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Applied Dynamics and Geometric Mechanics

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Abstract. This one week workshop was organized around several central subjects in applied dynamics and geometric mechanics. The specific organization with afternoons free for discussion led to intense exchanges of ideas. Bridges were forged between researchers representing different fields. Links were established between pure mathematical ideas and applications. The meeting was not restricted to any particular application area. One of the main goals of the meeting, like most others in this series for the past twenty years, has been to facilitate cross fertilization between various areas of mathematics, physics, and engineering. New collaborative projects emerged due to this meeting.

The workshop was well attended with participants from Europe, North America, and Asia. Young researchers (doctoral students, postdocs, junior faculty) formed about 30% of the participants.

Mathematics Subject Classification (2000): 37.-xx, 58.-xx, 70.-xx, 74.-xx,76.-xx, 85.-xx.

Introduction by the Organisers

This workshop on applied dynamics and geometric mechanics was introduced over 20 years ago by the late Klaus Kirchgässner and the late Jerrold E. Marsden. After Kirchgässner's retirement, this workshop continued to take place at regular intervals of three years under the leadership of Jerrold E. Marsden and Jürgen Scheurle. Every such meeting was inspired by new developments in the core fields of dynamical systems and geometric mechanics as well as recent exciting applications. The present meeting continued this tradition. The whole subject is scientifically extremely active and progressing in various new and promising directions. Each speaker and invitee presented a new mathematical or computational tool in

dynamical systems or geometric mechanics and linked it either to applications, or forged a bridge between various areas of pure dynamical systems and geometric mechanics and certain applications to physics, engineering, and other basic sciences.

A broad overview of these topics as covered in the meeting is as follows:

Dynamical Systems. The basic theory of dynamical systems is developing with numerous new ideas that have importance in applications. The meeting presented recent advances in this theory with an emphasis on applications in one of the following specific areas.

• *Astrodynamics.* There is a rich history of applications of the theory of dynamical systems to problems in astrophysics. The morning of the first day of the workshop was devoted entirely to problems in astrophysics and celestial mechanics. The speakers and posters emphasized the link between their own research problems to branches of dynamical systems and geometric mechanics.

• *Control Theory.* An important area of research that is closely connected with both dynamical systems and geometric mechanics is nonlinear control theory. Nonlinear control is naturally formulated on manifolds and has particular applications to mechanical systems where the control is studied on a Riemannian manifold. Basic problems include controllability, stabilization, and optimal control. A recent area of great interest is the simultaneous control of multiple systems (swarms). Such systems include groups of wheeled or legged robots or groups of submarine robotic vehicles. There are very interesting connections of this work with the study of biological swarming in birds or fish, for example. Another important topic is the control of interconnected systems which can be studied using the theory of Dirac structures. This is important for both electrical and mechanical networks. Several talks and posters on these topics were given during the workshop.

• *Multi-Agent Systems.* Many modern technical systems, such as multiple mobile robots in the same workspace, are composed out of many, relatively simple, subsystems (agents) that interact in a complicated way. Since the computational limitations of dealing with such complex interconnected systems have already been reached, new methods are being developed that treat such systems as strongly and weakly interconnected units. In other words, instead of thinking of these systems as huge systems of differential equations (ordinary or partial), one is organizing them in smaller units with massive message passing and information exchange between them. The speakers and posters presented new tools that could lead to the automatic determination of the strong or weak coupling between such subsystems; this then naturally leads to a hierarchy of corresponding dynamical computations. Another topic presented was about the development of cooperative distributed control strategies, both at the theoretical and computational/numerical level.

Geometric Mechanics. By now, geometric mechanics has matured to a main subject at the interface between several areas such as symplectic, Poisson, and Dirac geometry, dynamical systems, variational calculus, theoretical physics, numerical analysis, control theory, and various areas of engineering science. The

subject continues to thrive and develop, both by widening its core to include other theoretical fields such as integrable systems and conservative evolutionary PDEs and by reaching out to new applied areas such as imaging science, discrete differential geometry, stochastic analysis, or materials science. The following core subjects were specifically addressed at this workshop.

• *Nonholonomic Mechanics.* Nonholonomic mechanics is an important extension of Hamiltonian mechanics whose goal is the study of the dynamics of mechanical systems subject to nonintegrable constraints on the velocity (such as the rolling wheel, the ice skate, or the rolling ball). Such systems are endowed with a bracket that does not satisfy the Jacobi identity and have a dynamics that non-trivially generalizes that seen in Hamiltonian systems. For example, volume is not necessarily conserved in the phase space and it is possible to get asymptotic stability even in the absence of external friction. Also, there is an interesting generalization of Noether's theorem: Symmetry does not usually lead to momentum conservation but to a dynamic momentum equation. Some systems admit a "Hamiltonization", that is, one can produce a Poisson bracket such that relative to it and after a time reparametrization, the system becomes Hamiltonian. This then allows the study of the integrability of nonholonomic systems. There is also an interesting connection with control theory because nonintegrable constraints are related to the fact that a system remains controllable in the presence of constraints. There are many applications to robotic problems and problems in submarine and flight dynamics using these ideas. Several talks and posters addressed these fundamental questions and linked them to many applications.

• *Discrete Mechanics.* Discrete mechanics and the numerical analysis related to this area was another core subject represented at this workshop. Since the late 1980's, the field of geometric integration and structure preserving algorithms has seen spectacular development. It has produced and analyzed numerical methods for ordinary differential equations and, more recently, for partial differential equations, that preserve exactly (i.e., up to round-off error) as much of the underlying geometric structure as possible. Geometric mechanics has been one of the main beneficiaries of these geometric integration techniques which has led to new developments in the simulation of mechanical systems in particle and continuum mechanics as well as their stochastic counterparts. Several talks and posters addressed the above mentioned problems.

• *Stochastic Mechanics.* Randomness is ubiquitous in the description of dynamical phenomena for several reasons. It may express our lack of knowledge about the systems' parameters or components. It may arise intrinsically as non-determinism in a large spectrum of areas ranging from statistical mechanics to interacting systems of agents on financial markets. It also appears as an analytical tool in area of mathematics such as control theory and differential geometry. It may also be encountered as noise in mesoscopic limits of dynamical systems on different scales, arising in many different ways, from turbulence in ocean-atmosphere dynamics, to order book fluctuations governing price dynamics, in which the small scale component has good mixing properties. The talks and posters representing this

area underlined the achievements recently obtained in financial mathematics as well as stochastically perturbed conservative systems. In addition, the geometry induced by the addition of noise to a deterministic dynamical system was also presented.

• *Liquid Crystals.* The mathematical study of complex materials has seen an explosive growth in the past few years. These materials, both fluids and solids, are characterized by an additional internal structure of the particles which is encoded in an order parameter group. Liquid crystals are important representatives of complex materials. The dynamics of liquid crystals is dominated by two theories: Ericksen-Leslie order parameter theory and Eringen micropolar theory. No link between these theories has been established, in spite of the fact that the latter should naturally include the former. Worse, all attempts at proving this implication have failed due to errors of all papers addressing this problem in the literature. At this workshop, using sophisticated tools of geometric mechanics, a theorem was presented that proves such an inclusion.

Structure of the Meeting. Consistent with the general policy of Oberwolfach there were only twenty main lectures at the meeting. Twenty invitees were asked to speak and present their latest results. All participants were invited to present a poster. There were slots in the schedule specifically for advertising and viewing the posters, respectively, (teaser and presentation sessions). Wednesday evening an open discussion was held addressing the recent developments in the field of Geometric Mechanics and the new directions where it is supposed to develop.

Poster titles and poster presenters. The following posters have been presented at the workshop.

• Twisted structures in nonholonomic systems (Paula Balseiro)
• Stability of stationary fronts in inhomogeneous wave equations (Gianne Derks)
• Continuous and discrete Neumann systems on Stiefel varieties (Yuri Fedorov)
• Applications of Hamiltonization of nonholonomic systems (Oscar Fernandez)
• Solitary waves in a chain of coupled Fitzhugh-Nagumo neurons (Andreas Johann)
• Optimizing the stable behaviour of controlled dynamical systems (Peter Koltai)
• Global symplectic uncertainty propagation on Lie groups (Melvin Leok)
• Discrete Dirac mechanics and discrete Dirac geometry (Melvin Leok, Tomoki Ohsawa)
• Routh reduction for singular Lagrangians (Bavo Langerock)
• Moving framework and fiber bundle methods in nonholonomic mechanics (Jared Michael Maruskin)
• Involutive distributions and dynamical systems of second order type (Tom Mestag)
• Variational integration of constrained dynamics on different time scales (Sina Ober-Blöbaum, Sigrid Leyendecker)
• Nonholonomic Hamilton-Jacobi theory (Tomoki Ohsawa)
• On the topology of the double spherical pendulum (Manuele Santoprete)
• Discrete integrable dynamical systems (Yuri B. Suris)
• Invariant sets forced by symmetry (Sebastian Walcher)

Geometric Mechanics quo vadis? The discussion on Wednesday evening was one of the most interesting aspects of the meeting. Many topics that have become central to geometric mechanics or that use its tools in an essential way were identified. Here are some that were mentioned in this open discussion: Interplanetary missions, variational integrators, swimming theory, Lagrangian coherent structures, Euler-Poincaré theory, Lie-Poisson reduction, multisymplectic integrators, nonlinear stability, underwater vehicles, geometrical optimal control, computational anatomy, reduction by stages in both the Hamiltonian and Lagrangian setting, molecular oscillations, dynamics of asteroids pairs, dynamics of satellite with tethers, molecular strand theory, geometrically exact elasticity, robotics, solitons and peakons, various aspects of fluid dynamics, turbulence models, geometric formulation of complex fluid theory, liquid crystals, superfluids, plasmas, magnetohydrodynamics, geophysical fluid dynamics, general relativity, field theory, Lie groupoids and algebroids, swarming theory, telecommunications.

Several main directions for geometric mechanics were identified in this discussion:

• How does one deal with low regularity in geometric mechanics? The obvious example is compressible barotropic fluid flow that can be formally written as a Hamiltonian system, yet, after the first shock, it can be rigorously proven that the energy decays.

• Symmetric Hamiltonian Bifurcation Theory. Very little is known about this subject which remains, to these days, almost totally underdeveloped. The challenge here is to bring it to the level of the by now standard theory of symmetric bifurcation for generic vector fields developed by Golubitsky and his collaborators. One of the main technical tools in this development is the geometry of the momentum map.

• The Nature of Integrability. In spite of spectacular developments in the theory of integrable systems, the field itself is poorly developed. This entire area rests essentially on large classes of known integrable ODEs and PDEs. While Fomenko and his collaborators have developed a topological classification method, almost nothing is known about a symplectic classification. This in turn is essential in the study of semiclassical quantization and spectral analysis.

• Hybrid discrete and continuous systems. Hybrid systems can be described mathematically by a mixture of logic based switching and difference/ differential equations. Also, stochastic components can be included. Besides of continuously varying variables and parameters such systems additionally contain variables with a discrete range of values. Variations of these lead to sudden structural changes of the systems and thus to a rapid change in the systems' behaviour. Many systems in engineering and some physical systems can be modeled using such a mathematical framework. Examples are contact problems in mechanics, event driven systems and adaptive control. A general theory for this remains to be developed.

• Networks with varying connectivity/ topology. Complex networks play a central role in today's society. For example, communication, mobility and transportation are based and rely on networks. The question of how the network topology affects

the performance has not been addressed systematically. The topology of a network is determined by the nature of the coupling between its nodes (connectivity). The character of the coupling can change when structural parameters are varied. An interesting research topic is the extension of classical concepts from bifurcation and stability theory to such systems.

Workshop: Applied Dynamics and Geometric Mechanics

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Abstracts

Astrophysical Orbits and Random Hill's Equations

Fred C. Adams
(joint work with Anthony M. Bloch)

Overview. This work presents new mathematical results that are motivated by orbit problems in astrophysics. Most of the matter in our universe is thought to reside in the form of weakly interacting particles known as dark matter. These dark matter particles constitute enormous extended mass distributions, called dark matter halos, which generally exhibit triaxial forms. Note that the visible portions of galaxies are found at the centers of these halos. The orbits of dark matter particles through their halos represents the vast majority of orbital motion that takes place in the universe. Such orbits are found to be subject to a powerful orbit instability: When an orbit starts in any of the principle planes of the triaxial system, the motion is unstable to perturbations in the perpendicular direction. The development of this instability is described by a type of random Hill's equation, where the parameters of the differential equation vary from cycle to cycle. The time evolution of this stochastically forced Hill's equation can be studied by analyzing infinite products of random matrices. We find growth rates for these matrix products and hence for the original differential equations.

Hill's Equation with Random Forcing Parameters. As outlined above, orbit problems in extended mass distributions, such as dark matter halos and young embedded star clusters, give rise to stochastic Hill's equations [1]. In this context, Hill's equation takes the form

$$\frac{d^2y}{dt^2} + [\lambda_k + q_k \hat{Q}(t)]y = 0\,, \tag{1}$$

where the function $y(t)$ describes the perpendicular displacement of the orbit from its original principle plane. The Hill's equation is random in the sense that the parameters vary from cycle to cycle. The barrier shape function $\hat{Q}(t)$ is periodic, so that $\hat{Q}(t + \Delta\tau) = \hat{Q}(t)$, where $\Delta\tau$ is the period. The forcing strength q_k and the natural oscillation frequency λ_k change from cycle to cycle, and are drawn from a well-defined distribution. We note that the period $(\Delta\tau)_k$ could also vary from cycle to cycle, although such variations can be scaled out of the problem; in that case, the period variations change the distributions of the other parameters (λ_k, q_k).

Periodic differential equations in this class can be described by a discrete mapping of the coefficients of the principal solutions from one cycle to the next. The transformation matrix takes the form

$$\mathbf{M}_k = \begin{bmatrix} h_k & (h_k^2 - 1)/g_k \\ g_k & h_k \end{bmatrix}\,, \tag{2}$$

where the subscript denotes the cycle. The matrix elements for the kth cycle are given by

$$h_k = y_1(\Delta\tau) \qquad \text{and} \qquad g_k = \dot{y}_1(\Delta\tau)\,, \tag{3}$$

where y_1 and y_2 are the principal solutions for that cycle (and are evaluated at the end of the cycle). The index k indicates that the quantities (λ_k, q_k), and hence the solutions (h_k, g_k), vary from cycle to cycle. Throughout this work, the random variables are taken to be independent and identically distributed (iid).

The development of the solutions to the periodic differential equation (1) can thus be described by infinite products of matrices with the form given by equation (2), where the matrix elements are given by equation (3) and vary from cycle to cycle. The growth rates γ can be written in the form

$$\gamma = \lim_{N\to\infty} \frac{1}{N} \log ||\mathbf{M}^{(N)}|| \qquad \text{where} \qquad \mathbf{M}^{(N)} = \prod_{k=1}^{N} \mathbf{M}_k\,. \tag{4}$$

This result is independent of the choice of the norm $||\cdot||$, as shown in previous work [5, 6].

In the limit of strong forcing (e.g., when $q_k \gg 1$) the growth rates of the differential equation (1) and the corresponding matrices (2) have analytic forms [2]. These growth rates thus add to the collection of known, closed-form results for infinite products of random 2×2 matrices. We have developed a generalized analysis of these growth rates, including cases where all of the cycles are highly unstable, where some cycles are near the stability border, and where some cycles would be stable in the absence of fluctuations [3, 4]. More specifically, we have found expressions for the growth rates of the 2×2 matrices that describe the solutions. We found exact expressions — in terms of expectation values — for the growth rates for the full problem, first order corrections to the stable limit and the highly unstable limit, and for the case where the solutions are stable in the absence of random variations.

One result of including random forcing parameters is an increase in instability: For the standard case with constant parameters, Hill's equations generally display alternating bands of stability and instability in the (λ, q) plane of parameters [7]. In the presence of cycle-to-cycle parameter variations, however, the bands of stability essentially disappear [2, 3, 4].

Future work. These studies of random Hill's equations provide us with new examples where the infinite products of random matrices can be determined. It would be interesting to carry this work further. We can use our results obtained to date to find additional classes of matrices where the growth rates can be explicitly calculated. Turning the problem around, we can also explore how existing matrix examples imply properties of stochastic differential equations.

In many cases, an ensemble of stochastic systems of the type considered here can be described with a Fokker-Planck (FP) equation. However, the derivation of the FP equation is only valid in the limit of small stochastic perturbations (the validity of the FP approach for the limit $q_k \ll 1$ is described in [3]). On the other

hand, for the case of orbit instabilities, governed by the random Hill's equation (1), we are primarily interested in the opposite limit of large forcing terms where $q_k \gg 1$. This poses a number of related questions, including defining the regime of applicability of the FP treatment for this class of problems, and how solutions behave in the transition regime between small and large forcing terms.

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Brockett-Heisenberg Systems and Geometric Aspects of Control Communication Complexity

John Baillieul

(joint work with Wing-Shing Wong)

The interaction of information and control has been a topic of interest to system theorists that can be traced back to the 1950s when the fields of communications, control, and information theory were new but developing rapidly. Recent advances in our understanding of this interplay have emerged from work on the dynamical effect of state quantization and a corresponding understanding of how communication channel data rates affect system stability. While a large body of research has now emerged dealing with communication constrained feedback channels and optimal design of information flows in networks, less attention has been paid to ways in which control systems should be designed in order to optimally mediate computation and communication. Recently W.S. Wong has proposed the concept of control communication complexity (CCC) as a formal approach for understanding how a group of distributed agents can take independent actions that cooperatively realize common goals and objectives. A prototypical goal is the computation of a function, and CCC provides a promising new approach to understanding complexity in terms of the cost of information processing. This lecture introduces control communication complexity in terms of what are called standard parts optimal control problems. Such optimization problems are of interest in the context of quantum computing, and similar problems have recently been discussed

in connection with protocols for assembly of molecular components in synthetic biology.

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Torus Dynamics

James Binney

Massive observational resources, both ground- and space-based, are currently being devoted to surveying the contents of our Galaxy. The latter is of interest not merely because it is our home, but because it is typical of the galaxies that currently dominate the cosmic star-formation rate, and its luminosity lies precisely at the characteristic luminosity of galaxies, L^*.

We can measure all three components of the velocity of a star, the component $v_{\rm los}$ along the line of sight through Döppler shifts of spectral lines, and the transverse components by watching its "proper motion" μ across the sky. If the star is near enough, its distance s can be inferred by measuring the parallax $\varpi = {\rm AU}/s$ that arises from the Earth's motion about the Sun. The Gaia satellite, which will be launched by ESA in early 2013, will measure parallaxes with sufficient precision ($\delta\varpi < 5\times10^{-11}$) to determine the distances to stars as far away as the Galactic centre. By 2020 we will have useful measurements of the sky-positions, proper motions and parallaxes of $\sim 10^9$ stars and spectra for $> 10^8$ stars. From the spectra it is possible to determine not only $v_{\rm los}$ but also information about the chemical composition of the star, and, in favourable cases, information about the age and luminosity of the star. Given that even for the faintest stars we can measure the apparent brightness in a few wavebands, the space of observables never has dimension less than 7, and for brighter stars has dimension 12 or greater.

