discrete Elastic Rod

- The discrete Lagrangian takes the form

$$l_c = \sum_{\alpha=1}^{N} \underbrace{Tr(\Omega_{\alpha+1}^{k\;T} I_0)}_{\text{kinetic energy}} + \underbrace{Tr(\hat{\Omega}_{\alpha+1}^{k\;T} C_0)}_{\text{elastic potential energy}} - \underbrace{\langle \mathbf{p}_0, \mathbf{t}_\alpha^k \rangle}_{\text{extensibility constraint}}$$

- The Moser-Veselov integrator is

$$\boxed{\begin{aligned} M_\alpha^{k+1} &= Ad^*_{\Omega_\alpha^{k\;T}} M_\alpha^k + Ad^*_{\hat{\Omega}_\alpha^{k\;T}} N_\alpha^k - N_{\alpha+1}^k + 2\nabla_{\mathbf{t}_\alpha^k} l_{\mathbf{t}_\alpha^k} \diamond \mathbf{t}_\alpha^k, \\ \mathbf{t}_\alpha^{k+1} &= \Omega_\alpha^k \mathbf{t}_\alpha^k. \end{aligned}}$$

- $M := \frac{2}{h^2} skew\left((\nabla_{\Omega_\alpha^{k+1}} l_c)^T \Omega_\alpha^{k+1} \right)$ and
$N := \frac{2}{h^2} skew\left((\nabla_{\hat{\Omega}_{\alpha+1}^k} l_c)^T \hat{\Omega}_{\alpha+1}^k \right).$

The Dynamic Discrete Elastic Rod

Property (Discrete compatibility equation)

The time evolution of the discrete angular strain can be expressed interms of discrete angular velocities at consecutive spatial points through the relation

$$\boxed{\hat{\Omega}_{\alpha+1}^{k+1} = \Omega_{\alpha+1}^{k+1} \hat{\Omega}_{\alpha+1}^{k} \Omega_{\alpha}^{k+1}}$$

The Geometrically Exact Elastic Rod [SKM88]

- The discrete Lagrangian for an *extensible* and *shearable* rod

$$l_c = \sum_{\alpha=1}^{N} \underbrace{\frac{\rho_0}{2} A |\mathcal{V}_\alpha^k|^2 + Tr(I_0 \Omega_\alpha^{k+1\,T})}_{\text{kinetic energy}} - \underbrace{Tr(C_0^\wedge \hat{\Omega}_{\alpha+1}^{k}{}^{T}) - \langle \Gamma_\alpha^k, C_0^\phi \Gamma_\alpha^k \rangle}_{\text{potential energy}}$$

- Two momentum equations in the convected representation are

$$\begin{aligned} \mathfrak{m}_\alpha^{k+1} &= \Omega_\alpha^{k\,T} \mathfrak{m}_\alpha^k - \mathfrak{n}_{\alpha+1}^k + \hat{\Omega}_\alpha^{k\,T} \mathfrak{n}_\alpha^k, \\ M_\alpha^{k+1} &= Ad^*_{\Omega_\alpha^{k\,T}} M_\alpha^k + Ad^*_{\hat{\Omega}_\alpha^{k\,T}} N_\alpha^k - N_{\alpha+1}^k + 2\nabla_{\Gamma_\alpha^k} l_{\Gamma_\alpha^k} \diamond \Gamma_\alpha^k \end{aligned}$$

- The total spatial angular momentum and linear material momentum are conserved.

The Geometrically Exact Elastic Rod

	Axial material	Convected angular
Velocity	$\mathcal{V}_\alpha^k := \frac{\Lambda_\alpha^{k\,T}}{h}(\phi_\alpha^{k+1} - \phi_\alpha^k)$	$\Omega_\alpha^{k+1} := \Lambda_\alpha^{k\,T}\Lambda_\alpha^{k+1}$
Strain	$\Gamma_\alpha^k := \frac{\Lambda_\alpha^{k\,T}}{h}(\phi_{\alpha+1}^k - \phi_\alpha^k - h(\mathbf{d}_3)_\alpha^k)$	$\hat{\Omega}_{\alpha+1}^k := \Lambda_\alpha^{k\,T}\Lambda_{\alpha+1}^k$
Momentum	$\mathfrak{m}_\alpha^k := \rho_0 A \mathcal{V}_\alpha^k$	$M_\alpha^k := I_0 \Omega_\alpha^{k\,T} - \Omega_\alpha^k I_0$
Dual of strain	$\mathfrak{n}_\alpha^k := C_0 \Gamma_\alpha^k$	$N_\alpha^k := C_0 \hat{\Omega}_\alpha^{k\,T} - \hat{\Omega}_\alpha^k C_0$

