Melvin Leok: Bibliography

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Publications

Available for download at http://www.math.ucsd.edu/~mleok/

Refereed Journal Papers

1. *Estimating the Attractor Dimension of the Equatorial Weather System*, Acta Phys. Pol. A **85**, S27–S35, 1994.
2. *Discrete Poincaré Lemma* (with M. Desbrun, J.E. Marsden), Appl. Numer. Math. **53** (2–4), 231–248, 2005.
3. *Discrete Routh Reduction* (with S.M. Jalnapurkar, J.E. Marsden, M. West), J. Phys. A: Math. Gen. **39**, 5521-5544 (Geometric Integration Special Issue, invited paper), 2006.
4. *Lie Group Variational Integrators for the Full Body Problem* (with T. Lee, N.H. McClamroch), Comput. Methods Appl. Mech. Engrg. **196** (29-30), 2907–2924, 2007.
5. *Lie Group Variational Integrators for the Full Body Problem in Orbital Mechanics* (with T. Lee, N.H. McClamroch), Celestial Mechanics and Dynamical Astronomy **98** (2), 121–144, 2007.
6. *Global Optimal Attitude Estimation using Uncertainty Ellipsoids* (with T. Lee, A.K. Sanyal, N.H. McClamroch), Systems and Control Letters, **57** (3), 236–245, 2008.
7. *Optimal Attitude Control of a Rigid Body using Geometrically Exact Computations on SO(3)* (with T. Lee, N.H. McClamroch), Journal of Dynamical and Control Systems **14** (4), 465–487, 2008.
8. *Geometric Structure-Preserving Optimal Control of the Rigid Body* (with A.M. Bloch, I.I. Hussein, A.K. Sanyal), Journal of Dynamical and Control Systems **15** (3), 307–330, 2009.
9. *Computational Geometric Optimal Control of Rigid Bodies* (with T. Lee, N.H. McClamroch), Brockett Legacy Special Issue, Communications in Information and Systems **8** (4), 445–472, 2008.
10. *Controlled Lagrangians and Stabilization of Discrete Mechanical Systems* (with A.M. Bloch, J.E. Marsden, D.V. Zenkov), Discrete and Continuous Dynamical Systems – Series S (Nonholonomic Constraints in Mechanics and Optimal Control Theory Special Issue), **3** (1), 19–36, 2010.
11. *Lagrangian Mechanics and Variational Integrators on Two-Spheres* (with T. Lee, N.H. McClamroch), International Journal for Numerical Methods in Engineering **79** (9), 1147–1174, 2009.
12. *Nonlinear Dynamics of the 3D Pendulum* (with N.A. Chaturvedi, T. Lee, N.H. McClamroch), Journal of Nonlinear Science, **21** (1), 3–32, 2011.
13. *Discrete Hamiltonian Variational Integrators* (with J. Zhang), IMA Journal of Numerical Analysis, **31** (4), 1497–1532, 2011.
14. *Computational Dynamics of a 3D Elastic String Pendulum Attached to a Rigid Body and an Inertially Fixed Reel Mechanism* (with T. Lee, N.H. McClamroch), Nonlinear Dynamics, **64** (1-2), 97–115, 2011.
15. *On the Geometry of Multi-Dirac Structures and Gerstenhaber Algebras* (with J. Vankerschaver, H. Yoshimura), Journal of Geometry and Physics, **61** (8), 1415–1425, 2011.
16. *Variational and Geometric Structures of Discrete Dirac Mechanics* (with T. Ohsawa), Foundations of Computational Mathematics, **11** (5), 529–562, 2011.
17. *Discrete Hamilton–Jacobi Theory* (with A.M. Bloch, T. Ohsawa), SIAM Journal on Control and Optimization, **49** (4), 1829–1856, 2011.
18. *Prolongation–Collocation Variational Integrators* (with T. Shingel), IMA Journal of Numerical Analysis, **32** (3), 1194–1216, 2012.
19. *General Techniques for Constructing Variational Integrators* (with T. Shingel), Frontiers of Mathematics in China (Special issue on computational mathematics, invited paper), **7** (2), 273–303, 2012.
20. *The Hamilton–Pontryagin Principle and Multi-Dirac Structures for Classical Field Theories* (with J. Vankerschaver, H. Yoshimura), Journal of Mathematical Physics, **53** (7), 072903 (25 pages), 2012.
21. *Nonlinear Robust Tracking Control of a Quadrotor UAV on SE(3)* (with T. Lee, N.H. McClamroch), Asian Journal of Control, **15** (3), 1–18, 2013.
22. *Hamilton–Jacobi Theory for Degenerate Lagrangian Systems with Holonomic and Nonholonomic Constraints* (with T. Ohsawa, D. Sosa), Journal of Mathematical Physics, **53** (7), 072905 (29 pages), 2012.
23. *Dirac Structures and Hamilton-Jacobi Theory for Lagrangian Mechanics on Lie Algebroids* (with D. Sosa), Journal of Geometric Mechanics, **4** (4), 421–442, 2012.
24. *Generating functionals and Lagrangian partial differential equations* (with C. Liao, J. Vankerschaver), Journal of Mathematical Physics, **54** (8), 082901 (22 pages), 2013.
25. *A novel formulation of point vortex dynamics on the sphere: geometrical and numerical aspects* (with J. Vankerschaver), Journal of Nonlinear Science, **24** (1), 1–37, 2014.

Refereed Journal Papers (continued)

26. *Symplectic Semiclassical Wave Packet Dynamics* (with T. Ohsawa), Journal of Physics A, **46** (40), 405201 (28 pages), 2013.
27. *High-Fidelity Numerical Simulation of Complex Dynamics of Tethered Spacecraft* (with T. Lee, N.H. McClamroch), Acta Astronautica, **99**, June–July, 215–230, 2014.
28. *A Novel Variational Formulation for Thermoelastic Problems* (with Z. Ebrahimzadeh, M. Mahzoon), Communications in Nonlinear Science and Numerical Simulation, **22** (1–3), 263–268, 2015.
29. *Spectral Variational Integrators* (with J. Hall), Numerische Mathematik, **130** (4), 681–740, 2015.
30. *Lie Group Spectral Variational Integrators* (with J. Hall), Foundations of Computational Mathematics, accepted, 2015.
31. *Variational integrators for interconnected Lagrange–Dirac systems* (with H. Parks), Journal of Nonlinear Science, accepted pending minor revisions, 2016.

Refereed Book Chapters

32. *Discrete Control Systems* (with T. Lee, N. H. McClamroch), invited article for the Springer Encyclopedia of Complexity and Systems Science, 2002–2019, 2009. Reprinted in Mathematics of Complexity and Dynamical Systems, 143–159, 2011.
33. *Variational Integrators*, invited article for the Springer Encyclopedia of Applied and Computational Mathematics, 1519-1525, 2015.

Refereed Conference Papers

34. *A Lie Group Variational Integrator for the Attitude Dynamics of a Rigid Body with Applications to the 3D Pendulum* (with T. Lee, N.H. McClamroch), Proc. IEEE Conf. on Control Applications, 962–967, 2005.
35. *Controlled Lagrangians and Stabilization of the Discrete Cart-Pendulum System* (with A.M. Bloch, J.E. Marsden, D.V. Zenkov), Proc. IEEE Conf. on Decision and Control, 6579–6584, 2005.
36. *Attitude Maneuvers of a Rigid Spacecraft in a Circular Orbit* (with T. Lee, N.H McClamroch), Proc. American Control Conf., 1742–1747, 2006.
37. *Polyhedral Potential and Variational Integrator Computation of the Full Two Body Problem* (with E. Fahnestock, T. Lee, N.H. McClamroch, D. Scheeres), Proc. AIAA/AAS Astrodynamics Conf., AIAA-2006-6289, 2006.
38. *Optimal Control of a Rigid Body using Geometrically Exact Computations on SE(3)* (with T. Lee, N.H. McClamroch), Proc. IEEE Conf. on Decision and Control, 2710–2715, 2006.
39. *Deterministic Global Attitude Estimation* (with T. Lee, A.K. Sanyal, N.H. McClamroch), Proc. IEEE Conf. on Decision and Control, 3174–3179, 2006.
40. *Controlled Lagrangians and Potential Shaping for Stabilization of Discrete Mechanical Systems* (with A.M. Bloch, J.E. Marsden, D.V. Zenkov), Proc. IEEE Conf. on Decision and Control, 3333–3338, 2006.
41. *A Discrete Variational Integrator for Optimal Control Problems on SO(3)* (with A.M. Bloch, I.I. Hussein, A.K. Sanyal), Proc. IEEE Conf. on Decision and Control, 6636–6641, 2006.
42. *Global Attitude Estimation using Single Direction Measurements* (with T. Lee, N.H. McClamroch, A.K. Sanyal), Proc. American Control Conf., 3659–3664, 2007.
43. *Optimal Attitude Control for a Rigid Body with Symmetry* (with T. Lee, N.H. McClamroch), Proc. American Control Conf., 1073–1078, 2007.
44. *Propagation of Uncertainty in Rigid Body Attitude Flows* (with N.A. Chaturvedi, T. Lee, N.H. McClamroch, A.K. Sanyal), Proc. IEEE Conf. on Decision and Control, 2689–2694, 2007.
45. *A Combinatorial Optimization Problem for Spacecraft Formation Reconfiguration* (with T. Lee, N.H. McClamroch), Proc. IEEE Conf. on Decision and Control, 5370–5375, 2007.
46. *Matching and stabilization of discrete mechanical systems* (with A.M. Bloch, J.E. Marsden, D.V. Zenkov), Proc. Appl. Math. Mech. **7**, 1030603–1030604, 2007.
47. *Time Optimal Attitude Control for a Rigid Body* (with T. Lee, N.H. McClamroch), Proc. American Control Conf., 5210–5215, 2008.
48. *Global Symplectic Uncertainty Propagation on SO(3)* (with T. Lee, N.H. McClamroch), Proc. IEEE Conf. on Decision and Control, 61–66, 2008.
49. *Dynamics of Connected Rigid Bodies in a Perfect Fluid* (with T. Lee, N.H. McClamroch), Proc. American Control Conf., 408–413, 2009.
50. *Dynamics of a 3D Elastic String Pendulum* (with T. Lee, N.H. McClamroch), Proc. IEEE Conf. on Decision and Control, 3347–3352, 2009.
51. *Computational Geometric Optimal Control of Connected Rigid Bodies in a Perfect Fluid* (with T. Lee, N.H. McClamroch), Proc. American Control Conf., 5985–5990, 2010.

Refereed Conference Papers (continued)

52. *Discrete Dirac Structures and Implicit Discrete Lagrangian and Hamiltonian Systems* (with T. Ohsawa), XVIII International Fall Workshop on Geometry and Physics, 91–102, AIP Conference Proceedings 1260, 2010.
53. *Geometric Tracking Control of a Quadrotor UAV on SE(3)* (with T. Lee, N.H. McClamroch), Proc. IEEE Conf. on Decision and Control, 5420–5425, 2010.
54. *Discrete Hamilton-Jacobi Theory and Discrete Optimal Control* (with T. Ohsawa, A.M. Bloch), Proc. IEEE Conf. on Decision and Control, 5438–5443, 2010.
55. *Stokes-Dirac Structures through Reduction of Infinite-Dimensional Dirac Structures* (with J. Vankerschaver, H. Yoshimura, J.E. Marsden), Proc. IEEE Conf. on Decision and Control, 6265–6270, 2010.
56. *Geometric Numerical Integration of Complex Dynamics of Tethered Spacecraft* (with T. Lee, N.H. McClamroch), Proc. American Control Conf., 1885–1891, 2011.
57. *Stable Manifolds of Saddle Points for Pendulum Dynamics on S^2 and $SO(3)$* (with T. Lee, N.H. McClamroch), Proc. IEEE Conf. on Decision and Control, 3915–3921, 2011.
58. *Nonlinear Robust Tracking Control of a Quadrotor UAV on $SE(3)$* (with T. Lee, N.H. McClamroch), Proc. American Control Conf., 4649–4654, 2012.
59. *Dynamics and Control of a Chain Pendulum on a Cart* (with T. Lee, N.H. McClamroch), Proc. IEEE Conf. on Decision and Control, 2502–2508, 2012.
60. *Hamel's Formalism and Variational Integrators on a Sphere* (with A.M. Bloch, D.V Zenkov), Proc. IEEE Conf. on Decision and Control, 7504–7510, 2012.
61. *Space-Time Finite-Element Exterior Calculus and Variational Discretizations of Gauge Field Theories* (with J. Salamon, J. Moody), Proc. Mathematical Theory of Networks and Systems, 743–747, 2014.
62. *Global Formulations of Lagrangian and Hamiltonian Dynamics on Embedded Manifolds* (with T. Lee, N.H. McClamroch), Proc. IMA Conf. on Mathematics of Robotics, 2015.
63. *Global Formulations of Lagrangian and Hamiltonian Mechanics on Two-Spheres* (with T. Lee, N.H. McClamroch), Proc. IEEE Conf. on Decision and Control, 6010–6015, 2015.

Papers under Review

64. *Spectral-Collocation Variational Integrators* (with Y. Li, B. Wu), Journal of Computational Physics, submitted, 2015.
65. *Spectral variational integrators for semi-discrete Hamiltonian wave equations* (with Y. Li, B. Wu), Journal of Computational and Applied Mathematics, submitted, 2016.
66. *Taylor Variational Integrators* (with J.M. Schmitt, T. Shingel), under revision, 2016.
67. *Interpolation on Symmetric Spaces via the Generalized Polar Decomposition* (with E.S. Gawlik), Foundations of Computational Mathematics, submitted, 2016.
68. *Computing the Fréchet Derivative of the Polar Decomposition* (with E.S. Gawlik), SIAM Journal on Matrix Analysis and Applications, submitted, 2016.
69. *Embedding-Based Interpolation on the Special Orthogonal Group* (with E.S. Gawlik), Numerische Mathematik, submitted, 2016.
70. *Properties of Hamiltonian Variational Integrators* (with J.M. Schmitt), IMA Journal of Numerical Analysis, submitted, 2016.

Preprints

71. *Generalized Galerkin Variational Integrators*, 2004.
72. *A Discrete Theory of Connections on Principal Bundles* (with J.E. Marsden, A.D. Weinstein), 2004.
73. *Discrete Exterior Calculus* (with M. Desbrun, A.N. Hirani, J.E. Marsden), 2003.