Variables of physical interest, such as the distance and transverse velocity $v_\perp = \mu/\varpi$, are non-linearly related to the observed quantities, so we cannot profitably infer physical quantities directly from the data – for example, the measured parallax of a distant star will often be negative, and correspond to no distance. Yet a negative parallax does convey information, namely that the star is probably more distant than the inverse of the standard error on the parallax. In view of this situation we must proceed by comparing the data to probability density functions

(pdf) in the space of observables predicted by models. Traditional galaxy models, N-body and Schwarzschild orbit-superposition models, do not provide pdfs but discrete realisations of an unknown pdf. Moreover, it is hard to steer an N-body model towards a model that is consistent with the data, because the relation between the final model and the initial conditions is complex and ill-understood.

The most promising approach is best understood as a development of Schwarzschild modelling [1]. The key is to replace orbits as time series with orbital tori as three-dimensional submanifolds of phase space. Position on a torus is determined by three angle variables θ_i and the tori are labelled by their actions $J_i = (2\pi)^{-1} \oint_{\gamma_i} \mathrm{d}q \cdot p$, where γ_i are three closed paths on the torus that cannot be deformed into one another. We obtain our tori by choosing a canonical transformation that maps an analytic orbital torus of either the harmonic oscillator or the isochrone potential into the Galaxy's phase space. The general structure of the canonical transformation is specified a priori, and the coefficients in the generating function(s) of the transformation are adjusted to minimise (for given $\mathbf{J}$) the rms variation of the Galaxy's Hamiltonian H over the image torus [2].

After we have established the canonical transformation for all $\mathbf{J}$ in some region of action space, we can define an integrable Hamiltonian H_0 in that region by $H_0(\mathbf{J}) \equiv \langle H \rangle_\theta$ [3]. If our adjustment of the canonical transformation has been a complete success, H will be constant on the image tori so $H = H_0$. Generally H will fluctuate slightly on the the image tori, so there will be a small difference Hamiltonian $\Delta \equiv H - H_0$. Thus torus dynamics furnishes an integrable Hamiltonian, which can be used for preliminary modelling, and a perturbing Hamiltonian, which can be used to refine a model. Δ is typically very small, so first-order secular perturbation theory works much better than in traditional applications. In fact the smallness of Δ is such that we have to derive a refinement of the traditional pendulum equation for discussions of resonant trapping and the onset of chaos [4].

Our current galaxy models consist of analytic functions $f(\mathbf{J})$ for each cohort of physically distinguishable stars, for example old, metal-poor stars, and stars of approximately solar composition that were born $\sim 5\,\mathrm{Gyr}$ ago [5]. The functions f contain parameters and we choose these parameters by deriving from the fs and the known measurement errors the pdf of stars in the space of observables. Then we determine the likelihood of the data given the model by integrating the model pdf along the line of sight to each star through a plausible range of distances. The product of the individual stellar probabilities gives the likelihood of the data given the model, and a Markov-chain Monte-Carlo process is then used to determine the pdf of the parameters given the data [6].

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New Developments in Discrete Variational Calculus and Discrete Optimal Control Theory

David Martín de Diego

One of the main goals of numerical analysis and computational mathematics has been rendering physical phenomena into algorithms that produce sufficiently accurate, affordable, and robust numerical approximations. Therefore, numerical simulations are now an invaluable tool for exploring the dynamics of nonlinear differential equations. In the late 1980s, and throughout the 1990s, the field of Geometric Integration (GI) arose to design and to analyze numerical methods for ordinary differential equations and, more recently, for partial differential equations (PDEs), that preserve exactly (i.e. up to round-off error) as much of the underlying geometrical structures as possible [5]. In this sense, GI is concerned with producing numerical approximations preserving the qualitative attributes of the solution to the extent that it is possible (phase space, energy conservation, preservation of integrability under discretization, reversibility, symplecticity, volume preservation, etc) while not disregarding accuracy, affordability, and robustness. In particular, in many problems arising from science and engineering (such as solar system or molecular dynamics) the underlying geometric structure affects the qualitative behavior of solutions, and as such, numerical methods that preserve the geometry of a problem typically yield simulations that are qualitatively more accurate.

As a particular case of geometric integrators for lagrangian systems appears discrete variational integrators based on an appropriate discretization of the variational principle (see [9] and references therein). During the last decade, the effort has been concentrated to the case of discrete Lagrangian functions L on the cartesian product $Q \times Q$ of a differentiable manifold. This cartesian product plays the role of a "discretized version" of the standard velocity phase space TQ when we approach to vector by two nearby points. Applying a natural discrete variational principle, we obtain a recurrence law which is a second order recursion operator $\xi_d : Q \times Q \longrightarrow Q \times Q$ assigning to each input pair (x_{k-1}, x_k) the output pair (x_k, x_{k+1}). One interesting feature of this particular type of integrators is that automatically the derived numerical scheme inherits some of the geometric properties of the continuous Euler-Lagrange equations (symplecticity, momentum preservation, good energy behaviour, etc).

Although this type of geometric integrators have been mainly considered for conservative systems, the extension to geometric integrators for more involved situations is relatively easy knowing the geometry of the continuous counterpart. In this sense, it has been recently shown how discrete variational mechanics can include forced or dissipative systems, holonomic constraints, explicitly time-dependent

systems, frictional contact, nonholonomic constraints, multisymplectic fields theories... In the case of nonholonomic systems the induced numerical methods show a very good energy behavior and properties such as the preservation of the discrete nonholonomic momentum map [1].

Many of the previous examples are based on the discretization of the tangent bundle TQ as two copies of Q, $Q \times Q$. But, Moser and Veselov [10] consider also a discrete Lagrangian systems evolving on a Lie group, showing the possibility to extend discrete variational calculus to a more general class of examples, as the the case of Lie groups, as a dicrete version of lagrangians defined on Lie algebras (discrete Euler-Poincaré equations). All this plethora of examples induces to A. Weinstein [11] to study discrete mechanics on Lie groupoids, which is a structure that includes as particular examples the case of cartesian products $Q \times Q$ as well as Lie groups, but also many other examples which application to reduced Lagrangian and Hamiltonian mechanics. We recall that a Lie groupoid G is a natural generalization of the concept of a Lie group, where now not all elements are composable. The product $g_1 g_2$ of two elements is only defined on the set of composable pairs $G_2 = \{(g, h) \in G \times G \mid \beta(g) = \alpha(h)\}$ where $\alpha : G \longrightarrow M$ and $\beta : G \longrightarrow M$ are the source and target maps over a base manifold M.

In [6], we have described geometrically discrete Lagrangian and Hamiltonian Mechanics on Lie groupoids, in particular, the type of equations analyzed include the classical discrete Euler-Lagrange equations, the discrete Euler-Poincaré and discrete Lagrange-Poincaré equations. These results have applications for the construction of geometric integrators for continuous Lagrangian systems (reduced or not) Moreover, our methods have been extended to the case of discrete nonholonomic mechanics [2, 3] and discrete variational constrained problems including optimal control theory for reduced systems [7, 8]. The underlying structure of these discrete methods is analyzed following similar but adapted techniques than in the continuous setting, producing a new and promising derivation of numerical integrators. Additionally, these designs are applied to the treatment of dynamical and control systems with innovative applications to modern engineering systems (robotic arms, spacecrafts, underwater vehicles, quantum control systems, etc) [4].

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Geometry of Adding Noise to Dynamical Systems, and Decomposition of the Result

David Elworthy
(joint work with Yves LeJan and Xue-Mei Li)

1. addition of noise

There are a variety of reasons for adding noise to a given smooth dynamical system $\frac{dx_t}{dt} = A(x_t)$. The most obvious is that the noise may be necessary to improve the model, another could be to try to stabilise an unstable system; doing so can also be used as an aid to computation as done in Oliver Junge's talk. Here I shall consider only the addition of finite dimensional Gaussian white noise, the formal derivative of Brownian motion. We take A to be a vector field on a smooth n-dimensional manifold M.

There are two possible aproaches. A "diffusive" term could be added to yield a diffusion operator $\mathcal{A}$ of the form $\mathbb{L}_A + \Lambda$ where $\mathbb{L}_A$ refers to Lie differentiation in the direction A and Λ is a diffusion operator, by which we will mean a smooth second order semi-elliptic operator acting on real valued functions on M and with no zero order term. For example if M has a Riemannian metric, a constant multiple of the Laplace-Beltrami operator, Δ, might be a natural choice.

The other approach is to take a stochastic differential equation which has the vector field A as a "drift" in some sense. We can write this as

$$dx_t = A(x_t)dt + X(x_t) \circ dB_t \tag{1}$$

where $X : \underline{\mathbf{R}}^m \to TM$ is a vector bundle map from the trivial $\mathbf{R}^m$-bundle over M to the tangent bundle of M, and $\{B_t\}_{t\geq 0}$ is a Brownian motion on $\mathbf{R}^m$. We may have $m \neq n$. There is an underlying probability space, say $\{\Omega, \mathcal{F}, \mathbf{P}\}$ on which the Brownian motion is defined. Thus B_t and the solution x_t, which has values in M, are parametrised by elements of Ω. We will only consider the case of smooth X and will assume M to be compact, to ensure that solutions exist for all time and there is a solution flow of diffeomorphisms $\{\xi_t\}_{t\geq 0}$, a $Diff(M)$-valued process.

The solutions of our SDE form a Markov process with generator $\mathcal{A}$ with

$$\mathcal{A} = \mathbb{L}_A + \frac{1}{2}\Sigma_j \mathbb{L}_{X^j}\mathbb{L}_{X^j} \tag{2}$$

for $X^1, ..., X^m$ the vector fields given by $X(-)(e_j)$ for an orthonormal basis $\{e_j\}_{j=1}^m$ of $\mathbf{R}^m$. We say they form an $\mathcal{A}$-diffusion. In general there are many different ways to choose an SDE whose solutions form an $\mathcal{A}$-diffusion for a given $\mathcal{A}$.

Corresponding to these approaches there are two levels of geometric structure induced on the underlying manifold M:

- Having a diffusion operator $\mathcal{A}$ is equivalent to having a sample continuous Markov process, and being given the law of the one point motions of that process i.e. a measure on the space of continuous paths on M starting from a fixed point. It also determines and is determined by a semi-group of operators $\{P_t\}_{t>0}$ which we could write as $\{e^{t\mathcal{A}}\}_{t>0}$. The operator also has a (principal) *symbol*,

  $$\sigma^{\mathcal{A}} : T^*M \to TM.$$

  This is positive semi-definite and so determines an inner product $\langle -, - \rangle_x$ on each subspace $E_x := \sigma_x^{\mathcal{A}}[T_x^*M]$. In particular if $\mathcal{A}$ is elliptic, so $E_x = T_xM$, it determines a Riemannian structure on M.
- An SDE, $dx_t = X^0(x_t)\ dt + X(x_t) \circ\ dB_t$ determines a diffusion operator $\mathcal{A} = \mathbb{L}_X^0 + \frac{1}{2}\Sigma_j \mathbb{L}_{X^j}\mathbb{L}_{X^j}$ for which its solutions are $\mathcal{A}$-diffusions. Thus the choice of an SDE for given $\mathcal{A}$ corresponds to the choice of a Hormander form representation of A. Since Lie differentiation acts on sections of tensor bundles this determines operators on such sections.

  In our compact situation the SDE will have a smooth flow of solutions, a $Diff(M)$-valued process. This determines semi-groups on tensor fields defined by

  $$P_t\phi = \mathbb{E}\xi_t^*\phi.$$

  If we assume the image subspace space E of the symbol of $\mathcal{A}$ has constant rank and so is a sub-vector bundle of TM, we not only have a Riemannian metric on E but obtain an induced metric connection $\breve{\nabla}$ on E using the projection by X of the trivial connection on $\underline{\mathbf{R}}^m$.

A diffusion operator $\mathcal{A}$ is said to be *cohesive* if (i) the image E of its symbol has constant rank, p say, and (ii) it has a Hormander form representation involving only vector fields which are section of E. The "irrelevance of drift" , [7], asserts that in this situation, if $p > 1$, an SDE for $\mathcal{A}$ can be found of the form $dx_t = X(x_t) \circ dB_t$.

A useful notion is that of the *adjoint (semi)-connection* $\hat{\nabla}$. See [8], [7] following [4]. This gives a covariant derivative of vector fields and other tensor fields but only in the directions given by E. It is defined using the Lie bracket:

$$\hat{\nabla}_U V = \breve{\nabla}_V U + [U, V].$$

2. decomposition and filtering

Now suppose we have a smooth surjective map $p : N \to M$, and a diffusion operator $\mathcal{B}$ on N which lies over a cohesive diffusion operator $\mathcal{A}$ on M. There is a commutative diagram of symbols and using this there is a natural horizontal lift map $\mathfrak{h} : E_{p(u)} \to T_u N$ for each $u \in N$, a non-linear "semi-connection " over E. It would be a connection if $\mathcal{A}$ were elliptic, and a principal connection when also p is the projection of a principal bundle with $\mathcal{B}$ equivariant.

Using this one can show [8], [9] that there is a canonical decomposition of $\mathcal{B}$ into horizontal and vertical parts and corresponding skew-product type representations of the $\mathcal{B}$ -diffusion. In the Riemannian submersion case this goes back to [2] and [5]. See also [12], [1], [3]. Non-canonical decompositions are discussed in the context of Hamiltonian systems in [11].

Suppose now we have an SDE on M with a cohesive generator $\mathcal{A}$. Let $p : Diff(M) \to M$ be the evaluation map at some fixed $x_0 \in M$. It has a natural principal bundle structure. The flow of the SDE gives an operator $\mathcal{B}$ on $Diff(M)$ over $\mathcal{A}$ which is equivariant. It therefore determines a principal semi-connection over E on this diffeomorphism bundle, and hence on all natural bundles on M. The one induced on TM turns out to be the connection $\hat{\nabla}$ described above, [8],[9].

In particular we see from this that, when the symbol of $\mathcal{A}$ has constant rank, an SDE for an $\mathcal{A}$-diffusion not only induces a connection on E but also a semi-connection over E on any natural bundle over M.

For a more detailed study of the space of SDE see [10].

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Gauge Transformations, Twisted Poisson Brackets and Hamiltonization of Nonholonomic Systems

Luis García Naranjo
(joint work with Paula Balseiro)

It is well known that the equations of motion for a mechanical system with nonholonomic constraints do not arise from a variational principle in the usual sense. As a consequence, they cannot be formulated as a classical Hamiltonian system. Instead, they are written with respect to an *almost Poisson bracket* that fails to satisfy the Jacobi identity [3, 4].

On the other hand, after a symmetry reduction, the resulting equations of motion of a number of examples allow a Hamiltonian formulation (sometimes after a *time reparametrization*), in which case one talks about *Hamiltonization*.

In our research we employ recent ideas from Poisson geometry to study the Hamiltonization phenomenon from a geometric perspective. The main tool in our approach is the concept of *gauge transformation* of bivector fields (in the sense of Ševera and Weinstein [5]), an operation that uses differential 2-forms to modify bivector fields keeping their characteristic distribution unchanged.

Consider a nonholonomic system on a constraint phase space $\mathcal{M}$, equipped with the almost Poisson bracket $\{\cdot,\cdot\}_{\mathrm{nh}}$ [3, 4], known as the *nonholonomic bracket*, and Hamiltonian function $\mathcal{H}_{\mathcal{M}}$. The (almost) Hamiltonian vector field X_{nh}, defined by $\{\cdot,\cdot\}_{\mathrm{nh}}$ and $\mathcal{H}_{\mathcal{M}}$, governs the dynamics of the system. In our research we consider *new brackets* $\{\cdot,\cdot\}^B_{\mathrm{nh}}$ obtained by gauge transformations of $\{\cdot,\cdot\}_{\mathrm{nh}}$ with respect to suitably chosen 2-forms B on $\mathcal{M}$. Since gauge transformations do not modify the characteristic distribution, the (almost) Hamiltonian vector fields associated to $\{\cdot,\cdot\}^B_{\mathrm{nh}}$ satisfy the nonholonomic constraints. If, in addition, B verifies $\mathbf{i}_{X_{\mathrm{nh}}}B = 0$, we say that it defines a *dynamical gauge transformation*; the terminology reflects the fact that such gauge transformations do not affect the dynamics, in the sense that the (almost) Hamiltonian vector field defined by $\{\cdot,\cdot\}^B_{\mathrm{nh}}$ and $\mathcal{H}_{\mathcal{M}}$ is still X_{nh}. In this way, we distinguish a *family* $\mathfrak{F}$ of almost Poisson structures that describe the dynamics of our nonholonomic system.

Now suppose that our nonholonomic system possesses some symmetries described by the action of a Lie group G on $\mathcal{M}$. The main motivation to consider the family $\mathfrak{F}$ of almost Poisson brackets is to have a larger choice of structures to describe the reduced dynamics and hope to find one amongst them that Hamiltonizes the problem. More specifically, we consider the dynamics on the reduced space $\mathbb{R} := \mathcal{M}/G$. The reduction of the invariant brackets in $\mathfrak{F}$ yields a collection

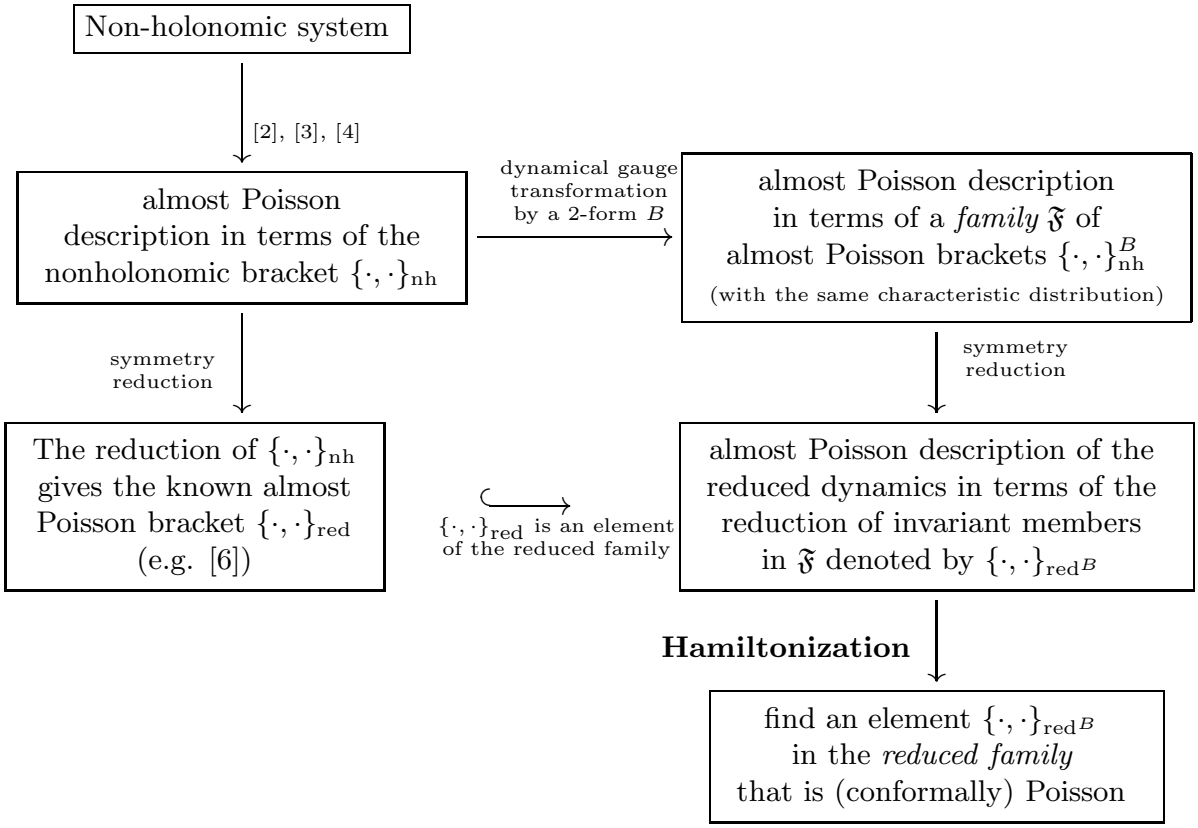

FIGURE 1. Summary of our approach to Hamiltonization.

of reduced brackets $\{\cdot,\cdot\}_{\mathrm{red}^B}$ on $\mathbb{R}$, and any member of this collection describes the reduced dynamics in (almost) Hamiltonian form with respect to the reduced Hamiltonian $\mathcal{H}_{\mathbb{R}}$. In particular, the reconstruction of the original dynamics on $\mathcal{M}$ is exactly the same regardless of the choice of bracket $\{\cdot,\cdot\}_{\mathrm{red}^B}$ on the reduced space.

