# Improving the accuracy of the discrete gradient method in the one-dimensional case

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We present two numerical schemes of high accuracy for one-dimensional dynamical systems. They are modifications of the discrete gradient method and keep its advantages, including stability and conservation of the energy integral. However, their accuracy is higher by several orders of magnitude.

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## I. INTRODUCTION

Discrete gradient methods were introduced many years ago in order to integrate numerically $N$-body systems of classical mechanics with possible applications in molecular dynamics and celestial mechanics [1] (see also [2]). In the present paper, we propose another numerical integrators (the so-called locally exact discrete gradient methods). The main idea of our approach consists in modifying a given numerical integrator (e.g., by replacing the time step $\varepsilon$ by some function depending on $\varepsilon$ and independent variables) in order to obtain a "locally exact" integrator (for instance, an integrator, which is locally equivalent to the exact discrete harmonic oscillator). The crucial point is to preserve "good" properties of the considered numerical scheme. In the case of the discrete gradient method, the locally exact modifications presented in this paper exactly preserve the energy integral. As a result, our methods inherit the excellent stability and the very good qualitative behavior of the discrete gradient method and, in the same time, are much more accurate.

In this paper, we confine ourselves to the one-dimensional case,

$$\dot{p} = -V'(x), \quad \dot{x} = p, \tag{1}$$

where $V(x)$ is a potential, and the dot and the prime denote differentiation with respect to $t$ and $x$, respectively. In this case, discrete gradient methods reduce to the so-called modified midpoint rule,

$$\frac{x_{n+1}-x_n}{\varepsilon} = \frac{1}{2}(p_{n+1}+p_n),$$

$$\frac{p_{n+1}-p_n}{\varepsilon} = -\frac{V(x_{n+1})-V(x_n)}{x_{n+1}-x_n}, \tag{2}$$

where $\varepsilon$ is the time step. One can easily prove that the total energy is preserved by this scheme,

$$\frac{1}{2}p_n^2 + V(x_n) = E = \text{const}. \tag{3}$$

The modified midpoint rule has been extended, in a natural way, on the three-dimensional case and on systems of particles, exactly preserving the total energy, the total linear momentum, and the total angular momentum of the system [1].

More recently, discrete gradient methods have been extended and developed in the context of geometric numerical integration [3] (see [4,5]). In particular, Quispel and coworkers constructed numerical integrators preserving integrals of motion of a given system of ordinary differential equations [6–8]. Similar ideas were applied in molecular-dynamics simulations of spin liquids [9].

In general, geometric numerical integrators are very good in preserving qualitative features of simulated differential equations, but it is not easy to enhance their accuracy. Symplectic algorithms can be improved using appropriate splitting methods [10–13]. Our research is concentrated on improving the efficiency of the discrete gradient method (which is not symplectic) without losing its outstanding qualitative advantages.

## II. MODIFIED DISCRETE GRADIENT SCHEME

In a recent paper, we compared several discretizations of the simple pendulum equation $[V(x)=-\cos x]$ with a special stress on the long-time behavior [14]. The discrete gradient scheme was among the best ones, especially when large energies (rotational motion) and the neighborhood of the separatrix were concerned. In the paper [14], we proposed a modification of the discrete gradient scheme (2). Assuming the stable equilibrium at $x=0$, we replaced $\varepsilon$ by the function $\delta_0=\delta_0(\varepsilon)$

$$\delta_0 = \frac{2}{\omega_0}\tan\frac{\omega_0\varepsilon}{2}, \tag{4}$$

where $\omega_0=\sqrt{V''(0)}$ (we point out, however, that the time step of the obtained numerical scheme is given still by $\varepsilon$). The motivation was to preserve (almost exactly) small oscillations around $x=0$, when the pendulum can be treated as a harmonic oscillator. The classical harmonic oscillator admits

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the so-called *exact* discretization (compare [15–17]; for more details, see the next section). The exact discretization of the harmonic-oscillator equation has been recently used to derive an orbit-preserving discretization of the classical Kepler problem [18]. The modified discrete gradient scheme, obtained in the paper [14], is quite satisfying: in the case of small oscillations, this method is better by 4 orders of magnitude than all other considered schemes (including the discrete gradient method). In the case of other initial conditions, the method is comparable with the discrete gradient method (by the way: both methods are of second order).

