Proposal Master/Bachelor Thesis
„Novel trends in Geometric Integration “

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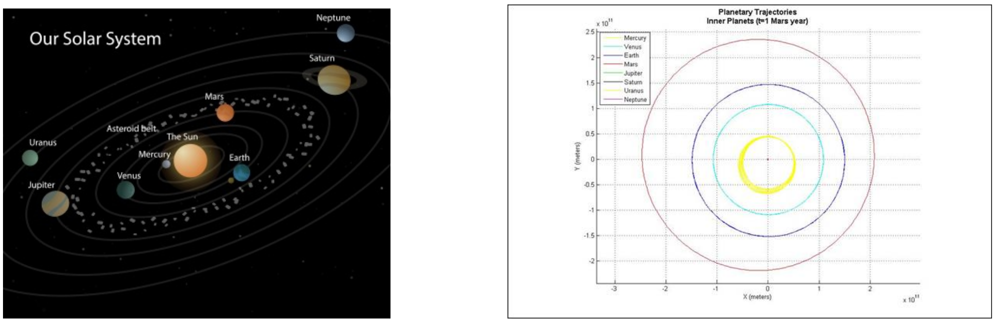
Summary:

The motivation of developing numerical methods which preserve the geometrical properties of the exact flow of a differential equation has been arising together with the developing and maturing the theory of numerical methods for general ordinary differential equations (ODEs). At some point it was realized that the structure preserving methods not only produce an improved qualitative behavior but also provide more accurate long -time integration. Such methods find there application in many types of problems from different areas such as molecular dynamics, mechanics, quantum physics and numerical analysis astronomy and many others.

Currently there have been published a great number of scientific articles representing different approaches to improve already existing methods. Since most of them differ form each other it would be interesting to investigate special properties of those integrators. Students will be offered to compare compare recently issued numerical schemes, find the "golden middle"between the accuracy and the computational effort and possibly to develop a state-of-art integrator.



(a) Solar System (b) Solar System Integration

Figure 1: N-Body Problem

Tasks:

- Geometric numerical integration of the system of ordinary differential equations, namely Hamiltonian equation of motions (programming in Matlab or C)
- **Bachelor:** Compare novel numerical integrators, testing on applications to celestial mechanics or molecular dynamics problems
- **Master:** Using recent developments construct more accurate or more computationally cheap numerical schemes

References:

- E. Hairer, C. Lubich, G. Wanner, Geometric Numerical Integration: Structure-Preserving Algorithms for Ordinary Differential Equations, Springer, Berlin, 2002.
- I.P. Omelyan, I.M. Mryglod, R. Folk, Symplectic analytically integrable decomposition algorithms: classification, derivation, and application to molecular dynamics, quantum and celestial mechanics, Comput. Phys. Commun. 151(2003), pp. 272–314.