In our approach, the issue of Hamiltonization is formulated by the requirement that one of the reduced brackets on $\mathbb{R}$, obtained as the reduction of an element in $\mathfrak{F}$, is *conformally Poisson*; in other words, there should exist a bracket $\{\cdot,\cdot\}_{\mathrm{red}^B}$ and a positive function φ such that $\varphi\{\cdot,\cdot\}_{\mathrm{red}^B}$ is a *Poisson bracket* on $\mathbb{R}$ (i.e., it satisfies the Jacobi identity).

The scaling of $\{\cdot,\cdot\}_{\mathrm{red}^B}$ by φ is dynamically interpreted as the time reparametrization $d\tau = \frac{1}{\varphi}\,dt$ (an idea that goes back to Chaplygin). In particular, the Hamiltonization of the celebrated *Chaplygin sphere problem* arises as the reduction of a dynamically gauged bracket $\{\cdot,\cdot\}^B_{\mathrm{nh}}$ that differs from the standard nonholonomic bracket $\{\cdot,\cdot\}_{\mathrm{nh}}$. Our approach to Hamiltonization is summarized in figure 1.

A key observation is that, although the brackets in $\mathfrak{F}$ are all gauge related, they may have fundamentally different features after reduction. For example, depending on the choice of the 2-form B, the characteristic distribution of the reduced almost Poisson bracket $\{\cdot,\cdot\}_{\mathrm{red}^B}$ may or may not be integrable. The

integrability of the characteristic distribution is of central importance, as it is a necessary condition for $\{\cdot,\cdot\}_{\mathrm{red}^B}$ to be conformally Poisson (and, hence, for the system to be Hamiltonizable).

An important class of almost Poisson brackets possessing an integrable characteristic distribution is given by the so-called *twisted Poisson structures* [5]. For these structures the failure of the Jacobi identity is controlled by a global closed 3-form ϕ as follows:

$$\{f,\{g,h\}\}+\{g,\{h,f\}\}+\{h,\{f,g\}\}+\phi(X_f,X_g,X_h)=0,$$

where X_f denotes the (almost) Hamiltonian vector field with Hamiltonian function f. In our research we have shown that any almost Poisson structure whose characteristic distribution is both integrable and regular is a twisted Poisson structure. As a consequence, we show that the reduced equations of some classical nonholonomic systems (the Veselova problem and the Chaplygin sphere) can be formulated in terms of twisted Poisson brackets in the original physical time (prior to any time reparametrization). To our knowledge, this establishes the first connection between twisted Poisson structures and nonholonomic mechanics. This should serve as a motivation to investigate the interplay between the rich geometrical properties of twisted Poisson brackets and the dynamical features of the corresponding (almost) Hamiltonian vector fields.

To illustrate the importance of our methods, we have introduced the problem of the motion of rigid bodies that are subject to *generalized rolling constraints*. These are nonholonomic constraints that relate the angular velocity $\boldsymbol{\omega}$ of the body and the linear velocity $\dot{\mathbf{x}}$ of its center of mass in a linear way, i.e., $\dot{\mathbf{x}}=A\boldsymbol{\omega}$ for a 3×3 matrix A satisfying certain properties. This type of constraints generalize the Chaplygin sphere problem. In fact, the constraints vary from *completely nonholonomic* if the rank of A equals 3, to (holonomic) classical free rigid body motion if $A=0$. For the Chaplygin sphere, the rank of A equals 2. By allowing gauge transformations, we prove that the problem is Hamiltonizable independently of the value of the rank of A. Using the Hamiltonian structure of the reduced system, we also show its complete integrability in the sense of Liouville.

For this explicit class of examples, the behavior of the reduced brackets, according to the rank of A, is illustrated in the table below. In our notation, $\{\cdot,\cdot\}_{\mathrm{red}}$ corresponds to the reduction of the classical nonholonomic bracket, while the bracket $\{\cdot,\cdot\}_{\mathrm{red}^B}$ corresponds to the reduction of a bracket obtained by a dynamical gauge transformation by a specific 2-form B.

Rank of A	0 (free rigid body)	1	2 (Chaplygin sphere)	3 (completely nonholonomic)
$\{\cdot,\cdot\}_{\mathrm{red}}$	Poisson	Conformally Poisson and Twisted Poisson	Non-integrable characteristic distribution	Non-integrable characteristic distribution
$\{\cdot,\cdot\}_{\mathrm{red}^B}$	Non-integrable characteristic distribution	Non-integrable characteristic distribution	Conformally Poisson and Twisted Poisson	Poisson

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Equivalent Theories of Liquid Crystal Dynamics

François Gay-Balmaz

(joint work with T. S. Ratiu and C. Tronci)

The Ericksen-Leslie equations for the dynamics of nematic liquid crystals are widely accepted and experimentally well-characterized through various measurements [2, 1, 13]. However, when orientational defects (*disclinations*) are present in the system, this model fails to provide a reliable description. For example, in the presence of defects, the liquid crystal molecules may undergo phase transitions, e.g., from uniaxial to biaxial, and the director field $\mathbf{n}$ is no longer an appropriate order parameter variable.

Among the various descriptions that incorporate defect dynamics, the micropolar theory developed by Eringen [4] appears promising to describe the motion of microfluids, including liquid crystals. Indeed, besides incorporating molecular shape changes into a microinertia tensor j, disclination dynamics is encoded in the so called *wryness tensor* γ, which is expressed in terms of $(\nabla\mathbf{n})\times\mathbf{n}$ when defects are absent [4].

However, while nematic liquid crystals are well known to be a typical example of microfluids, in spite of several attempts, it is not known how the Ericksen Leslie (EL) description arises from Eringen's micropolar theory. For example, the relation $\boldsymbol{\gamma} = (\nabla\mathbf{n})\times\mathbf{n}$ proposed by Eringen [4] fails to return the correct EL equations [11] as shown in [5] by two different methods (symmetry considerations and a direct computation). Thus it is not completely clear how $\boldsymbol{\gamma}$ may be expressed in terms of the director $\mathbf{n}$.

More recent developments in the understanding of defect dynamics are provided by the use of reduction theory [7, 5], which is behind the gauge-theory approach [3]. It applies to very general systems since it incorporates defect dynamics in different contexts, such as frustrated spin glasses [8, 3], for example. In this setting, one is naturally led to consider the wryness tensor $\boldsymbol{\gamma}$ as the magnetic potential of a Yang-Mills field (or, equivalently, a *connection one-form*) taking values in the

Lie algebra $\mathfrak{so}(3)$ of antisymmetric 3×3 matrices (usually identified with vectors in $\mathbb{R}^3$) of the rotation group $SO(3)$. The quantity $\boldsymbol{\gamma}$ is also known as 'spatial rotational strain' [7] and it expresses the amount by which a specified director field rotates under an infinitesimal displacement. Due to its tensorial nature, the gauge potential $\boldsymbol{\gamma}$ may be conveniently expressed in terms of an appropriate basis as

$$\boldsymbol{\gamma} = \boldsymbol{\gamma}_i \, \mathrm{d}x^i = \gamma_i^a \, \mathbf{e}_a \, \mathrm{d}x^i$$

where $\{\mathbf{e}_a\}$ is a fixed basis of $\mathbb{R}^3 \simeq \mathfrak{so}(3)$. Then, its corresponding magnetic vector field is given componentwise by

$$\boldsymbol{B}^i = \epsilon^{ijk}(\partial_j \boldsymbol{\gamma}_k + \boldsymbol{\gamma}_j \times \boldsymbol{\gamma}_k) \, .$$

In the gauge-theory approach developed in [3], the absence of disclinations is given by a vanishing magnetic field $\boldsymbol{B}$, rather than by a vanishing potential $\boldsymbol{\gamma}$. Thus, the presence of $\boldsymbol{\gamma}$ in a mathematical model must be compatible with EL dynamics, as long as $\boldsymbol{B} = 0$. In the context of reduction theory, one recognizes that a vanishing magnetic field $\boldsymbol{B} = 0$ simply amounts to the homogeneous initial condition $\boldsymbol{\gamma}_0 = 0$ [3]. If the latter condition is not satisfied, then the gauge-theory model would extend the EL formulation to incorporate non-trivial disclination dynamics.

On the other hand, Eringen's micropolar theory does not seem to possess a gauge-theory formulation, since the wryness tensor $(\nabla \mathbf{n}) \times \mathbf{n}$, as defined by Eringen, does not transform as a magnetic potential under gauge transformations; see [5]. Nevertheless, Eringen's theory still shares many analogies with gauge-theory models and the coexistence of the wryness and microinertia tensors in the dynamics provides an interesting opportunity to account for the shape evolution of the molecules interacting with disclination lines.

The considerations above represent the main motivation for the present work, which uses Euler-Poincaré variational methods to provide a unifying framework for incorporating defect dynamics in continuum systems with broken internal symmetry (e.g., liquid crystals) and shows that Eringen's micropolar theory comprises Ericksen-Leslie dynamics. This is done upon noticing that taking the gradient of the relation

$$\mathbf{n}(\mathbf{x}, t) = \chi(\mathbf{x}, t) \, \hat{\mathbf{z}},$$

relating director dynamics to the dynamics of the rotation matrix $\chi(\mathbf{x}, t) \in SO(3)$ in EL theory, immediately leads to

$$\nabla \mathbf{n} = (\nabla \chi) \hat{\mathbf{z}} = (\nabla \chi) \chi^{-1} \, \mathbf{n} \, .$$

Here $\hat{\mathbf{z}} := (0, 0, 1)$. Then, one observes that the new variable

$$\widehat{\boldsymbol{\gamma}} = -(\nabla \chi) \chi^{-1}$$

is precisely a connection one form taking values in $\mathfrak{so}(3)$ [7, 5]. It is straightforward to see that analogous relations hold independently of the order parameter space. Then, upon using the isomorphism $\mathfrak{so}(3) \simeq \mathbb{R}^3$ given by $a^k = -\epsilon^{kjl} \hat{a}_{jl}$, one can simply replace the relation $\nabla \mathbf{n} = \mathbf{n} \times \boldsymbol{\gamma}$ into the EL equations to account for the potential $\boldsymbol{\gamma}$ as an extra dynamical variable. Notice that, although the latter relation is satisfied by the choice $\boldsymbol{\gamma} = (\nabla \mathbf{n}) \times \mathbf{n}$, this expression is only defined up

to a component parallel to $\mathbf{n}$. Thus, $\boldsymbol{\gamma}$ cannot be entirely expressed in terms of the director $\mathbf{n}$ and it needs to be specified by all three columns of the matrix $\chi(\mathbf{x}, t)$.

The second key observation is that a different symmetry reduction of the same material Lagrangian yields a new set of equations for nematodynamics. We show that these are completely equivalent to the original Ericksen-Leslie equations. However, this new system allows for the description of disclinations, something that the Ericksen-Leslie equations could not handle, as discussed above.

Since all the above considerations hold regardless of the background fluid motion, we shall mainly confine our treatment to motion-less liquid crystal continua in order to emphasize the high points of the discussion.

More precisely, we start by showing how reduction theory can be applied to Ericksen-Leslie nematodynamics in two different fashions, thereby producing two different sets of equations of motion. The resulting dynamical systems are, however, completely equivalent. These two equivalent reduction methods are then formulated in a general context, for an arbitrary order parameter space. Then, Eringen's theory of micropolar media is shown to comprise Ericksen-Leslie nematodynamics. This requires a specified choice of the micropolar free energy, which in turn reduces to the Frank energy under the assumption of uniaxial molecules. We finally extend all the results to liquid crystal flows, thereby showing how the hydrodynamic Ericksen-Leslie equations possess a micropolar formulation.

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Waltzing Peakons and G-Strands

Darryl D. Holm
(joint work with Colin J. Cotter, Rossen I. Ivanov and James R. Percival)

We first considered singular solutions of a system of two cross-coupled Camassa-Holm (CCCH) equations. This CCCH system admits peakon solutions, but it is not in the two-component CH integrable hierarchy. The system is a pair of coupled Hamiltonian partial differential equations for two types of solutions on the real line, each of which separately possesses $\exp(-|x|)$ peakon solutions with a discontinuity in the first derivative at the peak. However, there are no self-interactions, so each of the two types of peakon solutions moves only under the induced velocity of the other type. We analyzed the 'waltzing' solution behaviour of the cases with a single bound peakon pair (a peakon couple), as well as the over-taking collisions of peakon couples and the antisymmetric case of the head-on collision of a peakon couple and a peakon anti-couple. We then presented numerical solutions of these collisions, which are *inelastic* because the waltzing peakon couples each possess an internal degree of freedom corresponding to their 'tempo' – that is, the period at which the two peakons of opposite type in the couple cycle around each other in phase space. Finally, we discussed compacton couple solutions of the cross-coupled Euler-Poincaré (CCEP) equations and illustrate the same types of collisions as for peakon couples, with triangular and parabolic compacton couples. We finished with a number of outstanding questions and challenges remaining for understanding couple dynamics of the CCCH and CCEP equations.

Next, we discussed G-strands. A G-strand is a map $g(t,x) : \mathbb{R}\times\mathbb{R} \to G$ for a Lie group G. For a certain Hamiltonian, the $SO(3)_K$-strand for ellipsoidal rotations is mapped here into a completely integrable generalization of the classical chiral model for the $SO(3)$-strand. The $SO(3)$-strand is the G-strand version of the rigid body equation and it may be regarded physically as a continuous spin chain. We derived the $SO(3)_K$-strand dynamics as an Euler-Poincaré system and recast it as a Lie-Poisson Hamiltonian system for coadjoint flow. Analogous results were discussed for an $Sp(2)$-strand. The $Sp(2)$-strand is the G-strand version of the $Sp(2)$ Bloch-Iserles ordinary differential equation, whose solutions exhibit dynamical sorting. Numerical solutions were shown that illustrated nonlinear interactions of coherent wave-like solutions in both cases. In addition, both the $SO(3)_K$-strand and the Bloch-Iserles partial differential equation represented by the $Sp(2)$-strand were shown to be completely integrable Hamiltonian systems that each admit soliton solutions. The latter was accomplished by finding transformations that take each of these systems into an extension of the chiral field model due to Yanovski (1998).

Rapid Expansions in Orthogonal Polynomials

Arieh Iserles
(joint work with María José Cantero)

The Fast Fourier Transform allows to approximate the first n terms of a Fourier expansion in $O(n\log n)$ operations, and this can be easily extended to the computation of the first terms of a Chebyshev expansion. This arguably is one of the most fundamental facts about modern scientific computing, which has revolutionised a raft of applications, from signal processing to numerical solution of differential equations. But what about fast computation of other orthogonal expansions?

The subject of this talk being rapid (i.e., $O(n\log n)$) computation of the first n terms of an expansion in an orthogonal polynomial system $\{p_n\}_{n\geq}$, say, with respect to an inner product induced by some complex-valued Borel measure $\mathrm{d}\mu$, we commence from the case $\mathrm{d}\mu(x)=(1-x^2)^\alpha$, $x\in(-1,1)$, $\alpha>-1$: the *ultraspherical polynomials* $p_n=\mathrm{P}_n^{(\alpha,\alpha)}$ [1]. Special cases are $\alpha=0$ (Legendre polynomials, already treated in [3]), $\alpha=-\frac{1}{2}$ (Chebyshev polynomials of the first kind) and $\alpha=\frac{1}{2}$ (Chebyshev polynomials of the second kind).