The modified discrete gradient scheme of [14] appeared independently, had a physical motivation (the harmonic oscillator), and was not influenced by existing numerical approaches. Now, after studying related literature, we see that analogical (or even identical) modifications could be achieved in the framework of at least three approaches: nonstandard finite difference schemes of Mickens [19,20], Gautschi's trigonometric methods [2,21], and exponential integrators [22]. However, according to our best knowledge, the discrete gradient method has never been treated or modified in the framework of these approaches. Our modifications resemble the Mickens approach because the time step $\varepsilon$ is replaced by some function $\delta(\varepsilon)$, but this replacement is a consequence of different principles than those used by Mickens.

## III. LOCALLY EXACT DISCRETE GRADIENT SCHEME AND ITS SYMMETRIC MODIFICATION

As the main result of this paper, we propose another (more powerful) modification of the discrete gradient scheme, namely, the *locally exact discrete gradient method*,

$$\frac{x_{n+1}-x_n}{\delta_n}=\frac{1}{2}(p_{n+1}+p_n),$$

$$\frac{p_{n+1}-p_n}{\delta_n}=-\frac{V(x_{n+1})-V(x_n)}{x_{n+1}-x_n}, \tag{5}$$

where $\delta_n$ is a function defined by

$$\delta_n=\frac{2}{\omega_n}\tan\frac{\varepsilon\omega_n}{2}, \quad [\text{if } V''(x_n)>0],$$

$$\delta_n=\varepsilon, \quad [\text{if } V''(x_n)=0],$$

$$\delta_n=\frac{2}{\omega_n}\tanh\frac{\varepsilon\omega_n}{2}, \quad [\text{if } V''(x_n)<0], \tag{6}$$

$\varepsilon$ denotes the time step, and, finally,

$$\omega_n=\sqrt{|V''(x_n)|}. \tag{7}$$

The first of formulas (6) imposes a restriction on the time step, namely, $\varepsilon\omega_n<\pi$. This condition is not very restrictive. For instance, in the simple pendulum case, we have $\omega_n\le\omega_0$, and, therefore it is sufficient to take $\varepsilon<\frac{1}{2}T_0$ (where $T_0$ is the period of small oscillations around the stable equilibrium).

In order to derive the locally exact numerical scheme (5), we recall that the classical harmonic oscillator driven by a constant force admits the exact discretization (like all linear ordinary differential equations, compare [15,16]). Namely, the system

$$\ddot{\xi}+\omega^2\xi=a, \quad \dot{\xi}=p, \tag{8}$$

where $\omega>0$ and $a$ are constant, admits the following exact discretization:

$$\xi_{n+1}-2\xi_n\cos\omega\varepsilon+\xi_{n-1}=\left(\frac{2}{\omega}\sin\frac{\omega\varepsilon}{2}\right)^2 a,$$

$$p_n=\frac{\omega}{\sin\omega\varepsilon}(\xi_{n+1}-\xi_n\cos\omega\varepsilon)-\frac{a}{\omega}\tan\frac{\omega\varepsilon}{2}, \tag{9}$$

which may be rewritten in the form of the first-order scheme,

$$\xi_{n+1}=\xi_n\cos\omega\varepsilon+\frac{\sin\omega\varepsilon}{\omega}p_n+\frac{2a}{\omega^2}\left(\sin\frac{\omega\varepsilon}{2}\right)^2,$$

$$p_{n+1}=p_n\cos\omega\varepsilon-\xi_n\omega\sin\omega\varepsilon+\frac{a}{\omega}\sin\omega\varepsilon. \tag{10}$$

The discretization (10) is called *exact* because $\xi_n=\xi(n\varepsilon)$, $p_n=p(n\varepsilon)$, where $\xi(t)$, $p(t)$ solve the system (8) [in particular, $\xi_0=\xi(0)$, $p_0=p(0)$]. The case $\omega^2\le 0$ can be treated in an analogous way (e.g., for $\omega^2<0$, we can formally put $\omega=i\sqrt{|\omega^2|}$ obtaining hyperbolic functions).

