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A new SOR-type iteration method for solving linear systems[☆]

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ABSTRACT

Many discretization methods for continuous dynamical systems have the iterative nature and therefore can provide iterative techniques for solving problems in numerical linear algebra. In this paper, based on the discrete gradient and the variation-of-constants formula for ordinary differential equations, a new SOR-type iteration method is proposed for solving the linear system $Ax = b$. The convergence of the new method is guaranteed by the decay of the Liapunov function. Numerical experiments are carried out to show the effectiveness of the new method.

1. Introduction

In this paper, we consider iterative methods for the linear system

$$Ax = b, \tag{1}$$

where $A = (a_{ij}) \in \mathcal{R}^{n\times n}$ is a nonsingular matrix, and $x, b \in \mathcal{R}^n$.

The linear system (1) plays an important role in scientific and engineering computations. Many stationary iterative methods including Jacobi, Gauss–Seidel (GS), and successive over-relaxation (SOR) method [1,2] are designed to approximately solve the linear systems under special conditions. On some classes of problems, such iterative methods compete well with direct methods.

Many iterative numerical methods for linear system (1), especially one-step processes, are formulated as

$$x^{n+1} = Gx^n + c. \tag{2}$$

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Since 1970s, the connections between iterative numerical methods in numerical linear algebra and continuous dynamic systems have been studied [3,4]. For example, the method of steepest descent can be achieved by applying explicit Euler methods with variable stepsize to the first-order ordinary differential equations $\frac{dx}{dt} = b - Ax, x(0) = x^0$. Applying explicit Euler methods with fixed stepsize $h = 1$ to the differential equations $\frac{dx}{dt} = A^{-1}(b - Ax), x(0) = x^0$ gives the well-known Wilkinson's iterative refinement [5] for ill-conditioned linear systems. Based on the discrete gradient method, Miyatake [6] presents a new connection between SOR methods and gradient systems. The link between iteration methods and continuous dynamic systems leads to the development of so-called dynamic system methods [7], which become fruitfully alternative methods. In contrast to discrete methods, dynamic system methods have some superiors to discrete ones since the theoretical techniques of ordinary differential equations often offer better understanding about the convergence conditions for the corresponding discrete method. Moreover, there are many state-of-the-art numerical techniques available for following the associated solution flows.

In recent years, a relatively new and increasingly important area in numerical integration methods is that of geometric integrator. A numerical integration method is called geometric if it exactly preserves one or more physical/geometric properties such as first integrals, symplectic structure, symmetries, phase-space volume, Liapunov functions etc. of the system. We refer the reader to [8,9] for recent surveys of this research. The study of geometric numerical integration provides us a variety of numerical tools for solving the continuous dynamic systems. It is much likely that using state-of-the-art numerical methods could lead to better iterative numerical methods.

In light of the connection between SOR-type methods and gradient systems, we will propose a new stationary iteration method for the linear system (1) based on the gradient system. The key idea is to use energy-preserving exponential integrators [10,11] as the underlying numerical methods for the continuous dynamic system. The energy-preserving exponential integrator is a combination of exponential integrator [12] and discrete gradient method [13,14]. It can preserve the energy of the continuous system while dealing with the stiffness of the system efficiently.

The rest of the paper is organized as follows. In Section 2, the discrete gradient method as a numerical method in geometric numerical integration is introduced together with its extension, i.e., the energy-preserving exponential integrator. The new SOR-type iteration method is derived and analyzed in Section 3. In Section 4, we present some numerical examples to show the effectiveness of the new method.

2. Discrete gradient method for gradient systems and its exponential form

Discrete gradient methods for ordinary differential equations were introduced by Gonzalez [15]. See also [13,14,16–18].

Definition 2.1. Let $f : \mathcal{R}^n \to \mathcal{R}$ be continuously differentiable function. Then $\overline{\nabla} f : \mathcal{R}^n \times \mathcal{R}^n \to \mathcal{R}^n$ is a discrete gradient of f provided it is continuous and satisfies

$$\begin{cases} \overline{\nabla} f(x, x') \cdot (x' - x) = f(x') - f(x), \\ \overline{\nabla} f(x, x) = \nabla f(x). \end{cases} \tag{3}$$

Three well-known discrete gradients are the mean value discrete gradient, the midpoint discrete gradient and the coordinate increment discrete gradient, which are defined as follows.

