FOCM 2014 - Workshop B4
Geometric Integration and Computational Mechanics

B4 - December 15, 14:30 – 14:55

Post-Lie algebras in differential geometry and applications

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Algebraic combinatorics has become a powerful tool in the study of geometric properties of differential equations, with applications in diverse areas such as control theory, stochastic differential equations, geometric numerical integration algorithms and renormalisation theory.

Pre-Lie algebras describe algebras of flat and torsion-free connections on (mostly) euclidean spaces (Vinberg 1963). This is the algebraic foundation of Butchers B-series (Butcher 1963-72) and is closely related to a Hopf algebra appearing in renormalisation theory and non-commutative geometry (Connes-Kreimer 1999). Pre-Lie structures also appear in algebraic deformation theory (Gerstenhaber 1963). Unfortunately, pre-Lie connections do only exist on very special Lie groups, such as Euclidean spaces and certain nil-potent groups, and they are therefore not applicable for the analysis of many geometric structures appearing in mechanics and gauge field theories (principal bundles).

Post-Lie algebras is a recent invention from the last decade. The differential geometric view is the algebra of a flat connection with constant torsion. This view, with applications to numerical analysis, has been explored in a series of papers by our research group (MK-Wright 2006), MK-Lundervold 2013, Lundervold-EbrahimiFard-MK 2014). The same algebraic structure (and the name post-Lie) also appears in operad theory (Vallette 2007), where it arises as a Koszul dual of a commutative trialgebra.

Post-Lie algebras is a powerful algebraic abstraction which encodes both infinitesimal and finite aspects of flows (vector fields and their analytical or numerical flows) as well as geometric aspects such as parallel transport and curvature. There are natural post-Lie structures associated with any Lie group and more generally with homogeneous spaces and Klein geometries, where the post-Lie structure describes a connection on the Atiyah Lie algebroid.

In the talk we will survey recent developments in this field, focus on some applications in numerical integration and point out some important open research areas.

Joint work with Alexander Lundervold (Bergen University College), Olivier Verdier (Bergen University College) and Kurusch Ebrahimi-Fard (ICMAT Madrid).

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The Butcher group is a Lie group

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The concept of B-series, formal expansions of numerical methods for ordinary differential equations, has been an important tool for numerical analysts over the last decades.

In 1972, Butcher showed that numerical integrators which allow a B-series expansion, form an infinite-dimensional group under composition.

In 1998, the Butcher group was rediscovered by Connes and Kreimer in the context of renormalization in Quantum Field Theory. Connes and Kreimer also showed that, algebraically, the Butcher group is associated with a Lie algebra.

We show that the Butcher group is a Lie group modeled on a Fréchet space. The Lie algebra of Connes and Kreimer reappears as a dense subalgebra of the tangent space at the identity of this group.

We explore the properties of the Butcher group from the point of infinite dimensional Lie group, thus complementing the algebraic tretament by Connes and Kreimer.

Joint work with Alexander Schmeding (Norwegian University of Science and Technology).

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Discrete inequalities for central-difference type operators

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One advantage of the energy-preserving methods is that sometimes the energy gives an a priori estimate for the (numerical) solution. For example, in the cubic nonlinear Schroedinger equation, the quartic energy function (the Hamiltonian) yields an estimate $\|u\|_\infty < \infty$ for all $t > 0$, with the aid of the discrete Gagliardo–Nirenberg and Sobolev inequalities.

Although such discrete inequalities have been known for the simplest forward (i.e. one-sided) finite difference operator, it remained open for more general operators including the standard central-difference operator, as far as the authors know. Accordingly, the analyses of energy-preserving methods with such operators remained open as well.

Recently, we found a unified way of establishing discrete inequalities for a certain range of central-difference type operators. In this talk, we show some results, and illustrate them through applications to some structure-preserving numerical schemes.

Joint work with Daisuke Furihata (Osaka University) and Hiroki Kojima (University of Tokyo).

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Spherical midpoint method

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In this talk I will discuss a novel symplectic integrator for Hamiltonian systems on direct products of 2-spheres. Such systems are called spin systems and occur frequently in physics; examples include the free rigid body, point vortex dynamics on the sphere, the classical Heisenberg spin chain, and the Landau-Lifshitz equation of micromagnetics. The new method is simple, works for all Hamiltonians, and is $O(3)$-equivariant. I will explain how the method is related to the classical midpoint method and to the recent concept of collective symplectic integrators.