The numerical scheme (5) can be derived as follows. First, we replace $\varepsilon$, appearing in formulas (2), by a variable $\delta_n$ depending not only on $\varepsilon$ but also on $x_n$. Similar replacements, $\varepsilon\to\delta(\varepsilon)$, are characteristic for the so-called nonstandard finite difference schemes [20], but here we allow also a dependence on $x_n$. Then, we compute the form of the function $\delta_n$ requiring that the modified scheme (5) is *locally exact*. By local exactness, we mean that the linearization of the scheme (5) around $x_n$, i.e.,

$$\frac{x_{n+1}-x_n}{\delta_n}=\frac{1}{2}(p_{n+1}+p_n),$$

$$\frac{p_{n+1}-p_n}{\delta_n}=-V'(x_n)-\frac{1}{2}(x_{n+1}-x_n)V''(x_n), \tag{11}$$

coincides with the *exact discretization* of the linearization of the considered system (1) around $x_n$. This linearization is given by

$$\frac{dp}{dt}=-V'(x_n)-V''(x_n)\xi, \quad \frac{d\xi}{dt}=p, \tag{12}$$

where $\xi=x-x_n$ and $x_n$ is fixed (i.e., it is treated as a constant). Comparing Eq. (12) with Eq. (8), we obtain

$$\omega^2=V''(x_n), \quad a=-V'(x_n). \tag{13}$$

Moreover, $\xi_n=x_n-x_n=0$ and $\xi_{n+1}=x_{n+1}-x_n$. To fix an attention, we confine ourselves to the case $\omega^2>0$. Then Eqs. (10) assume the form

$$x_{n+1} = x_n + \frac{\sin \omega\varepsilon}{\omega} p_n + \frac{2a}{\omega^2}\left(\sin\frac{\omega\varepsilon}{2}\right)^2,$$

$$p_{n+1} = p_n \cos \omega\varepsilon + \frac{a}{\omega}\sin \omega\varepsilon. \tag{14}$$

Therefore, the exact discretization of Eq. (12) is given by Eqs. (14) with $\omega$ and $a$ defined by Eq. (13). In order to compare Eqs. (11) with Eqs. (13) and (14), we rewrite Eqs. (11) as follows:

$$x_{n+1} = x_n + \frac{\delta_n p_n}{1 + \frac{1}{4}\delta_n^2 V''(x_n)} - \frac{\frac{1}{2}\delta_n^2 V'(x_n)}{1 + \frac{1}{4}\delta_n^2 V''(x_n)},$$

$$p_{n+1} = \frac{1 - \frac{1}{4}\delta_n^2 V''(x_n)}{1 + \frac{1}{4}\delta_n^2 V''(x_n)} p_n - \frac{\delta_n V'(x_n)}{1 + \frac{1}{4}\delta_n^2 V''(x_n)}. \tag{15}$$

Now, we compare Eqs. (15) with Eqs. (13) and (14). Looking at the last terms, we immediately get $\delta_n = \frac{2}{\omega}\tan\frac{\varepsilon\omega}{2}$. Hence, $\delta_n^2 V''(x_n) = 4\tan^2\frac{\varepsilon\omega}{2}$ and one can easily check that Eqs. (15) coincide with Eqs. (14). Thus, we derived the first equation of Eqs. (6). The remaining subcases of Eqs. (6) can be derived in a similar way.

We point out that $\delta_n$ is a function which is almost constant, $\delta_n = \varepsilon + O(\varepsilon^3)$, but we are going to show that these very small variations have surprisingly strong positive influence on the accuracy of the obtained numerical scheme.

