This seminar is about simulating dynamical systems, especially conservative systems such as arise in celestial mechanics and molecular models. The time integrator is the core of any dynamical simulation; it replaces a differential equation in continuous time by a difference equation defining approximate snapshots of the solution at discrete timesteps. As computers grow in power, approximate solutions are computed over ever-longer time intervals, and the integrator may be iterated many millions or even billions of times; in such cases, the qualitative properties of the integrator itself can become critical to the success of a simulation. Geometric integrators are methods that exactly (i.e. up to rounding errors) conserve qualitative properties associated to the solutions of the dynamical system under study.

The increase in the use of simulation in applications has mirrored rising interest in the theory of dynamical systems. Many of the recent developments in mathematics have followed from the appreciation of the fundamentally chaotic nature of physical systems, a consequence of nonlinearities present in even the simplest useful models. In a chaotic system the individual trajectories are by definition inherently unpredictable in the exact sense: solutions depend sensitively on the initial data. In some ways, this observation has limited the scope and usefulness of results obtainable from mathematical theory. Most of the common techniques rely on local approximation and perturbation expansions, methods best suited for understanding problems which are almost linear, while the new mathematics that would be needed to answer even the most basic questions regarding chaotic systems is still in its infancy. In the absence of a useful general theoretical method for analyzing complex nonlinear phenomena, simulation is increasingly pushed to the fore. It provides one of the few broadly applicable and practical means of shedding light on the behavior of complex nonlinear systems, and is now a standard tool in everything from materials modeling to bioengineering, from atomic theory to cosmology.

Beginning with the idea of splitting we will see how many simple but effective integrators can be generated by using a few building blocks. The same techniques can be used to derive more sophisticated schemes. For example, explicit higher order methods have a very natural derivation in the case of canonical mechanical systems developed in terms of the kinetic+potential form of the energy. We survey recent work on methods for constrained systems and consider various approaches to the simulation of rigid body systems, methods which offer an efficient and in many cases demonstrably superior geometric alternative to more widespread schemes. Molecular dynamics applications are an important source of challenging problems for geometric integration, so we devote some time to their particular characteristics, as well as drawing on examples from this field for motivation and for evaluation of concepts and methods.
Literature

The seminar topics will mainly be taken from the following textbook:


Other good references on the topic include


First Meeting: Tuesday, 15th October 2019, 11:15, Mathematikon, SR1.

If you have any questions please address them via email to:

r.scheichl@uni-heidelberg.de or a.strehlow@uni-heidelberg.de