Let a function f be analytic in a Bernstein ellipse $\mathcal{B}_r=\{r\mathrm{e}^{\mathrm{i}\theta}+r^{-1}\mathrm{e}^{-\mathrm{i}\theta}\,:\,\theta\in[-\pi,\pi]\}$, $r\in(0,1)$. Instead of representing the nth expansion coefficient $\hat{f}_n$ in the usual way, we write it as an infinite linear combination of derivatives of f. Thus, we represent explicitly x^m in the basis $\{p_1,p_1,\ldots,p_m\}$, $x^m=\sum_{n=0}^m a_{m,n}p_n(z)$, say, whence we can write

$$f(z)=\sum_{m=0}^\infty\frac{f^{(m)}(0)}{m!}\sum_{n=0}^m a_{m,n}p_n(z)=\sum_{n=0}^m\left[\sum_{m=n}^\infty\frac{a_{m,n}f^{(m)}(0)}{m!}\right]p_n(z).$$

Next, using explicit expressions for the $a_{m,n}$s and the Cauchy Integral Theorem for derivatives, we prove that

$$\hat{f}_n=\frac{c_n}{2\pi\mathrm{i}}\int_\gamma\frac{f(z)}{z^{n+1}}\varphi_n(z)\mathrm{d}z,\qquad n\geq 0,$$

where γ is a simple, closed, positively-oriented Jordan curve in $\mathcal{B}_r$ which does not intersect $[-1,1]$, while

$$c_n=\frac{(1+2\alpha)_n n!}{2^n(1+\alpha)_n(\alpha+\frac{1}{2})_n},\qquad \varphi_n(z)={}_2\mathrm{F}_1\left[\begin{array}{l}\frac{n+1}{2},\frac{n+2}{2};\\ \alpha+n+\frac{3}{2};\end{array}\;\frac{1}{z^2}\right].$$

The above hypergeometric function converges very slowly, rendering it of little use in direct computation. Instead, we use the transformation

$${}_2\mathrm{F}_1\left[\begin{array}{l}a,a+\frac{1}{2};\\ c;\end{array}\;2\zeta-\zeta^2\right]=\frac{1}{1-\frac{1}{2}\zeta)^{2a}}{}_2\mathrm{F}_1\left[\begin{array}{l}2a,2a-c+1;\\ c;\end{array}\;\frac{\zeta}{2-\zeta}\right]$$

with $a=\frac{n+1}{2}$, $c=\alpha+n+\frac{3}{2}$ and $\zeta/(2-\zeta)$ on the Bernstein ellipse $\mathcal{B}_\rho$ for some $\rho\in(r,1)$. After much algebra, this results in

$$\hat{f}_n=\frac{c_n(2\rho)^n}{2\pi}\int_{-\pi}^\pi(1-\rho^2\mathrm{e}^{2\mathrm{i}\theta})f(\tfrac{1}{2}(\rho\mathrm{e}^{\mathrm{i}\theta}+\rho^{-1}\mathrm{e}^{-\mathrm{i}\theta}))\mathrm{e}^{\mathrm{i}n\theta}\chi_n(\rho^2\mathrm{e}^{2\mathrm{i}\theta})\mathrm{d}\theta,\qquad n\geq 0,$$

where

$$\chi_n(z) = {}_2\mathrm{F}_1\left[\begin{array}{l} n+1, \frac{1}{2}-\alpha; \\ n+\alpha+\frac{3}{2}; \end{array} z\right] = \sum_{m=0}^{\infty} \chi_{n,m} z^m$$

has a rapidly-convergent Taylor expansion. Truncating, we thus have

$$\hat{f}_n \approx \hat{f}_n^{[M]} = c_n (2\rho)^n \sum_{m=0}^{M} \chi_{n,m} \rho^{2m} \hat{v}_{n+2m},$$

where $M \geq 0$ is a suitable integer and

$$\hat{v}_n = \frac{1}{2\pi} \int_{-\pi}^{\pi} (1 - \rho^2 \mathrm{e}^{2\mathrm{i}\theta}) f(\tfrac{1}{2}(\rho \mathrm{e}^{\mathrm{i}\theta} + \rho^{-1} \mathrm{e}^{-\mathrm{i}\theta})) \mathrm{e}^{\mathrm{i}n\theta} \mathrm{d}\theta$$

can be computed rapidly with FFT for relevant values of n.

Given $\varepsilon > 0$, we prove that we can choose M so that $|\hat{f}_n - \hat{f}_n^{[M]}| < \varepsilon$ for all $n \geq 0$. The outcome is an algorithm where the $O(n \log n)$ cost of FFT is complemented by further $O(n)$ operations: a fast algorithm for ultraspherical expansions [1].

Further, assuming $\alpha > -\frac{1}{2}$, it is possible to prove that the algorithm 'survives' when $\rho \to 1$ and the Bernstein ellipse collapses to the interval $[-1, 1]$. In that case we can express $\hat{f}_n$ as a linear combination of Chebyshev coefficients of f.

In the second part of the talk we extend the first two stages in the development of the above algorithm—expressing x^m in an orthogonal polynomial basis and $\hat{f}_n$ as an integral transform—to general orthogonal polynomial expansions. Thus, suppose first that $\{p_n\}_{n\geq 0}$ are a monic *OPRL* (orthogonal polynomials on the real line) system,

$$\int_{-\infty}^{\infty} p_m(x) p_n(x) \mathrm{d}x = \begin{cases} \lambda_n > 0, & m = n, \\ 0, & m \neq n. \end{cases}$$

Since

$$x^m = \sum_{n=0}^{m} d_{m,n} p_n(x), \quad \text{where} \quad d_{m,n} = \frac{1}{\lambda_n} \int_{-\infty}^{\infty} x^m p_n(x) \mathrm{d}\mu(x),$$

using the three-term recurrence relation

$$p_{n+1}(x) = (x - a_n) p_n(x) - b_n p_{n-1}(x)$$

we obtain the mixed recurrence

$$\tilde{d}_{m+1,n} = b_n \tilde{d}_{m,n-1} + a_n \tilde{d}_{m,n} + \tilde{d}_{m,n+1}$$

or, in a matrix form, padding $\tilde{\mathbf{d}}_m$ with zeros, $\tilde{\mathbf{d}}_m = \mathcal{H} \tilde{\mathbf{d}}_n$, where $\mathcal{H}$ is an infinite tridiagonal matrix with a_k along the main diagonal, b_k in the subdiagonal and ones in the superdiagonal. We deduce that $\tilde{\mathbf{d}}_m = \mathcal{H}^m \mathbf{e}_0$, where $\mathbf{e}_k$ is the kth unit vector. An important observation is that $\mathcal{H}$ is similar to the *Jacobi matrix* $\mathcal{J}$ of the OPRL. Since the spectrum of the latter is known to reside in the least closed interval supporting $\mathrm{d}\mu$, we deduce that the resolvent of $\mathcal{H}$ is analytic outside that interval.

Similar argument can be extended to *orthogonal polynomials on the unit circle* and to *Laurent orthogonal polynomials on the unit circle*: we omit the details.

Assume next that the support is in a compact interval $[a,b]$ and that w.l.o.g. $0 \in [a,b]$. Expand $f(z) = \sum_{m=0}^{\infty} f_m z^m$. As for ultraspherical polynomials,

$$f(z) = \sum_{n=0}^{\infty} \left(\sum_{m=n}^{\infty} f_m d_{m,n} \right) p_n(z) \qquad \Rightarrow \qquad \hat{f}_n = \frac{\lambda_0}{\lambda_n} \sum_{m=n}^{\infty} \frac{f^{(m)}(0)}{m!} \tilde{d}_{m,n}, \quad n \geq 0.$$

Let γ be a simple, positively-oriented, closed Jordan curve in $\Omega \setminus [a,b]$ and assume that f is analytic in Ω. Using again the Cauchy theorem,

$$\begin{aligned} \hat{f}_n &= \frac{\lambda_0}{\lambda_n} \frac{1}{2\pi \mathrm{i}} \int_\gamma f(z) \sum_{m=n}^{\infty} \frac{\tilde{d}_{m,n}}{z^{m+1}} \mathrm{d}z = \frac{\lambda_0}{\lambda_n} \frac{1}{2\pi \mathrm{i}} \int_\gamma \frac{f(z)}{z} \mathbf{e}_n^\top \left(\sum_{m=n}^{\infty} \mathcal{H}^m z^{-m} \right) \mathbf{e}_0 \mathrm{d}z \\ &= \frac{\lambda_0}{\lambda_n} \frac{1}{2\pi \mathrm{i}} \int_\gamma \frac{f(z)}{z^{n+1}} \mathbf{e}_n^\top (I - z^{-1}\mathcal{H})^{-1} \mathbf{e}_0 \mathrm{d}z, \qquad n \geq 0. \end{aligned}$$

Bearing in mind the analyticity of the resolvent in $\Omega \setminus [a,b]$, the integral is well defined. Thus, we have completed two—out of three—conceptual steps leading to a fast algorithm in a general setting of OPRL, with similar results available for polynomials and Laurent polynomials orthogonal on the unit circle.

There is a remaining step in designing an algorithm for rapid evaluation of expansion coefficients: accelerating the convergence of the integral kernel and choosing an appropriate path γ to reduce the calculations to FFT. This is a matter for active current research.

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Estimating Long Term Behavior of Flows Without Trajectory Integration: The Infinitesimal Generator Approach

Oliver Junge

(joint work with Gary Froyland and Péter Koltai)

The long-term distributions of trajectories of a flow are described by invariant densities, i.e. fixed points of an associated transfer operator. In addition, global slowly mixing structures, such as almost-invariant sets, which partition phase space into regions that are almost dynamically disconnected, can also be identified by certain eigenfunctions of this operator. Indeed, these structures are often hard to obtain by brute-force trajectory-based analyses. In a wide variety of applications, transfer operators have proven to be very efficient tools for an analysis of the global behavior of a dynamical system.

The computationally most expensive step in the construction of an approximate transfer operator is the numerical integration of many short term trajectories. In this paper, we propose to directly work with the *infinitesimal generator* instead of the operator, completely avoiding trajectory integration. We propose two different discretization schemes; a cell based discretization and a spectral collocation approach. Convergence can be shown in certain circumstances. We demonstrate numerically that our approach is much more efficient than the operator approach, sometimes by several orders of magnitude.

Transfer operators. Let the domain $M \subset \mathbb{R}^d$ of our flow be a smooth compact manifold and m the (normalized) Lebesgue measure on M. Denote by $F : M \to \mathbb{R}^d$ the vector field generating the flow and by $\Phi^t : M \to M$, $t \in \mathbb{R}$, the flow.

One asks how the flow changes probability measures. Sample x according to a probability measure μ; the distribution of $\Phi^t x$ is then given by $\mu \circ \Phi^{-t}$. Special attention is to be drawn to *invariant measures*, which do not change under the dynamics ($\mu = \mu \circ \Phi^{-t}$). Invariant measures μ are called *ergodic* if invariant sets have either zero or full measure, i.e. if $A \subset M$ satisfies $\Phi^{-t}A = A$ then $\mu(A) \in \{0, 1\}$. One has that absolutely continuous ergodic measures are natural invariant measures. The density of an invariant measure is called the *invariant density*. When looking for invariant densities, one can rephrase the action of the flow on measures as an action on densities. If f denotes the density of μ, then f is evolved by the flow as

$$\mathcal{P}^t f\ (x) = f\left(\Phi^{-t}x\right) |D\Phi^{-t}x|,$$

where $|B|$ denotes $|\det B|$ for a matrix B. The linear operator $\mathcal{P}^t : L^1(M) \circlearrowleft$ is known as a *transfer operator* or the *Perron-Frobenius operator* associated with the flow Φ. Note that invariant densities are fixed points of $\mathcal{P}^t$.

The infintesimal generator. The transfer operator also inherits some (semi) group properties of the flow Φ^t: The transfer operator $\mathcal{P}^t$ is a C_0 semigroup of contractions on L^1, see [5] for a proof (in particular Remark 7.6.2 for the continuity).

Definition 1. For a semigroup $\mathcal{T}^t$ we define the operator $\mathcal{A} : \mathcal{D}(\mathcal{A}) \to X$ by

$$\mathcal{A}f = \lim_{t \to 0} \frac{\mathcal{T}^t f - f}{t}, \qquad f \in \mathcal{D}(\mathcal{A}),$$

with $\mathcal{D}(\mathcal{A}) \subset X$ being the linear subspace of X where the above limit exists. The operator $\mathcal{A}$ is called the *infinitesimal generator* of the semigroup.

For $\mathcal{P}^t$, the infinitesimal generator turns out to be (provided the F_i are continuously differentiable) $\mathcal{A}_{PF} f = -\operatorname{div}(fF)$, see [5]. The following result (see eg. Theorem 2.2.4 [7]) shows the connection between the eigenvalues of the semigroup operators and their infinitesimal generator:

Theorem 1 (Spectral mapping theorem)**.** *Let $\mathcal{T}^t$ be a C_0 semigroup and let $\mathcal{A}$ be its infinitesimal generator. Then $e^{t\sigma(\mathcal{A})} \subset \sigma\left(\mathcal{T}^t\right) \subset e^{t\sigma(\mathcal{A})} \cup \{0\}$, where $\sigma(\cdot)$ denotes the point spectrum of the operator. The corresponding eigenvectors are identical.*

Ulam's method. We describe here the "standard" Ulam approach. We partition M into d-dimensional connected, positive volume subsets $\{B_1, \ldots, B_n\}$. Typically, each B_i will be a hyperrectangle or simplex to simplify computations. As an approximation space we consider the space $\Delta_n = \mathrm{sp}\{\chi_{B_1}, \ldots, \chi_{B_n}\}$ of functions which are piecewise constant on the cells of the partition. Let $\pi_n : L^1 \to \Delta_n$, $\pi_n f = \sum_{i=1}^n \frac{1}{m(B_i)} \int_{B_i} f \; dm \; \chi_{B_i}$, be the L^2-orthogonal projection onto Δ_n. We let $\mathcal{P}_n^t : \Delta_n \to \Delta_n$, $\mathcal{P}_n^t := \pi_n \mathcal{P}^t$, be the approximate Frobenius-Perron operator. Note that $\mathcal{P}_n^t \chi_{B_i} = \pi_n \mathcal{P}^t \chi_{B_i} = \sum_{j=1}^n \frac{1}{m(B_j)} \int_{B_j} \mathcal{P}^t \chi_{B_i} \; dm \; \chi_{B_j}$, i.e. the matrix representation $P_n^t \in \mathbb{R}^{n \times n}$ of $\mathcal{P}_n^t$ with respect to the basis $\chi_{B_1}, \ldots, \chi_{B_n}$ and multiplication on the left is

$$(P_n^t)_{ij} = \frac{1}{m(B_j)} \int_{B_j} \mathcal{P}^t \chi_{B_i} \; dm = \frac{m(B_i \cap \Phi^{-t} B_j)}{m(B_j)}.$$

This matrix is easily constructed numerically using eg. GAIO [3].

Ulam's method for the generator. We partition M as in the standard Ulam's method. Our candidate approximate operator is

$$\mathcal{A}_n f := \lim_{t \to 0} \left(\frac{\pi_n \mathcal{P}^t \pi_n f - \pi_n f}{t} \right). \tag{1}$$

The following lemma allows us to construct $\mathcal{A}_n$ without the computation of the flow Φ^t.

Lemma 2. *For $i \neq j$, define $\mathbf{n}_{ij}$ to be the the unit normal vector pointing out of B_i into B_j if $B_i \cap B_j$ is a $d-1$-dimensional face, and the zero vector otherwise. The matrix representation of $\mathcal{A}_n : \Delta_n \circlearrowleft$ with respect to the basis $\chi_1, \ldots, \chi_n$ under multiplication on the left is*

$$(A_n)_{ij} = \begin{cases} \dfrac{1}{m(B_j)} \displaystyle\int_{B_i \cap B_j} \max\{F(x) \cdot \mathbf{n}_{ij}, 0\} \; dm_{d-1}(x), & i \neq j; \\ -\displaystyle\sum_{j \neq i} \dfrac{m(B_j)}{m(B_i)} (A_n)_{ij}, & \text{otherwise.} \end{cases} \tag{2}$$

Spectral collocation for the generator. In many real world situations, a deterministic model of some physical system is not appropriate. Instead of an ordinary differential equation, we now deal with a stochastic differential equation. If the vector field F is smooth enough, the evolution of densities is governed by the *Fokker-Planck* or *Kolmogorov forward equation*:

$$\frac{\partial f}{\partial t} = \frac{\varepsilon^2}{2} \Delta f - \mathrm{div}(fF) =: \mathcal{A}_\varepsilon f. \tag{3}$$

One knows that the operator $\mathcal{A}_\varepsilon$ (with Neumann boundary conditions) is the infinitesimal generator of a C_0 semigroup $\mathcal{P}_{\varepsilon,1}^t$ on L^1, cf. [1, 6].

The eigenfunctions of $\mathcal{A}_\varepsilon$ are smooth. We choose a family of smooth approximation spaces $\{V_n\}_{n \in \mathbb{N}}$, such that $V_n \subset C^\infty(M)$ for all n. Depending on the type of the phase space, we use two different approximation spaces:

- *Periodic domain/uniform grid.* We have $M = \mathbb{T}^1$ and restrict ourselves to odd values of n. Then the basis we choose for V_n is $\left\{e^{ikx}\right\}_{-n/2-1\leq k\leq n/2}$. The associated collocation nodes are $\{0, 1/n, \ldots, (n-1)/n\}$.
- *Standard domain/Chebyshev grid.* Here, $M = [-1, 1]$. The space V_n is spanned by the monomials of order 0 to n. We use Chebyshev polynomials as basis functions: $\{\cos(k \arccos(x))\}_{0\leq k\leq n}$, together with the Chebyshev grid $\{-\cos(2\pi j/n), j = 0, \ldots, n\}$, as collocation nodes.

Let $f \in V_n$ and $\mathcal{I}_n : C^\infty \to V_n$ be the interpolation operator for the given collocation nodes. We define the approximate generator by $\mathcal{A}_{\varepsilon,n} f := \mathcal{I}_n \mathcal{A}_\varepsilon f$. For both cases we have following:

Theorem 3 (Spectral accuracy, [2]). *For $f \in C^\infty(M)$ let f_n be the best approximation of f in V_n w.r.t. the supremum norm $\|\cdot\|_\infty$. Then for each $k \in \mathbb{N}$ there is a $c_k > 0$ such that $\|f - f_n\|_\infty \leq c_k\, n^{-k}$ for all $n \in \mathbb{N}$.*

Convergence then follows from standard results on the analysis of Galerkin methods for elliptic differential operators and spectral approximation (cf. also [4]).

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Control of Collectives

P. S. Krishnaprasad

1. Talk Summary: In this talk we discussed ways to generate collective behavior from building blocks of pursuit behavior found in nature (e.g. prey capture, seeking mates, and aggressive territorial battles). With the study of collectives of starlings *Sturnus vulgaris* as a motivating problem, the talk centered on models of planar pursuit, a set of pursuit strategies, and collective strategies synthesized from these with directed graphs (specifically cycles). A particular collective strategy, known as constant bearing (CB) cyclic pursuit, and feedback laws to execute

it, was discussed. The resulting closed loop system admits a rich variety of solutions with symmetry, that can be spliced together to produce complex collective behavior.

While general results on relative equilibria (of rectilinear and circling type) and spiraling solutions were stated for n-particle cyclic CB pursuit, detailed phase portraits were obtained when $n = 3$, through reduction by symmetry.

2. Models: Consider a planar system of n particles each of unit mass, subject to gyroscopic interactions in a cycle, governed by the equations:

$$\begin{aligned} \dot{r}_i &= \nu_i x_i, \\ \dot{x}_i &= \nu_i y_i u_i, \\ \dot{y}_i &= -\nu_i x_i u_i, \;\; i = 1, 2, ..., n, \end{aligned}$$

where the speed ν_i is assumed to be unity for all particles. The curvature u_i of each paricle is governed by a *cyclic* feedback law of the form

$$u_i = u_{i,CB(\alpha)} = -\mu \left(Rot(\alpha) y_i \cdot \frac{r_{i,i+1}}{|r_{i,i+1}|} \right) - \frac{1}{|r_{i,i+1}|} \left(\frac{r_{i,i+1}}{|r_{i,i+1}|} \cdot \dot{r}^{\perp}_{i,i+1} \right)$$

where μ is a positive gain, the line-of-sight vector $r_{i,i+1} = r_i - r_{i+1}$, $Rot(\alpha)$ denotes counter-clockwise rotations by α, the superscript $\perp$ denotes the operation of counter-clockwise rotation by $\pi/2$, and the particle indices are defined mod n, in the formula for the feedback law. The bearing α is allowed to depend on the particle index i and the cyclic feedback law asymptotically realizes the collective CB strategy (with an n-tuple of bearings α_i), specified by the constraint:

$$\left(Rot(\alpha_i) x_i \cdot \frac{r_{i,i+1}}{|r_{i,i+1}|} \right) = -1, \;\; i = 1, 2, 3, ..., n.$$

The state space for n-particle cyclic CB pursuit is given in terms of the Euclidean group SE(2) as:

$$\mathrm{M}_{state} = \underbrace{(SE(2) \times SE(2) \times \cdots \times SE(2))}_{n \text{ times}} - \Delta$$

where the excluded subset Δ contains one or more sequential colocations, *i.e.*, $|r_{i,i+1}| = 0$ for some i. The Euclidean invariance of the CB feedback law implies passage of the dynamics to a shape space $\mathrm{M}_{state}/SE(2)$ denoted as M_{shape}, with redundant coordinates $\kappa_i, \theta_i, \rho_i$ given by

$$\begin{aligned} Rot(\kappa_i)\, x_i \cdot \frac{r_{i,i+1}}{|r_{i,i+1}|} &= -1 \\ Rot(\theta_i)\, x_i \cdot \frac{r_{i-1,i}}{|r_{i-1,i}|} &= 1 \\ \rho_i &= |r_{i,i+1}| \qquad\qquad i = 1, 2, ..., n, \end{aligned}$$

subject to the closure constraints that particle indexed n pursues particle indexed 1.