Books

74. *Global Formulation of Lagrangian and Hamiltonian Mechanics on Manifolds: A Geometric Approach to Modeling and Analysis*, Volume I (with T. Lee, N.H. McClamroch), Springer, 2015 (contract signed).
75. *Global Formulation of Lagrangian and Hamiltonian Mechanics on Manifolds: A Geometric Approach to Modeling and Analysis*, Volume II (with T. Lee, N.H. McClamroch), Springer, 2017 (contract signed).

Thesis

76. *Foundations of Computational Geometric Mechanics*, Ph.D. thesis, California Institute of Technology, 2004.
    A preliminary version of this thesis received the *SIAM Student Paper Prize*, and the *Leslie Fox Prize in Numerical Analysis* (second prize) in 2003.

Melvin Leok: Bibliography

Abstracts

1. **Estimating the Attractor Dimension of the Equatorial Weather System**
   Acta Phys. Pol. A **85**, 1994.

   The correlation dimension and limit capacity serve theoretically as lower and upper bounds, respectively, of the fractal dimension of attractors of dynamic systems. In this paper we show that estimates of the correlation dimension grow rapidly with increasing noise level in the time-series, while estimates of the limit capacity remain relatively unaffected. It is therefore proposed that the limit capacity can be used in studies of noisy data, despite its heavier computational requirements. An analysis of Singapore wind data with the limit capacity estimate revealed a surprisingly low dimension (≈ 2.5). It is suggested that further studies can be made with comprehensive equatorial weather data.

2. **Discrete Poincaré Lemma** *(with M. Desbrun, and J.E. Marsden)*
   Appl. Numer. Math. **53** (2–4), 231–248, 2005.

   This paper proves a discrete analogue of the Poincaré lemma in the context of a discrete exterior calculus based on simplicial cochains. The proof requires the construction of a generalized cone operator, $p : C_k(K) \to C_{k+1}(K)$, as the geometric cone of a simplex cannot, in general, be interpreted as a chain in the simplicial complex. The corresponding cocone operator $H : C^k(K) \to C^{k-1}(K)$ can be shown to be a homotopy operator, and this yields the discrete Poincaré lemma.

   The generalized cone operator is a combinatorial operator that can be constructed for any simplicial complex that can be grown by a process of local augmentation. In particular, regular triangulations and tetrahedralizations of $\mathbb{R}^2$ and $\mathbb{R}^3$ are presented, for which the discrete Poincaré lemma is globally valid.
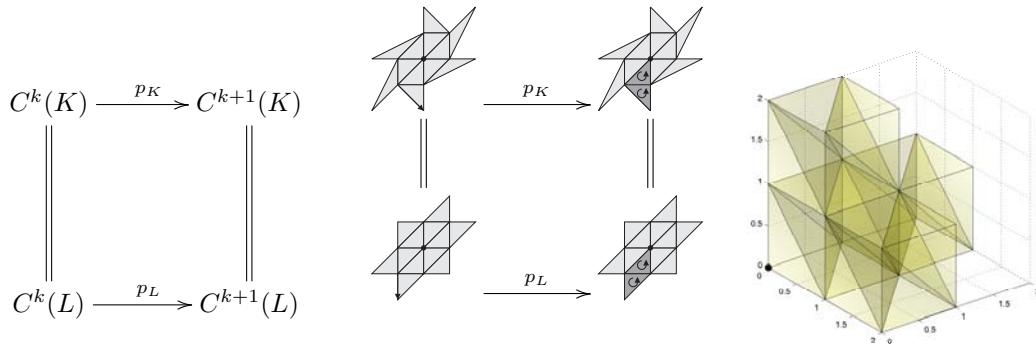
3. **Discrete Routh Reduction** *(with S.M. Jalnapurkar, J.E. Marsden, and M. West)*
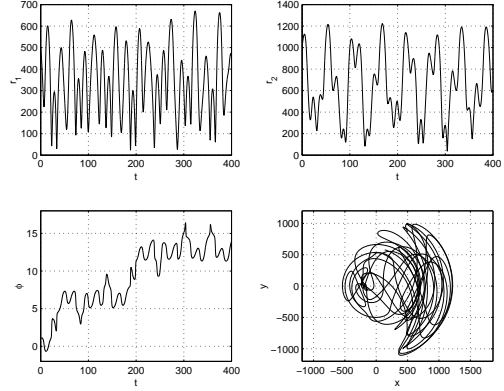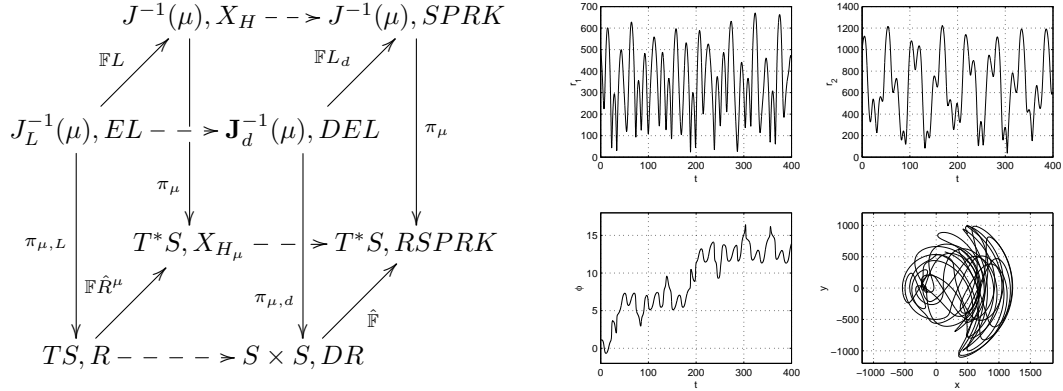   J. Phys. A: Math. Gen. **39**, 5521–5544 (Geometric Integration Special Issue, invited paper), 2006.

   This paper develops the theory of abelian Routh reduction for discrete mechanical systems and applies it to the variational integration of mechanical systems with abelian symmetry. The reduction of variational Runge-Kutta discretizations is considered, as well as the extent to which symmetry reduction and discretization commute. These reduced methods allow the direct simulation of dynamical features such as relative equilibria and relative periodic orbits that can be obscured or difficult to identify in the unreduced dynamics.

   The methods are demonstrated for the dynamics of an Earth orbiting satellite with a non-spherical J_2 correction, as well as the double spherical pendulum. The J_2 problem is interesting because in the unreduced picture, geometric phases inherent in the model and those due to numerical discretization can be hard to distinguish, but this issue does not appear in the reduced algorithm, where one can directly observe interesting dynamical structures in the reduced phase space (the cotangent bundle of shape space), in which the geometric phases have been removed.

   The main feature of the double spherical pendulum example is that it has a nontrivial magnetic term in its reduced symplectic form. Our method is still efficient as it can directly handle the essential non-canonical nature of the symplectic structure. In contrast, a traditional symplectic method for canonical systems could require repeated coordinate changes if one is evoking Darboux' theorem to transform the symplectic structure into canonical form, thereby incurring additional computational cost. Our method allows one to design reduced symplectic integrators in a natural way, despite the noncanonical nature of the symplectic structure.

$$J^{-1}(\mu), X_H \dashrightarrow J^{-1}(\mu), SPRK$$

$$\mathbb{F}L \qquad \mathbb{F}L_d$$

$$J_L^{-1}(\mu), EL \dashrightarrow \mathbf{J}_d^{-1}(\mu), DEL \qquad \pi_\mu$$

$$\pi_\mu$$

$$\pi_{\mu,L} \qquad T^*S, X_{H_\mu} \dashrightarrow T^*S, RSPRK$$

$$\mathbb{F}\hat{R}^\mu \qquad \pi_{\mu,d} \qquad \hat{\mathbb{F}}$$

$$TS, R \dashrightarrow S \times S, DR$$

4. **Lie Group Variational Integrators for the Full Body Problem** *(with T. Lee, and N.H. McClamroch)*
Comput. Methods Appl. Mech. Engrg., **196** (29-30), 2907–2924, 2007.

We develop the equations of motion for full body models that describe the dynamics of rigid bodies, acting under their mutual gravity. The equations are derived using a variational approach where variations are defined on the Lie group of rigid body configurations. Both continuous equations of motion and variational integrators are developed in Lagrangian and Hamiltonian forms, and the reduction from the inertial frame to a relative coordinate system is also carried out. The Lie group variational integrators are shown to be symplectic, to preserve conserved quantities, and to guarantee exact evolution on the configuration space. One of these variational integrators is used to simulate the dynamics of two rigid dumbbell bodies.
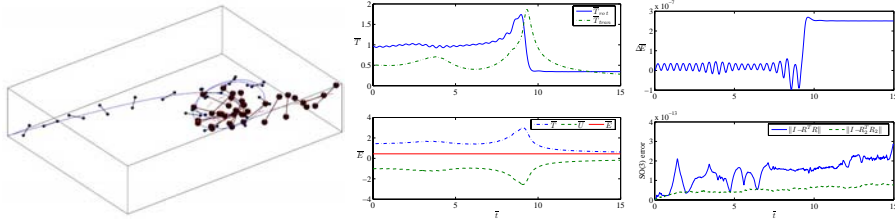
5. **Lie Group Variational Integrators for the Full Body Problem in Orbital Mechanics**
(with T. Lee, and N.H. McClamroch)
Celestial Mechanics and Dynamical Astronomy, **98** (2), 121–144, 2007.

Equations of motion, referred to as full body models, are developed to describe the dynamics of rigid bodies acting under their mutual gravitational potential. Continuous equations of motion and discrete equations of motion are derived using Hamilton's principle. These equations are expressed in an inertial frame and in relative coordinates. The discrete equations of motion, referred to as a Lie group variational integrator, provide a geometrically exact and numerically efficient computational method for simulating full body dynamics in orbital mechanics; they are symplectic and momentum preserving, and they exhibit good energy behavior for exponentially long time periods. They are also efficient in only requiring a single evaluation of the gravity forces and moments per time step. The Lie group variational integrator also preserves the group structure without the use of local charts, reprojection, or constraints. Computational results are given for the dynamics of two rigid dumbbell bodies acting under their mutual gravity; these computational results demonstrate the superiority of the Lie group variational integrator compared with integrators that are not symplectic or do not preserve the Lie group structure.
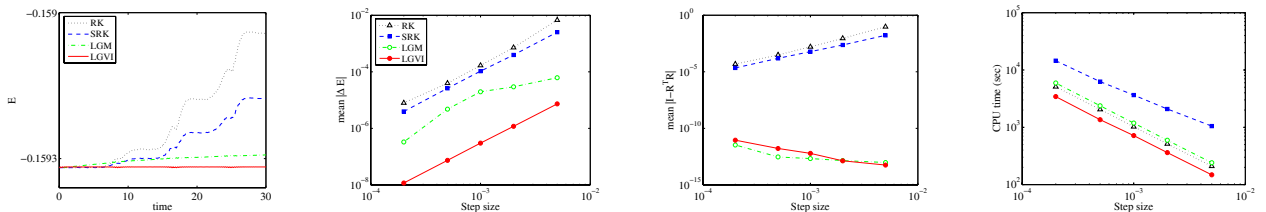
Computational properties of explicit Runge-Kutta (RK), symplectic Runge-Kutta (SRK), Lie group method (LGM), and Lie group variational integrator (LGVI).

6. **Global Optimal Attitude Estimation using Uncertainty Ellipsoids**
(with T. Lee, A.K. Sanyal, N.H. McClamroch)
Systems and Control Letters, **57** (3), 236–245, 2007.

A deterministic attitude estimation problem for a rigid body in a potential field, with bounded attitude and angular velocity measurement errors is considered. An attitude estimation algorithm that globally minimizes the attitude estimation error is obtained. Assuming that the initial attitude, the initial angular velocity and measurement noise lie within given ellipsoidal bounds, an uncertainty ellipsoid that bounds the attitude and the angular velocity of the rigid body is obtained. The center of the uncertainty ellipsoid provides point estimates, and the size of the uncertainty ellipsoid measures the accuracy of the estimates. The point estimates and the uncertainty ellipsoids are propagated using a Lie group variational integrator and its linearization, respectively. The attitude and angular velocity estimates are optimal in the sense that the sizes of the uncertainty ellipsoids are minimized.

7. **Optimal Attitude Control of a Rigid Body using Geometrically Exact Computations on $SO(3)$**
(with T. Lee, and N.H. McClamroch)
Journal of Dynamical and Control Systems, **14** (4), 465–487, 2008.

An efficient and accurate computational approach is proposed for optimal attitude control of a rigid body. The problem is formulated directly as a discrete time optimization problem using a Lie group variational integrator. Discrete necessary conditions for optimality are derived, and an efficient computational approach is proposed to solve the resulting two point boundary value problem. The use of geometrically exact computations on $SO(3)$ guarantees that this optimal control approach has excellent convergence properties even for highly nonlinear large angle attitude maneuvers. Numerical results are presented for attitude maneuvers of a 3D pendulum and a spacecraft in a circular orbit.
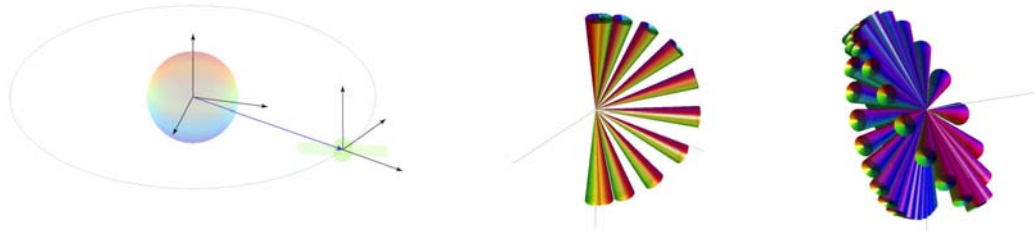
8. **Geometric Structure-Preserving Optimal Control of the Rigid Body**
*(with A.M. Bloch, I.I. Hussein, A.K. Sanyal)*
Journal of Dynamical and Control Systems, **15** (3), 307–330, 2009.

In this paper we study a discrete variational optimal control problem for the rigid body. The cost to be minimized is the external torque applied to move the rigid body from an initial condition to a pre-specified terminal condition. Instead of discretizing the equations of motion, we use the discrete equations obtained from the discrete Lagrange–d'Alembert principle, a process that better approximates the equations of motion. Within the discrete-time setting, these two approaches are not equivalent in general. The kinematics are discretized using a natural Lie-algebraic formulation that guarantees that the flow remains on the Lie group $SO(3)$ and its algebra $\mathfrak{so}(3)$. We use Lagranges method for constrained problems in the calculus of variations to derive the discrete-time necessary conditions. We give a numerical example for a three-dimensional rigid body maneuver.

