Design of geometric integrators *

María Barbero Liñán † **Kurusch Ebrahimi-Fard** ‡

Instituto de Ciencias Matemáticas (CSIC-UAM-UC3M-UCM), Madrid, Spain
(joint partner Department of Mathematics, University of Bergen, Norway)

Objective: Computational solutions of differential equations are essential in natural sciences and technology. Geometric integration algorithms, designed to preserve geometric structures of dynamical systems, is a very active research field. Recent remarkable developments have culminated in the unveiling of hitherto hidden connections between numerical analysis, discrete mechanics and algebraic combinatorics. This project has focused on deep connections between two rather complementary approaches to geometric integration methods by combining advanced differential geometry and modern algebraic combinatorics.

1 Work packages

1. **B-series methods for geometric integration and its connections to algebraic combinatorics:** Following the pioneering work of Arthur Cayley, John Butcher used rooted trees to describe a wide and important class of numerical integration schemes, including Runge-Kutta methods. Today, Butcher's so-called B-series provide a particularly nice and successful framework for discussing geometric integrators, with a large and active international community. Indeed, B-series can be used especially to elaborate on numerical and algebraic aspects of structure preserving numerical integrators.

PURSUED PROBLEMS:
- Understand **looped tree** in the context of symmetries on homogeneous spaces, symmetric manifolds and Lie algebroids.
- Understand **subalgebras** arising from symplectic vector fields on Poisson manifolds.
- Investigate the possibility of constructing numerical integrators, which are at the same time **affinely equivariant maps via aromatic trees**.
- Study the structure of the **sub-complex of the variational bi-complex spanned by the exterior algebra of aromatic trees** in the pre-Lie and post-Lie algebraic setting.

2. **Discrete variational integrators:** Discretization of continuous settings is one of the fundamental aspects of geometric integration methods for differential equations. It is known that variational integrators are easily adaptable to different classes of mechanical systems, and in the context of discrete mechanics this may be employed to derive geometric integrators. Connes' tangent groupoid can be considered as a geometric structure that combines in a differentiable manner the continuous and discrete settings. In fact, it encodes the smooth deformation of a Lie groupoid to its corresponding Lie algebroid.

PURSUED PROBLEMS:
- Construct **variational integrators** preserving the integrability of the continuous system.
- Interpret a numerical method as a **family of submanifolds of a Lie groupoid** (for instance, Lagrangian submanifolds for symplectic methods).
- **Implement geometric integrators** and study their performance versus non geometric numerical methods.

2 Background

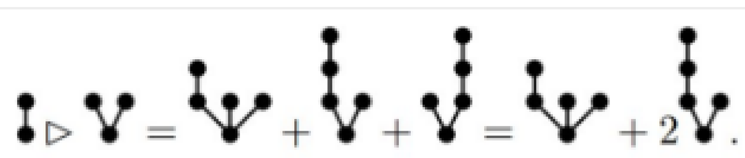
B-SERIES METHODS.

Let $y' = f(y)$, $y_0 = y(0)$ be a differential equation on $\mathbb{R}^n$. The derivatives of f can be associated with rooted trees. **Butcher series:** $y = \sum_{\tau\in\mathcal{T}} \alpha(\tau)\mathcal{F}(\tau)$, where $\mathcal{T}$ is a family of trees.

Numerical methods such as the midpoint method can be represented as a **B-series**: $y_{k+1} = y_k + h\, f(y_k) + \frac{h^2}{2} f'(y_k)\, f(y_k) + O(h^3)$.

B-series methods are exactly the local, affine equivariant methods (2014). B-series are**useful for order theory, structure-preservation** (such as Hamiltonian, symplectic, etc), **discovering connections to other fields** such as pre-Lie algebras.

Pre-Lie algebra of trees: The set of rooted nonplanar trees $\mathcal{T}$ with the grafting product.



Lie-Butcher series approximate differential equations $y' = F(y) = f(y)\cdot y$, $y(0) = y_0$ (Lie group methods).

DISCRETE VARIATIONAL INTEGRATORS.

AIM: Let $L\colon TQ \to \mathbb{R}$ be a Lagrangian function, to extremize

$$\begin{aligned} \mathcal{S}\colon\ \mathcal{C} &\longrightarrow \mathbb{R} \\ q &\longmapsto \mathcal{S}[q] = \int_0^T L(q(t), \dot q(t))\mathrm{d}t, \end{aligned}$$

where $\mathcal{C}$ is the space of all the $\mathcal{C}^2$-curves $q\colon [0,T] \to Q$ such that $q(0) = q_0$ and $q(T) = q_T$.