The replacement $\varepsilon \to \delta_n$ works very well for the first-order systems (5). However, if we try to replace $\varepsilon$ by $\delta_n$ in the second-order discrete equation for $x_n$ [see Eq. (46) in the paper [14]], then we get a difference scheme which is only a little bit better than the scheme with constant $\delta = \delta_0$ and is much worse than the numerical scheme (5). We point out that the second-order consequence of Eqs. (5) is

$$\frac{x_{n+1} - x_n}{\delta_n} - \frac{x_n - x_{n-1}}{\delta_{n-1}} = -\frac{\delta_n}{2}\left(\frac{V_{n+1} - V_n}{x_{n+1} - x_n}\right) - \frac{\delta_{n-1}}{2}\left(\frac{V_n - V_{n-1}}{x_n - x_{n-1}}\right), \tag{16}$$

where $V_n := V(x_n)$. Equation (16) contains both $\delta_n$ and $\delta_{n-1}$. Thus, it cannot be obtained from Eq. (46) by the simple replacement $\varepsilon \to \delta_n$. However, for $\varepsilon \approx 0$, we have $\delta_n \approx \delta_{n-1} \approx \varepsilon$ and, in this limit, Eq. (16) coincides with Eq. (46) from [14].

The system (1) is obviously symmetric (time reversible), while its locally exact discretization (5) are not time reversible. Changing a little bit the definition of $\omega_n$, namely,

$$\omega_n = \sqrt{\left|V''\left(\frac{x_n + x_{n+1}}{2}\right)\right|}, \tag{17}$$

we get another integrator, which is time reversible. In what follows, this integrator [defined by Eqs. (5), (6), and (17)] will be referred to as the *symmetric modification* of the locally exact discrete gradient scheme.

## IV. ORDER OF THE CONSIDERED DISCRETE GRADIENT METHODS

The order of a numerical scheme is $N$ if $|\vec{x}_{n+1} - \vec{x}(t+\varepsilon)| = O(\varepsilon^{N+1})$ provided that $\vec{x}_n = \vec{x}(t)$, where $\vec{x} = \vec{x}(t)$ is an exact solution and, in our case, $\vec{x} = (x, p)$.

The system (5) (where $x_n \equiv x$ and $p_n \equiv p$ are given and $\delta_n \equiv \delta$ is a small parameter) implicitly defines $x_{n+1}$ and $p_{n+1}$. Therefore, using implicit differentiation, we can write down the corresponding Taylor series,

$$x_{n+1} = x + p\delta - \frac{1}{2}V'\delta^2 - \frac{1}{4}pV''\delta^3 + \frac{1}{24}(3V'V'' - 2p^2V''')\delta^4 + O(\delta^5),$$

$$p_{n+1} = p - V'\delta - \frac{1}{2}pV''\delta^2 + \frac{1}{12}(3V'V'' - 2V'''p^2)\delta^3 - \frac{1}{24}[4pV'V''' + 3p(V'')^2 - p^3V^{(4)}]\delta^4 + O(\delta^5). \tag{18}$$

Then, we use Eq. (1) in order to expand $x(t+\varepsilon)$ and $p(t+\varepsilon)$,

$$x(t+\varepsilon) = x + p\varepsilon - \frac{1}{2}V'\varepsilon^2 - \frac{1}{6}pV''\varepsilon^3 + \frac{1}{24}(V'V'' - V'''p^2)\varepsilon^4 + O(\varepsilon^5),$$

$$p(t+\varepsilon) = p - V'\varepsilon - \frac{1}{2}pV''\varepsilon^2 + \frac{1}{6}(V'V'' - V'''p^2)\varepsilon^3 + \frac{1}{24}[3pV'V''' + p(V'')^2 - p^3V^{(4)}]\varepsilon^4 + O(\varepsilon^5). \tag{19}$$

The last step is to substitute an appropriate expression for $\delta = \delta(\varepsilon)$ into Eqs. (18) and to compare the obtained $\varepsilon$ series with Eqs. (19).

The conventional discrete gradient method corresponds to $\delta(\varepsilon) = \varepsilon$. In this case,

$$x_{n+1} - x(t+\varepsilon) = -\frac{1}{12}pV''\varepsilon^3 + O(\varepsilon^4),$$

$$p_{n+1} - p(t+\varepsilon) = \frac{1}{12}V'V''\varepsilon^3 + O(\varepsilon^4). \tag{20}$$

Therefore, the discrete gradient method is of the second order for $V'' \neq 0$ (and for $V$ linear in $x$, one can easily check that the discrete gradient method is exact, i.e., its order is infinite).