The dynamics in these coordinates are

$$\begin{aligned}
\dot{\kappa}_i &= -\mu_i \sin\,(\kappa_i - \alpha_i) \\
\dot{\theta}_i &= -\mu_i \sin\,(\kappa_i - \alpha_i) \\
&\quad + \frac{1}{\rho_{i-1}}\,(\sin\,(\kappa_{i-1}) + \sin\,(\theta_i)) \\
&\quad - \frac{1}{\rho_i}\,(\sin\,(\kappa_i) + \sin\,(\theta_{i+1})) \\
\dot{\rho}_i &= -\cos\,(\kappa_i) - \cos\,(\theta_{i+1}) \qquad i = 1, 2, ..., n.
\end{aligned}$$

This system admits an attracting invariant manifold $\kappa_i \equiv \alpha_i \quad i = 1, 2, ..., n$, and in the invariant manifold, the dynamics is subject to the closure constraints

$$Rot\left(\sum_{i=1}^{n} (\pi + \alpha_i - \theta_i)\right) = I \ \text{ the identity}$$

and

$$\sum_{i=1}^{n} \rho_i \ Rot\ \left(\sum_{j=1}^{i} (\pi + \alpha_j - \theta_j)\right) = 0$$

3. Symmetric Solutions Under suitable conditions on the parameters α_i, $SE(2)$ relative equilibria (and hence equilibria on the invariant manifold $\kappa_i \equiv \alpha_i$ $i = 1, 2, ..., n$ of shape space dynamics) arise. In addition spiraling solutions are possible.

4. Phase portraits for n=3. In the 3-particle case there arises a rather complete characterization of the phase portrait for a family of parameters, $\alpha_1 = \alpha_2 = \alpha = \pi + \alpha_3$ for $\alpha \in [0, 2\pi]$. In particular $\alpha = \pi/2$ allows an additional discrete symmetry leading to periodic solutions in a reduced phase space.

5. Notes on References: The cyclic CB pursuit work sketched here is the joint work of Kevin Galloway, Eric Justh and P. S. Krishnaprasad (2009, 2010, 2011) culminating in the Ph.D. thesis Kevin Galloway (2011). The CB pursuit feedback law was first discussed in Wei - Justh - Krishnaprasad (2009).

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General Techniques for Constructing Variational Integrators

Melvin Leok
(joint work with Tatiana Shingel)

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. 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. This approach is described in detail in [1, 2].

Shooting-based Variational Integrators. The *discrete Lagrangian*, $L_d : Q \times Q \to \mathbb{R}$, is a generating function of the symplectic flow, and is an approximation to the *exact discrete Lagrangian*,

$$L_d^E(q_0, q_1; h) = \int_0^h L(q_{01}(t), \dot{q}_{01}(t))dt,$$

where $q_{01}(0) = q_0$, $q_{01}(h) = q_1$, and q_{01} satisfies the Euler–Lagrange equation in the time interval $(0, h)$. The exact discrete Lagrangian is related to the Jacobi solution of the Hamilton–Jacobi equation, and can be interpreted as the action integral evaluated on a solution of a two-point boundary-value problem. As such, a computable approximation to the exact discrete Lagrangian can be obtained in two stages: (i) apply a numerical quadrature formula to the action integral, evaluated along the exact solution of the Euler–Lagrange boundary-value problem; (ii) replace the exact solution of the Euler–Lagrange boundary-value problem with a numerical solution of the boundary-value problem, in particular, by a converged shooting solution associated with a given one-step method. More generally, the shooting-based solution of the Euler–Lagrange boundary-value problem can also be replaced with approximate solutions based on other numerical schemes, including Taylor integrators, and collocation methods applied to either the Euler–Lagrange vector field or its prolongation.

Given a one-step method $\Psi_h : TQ \to TQ$, and a numerical quadrature formula $\int_0^h f(x)dx \approx h \sum_{i=0}^n b_i f(x(c_i h))$, with quadrature weights b_i and quadrature nodes

$0 = c_0 < c_1 < \ldots < c_{n-1} < c_n = 1$, we construct the *shooting-based discrete Lagrangian*,

$$L_d(q_0, q_1; h) = h \sum\nolimits_{i=0}^{n} b_i L(q^i, v^i),$$

where

$$(q^{i+1}, v^{i+1}) = \Psi_{(c_{i+1}-c_i)h}(q^i, v^i), \qquad q^0 = q_0, \qquad q^n = q_1.$$

These equations, together with the implicit discrete Euler–Lagrange equations,

$$p_k = -D_1 L_d(q_k, q_{k+1}), \qquad p_{k+1} = D_2 L_d(q_k, q_{k+1}),$$

can be solved iteratively using a shooting method. If one uses a p-th order accurate one-step method, and a q-th order accurate quadrature formula to construct the variational integrator, then the resulting variational integrator will have order of accuracy $\min(p, q)$.

Galerkin Variational Integrators. The variational characterization of the exact discrete Lagrangian,

$$L_d^E(q_0, q_1; h) = \operatorname*{ext}_{\substack{q \in C^2([0,h],Q) \\ q(0)=q_0, q(h)=q_1}} \int_0^h L(q(t), \dot{q}(t))dt,$$

leads to a class of Galerkin variational integrators, where one replaces the integral with a quadrature formula, and replaces the space of C^2 curves with a finite-dimensional function space.

Let $\{\psi_i(\tau)\}_{i=1}^s$, $\tau \in [0, 1]$, be a set of basis functions for a s-dimensional function space C_d^s, and choose a numerical quadrature formula with quadrature weights b_i, and quadrature nodes c_i.

$$\begin{aligned}
q_1 &= q_0 + h \sum_{i=1}^{s} B_i V^i, \\
p_1 &= p_0 + h \sum_{i=1}^{s} b_i \frac{\partial L}{\partial q}(Q^i, \dot{Q}^i), \\
Q^i &= q_0 + h \sum_{j=1}^{s} A_{ij} V^j, \\
0 &= \sum_{i=1}^{s} b_i \frac{\partial L}{\partial \dot{q}}(Q^i, \dot{Q}^i)\psi_j(c_i) - p_0 B_j - h \sum_{i=1}^{s} (b_i B_j - b_i A_{ij}) \frac{\partial L}{\partial q}(Q^i, \dot{Q}^i), \\
0 &= \sum_{i=1}^{s} \psi_i(c_j) V^i - \dot{Q}^j,
\end{aligned}$$

where (b_i, c_i) are the quadrature weights and quadrature points, $B_i = \int_0^1 \psi_i(\tau)d\tau$, $A_{ij} = \int_0^{c_i} \psi_j(\tau)d\tau$. When the chosen basis functions satisfy a Kronecker delta property, the last equation states that $V^i = \dot{Q}^i$, and the method reduces to a *symplectic-partitioned Runge–Kutta method*.

An analogous theory of variational integrators formulated in terms of the Hamiltonian was developed in [3]. When the Lagrangian and Hamiltonian are hyperregular, these two approaches yield equivalent variational integrators, but the Hamiltonian approach remains valid even in the case of degenerate Hamiltonian systems, when there is no Lagrangian analogue.

Conclusions. We presented two general techniques for constructing discrete Lagrangians: (i) the Galerkin approach, which depends on a choice of a quadrature formula, and a finite-dimensional function space; (ii) the shooting-based approach, which depends on a choice of a quadrature formula, and a one-step method.

The order of approximation and momentum-conservation properties of a variational integrator are related to the order of approximation and the group-invariance of the discrete Lagrangian, respectively. This results in a substantial simplification in the analysis of variational integrators, since it is easier to verify the approximation and group-invariance properties of the discrete Lagrangian than it is to directly verify the order of accuracy and momentum-conservation properties of the associated variational integrator.

For Galerkin variational integrators, the group-invariance of the discrete Lagrangian can further be reduced to the group-equivariance of the finite-dimensional function space. For shooting-based variational integrators, the order of the discrete Lagrangian is related to the order of the quadrature formula and one-step method, and the group-invariance of the discrete Lagrangian is related to the group-equivariance of the one-step method. Furthermore, the shooting-based implementation allows the variational integrator to partially inherit the computational efficiencies of the underlying one-step method. In particular, a shooting-based variational integrator constructed from an explicit one-step method will be more computationally efficient than one based on an implicit one-step method.

These two approaches provide an explicit link between the construction of variational integrators, approximation theory, and one-step methods for ordinary differential equations. In particular, this allows one to leverage existing theoretical results and techniques in approximation theory and the numerical analysis of time-integration methods in the construction and analysis of variational integrators.

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A Variational Approach to Multirate Integration for Constrained Systems

Sigrid Leyendecker and Sina Ober-Blöbaum

The simulation of systems with dynamics on strongly varying time scales is quite challenging and demanding with regard to possible numerical methods and computational costs. Multirate methods integrate the slow part of the system with a relatively large step size while the fast part is integrated with a small time step (see e.g. Ref. [1, 2, 3, 5]). In this work, a multirate integrator for constrained dynamical systems is derived in closed form via a discrete variational principle on a time grid consisting of macro and micro time nodes. Being based on a discrete version of Hamilton's principle, the resulting variational multirate integrator is structure preserving. Depending on the discrete approximations for the Lagrangian function, one obtains different integrators with varying convergence properties, e.g. purely implicit second order or purely explicit first order schemes, or methods that treat the fast and slow parts in different ways.

1. Variational multirate integrator

Slow and fast potential and constraints Consider a mechanical system on a manifold $\mathcal{Q} \subseteq \mathbb{R}^n$ with the Lagrangian $L : T\mathcal{Q} \to \mathbb{R}$ given by $L(q, \dot{q}) = T(\dot{q}) - U(q)$ being the difference between the kinetic energy T and a potential U. Let the fact that the Lagrangian contains slow and fast dynamics be characterised by the possibility to additively split the potential energy $U(q) = V(q) + W(q)$ into a slow potential V and a fast potential W. Furthermore, let the configuration be constrained to the $(n-m)$-dimensional constraint manifold $\mathcal{C} = \{q \in \mathcal{Q} | g(q) = 0\}$ defined by the holonomic constraint function $g : \mathcal{Q} \to \mathbb{R}^m$. Then, the constrained Euler-Lagrange equations of motion on a time interval $[t_0, t_N] \subset \mathbb{R}$ can be derived via variation of the action integral, i.e. $\delta\mathfrak{S} = \delta \int_{t_0}^{t_N} L(q, \dot{q}) - g(q)^T \cdot \lambda \, dt = 0$. Here, $\lambda \in \mathbb{R}^m$ denotes the Lagrange multiplier.

Slow and fast variables We further assume that the n-dimensional configuration variable q can be divided into n^s slow variables $q^s \in \mathcal{Q}^s$ and n^f fast variables $q^f \in \mathcal{Q}^f$ such that $\mathcal{Q}^s \times \mathcal{Q}^f = \mathcal{Q}$ and $q = (q^s, q^f)$ with $n^f + n^s = n$. Let the fast potential depend of the fast degrees of freedom only, i.e. $W = W(q^f)$ while the slow potential $V = V(q)$ depends on the complete configuration variable

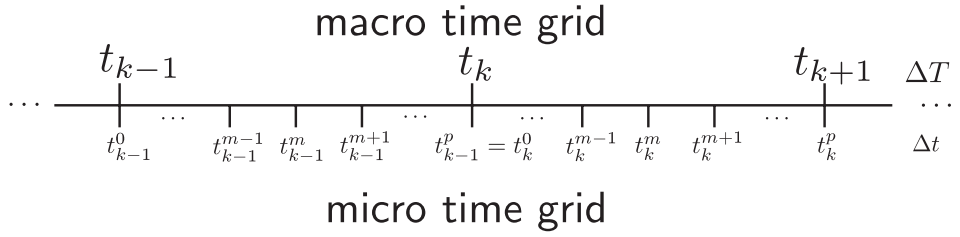

Figure 1. Macro and micro time grid.

as does the constraint function $g = g(q)$.

Variational multirate integrator In the framework of variational integrators [4], a discrete Lagrangian is defined as an approximation of the action functional on a short time span ΔT. Rather than choosing one time grid for the approximation as for standard variational integrators, for the multirate integrator, two different time grids are introduced, see Fig. 1. With time steps ΔT and Δt (where $\Delta T \geq \Delta t$), a macro time grid $\{t_k = k\Delta T \,|\, k = 0, \ldots, N\}$ and a micro time grid $\{t_k^m = k\Delta T + m\Delta t \,|\, k = 0, \ldots, N-1, m = 0, \ldots, p\}$ are defined. These provide the domains for the discrete macro trajectory $q_d^s = \{q_k^s\}_{k=0}^N$ with $q_k^s \approx q^s(t_k)$ and the discrete micro trajectory $q_d^f = \{\{q_k^{f,m}\}_{m=0}^p\}_{k=0}^{N-1}$ with $q_k^{f,m} \approx q^f(t_k^m)$ and Lagrange multipliers $\lambda_d = \{\lambda_k\}_{k=0}^{N-1} = \{\{\lambda_k^m\}_{m=0}^p\}_{k=0}^{N-1}$ with $\lambda_k^m \approx \lambda(t_k^m)$. The discrete action is defined as

$$\mathfrak{S}_d\left(q_d^s, q_d^f, \lambda_d\right) = \sum_{k=0}^{N-1} \left[L_d(q_k^s, q_{k+1}^s, q_k^f) - h_d(q_k^s, q_{k+1}^s, q_k^f, \lambda_k)\right]$$

On the multirate configuration space $\mathcal{Q}^{sf} = \mathcal{Q}^s \times \mathcal{Q}^s \times \left(\mathcal{Q}^f\right)^{p+1}$, the discrete Lagrangian $L_d : \mathcal{Q}^{sf} \to \mathbb{R}$ approximates $\int_{t_k}^{t_{k+1}} L(q, \dot{q})\, dt$ while $h_d : \mathcal{Q}^{sf} \times (\mathbb{R}^m)^{p+1} \to \mathbb{R}$ is approximating $\int_{t_k}^{t_{k+1}} g(q)^T \cdot \lambda\, dt$. Stationarity of the discrete action yields the discrete Euler-Lagrange equations. Their solution propagates the discrete variables forward in time via the multirate discrete Lagrangian flow $F_{L_d}^{\Delta T} : \mathcal{Q}^{sf} \to \mathcal{Q}^{sf}$ reading $F_{L_d}^{\Delta T}(q_{k-1}^s, q_k^s, \{q_{k-1}^{f,m}\}_{m=0}^p) = (q_k^s, q_{k+1}^s, \{q_k^{f,m}\}_{m=0}^p)$. Due to the variational derivation of the multirate integrator, we can state that it has the following two properties which classify it as being structure preserving. Let Ω_{L_d} denote the discrete symplectic form on $\mathcal{Q}^{sf}$, then it is preserved along the discrete solution trajectory, i.e. $\left(F_{L_d}^{\Delta T}\right)^* \Omega_{L_d} = \Omega_{L_d}$. Furthermore, if the discrete Lagrangian is invariant under the (appropriately lifted) group action $\psi_g^{\mathcal{Q}^{sf}}$, i.e. $L_d \circ \psi_g^{\mathcal{Q}^{sf}} = L_d$ holds for all elements g in a Lie group G, then $J_{L_d} \circ F_{L_d}^{\Delta T} = J_{L_d}$ and the corresponding momentum map J_{L_d} is preserved. This follows from the discrete Noether Theorem, see Ref. [4]. For variational integrators, the approximation order of the schemes coincides with the order of accuracy to which the discrete Lagrangian approximates the continuous action. For the variational multirate scheme at hand, the approximation error of the discrete Lagrangian

$$\begin{aligned} e_{L_d}^{\Delta T} &= \left\| \int_0^{\Delta T} L(q^s(t), q^f(t), \dot{q}^s(t), \dot{q}^f(t))\, dt - L_d(q^s(0), q^s(\Delta t), \{q^f(m\Delta t)\}_{m=0}^p) \right\| \\ &\leq \underbrace{p\mathcal{O}(\Delta t^{q+1})}_{\text{quadrature}} + \underbrace{p\mathcal{O}(\Delta t^{b+1})}_{\text{interpolation fast}} + \underbrace{\mathcal{O}(\Delta T^{a+1})}_{\text{interpolation slow}} \end{aligned}$$

is composed by errors due to the quadrature of the integral (of order q) and by errors stemming from the interpolation of the fast variables on the micro grid (of order b) and that of the slow variable on the macro grid (of order a). Note

that the number of micro nodes per macro interval p plays a relevant role when identifying the dominant terms, e.g. let $p = const$ and both $\Delta t \to 0, \Delta T \to 0$, then for the combination of midpoint quadrature with linear interpolation, the scheme converges quadratically as illustrated for the Fermi-Pasta-Ulam problem in Fig. 2. Furthermore, the quadrature rule in use for the discrete Lagrangian determines the degree of coupling between the discrete equations. This can range from a fully implicit scheme over variants being explicit in the macro and implicit in the micro quantities to fully explicit schemes. The two plots in Fig. 3 show the evolution of the configuration and conjugate momentum of m_3^{fast} in a triple pendulum, whereby the lines connect the values at the marco nodes and the intermediate micro node values are indicated by little crosses. One can see clearly, that the macro grid is too coarse to resolve the fast motion.

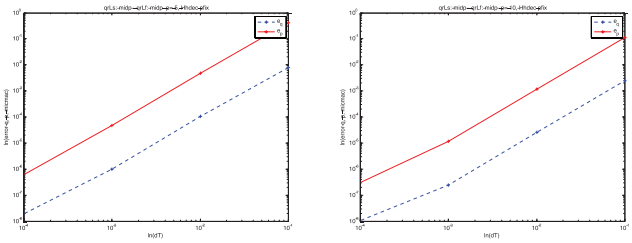

FIGURE 2. Fermi-Pasta-Ulam: quadratic convergence for $p = 5$ (left) and $p = 10$ (right).

