# THE SPLIT INTEGRATION SYMPLECTIC METHOD

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**Abstract:** The split integration symplectic method (SISM) for Hamiltonian systems based on factorization of the Liouville propagator is presented.

**Key Words:** Hamiltonian System, Symplectic Integration Methods.

## INTRODUCTION

Hamiltonian systems posses a unique property, symplecticness, which is the preservation of an oriented area in the one-degree-of-freedom example. Symplectic integration methods retain this property.
Here we describe the SISM, a technique derived in terms of the Lie algebraic theory, which uses an analytical treatment of high-frequency motions within a second order generalized leapfrog scheme.

## METHOD

The explicit symplectic integrator can be derived in terms of the Lie algebra approach in which the Hamilton equation is written in the form

$$\frac{d\vec{x}}{dt} = \{\vec{x}, H\} = \hat{L}_H \vec{x}$$

where $\{\vec{x}, H\}$ denotes the Poisson bracket, $\hat{L}_H$ is the Poisson bracket operator, and $\vec{x} = (\vec{q}, \vec{p})$ is a vector of the coordinates and momenta of all particles.
The Hamiltonian $H$ is split as

$$H = H_0 + H_r$$

where $H_0$ is the pure harmonic part and $H_r$ is the remaining part. This splitting, incorporated in the second order generalized leapfrog scheme, gives the following approximation for the solution operator of the Hamiltonian system

$$\vec{x}|_{t_0+\Delta t} \approx \exp\left(\tfrac{\Delta t}{2}\hat{L}_{H_0}\right)\exp\left(\Delta t\hat{L}_{H_r}\right)\exp\left(\tfrac{\Delta t}{2}\hat{L}_{H_0}\right)\vec{x}|_{t_0}$$

which prescribes how to propagate from one point in the phase space to another. The system is first propagated by $H_0$ for a half integration step, then for a whole step by $H_1$, and finally for another half step by $H_0$. This integration scheme was employed in the development of the SISM, a second order symplectic

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integration algorithm for Hamiltonian systems [1, 2].
Knowing $H_0$, which represents the dynamically leading contribution, we treat the high-frequency terms analytically, i.e., independently of the size of the integration step. The whole integration step thus combines the analytical evolution of the harmonic part of the Hamiltonian with a correction arising from the remaining part performed by numerical integration.

## RESULTS AND DISCUSSION

The SISM described above was evaluated on simple systems of the pendulum, Duffing equation (weakly nonlinear oscillator), and Hénon-Heiles Hamiltonians. In order to compare the efficiency of the SISM with the standard second order symplectic leapfrog-Verlet method (LFV), we compared computational performances for the same level of accuracy. To study the error accumulation and numerical stability, we monitored the error in total energy [1, 2]. The results using two different methods (LFV and SISM) are presented in Fig.1. It can be seen that the SISM can use a much larger time step than the LFV for the same level of accuracy and computational complexity.

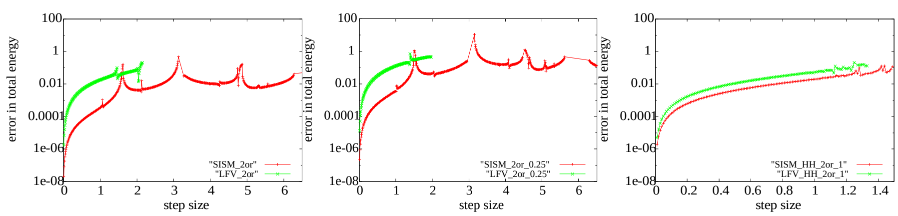


Fig.1. Error in total energy for the LFV and SISM of systems of the pendulum, Duffing equation (weakly nonlinear oscillator), and Hénon-Heiles Hamiltonians.

The SISM, which uses an analytical treatment of high-frequency motions representing the main restriction on step size, is up to an order of magnitude faster than the commonly used LFV algorithm.

## REFERENCES

1. Janežič, D. and Merzel, F. An efficient symplectic integration algorithm for molecular dynamics simulations. **J. Chem. Inf. Comput. Sci.** 35 (1995) 321-326.
2. Janežič, D. and Praprotnik, M. Symplectic molecular dynamics integration using normal mode analysis. **Int. J. Quantum Chem.** 84 (2001) 2-12.