The Taylor series of $\delta_n$ defined by Eqs. (6) is given by the following single expression:

$$\delta(\varepsilon) = \varepsilon + \frac{1}{12}V''\varepsilon^3 + \frac{1}{120}(V'')^2\varepsilon^5 + O(\varepsilon^7), \tag{21}$$

and then Eqs. (18) expand with respect to $\varepsilon$ as follows:

$$x_{n+1} = x + p\varepsilon - \frac{1}{2}V'\varepsilon^2 - \frac{1}{6}pV''\varepsilon^3 + \frac{1}{24}(V'V'' - 2p^2V''')\varepsilon^4 + O(\varepsilon^5),$$

$$p_{n+1} = p - V'\varepsilon - \frac{1}{2}pV''\varepsilon^2 + \frac{1}{6}(V'V'' - V'''p^2)\varepsilon^3 + \frac{1}{24}[4pV'V''' + p(V'')^2 - p^3V^{(4)}]\varepsilon^4 + O(\varepsilon^5). \tag{22}$$

Therefore,

$$x_{n+1} - x(t+\varepsilon) = -\frac{1}{24}p^2V'''\varepsilon^4 + O(\varepsilon^5),$$

$$p_{n+1} - p(t+\varepsilon) = \frac{1}{24}pV'V'''\varepsilon^4 + O(\varepsilon^5). \tag{23}$$

and we conclude that the locally exact dicrete gradient method is of the third order.

In case of the modified discrete gradient scheme $\delta = \delta_0$ [see Eq. (4)] and then

$$\delta(\varepsilon) = \varepsilon + \frac{1}{12}V_0''\varepsilon^3 + \frac{1}{120}(V_0'')^2\varepsilon^5 + O(\varepsilon^7), \tag{24}$$

where $V_0'' \equiv V''(0)$. In this case, Eqs. (18) become

$$x_{n+1} = x + p\varepsilon - \frac{1}{2}V'\varepsilon^2 - \frac{1}{12}p(3V'' - V_0'')\varepsilon^3 + O(\varepsilon^4),$$

$$p_{n+1} = p - V'\varepsilon - \frac{1}{2}pV''\varepsilon^2 + \frac{1}{12}(3V'V'' - V'V_0'' - 2V'''p^2)\varepsilon^3 + O(\varepsilon^4), \tag{25}$$

and, finally,

$$x_{n+1} - x(t+\varepsilon) = \frac{1}{12}p(V_0'' - V'')\varepsilon^3 + O(\varepsilon^4),$$

$$p_{n+1} - p(t+\varepsilon) = \frac{1}{12}V'(V'' - V_0'')\varepsilon^3 + O(\varepsilon^4). \tag{26}$$

Hence, the modified discrete gradient scheme is of the second order.

Finally, we consider the symmetric modification of the locally exact discrete gradient scheme with $\omega_n$ given by Eq. (17). In this case,

$$\delta = \varepsilon + \frac{1}{12}V''\varepsilon^3 + \frac{1}{24}pV'''\varepsilon^4 + \frac{1}{24}\varepsilon^5\left[\frac{1}{5}(V'')^2 + \frac{1}{4}p^2V^{(4)} - \frac{1}{2}V'V'''\right] + O(\varepsilon^6), \tag{27}$$

and we get $x_{n+1} - x(t+\varepsilon) = O(\varepsilon^5)$ and $p_{n+1} - p(t+\varepsilon) = O(\varepsilon^5)$. Therefore, the numerical scheme defined by Eqs. (5), (6), and (17) is of the fourth order.