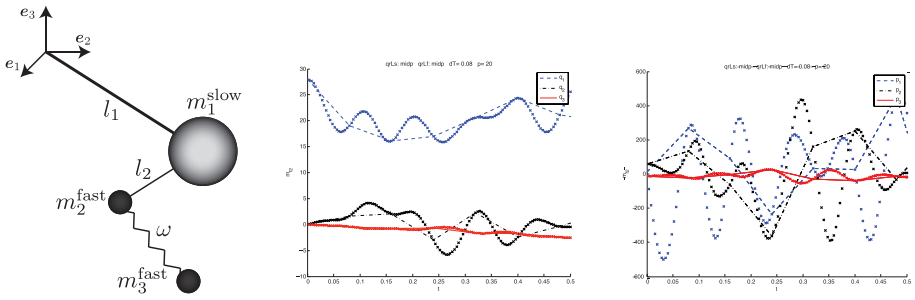

FIGURE 3. Triple pendulum: evolution of configuration (middle) and momentum (right) of m_3^{fast} ($\Delta T = 0.08$, $p = 20$).

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Invariant Measures in Nonholonomic Mechanics

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(joint work with Yuri N. Fedorov and Luis García-Naranjo)

The existence of an invariant measure for a system of differential equations is a very important property. From the point of view of dynamical systems, it is a key ingredient for the application of ergodic theory. It is also a crucial hypothesis in Jacobi's theorem of the last multiplier that establishes integrability of the system via quadratures, see e.g. [2]. Moreover, the existence of a smooth invariant measure imposes certain restrictions on the qualitative nature of the fixed points of the system; namely, it prohibits the existence of asymptotic equilibria. Our methods address the general question of the existence of an invariant measure for nonholonomic mechanical systems.

Unimodularity and measure preservation in mechanics. The well known theorem of Liouville states that a Hamiltonian system on a symplectic manifold preserves the symplectic volume, see e.g. [1]. The situation is not so simple for a Hamiltonian system on a Poisson manifold. For instance, if the Poisson manifold is the dual space $\mathfrak{g}^*$ of a Lie algebra $\mathfrak{g}$ equipped with the Lie-Poisson structure, then Kozlov [10] showed that the flow of a Hamiltonian of kinetic energy type on $\mathfrak{g}^*$ preserves a smooth measure if and only if the Lie algebra $\mathfrak{g}$ is unimodular.

More generally, a sufficient condition for the existence of a smooth measure for a Hamiltonian system on an abstract Poisson manifold, is that the first element in the cohomology of the Poisson manifold, which is called the *modular class of the Poisson manifold*, vanishes, see e.g. [15].

A large number of Poisson manifolds that appear in classical mechanics, for example after reduction, can be interpreted as the natural linear Poisson structure on the dual bundle A^* of a Lie algebroid $\tau_A : A \to Q$. Recall that a Lie algebroid $\tau_A : A \to Q$ is a vector bundle over the manifold Q that is equipped with an $\mathbf{R}$-linear Lie bracket $[\![\cdot, \cdot]\!]_A$ on the sections of A, and an anchor map $\rho_A : A \to TQ$ that is a Lie algebra morphism between the sections of A and the vector fields on Q, where TQ is equipped with the usual commutator of vector fields. A Lie algebroid generalizes at the same time the notions of the tangent bundle of a manifold and of the Lie algebra of a Lie group.

The modular class of a Lie algebroid $\tau_A : A \to Q$ was introduced in [5] and generalizes the modular character of a Lie algebra. In Marrero [12] the results of Kozlov [10] are generalized to consider the preservation of volumes for Hamiltonian systems of mechanical type on the dual space of a Lie algebroid. We say that a Hamiltonian $H : A^* \to \mathbf{R}$ is mechanical if it can be expressed as the sum of the kinetic and potential energies, where the kinetic energy defines a fibered metric on A and the potential energy is a real valued function on Q. Just as in the case studied by Kozlov, the unimodularity of the Lie algebroid is intimately related with necessary and sufficient conditions for the existence of an invariant measure.

We will follow the research line of [12] but we consider the preservation of volumes for mechanical systems subject to affine and linear nonholonomic constraints.

There is a major complication in doing this since the equations of motion for nonholonomic systems are not Hamiltonian. In the case of linear constraints, they can however be formulated with respect to an almost Poisson bracket that fails to satisfy the Jacobi identity. This formulation has its origins in [13, 11] and others.

In analogy to what happens with classical unconstrained mechanical systems, the almost Poisson structure associated with a nonholonomic system with linear constraints, before and after reduction, coincides with the linear almost Poisson structure on the dual bundle D^* of an appropriate skew-symmetric algebroid D [7]. Roughly speaking, a skew-symmetric algebroid $\tau_D : D \to Q$ is a vector bundle over the manifold Q satisfying all the properties of a Lie algebroid except that the bracket $[\![\cdot, \cdot]\!]_D$ of sections of D does not satisfy the Jacobi identity.

It is thus natural to consider the dynamics of a nonholonomic system with linear constraints as a Hamiltonian flow on D^* with respect to its linear almost Poisson structure. If the constraints are affine, the description of the dynamics is more intricate [7], but it still involves a Hamiltonian vector field on the dual space of a skew-symmetric algebroid.

Since the bracket $[\![\cdot, \cdot]\!]_D$ on a skew-symmetric algebroid $\tau_D : D \to Q$ fails to satisfy the Jacobi identity, it is not possible to define the modular class of D. However, one can introduce the notion of *unimodularity of a skew-symmetric algebroid*. This concept has recently been studied by Grabowski in [6]. From an abstract perspective, our main results relate the unimodularity of D with necessary and sufficient conditions for the existence of a preserved measure for the flow of mechanical Hamiltonian vector fields on the dual bundle D^*. We also obtain the corresponding results which may be applied to the dynamics in the presence of affine constraints.

Known results on the existence of invariant measures for nonholonomic systems. The existence of a smooth invariant measure for nonholonomic systems had been considered in the past but always specialized to particular kinds of systems possessing some type of symmetries.

Let Q be the configuration manifold of a nonholonomic mechanical system with linear constraints that are defined by the non-integrable subbundle $D \subset TQ$. The following works consider the existence of a preserved measure in the presence of symmetries. It is assumed that the symmetry group G acts (free and properly) on the left on Q and its lift to TQ preserves both the Lagrangian of the system and the constraint distribution D.

1. *Kozlov and Jovanovic on LL systems* [10, 9]. In this case $Q = G$, i.e. the configuration space is a Lie group, and both the constraints and the kinetic energy metric are left invariant. The case where the group is compact was treated by V.V. Kozlov in [10]. He obtained a necessary and sufficient condition for the existence of an invariant measure in terms of the structure constants of the corresponding Lie algebra and the metric tensor at the identity (commonly referred to as the inertia tensor). These results were extended to non-compact Lie groups by B. Jovanovic in [9].

2. *Cantrijn, Cortés, de León, and Martín de Diego on generalized Chaplygin systems* [4]. In this kind of systems the orbits of the symmetry group exactly complement the constraint space. That is $T_q\mathrm{Orb}(q) \oplus D_q = T_qQ$ for all $q \in Q$. The authors give a necessary and sufficient condition for the existence of an invariant measure. They also exhibit an example of a generalized Chaplygin system that does not have an invariant measure, thereby proving false a conjecture of J. Koiller [8], who suggested that systems of this type always possess an invariant measure.
3. *Zenkov and Bloch on nonholonomic flows with internal degrees of freedom* [16]. This case contains both LL and generalized Chaplygin systems as special cases. The authors assume that the sum of the tangent space to the orbits of the symmetry group and the constraint distribution span the tangent space of the configuration manifold, $T_q\mathrm{Orb}(q) + D_q = T_qQ$ for all $q \in Q$ (this is sometimes called the *dimension assumption*). However, contrary to generalized Chaplygin systems, they permit a non-trivial intersection of the tangent space to the group orbits and the constraint distribution ($T_q\mathrm{Orb}(q) \cap D_q \neq \{0\}$). Such intersection is assumed to be of constant dimension. In contrast with LL systems, they also allow for a non-trivial *shape space* Q/G containing the internal degrees of freedom. The authors obtain necessary and sufficient conditions for the existence of an invariant measure. These conditions are expressed in terms of the coefficients appearing in the local expression of the Lagrange-D'Alembert-Poincaré equations, see [3].

Another important result where there is a different type of symmetries is given by

4. *Veselov and Veselova on LR systems* [14]. Here the configuration space is a Lie group and the kinetic energy metric is left invariant. However, in this case the constraints are right invariant. The authors show that if the Lie algebra of the configuration group is unitary, then the system preserves an invariant measure. Moreover, the authors give an explicit formula for the measure.

Our approach to the problem of existence of an invariant measure in terms of unimodularity of skew-symmetric algebroids allows us to unify the study of the above results. Indeed, our results apply to all of them provided that one formulates the reduced problem on the appropriate skew-symmetric algebroid. Moreover, we present some new results that are summarized below.

New results on the existence of invariant measures for nonholonomic systems. We present our original contributions to the problem according to the list of results given above.

1. We generalize the results of Kozlov [10] and Jovanovic [9] by deriving necessary and sufficient conditions for the existence of an invariant measure in the presence of affine constraints. Moreover, in the case when several constraints are present, we present the condition for the existence of an invariant measure in an explicit form.

2. We refine the results of Cantrijn, Cortés, de León, and Martín de Diego on generalized Chaplygin systems [4] in two ways. First of all, we propose a candidate for the preserved measure and give necessary and sufficient conditions under which it is indeed conserved. This measure on the reduced space is expressed intrinsically in terms of the geometric data of the problem and is shown to be invariant for the nonholonomic particle and the Chaplygin sphere. The other contribution is to give a mechanical example of a generalized Chaplygin system that does not possess a smooth preserved measure. Such example is provided by the two-wheel cart. The example given in [4] concerns a generalization of the nonholonomic particle whose physical realization is not immediate.
3. We express the necessary and sufficient conditions for the existence of an invariant measure in the presence of internal degrees of freedom given by Zenkov and Bloch [16] in an intrinsic way, without relying on the local expression of the evolution equations for the variables in the shape space Q/G. Moreover, our approach allows us to drop the dimension assumption.
4. We generalize the result of Veselov and Veselova on LR systems [14] by showing that an arbitrary LR system possesses an invariant measure, i.e. without requiring the Lie algebra $\mathfrak{g}$ of the configuration group G to be unimodular. We also give a formula for the invariant measure in this case. Moreover, our construction takes place on the constraint space D^*. This contrasts with the results of [14] where it is first shown that the system preserves a measure on the extended space $\mathfrak{g}^* \times (\mathfrak{g}^*)^k$ where k is the number of constraints, and later it is proved that there is a conserved measure on the cotangent bundle T^*G. Our results concern a smaller phase space since there is a natural inclusion $D^* \hookrightarrow T^*G$.

Finally we mention that our approach considers for the first time the conservation of measures for nonholonomic systems subject to affine constraints.

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Geometry and Thermodynamics for the Coupling of Quantum Mechanics and Dissipative Systems

Alexander Mielke

We report on the ongoing work [MiN11] that is based on the papers [Ött10b, Ött10a] giving a thermodynamical consistent coupling between classical dissipative systems and reversible quantum systems. The basis is the theory of GENERIC, which is an acronym for *General Equations for Non-Equilibrium Reversible Irreversible Coupling*. It provides systems that are thermodynamically correct in the sense that the total energy is preserved while the total entropy is nondecreasing. However, the theory has more structure in the sense that the reversible dynamics is driven by a Poisson structure acting on the differential of the energy while the dissipative structure is given as a gradient flow with the total entropy as the driving functional.

The aim of the work [MiN11] is to identify conditions under which the systems introduced in [Ött10b, Ött10a] are well-posed. By this, we mean existence of solutions as well as the proper positivity conditions, energy conservation and entropy production and possible convergence to the thermodynamic equilibrium state.

1. The GENERIC framework

The framework of GENERIC was introduced by Öttinger and Grmela in [GrÖ97, ÖtG97], see also [Mie11] for a more mathematical presentation with application to viscoplasticity. It is based on a quintuple $(\mathcal{X}, \mathcal{E}, \mathcal{S}, L, K)$, where the smooth functionals $\mathcal{E}$ and $\mathcal{S}$ on a smooth manifold $\mathcal{X}$, where $\mathcal{E}$ denotes the total energy and the $\mathcal{S}$ the total entropy. Moreover, on $\mathcal{X}$ we have given a Poisson structure L and a dissipative structure K, i.e.

$$\begin{aligned} &L(X) = -L(X)^* \text{ and } L \text{ satisfies Jacobi's identity,} \\ &K(X) = K(X)^* \geq 0, \text{ i.e., } \langle \xi, K(X)\xi \rangle \geq 0. \end{aligned} \tag{1}$$

The evolution of the system is given by the differential equation

$$\dot{X} = L(X)\mathrm{D}\mathcal{E}(X) + K(X)\mathrm{D}\mathcal{S}(X), \tag{2}$$

where $L\mathrm{D}\mathcal{E}$ is the reversible (Hamiltonian) part and $K\mathrm{D}\mathcal{S}$ the irreversible (dissipative) part. The central condition states that the energy functional does not contribute to dissipative mechanisms and that the entropy functional does not contribute to reversible dynamics, which is the following *non-interaction condition*:

$$\textbf{(NIC)} \qquad \forall\, X \in \mathcal{X}: \quad L(X)\mathrm{D}\mathcal{S}(X) = 0 \quad \text{and} \quad K(X)\mathrm{D}\mathcal{E}(X) = 0.$$

Trivial consequences of the GENERIC structure are $\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{E}(X(t)) = 0$ and $\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{S}(X(t)) = \langle \mathrm{D}\mathcal{S}, K\mathrm{D}\mathcal{S}\rangle \geq 0$ along solutions. Moreover, the *maximum entropy principle* holds: If X_{eq} maximizes $\mathcal{S}$ under the constraint $\mathcal{E}(X) = E_0$, then X_{eq} is a steady state for (2).

2. GENERIC of a quantum mechanical and a dissipative system

The quantum mechanical system is described by states ψ in a Hilbert space $\boldsymbol{H}$ and a selfadjoint and semi-bounded Hamiltonian (operator) $H : D(H) \to \boldsymbol{H}$. The single-state equation is $\dot{\psi} = \jmath H\psi$, where $\jmath = 1/(\mathrm{i}\hbar)$. For the coupling to dissipative systems we use density matrices

$$\rho \in \mathcal{R} := \left\{\, \rho \in \mathfrak{S}^1(\boldsymbol{H}) \;\middle|\; \rho = \rho^* \geq 0,\ \mathrm{trace}\rho = 1 \,\right\}.$$

The Hamiltonian evolution of ρ is given in terms of Liouville's equation

$$\dot{\rho} = \jmath\,[H, \rho] := \jmath\,(H\rho - \rho H). \tag{3}$$

Obviously, the von Neumann's entropy $S_{\mathrm{qm}}(\rho) = -k_{\mathrm{B}}\mathrm{trace}(\rho \log \rho)$ remains constant in the Hamiltonian case, because ρ commutes with $\log \rho$.

We assume that an additional variable z is present in the model that is dissipative. For simplicity, we assume that z lies in a closed subset $\mathcal{Z} \subset \boldsymbol{Z}$. The evolution is assumed to be purely dissipative in the sense that it is a gradient flow with respect to the entropy $S : \mathcal{Z} \to \mathbb{R}$, namely

$$\dot{z} = K_{\mathcal{Z}}(z)\mathrm{D}S(z), \text{ where } K(z) = K(z)^* \geq 0. \tag{4}$$

We assume that there is a conserved energy $E(z)$ satisfying $K(z)\mathrm{D}E(z) \equiv 0$.

We now couple these two systems in the GENERIC framework with the joint state space is $\mathcal{X} = \mathcal{R} \times \mathcal{Z} \subset \mathfrak{S}^1_{\mathrm{S}}(\boldsymbol{H}) \times \boldsymbol{Z}$, where the state is given by the pairs $X = (\rho, z)$. The energy functional $\mathcal{E}$ and the entropy functional $\mathcal{S}$ take the form

$$\mathcal{E}(\rho, z) = \mathrm{trace}(\rho\, H(z)) + E(z) \quad \text{and} \quad \mathcal{S}(\rho, z) = -k_{\mathrm{B}}\mathrm{trace}\big(\rho \log \rho\big) + S(z),$$

where the Hamiltonian H may depend on the dissipative variable z.

For the Poisson structure we assume that the variable z is totally dissipative, which means that L has block structure in the form

$$L(\rho, z) = \begin{pmatrix} \jmath[\,\square\,, \rho] & 0 \\ 0 & 0 \end{pmatrix} : \begin{pmatrix} \mu \\ \zeta \end{pmatrix} \mapsto \begin{pmatrix} \jmath[\mu, \rho] \\ 0 \end{pmatrix}.$$

Clearly, we have $(\mathrm{NIC})_1$, namely $L(X)\mathrm{D}\mathcal{S}(X) = 0$ as $\log \rho$ commutes with ρ.

Following [Ött10b, Ött10a] we use a special ansatz for the dissipative structure that is based on the physical fact that the interaction of a quantum mechanical system interacts with its environment only via commutators with respect to suitable observables $Q_m(z) \in \mathfrak{S}^\infty_{\mathrm{S}}(\boldsymbol{H})$. This leads to

$$\Big\langle K(\rho,z)\begin{pmatrix}\mu\\ \zeta\end{pmatrix}\Big|\begin{pmatrix}\mu\\ \zeta\end{pmatrix}\Big\rangle = \langle\zeta, K_{\mathcal{Z}}(z)\zeta\rangle_{\boldsymbol{Z}} + \sum_{m=1}^{M} \|\!|[Q_m(z), \mu - \langle\zeta, \alpha_m(\rho,z)\rangle_{\boldsymbol{Z}} H(z)]|\!\|^2_{\mathcal{C}_\rho},$$

where $\alpha_m(\rho,z) \in \boldsymbol{Z}$ such that $\langle \mathrm{D}E(z), \alpha_m(\rho,z)\rangle_{\boldsymbol{Z}} \equiv 1$. By construction we see that $(\mathrm{NIC})_2$ holds, namely $K\mathrm{D}\mathcal{E} \equiv 0$.

The canonical correlation operator $\mathcal{C}_\rho$ (the inverse of which defines the Kubo-Mori metric on density matrices) and the associated norm $\|\!|\cdot|\!\|_{\mathcal{C}_\rho}$ are defined via

$$\mathcal{C}_\rho A := \int_0^1 \rho^s A \rho^{1-s}\,\mathrm{d}s \quad \text{and} \quad \|\!|A|\!\|^2_{\mathcal{C}_\rho} := \mathrm{trace}(A\,\mathcal{C}_\rho A), \tag{5}$$

see [Gra82, KTH91, Ött10a]. The fundamental identities

$$\big[\mathcal{C}_\rho A, \log\rho\big] \;=\; \big[A,\rho\big] \;=\; \mathcal{C}_\rho\big[A,\log\rho\big],$$

which go back to [Kub66], play a central role in the field of dissipative effects in quantum mechanics, because they relate the derivative of von Neumann's logarithmic entropy via commutators to the canonical correlation operator $\mathcal{C}_\rho$.