◂ Diagram

Experiment 1: Initial Conditions

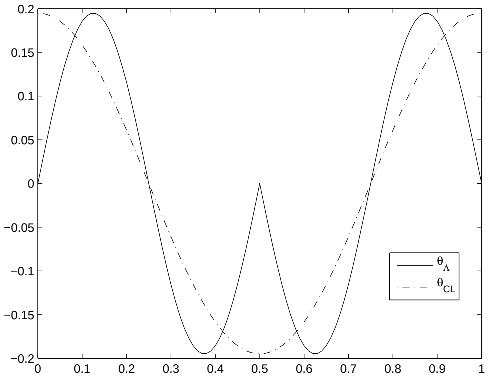
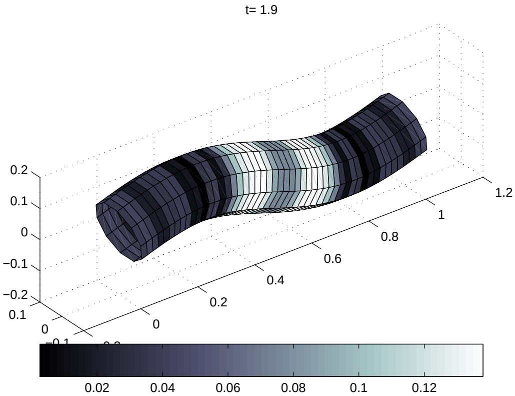


Figure: $\Delta t = 0.01$, $N = 50$ and $\phi_i(t_0) = \{0, 0, a_0 sin(\frac{2\pi}{L} S_i)\}$, $a_0 = 2\pi \times 10^{-2}$ and $\Lambda_1^k = \Lambda_N^k = I_d$, $\forall k$.

Numerical Simulation: Shearing motion



animate 1 animate 2[a]

[a] Colormap variable: $|\phi' - d_3|$ is a measure of shear.

Numerical Simulation: Angular Momentum Distribution

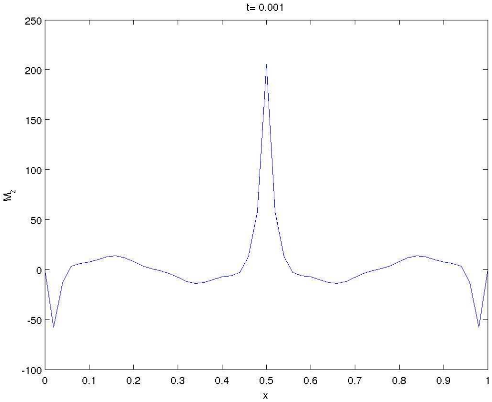
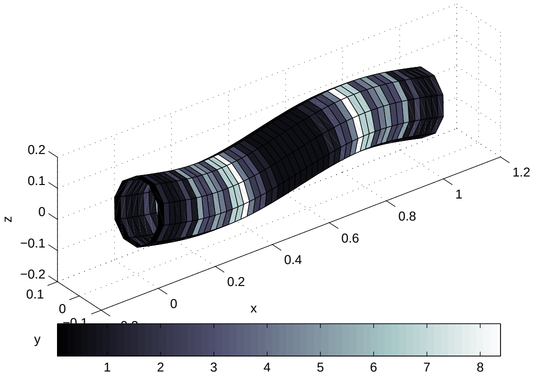


Figure: $\Delta t = 0.01$, $N = 50$ and $\phi_i(t_0) = \{0, 0, a_0 sin(\frac{2\pi}{L} S_i)\}$, $a_0 = 2\pi \times 10^{-2}$ and $\Lambda_1^k = \Lambda_N^k = I_d$, $\forall k$.

animate

Numerical Simulation: Time constraint



animate[a]

[a] Colormap variable is t_k^s.

