Computations with Formal Lie Series and Symplectic Integration

Nickolay Vassiliev, Steklov Mathematical Institute at St.Petersburg
Russian Academy of Sciences
e-mail: vasiliev@pdmi.ras.ru

April 23, 2003

We consider different applications of symbolic computations with formal Lie series. The first example is symplectic integration. Construction of most known symplectic methods, like the Yoshida method, is based on iterating the process of superpositions of Lie transformations. We show how to construct implicit symplectic methods for numerical integration of a hamiltonian ODE if the hamiltonian does not have the form $H(P,Q) = U(P) + V(Q)$. Another problem which is also connected with application of symplectic methods is computation of the perturbation of the hamiltonian due to the concrete symplectic method for numerical integration. Usually formulas for such perturbations are given only for the next order relative to the order of the integrator. But, if we need to develop the difference of modeled solutions from real ones with high accuracy, we have to use the terms of highest orders in the perturbed hamiltonian. It is impossible to get such exact formulas in highest orders on the basis of the Baker-Hausdorf formula, because of computational complexity. Nevertheless using Lie transformations we can construct an iterative procedure to get the perturbed hamiltonian with high accuracy.

Another theme is the nonconservative effects of modeling of hamiltonian dynamical systems via orthodox methods. We show how the nonsymplectic methods of integration globally disturb the topology of the phase space. Some results about modeling the Henon-Heyles system via symplectic and nonsymplectic methods are presented. Application of the Lie transformations technique to normalization of ODE's is also discussed.

We also discuss some algorithms for processing with formal Lie series, the problem of computer construction of special bases in free Lie algebra, and methods for representation of Lie series which allow effective realization of such algorithms.