9. **Computational Geometric Optimal Control of Rigid Bodies** *(with T. Lee, N.H. McClamroch)*
Brockett Legacy Special Issue, Communications in Information and Systems, **8** (4), 445–472, 2008.

   This paper formulates optimal control problems for rigid bodies in a geometric manner and it presents computational procedures based on this geometric formulation for numerically solving these optimal control problems. The dynamics of each rigid body is viewed as evolving on a configuration manifold that is a Lie group. Discrete-time dynamics of each rigid body are developed that evolve on the configuration manifold according to a discrete version of Hamilton's principle so that the computations preserve geometric features of the dynamics and guarantee evolution on the configuration manifold; these discrete-time dynamics are referred to as Lie group variational integrators. Rigid body optimal control problems are formulated as discrete-time optimization problems for discrete Lagrangian/Hamiltonian dynamics, to which standard numerical optimization algorithms can be applied. This general approach is illustrated by presenting results for several different optimal control problems for a single rigid body and for multiple interacting rigid bodies. The computational advantages of the approach, that arise from correctly modeling the geometry, are discussed.
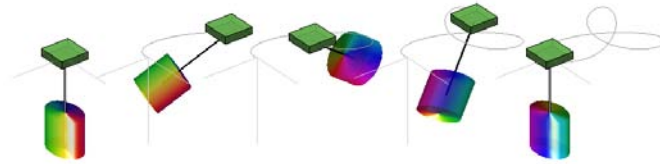
10. **Controlled Lagrangians and Stabilization of Discrete Mechanical Systems**
(with A.M. Bloch, J.E. Marsden, D.V. Zenkov)
Discrete and Continuous Dynamical Systems – Series S (Nonholonomic Constraints in Mechanics and Optimal Control Theory Special Issue), **3** (1), 19–36, 2010.

    Controlled Lagrangian and matching techniques are developed for the stabilization of relative equilibria of discrete mechanical systems with symmetry and equilibria of discrete mechanical systems with broken symmetry. Unexpected phenomena arise in the controlled Lagrangian approach in the discrete context that are not present in the continuous theory. In particular, to make the discrete theory effective, one can make an appropriate selection of momentum levels or, alternatively, introduce a new parameter into the controlled Lagrangian to complete the kinetic matching procedure. New terms in the controlled shape equation that are necessary for potential matching in the discrete setting are introduced. The theory is illustrated with the problem of stabilization of the cart-pendulum system on an incline, and the application of the theory to the construction of digital feedback controllers is also discussed.

11. **Lagrangian Mechanics and Variational Integrators on Two-Spheres**
(with T. Lee and N.H. McClamroch)
International Journal for Numerical Methods in Engineering, **79** (9), 1147–1174, 2009.

    Euler-Lagrange equations and variational integrators are developed for Lagrangian mechanical systems evolving on a product of two-spheres. The geometric structure of a product of two-spheres is carefully considered in order to obtain global equations of motion. Both continuous equations of motion and variational integrators completely avoid the singularities and complexities introduced by local parameterizations or explicit constraints. We derive global expressions for the Euler-Lagrange equations on two-spheres which are more compact than existing equations written in terms of angles. Since the variational integrators are derived from Hamilton's principle, they preserve the geometric features of the dynamics such as symplecticity, momentum maps, or total energy, as well as the structure of the configuration manifold. Computational properties of the variational integrators are illustrated for several mechanical systems. In addition, we describe how Lie group variational integrators can be used to integrate Lagrangian flows on more general homogeneous spaces by lifting the discrete Hamilton's principle on homogeneous spaces to a constrained discrete variational principle on the Lie group by choosing a discrete connection.

12. **Nonlinear Dynamics of the 3D Pendulum** *(with N.A. Chaturvedi, T. Lee, N.H. McClamroch)*
    Journal of Nonlinear Science, **21** (1), 3–32, 2011.

    A 3D pendulum consists of a rigid body, supported at a fixed pivot, with three rotational degrees of freedom. The pendulum is acted on by a gravitational force. 3D pendulum dynamics have been much studied in integrable cases that arise when certain physical symmetry assumptions are made. This paper treats the non-integrable case of the 3D pendulum dynamics when the rigid body is asymmetric and the center of mass is distinct from the pivot location. Full and reduced models of the 3D pendulum are introduced and used to study important features of the nonlinear dynamics: conserved quantities, equilibria, relative equilibria, invariant manifolds, local dynamics, and presence of chaotic motions. The paper provides a unified treatment of the 3D pendulum dynamics that includes prior results and new results expressed in the framework of geometric mechanics. These results demonstrate the rich and complex dynamics of the 3D pendulum.

(a) 3D view   (b) Top view   (c) Bottom view
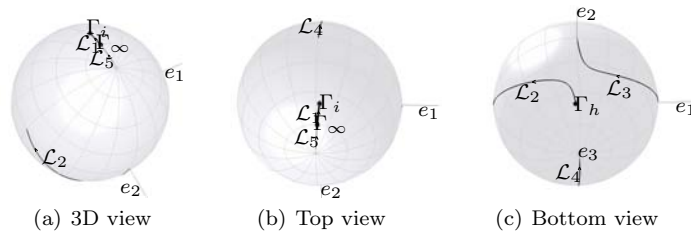
Relative equilibria attitudes for an elliptic cylinder 3D pendulum model

(d) $E = -2.65$ (e) $E = 0$ (f) $E = 2.03$ (g) $E = 8.83$ (h) $E = 11.95$
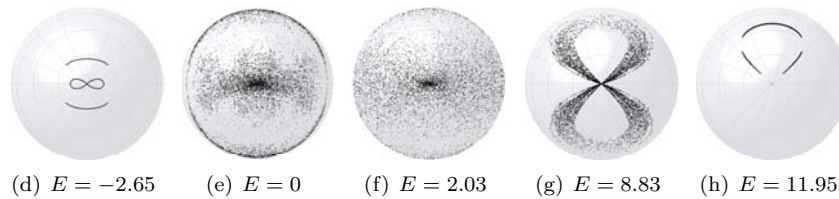
Poincaré maps for 3D pendulum with varying total energy

13. **Discrete Hamiltonian Variational Integrators** *(with J. Zhang)*
    IMA Journal of Nonlinear Analysis, **31** (4), 1497–1532, 2011.

    We consider the continuous and discrete-time Hamilton's variational principle on phase space, and characterize the exact discrete Hamiltonian which provides an exact correspondence between discrete and continuous Hamiltonian mechanics. The variational characterization of the exact discrete Hamiltonian naturally leads to a class of generalized Galerkin Hamiltonian variational integrators, which include the symplectic partitioned Runge–Kutta methods. We also characterize the group invariance properties of discrete Hamiltonians which lead to a discrete Noether's theorem.

14. **Computational Dynamics of a 3D Elastic String Pendulum Attached to a Rigid Body and an Inertially Fixed Reel Mechanism** *(with T. Lee, N.H. McClamroch)*
    Nonlinear Dynamics, **64** (1-2), 97–115, 2011.

    A high fidelity model is developed for an elastic string pendulum, one end of which is attached to a rigid body while the other end is attached to an inertially fixed reel mechanism which allows the unstretched length of the string to be dynamically varied. The string is assumed to have distributed mass and elasticity that permits axial deformations. The rigid body is attached to the string at an arbitrary point, and the resulting string pendulum system exhibits nontrivial coupling between the elastic wave propagation in the string and the rigid body dynamics. Variational methods are used to develop coupled ordinary and partial differential equations of motion. Computational methods, referred to as Lie group variational integrators, are then developed, based on a finite element approximation and the use of variational methods in a discrete-time setting to obtain discrete-time equations of motion. This approach preserves the geometry of the configurations, and leads to accurate and efficient algorithms that have guaranteed accuracy properties that make them suitable for many dynamic simulations, especially over long simulation times. Numerical results are presented for typical examples involving a constant length string, string deployment, and string retrieval. These demonstrate the complicated dynamics that arise in a string pendulum from the interaction of the rigid body motion, elastic wave dynamics in the string, and the disturbances introduced by the reeling mechanism. Such interactions are dynamically important in many engineering problems, but tend be obscured in lower fidelity models.
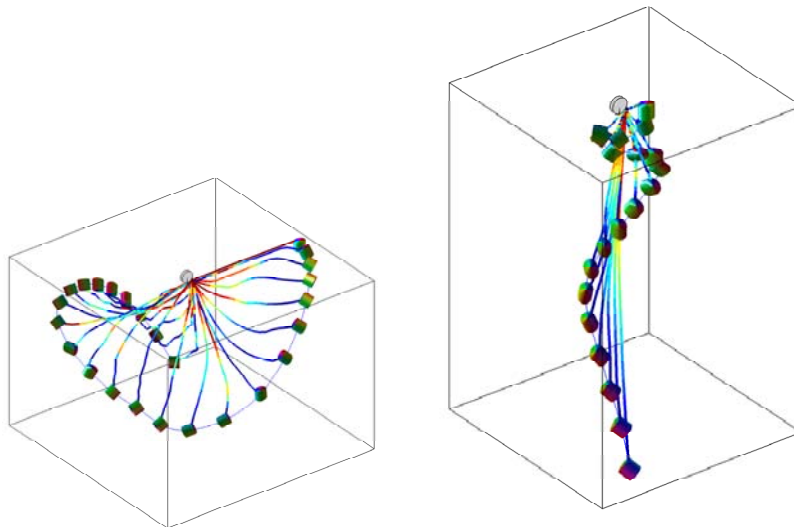

15. **On the Geometry of Multi-Dirac Structures and Gerstenhaber Algebras** *(with J. Vankerschaver, H. Yoshimura)*
    Journal of Geometry and Physics, **61** (8), 1415–1425, 2011.

    In a companion paper, we introduced a notion of multi-Dirac structures, a graded version of Dirac structures, and we discussed their relevance for classical field theories. In the current paper we focus on the geometry of multi-Dirac structures. After recalling the basic definitions, we introduce a graded multiplication and a multi-Courant bracket on the space of sections of a multi-Dirac structure, so that the space of sections has the structure of a Gerstenhaber algebra. We then show that the graph of a k-form on a manifold gives rise to a multi-Dirac structure and also that this multi-Dirac structure is integrable if and only if the corresponding form is closed. Finally, we show that the multi-Courant bracket endows a subset of the ring of differential forms with a graded Poisson bracket, and we relate this bracket to some of the multisymplectic brackets found in the literature.
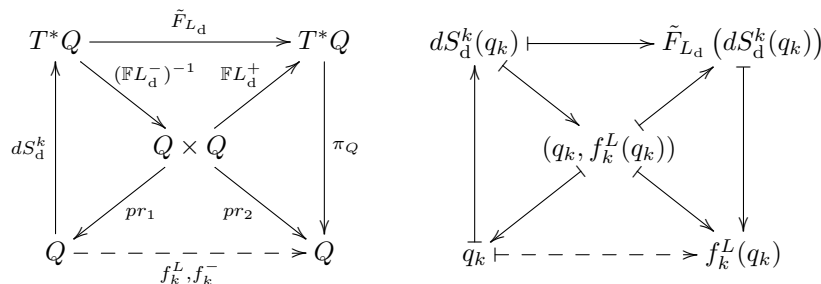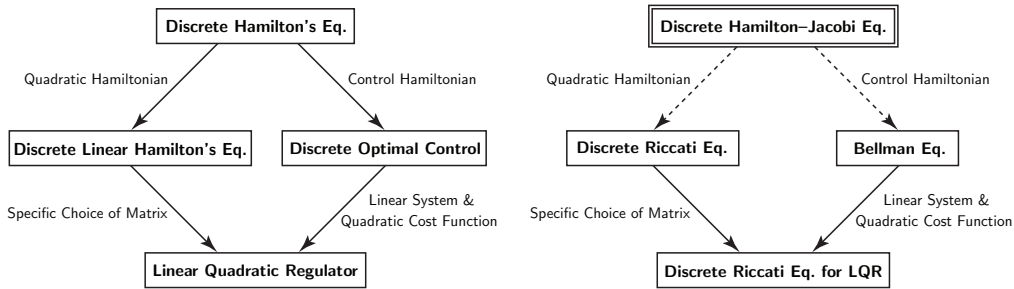
16. **Variational and Geometric Structures of Discrete Dirac Mechanics** *(with T. Ohsawa)*
Foundations of Computational Mathematics, **11** (5), 529–562, 2011.

In this paper, we develop the theoretical foundations of discrete Dirac mechanics, that is, discrete mechanics of degenerate Lagrangian/Hamiltonian systems with constraints. We first construct discrete analogues of Tulczyjew's triple and induced Dirac structures by considering the geometry of symplectic maps and their associated generating functions. We demonstrate that this framework provides a means of deriving discrete Lagrange–Dirac and nonholonomic Hamiltonian systems. In particular, this yields nonholonomic Lagrangian and Hamiltonian integrators. We also introduce discrete Lagrange–d'Alembert–Pontryagin and Hamilton–d'Alembert variational principles, which provide an alternative derivation of the same set of integration algorithms. The paper provides a unified treatment of discrete Lagrangian and Hamiltonian mechanics in the more general setting of discrete Dirac mechanics, as well as a generalization of symplectic and Poisson integrators to the broader category of Dirac integrators.
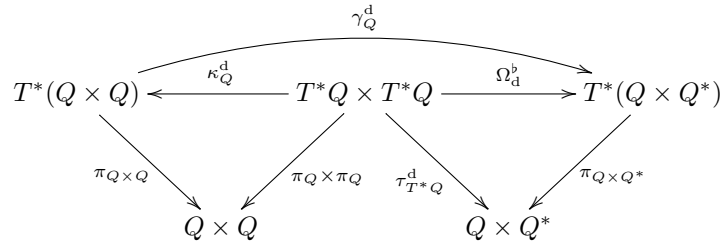
17. **Discrete Hamilton–Jacobi Theory** *(with T. Ohsawa, A.M. Bloch)*
SIAM Journal on Control and Optimization, **49** (4), 1829–1856, 2011.

We develop a discrete analogue of the Hamilton–Jacobi theory in the framework of the discrete Hamiltonian mechanics. We first reinterpret the discrete Hamilton-Jacobi equation derived by Elnatanov and Schiff in the language of discrete mechanics. The resulting discrete Hamilton–Jacobi equation is discrete only in time, and is shown to recover the Hamilton–Jacobi equation in the continuous-time limit. The correspondence between discrete and continuous Hamiltonian mechanics naturally gives rise to a discrete analogue of Jacobi's solution to the Hamilton-Jacobi equation. We also prove a discrete analogue of the geometric Hamilton–Jacobi theorem of Abraham and Marsden. These results are readily applied to discrete optimal control setting, and some well-known results in discrete optimal control theory, such as the Bellman equation (discrete-time Hamilton–Jacobi–Bellman equation) of dynamic programming, follow immediately. We also apply the theory to discrete linear Hamiltonian systems, and show that the discrete Riccati equation follows as a special case of the discrete Hamilton–Jacobi equation.