Experiment 2: Energy Conservation

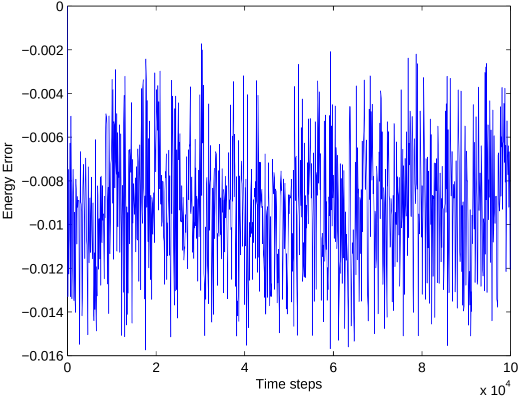


Figure: $\Delta t = 0.1$, $N = 50$ and $\phi_i(t_0) = 0.1\{sin(\frac{\pi}{2}S_i), 0, sin(\frac{\pi}{2}S_i)\}$

Numerical Results: Linear Momentum Conservation

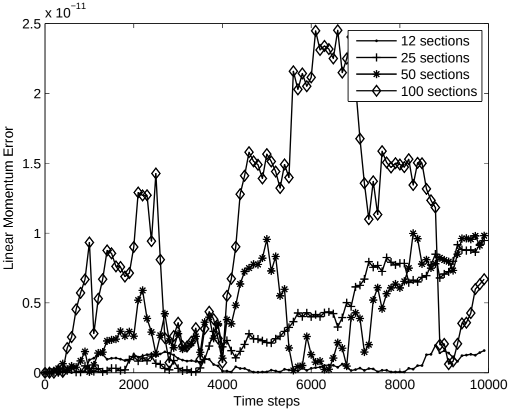


Figure: $\Delta t = 0.1$, $N \in \{12, 25, 50, 100\}$ and $\phi_i(t_0) = 0.1\{sin(\frac{\pi}{2}S_i), 0, sin(\frac{\pi}{2}S_i)\}$

Numerical Results: Angular Momentum Conservation

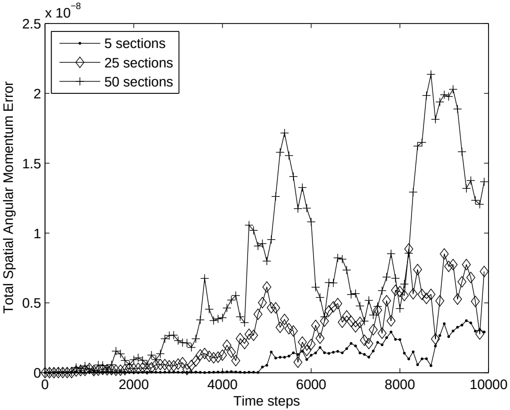


Figure: $\Delta t = 0.1$, $N \in \{5, 25, 50\}$ and $\phi_i(t_0) = 0.1\{sin(\frac{\pi}{2} S_i), 0, sin(\frac{\pi}{2} S_i)\}$

Summary

- Used a discrete Kirchhoff analogy to extend MV integrators to elastic rod motions
- Adaptive time stepping is the key to running high resolution long-time simulations
- The MV integrator remains robust under large shearing and bending potential gradients across the geometrically exact rod model without adding numerical dissipation
- The MV integrator for the geometrically exact rod preserves energy to $\mathcal{O}(\Delta t)$ and angular and linear momentum to numerical round-off

Future Work

- Future work to apply a ▸ $SU(2)$ DMV algorithm to the quaternionic formulation of the rod model
- Extend the approach to geometrically exact thin shells and plate models [a]
- Apply MV integrators to study the dynamics of charged molecular strands[b]

---

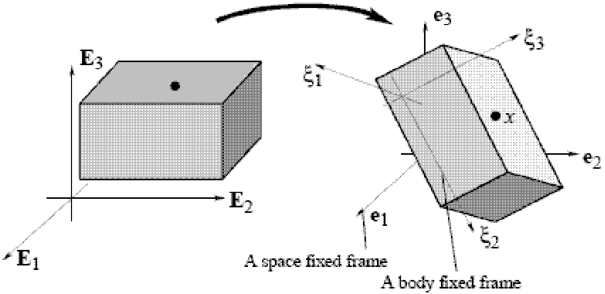
[a] J.C. Simo, P.S. Krishnaprasad and J.E. Marsden [1988], *The Hamiltonian Structure of Nonlinear Elasticity: The convected Representation of Solids, Rods, and Plates*, Arch. Rat. Mech.