## V. NUMERICAL EXPERIMENTS

The accuracy of our numerical schemes was tested on the case of the simple pendulum equation $[V(x) = -\cos x]$. We compared them with the standard leap-frog scheme, the discrete gradient method, and modified discrete gradient method (introduced in [14]). All motions of the simple pendulum are periodic, so we focus our attention on the relative error of the period of considered discretizations. Numerical experiments show that both discrete gradient methods studied in [14] are very stable. Our methods, the locally exact discrete gradient scheme, and its symmetric modification share this property as well. The details of numerical computations of the period are explained in [14]. For simplicity, we assume $x_0 = 0$. In this case, $p_0^2 = 2E + 2$ and the exact solution of the continuous problem is given by $\sin\frac{x}{2} = \frac{p_0}{2}\mathrm{sn}(t, \frac{p_0}{2})$ for $p_0 < 2$ and $\sin\frac{x}{2} = \mathrm{sn}(\frac{p_0 t}{2}, \frac{2}{p_0})$ for $p_0 > 2$, where $\mathrm{sn}(u,k)$ denotes one of Jacobi elliptic functions with the modulus $k$ (see, for instance, [23]). In the limiting case $p_0 = 2$, we have $\sin\frac{x}{2} = \tanh t$.

### A. Locally exact predictor

In practical implementation, we use the implicit scheme (5) as the corrector, while taking as the predictor the explicit scheme,

$$x_{n+1} = x_n + \frac{\sin(\omega_n\varepsilon)}{\omega_n}p_n - \frac{1-\cos(\omega_n\varepsilon)}{\omega_n^2}V'(x_n), \quad [\text{if } V''(x_n) > 0],$$

$$x_{n+1} = x_n + \varepsilon p_n - \frac{1}{2}\varepsilon^2 V'(x_n), \quad [\text{if } V''(x_n) = 0],$$

$$x_{n+1} = x_n + \frac{\sinh(\omega_n\varepsilon)}{\omega_n}p_n - \frac{1-\cosh(\omega_n\varepsilon)}{\omega_n^2}V'(x_n), \quad [\text{if } V''(x_n) < 0]. \tag{28}$$

In order to obtain Eqs. (28), one has to eliminate $p_{n+1}$ from the system (5) and expand the result in the Taylor series with respect to $x_{n+1} - x_n$, leaving only linear terms. The numerical scheme (28) has the same order (third) as Eqs. (5). What is more, these both difference schemes are locally exact. However, this is of some advantage only for very small $\varepsilon$ and for very short times [thus, Eqs. (28) can serve as a very good predictor]. If the long-time behavior is concerned, the scheme (28) is not good and yields solutions with wrong qualitative behavior.

### B. Iterative solution of implicit equations

Here we add more details concerning the numerical solution of Eqs. (5). All discrete gradient schemes are implicit. To solve these implicit equations, we apply both the fixed-point method and the Newton method. These procedures are iterated until the acuracy $10^{-16}$ is obtained. At some points [where the function $x = x(t)$ is almost flat], the problem seems to be somewhat ill conditioned and the iterations oscillate

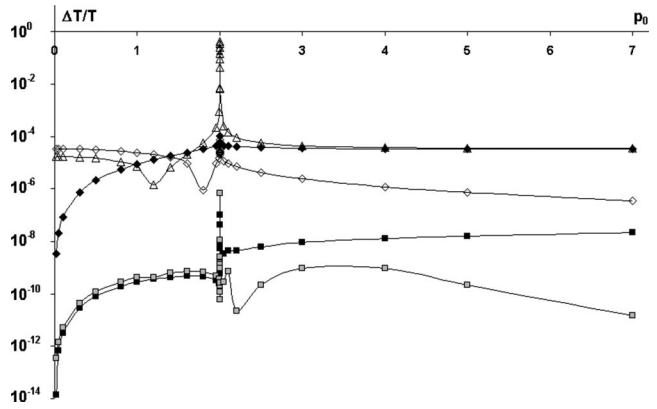


FIG. 1. Relative error of the period for $\varepsilon=0.02$ as a function of $p_0$. White triangles: leap frog; white diamonds: discrete gradient; black diamonds: modified discrete gradient ($\delta=$const); black squares: locally exact discrete gradient; gray squares: symmetric modification of the locally exact discrete gradient.

