Courses 2018-19

# Geometric Numerical Integration

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**20-24 May 2019 (5 sessions) l 10:00 - 12:00 (a total of 10 hours)**

This course is devoted to the study of numerical techniques used for simulating dynamical systems, especially conservative systems such as those in celestial mechanics and molecular models. In a dynamical simulation, an integrator replaces a differential equation in continuous time by a difference equation defining approximate captures of the solution at discrete time steps. More precisely, geometric integrators are numerical methods that preserve geometric properties of the exact flow of a differential equation.

Molecular dynamics is a rich source of applications for geometric integration and, in the course, the examples illustrating the numerical methods will be mainly drawn from this field. However, geometric integration has a vast range of applications: from weather prediction to robotics, or from the study of the Schrödinger equation to computational statistics. Since in the course the emphasis will be put on the methods rather than on the applications, it may be of interest to a very broad audience.

**PROGRAMME:**

1. Hamiltonian mechanics and numerical methods**.**
2. Symplectic integration.
3. Modified equations.
4. Constrained mechanical systems.
5. Adaptive geometric integrators

**OBJECTIVES:**

The purpose of this course is to survey well-known techniques in the field of geometric numerical integration with special attention to the solution of numerical Hamiltonian problems.

**PREREQUISITES:**

There are no formal prerequisites, but some basic knowledge of numerical analysis, linear algebra and differential equations is expected.

**REFERENCES:**

[1] Hairer, Ernst; Lubich, Christian; Wanner, Gerhard (2002). Geometric Numerical Integration: Structure-Preserving Algorithms for Ordinary Differential Equations. Springer-Verlag.

[2] Leimkuhler, Ben; Reich, Sebastian (2005). Simulating Hamiltonian Dynamics. Cambridge University Press**.**

[3] Sanz-Serna, J.M.; Bou-Rabee, Nawaf (2018). Geometric Integrators and the Hamiltonian Monte Carlo method. Acta Numerica. https://arxiv.org/pdf/1711.05337.pdf

[4] Sanz-Serna, J.M.; Calvo, Mari Paz (1994). Numerical Hamiltonian problems. Chapman & Hall.

***Registration is free but required before May 17th.** Go to https://bit.ly/2CqcLhJ and fill the form to register**. Student grants will be available until April 15th**. Please, let us know if you need support for travel and accommodation expenses when you fill the form.