[b] D. C. P. Ellis, F. Gay-Balmaz, D. D. Holm, V. Putkaradze and T. S. Ratiu [2009], *Dynamics of charged molecular strands*, arXiv.org:0901.2959

Extra frames

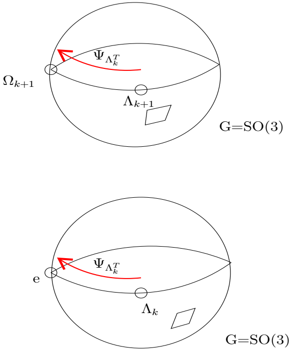
Material, Body and Spatial Coordinates

Back



Aside: The Principal G-Bundle[LMW04]

Back



The principle G-bundle consists of a bundle space $Q = G \times G$, a shape space $S = G \simeq G \times G/G$ (not shown on the Figure) and a projection $\pi : Q \longrightarrow S$ which is isomorphic to the natural projection $\pi_{Q/G} = Q \longrightarrow G \times G/G$. At time t_k, this natural projection is defined by the diagonal action of Λ_k^T on $(\Lambda_k, \Lambda_{k+1})$ and is illustrated by the two curved arrows.

Momentum Map

Back

Definition (Momentum Map (MR99))

Let G act canonically on a Poisson manifold P. A momentum map for this action is a map $J : P \to \mathfrak{g}^*$ such that the map

$$J_\zeta : P \to \mathfrak{F}(P) \ : \ J_\zeta(\mathbf{z}) = \langle J(\mathbf{z}), \zeta \rangle$$

satisfies

$$X_{J_\zeta} = \zeta_P, \quad \forall \zeta.$$

Symmetry Reduction to the Spatial Representation

Back

- Consider the Lagrangian defined on the *augmented* space,

$$L_{I_0} : SO(3)\times SO(3)\times V^* \to \mathbb{R} \mid L_{I_0}(\Lambda_k, \Lambda_{k+1}, I_0) = Tr(\Lambda_k I_0 \Lambda_{k+1}^T)$$

Definition

The (right) ***augmented diagonal action*** *of* G *on* $G \times G \times V^*$ *is defined as* $\hat{\Psi}_f : (G \times G \times V^*) \times G \to G \times G \times V^* \mid \hat{\Psi}((g, h, a), f) = (g, h, a) \cdot f = (gf, hf, f^{-1}af^{-T})$.

- Reduce L by $\hat{\Psi}$ to give

$$l_{I_k}(\omega_{k+1}, I_k) = Tr(\omega_{k+1} I_k).$$

- ω_{k+1} is the (right invariant) spatial angular "velocity" and I_k is the inertia matrix in the spatial frame.

Clebsch Potentials and Momentum Maps

Back

- The spatial representation of the Lagrangian with Clebsch potentials is

$$\tilde{l}_{l_k} := Tr\,(I_k\omega_{k+1}) + \underbrace{\frac{Tr}{2}(P_{k+1}^T(\Lambda_{k+1} - \omega_{k+1}\Lambda_k)}_{\text{Clebsch constraint for } \Lambda_k}$$

$$+ \underbrace{\frac{Tr}{2}(J_{k+1}(I_{k+1} - \omega_{k+1}I_k\omega_{k+1}^T))}_{\text{Clebsch constraint for } I_k} - Tr\left(\Theta_{k+1}(\omega_{k+1}\omega_{k+1}^T - I_d)\right).$$

Clebsch Potentials and Momentum Maps

Back

- Extremising the discrete action principle gives the recursion relations

$$P_{k+1} = \omega_{k+1}^{-T} P_k \, ,$$
$$J_{k+1} = \omega_{k+1} (2 \nabla_{l_k} l_{l_k} + J_k) \omega_{k+1}^T \, .$$

- The infinitesimally equivariant *left* momentum map of the general form

$$J_{k+1}^L = \Lambda_k \diamond P_k + J_k \diamond l_k \, ,$$

for cotangent lifted actions of $\zeta \in \mathfrak{g}$ on the augmented cotangent bundle $T^*(G \times V^*)$.