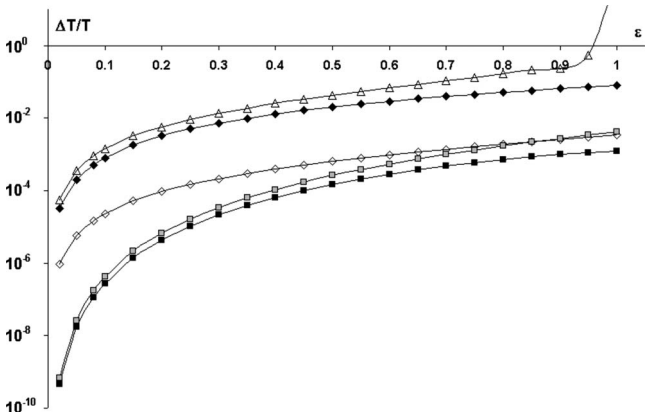


FIG. 2. Relative error of the period for $p_0=1.8$ as a function of $\varepsilon$ (theoretical period $T_{th}=9.122\ 196\ 554$). Symbols: the same as in Fig. 1.

without reaching the limit (the amplitude of these small oscillations is at most of order $10^{-15}$). In such cases, we stop the iterating procedure after 100 iterations (in the case of the fixed-point method) or 15 iterations (in the case of the Newton method). Choosing higher values for these maximal numbers of iterations, we get the same final results. The average number of iterations strongly depends on $\varepsilon$ and shows some dependence on $p_0$ as well. For small $\varepsilon$ (e.g., $\varepsilon=0.02$), we need only 2 iterations using the Newton method and 5 iterations using the fixed-point method. These numbers grow with $\varepsilon$, e.g., for $\varepsilon=0.2$ we need 3 and 12-13 iterations, respectively (the exact average number of iterations depends on $p_0$), and for $\varepsilon=0.5$ we need 3-4 and 21-24 iterations, respectively. We estimate that the Newton method needs about 3.3 times more time for one iteration than the fixed-point method. Therefore, in our case, both these basic iteration methods work with a similar speed. It turns out that for small time steps (say, $\varepsilon<0.2$), both methods have almost the same computational cost (which is only 6–10 times higher than the cost of the leap-frog scheme). Actually, for smaller time steps (e.g., for $\varepsilon=0.02$), the fixed-point method is even slightly faster. For larger $\varepsilon$, the Newton method becomes relatively more effective (e.g., for $\varepsilon=0.9$, the fixed-point method works over 2 times slower).

### C. Relative error of the period

The accuracy of our schemes is surprisingly high, especially for small (but not necessarily very small) time steps. As an example, we present the case $\varepsilon=0.02$ (see Fig. 1). For small oscillations (e.g., $p_0=0.02$), the accuracy of the locally exact discrete gradient scheme is greater by 5 orders of magnitude as compared to the modified discrete gradient method, and by 9 (nine) orders of magnitude better than the leap-frog or discrete gradient method. Actually, the locally exact discrete gradient method and its symmetric modification are much more accurate than any other considered method for any initial conditions (see Fig. 1) (note that the scale on the vertical axis is logarithmic). In the case of oscillating motions, the methods proposed in this paper are better by about 4 orders of magnitude. The symmetric modification of the locally exact discrete gradient scheme beats all other methods in the large energies region ($p_0>2$).

We present also the time-step dependence of the considered numerical schemes for $p_0=1.8$ (see Fig. 2, this graph is also semilogarithmic). The locally exact discrete gradient scheme is clearly the best. The symmetric modification is slightly less accurate. The discrete gradient scheme is comparable with our methods only for large time steps. Taking into account the computational cost of the methods (which reduces, in practice, to allowing smaller time step for the leap-frog scheme), we see that for $p_0=1.8$ the corrected leap-frog scheme yields results similar to the discrete gradient method. Both methods presented in this paper are much better. Only in some exceptional cases (e.g., the "resonance value" $p_0=1.21$, see [14]) the corrected leap-frog scheme is a little bit better than locally exact modifications of the discrete gradient method.

