Recent advances in the numerical solution of Hamiltonian problems

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Abstract

The numerical solution of conservative problems is an active field of investigation dealing with the geometrical properties of the discrete vector field induced by numerical methods. The final goal is to reproduce, in the discrete setting, a number of geometrical properties shared by the original continuous problem. Because of this reason, it has become customary to refer to this field of investigation as geometric integration. In particular, we shall deal with the numerical solution of Hamiltonian problems, which are encountered in many real-life applications, ranging from the nano-scale of molecular dynamics to the macro-scale of celestial mechanics. Such problems are characterized by the conservation of the associated Hamiltonian function. Often, the Hamiltonian is also called the energy, since for isolated mechanical systems it has the physical meaning of total energy. Consequently, energy conservation is an important feature in the correct simulation of such problems. In this talk we review the main facts about the recently introduced family of energy-conserving Runge-Kutta-type methods named Hamiltonian Boundary Value Methods (HBVMs), and sketch their application to both Hamiltonian ODE and PDE problems.

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