The Spatial Moser-Veselov Integrator

Back

- The spatial Moser-Veselov integrator

$$Ad^*_{\omega_{k+1}} m_{k+1} = m_k + 2\nabla_{l_k} l_{l_k} \diamond l_k\,,$$
$$l_{k+1} = \phi_{\omega_{k+1}}(l_k),$$

  where $\diamond : V \times V^* \to \mathfrak{so}(3)^*$.
- Spatial angular momentum is conserved $m_{k+1} = m_k$.
- Equivalent to the discrete Euler-Poincaré equations with an advected quantity (Bobenko and Suris, 1999).

Semi-direct Product Lie-Poisson Structure

Back

- The map

$$(m_k, l_k) \mapsto (m_{k+1}, l_{k+1}) \ \in \mathfrak{g}^* \times V^*$$

is Poisson with respect to the Lie-Poisson bracket on $[\mathfrak{s}^* = \mathfrak{g}^* \circledS V^*]_\pm$

$$\{F_1, F_2\}_\pm(m, l) \\ = \pm\langle m, [\nabla_m F_1, \nabla_m F_2]\rangle \pm \langle l, \nabla_m F_1 \cdot \nabla_l F_2 - \nabla_m F_2 \cdot \nabla_l F_1\rangle.$$

- $det(l)$ and $||l||_2$ are Casimirs of this Lie-Poisson bracket.

The Spatial Representation in Continuous and Discrete Time

Back

Property	Continuous	Discrete
Body attitude	$\Lambda(t) \in SO(N)$	$\Lambda_k \in SO(N)$
Angular velocity	$\omega = \dot{\Lambda}\Lambda^T = -\omega^T$	$\omega_{k+1} = \Lambda_{k+1}\Lambda_k^T$
Inertia Matrix	$I = \Lambda I_0 \Lambda^T$	$I_k = \Lambda_k I_0 \Lambda_k^T$
Angular momentum	$m = I\omega - \omega^T I$	$m_k = I_k \omega_k^T - \omega_k I_k$
Equations of motion	$\dot{m} = ad^*_\omega m - \nabla_I L \diamond I = 0$, $\dot{I} = [\omega, I]$	$m_{k+1} = Ad^*_{\omega_k^T} m_k + 2\nabla_{I_k} l_{I_k} \diamond I_{k+1}$, $I_{k+1} = \omega_{k+1} I_k \omega_{k+1}^T$
Left momentum map	$J_L = P \diamond \Lambda + J \diamond I$	$J_L^{k+1} = P_k \diamond \Lambda_k + G_k \diamond I_k$

Numerical Results: $I_1 = I_2 > I_3$

Back

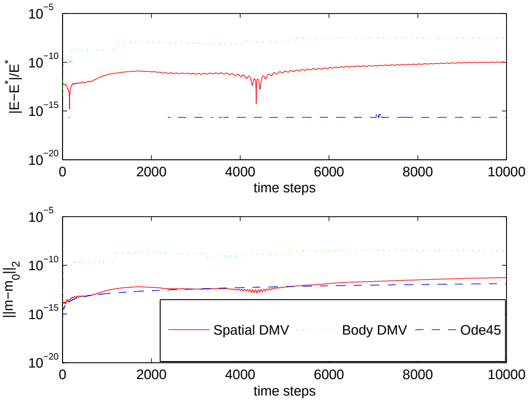


Figure: $I_1 = 2,\ I_2 = 2,\ I_3 = 1, M_1(0) = 0.1,\ M_2(0) = 0,\ M_3(0) = 1$ and $\Delta t = 0.1$.