Joint work with Robert McLachlan (Massey University, New Zealand) and Olivier Verdier (Umeå University, Sweden).

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Symplectic Runge-Kutta methods for nonsymplectic problems

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Symplectic Runge-Kutta and Partitioned Runge-Kutta methods exactly preserve quadratic first integrals (invariants of motion) of the system being integrated. While this property is often seen as a mere curiosity (it does not hold for arbitrary first integrals), it plays an important role in the computation of numerical sensitivities, optimal control theory and Lagrangian mechanics. Some widely used procedures, such as the direct method in optimal control theory and the computation of sensitivities via reverse accumulation imply hidden integrations with symplectic Partitioned Runge-Kutta schemes.

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Algebra and structure-preserving integrators

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Since the pioneering work of Butcher, it is known that a large class of numerical integration schemes for ordinary differential equations may be encoded algebraically using trees. Order conditions, composition of schemes and other useful properties may then be studied at the algebraic level. In applications, it is often desirable that numerical schemes retain certain structural properties of the underlying equation, such as symplecticity. These constraints may be encoded at the algebraic level. In many cases the algebraic structure simplifies accordingly. We explore the algebraic encoding of such simplifications and their implications for the study of structure-preserving numerical methods.

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The exact discrete Lagrangian function on the Lie algebroid of a Lie groupoid

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In this talk, I will present a definition of the exact discrete Lagrangian function associated with a continuous regular Lagrangian function on the Lie algebroid of a Lie groupoid. Some applications on variational analysis error in this setting will also be presented. In order to define the exact discrete Lagrangian function, I will use some results on second order differential equations on the vertical bundle of a fibration. These results may be proved using classical theorems on second order differential equations.

Joint work with D Martín de Diego (ICMAT, Spain) and E Martínez (University of Zaragoza, Spain).

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Reduction by stages of discrete mechanical systems: a discrete Lagrange-Poincare approach

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Discrete mechanical systems (DMS) are a type of dynamical system whose trajectories are the extrema of a discrete variational problem determined by a discrete Lagrangian function. Those trajectories provide interesting numerical integrators. Under fairly reasonable conditions symmetric DMSs can be reduced, that is, a new dynamical system can be constructed whose dynamics captures the essential features of the original one. In some cases, it is convenient to perform the reduction procedure in more than one step, what is generically known as reduction by stages. Unfortunately, the reduced systems are usually not DMSs so that a second reduction may not be possible within the standard DMS theory.

In this talk we expand the family of DMSs to a new family, the discrete Lagrange-Poincare systems, that is closed under reduction. As a consequence, the reduction by stages can be satisfactorily performed.

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Geometric Numerical Integration and Computational Geometric Mechanics

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Symmetry, and the study of invariant and equivariant objects, is a deep and unifying principle underlying a variety of mathematical fields. In particular, geometric mechanics is characterized by the application of symmetry and differential geometric techniques to Lagrangian and Hamiltonian mechanics, and geometric integration is concerned with the construction of numerical methods with geometric invariant and equivariant properties. Computational geometric mechanics blends these fields, and uses a self-consistent discretization of geometry and mechanics to systematically construct geometric structure-preserving numerical schemes.

In this talk, we will introduce a systematic method of constructing geometric integrators based on a discrete Hamilton's variational principle. This involves the construction of discrete Lagrangians that approximate Jacobi's solution to the Hamilton-Jacobi equation. Jacobi's solution can be characterized either in terms of a boundary-value problem or variationally, and these lead to shooting-based variational integrators and Galerkin variational integrators, respectively. We prove that the resulting variational integrator is order-optimal, and when spectral basis elements are used in the Galerkin formulation, one obtains geometrically convergent variational integrators.

We will also introduce the notion of a boundary Lagrangian, which is analogue of Jacobi's solution in the setting of Lagrangian PDEs. This provides the basis for developing a theory of variational error analysis for multisymplectic discretizations of Lagrangian PDEs. Equivariant approximation spaces will play an important role in the construction of geometric integrators that exhibit multimomentum conservation properties, and we will describe two approaches based on spacetime generalizations of Finite-Element Exterior Calculus, and Geodesic Finite Elements on the space of Lorentzian metrics.