- The *mean value discrete gradient* (Harten et al. [19]) :

$$\overline{\nabla}_1 f(x, x') := \int_0^1 \nabla f((1-\tau)x + \tau x')d\tau, \quad x \neq x'. \tag{4}$$

- The *midpoint discrete gradient* (Gonzalez [15]):

$$\overline{\nabla}_2 f(x,x') := \nabla f(\frac{1}{2}(x+x')) + \frac{f(x') - f(x) - \nabla f(\frac{1}{2}(x+x'))\cdot(x'-x)}{|x'-x|^2}(x'-x), \quad x \neq x'. \tag{5}$$

- The *coordinate increment discrete gradient* (Itoh and Abe [16]):

$$\overline{\nabla}_3 f(x,x') := \begin{pmatrix} \frac{f(x_1',x_2,x_3,\ldots,x_n)-f(x_1,x_2,x_3,\ldots,x_n)}{x_1'-x_1} \\ \frac{f(x_1',x_2',x_3,\ldots,x_n)-f(x_1',x_2,x_3,\ldots,x_n)}{x_2'-x_2} \\ \vdots \\ \frac{f(x_1',\ldots,x_{n-2}',x_{n-1}',x_n)-f(x_1',\ldots,x_{n-2}',x_{n-1},x_n)}{x_{n-1}'-x_{n-1}} \\ \frac{f(x_1',\ldots,x_{n-2}',x_{n-1}',x_n')-f(x_1',\ldots,x_{n-2}',x_{n-1}',x_n)}{x_n'-x_n} \end{pmatrix}, x_i' \neq x_i,\ i=1,2,\ldots,n \tag{6}$$

For the gradient system

$$\dot{x} = -\nabla f(x), x(0) = x^0, \tag{7}$$

every discrete gradient leads to an associated discrete gradient method

$$\frac{x^{k+1}-x^k}{h} = -\overline{\nabla} f(x^k, x^{k+1}). \tag{8}$$

According to Definition 2.1, discrete gradient method (8) preserves the energy-dissipation property of the gradient system. More precisely, we have

$$f(x^{k+1}) - f(x^k) = \overline{\nabla} f(x^k,x^{k+1})\cdot(x^{k+1}-x^k) = -h\overline{\nabla} f(x^k,x^{k+1})^T\overline{\nabla} f(x^k,x^{k+1}) \leqslant 0,$$

which is a discrete analogue to the decay of the Liapunov function $f(x)$:

$$\frac{d}{dt}f(x(t)) = -\nabla f(x)^T\dot{x} = -\nabla f(x)^T\nabla f(x) \leqslant 0.$$

For the special case that the Liapunov function has the form $f(x) = \frac{1}{2}x^T Dx + g(x)$, where D is a symmetric and semi-positive definite matrix, the gradient system (7) can be reformulated as

$$\dot{x} + Dx = -\nabla g(x), x(0) = x^0. \tag{9}$$

System (9) usually exhibits a stiffness property because of the presence of Dx, especially when the coefficient matrix D has a large spectral radius. The exponential integrator was introduced to resolve the stiffness in the solution. It exhibits long time stability, allow for relatively larger stepsizes for the stiff system. The construction of exponential integrators starts from the variation-of-constants formula

$$x(t) = \exp\big(-tD\big)x^0 - \int_0^t \exp\big(-(t-\xi)D\big)\nabla g(x(\xi))\mathrm{d}\xi.$$

It follows immediately that

$$x(t_k+h) = \exp\big(-hD\big)x(t_n) - \int_0^h \exp\big(-\xi D\big)\nabla g(x(t_k+\xi))\mathrm{d}\xi. \tag{10}$$

Replacing the gradient $\nabla g(x(t_k+\xi))$ in (10) by its corresponding discrete gradient at (x^k, x^{k+1}) yields the integrator

$$x^{k+1} = \exp\big(-hD\big)x^k - h\varphi(-hD)\overline{\nabla} g(x^k, x^{k+1}), \tag{11}$$

where the scalar function is given by $\varphi(z) = (\exp(z)-1)/z$. The integrator (11) also preserves the energy-dissipation property of the gradient system (9). We refer the reader to [10] for a detailed proof.