Numerical Results: $I_1 > I_2 > I_3$

Back

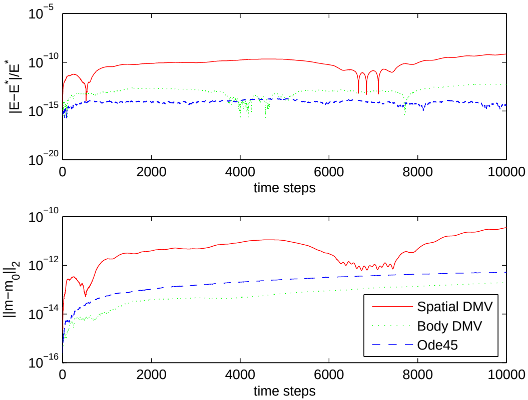
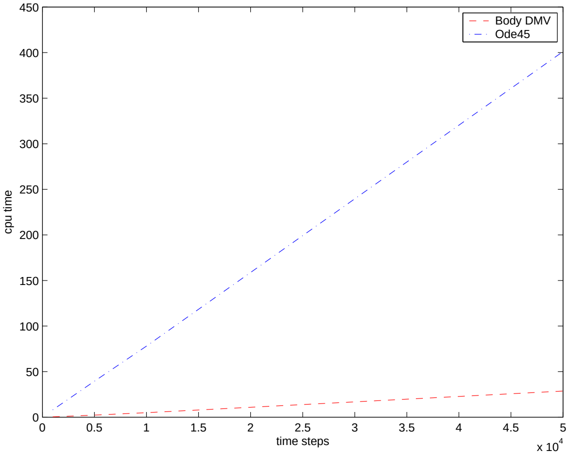


Figure: $I_1 = 3.5,\ I_2 = 2.5,\ I_3 = 2, M_1(0) = -0.5,\ M_2(0) = 0,\ M_3(0) = 1$ and $\Delta t = 0.1$.

CPU Time

Back



Convective and Spatial Representations of Ellipsoidal Motion

- In convective variables

$$l_{C_t}(\Gamma) = l(\Gamma, C_t) = \frac{1}{2} Tr(\Gamma I_0 \Gamma^T C_t),$$

where $\Gamma := Q^{-1}\dot{Q}$ is (minus) the left Q invariant *convective velocity*.

- In spatial variables

$$l_{I_t}(\gamma) = l(\Gamma, I_t) = \frac{1}{2} Tr(\gamma I_t \gamma^T C_0),$$

where $\gamma := \dot{Q}Q^{-1}$ is the right Q invariant *spatial velocity*.

Convective and Spatial Representations of Ellipsoidal Motion

- Convective:

$$\begin{aligned} Ad^*_{\Gamma_k^{-1}} M_{k+1} &= M_k + C_{k-1} \diamond \nabla_{C_{k-1}} l_{C_{k-1}}, \\ C_k &= \phi^*_{\Gamma_k}(C_{k-1}), \end{aligned} \tag{1}$$

- Spatial:

$$\begin{aligned} Ad^*_{\gamma_k} m_{k+1} &= m_k + 2\nabla_{I_{k-1}} l_{I_{k-1}} I_{k-1}, \\ I_k &= \phi_{\gamma_k}(I_{k-1}), \end{aligned} \tag{2}$$

Momentum maps for the discrete Isotropic Pseudo-Rigid Body

- The momentum map $M_{k+1} : T^*SO(3) \to \mathfrak{so}(3)^*$ takes the form

$$M_{k+1} := \mathfrak{s}_{k+1}\Omega_{k+1}^T - \Omega_{k+1}\mathfrak{s}_{k+1}^T = S_{k+1}(Q_k^T P_k - P_k^T Q_k)S_{k+1}^T,$$

- The angular momentum $m_{k+1} = R_{k+1}^T M_{k+1} R_{k+1}$ is conserved.
- The momentum map $N_{k+1} : T^*SO(3) \to \mathfrak{so}(3)^*$ takes the form

$$N_{k+1} := \Omega_{k+1}\mathfrak{s}_{k+1}^T - \mathfrak{s}_{k+1}\Omega_{k+1}^T = \mathfrak{s}_{k+1}R_k(Q_k P_k^T - P_k Q_k^T)R_k^T \mathfrak{s}_{k+1}^T.$$

The vorticity $n_{k+1} = S_{k+1}^T N_{k+1} S_{k+1}$ is conserved.

