A TECHNIQUE OF CONSTRUCTING EXPLICIT-IMPLICIT SIMPLECTIC NUMERICAL SCHEMES FOR SOLVING OF HAMILTON SYSTEM OF EQUATIONS

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Actively used in various fields of science and technologies for complex systems simulations molecular dynamics methods are based on an every time step solution of the Hamilton system of equations. Requirements to be more realistic for simulations leads to order increasing for the system of molecular dynamics equations. Efficiency enhancement of numerical methods at every time step could bring important improvement of numerical simulation economy. In our work, self-consistent technique of constructing explicit-implicit simplectic numerical schemes of arbitrary approximation order for solving of molecular dynamics equations in Hamilton form is proposed. It based on using of generating function and Taylor expansion of approximate solution. Computational experiments show both numerical efficiency and geometric properties conservation with necessary accuracy of initial Hamilton system.