18. **Prolongation-Collocation Variational Integrators** *(with T. Shingel)*
IMA Journal of Numerical Analysis, **32** (3), 1194-1216, 2011.

We introduce a novel technique for constructing higher-order variational integrators for Hamiltonian systems of ODEs. In particular, we are concerned with generating globally smooth approximations to solutions of a Hamiltonian system. Our construction of the discrete Lagrangian adopts Hermite interpolation polynomials and the Euler–Maclaurin quadrature formula, and involves applying collocation to the Euler–Lagrange equation and its prolongation. Considerable attention is devoted to the order analysis of the resulting variational integrators in terms of approximation properties of the Hermite polynomials and quadrature errors. A performance comparison is presented on a selection of these integrators.

19. **General Techniques for Constructing Variational Integrators***(with T. Shingel)*
Frontiers of Mathematics in China (Special issue on computational mathematics, invited), **7** (2), 273–303, 2012.

The numerical analysis of variational integrators relies on variational error analysis, which relates the order of accuracy of a variational integrator with the order of approximation of the exact discrete Lagrangian by a computable discrete Lagrangian. The exact discrete Lagrangian can either be characterized variationally, or in terms of Jacobi's solution of the Hamilton–Jacobi equation. These two characterizations lead to the Galerkin and shooting-based constructions for discrete Lagrangians, which depend on a choice of a numerical quadrature formula, together with either a finite-dimensional function space or a one-step method. We prove that the properties of the quadrature formula, finite-dimensional function space, and underlying one-step method determine the order of accuracy and momentum-conservation properties of the associated variational integrators. We also illustrate these systematic methods for constructing variational integrators with numerical examples.

20. **The Hamilton–Pontryagin Principle and Multi-Dirac Structures for Classical Field Theories** (with H. Yoshimura, J. Vankerschaver)
Journal of Mathematical Physics, **53** (7), 072903 (25 pages), 2012.

We introduce a variational principle for field theories, referred to as the Hamilton-Pontryagin principle, and we show that the resulting field equations are the Euler-Lagrange equations in implicit form. Secondly, we introduce multi-Dirac structures as a graded analog of standard Dirac structures, and we show that the graph of a multisymplectic form determines a multi-Dirac structure. We then discuss the role of multi-Dirac structures in field theory by showing that the implicit Euler-Lagrange equations for fields obtained from the Hamilton-Pontryagin principle can be described intrinsically using multi-Dirac structures. Lastly, we show a number of illustrative examples, including time-dependent mechanics, nonlinear scalar fields, Maxwell's equations, and elastostatics.

21. **Nonlinear Robust Tracking Control of a Quadrotor UAV on** $SE(3)$
(with T. Lee, N. H. McClamroch)
Asian Journal of Control, **15** (3), 1–18, 2013.

This paper provides nonlinear tracking control systems for a quadrotor unmanned aerial vehicle (UAV) that are robust to bounded uncertainties. A mathematical model of a quadrotor UAV is defined on the special Euclidean group, and nonlinear output-tracking controllers are developed to follow (1) an attitude command, and (2) a position command for the vehicle center of mass. The controlled system has the desirable properties that the tracking errors are uniformly ultimately bounded, and the size of the ultimate bound can be arbitrarily reduced by control system parameters. Numerical examples illustrating complex maneuvers are provided.

22. **Hamilton–Jacobi Theory of Degenerate Lagrangian Systems with Holonomic and Nonholonomic Constraints** *(with T. Ohsawa, D. Sosa)*
Journal of Mathematical Physics, **53** (7), 072905 (29 pages), 2012.

We extend Hamilton–Jacobi theory to Lagrange–Dirac (or implicit Lagrangian) systems, a generalized formulation of Lagrangian mechanics that can incorporate degenerate Lagrangians as well as holonomic and non-holonomic constraints. We refer to the generalized Hamilton–Jacobi equation as the *Dirac–Hamilton–Jacobi equation*. For non-degenerate Lagrangian systems with nonholonomic constraints, the theory specializes to the recently developed nonholonomic Hamilton–Jacobi theory. We are particularly interested in applications to a certain class of degenerate nonholonomic Lagrangian systems with symmetries that arise as simplified models of nonholonomic mechanical systems; these systems are shown to reduce to non-degenerate nonholonomic Lagrangian (and hence nonholonomic Hamiltonian) systems. Accordingly, the Dirac–Hamilton–Jacobi equation reduces to the nonholonomic Hamilton–Jacobi equation associated with the reduced system. We illustrate through a few examples how the Dirac–Hamilton–Jacobi equation can be used to exactly integrate the equations of motion.

23. **Dirac Structures and Hamilton–Jacobi Theory for Lagrangian Mechanics on Lie Algebroids** *(with D. Sosa)*
Journal of Geometric Mechanics, **4** (4), 421–442, 2012.

This paper develops the notion of implicit Lagrangian systems on Lie algebroids and a Hamilton–Jacobi theory for this type of system. The Lie algebroid framework provides a natural generalization of classical tangent bundle geometry. We define the notion of an implicit Lagrangian system on a Lie algebroid E using Dirac structures on the Lie algebroid prolongation $\mathcal{T}^E E^*$. This setting includes degenerate Lagrangian systems with nonholonomic constraints on Lie algebroids.

24. **Generating Functionals and Lagrangian PDEs** *(with J. Vankerschaver, C. Liao)*
Journal of Mathematical Physics, **54** (8), 082901 (22 pages), 2013.

We introduce the concept of Type-I/II generating functionals defined on the space of boundary data of a Lagrangian field theory. On the Lagrangian side, we define an analogue of Jacobi's solution to the Hamilton-Jacobi equation for field theories, and we show that by taking variational derivatives of this functional, we obtain an isotropic submanifold of the space of Cauchy data, described by the so-called multisymplectic form formula. We also define a Hamiltonian analogue of Jacobi's solution, and we show that this functional is a Type-II generating functional. We finish the paper by defining a similar framework of generating functions for discrete field theories, and we show that for the linear wave equation, we recover the multisymplectic conservation law of Bridges.

25. **A novel formulation of point vortex dynamics on the sphere: geometrical and numerical aspects** *(with J. Vankerschaver)*
Journal of Nonlinear Science, **24** (1), 1–37, 2014.

In this paper, we present a novel Lagrangian formulation of the equations of motion for point vortices on the unit 2-sphere. We show first that no linear Lagrangian formulation exists directly on the 2-sphere but that a Lagrangian may be constructed by pulling back the dynamics to the 3-sphere by means of the Hopf fibration. We then use the isomorphism of the 3-sphere with the Lie group $SU(2)$ to derive a variational Lie group integrator for point vortices which is symplectic, second-order, and preserves the unit-length constraint. At the end of the paper, we compare our integrator with classical fourth-order Runge–Kutta, the second-order midpoint method, and a standard Lie group Munthe-Kaas method.

26. **Symplectic Semiclassical Wave Packet Dynamics** *(with T. Ohsawa)*
Journal of Physics A, **46** (40), 405201 (28 pages), 2013.

The paper gives a symplectic-geometric account of semiclassical Gaussian wave packet dynamics. We employ geometric techniques to "strip away" the symplectic structure behind the time-dependent Schrödinger equation and incorporate it into semiclassical wave packet dynamics. We show that the Gaussian wave packet dynamics of Heller is a Hamiltonian system with respect to the symplectic structure, apply the theory of symplectic reduction and reconstruction to the dynamics, and discuss dynamic and geometric phases in semiclassical mechanics. We also propose an asymptotic approximation of the potential term that provides a practical semiclassical correction term to the approximation by Heller. A simple harmonic oscillator example is worked out to illustrate the results, along with the canonical and action–angle coordinates for the system. Finally, we look into the geometry behind the Hagedorn parametrization of Gaussian wave packet dynamics.

27. **High-Fidelity Numerical Simulation of Complex Dynamics of Tethered Spacecraft**
(with T. Lee, N.H. McClamroch)
Acta Astronautica, **99**, June–July, 215–230, 2014.

This paper presents an analytical model and a geometric numerical integrator for a tethered spacecraft model that is composed of two rigid bodies connected by an elastic tether. This high-fidelity model includes important dynamic characteristics of tethered spacecraft in orbit, namely the nonlinear coupling among tether deformations, rigid body rotational dynamics, a reeling mechanism, and orbital dynamics. A geometric numerical integrator, referred to as a Lie group variational integrator, is developed to numerically preserve the Hamiltonian structure of the presented model and its Lie group configuration manifold. This approach preserves the geometry of the configurations, and leads to accurate and efficient algorithms that have guaranteed accuracy properties that make them suitable for many dynamic simulations, especially over long simulation times. These analytical and computational models provide a reliable benchmark for testing the validity and applicability of the many simplified models in the existing literature, which have hitherto been used without careful verification that the simplifying assumptions employed are valid in physically realistic parameter regimes. We present numerical simulations which illustrate the important qualitative differences in the tethered spacecraft dynamics when the high-fidelity model is employed, as compared to models with additional simplifying assumptions.

28. **A Novel Variational Formulation for Thermoelastic Problems** *(with Z. Ebrahimzadeh, M. Mahzoon)*
Communications in Nonlinear Science and Numerical Simulation, **22** (1–3), 263–268, 2015.

A novel variational formulation for thermoelasticity is proposed in this paper. The formulation is based on the Hamilton–Pontryagin principle and the concept of temperature displacement. Although there are many other papers that have a similar goal, most of the proposed approaches are quite complicated, and contain assumptions that curtail their applicability. The proposed variational principle in this paper is straightforward with no extra assumptions and it is in conformity with the Clausius–Duhem inequality as a statement of the second law of thermodynamics. Conservation laws for linear momentum and energy, and the constitutive equation for thermoelasticity are consequences of this variational formulation.

29. **Spectral Variational Integrators** *(with J. Hall)*
Numerische Mathematik, **130** (4), 681–740, 2015.

In this paper, we present a new variational integrator for problems in Lagrangian mechanics. Using techniques from Galerkin variational integrators, we construct a scheme for numerical integration that converges geometrically, and is symplectic and momentum preserving. Furthermore, we prove that under appropriate assumptions, variational integrators constructed using Galerkin techniques will yield numerical methods that are arbitrarily high-order. In particular, if the quadrature formula used is sufficiently accurate, then the resulting Galerkin variational integrator has a rate of convergence at the discrete time-steps that is bounded below by the approximation order of the finite-dimensional function space. In addition, we show that the continuous approximating curve that arises from the Galerkin construction converges on the interior of the time-step at half the convergence rate of the solution at the discrete time-steps. We further prove that certain geometric invariants also converge with high-order, and that the error associated with these geometric invariants is independent of the number of steps taken. We close with several numerical examples that demonstrate the predicted rates of convergence.

30. **Lie Group Spectral Variational Integrators** *(with J. Hall)*
Foundations of Computational Mathematics, accepted, 2015.

We present a new class of high-order variational integrators on Lie groups. We show that these integrators are symplectic, momentum preserving, and can be constructed to be of arbitrarily high-order, or can be made to converge geometrically. Furthermore, these methods are capable of taking very large timesteps. We demonstrate the construction of one such variational integrator for the rigid body, and discuss how this construction could be generalized to other related Lie group problems. We close with several numerical examples which demonstrate our claims, and discuss further extensions of our work.

31. **Variational integrators for interconnected Lagrange–Dirac systems** *(with H. Parks)*
Journal of Nonlinear Science, accepted pending minor revisions, 2016.

Interconnected systems are an important class of mathematical models, as they allow for the construction of complex, hierarchical, multiphysics, and multiscale models by the interconnection of simpler subsystems. LagrangeDirac mechanical systems provide a broad category of mathematical models that are closed under interconnection, and in this paper, we develop a framework for the interconnection of discrete LagrangeDirac mechanical systems, with a view towards constructing geometric structure-preserving discretizations of interconnected systems. This work builds on previous work on the interconnection of continuous LagrangeDirac systems and discrete Dirac variational integrators. We test our results by simulating some of the continuous examples given in Jacobs and Yoshimura 2014.

32. **Discrete Control Systems** *(with T. Lee and N.H. McClamroch)*
Invited article for the Springer Encyclopedia of Complexity and Systems Science, 2002–2019, 2009.

Discrete control systems, as considered here, refer to the control theory of discrete-time Lagrangian or Hamiltonian systems. These discrete-time models are based on a discrete variational principle, and are part of the broader field of geometric integration. Geometric integrators are numerical integration methods that preserve geometric properties of continuous systems, such as conservation of the symplectic form, momentum, and energy. They also guarantee that the discrete flow remains on the manifold on which the continuous system evolves, an important property in the case of rigid-body dynamics.

In nonlinear control, one typically relies on differential geometric and dynamical systems techniques to prove properties such as stability, controllability, and optimality. More generally, the geometric structure of such systems plays a critical role in the nonlinear analysis of the corresponding control problems. Despite the critical role of geometry and mechanics in the analysis of nonlinear control systems, nonlinear control algorithms have typically been implemented using numerical schemes that ignore the underlying geometry.

The field of discrete control system aims to address this deficiency by restricting the approximation to choice of a discrete-time model, and developing an associated control theory that does not introduce any additional approximation. In particular, this involves the construction of a control theory for discrete-time models based on geometric integrators that yields numerical implementations of nonlinear and geometric control algorithms that preserve the crucial underlying geometric structure.

33. **Variational Integrators**
Invited article for Springer Encyclopedia of Applied and Computational Mathematics, 1519–1525, 2015.

Variational integrators are a class of geometric structure-preserving numerical methods that are based on a discrete Hamilton's variational principle, and are automatically symplectic and momentum preserving.

Geometric numerical integrators are numerical methods that preserve the geometric structure of a continuous dynamical system, and variational integrators provide a systematic framework for constructing numerical integrators that preserve the symplectic structure and momentum, of Lagrangian and Hamiltonian systems, while exhibiting good energy stability for exponentially long times.

In many problems, the underlying geometric structure affects the qualitative behavior of solutions, and as such, numerical methods that preserve the geometry of a problem typically yield more qualitatively accurate simulations. This qualitative property of geometric integrators can be better understood by viewing a numerical method as a discrete dynamical system that approximates the flow map of the continuous system, as opposed to the traditional view that a numerical method approximates individual trajectories. In particular, this viewpoint allows questions about long-time stability to be addressed, which would otherwise be difficult to answer.