Euler-Lagrange equations: $\frac{\mathrm{d}}{\mathrm{d}\,t}\frac{\partial L}{\partial \dot q} - \frac{\partial L}{\partial q} = 0\,.$

AIM: Let $L_d\colon Q\times Q \to \mathbb{R}$ be the **discrete Lagrangian function**, to minimize

$$\begin{aligned} \mathcal{S}_d\colon\quad \mathcal{C}_d &\longrightarrow \mathbb{R} \\ (q_0, q_1, \ldots, q_N) &\longmapsto \mathcal{S}(q_0, q_1, \ldots, q_N) = \\ & \qquad L_d(q_0,q_1) + L_d(q_1,q_2) + \cdots + L_d(q_{N-1}, q_N)\,, \end{aligned}$$

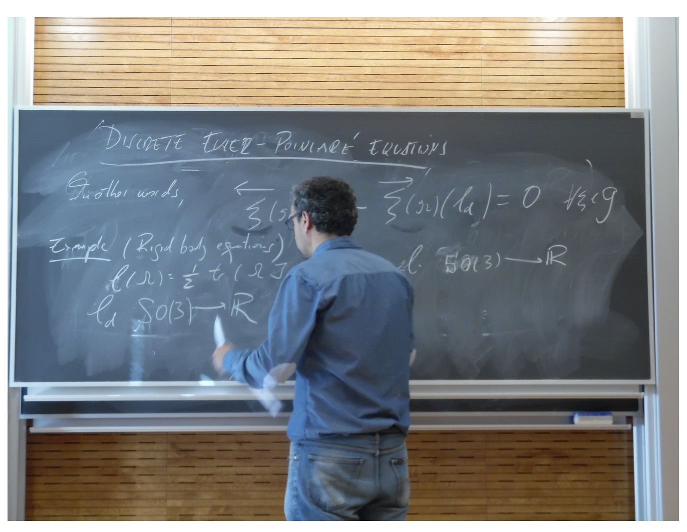
where $\mathcal{C}_d$ is the set of admissible curves which are sequence of points with fixed end-points.

Discrete Euler-Lagrange equations: $D_1L_d(q_k, q_{k+1}) + D_2L_d(q_{k-1}, q_k) = 0\,,\quad k = 1, \ldots, N-1\,.$

3 Methodology

READ, THINK, DISCUSS, READ, THINK DISCUSS,...

We have organized:
- **Seminars** in both institutions to introduce each other the common foundations to progress.
- **10 research visits to ICMAT** by the Norwegian partner, **11 research visits to University of Bergen** by the Spanish partner.
- **Brainstorming workshop on New Developments in Discrete Mechanics, Geometric Integration and Lie-Butcher Series, ICMAT, May 25-28, 2015** (partially supported by 010-BBRR).



4 Achieved results

- **Intrinsic construction of Lie-Poisson integrators that preserve the integrability of the systems** in the discrete setting.
- "**On the Lie enveloping algebra of a post-Lie algebra**" by K. Ebrahimi-Fard, A. Lundervold, H. Munthe-Kaas. To appear in *J. Lie Theory*, **25**(4) (2015) 1139–1165.
- "**Post-Lie algebras and isospectral flows**" by K. Ebrahimi-Fard, A. Lundervold, I. Mencattini, H. Z. Munthe-Kaas. *SIGMA* **11** (2015), 093, 16 pages.
- Establish **contact with members in the Norwegian University of Science and Technology at Trodheim** where there is a strong group working on geometric integrators and with industrial partners.
- In preparation a **volume of research papers (surveys and new contributions) in Springer Proceedings in Mathematics & Statistics** (http://www.springer.com/series/10533). This volume includes papers by researchers at University of Bergen (1 paper) and at ICMAT (3 papers), plus some other participants in the activity "Brainstorming Workshop on New Developments in Discrete Mechanics, Geometric Integration and Lie-Butcher series". Moreover, the volume will have a special survey paper written by A. Iserles and R. Quispel, top researchers in the area of numerical integrators.

5 Future work/activities/projects

RESEARCH LINES: on Lie triple systems/symmetric spaces; on geometric integrators and stochastic dynamics; on discrete-time Chen-Fliess series and efficient approximation methods.

ACTIVITIES/PROJECTS:
- **Abel Symposium 2016 "Computation and Combinatorics in Dynamics, Stochastics and Control"**, which is taking place from August 16-19, 2016, at Barony Rosendal in Norway.
- Elena Celledoni (Norwegian University of Science and Technology, Norway) has just got a **RISE network**, which includes a company partner from Cambridge (UK).

*010-ABEL-CM-2014A. Discrete Mechanics, Geometric Integration and Lie-Butcher Series. Supported by a grant from Iceland, Liechtenstein and Norway through the EEA Financial Mechanism. Operated by Universidad Complutense de Madrid.
†mbarbero@icmat.es
‡kurusch@icmat.es.