3. The new SOR-type iteration method for (1)

For now, we restrict A to be symmetric positive definite and let $f(x) = \frac{1}{2}x^T Ax - x^T b$. Consider the following gradient system

$$\begin{cases} \dot{x} = -\nabla f(x) = b - Ax, \\ x(0) = x^0, x^0 \in \mathcal{R}^n. \end{cases} \tag{12}$$

Theorem 3.1. *The solution $x^* = A^{-1}b$ of linear system (1) is a unique globally asymptotically stable equilibrium point of the gradient system (12).*

Proof. Let $H(x) = \dfrac{1}{2}(Ax-b)^T(Ax-b)$. We have

$$\frac{dH}{dt} = \frac{dH}{dx}\frac{dx}{dt} = (Ax-b)^T A\frac{dx}{dt} = -(Ax-b)^T A(Ax-b) < 0,$$

provided $x \neq x^*$. Moreover, we have $H(x^*) = 0$ and $H(x) \neq 0$, for any $x \neq x^*$. Therefore, $H(x)$ is a strict Liapunov function of dynamic system (12). Therefore, the unique root of $H(x)$, $x = x^*$ is a unique globally asymptotically stable equilibrium point of gradient system (12). □

It can be seen from Theorem 3.1 that if $x(t, x^0)$ is the exact flow of the gradient system (12), then we have

$$\lim_{t\to\infty} x(t, x^0) = A^{-1}b.$$

Note that the equilibrium of the gradient system (12) is the unique optimal solution to the unconditioned optimization problem $\min_{x\in\mathcal{R}^n} f(x)$, or equivalently, the solution to $\nabla f(x) = 0$. Along the exact flow, $f(x(t))$ decreases to its minimum as $t \to \infty$. Therefore applying discrete gradient method which preserves the decay of $f(x)$ to the gradient system (12) results in an iteration method that converges to the unique solution $x^* = A^{-1}b$ [6].

Now, let us express the matrix A as the matrix sum $A = D - L - U$, where D is the diagonal matrix whose diagonal entries are those of A, $-L$ is the strictly lower-triangular part of A, and $-U$ is the strictly upper-triangular part of A. Notice that $U = L^T$ since A is symmetric. With these notations, the gradient system (12) can be reformulated as

$$\begin{cases} \dfrac{dx}{dt} + Dx = -\nabla g(x) = Lx + Ux + b, \\ x(0) = x^0, x^0 \in \mathcal{R}^n \end{cases} \tag{13}$$

with $g(x) = \dfrac{1}{2}x^T(-L-U)x - x^T b$.

Now we apply the energy-preserving exponential integrator (11) to the gradient system (13). Note that the coordinate increment discrete gradient is derivative-free and hence its computational realization relatively cheap. Let us employ the coordinate increment discrete gradient (6). In this case, the ith component of the discrete gradient of $g(x)$ is calculated to be

$$\left(\overline{\nabla}_3 g(x^k, x^{k+1})\right)_i = \sum_{j=1}^{i-1} a_{ij}x_j^k + \sum_{j=i+1}^{n} a_{ij}x_j^{k+1} - b_i.$$

Therefore, the energy-preserving exponential integrator (11) with the coordinate increment discrete gradient (6) yields the following iteration method:

$$x_i^{k+1} = \exp\left(-ha_{ii}\right)x_i^k + h\varphi(-ha_{ii})\left(-\sum_{j=1}^{i-1} a_{ij}x_j^{k+1} - \sum_{j=i+1}^{n} a_{ij}x_j^k + b_i\right). \tag{14}$$

Bearing $\varphi(z) = (\exp(z) - 1)/z$ in mind, the method (14) can be represented in matrix form as

$$x^{k+1} = (I - \Omega)x^k + \Omega D^{-1}\left(Lx^{k+1} + Ux^k + b\right), \tag{15}$$

where $\Omega = I - \exp\bigl(-hD\bigr)$. The formation of the iteration method (15) is exactly the same as the relaxation method

$$x^{k+1} = (1 - \omega)x^k + \omega D^{-1}\left(Lx^{k+1} + Ux^k + b\right) \tag{16}$$

except that for the standard relaxation method, $0 < \omega < 2$ is a scalar while in our case Ω is a diagonal matrix. For choices of ω with $0 < \omega < 1$, (16) is called under-relaxation method. The choices of ω with $1 < \omega < 2$ result in over-relaxation method. It is used to accelerate the convergence for systems that are convergent by the Gauss–Seidel method [2].