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Solvability of Geometric Integrators for Multi-body Systems

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This work is concerned with the solvability of implicit time-stepping methods for simulating the dynamics of multi-body systems. The standard approach is to select a time-step based on desired level of accuracy and computational efficiency of integration. Implicit methods impose an additional but often overlooked requirement that the resulting nonlinear root-finding problem is solvable and has a unique solution. Motivated by empirically observed integrator failures when using large time-steps this work develops bounds on the chosen time-step which guarantee convergence of the root-finding problem solved with Newton's method. Second-order geometric variational integrators are used as a basis for the numerical scheme due to their favorable numerical behavior. In addition to developing solvability conditions for systems described by local coordinates, this work initiates a similar discussion for Lie group integrators which are a favored choice for floating-base systems such as robotic vehicles or molecular structures.

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Structure preserving integration of hybrid dynamical systems and optimal control

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The optimal control of human walking movements requires simulation techniques, which handle the contact's establishing and releasing between the foot and the ground. The system's dynamics switches non-smoothly between phases with and without contact making the system hybrid.

During motion phases without switch, the direct transcription method Discrete Mechanics and Optimal Control (DMOCC) is used to transform the optimal control problem into a constrained optimisation problem. It involves a mechanical integrator based on a discrete constrained version of the Lagrange-d'Alembert principle. This integrator represents exactly the behaviour of the analytical solution concerning the consistency of momentum maps and symplecticity. To guarantee the structure preservation and the geometrical correctness during the establishing and releasing of contacts, the non-smooth problem is solved including the computation of the contact or contact release configuration as well as the contact time and force, instead of relying on a smooth approximation of the contact problem via a penalty potential.

While in a first approach, the sequence (not the switching time) in which the closing and opening of contacts follow each other is considered as known, a more general approach is the optimisation of the whole locomotion requiring a combined model including transitions between the different dynamical systems. Integer valued functions can be used to control if and when the switch to another dynamical system occurs, i.e. they permit to control the sequence and switching times of the dynamical systems. A variable time transformation allows to eliminate the integer valued functions and therefore to apply gradient based optimisation methods to approximate the mixed integer optimal control problem.

Joint work with Michael W. Koch (Chair of Applied Dynamics, University of Erlangen-Nuremberg), Maik Ringkamp (Chair of Applied Dynamics, University of Erlangen-Nuremberg) and Sina Ober-Blöbaum (Computational Dynamics and Optimal Control, Department of Mathematics, University of Paderborn).

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Higher order variational integrators in the optimal control of mechanical systems

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In recent years, much effort in designing numerical methods for the simulation and optimization has been put into schemes which are structure preserving. One particular class are variational integrators which are momentum preserving and symplectic. In this talk, we develop a convergence theory on high order variational integrators applied to finite-dimensional optimal control problems posed with mechanical systems.

In the first part of the talk, we derive two different kinds of high order variational integrators based on different dimensions of the underlying approximation space. While the first well-known integrator is equivalent to a symplectic partitioned Runge-Kutta method, the second integrator, denoted as symplectic Galerkin integrator, yields a method which in general, cannot be written as a standard symplectic Runge-Kutta scheme.

In the second part of the talk, we use these integrators for the discretization of optimal control problems. By analyzing the adjoint systems of the optimal control problem and its discretized counterpart, we prove that for these particular integrators dualization and discretization commute. This property guarantees that the convergence rates are preserved for the adjoint system which is also referred to as the Covector Mapping Principle.

Joint work with Cédric M. Campos (Universidad de Valladolid, Spain).

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Geometric Integration for High Fidelity Visual Computing Applications

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To be able to take into account a multitude of physical effects, high fidelity simulations are nowadays of growing interest for analysing and synthesising visual data. In contrast to most numerical simulations in engineering, local accuracy is secondary to the global visual plausibility. Global accuracy can be achieved by preserving the geometric nature and physical quantities of the simulated systems for which reason geometric integration algorithms like symplectic methods are often considered as a natural choice. Additionally, if the underlying phenomena behaves numerically stiff, a non-geometric nature comes into play requiring for strategies to capture different timescales accurately. In this contribution, a hybrid semi-analytical, semi-numerical Gautschi-type exponential integrator for modeling and design applications is presented. It is based on the idea to handle strong forces through analytical expressions to allow for long-term stability in stiff cases. By using an appropriate set of analytical filter functions, this explicit scheme is symplectic as well as time-reversible. It is further parallelizable exploiting the power of up-to-date hardware. To demonstrate its applicability in the field of visual computing, various examples including collision scenarios and molecular modeling are presented.

