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Improving the accuracy of the AVF method

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ABSTRACT

The average vector field (AVF) method is a *B*-series scheme of the second order. As a discrete gradient method, it preserves exactly the energy integral for any canonical Hamiltonian system. We present and discuss two locally exact and energy-preserving modifications of the AVF method: AVF–LEX (of the third order) and AVF–SLEX (of the fourth order). Applications to spherically symmetric potentials are given, including a compact explicit expression for the AVF scheme for the Coulomb–Kepler problem.

1. Introduction

Discrete gradient methods were developed many years ago for molecular dynamics simulations [1]. They preserve exactly the energy integral, which is of considerable advantage [2]. More recently, discrete gradient methods have been essentially developed by McLachlan, Quispel and their collaborators [3–5]. In particular, discrete gradient schemes preserving any first integrals for any ordinary differential equations were constructed [6].

A discrete gradient is a function of two vector variables $(\boldsymbol{y}_n, \boldsymbol{y}_{n+1})$ and has to satisfy (see [3])

$$\begin{aligned} &\bar{\nabla} H(\boldsymbol{y}_n, \boldsymbol{y}_{n+1}) \cdot (\boldsymbol{y}_{n+1} - \boldsymbol{y}_n) = H(\boldsymbol{y}_{n+1}) - H(\boldsymbol{y}_n) \\ &\bar{\nabla} H(\boldsymbol{y}_n, \boldsymbol{y}_{n+1}) \to \nabla H(\boldsymbol{y}) \quad \text{for } \boldsymbol{y}_n \to \boldsymbol{y}, \end{aligned} \tag{1.1}$$

where H is a function of $\boldsymbol{y}$ (we will confine ourselves to a particular case where H is a Hamiltonian). We will consider only symmetric discrete gradients, i.e., such that $\bar{\nabla} H(\boldsymbol{y}_n, \boldsymbol{y}_{n+1}) = \bar{\nabla} H(\boldsymbol{y}_{n+1}, \boldsymbol{y}_n)$. Discrete gradients are highly non-unique. An important special case of the average vector field discrete gradient (AVF) was introduced in [3]. Later, the AVF scheme was identified as a *B*-series method [5], which prompted intensive studies on energy-preserving *B*-series methods [7–9].

In this paper we derive simple explicit formulas for the AVF discrete gradient for two important cases: the Coulomb–Kepler problem and a three-dimensional anharmonic oscillator; see Section 2. We also propose two "locally exact" modifications of the AVF method: AVF–LEX and AVF–SLEX. They preserve the energy integral and have much higher accuracy than the original AVF scheme. Although such modifications can be constructed for any Hamiltonian and any discrete gradient (see [10]), in this paper we focus on discrete gradient schemes for Hamiltonians of the form $H = \frac{1}{2}\boldsymbol{p}^2 + V(\boldsymbol{x})$; see Section 4. More general results can be found in Section 5.

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A numerical scheme for solving an ordinary differential equation $\dot{\boldsymbol{y}} = F(\boldsymbol{y})$ is *locally exact* if there exists a sequence $(\bar{\boldsymbol{y}}_n)$ such that the linearization of the scheme around $\bar{\boldsymbol{y}}_n$ is identical with the exact discretization of the differential equation linearized around $\bar{\boldsymbol{y}}_n$; see [11,12]. In this paper we consider two kinds of locally exact modifications: $\bar{\boldsymbol{y}}_n = \boldsymbol{y}_n$ (LEX) and $\bar{\boldsymbol{y}}_n = \frac{1}{2}(\boldsymbol{y}_n + \boldsymbol{y}_{n+1})$ (SLEX). Our approach consists in considering a class of non-standard modifications of a numerical scheme (compare [13]) parameterized by some functions (e.g., matrices denoted by $\boldsymbol{\delta}_n$). Requiring local exactness, we can determine these functions (another possibility is proposed in [12,14]). We point out that any linear ordinary differential equation with constant coefficients admits the exact discretization in an explicit form; see [15,16,13,17]. The exact discretization of linearized equations is known as the exponential Euler method [18]. A similar notion (preservation of the linearization at all fixed points) appeared in [4]; see also [19].