It should be noted that the choices of $\Omega = I - \exp\bigl(-hD\bigr)$ restrict the iteration method (15) to be under relaxed for any $h > 0$. Whereas, we are mostly interested in the case of over relaxation. This motivates us to consider the choices of $\Omega = I + \exp\bigl(-hD\bigr)$, which gives the following iteration method:

$$x_i^{k+1} = -\exp\bigl(-ha_{ii}\bigr)x_i^k + h\phi(-ha_{ii})\left(-\sum_{j=1}^{i-1} a_{ij}x_j^{k+1} - \sum_{j=i+1}^{n} a_{ij}x_j^k + b_i\right). \tag{17}$$

Here the scalar function is given by $\phi(z) = -(\exp(z)+1)/z$. We refer (17) as an *exponential discrete gradient iteration method* and denote it by *EDG*.

Theorem 3.2. *Assume that the matrix A is positive definite. The exponential discrete gradient iteration method (17) with stepsize $h > 0$ converges to the solution of the linear system (1) for any initial value x^0.*

Proof. To show that the exponential discrete gradient iteration method gives a sequence $\{x^k\}_{k=0}^{\infty}$ that converges to the solution of linear system (1), one only need to verify that the Liapunov function $f(x) = \frac{1}{2}x^T Ax - x^T b$ is decreased with respect to the sequence $\{x^k\}_{k=0}^{\infty}$ generated by (17). This is verified by the following inequality:

$$f(x^{k+1}) - f(x^k) = (x^{k+1} - x^k)^T \left(D\left(\frac{1}{2}I - (I + \exp(-hD))^{-1}\right)\right)(x^{k+1} - x^k) < 0. \quad \square$$

Remark 3.1. Under the assumption $a_{ii} > 0, i = 1, \ldots, n$. The exponential discrete gradient iteration methods (14) and (17) both reduce to the Gauss–Seidel iteration method as $h \to +\infty$:

$$x_i^{k+1} = \frac{1}{a_{ii}}\left(-\sum_{j=1}^{i-1} a_{ij}x_j^{k+1} - \sum_{j=i+1}^{n} a_{ij}x_j^k + b_i\right). \tag{18}$$

Remark 3.2. Suppose that A is in the $p \times p$ block partitioned form

$$A = \begin{pmatrix} A_{11} & A_{12} & \cdots & A_{1p} \\ A_{21} & A_{22} & \cdots & A_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ A_{p1} & A_{p2} & \cdots & A_{pp} \end{pmatrix}$$

Correspondingly, the vector x is also divided into p parts: $x = (x_1^T, x_2^T, \ldots, x_p^T)$. Then the exponential discrete gradient iteration method can be extended to the blockwise fashion as follows.

$$x_i^{k+1} = -\exp\bigl(-hA_{ii}\bigr)x_i^k + h\phi(-hA_{ii})\left(-\sum_{j=1}^{i-1} A_{ij}x_j^{k+1} - \sum_{j=i+1}^{n} A_{ij}x_j^k + b_i\right), i = 1, \ldots, p. \tag{19}$$

Remark 3.3. If the diagonal entries of the coefficient matrix A satisfy $a_{ii} = a, i = 1, \ldots, n$, then the exponential discrete gradient iteration method (17) is exactly the successive over-relaxation method with $\omega = 1 + \exp(-ha)$.

4. Numerical experiments

In this section, two numerical examples are performed to show the effectiveness of the proposed method. All experiments are executed by using the MATLAB programming package with double precision by default. In all the numerical experiments, the initial approximation x^0 is taken as the zero vector, and the right-hand-side vector b is chosen so that $x^* = (1, \ldots, 1)^T$ is the solution of the considered system. The Gauss–Seidel method, the successive over-relaxation method and the exponential discrete gradient iteration method are applied to solving the linear system. The parameter ω in SOR method and the parameter h in the exponential discrete gradient iteration method are both chosen to be the optimal in the sense that the spectral radii of the iteration matrices for the methods are minimum.

Example 4.1. Let

$$A = \begin{pmatrix} 2+q_1 & -1 & & \\ -1 & 2+q_2 & \ddots & \\ & \ddots & \ddots & -1 \\ & & -1 & 2+q_n \end{pmatrix} \in \mathcal{R}^{n\times n}.$$

This matrix arises from the two-point boundary value problem $y''(x) = q(x)y(x) + r(x)$. Here, we choose $q_i = 2\cos^2\left(\frac{2\pi i}{n}\right), i = 1, \ldots, n$ with $n = 100, 200$.