3. A simple fully consistent example with one heat bath

We simplify the above problem even further, by assuming that there is only one dissipative interaction term (i.e. $m = 1$) and by assuming that H, Q, α, and $K_{\mathcal{Z}}$ are independent of (ρ, z). Further, we assume that z is scalar and equals the absolute temperature, viz. $z = \theta \in [0,\infty[\in \mathbb{R}$. With $E(z) = c\theta$ and $S(z) = c\log\theta$ the total energy and the total entropy are given by

$$\mathcal{E}(\rho,\theta) = \mathrm{trace}(\rho\,H) + c\theta \quad \text{and} \quad \mathcal{S}(\rho,\theta) = -k_{\mathrm{B}}\mathrm{trace}(\rho\log\rho) + c\log\theta$$

To obtain the fundamental (NIC) we use $\alpha = 1/c$ and $K_{\mathcal{Z}} = 0$ and find the system

$$\begin{aligned}\dot\rho &= \jmath\big[H,\rho\big] - \Big[Q, k_{\mathrm{B}}\big[Q,\rho\big] + \frac{1}{\theta}\mathcal{C}_\rho\big[Q,H\big]\Big],\\ \dot\theta &= \frac{1}{c}\mathrm{trace}\Big(\big(k_{\mathrm{B}}\big[Q,\rho\big] + \frac{1}{\theta}\mathcal{C}_\rho\big[Q,H\big]\,\big)\big[Q,H\big]\Big).\end{aligned} \tag{6}$$

The following result is established in [MiN11].

Theorem. *If $\boldsymbol{H}$ is finite dimensional, then for each $X_0 = (\rho_0,\theta_0) \in \mathcal{X}$ system* (6) *has a global solution $X : [0,\infty[\to \mathcal{X}$.*

Moreover, under suitable commutator conditions on H and Q, it is shown that all solutions converge for $t \to \infty$ to the unique steady state given by the maximum entropy principle, namely $X_{\mathrm{eq}} = (\exp(-\frac{1}{k_{\mathrm{B}}\theta_{\mathrm{eq}}}H), \theta_{\mathrm{eq}})$.

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A Zoo of Bifurcations in Point Vortex Systems on the Sphere

James Montaldi

(joint work with Mark Roberts and Frédéric Laurent-Polz)

The system of point vortices on the sphere is a very rich source of bifurcations for Hamiltonian systems with symmetry. The system is described as follows. A point vortex is a point on the sphere S^2, considered as the unit sphere in $\mathbb{R}^3$, with a non-zero real number κ ascribed to it, called the vortex strength or vorticity. A system of N vortices evolves via the differential equation

$$\dot{\mathbf{x}}_i = \sum_{j\neq i} \kappa_j \frac{\mathbf{x}_j \times \mathbf{x}_i}{1 - \mathbf{x}_i \cdot \mathbf{x}_j}, \qquad (i = 1, \dots, N).$$

This equation is Hamiltonian, with symplectic from $\omega = \oplus_j \kappa_j \omega_j$ (where ω_j is the natural symplectic form on the j^{th} copy of S^2 with area 4π), and with Hamiltonian function

$$H(\mathbf{x}_1, \dots, \mathbf{x}_N) = -\sum_{i<j} \kappa_i \kappa_j \ln(\|\mathbf{x}_i - \mathbf{x}_j\|^2).$$

The system has the symmetry $\mathsf{SO}(3)$ acting as rotations of the sphere, and the associated conserved quantities are the components of the momentum map

$$\mathbf{J}(\mathbf{x}_1, \dots, \mathbf{x}_N) = \sum_j \kappa_j \mathbf{x}_j \in \mathbb{R}^3.$$

In this talk, I report on some results from [3] on the stability of relative equilibria with dihedral symmetry, so consisting of rings of vortices lying on circles of constant latitude with possibly a polar vortex or two at the North (and South) poles. The dihedral symmetry implies that each ring has the same number of vortices, denoted n, and within each ring the vortex strengths are identical. Using

Cartesian coordinates in $\mathbb{R}^3$, we choose the axis of symmetry to be the z-axis, so the poles are at $z = \pm 1$, and a ring lies in the circle of colatitude θ (so the intersection of the unit sphere with the plane $z = \cos\theta$).

A single ring For a single ring at colatitude θ and with no other vortices, the stability depends on θ. The linear stability was first calculated by Polvani & Dritschel [5]:

n	condition for stability	n	condition for stability
2, 3	all θ	4	$\cos^2\theta > 1/3$
5	$\cos^2\theta > 1/2$	6	$\cos^2\theta > 4/5$

while for $n \geq 7$ it is always linearly unstable. It was later shown by Boatto and Cabral [1] that the same criteria guarantee full nonlinear stability. As θ is increased, the relative equilibrium loses stability through a pitchfork bifurcation with dihedral symmetry, where a pair of imaginary eigenvalues collide at 0 and become real (the so-called splitting type of pitchfork). When $n = 4$ or 6 this is the traditional pitchfork bifurcation with a reflectional symmetry, and the bifurcation solutions will both be stable, while if $n = 5$ the pitchfork has $\mathbf{D}_5$-symmetry, so giving rise to 5 stable and 5 unstable bifurcating solutions.

A single ring and a pole The stability of configurations consisting of a single ring at colatitude θ and a single polar vortex of strength κ were studied in [2] (with some errors which are corrected in [3]) and demonstrate a complex stability diagram: we show the diagram for $n = 3$ below (the most complex one). The dark regions represent configurations that are Lyaponov stable, the lighter gray regions correspond to just linear stability while white regions correspond to the configuration having eigenvalues with nonzero real part (so linearly unstable). For these configurations, the momentum $\mathbf{J} = (0, 0, \mu)$ with $\mu = \kappa + n\cos\theta$ (here $n = 3$). The angular velocity is $\xi = ((2 + \kappa)\cos\theta + \kappa) / \sin^2\theta$.

Several notable bifurcations take place in this example.

- Crossing the curve $\mu = 0$ one finds Lyapounov stable configurations on one side and linearly stable ones on the other. When a relative equilibrium with zero momentum is Lyapounov stable then this is the typical transition to be found (provided the generic hypothesis of "no rovibration resonance" is satisfied), see [4] for a full explanation, and the second example below.
- There is also a change from Lyapounov to linear stability when crossing the $\kappa = 0$ line. This is not strictly a Hamiltonian bifurcation as the system fails to be Hamiltnoian when $\kappa = 0$ (the symplectic form becomes degenerate). Such bifurcations have not been studied in general.
- Each white region (of linearly unstable configurations) is bounded by a narrow light gray region and continuing one then passes into a dark region. Reversing this path, one starts with a Lyapounov stable configuration, which then becomes degenerate when a pair of imaginary eigenvalues meet at the origin. However they pass through the origin and remain on the imaginary axis, so the configuration becomes merely linear stable (a pitchfork of *passing* type). Continuing the path into the unstable region, the eigenvalue that passed through the origin increases in magnitude until

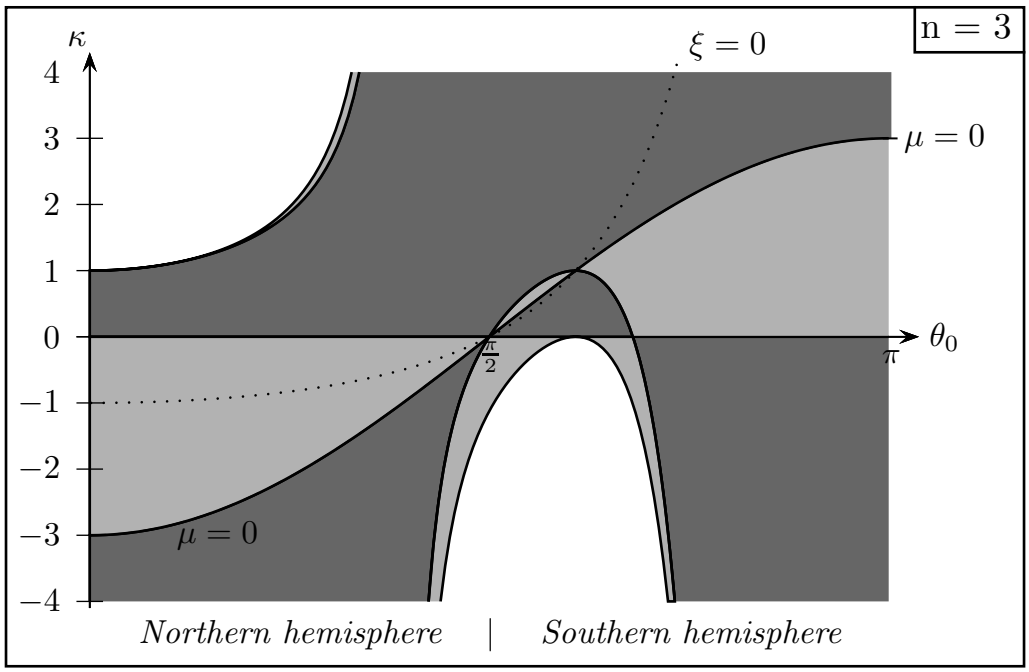


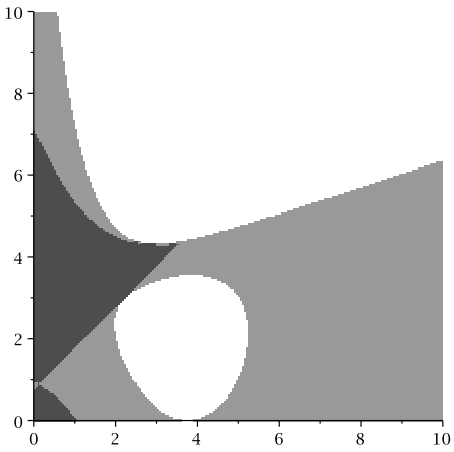
FIGURE 1. Bifurcation diagram for a 3-ring plus a polar vortex

it collides with another imaginary eigenvalue. The two then split off the imagniary axis to form a "real conjugate" pair, so a quadruplet of eigenvalues altogether. This the the well-known Hamiltonian-Hopf bifurcation.

- At the point where $\xi = \mu = 0$ (but $\kappa \neq 0$) there is an interesting meeting of 4 different regions. At this configuration, the 4 vortices all have the same strength, and the system has tetrahedral symmetry; however a full analysis of the unfolding of this situation has not been undertaken.

A single ring and two poles A second very rich collection of bifurcations is shown in the system with a ring with 2 polar vortices. This system has 3 natural parameters: the colatitude of the ring and the strength of each vortex. Below we have the diagram for $n = 3$ vortices in the ring and for the fixed colatitude of $\theta = 1.3$ (radians). The horizontal and vertical axes are the strengths of the North and South polar vortices, respectively; we just see the diagram for positive vortex strengths (see [3] for further information). The momentum is again $\mathbf{J} = (0, 0, \mu)$ with now $\mu = \kappa_1 - \kappa_2 + n\cos\theta$. Similar bifurcations to those described above occur

here. The straight line $\kappa_2 = \kappa_1 + \cos(1.3)$ (so $\mu = 0$) shows the same Lyapounov to linearly stable transition described above. The end of that line at the top right occurs when the zero-momentum relative equilibrium loses stability through a pitchfork bifurcation. However there is one further point of interest, where the white oval meets that line. The transition from the elliptic to unstable region is via a Hamiltonian-Hopf bifurcation and at the point where the oval unstable region is tangent to the $\mu = 0$ line there is a "rovibration" resonance, where one of the eigenvalues of the reduced equilibrium coincides with the eigenvalue for the rotational motion (i.e. the angular velocity): this bifurcation has yet to be investigated in detail.



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Dynamical Systems Approach to Data Assimilation for Mechanical Systems

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(joint work with Georg Gottwald, Kay Bergemann, Eugenia Kalnay, Javier Amezcua and Kayo Ide)

The basic task of data assimilation (nonlinear filtering) for a mechanical system

$$\frac{dQ}{dt} = \mathcal{M}^{-1} P, \qquad \frac{dP}{dt} = -\nabla_Q V(Q) \tag{1}$$

with coordinates $Q \in \mathbb{R}^N$, momenta $P \in \mathbb{R}^N$, $N \gg 1$, symmetric mass matrix $\mathcal{M}$ and potential energy $V(Q)$ can be phrased as follows. Often the full mechanical model (the "truth") is not directly accessible and the phenomena of interest is instead modeled by a reduced second-order stochastic Langevin dynamics model

$$dq = M^{-1} p dt, \tag{2}$$

$$dp = -\nabla_q U(q) dt - \gamma p dt + \sqrt{\sigma} dw(t) \tag{3}$$

in distinguished degrees of freedom (q, p) which arise as linear combinations $q = LQ, p = LP$ from the full set of model variables, where L is an appropriate linear operator and $w(t)$ denotes standard Brownian motion. The parameters $\gamma > 0$ and $\sigma > 0$ are often unknown while the reduced potential $U(q)$, the reduces mass matrix M as well as the initial conditions $q(0)$ and $v(0)$ are assumed to be known.

Using data assimilation, we wish to find parameter values (γ, σ) and solutions of (2)-(3) that stay close to partially observed reference trajectories of the full mechanical model (1). We now assume for simplicity that $q, p \in \mathbb{R}$ and that partial observations are given by "measurements" $d\mathrm{q}(t) \in \mathbb{R}$, which satisfy the stochastic differential equation

$$d\mathrm{q}(t) = L\mathcal{M}^{-1}P_T(t)dt + \sqrt{r}du(t). \tag{4}$$

Here $u(t)$ denotes again Brownian motion, $r > 0$ is a known parameter, and $(Q_T(t), P_T(t))$, $t \geq 0$, denotes an unknown reference solution (the "truth") from the full mechanical model (1).

Both naive approaches of either solving (2)-(3) with the given initial conditions or integrating (4) to obtain $\mathrm{q}(t)$ are able to track the reference solution $q_T(t) = LQ_T(t)$ over long periods of time. Instead one has to resort to filtering or smoothing techniques to combine (2)-(4) in an optimal manner.

In recent year, the ensemble Kalman filter (EnKF) [1] has emerged as a powerful nonlinear filter for intermittent data assimilation. For simplicity we restrict to the case of only estimating the model state while all model parameters are assumed to be known. We have extended the EnKF technique to continuous data assimilation problems as outlined above. In particular, the ensemble Kalman-Bucy filter [5, 7] leads to the following augmented system of stochastic differential equations. We first rewrite (2)-(4) in more abstract form as

$$dx = f(x,t)dt + \Sigma^{1/2}dw(t), \tag{5}$$

$$dy = Hxdt + R^{1/2}du(t) \tag{6}$$

Then the ensemble Kalman-Bucy filter equations for an ensemble of m members $x_i(t)$ are

$$dx_i = f(x_i,t)dt + \Sigma^{1/2}dw_i(t) - \mathrm{P}H^TR^{-1}(Hx_idt - dy(t) + R^{1/2}du_i(t))$$

with empirical covariance matrix

$$\mathrm{P} = \frac{1}{m-1}\sum_i (x_i - \bar{x})(x_i - \bar{x})^T, \quad \bar{x} = \frac{1}{m}\sum_i x_i$$

and mutually independent Brownian motions $w_i(t)$, $u_i(t)$, $i = 1, \ldots, m$.

To make progress towards more general and accuracte filters for nonlinear problems we consider intermittent data assimilation where (6) is replaced by

$$y_q = Hx(t_q) + R^{1/2}\eta_q \tag{7}$$

at discrete times t_q, $q = 1, \ldots, K$ with random variables $\eta_q \sim \mathrm{N}(0, I)$ and H denoting an appropriate forward operator. We also set $\Sigma = 0$ in (5). The ensemble

Kalman-Bucy filter can also be applied to such filter problems and leads to efficient implementation of ensemble Kalman filters [2, 3, 4, 7].

On a more general level, one can reformulate the data assimilation problem for model (5) with $\Sigma = 0$ and observations (7) as a Vlasov-McKean system [5]

$$\dot{x} = f(x,t) + \sum_q \delta(t-t_q)\mathrm{M}\nabla_x \psi(x,\rho) \tag{8}$$

$$\rho_t = -\nabla_x \cdot (\rho \dot{x}), \tag{9}$$

where $\delta(\cdot)$ denotes the Dirac delta function, M is a positive definite matrix, and the potential ψ is determined from

$$\nabla_x \cdot (\rho \mathrm{M}\nabla_x \psi) = \rho(L - E_\rho[L]) \tag{10}$$

where

$$L(y_q; x) = \frac{1}{2}(Hx - y_q)^T R^{-1}(Hx - y_q)$$

is the negative log-likelihood associated with the measurement (7) and $E_\rho[L]$ denotes expectation of L with respect to the probability density ρ. Numerical approximations based on (8)-(9) including Gaussian mixture approximations and Gaussian kernel density estimators for ρ have been discussed in [6]. The key idea is to approximate (8)-(9) using Lagrangian particle methods. The ensemble at time t_q is converted into a statistical model yielding a density approximation $\tilde{\rho}$ which is then used in (10) in place of ρ to find the potential ψ in (8).

Interesting questions for further research include exploration of the geometric structure of the Vlasov-McKean filter equations (8)-(9), the importance of geometric integration methods for solving (8)-(9), and efficient numerical methods for solving (8)-(9) in the presence of highly oscillatory solution components.

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Minimum Energy Configurations in the *N*-Body Problem and the Celestial Mechanics of Granular Systems

Daniel J. Scheeres

Celestial Mechanics systems have two fundamental conservation principles that enable their deeper analysis: conservation of momentum and conservation of (mechanical) energy. Of the two, conservation of momentum provides the most constraints on a general system, with three translational symmetries (which can be trivially removed) and three rotational symmetries. If no external force acts on the system, these quantities are always conserved independent of the internal interactions of the system. Conservation of energy instead involves assumptions on both the lack of exogenous forces and on the nature of internal interactions within the system. For this reason energy is often not conserved for "real" systems that involve internal interactions, such as tidal deformations or impacts, even though they may conserve their total momentum. Thus mechanical energy generally decays through dissipation until the system has found a local or global minimum energy configuration that corresponds to its constant level of angular momentum. This observation motivates a fundamental question for celestial mechanics:

What is the minimum energy configuration of a N-body system with a fixed level of angular momentum?

For a system of point masses this question cannot be fully answered. If $N = 2$, then there exists a well defined minimum energy configuration for any non-zero angular momentum – the circular orbit. If $N \geq 3$ there is no well defined minimum energy configuration and, in fact, it can be shown that at a fixed level of angular momentum a configuration of the system can always be found for which the energy $E \to -\infty$.

Introduction of physically valid constraints can remove this dichotomy. Real systems always have a finite density and, hence, any particle in a celestial mechanics system has a finite radius. We call such a physically corrected system the "Full N-Body Problem," as inclusion of finite density also necessitates the modeling of the rotational motion of the components, which is not needed for consideration of point masses. Thus their mass centers cannot come arbitrarily close to each other, as at some distance they will rest on each other. Introduction of this correction allows the minimum energy configurations for an N-body system to be explicitly defined and computed for a given level of angular momentum.