34. **A Lie Group Variational Integrator for the Attitude Dynamics of a Rigid Body with Applications to the 3D Pendulum** *(with T. Lee, and N.H. McClamroch)*
Proc. IEEE Conf. on Control Applications, 962–967, 2005.

A numerical integrator is derived for a class of models that describe the attitude dynamics of a rigid body in the presence of an attitude dependent potential. The numerical integrator is obtained from a discrete variational principle, and exhibits excellent geometric conservation properties. In particular, by performing computations at the level of the Lie algebra, and updating the solution using the matrix exponential, the attitude automatically evolves on the rotation group embedded in the space of matrices. The geometric conservation properties of the numerical integrator imply long time numerical stability. We apply this variational integrator to the uncontrolled 3D pendulum, that is a rigid asymmetric body supported at a frictionless pivot acting under the influence of uniform gravity. Interesting dynamics of the 3D pendulum are exposed.
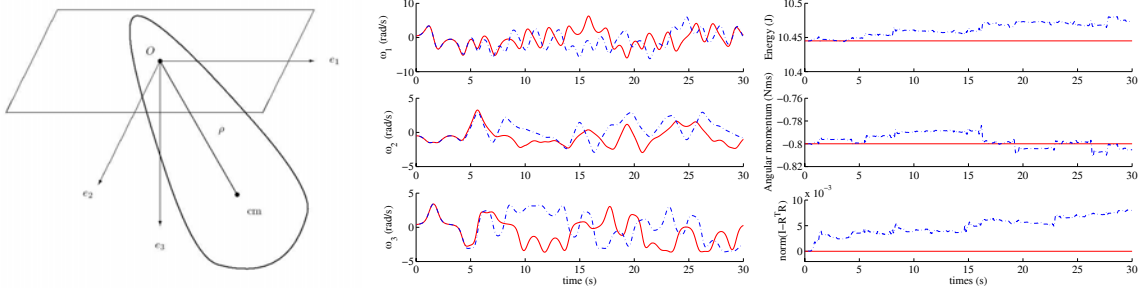
35. **Controlled Lagrangians and Stabilization of the Discrete Cart-Pendulum System**
(with A.M. Bloch, J.E. Marsden, and D.V. Zenkov)
Proc. IEEE Conf. on Decision and Control, 6579–6584, 2005.

Matching techniques are developed for discrete mechanical systems with symmetry. We describe new phenomena that arise in the controlled Lagrangian approach for mechanical systems in the discrete context. In particular, one needs to either make an appropriate selection of momentum levels or introduce a new parameter into the controlled Lagrangian to complete the matching procedure. We also discuss digital and model predictive control.
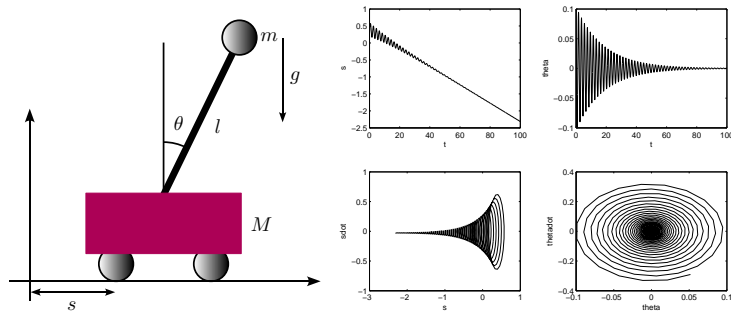
36. **Attitude Maneuvers of a Rigid Spacecraft in a Circular Orbit** *(with T. Lee, and N.H. McClamroch)*
    Proc. American Control Conf., 1742–1747, 2006.

    A global model is presented that can be used to study attitude maneuvers of a rigid spacecraft in a circular orbit about a large central body. The model includes gravity gradient effects that arise from the non-uniform gravity field and characterizes the spacecraft attitude with respect to the uniformly rotating local vertical local horizontal coordinate frame. The model is globally defined and provides the basis for development and analysis of various attitude maneuvers. An accurate computational approach for solving a nonlinear boundary value problem, with given initial attitude, given terminal attitude and given maneuver time, is proposed, assuming that control torque impulses can be applied at initiation and at termination of the maneuver. If the terminal attitude condition is relaxed, then an accurate computational approach for solving the minimal impulse optimal control problem is presented.
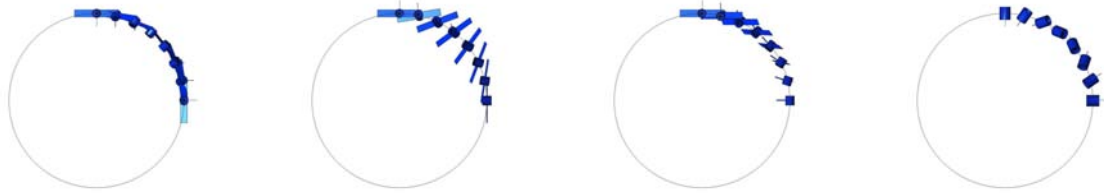
37. **Polyhedral Potential and Variational Integrator Computation of the Full Two Body Problem**,
    (with E. Fahnestock, T. Lee, N.H. McClamroch, and D. Scheeres)
    Proc. AIAA/AAS Astrodynamics Specialist Conf., AIAA-2006-6289, 2006.

    We present a combination of tools which allows for investigation of the coupled orbital and rotational dynamics of two rigid bodies with nearly arbitrary shape and mass distribution, under the influence of their mutual gravitational potential. Methods for calculating that mutual potential and resulting forces and moments for a polyhedral body representation are simple and efficient. Discrete equations of motion, referred to as the Lie Group Variational Integrator (LGVI), preserve the structure of the configuration space, SE(3), as well as the geometric features represented by the total energy and the total angular momentum. The synthesis of these approaches allows us to simulate the full two body problem accurately and efficiently. Simulation results are given for two octahedral rigid bodies for comparison with other integration methods and to show the qualities of the results thus obtained. A significant improvement is seen over other integration methods while correctly capturing the interesting effects of strong orbit and attitude dynamics coupling, in multiple scenarios.
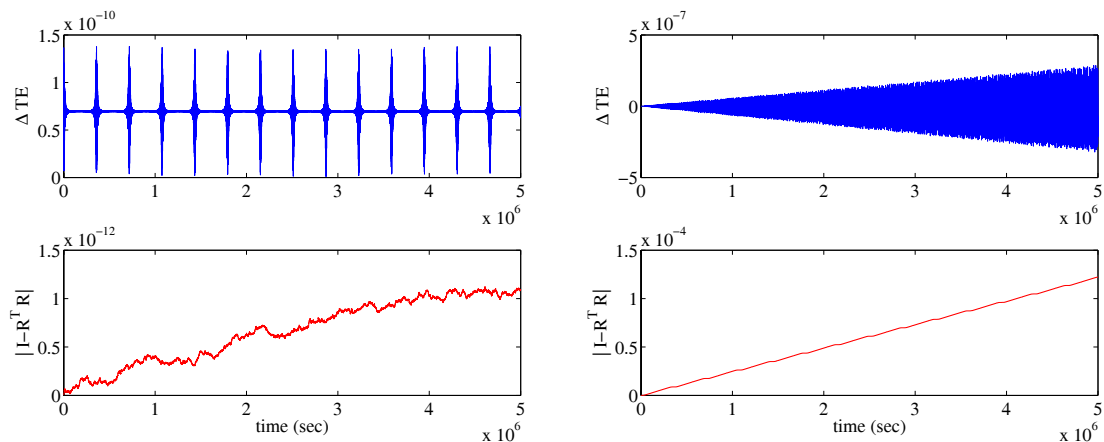
Qualitative comparisons of behavior of deviation in total energy and rotation matrix
error over time with similar computational load for LGVI and RKF7(8).

38. **Optimal Control of a Rigid Body using Geometrically Exact Computations on SE(3)**
    (with T. Lee, and N.H. McClamroch)
    Proc. IEEE Conf. on Decision and Control, 2710–2715, 2006.

    Optimal control problems are formulated and efficient computational procedures are proposed for combined orbital and rotational maneuvers of a rigid body in three dimensions. The rigid body is assumed to act under the influence of forces and moments that arise from a potential and from control forces and moments. The key features of this paper are its use of computational procedures that are guaranteed to preserve the geometry of the optimal solutions. The theoretical basis for the computational procedures is summarized, and examples of optimal spacecraft maneuvers are presented.
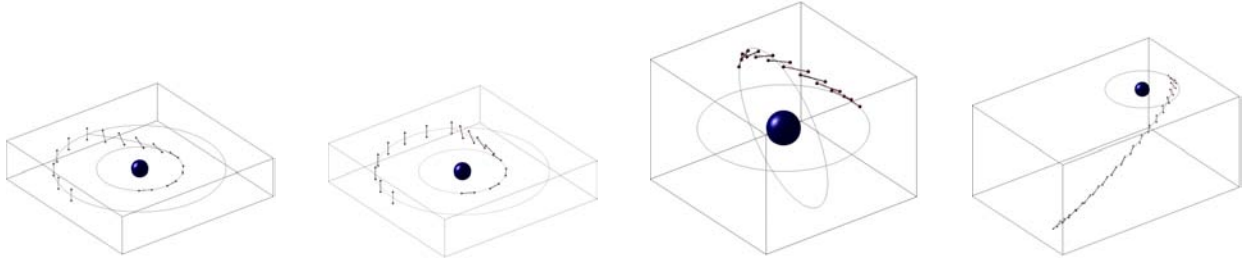
39. **Deterministic Global Attitude Estimation** *(with T. Lee, A.K. Sanyal, N.H. McClamroch)*
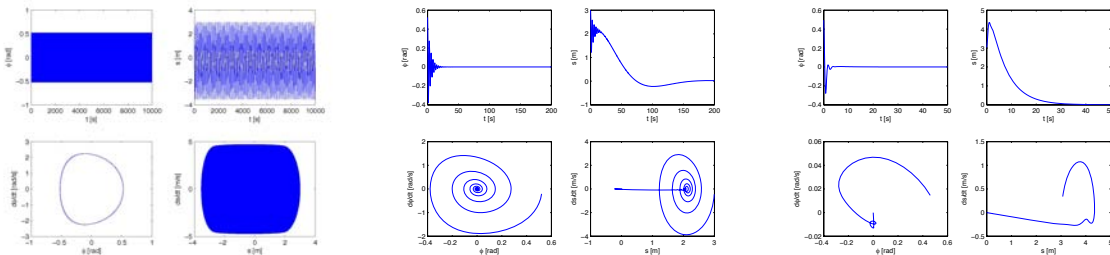   Proc. IEEE Conf. on Decision and Control, 3174–3179, 2006.

    A deterministic attitude estimation problem for a rigid body in an attitude dependent potential field with bounded measurement errors is studied. An attitude estimation scheme that does not use generalized coordinate representations of the attitude is presented here. Assuming that the initial attitude, angular velocity and measurement noise lie within given ellipsoidal bounds, an uncertainty ellipsoid that bounds the attitude and the angular velocity of the rigid body is obtained. The center of the uncertainty ellipsoid provides point estimates, and its size gives the accuracy of the estimates. The point estimates and the uncertainty ellipsoids are propagated using a Lie group variational integrator and its linearization, respectively. The estimation scheme is optimal in the sense that the attitude estimation error and the size of the uncertainty ellipsoid is minimized at each measurement instant, and it is global since the attitude is represented by a rotation matrix.

40. **Controlled Lagrangians and Potential Shaping for Stabilization of Discrete Mechanical Systems**
    (with A.M. Bloch, J.E. Marsden, D.V. Zenkov)
    Proc. IEEE Conf. on Decision and Control, 3333–3338, 2006.

    The method of controlled Lagrangians for discrete mechanical systems is extended to include potential shaping in order to achieve complete state-space asymptotic stabilization. New terms in the controlled shape equation that are necessary for matching in the discrete context are introduced. The theory is illustrated with the problem of stabilization of the cartpendulum system on an incline. We also discuss digital and model predictive control.

41. **A Discrete Variational Integrator for Optimal Control Problems on SO(3)** *(with A.M. Bloch, I.I. Hussein, A.K. Sanyal)*
Proc. IEEE Conf. on Decision and Control, 6636–6641, 2006.

In this paper we study a discrete variational optimal control problem for the rigid body. The cost to be minimized is the external torque applied to move the rigid body from an initial condition to a pre-specified terminal condition. Instead of discretizing the equations of motion, we use the discrete equations obtained from the discrete Lagrange–d'Alembert principle, a process that better approximates the equations of motion. Within the discrete-time setting, these two approaches are not equivalent in general. The kinematics are discretized using a natural Lie-algebraic formulation that guarantees that the flow remains on the Lie group $SO(3)$ and its algebra $\mathfrak{so}(3)$. We use Lagrange's method for constrained problems in the calculus of variations to derive the discretetime necessary conditions. We give a numerical example for a three-dimensional rigid body maneuver.

42. **Global Attitude Estimation using Single Direction Measurements**
(with T. Lee, N.H. McClamroch, A.K. Sanyal)
Proc. American Control Conf., 3659–3664, 2007.

A deterministic attitude estimator for a rigid body under an attitude dependent potential is studied. This estimator requires only a single direction measurement to a known reference point at each measurement instant. The measurement cannot completely determine the attitude, but an attitude estimation scheme based on this measurement is developed; a feasible set compatible with the measurement is described and it is combined with an attitude dynamics model to obtain an attitude estimate. The attitude is globally represented by a rotation matrix, and the uncertainties are described by ellipsoidal sets. A numerical example for a spacecraft in a circular orbit is presented.
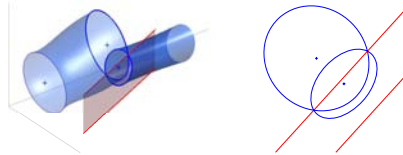
43. **Optimal Attitude Control for a Rigid Body with Symmetry** *(with T. Lee, N.H. McClamroch)*
Proc. American Control Conf., 1073–1078, 2007.