Example 4.2. When the standard five-point finite difference scheme on a uniform grid with $m \times m$ interior nodes is applied to the discretization of the two-dimensional elliptic partial differential equation

$$-\Delta u + p(x)u = f(x, y)$$

in the unit square $[0, 1] \times [0, 1] \subset \mathcal{R}^2$ with homogeneous Dirichlet boundary conditions, we get a system of linear equations with the coefficient matrix

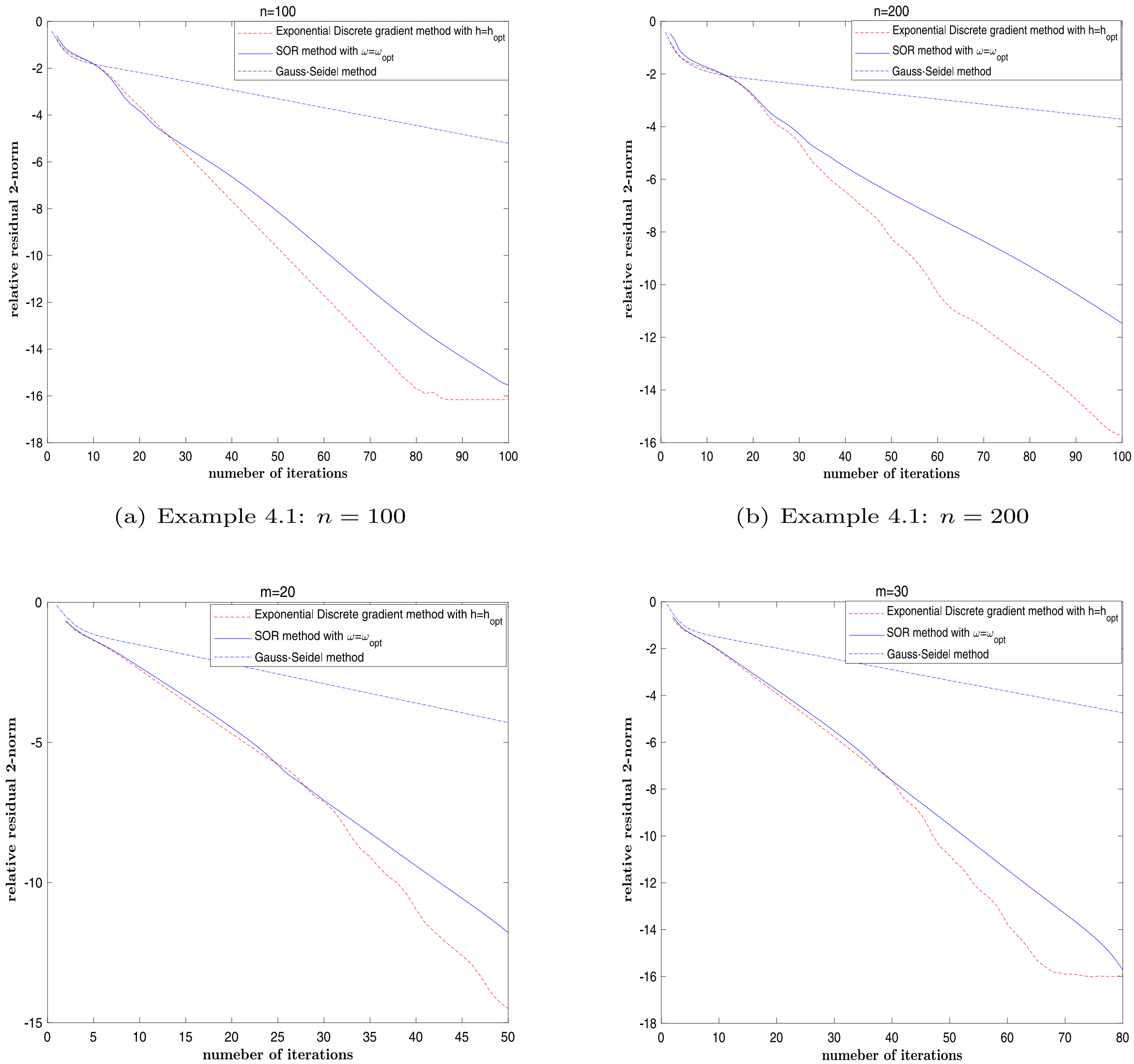
$$A = (I + P) \otimes I - \frac{1}{4} B \otimes I - \frac{1}{4} I \otimes B$$