A Discrete Kelvin Circulation Theorem

Theorem (Discrete time Kelvin circulation)

The change in the exterior derivative of the circulation one-form about a closed loop $c(\mathbf{x}_{k+1})$ is

$$\Delta_t d(\mathbf{x}_{k+1} \cdot d\mathbf{x}_k) = 0 \quad \text{along} \quad \mathbf{x}_{k+1} = \mathfrak{u}_k \mathbf{x}_k .$$

Proof

Substituting the reconstruction formula $\mathbf{x}_{k+1} = \mathfrak{u}_{k+1}\mathbf{x}_k$ into the differential two-form gives

$$\begin{aligned} d(\mathfrak{u}_{k+1}\mathbf{x}_k \cdot d\mathbf{x}_k) &= (Q_{k+1}Q_k^{-1})_{ij} dx_k^j \wedge dx_k^i \\ &= \frac{1}{2}(Q_{k+1}^T Q_k - Q_k^T Q_{k+1})_{ab} d\ell^a \wedge d\ell^b . \end{aligned}$$

A DMV Algorithm for the Pseudo-Rigid Body

- The coupled MV integrator for the momentum components takes the form

$$
\begin{aligned}
M_1 &= M_1' + J(\Omega_2)\Omega_1^T - \Omega_1 J(\Omega_2)^T,\\
M_2 &= M_2' + J(\Omega_1)\Omega_2^T - \Omega_2 J(\Omega_1)^T,
\end{aligned}
$$

- Introduce a splitting

$$
\begin{aligned}
M_1 &= M_1' + J(\tilde{\Omega}_2)\Omega_1^T - \Omega_1 J(\tilde{\Omega}_2)^T,\\
M_2 &= M_2' + J(\tilde{\Omega}_1)\Omega_2^T - \Omega_2 J(\tilde{\Omega}_1)^T,
\end{aligned}
$$

MV integrators for the Cayley-Klein Parameterisation of Rigid Body Motion

Back

- Define the discrete Lagrangian $\mathbf{l}^k : SU(2) \times SU(2) \to \mathbb{R}$ given by

$$\mathbf{l}^k = Tr\left(\Omega_{k+1}^{\dagger}\mathbb{J}(\Omega_{k+1})\right).$$

where $\mathbb{J}(\Omega_{k+1}) = I_d - (1 - I_i)\Omega_{k+1} Tr^2\left(\tilde{E}_i^{\dagger}\Omega_{k+1}\right)$.

- The *tilde map* $\tilde{}$ is given by

$$\mathbf{x} \mapsto \tilde{\mathbf{x}} = \frac{1}{2\imath}\sigma_j x_j,$$

where $\frac{\sigma_j}{2\imath}$ are the Pauli spin matrices which form the basis of $\mathfrak{su}(2)$.

Cayley-Klein Parameterisation and Quaternionic formulation of Rigid Body Motion

Back

Property	$SU(2) = h(Q)$	Q
Body attitude	$\Lambda_k \in SU(2)$	$q_k \in Q$
Angular 'velocity'	$\Omega_{k+1} = \Lambda_k^\dagger \Lambda_{k+1}$	$\Omega_{k+1} = \bar{q}_k * q_{k+1}$
Moments of inertia	$I_j,\ j := 1 \to 3$	
Inertia matrix	$A_k = I_d - I_i Tr\left(\Omega_k^\dagger \tilde{E}_i\right)\tilde{E}_i$	$A_k = [1, \mathbf{A}_v(t_k)]$
		$\mathbf{A}_v = \imath_j I_j \Omega(t_k)_j$
Angular momentum	$M_{k+1} = A_{k+1}\Omega_{k+1}^\dagger - \Omega_{k+1}A_{k+1}^\dagger$	$M_{k+1} = \frac{1}{2}A_{k+1} * \bar{\Omega}_{k+1} - \frac{1}{2}\Omega_{k+1} * \bar{A}_{k+1}$
Equations of motion	$M_{k+1} = Ad^*_{\Omega_k^T} M_k$	$M_{k+1} = \Omega_k * M_k * \bar{\Omega}_k$
Right mom. map	$J_R^{k+1} = P_k \diamond \Lambda_k$	$J_R^{k+1} = p_k \diamond q_k$