Optimal control problems are formulated and efficient computational procedures are proposed for attitude dynamics of a rigid body with symmetry. The rigid body is assumed to act under a gravitational potential and under a structured control moment that respects the symmetry. The symmetry in the attitude dynamics system yields a conserved quantity, and it causes a fundamental singularity in the optimal control problem. The key feature of this paper is its use of computational procedures that are guaranteed to avoid the numerical ill-conditioning that originates from this symmetry. It also preserves the geometry of the attitude dynamics. The theoretical basis for the computational procedures is summarized, and examples of optimal attitude maneuvers for a 3D pendulum are presented.
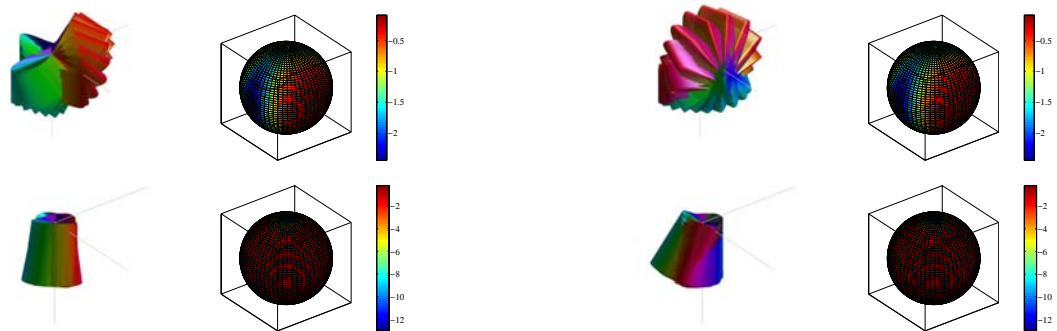
44. **Propagation of Uncertainty in Rigid Body Attitude Flows**
(with N.A. Chaturvedi, T. Lee, A.K. Sanyal and N.H. McClamroch)
Proc. IEEE Conf. on Decision and Control, 2689–2694, 2007.

Motivated by attitude control and attitude estimation problems for a rigid body, computational methods are proposed to propagate uncertainties in the angular velocity and the attitude. The nonlinear attitude flow is determined by Euler-Poincaré equations that describe the rotational dynamics of the rigid body acting under the influence of an attitude dependent potential and by a reconstruction equation that describes the kinematics expressed in terms of an orthogonal matrix representing the rigid body attitude. Uncertainties in the angular velocity and attitude are described in terms of ellipsoidal sets that are propagated through this highly nonlinear attitude flow. Computational methods are proposed, one method based on a local linearization of the attitude flow and two methods based on propagation of a small (unscented) sample selected from the initial uncertainty ellipsoid. Each of these computational methods is constructed using the Lie group variational integrator algorithm, viewed as a discretization of the attitude flow dynamics. Computational results are obtained that indicate (1) the strongly nonlinear attitude flow characteristics and (2) the limitations of each of these methods, and indeed any method, in providing effective global bounds on the nonlinear attitude flow.

Linearization

Unscented method

Unscented with re-sampling
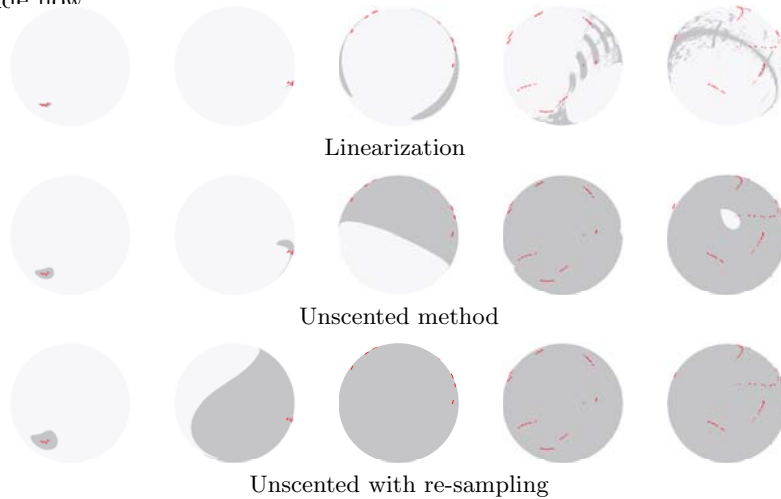
Uncertainty projected onto the reduced attitude on S^2 for irregular attitude flow.

45. **A Combinatorial Optimization Problem for Spacecraft Formation Reconfiguration**
(with T. Lee, and N.H. McClamroch)
Proc. IEEE Conf. on Decision and Control, 5370–5375, 2007.

We consider a spacecraft formation reconfiguration problem in the case of identical spacecraft. This introduces in the optimal reconfiguration problem a permutational degree of freedom, in addition to the choice of individual spacecraft trajectories. We approach this using a coupled combinatorial and continuous optimization framework, in which the inner loop consists of computing the costs associated with a particular assignment by using a geometrically exact and numerically efficient discrete optimal control method based on Lie group variational integrators. In the outer optimization loop, combinatorial techniques are used to determine the optimal assignments based on the costs computed in the inner loop. The proposed method is demonstrated on the optimal reconfiguration problem for 5 identical spacecraft to go from an inline configuration to one equally spaced on a circle.
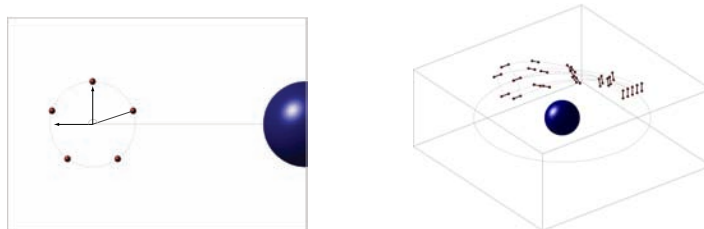
46. **Matching and stabilization of discrete mechanical systems**
   *(with A.M. Bloch, J.E. Marsden, and D.V. Zenkov)*
    Proc. Appl. Math. Mech. **7**, 1030603–1030604, 2007.

    Controlled Lagrangian and matching techniques are developed for the stabilization of equilibria of discrete mechanical systems with symmetry as well as broken symmetry. Interesting new phenomena arise in the controlled Lagrangian approach in the discrete context that are not present in the continuous theory. Specifically, a nonconservative force that is necessary for matching in the discrete setting is introduced. The paper also discusses digital and model predictive controllers.

47. **Time Optimal Attitude Control for a Rigid Body** *(with T. Lee and N.H. McClamroch)*
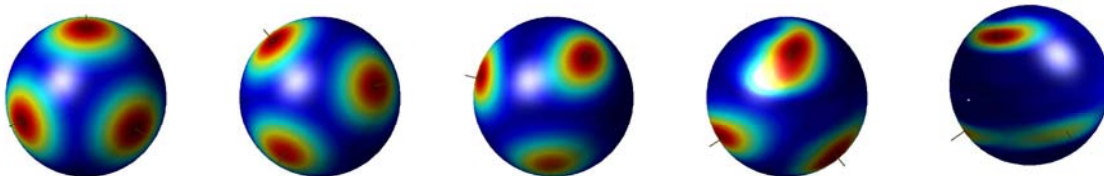   Proc. American Control Conf., 5210–5215, 2008.

    A time optimal attitude control problem is studied for the dynamics of a rigid body. The objective is to minimize the time to rotate the rigid body to a desired attitude and angular velocity while subject to constraints on the control input. Necessary conditions for optimality are developed directly on the special orthogonal group using rotation matrices. They completely avoid singularities associated with local parameterizations such as Euler angles, and they are expressed as compact vector equations. In addition, a discrete control method based on a geometric numerical integrator, referred to as a Lie group variational integrator, is proposed to compute the optimal control input. The computational approach is geometrically exact and numerically efficient. The proposed method is demonstrated by a large-angle maneuver for an elliptic cylinder rigid body.
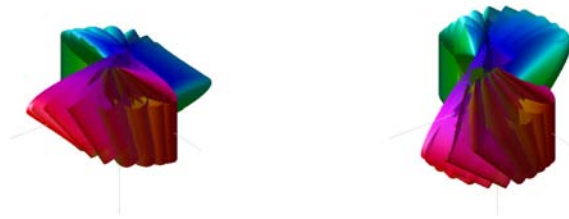
48. **Global Symplectic Uncertainty Propagation on** $SO(3)$ *(with T. Lee and N.H. McClamroch*
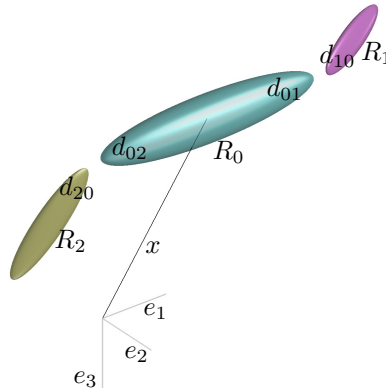   Proc. IEEE Conf. on Decision and Control, 61–66, 2008.

    This paper introduces a global uncertainty propagation scheme for rigid body dynamics, through a combination of numerical parametric uncertainty techniques, noncommutative harmonic analysis, and geometric numerical integration. This method is distinguished from prior approaches, as it allows one to consider probability densities that are global, and are not supported on only a single coordinate chart on the manifold. The use of Lie group variational integrators, that are symplectic and stay on the Lie group, as the underlying numerical propagator ensures that the advected probability densities respect the geometric properties of uncertainty propagation in Hamiltonian systems, which arise as consequence of the Gromov nonsqueezing theorem from symplectic geometry. We also describe how the global uncertainty propagation scheme can be applied to the problem of global attitude estimation.

49. **Dynamics of Connected Rigid Bodies in a Perfect Fluid** *(with T. Lee, N.H. McClamroch)*
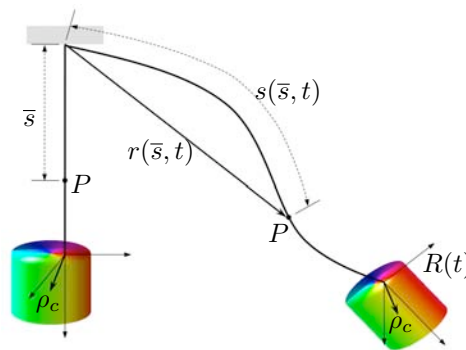Proc. American Control Conf., 408–413, 2009.

This paper presents an analytical model and a geometric numerical integrator for a system of rigid bodies connected by ball joints, immersed in an irrotational and incompressible fluid. The rigid bodies can translate and rotate in three-dimensional space, and each joint has three rotational degrees of freedom. This model characterizes the qualitative behavior of three-dimensional fish locomotion. A geometric numerical integrator, refereed to as a Lie group variational integrator, preserves Hamiltonian structures of the presented model and its Lie group configuration manifold. These properties are illustrated by a numerical simulation for a system of three connected rigid bodies.
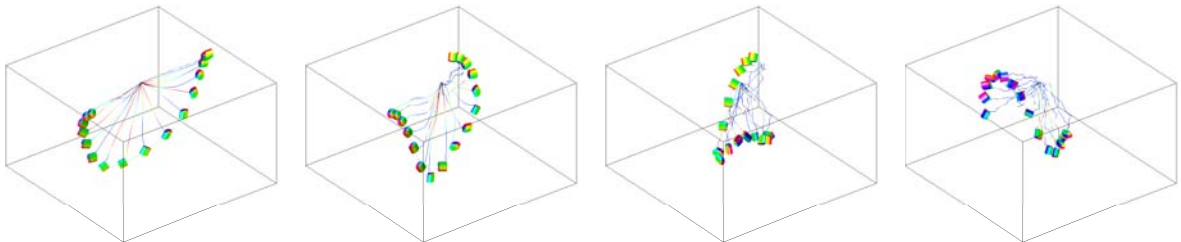

Connected Rigid Bodies Immersed in a Perfect Fluid

50. **Dynamics of a 3D Elastic String Pendulum** *(with T. Lee, N.H. McClamroch)*
Proc. IEEE Conf. on Decision and Control, 3347–3352, 2009.

This paper presents an analytical model and a geometric numerical integrator for a rigid body connected to an elastic string, acting under a gravitational potential. Since the point where the string is attached to the rigid body is displaced from the center of mass of the rigid body, there exist nonlinear coupling effects between the string deformation and the rigid body dynamics. A geometric numerical integrator, referred to as a Lie group variational integrator, is developed to numerically preserve the Hamiltonian structure of the presented model and its Lie group configuration manifold. These properties are illustrated by a numerical simulation.

Reference configuration   Deformed configuration

51. **Computational Geometric Optimal Control of Connected Rigid Bodies in a Perfect Fluid**
    (with T. Lee, N. H. McClamroch)
    Proc. American Control Conf., 5985–5990, 2010.

    This paper formulates an optimal control problem for a system of rigid bodies that are connected by ball joints and immersed in an irrotational and incompressible fluid. The rigid bodies can translate and rotate in three-dimensional space, and each joint has three rotational degrees of freedom. We assume that internal control moments are applied at each joint. We present a computational procedure for numerically solving this optimal control problem, based on a geometric numerical integrator referred to as a Lie group variational integrator. This computational approach preserves the Hamiltonian structure of the controlled system and the Lie group configuration manifold of the connected rigid bodies, thereby finding complex optimal maneuvers of connected rigid bodies accurately and efficiently. This is illustrated by numerical computations.

52. **Discrete Dirac Structures and Implicit Discrete Lagrangian and Hamiltonian Systems**
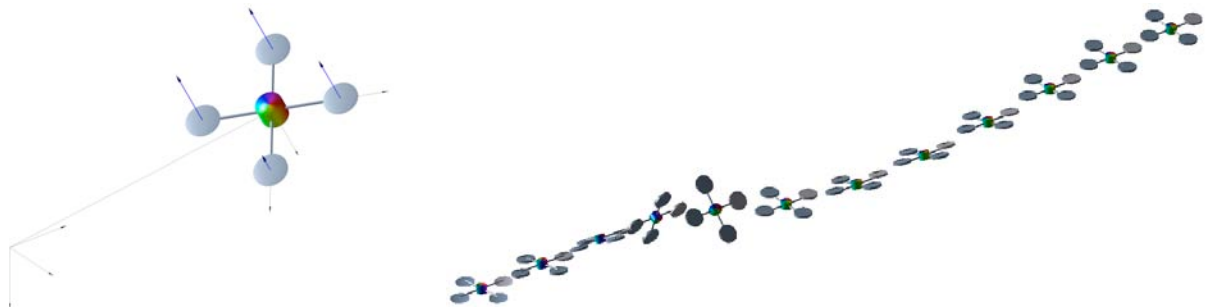   *(with T. Ohsawa)*
    Proc. XVIII International Fall Workshop on Geometry and Physics, 92–102, AIP Conference Proceedings 1260, 2010.