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On a problem in quantum control with unknown initial conditions

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We consider the problem of controlling solutions of the linear Schroedinger equation using linear lasers. The initial condition is not exactly known, but it is known that it can be generated within a range of initial conditions. Is it possible to construct a laser that drives all these initial conditions to a detectable wave? We formulate the problem mathematically and discuss a numerical method to approximate the laser. This problem is relevant in the experimental physics setting to detect whether antimatter is subject to the same gravitational force as matter or not.

Joint work with Jan Petter Hansen (University of Bergen).

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Simulation of Wind Instruments and a Geometric Invariance of the Discrete Gradient Method

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In this talk we consider simulation of wind instruments by using the Webster equation. The Webster equation is a model equation of sound waves in tubes such as vocal tracts and bodies of wind instruments. Simulation of sound waves requires long-time calculation compared to the time scale of wave propagation phenomena and hence we need structure-preserving methods to obtain meaningful results.

We apply the discrete gradient method to this equation. Because a gradient is defined by using an inner product, we must introduce a suitable Riemannian structure to the phase space. We used two different inner products to design numerical schemes by the discrete gradient method; however, it turned out that the schemes do not depend on the choice of the inner product.

By extending this result, we show a theorem that states a geometric invariance of the discrete gradient method under the change of the Riemannian structure.

Joint work with Ai Ishikawa (Kobe University).

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Asymptotic exponential splitting for the linear, time-dependant Schrödinger equation

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This talk is about recent results obtained in numerical approximation of linear, time-dependant Schrödinger equation. The main difficulty lies in a minute size of Planck constant and in the time-dependant potential. The outcome of our investigation is an asymptotic exponential splitting, which features two significant advantages: it separates scales of the frequency and every successive term in this splitting is of increasingly higher order. This means that the accuracy of proposed methods scales linearly with their cost. These results were obtained, working at a level of differential operators, by combining Magnus expansion, the sBCH formula and Zassenhaus splitting. Additionally, to render the method more efficient, we are following the Munthe-Kaas – Owren approach of changing the basis at the stage of Magnus expansion.

Joint work with Arieh Iserles (University of Cambridge, UK) and Pranav Singh (University of Cambridge, UK).

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Energy preservation for moving mesh PDEs

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Recently, there has been a growing interest in designing integral preserving schemes for PDEs which use well-known ideas from ordinary differential equations, such as discrete gradient methods and the averaged vector field method. Although adapting such schemes to simple finite difference or finite element methods on constant uniform grids is straightforward, the situation becomes much more challenging when the spatial mesh is non-uniform or even changing with time. In the latter case it is not even very clear what should be meant by an integral being preserved. In this talk we shall look at various possible ways of giving meaning to the concept of integral preservation of moving mesh PDEs and we provide some promising numerical results.

Joint work with Sølve Eidnes (Norwegian University of Science and Technology).

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Geometric data assimilation: a thermostat-based particle filter

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Particle filters used in data assimilation are nonintrusive in the sense that they do not alter the trajectories of individual ensemble members. For this reason they offer a simple means of preserving geometric features of the dynamics to effect 'data assimilation on manifolds'. However they suffer from degeneracy of the ensemble, in which all of the ensemble weight gets assigned to a single sample, and have no mechanism for correcting ensemble drift. Thermostats have traditionally been used to perturb trajectories of molecular gases to ergodically sample equilibrium (Gibbs) measures. However they can be easily implemented to preserve additional (e.g. structural) invariants. Recent experience with thermostats also indicates they can be used to sample a nonstationary measures conditioned on data, making them a potential compromise for particle filtering.

Joint work with Keith Myerscough (CWI, Amsterdam) and Ben Leimkuhler (U. Edinburgh).

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Collocation method for solving singular ODEs and higher index DAEs

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During recent years, a lot of scientific work concentrated on the analysis and numerical treatment of boundary value problems (BVP) in ordinary differential equations (ODEs) which can exhibit singularities. Such problems have often the following form:

$$y'(t) = \frac{1}{t^\alpha} M(t)y(t) + f(t, y(t)), \quad t \in (0,1], \quad b(y(0), y(1)) = 0.$$

For $\alpha = 1$ the problem is called singular with a singularity of the first kind, for $\alpha > 1$ it is essentially singular (singularity of the second kind).

The search for efficient numerical methods to solve the above BVP is strongly motivated by numerous applications from physics, chemistry, mechanics, ecology, or economy. In particular, problems posed on infinite intervals are frequently transformed to a finite domain taking above form with $\alpha > 1$. Also, research activities in related fields, like differential algebraic equations (DAEs) or singular Sturm-Liouville eigenvalue problems benefit from techniques developed for singular BVPs.

