Modified differential equations

Ernst HAIRER, Université de Genève
Philippe CHARTIER, INRIA Rennes
Gilles VILMART, INRIA Rennes et Université de Genève

The aim of this talk is to combine the ideas of two well-established topics in *geometric numerical integration* concerning the structure-preserving long-time integration of ordinary differential equations. This will be the basis for the design of new efficient integrators that preserve geometric properties of the exact flow. The two techniques are:

- *Backward error analysis* (e.g., [2, Chap. IX]). The idea is to interpret (on a formal level) the numerical solution for a problem $\dot{y} = f(y)$ as the exact solution of a modified differential equation

$$\dot{y} = f(y) + hf_2(y) + h^2 f_3(y) + h^3 f_4(y) + \dots \ . \tag{1}$$

  Geometric properties of the discrete numerical method are transfered to the vector field of the modified equation (1). For example, symplectic methods give rise to Hamiltonian modified equations.

- *Hamilton–Jacobi theory and generating functions* (e.g., [2, Sect. VI.5]). The exact time t flow $(P, Q) = \varphi_t(p, q)$ of a Hamiltonian system $\dot{p} = -\nabla_q H(p, q)$, $\dot{q} = \nabla_p H(p, q)$ can be computed from the relation

$$P = p - \nabla_q S(t, P, q), \qquad Q = q + \nabla_p S(t, P, q), \tag{2}$$

  where the function $S(t, p, q)$ is a solution of the Hamilton–Jacobi differential equation

$$\frac{\partial S}{\partial t}(t, p, q) = H\Big(p, q + \frac{\partial S}{\partial p}(t, p, q)\Big), \qquad S(0, p, q) = 0 \tag{3}$$

  whose solution can formally be expanded as $S(t, p, q) = tH(p, q) + t^2 S_2(p, q) + t^3 S_3(p, q) + \dots$. If we replace $S(t, p, q)$ by $tH(p, q)$ in the formula (2), we recognize a numerical scheme, namely the symplectic Euler discretization. Consequently, this numerical scheme applied to the Hamiltonian system with Hamiltonian $S(t, p, q)$ yields the exact solution of the original problem.

Both apparently different theoretical tools are special cases of the following more general situation: for two numerical integrators, consider the modified equation (1) such that
the numerical solution of the first method applied to $\dot{y} = f(y)$ gives precisely
the numerical solution of the second method applied to the modified differential equation (1).
In the case of backward error analysis, the second "method" is the exact flow of the original problem; in the case of Hamilton–Jacobi theory, the first "method" is the exact flow of the original problem (in the context of symplectic methods and Hamiltonian systems). All results of backward error analysis can be extended more or less straight-forwardly to this situation (see [1]).

Applying a simple numerical integrator to the truncated modified differential equation (in the sense of Hamilton–Jacobi theory), high order methods are obtained that conserve the geometric properties of the exact flow. As an application we develop new efficient integrators for the simulation of the full dynamics of rigid bodies (see [3]).

References

[1] P. Chartier, E. Hairer, G. Vilmart, *Modified differential equations for pairs of numerical integrators*, Submitted for publication, 2005.

[2] E. Hairer, C. Lubich, G. Wanner, *Geometric Numerical Integration. Structure-Preserving Algorithms for Ordinary Differential Equations*, Second edition, Springer, 2006.

[3] E. Hairer, G. Vilmart, *Preprocessed RATTLE algorithm for the full dynamics of the rigid body*, In preparation, 2006.

Ernst HAIRER – Ernst.Hairer@math.unige.ch
Section de Mathématiques, Université de Genève, 2–4 rue du Lièvre, CH-1211 Genève 4, Switzerland