    We present discrete analogues of Dirac structures and the Tulczyjew's triple by considering the geometry of symplectic maps and their associated generating functions. We demonstrate that this framework provides a means of deriving discrete analogues of implicit Lagrangian and Hamiltonian systems. In particular, this yields implicit nonholonomic Lagrangian and Hamiltonian integrators. We also introduce discrete Lagrange–d'Alembert–Pontryagin and Hamilton–d'Alembert variational principles, which provide an alternative derivation of the same set of integration algorithms. In addition to providing a unified treatment of discrete Lagrangian and Hamiltonian mechanics in the more general setting of Dirac mechanics, it provides a generalization of symplectic and Poisson integrators to the broader category of Dirac integrators.

53. **Geometric Tracking Control of a Quadrotor UAV on** $SE(3)$ *(with T. Lee, N.H. McClamroch)*
    Proc. IEEE Conf. on Decision and Control, 5420–5426, 2010.

    This paper provides new results for the tracking control of a quadrotor unmanned aerial vehicle (UAV). The UAV has four input degrees of freedom, namely the magnitudes of the four rotor thrusts, that are used to control the six translational and rotational degrees of freedom, and to achieve asymptotic tracking of four outputs, namely, three position variables for the vehicle center of mass and the direction of one vehicle body-fixed axis. A globally defined model of the quadrotor UAV rigid body dynamics is introduced as a basis for the analysis. A nonlinear tracking controller is developed on the special Euclidean group $SE(3)$ and it is shown to have desirable closed loop properties that are almost global. Several numerical examples, including an example in which the quadrotor recovers from being initially upside down, illustrate the versatility of the controller.

54. **Discrete Hamilton–Jacobi Theory and Discrete Optimal Control**
    (with T. Ohsawa, A.M. Bloch)
    Proc. IEEE Conf. on Decision and Control, 5438–5443, 2010.

    We develop a discrete analogue of Hamilton–Jacobi theory in the framework of discrete Hamiltonian mechanics. The resulting discrete Hamilton–Jacobi equation is discrete only in time. The correspondence between discrete and continuous Hamiltonian mechanics naturally gives rise to a discrete analogue of Jacobi's solution to the Hamilton–Jacobi equation. We prove discrete analogues of Jacobi's solution to the Hamilton–Jacobi equation and of the geometric Hamilton–Jacobi theorem of Abraham and Marsden. These results are readily applied to the discrete optimal control setting, and some well-known results in discrete optimal control theory, such as the Bellman equation (discrete-time Hamilton–Jacobi–Bellman equation) of dynamic programming, follow immediately. We also apply the theory to discrete linear Hamiltonian systems, and show that the discrete Riccati equation follows as a special case of the discrete Hamilton–Jacobi equation.

55. **Stokes–Dirac Structures through Reduction of Infinite-Dimensional Dirac Structures**
    (with J. Vankerschaver, H. Yoshimura, J.E. Marsden)
    Proc. IEEE on Decision and Control, 6265–6270, 2010.

    We consider the concept of Stokes-Dirac structures in boundary control theory proposed by van der Schaft and Maschke. We introduce Poisson reduction in this context and show how Stokes-Dirac structures can be derived through symmetry reduction from a canonical Dirac structure on the unreduced phase space. In this way, we recover not only the standard structure matrix of Stokes-Dirac structures, but also the typical non-canonical advection terms in (for instance) the Euler equation.

56. **Geometric Numerical Integration of Complex Dynamics of Tethered Spacecraft**
    (with T. Lee, N.H. McClamroch)
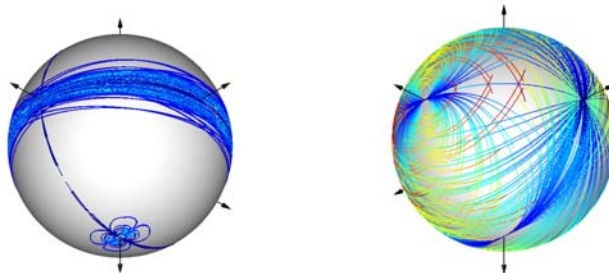   Proc. American Control Conf., 1885-1891, 2011.

    This paper presents an analytical model and a geometric numerical integrator for a tethered spacecraft model that is composed of two rigid bodies connected by an elastic tether. This model includes important dynamic characteristics of tethered spacecraft in orbit, namely the nonlinear coupling between deformations of tether, rotational dynamics of rigid bodies, a reeling mechanism, and orbital dynamics. A geometric numerical integrator, referred to as a Lie group variational integrator, is developed to numerically preserve the Hamiltonian structure of the presented model and its Lie group configuration manifold. The structure-preserving properties are particularly useful for studying complex dynamics of a tethered spacecraft over a long period of time. These properties are illustrated by numerical simulations.

57. **Stable Manifolds of Saddle Points for Pendulum Dynamics on S^2 and $SO(3)$**
    (with T. Lee, N. H. McClamroch)
    Proc. IEEE Conf. on Decision and Control, 3915–3921, 2011.

    Interesting and complicated nonlinear dynamics arise in studying closed loop attitude control systems. In this paper, we describe stable manifolds of hyperbolic equilibria that necessarily arise from closed loop attitude control systems. The concepts are illustrated by studying the dynamics of two distinct closed loop attitude control systems: a spherical pendulum with configurations in S^2 and a 3D pendulum with configurations in $SO(3)$.

58. **Nonlinear Robust Tracking Control of a Quadrotor UAV on SE(3)** *(with T. Lee, N. H. McClamroch)*
Proc. American Control Conf., 4649–4654, 2012.

This paper provides nonlinear tracking control systems for a quadrotor unmanned aerial vehicle (UAV) that are robust to bounded uncertainties. A mathematical model of a quadrotor UAV is defined on the special Euclidean group, and nonlinear output-tracking controllers are developed to follow (1) an attitude command, and (2) a position command for the vehicle center of mass. The controlled system has the desirable properties that the tracking errors are uniformly ultimately bounded, and the size of the ultimate bound can be arbitrarily reduced by control system parameters. Numerical examples illustrating complex maneuvers are provided.

59. **Dynamics and Control of a Chain Pendulum on a Cart** *(with T. Lee, N. H. McClamroch)*
Proc. IEEE Conf. on Decision and Control, 2502–2508, 2012.

A geometric form of Euler-Lagrange equations is developed for a chain pendulum, a serial connection of n rigid links connected by spherical joints, that is attached to a rigid cart. The cart can translate in a horizontal plane acted on by a horizontal control force while the chain pendulum can undergo complex motion in 3D due to gravity. The configuration of the system is in $(S^2)^n \times \mathbb{R}^2$. We examine the rich structure of the uncontrolled system dynamics: the equilibria of the system correspond to any one of 2^n different chain pendulum configurations and any cart location. A linearization about each equilibrium, and the corresponding controllability criterion is provided. We also show that any equilibrium can be asymptotically stabilized by using a proportional-derivative type controller, and we provide a few numerical examples.
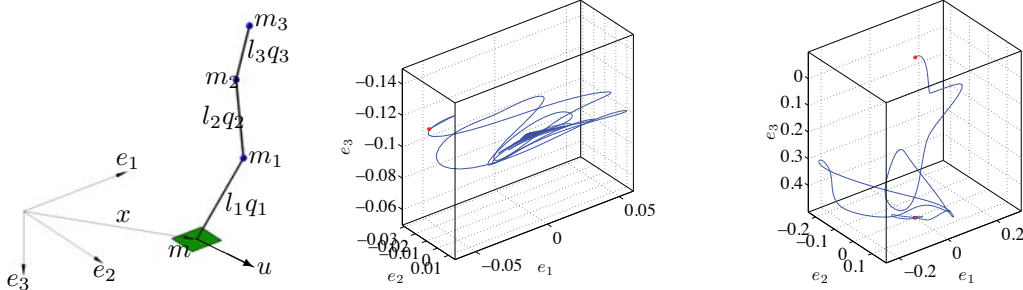

60. **Hamel's Formalism and Variational Integrators on a Sphere** *(with A. M. Bloch, D. V. Zenkov)*
Proc. IEEE Conf. on Decision and Control, 7504–7510, 2012.

This paper discusses Hamel's formalism and its applications to structure-preserving integration of mechanical systems. It utilizes redundant coordinates in order to eliminate multiple charts on the configuration space as well as nonphysical artificial singularities induced by local coordinates, while keeping the minimal possible degree of redundancy and avoiding integration of differential-algebraic equations.

61. **Space-Time Finite-Element Exterior Calculus and Variational Discretizations of Gauge Field Theories** *(with J. Salamon, J. Moody)*
Proc. Mathematical Theory of Networks and Systems, 743–747, 2014.

Many gauge field theories can be described using a multisymplectic Lagrangian formulation, where the Lagrangian density involves space-time differential forms. While there has been much work on finite-element exterior calculus for spatial and tensor product space-time domains, there has been less done from the perspective of space-time simplicial complexes. One critical aspect is that the Hodge star is now taken with respect to a pseudo-Riemannian metric, and this is most naturally expressed in space-time adapted coordinates, as opposed to the barycentric coordinates that the Whitney forms (and their higher-degree generalizations) are typically expressed in terms of.

We introduce a novel characterization of Whitney forms and their Hodge dual with respect to a pseudo-Riemannian metric that is independent of the choice of coordinates, and then apply it to a variational discretization of the covariant formulation of Maxwells equations. Since the Lagrangian density for this is expressed in terms of the exterior derivative of the four-potential, the use of finite-dimensional function spaces that respects the de Rham cohomology results in a discretization that inherits the gauge symmetries of the continuous problem. This then yields a variational discretization that exhibits a discrete Noethers theorem, which implies that an associated multimomentum is automatically conserved by the discretization.
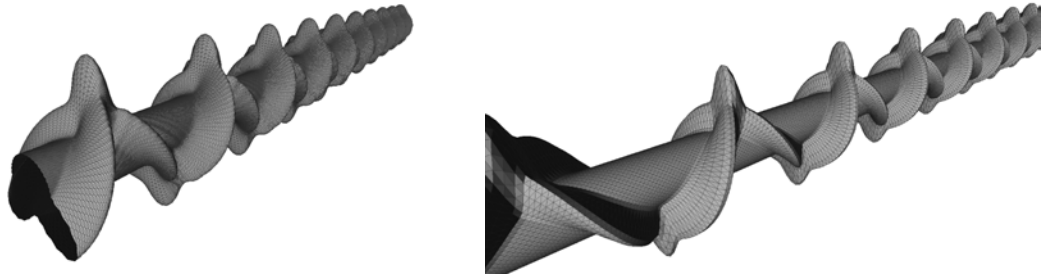
62. **Global Formulations of Lagrangian and Hamiltonian Dynamics on Embedded Manifolds** *(with T. Lee, N.H. McClamroch)*
Proc. IMA Conf. on Mathematics of Robotics, accepted, 2015.

This paper provides global formulations of Lagrangian and Hamiltonian variational dynamics evolving on a manifold embedded in $\mathbb{R}^n$, which appears often in robotics and multi body dynamics. Euler–Lagrange equations and Hamiltons equations are developed in a coordinate-free fashion on a manifold, without relying on local parameterizations that may lead to singularities and cumbersome equations of motion. The proposed intrinsic formulations of Lagrangian and Hamiltonian dynamics are expressed compactly, and they are useful in analysis and computation of the global dynamics. These are illustrated by dynamic systems on the unit-spheres and the special orthogonal group.

63. **Global Formulations of Lagrangian and Hamiltonian Mechanics on Two-Spheres** *(with T. Lee, N.H. McClamroch)*
Proc. IEEE Conf. on Decision and Control, accepted, 2015.

This paper provides global formulations of Lagrangian and Hamiltonian variational dynamics evolving on the product of an arbitrary number of two-spheres. Four types of Euler-Lagrange equations and Hamiltons equations are developed in a coordinate-free fashion on two-spheres, without relying on local parameterizations that may lead to singularities and cumbersome equations of motion. The proposed intrinsic formulations of Lagrangian and Hamiltonian dynamics are novel in that they incorporate the geometry of two-spheres, resulting in equations of motion that are expressed compactly, and they are useful in analysis and computation of the global dynamics.

64. **Spectral-Collocation Variational Integrators** *(with Y. Li, B. Wu)*
    Journal of Computational Physics, submitted, 2015.

    Spectral methods are a popular choice for constructing numerical approximations for smooth problems, as they can achieve geometric rates of convergence and have a relatively small memory footprint. In this paper, we recall the method for constructing Galerkin spectral variational integrators and introduce a general framework to convert a spectral-collocation method into a shooting-based variational integrator for Hamiltonian systems. We also present a systematic comparison of how spectral-collocation methods, Galerkin spectral variational integrators, and shooting-based variational integrators derived from spectral-collocation methods perform in terms of their ability to reproduce accurate trajectories in configuration and phase space, their ability to conserve momentum and energy, as well as the relative computational efficiency of these methods when applied to some classical Hamiltonian systems. In particular, we note that spectrally-accurate variational integrators, such as the Galerkin spectral variational integrator and the spectral-collocation variational integrator, combine the computational efficiency of spectral methods together with the geometric structure-preserving and long-time structural stability properties of symplectic integrators.

65. **Spectral variational integrators for semi-discrete Hamiltonian wave equations**
    (with Y. Li, B. Wu)
    Journal of Computational and Applied Mathematics, submitted, 2016.

    In this paper, we present a highly accurate Hamiltonian structure-preserving numerical method for simulating Hamiltonian wave equations. This method is obtained by applying spectral variational integrators (SVI) to the system of Hamiltonian ODEs which are derived from the spatial semi-discretization of the Hamiltonian PDE. The spatial variable is discretized by using high-order symmetric finite-differences. An efficient implementation of SVI for high-dimensional systems of ODEs is presented.
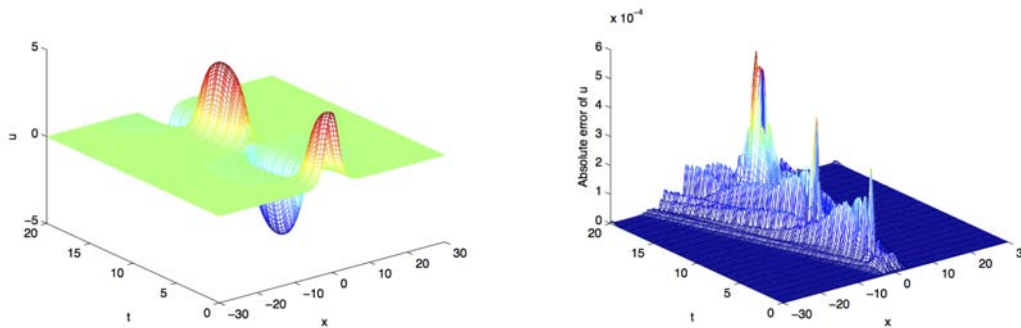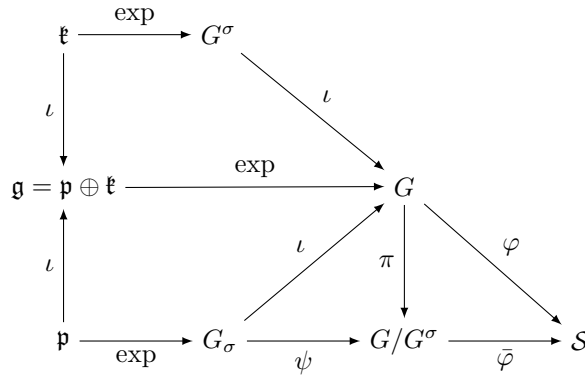

66. **Taylor Variational Integrators** *(with J. Schmitt, T. Shingel)*
    IMA Journal of Numerical Analysis, under revision, 2015.

