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Tuning Symplectic Integrators is Easy and Worthwhile

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Abstract. Many applications in computational physics that use numerical integrators based on splitting and composition can benefit from the development of optimized algorithms and from choosing the best ordering of terms. The cost in programming and execution time is minimal, while the performance improvements can be large. In this note we report the influence of term ordering for random systems and for two systems from celestial mechanics that describe particle paths near black holes, quantifying its significance for both optimized and unoptimized methods. We also present a method for the computation of solutions of integrable monomial Hamiltonians that minimizes roundoff error and allows the effective use of compensation summation.

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1 Introduction

Symplectic numerical integration by splitting the Hamiltonian and composing the flows of the associated vector fields has become an extremely widely used technique in computational science, especially computational physics and chemistry. A splitting into two parts, $H = H_1 + H_2$, together with the 3-term composition

$$\mathrm{e}^{\frac{1}{2}hX_1}\mathrm{e}^{hX_2}\mathrm{e}^{\frac{1}{2}hX_1},$$

is the most common and is often all that is needed. It is variously called the leapfrog, Störmer–Verlet, or Strang splitting method. (Here X_i is the Hamiltonian vector field associated with Hamiltonian H_i, e^{hX} is the time-h flow of the vector field X, and h is the time step.) For example, it is the basic building block of the Hamiltonian Monte Carlo method (see [6] for refinements).

Some Hamiltonians can only be written as the sum of more than two explicitly integrable terms, say $H = \sum_{i=1}^{n} H_i$. In addition, some applications need order higher than two

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to achieve the required accuracy for a given amount of computational effort. Methods of all orders exist, but are progressively more expensive. Optimized methods have been develop that can significantly reduce discretization errors at fixed cost [4].

However, an informal survey of the current literature suggests that unoptimized composition methods of order 4, 6, and 8 [43] are in common use in cosmology, celestial mechanics, quantum mechanics, quantum statistical mechanics, solid state physics, kinetic theory, plasma physics, molecular dynamics, optics, neural networks, and fluid mechanics [2,7–9,11–13,15,16,19–22,25,28,30–32,34,36–39,41,42]. Computations in these fields could benefit from experience gained in numerical analysis to reduce errors and error growth at little cost either in programming or execution time.

In this note we consider four such techniques: optimized composition coefficients; the effect of term ordering; compensated summation to reduce round-off error; and methods with processing. We report the influence of term ordering for random systems and for two systems from celestial mechanics that describe particle paths near black holes, confirming and quantifying its significance in both cases for both optimized and unoptimized methods. We also present a method for the computation of solutions of integrable monomial Hamiltonians that minimizes roundoff error and allows the effective use of compensation summation.

2 Optimized methods for multi-term splittings

Let the vector field $X=\sum_{i=1}^{n} X_i$ be split into n parts, each explicitly integrable and let

$$\chi_h = \mathrm{e}^{hX_n}\circ\cdots\circ\mathrm{e}^{hX_1}$$

be a first-order integrator for X. We define the adjoint χ_h^* of χ_h by $\chi_h^*=(\chi^{-1})_{-h}$; that is,

$$\chi_h^* = \mathrm{e}^{hX_1}\circ\cdots\circ\mathrm{e}^{hX_n}.$$

Let

$$\psi_h(\alpha) = \chi_{\alpha_s h}\circ\chi^*_{\alpha_{(s-1)}h}\circ\cdots\circ\chi_{\alpha_2 h}\circ\chi^*_{\alpha_1 h}. \tag{2.1}$$

The second-order leapfrog method is $S_{2,h}=\psi_h(\frac{1}{2},\frac{1}{2})$. Note that when $n=2$, this reduces to a composition that alternates steps of X_1 and X_2. Methods of this type designed for $n=2$ and for arbitrary n have the same order [23], although the optimal coefficients may not be the same. Nevertheless, coefficients optimised for the method (2.1) can reduce the error significantly.

In particular, the minimal-s methods formed by recursively increasing the order from k to $k+2$ by $S_{k,ch}\circ S_{k,(1-2c)h}\circ S_{k,ch}$ with $c=1/(2-2^{1/(2k+1)})$ have very large error constants and poor stability and should be avoided. The 3-stage method with $k=2$, called $\mathrm{S}_3 4$, will be used as a reference method here. (The notation indicates that it has order 4 and uses work equivalent to 3 leapfrog steps.) Its large substeps, $1.35h$, $-1.70h$, and $1.35h$, contribute to its large error constants and poor stability.