For $N \geq 3$ it can be shown that minimum energy configurations of Full Body problems involve condensation of the particles into either one or two collections. A reasonable hypothesis, still to be fully proven, is that all minimum energy configurations of Full Body problems result in one of two general states: i) All the particles rest on each other in one collection and spin at a uniform rate; ii) All the particles separate into two collections in a mutually circular orbit about each other with doubly-synchronous rotation.

As the angular momentum of a system is increased we find distinct transitions in the minimum energy configurations within each of the above two classes and, at some point, between these two classes. It is significant to note that during the transition between Class i and ii there is a significant change in the energy available for the dynamical evolution of the system. Thus, we find that immediately after fission of a collection of particles in Class i they can have sufficient energy for the bodies to mutually escape from each other – this escape will never constitute a minimum energy configuration of the Class ii system, although for a large class of Full Body systems it can be shown to be the most likely outcome once a finite rate of energy dissipation in the system is included.

Given this perspective, an interesting problem is to track the absolute minimum energy configuration of a collection of N particles as the system angular momentum increases from zero. This is, essentially, an investigation of the celestial mechanics of granular systems as a function of total angular momentum. This problem has been shown to be relevant to the understanding of solar system bodies, especially among asteroids whose size is small enough so that when their components rest on each other they have insufficient gravitational attraction to overcome material strength, and thus retain the physical characteristics of rigid bodies resting on each other. Due to the celebrated YORP effect, which has established that non-symmetrically shaped bodies subject to solar radiation will change their spin rates over time, this question has several practical applications and has been implicated in how small asteroids form binary systems [1]. The question of stable minimum energy configurations for the $N = 2$ particle Full Body problem has been worked out in detail [2], and has been verified as a viable physical model via astronomical observations of asteroids [3].

Current research has expanded the analysis beyond two particle systems and is investigating the minimum energy configurations of $N \geq 3$ particle systems as a function of total angular momentum using both analytical and numerical methods (as described in [4]). Our results show a surprising complexity in the evolution of minimum energy states as a function of angular momentum, with distinctly different pathways arising as the number of particles in the system increases. There also exist fundamental relationships between this problem and the central configurations of the classical N-body problem. This work is currently being written up for submission to a mathematically-oriented journal.

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Geometry of Option Price Surface Models

Josef Teichmann

We show that Markovian models in the Carmona-Nadtochiy-Kallsen-Krühner framework for the time evolution of volatility surfaces admit finite dimensional realization only if the time evolution is driven by an underlying finite dimensional time-inhomogenous affine process. The result also allows to transfer the methodology of Hull-White extensions and is another justification for the importance of affine stochastic processes.

Let me outline in the sequel on the background of the result and on the result itself: A (markovian) finite-dimensional factor model for option pricing is defined by specifying a state space, the functional dependence of the local characteristics ("model-parameters") of the Markov process on the state variable, and the relations between the underlying(s) and the factor process. In such a setting the state variable apparently follows a dynamics and can change over time, whereas the model parameters are assumed to be constant. Option prices are then usually described by appropriate solutions of backward Kolmogorov equations, which depend on the current state of the factor process and on the model parameters. *Calibration* is a choice of model parameters and a choice of a state variable, such that market prices are optimally reproduced by the factor model. *Recalibration* in this setting is the (delicate) procedure to fit next day's market prices to model prices by only changing the state variables, whereas the model parameters have to be kept constant for consistency reasons.

The term structure approach – in contrast – considers the *liquid market prices* as (part of the) state variable and faces the challenging task to write a stochastic evolution on the set of *liquid market prices*. Since the set of liquid market prices is subject to several constraints, it is of utmost importance to carefully choose a tractable parametrization of this set (choice of a codebook). In the last years several approaches have been suggested, taking implied volatility, local volatility or time-dependent Lévy processes as respective parameters.

- Implied volatility appears as a natural candidate for parametrization, since it is industry standard to quote option prices in terms of their implied volatility. However, the static and dynamic constraints on implied volatility are so awkward that it is very hard to analyze geometrically and analytically time evolutions of implied volatility surfaces, see [7, 8, 9]. Additionally it would be difficult to express stochastic interest rates or multivariate situations within this framework of the implied volatility codebook.
- Local volatility constitutes an industry standard to construct interpolations of (implied) volatility surfaces. It seems therefore natural to construct time evolutions of local volatility functions, see [1]. This is even more attractive, since it is much easier to tell whether a function is a local volatility than an implied volatility. However, the description of the time evolution of local volatilities contains extremely non-linear and non-continuous operations, so that this parametrization also appears less

useful. Additionally the extension towards stochastic interest rates is not well understood within the local volatility codebook.

- A last approach was independently and in parallel proposed by Carmona-Nadtochiy (see [2, 3]) and Kallsen-Krühner (see [6]), where option prices are parametrized by a time-dependent Lévy processes with characteristics absolutely continuous with respect to Lebesgue measure. From an analytic point of view it seems a bit more delicate to describe this set of parameters, however, the drift conditions are considerably less complicated in the Lévy codebook.

Following the approaches of Carmona-Nadtochiy and Kallsen-Krühner, subsequently abbreviated by CNKK-approach, we are equipped with tractable parameterizations. In this talk we prefer the KK-approach to the CN-approach, since we see the following two advantages:

- In contrast to CN the time-inhomogenous Lévy process is encoded by its Lévy exponent, i.e. the logarithm of its Fourier-Laplace transform. CN choose the Lévy-Khintchine triplet (and assume the absence of volatility), which seems – from a purely analytic point of view – more appropriate, since the set of Lévy-Khintchine triplets is more easy to describe analytically than the set of Lévy exponents. On the other hand, and that is a main insight, the necessary martingale conditions, which express the lack of dynamic arbitrage, can be formulated again easier in the Lévy exponent parametrization.
- Dependence between increments of the underlying(s) and the increments of option prices ("leverage effect") are easily included into the KK-framework since this effect is easily expressed in the language of Lévy exponents.

Having fixed the Lévy codebook the geometric and analytic approaches of [5] can be performed and due to several structural similarities the conclusions are of a very similar nature.

Let me describe the main result in words: if we assume that the term structure evolution of Lévy exponents, which describes the liquid option market prices, allows for regular finite dimensional realizations (i.e. we have a regular finite dimensional foliation on a subset of the state Hilbert space), then each leaf of this foliation is a ruled surface, i.e. an affine subspace moving transversally along a one-dimensional trajectory in Hilbert space. This means in particular that factor models in terms of affine processes play a particular role in mathematical finance (for general information on general affine processes see [4]).

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Interconnection, Dirac Structures and Dirac Systems in Mechanics

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(joint work with Henry Jacobs)

Dirac structures unifying both presymplectic and Poisson structures provide an implicit generalization of Lagrangian and Hamiltonian systems including the cases of nonholonomic systems as well as degenerate Lagrangian systems in mechanics; a Dirac structure on the cotangent bundle of a configuration manifold induced from a smooth distribution denotes a power conserving structure between physical elements, which is called an "interconnection". Namely, the Dirac structure plays an essential role in modeling of complicated electric circuits and multibody systems as an interconnected dynamical system. In this study, we primarily consider how distinct Dirac structures D_1 and D_2 on the cotangent bundles can be interconnected through a Dirac structure D_{int}. To do this, we introduce a tensor product $\bowtie$ of Dirac structures D_1, D_2 and D_{int} such that the interconnection of Dirac structures can be given by $(D_1 \oplus D_2) \bowtie D_{\text{int}}$. Finally, we also show an interconnection of Dirac-Lagrange dynamical systems by using $(D_1 \oplus D_2) \bowtie D_{\text{int}}$.

Dirac–Lagrange Dynamical Systems. Let $L : TQ \to \mathbb{R}$ be a Lagrangian, possibly degenerate. Let $\Delta_Q \subset TQ$ be a smooth distribution on Q and let $\Delta_{T^*Q} = T\pi_Q^{-1}(\Delta_Q)$ be a lifted distribution on Q, where $\pi_Q : T^*Q \to Q$. Define a Dirac structure on T^*Q by, for each point $z \in T^*Q$,

$$D(z) = \{(v, \alpha) \in T_z T^*Q \times T_z^* T^*Q \mid v \in \Delta_{T^*Q}(z), \\ \text{and } \alpha - \Omega^\flat(z) \cdot v \in \Delta^\circ_{T^*Q}(z)\}.$$

Recall that a *partial vector field* $X : TQ \oplus T^*Q \to TT^*Q$ is defined as a map that assigns to each point $(q, v, p) \in TQ \oplus T^*Q$, a vector in TT^*Q at the point $(q, p) \in T^*Q$; we write X as $X(q, v, p) = (q, p, \dot{q}, \dot{p})$. Let $E_L : TQ \oplus T^*Q \to \mathbb{R}$ be the *generalized energy* given by $E_L(q, v, p) := \langle p, v \rangle - L(q, v)$.

A **Dirac–Lagrange dynamical system** is a triple (E_L, D, X) that satisfies, for each $(q, v, p) \in TQ \oplus T^*Q$,

$$(X(q,v,p), \mathbf{d}E_L(q,v,p)|_{T_{(q,p)}P}) \in D(\phi(q,v,p)),$$

where $(q, p = \partial L/\partial v) \in P = \mathbb{F}L(\Delta_Q) \subset T^*Q$ and $\phi : TQ \oplus T^*Q \to T^*Q$ ia a natural projection.

Tensor Product of Dirac Structures. Let $P = M \times M$ and let $d : M \hookrightarrow P$ be the diagonal embedding by $M = \{(m, n) \in P \mid m = n\}$. Given Dirac structures D_a, D_b on M, define the direct product of Dirac structures D_a and D_b by $D_a \oplus D_b$ on P. One may pull back the Dirac structure $D_a \oplus D_b \subset TP \oplus T^*P$ on P to M as

$$d^*(D_a \oplus D_b) = \frac{(D_a \oplus D_b) \cap (TM \oplus T^*P|_M)}{(D_a \oplus D_b) \cap (\{0\} \oplus TM^\circ)},$$

where we assume $(D_a \oplus D_b) \cap (TM \oplus T^*P_M)$ has constant dimension, and the subbundle $d^*(D_a \oplus D_b)$ is a Dirac structure on M. Let us rewrite the above as

$$D_a \bowtie D_b := d^*(D_a \oplus D_b).$$

Let D_1 and D_2 be Dirac structures on the cotangent bundles over distinct manifolds Q_1 and Q_2, which are induced from smooth constraint distributions $\Delta_{Q_1} \subset TQ_1$ and $\Delta_{Q_2} \subset TQ_2$ as before. Let Δ_c be a given distribution on $Q = Q_1 \times Q_2$ due to the interconnection of D_1 and D_2. Recall that an interconnection Dirac structure is given by $D_{\text{int}} = \Delta_{\text{int}} \oplus \Delta_{\text{int}}^\circ$, where $\Delta_{\text{int}} = (T\pi_Q)^{-1}(\Delta_c) \subset TT^*Q$ is the constraint distribution associated to the interconnection. Here, we utilize the bowtie operator $\bowtie$ for *interconnecting* the induced Dirac structures D_1 and D_2 through the interconnection Dirac structure D_{int} on T^*Q, which may be constructed from $\Delta = (\Delta_{Q_1} \times \Delta_{Q_2}) \cap \Delta_c$ and $\Omega = \Omega_1 \oplus \Omega_2$, where Ω_1 and Ω_2 are respectively the canonical two-forms on T^*Q_1 and T^*Q_2. Assuming Δ has constant rank, the **interconnection of two distinct induced Dirac structures** D_1 and D_2 through $D_{\text{int}} = \Delta_{\text{int}} \oplus \Delta_{\text{int}}^\circ$ is given by

$$\mathcal{D} = (D_1 \oplus D_2) \bowtie D_{\text{int}}.$$

Interconnected Dirac-Lagrange Systems. Let (E_{L_1}, D_1, X_1) and (E_{L_2}, D_2, X_2) be distinct Dirac-Lagrange dynamical systems on T^*Q_1 and T^*Q_2. Let $\mathcal{Q} = Q_1 \times Q_2$. Define the Lagrangian $\mathcal{L} : T\mathcal{Q} \to \mathbb{R}$ for the interconnected system by $\mathcal{L} = L_1 + L_2$ and define the associated generalized energy by $\mathcal{E}_\mathcal{L} = E_{L_1} + E_{L_2} : T\mathcal{Q} \oplus T^*\mathcal{Q} \to \mathbb{R}$. Set a partial vector field by $\mathcal{X} = X_1 \oplus X_2 : T\mathcal{Q} \oplus T^*\mathcal{Q} \to TT^*\mathcal{Q}$. Then, the interconnection of Dirac-Lagrange dynamical systems can be given by, for each $(q, v, p) \in TQ \oplus T^*Q$,

$$(\mathcal{X}(q,v,p), \mathbf{d}\mathcal{E}(q,v,p)|_{T_{(q,p)}\mathcal{P}}) \in \mathcal{D}(\varphi(q,v,p)),$$

where $(q, p = \partial L/\partial v) \in \mathcal{P} = \mathbb{F}\mathcal{L}(\Delta) \subset T^*Q$ and $\varphi : TQ \oplus T^*Q \to T^*Q$.

In the talk, we further develop variational structures associated with the interconnection of associated Dirac-Lagrange dynamical systems. Lastly, we demonstrate the theory of interconnection of Dirac structures and associated Lagrange-Dirac dynamical systems by some examples including electric circuits, nonholonomic mechanical systems, and simple mass-spring mechanical systems.

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Stability of Relative Equilibria of Discrete Chaplygin Systems

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(joint work with Cameron Lynch and Kenneth Ball)

Chaplygin systems are nonholonomic mechanical systems with symmetry whose group dynamics is completely determined by constraints. We study stability of relative equilibria of discrete commutative Chaplygin systems. That is, we assume that the group in the definition of a Chaplygin system is commutative. In addition, we assume that the reduced system has its own commutative symmetry group. Many systems, such as the rattleback, the rolling disk, and the roller racer, are invariant with respect to the semidirect product of the said two groups. Stability in the continuous-time setting has been studied by Karapetyan [3].

A discrete analogue of Lagrangian mechanics can be obtained by considering a discretization of Hamilton's principle; this approach underlies the construction of variational integrators. The origins of discrete mechanics can be found in the control literature of the 1960s. See Marsden and West [6], and references therein, for a more detailed discussion of variational integrators, discrete mechanics, and history.

Variational integrators are known to adequately represent the dynamics of continuous-time Lagrangian systems over long time intervals. Moreover, algorithms obtained this way are structure-preserving: They conserve the volume in the momentum phase space and conserve momentum if the continuous-time system has symmetry. They also are known to accurately track the system's energy over long time intervals, i.e., they are free from the so-called numerical dissipation (an artificial dissipation introduced by some numerical methods).

Cortés and Martínez [2] extend this formalism to the nonholonomic setting by replacing Hamilton's principle with a discrete version of the Lagrange–d'Alembert

principle and approximating nonholonomic constraints with a suitable submanifold of the phase space of the discrete system. They also consider an alternative discrete model, in which the constraints are replaced with a suitable discretization of the reaction force of continuous-time constraints. They point out that, contrary to the continuous-time case, these two discrete model are typically not the same for ideal constraints. In other words, the discrete Lagrange–d'Alembert principle introduced by Cortés and Martínez is incompatible with the concept of ideal constraints. Below these two discrete models are referred to as "nonholonomic discretization" and "forced discretization", respectively. Our study of these discretizations reveales that the former one may not preserve the manifold of relative equilibria of the continuous-time system, and thus may fail to be structurally stable, while the latter one always preserves relative equilibria as well as their stability types.

It is well-known that, in the absence of external dissipation, relative equilibria of continuous-time nonholonomic systems may be partially asymptotically stable, i.e., Lyapunov-stable as well as asymptotically stable in some directions in the phase space. Here by stability we understand orbital stability, i.e., a relative equilibrium is stable if the corresponding equilibrium of the reduced system is stable. Spectral stability in nonholonomic setting is discussed in Routh [7], the nonlinear stability is established by Karapetyan [3]. It is also well-known (see e.g. Bloch, Krishnaprasad, Masden, and Murray [1] and references therein) that generically momentum is not preserved in nonholonomic systems with symmetry. It is however preserved for so-called horizontal symmetries. Cortés and Martínez prove that in their discrete models momentum is preserved for horizontal symmetries, just like in the continuous time case. One should keep in mind that horizontal symmetries are not observed in a number of interesting examples. One cannot also expect that an invariant measure exists generically in the discrete setting; this is confirmed below by the existence of partially asymptotically stable relative equilibria in the discrete setting.

Since nonholonomic flows, in general, are not symplectic, volume, or momentum preserving, structure-preservation in the discrete nonholonomic setting should be understood in a different way. Relative equilibria of nonholonomic systems with symmetry are never isolated and often are partially asymptotically stable. Motivated by these observations, we ask for a discretization to preserve the manifold of equilibria of the reduced system and their stability type. Otherwise, one ends up with structurally-unstable discretizations. Indeed, if the manifold and stability types of equilibria of the reduced continuous-time system are not preserved by the discretization, the α and/or ω limit sets of the continuous-time system and its discretization are certain to be different, and the continuous-time and discrete dynamics are certain to have inconsistent asymptotic behavior. We emphasize that while the change in the structure of the limit sets may be local, the influence of this change on the dynamics is global.

Assuming that the reduced discrete nonholonomic system has a manifold of equilibria, we utilize the center manifold stability analysis technique and establish

conditions for partial asymptotic stability of equilibria of this system, thus obtaining a discrete analogue of Karapetyan's stability result. The key observation is that the manifold of equilibria and center manifold of the reduced discrete dynamics coincide. The stability result then follows from spectral stability condition. Indeed, if the spectrum of the linearization at the equilibrium of interest has maximal possible number of eigenvalues in the open unit disc, the phase space of the reduced system in a neighborhood of the said equilibrium is foliated by the stable manifolds. Any small perturbation then will give rise to a solution that belongs to one of these stable manifolds, and thus the equilibrium of interest is stable and in addition asymptotically stable along these stable manifolds.

We then prove that the manifolds of equilibria of the reduced continuous-time system and of its forced discretization are identical. Next, we prove that the stability conditions of relative equilibria for the forced discretization are identical to Karapetyan's stability conditions for the associated continuous-time system. By constructing an example, it is shown that the dimension of the manifold of equilibria of the reduced discrete dynamics, obtained by the nonholonomic discretization, may be different from the dimension of equilibria of the associated continuous-time system. See [4] for details.

A careful analysis shows that when the manifolds of equilibria of the reduced continuous-time system and of its nonholonomic discretization are identical, the stable manifolds at an equilibrium of the reduced continuous time system and of its discretization may intersect transversally at the said equilibrium.

It follows from the analysis above that the forced discretization is in a better agreement with the continuous-time dynamics than the nonholonomic one.

We also discuss (see [5]) conditions for the nonholonomic discretization to preserve equilibria of the associated reduced continuous-time system. These conditions are shown to be satisfied for the practically important case of planar Euclidean symmetry.

The theory is illustrated with the stability analysis of relative equilibria of the discrete roller racer.

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