    The shooting-based variational integrator approach provided a means of converting any one-step numerical integrator into a symplectic and variational integrator with the same order of accuracy. This is achieved by relating the exact generating function for the symplectic time-h flow map of Hamilton's equations with the action integral evaluated on the solution of the Euler–Lagrange boundary-value problem. However, this required the use of a sufficiently accurate numerical quadrature rule, and in practice, that meant that in order to construct a high-order variational integrator using this approach, one would have to apply the underlying one-step method multiple times in order to generate the discrete solution of the Euler–Lagrange boundary value problem at the requisite quadrature nodes. In this paper, we present a variational integrator that is based on an approximation of the Euler–Lagrange boundary-value problem that is obtained using Taylor's method. This method is more efficient, since Taylor's method can be used to compute the discrete solution at the quadrature nodes at the cost of a polynomial evaluation once the prolongation of the Euler–Lagrange vector field is computed at the initial time. In addition, the resulting symplectic and variational integrator is one order higher than the order of the underlying Taylor's method.

67. **Interpolation on Symmetric Spaces via the Generalized Polar Decomposition** *(with E. Gawlik)*
    Foundations of Computational Mathematics, submitted, 2016.

    We construct interpolation operators for functions taking values in a symmetric space a smooth manifold with an inversion symmetry about every point. Key to our construction is the observation that every symmetric space can be realized as a homogeneous space whose cosets have canonical representatives by virtue of the generalized polar decomposition a generalization of the well-known factorization of a real nonsingular matrix into the product of a symmetric positive-definite matrix times an orthogonal matrix. By interpolating these canonical coset representatives, we derive a family of structure-preserving interpolation operators for symmetric space-valued functions. As applications, we construct interpolation operators for the space of Lorentzian metrics, the space of symmetric positive-definite matrices, and the Grassmannian. In the case of Lorentzian metrics, our interpolation operators provide a family of finite elements for numerical relativity that are frame-invariant and have signature which is guaranteed to be Lorentzian pointwise. We illustrate their potential utility by interpolating the Schwarzschild metric numerically.
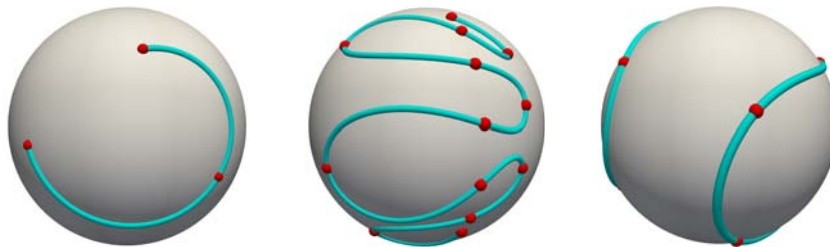
$$
\begin{array}{ccc}
\mathfrak{k} & \xrightarrow{\ \exp\ } & G^\sigma \\
\downarrow{\scriptstyle\iota} & & \searrow{\scriptstyle\iota} \\
\mathfrak{g} = \mathfrak{p} \oplus \mathfrak{k} & \xrightarrow{\ \exp\ } & G \\
\uparrow{\scriptstyle\iota} & {\scriptstyle\iota}\nearrow \quad {\scriptstyle\pi}\downarrow \quad {\scriptstyle\varphi}\searrow & \\
\mathfrak{p} & \xrightarrow[\ \exp\ ]{} G_\sigma \xrightarrow[\ \psi\ ]{} G/G^\sigma \xrightarrow[\ \bar\varphi\ ]{} \mathcal{S}
\end{array}
$$

68. **Computing the Fréchet Derivative of the Polar Decomposition** *(with E. Gawlik)*
    SIAM Journal on Matrix Analysis and Applications, submitted, 2016.

    We derive iterative methods for computing the Fréchet derivative of the map which sends a full-rank matrix A to the factor U in its polar decomposition $A = UH$, where U has orthonormal columns and H is Hermitian positive definite. The methods apply to square matrices as well as rectangular matrices having more rows than columns. Our derivation relies on a novel identity that relates the Fréchet derivative of the polar decomposition to the matrix sign function $\mathrm{sign}(X) = X(X^2)^{-1/2}$ applied to a certain block matrix X.

69. **Embedding-Based Interpolation on the Special Orthogonal Group** *(with E. Gawlik)*
    Numerische Mathematik, submitted, 2016.

    We study schemes for interpolating functions that take values in the special orthogonal group $SO(n)$. Our focus is on interpolation schemes obtained by embedding $SO(n)$ in a linear space, interpolating in the linear space, and mapping the result onto $SO(n)$ via the closest point projection. The resulting interpolants inherit both the order of accuracy and the regularity of the underlying interpolants on the linear space. The values and derivatives of the interpolants admit efficient evaluation via either explicit formulas or iterative algorithms, which we detail for two choices of embeddings: the embedding of $SO(n)$ in the space of $n \times n$ matrices and, when $n = 3$, the identification of $SO(3)$ with the set of unit quaternions. Along the way, we point out a connection between these interpolation schemes and geodesic finite elements. We illustrate the utility of these interpolation schemes by numerically computing minimum acceleration curves on $SO(n)$, a task which is handled naturally with $SO(n)$-valued finite elements having C^1-continuity.

70. **Properties of Hamiltonian Variational Integrators** *(with J. Schmitt)*
    IMA Journal of Numerical Analysis, submitted, 2016.

    Discrete Hamiltonian variational integrators are derived from Type II and Type III generating functions for symplectic maps, and in this paper we establish a variational error analysis result that relates the order of accuracy of the associated numerical methods with the extent to which these generating functions approximate the exact discrete Hamiltonians. We also introduce the notion of an adjoint discrete Hamiltonian, and relate it to the adjoint of the associated symplectic integrator. We show that when constructing discrete Lagrangians and discrete Hamiltonians using the Taylor variational integrator approach, the same underlying one-step method and quadrature rule does not necessarily lead to the same symplectic integrator, and the same observation holds when developing variational integrators based on averaging techniques. Numerical experiments also indicate that the resonance behavior of variational integrators also depend on the type of generating functions used, and we relate this resonance behavior to the ill-posedness of the boundary-value problems used to define the exact discrete Lagrangian and exact discrete Hamiltonian.

71. **Generalized Galerkin Variational Integrators**
    Preprint, 2004.

    We introduce generalized Galerkin variational integrators, which are a natural generalization of discrete variational mechanics, whereby the discrete action, as opposed to the discrete Lagrangian, is the fundamental object. This is achieved by approximating the action integral with appropriate choices of a finite-dimensional function space that approximate sections of the configuration bundle and numerical quadrature to approximate the integral. We discuss how this general framework allows us to recover higher-order Galerkin variational integrators, asynchronous variational integrators, and symplectic-energy-momentum integrators. In addition, we will consider function spaces that are not parameterized by field values evaluated at nodal points, which allows the construction of Lie group, multiscale, and pseudospectral variational integrators. The construction of pseudospectral variational integrators is illustrated by applying it to the (linear) Schrödinger equation. G-invariant discrete Lagrangians are constructed in the context of Lie group methods through the use of natural charts and interpolation at the level of the Lie algebra. The reduction of these G-invariant Lagrangians yield a higher-order analogue of discrete Euler–Poincaré reduction. By considering nonlinear approximation spaces, spatio-temporally adaptive variational integrators can be introduced as well.
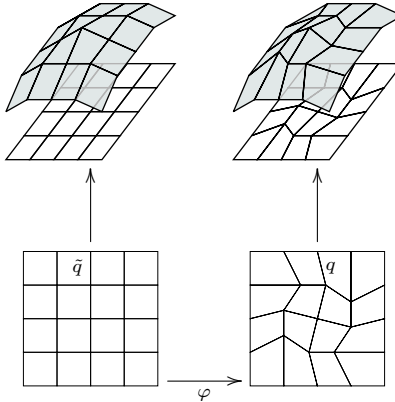
72. **A Discrete Theory of Connections on Principal Bundles** *(with J.E. Marsden, and A.D. Weinstein)*
Preprint, 2004.

Connections on principal bundles play a fundamental role in expressing the equations of motion for mechanical systems with symmetry in an intrinsic fashion. A discrete theory of connections on principal bundles is constructed by introducing the discrete analogue of the Atiyah sequence, with a connection corresponding to the choice of a splitting of the short exact sequence. Equivalent representations of a discrete connection are considered, and an extension of the pair groupoid composition, that takes into account the principal bundle structure, is introduced. Computational issues, such as the order of approximation, are also addressed. Discrete connections provide an intrinsic method for introducing coordinates on the reduced space for discrete mechanics, and provide the necessary discrete geometry to introduce more general discrete symmetry reduction. In addition, discrete analogues of the Levi-Civita connection, and its curvature, are introduced by using the machinery of discrete exterior calculus, and discrete connections.

$$0 \longrightarrow \tilde{G} \xrightarrow[\substack{(q,gq) \\ (\pi_1,\mathcal{A}_d)}]{} (Q \times Q)/G \xrightarrow[\substack{(\pi,\pi) \\ (\cdot,\cdot)^h}]{} S \times S \longrightarrow 0$$

$$0 \longrightarrow \tilde{G} \xrightarrow[\substack{i_1 \\ \pi_1}]{} \tilde{G} \oplus (S \times S) \xrightarrow[\substack{\pi_2 \\ i_2}]{} S \times S \longrightarrow 0$$

73. **Discrete Exterior Calculus** *(with M. Desbrun, A.N. Hirani, J.E. Marsden)*
Preprint, 2003.

We present a theory and applications of discrete exterior calculus on simplicial complexes of arbitrary finite dimension. This can be thought of as calculus on a discrete space. Our theory includes not only discrete differential forms but also discrete vector fields and the operators acting on these objects. This allows us to address the various interactions between forms and vector fields (such as Lie derivatives) which are important in applications. Previous attempts at discrete exterior calculus have addressed only differential forms. We also introduce the notion of a circumcentric dual of a simplicial complex. The importance of dual complexes in this field has been well understood, but previous researchers have used barycentric subdivision or barycentric duals. We show that the use of circumcentric duals is crucial in arriving at a theory of discrete exterior calculus that admits both vector fields and forms.
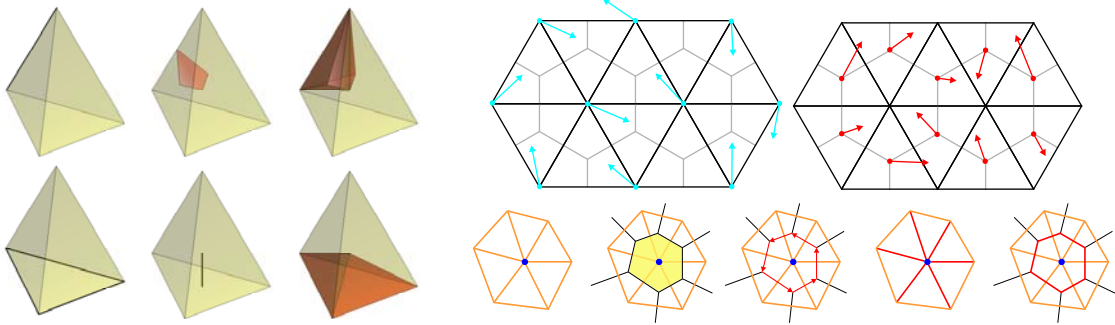
Thesis Abstract

Foundations of Computational Geometric Mechanics
Ph.D., Control and Dynamical Systems, California Institute of Technology, 2004.
Thesis Advisor: Jerrold E. Marsden

A preliminary version of this thesis received the **SIAM Student Paper Prize**
and the **Leslie Fox Prize in Numerical Analysis** *(second prize).*

Geometric mechanics involves the study of Lagrangian and Hamiltonian mechanics using geometric and symmetry techniques. Computational algorithms obtained from a discrete Hamilton's principle yield a discrete analogue of Lagrangian mechanics, and they exhibit excellent structure-preserving properties that can be ascribed to their variational derivation.

We construct discrete analogues of the geometric and symmetry methods underlying geometric mechanics to enable the systematic development of computational geometric mechanics. In particular, we develop discrete theories of reduction by symmetry, exterior calculus, connections on principal bundles, as well as generalizations of variational integrators.

Discrete Routh reduction is developed for abelian symmetries, and extended to systems with constraints and forcing. Variational Runge–Kutta discretizations are considered in detail, including the extent to which symmetry reduction and discretization commute. In addition, we obtain the Reduced Symplectic Runge–Kutta algorithm, which is a discrete analogue of cotangent bundle reduction.

Discrete exterior calculus is modeled on a primal simplicial complex, and a dual circumcentric cell complex. Discrete notions of differential forms, exterior derivatives, Hodge stars, codifferentials, sharps, flats, wedge products, contraction, Lie derivative, and the Poincaré lemma are introduced, and their discrete properties are analyzed. In examples such as harmonic maps and electromagnetism, discretizations arising from discrete exterior calculus commute with taking variations in Hamilton's principle, which implies that directly discretizing these equations yield numerical schemes that have the structure-preserving properties associated with variational schemes.

Discrete connections on principal bundles are obtained by introducing the discrete Atiyah sequence, and considering splittings of the sequence. Equivalent representations of a discrete connection are considered, and an extension of the pair groupoid composition that takes into account the principal bundle structure is introduced. Discrete connections provide an intrinsic coordinatization of the reduced discrete space, and the necessary discrete geometry to develop more general discrete symmetry reduction techniques.

Generalized Galerkin variational integrators are obtained by discretizing the action integral through appropriate choices of finite-dimensional function space and numerical quadrature. Explicit expressions for Lie group, higher-order Euler–Poincaré, higher-order symplectic-energy-momentum, and pseudospectral variational integrators are presented, and extensions such as spatio-temporally adaptive and multiscale variational integrators are briefly described.