Locally exact modifications of the discrete gradient method for Hamiltonian systems were studied in [11,20,10,21,12]. Discrete gradient schemes were modified without changing their most important property: the exact conservation of the energy integral. Locally exact modifications improve the accuracy (especially in the neighbourhood of a stable equilibrium) although their order is not always higher. In the case of one degree of freedom the symmetric discrete gradient scheme (of second order) has locally exact modifications of third (LEX) and fourth (SLEX) order, respectively [21,12]. In the multidimensional case the order is usually unchanged; see [20]. The AVF method turns out to be an exception: locally exact modifications, AVF–LEX and AVF–SLEX, are of third and fourth order, respectively. Numerical experiments confirm the advantages of the proposed modifications; see Section 6. Locally exact modifications increase the accuracy by several orders of magnitude.

2. The average vector field method

We consider a Hamiltonian system of the form

$$\dot{\boldsymbol{y}} = F(\boldsymbol{y}), \qquad F(\boldsymbol{y}) = S\nabla H, \quad S = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix} \tag{2.1}$$

where $\boldsymbol{y} \in \mathbb{R}^{2m}$, $H = H(\boldsymbol{y})$ is a Hamiltonian, and I is an $m \times m$ unit matrix. The average vector field method is defined by

$$\frac{\boldsymbol{y}_{n+1} - \boldsymbol{y}_n}{h_n} = \int_0^1 F(\boldsymbol{y}_n + \xi\,\Delta\boldsymbol{y}_n)d\xi, \tag{2.2}$$

where h_n is a variable time step and $\Delta\boldsymbol{y}_n := \boldsymbol{y}_{n+1} - \boldsymbol{y}_n$. The AVF method exactly preserves the energy integral H, is a symmetric B-series method of the second order, and is affine-covariant and self-adjoint [7].

We denote $\boldsymbol{y} = (\boldsymbol{x}, \boldsymbol{p}) = (x^1, \ldots, x^m, p^1, \ldots, p^m)$. In this paper we often confine ourselves to the case

$$H = \frac{1}{2}\boldsymbol{p}^2 + V(\boldsymbol{x}). \tag{2.3}$$

Then

$$F(\boldsymbol{y}) = \begin{pmatrix} \boldsymbol{p} \\ -V_{\boldsymbol{x}} \end{pmatrix} \equiv \left(p^1, \ldots, p^m, -\frac{\partial V}{\partial x^1}, \ldots, -\frac{\partial V}{\partial x^m} \right)^T \tag{2.4}$$

and the AVF method (2.2) can be rewritten as

$$\frac{\boldsymbol{x}_{n+1} - \boldsymbol{x}_n}{h_n} = \frac{\boldsymbol{p}_n + \boldsymbol{p}_{n+1}}{2}, \qquad \frac{\boldsymbol{p}_{n+1} - \boldsymbol{p}_n}{h_n} = \int_0^1 \boldsymbol{f}(\boldsymbol{x}_n + \xi\,\Delta\boldsymbol{x}_n)d\xi, \tag{2.5}$$

where $\boldsymbol{f}(\boldsymbol{x}) := -V_{\boldsymbol{x}}(\boldsymbol{x})$ and $\Delta\boldsymbol{x}_n := \boldsymbol{x}_{n+1} - \boldsymbol{x}_n$. Therefore, it is natural to define the AVF discrete gradient as

$$\bar{\nabla}^{\mathrm{AVF}} V \equiv \bar{\nabla}^{\mathrm{AVF}} V(\boldsymbol{x}_n, \boldsymbol{x}_{n+1}) := -\int_0^1 \boldsymbol{f}(\boldsymbol{x}_n + \xi\,\Delta\boldsymbol{x}_n)d\xi. \tag{2.6}$$

In some special cases the integral defining the AVF discrete gradient can be explicitly calculated. We will consider the important case of a spherically symmetric anharmonic oscillator and the Coulomb–Kepler potential.

Lemma 2.1. *The AVF discrete gradient for an anharmonic oscillator potential $V(r) = \alpha r^2 - \beta r^4$ (where $r = |\boldsymbol{x}|$) can be explicitly computed by using the Simpson rule:*

$$\bar{\nabla}^{\mathrm{AVF}} V = -\frac{1}{6}\left(\boldsymbol{f}(\boldsymbol{x}_n) + 4\boldsymbol{f}\left(\frac{\boldsymbol{x}_n + \boldsymbol{x}_{n+1}}{2} \right) + \boldsymbol{f}(\boldsymbol{x}_{n+1}) \right) \tag{2.7}$$

where $\boldsymbol{f}(\boldsymbol{x}) = -V_{\boldsymbol{x}}(\boldsymbol{x})$.