While collocation stays robust and shows advantageous convergence properties in context of singular problems, other high order methods suffer from instabilities and order reductions. It turns out that for singular BVPs with smooth solutions, the convergence order of the polynomial collocation is at least equal to the so-called stage order of the method. For collocation at equidistant points or Gaussian points this convergence result means that the scheme with m inner collocation points constitutes a high order basic solver whose global error is $O(h^m)$ uniformly in t [5].

Clearly, in order to solve an ODE system efficiently, the error estimate and the mesh adaptation strategy have to be provided to correctly reflect the solution behavior. Due to the robustness of collocation, this method was used in one of the best established standard FORTRAN codes for (regular) BVPs, COLSYS [1], as well as in Matlab codes bvp4c [7], the standard module for (regular) ODEs with an option for singular problems, BVP SOLVER [8], sbvp [2], and bvpsuite [6]. The scope of bvpsuite includes fully implicit form of the ODE system with multi-point boundary conditions, arbitrary mixed order of the differential equations including zero, module for dealing with infinite intervals, module for eigenvalue problems, free parameters, and a path-following strategy for parameter-dependent problems with turning points.

We will illustrate how bvpsuite can be used to solve BVPs from applications, Complex Ginzburg-Landau equations, density profile in hydrodynamics, and generalized Korteweg-de Vries equation [3].

Finally, we turn to higher index DAEs. Higher index DAEs constitute a really challenging class of problems due to the involved differentiation which is a critical operation to carry out numerically. A possible technique to master the problem is to pre-handle the DAE system in such a way that the transformed problem is of index one and less difficult to solve. Since this approach is technically involved, it is worth to try to avoid it and provide a method which can be applied directly to the original DAE system of high index. At present, there are only some experimental results available, but they are quite encouraging and therefore, we shall briefly discuss them during the presentation [4].

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B4 - Poster

Some results on invariant measures of reduced discrete mechanical systems

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The interest in discrete (time) mechanical systems is highly motivated by the construction of structure preserving numerical integrators for the continuous ones [MW01]. For instance, one of the features of their discrete evolution consists in the invariance of a Liouville measure, which is associated to an invariant canonical symplectic form on the discrete phase space; the latter is formed by pairs of positions in the configuration space (a differentiable manifold).

Another known fact about discrete mechanical systems is the momentum preservation in the presence of symmetries. Moreover, there is a well developed discrete counterpart of reduction theory of continuous systems. When passing to a dynamical system on a quotient space in order to remove the symmetries, it is worth saying that the latter result in hamiltonian systems on a Poisson manifold. In this sense, they preserve a Poisson bracket but not necessarily a symplectic form, and, thus, it is not guaranteed the existence of an invariant measure as in the previous case; the situation is analogue for discrete systems.

When satisfied, the property of unimodularity of a Poisson manifold gives an affirmative answer to the question of whether such a reduced continuous system preserves a measure. This is due to the equivalence between the notion of unimodularity and the existence of a volume form that is invariant by all hamiltonian flows [Wei97,FGM13].

It is the purpose of this work to study sufficient conditions to relate the concept of unimodulatiry of a Poisson manifold to the existence of invariant measures of reduced discrete mechanical systems. To this end, we firstly address the problem for the discrete Euler-Poincaré equations under quite general conditions. These equations describe the reduced dynamics of discrete systems whose configuration space, G, is simultaneously a group of symmetries acting on the discrete phase space, $G \times G$, by the diagonal action induced by the left multiplication [BS99]. Reinterpreting the idea of unimodularity as the unimodularity of $(G \times G)/G \cong G$ as a Lie group [Koz88], we use results from Lie algebra theory to show that this is sufficient to prove the invariance of a certain measure.

Finally, towards a more general result, we tackle the problem of existence of invariant measures of reduced discrete mechanical systems by means of geometric arguments, instead of dealing with their equations of motion. These take into account the presevation of the reduced Poisson structure on the reduced discrete space and, also, the symplectic leaves associated to it. Although this work-in-progress technique requires stronger hypotheses when it is applied and compared to the previous particular situation, it is intended to cover a wider range of systems. As future work, our next step will be to extend the current approach to include (nonholonomic) constraints.

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Joint work with Javier Fernández (Instituto Balseiro, Universidad Nacional de Cuyo - CNEA, Argentina) and Marcela Zuccalli (Depto. de Matemática (FCE), Universidad Nacional de La Plata, Argentina).