### D. Neighborhood of the separatrix

The neighborhood of the separatrix ($p_0\approx 2$) is most difficult to be simulated numerically. The discrete gradient method turns out to be relatively good in this region (see [14]). The locally exact discrete gradient method is excellent also in that case (see Fig. 3). Its symmetric modification yields practically the same results. We point out that the trajectory is very close to the separatrix ($|p_0-2|=10^{-10}$) and $\varepsilon$ is very large but, nevertheless, our methods simulate very accurately the motion of the pendulum. Discrete points $x_n$ practically lie on the continuous curve of the exact solution. The other two discrete gradient methods also yield quite good results (at least qualitatively), while the leap-frog scheme fails to reproduce even the qualitative behavior. The computational cost of the proposed implicit algorithms is higher than the cost of explicit schemes: we estimate that in the case presented at Fig. 3, one step of discrete gradient schemes iterated by the Newton method costs approximately 13 times more than one step of the leap-frog scheme (for the fixed-point method, the corresponding factor is close to 29). How-

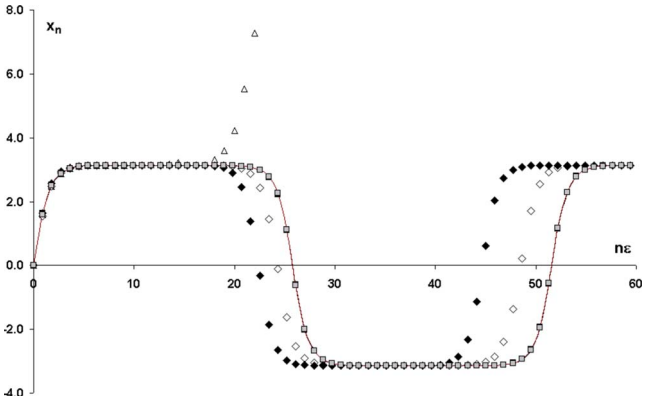


FIG. 3. (Color online) $x_n$ as a function of $n$, very near the separatrix ($p_0$=1.999 999 999 9), $\varepsilon$=0.9 for all gradient schemes, and $\varepsilon$=0.001 for the leap-frog scheme. Symbols: the same as in Fig. 1 (black squares are hidden under gray squares). The solid line corresponds to the exact (continuous) solution (theoretical period $T_{th}$=51.596 879 14).

ever, in this case the leap-frog scheme cannot be essentially improved even by very serious decreasing of the time step. Note that on Fig. 3, the time step for the leap-frog scheme ($\varepsilon$=0.001) is much smaller than the time step for gradient schemes ($\varepsilon$=0.9) and, therefore, the computational cost of the leap-frog scheme is much higher in comparison with the discrete gradient method and its modifications. Therefore, in the neighborhood of the separatrix, the leap-frog scheme is much worse than all discrete gradient methods.

## VI. CONCLUSIONS

The proposed numerical integrators (5) and (6) [the locally exact discrete gradient method and its symmetric modification, corresponding to Eqs. (7) and (17), respectively] have important advantages:

(i) exact conservation of the energy integral [i.e., Eq. (3) holds],

(ii) higher order (third and fourth, respectively) as compared with the discrete gradient method,

(iii) high stability and accuracy,

(iv) very good long-time behavior of numerical solutions.

Therefore, modifications presented in this paper essentially improve the discrete gradient method (at least in the one-dimensional case) keeping all its advantages.

We point out, however, that numerical schemes (5), like all discrete gradient methods, are neither symplectic nor volume preserving. Moreover, in the case defined by Eq. (7), the scheme (5) is not time reversible. The symmetric (time-reversible) modification of Eqs. (5), although of higher order (fourth), is not much more accurate than the locally exact discrete gradient method (actually, for oscillating motions, it is less accurate). It may suggest that the local exactness is of considerable advantage, perhaps worthwhile to be preserved even at the cost of breaking the symmetry of a numerical scheme. This point deserves further studies.

We plan to generalize the approach presented in this paper on some multidimensional cases and to extend the range of its applications on some other numerical integrators (including the implicit midpoint rule) [24]. Note that the time step of the locally exact discrete gradient schemes (5) is equal to $\varepsilon$ and is assumed to be constant. However, there are no obstacles to use the variable time step and it is worthwhile to examinate this possibility in the future.

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