with $P = diag(p_1, p_2, \ldots, p_m)$, which is related to the space step and the variable coefficient $p(x)$ in the equation. And

$$B = \begin{pmatrix} 0 & 1 & & \\ 1 & \ddots & \ddots & \\ & \ddots & \ddots & 1 \\ & & 1 & 0 \end{pmatrix} \in \mathcal{R}^{m\times m}.$$

In this example, we choose $p_i = \frac{1}{2}\left(1 + \sin\left(\frac{2\pi i}{n}\right)\right), i = 1, \ldots, m$ with $m = 20, 30$. Then the dimension of the corresponding linear system is $n = 400$ and $n = 900$, respectively.

The relative residual 2-norm versus iteration steps for the three methods are plotted for the two examples. The results are shown in Fig. 1. We observe that the convergence of the new method and the SOR method is much faster than that of the Gauss–Seidel method. Moreover, the convergence of the new method with



(a) Example 4.1: $n = 100$

(b) Example 4.1: $n = 200$

(c) Example 4.2: $m = 20$

(d) Example 4.2: $m = 30$

Fig. 1. The relative residual 2-norm versus number of iterations.

optimal parameter is faster than that of the SOR method with optimal relaxation parameter. It should be noted that the choice of relaxation parameter is very subtle. Generally speaking, the optimal parameter is not attainable in practice. However, the new method still provides us a potentially better alternative of the traditional successive over-relaxation method.

References

[1] S. Agmon, The relaxation method for linear inequalities, Canad. J. Math. 66 (1954) 382–392.
[2] C.T. Kelley, Iterative Methods for Linear and Nonlinear Equations, SIAM, Philadelphia, 1995.
[3] M.T. Chu, On the continuous realization of iterative processes, SIAM Rev. 30 (1988) 375–387.
[4] M.T. Chu, Linear algebra algorithms as dynamical systems, Acta Numer. 19 (2008) 1–86.
[5] X.Y. Wu, X. You, Extended version with the analysis of dynamic system for iterative refinement of solution, Int. J. Comput. Math. 87 (2010) 920–934.

[6] Y. Miyatake, T. Sogabe, S.L. Zhang, On the equivalence between SOR-type methods for linear systems and the discrete gradient methods for gradient systems, J. Comput. Appl. Math. 342 (2018) 58–69.
[7] A.G. Ramm, Dynamical systems method for solving operator equations, Commun. Nonlinear Sci. Numer. Simul. 9 (2004) 383–402.
[8] E. Hairer, C. Lubich, G. Wanner, Geometric Numerical Integration: Structure-preserving Algorithms, second ed., Springer-Verlag, Berlin, Heidelberg, 2006.
[9] J.M. Sanz-Serna, Symplectic integrators for Hamiltonian problems: an overview, Acta Numer. 1 (1992) 243–286.
[10] Y.W. Li, X. Wu, Exponential integrators preserving first integrals or lyapunov functions for conservative or dissipative systems, SIAM J. Sci. Comput. 3 (2016) A1876–A1895.
[11] X.F. Shen, M. Leok, Geometric exponential integrators, SIAM J. Sci. Comput. 382 (2019) 27–42.
[12] M. Hochbruck, C. Lubich, A Gautschi-type method for oscillatory second-order differential equations, Numer. Math. 83 (1999) 403–426.
[13] G.R.W. Quispel, H.W. Capel, Solving ODEs numerically while preserving a first integral, Phys. Lett. A 218 (1996) 223–228.
[14] R.I. McLachlan, G.R.W. Quispel, N. Robidoux, Geometric integration using discrete gradients, Phil. Trans. R. Soc. A 357 (1999) 1021–1045.
[15] O. Gonzalez, Time integration and discrete Hamiltonian systems, J. Nonlinear Sci. 6 (1996) 449–467.
[16] T. Itoh, K. Abe, Hamiltonian conserving discrete canonical equations based on variational difference quotients, J. Comput. Phys. 77 (1988) 85–102.
[17] G.R.W. Quispel, D.I. McLaren, A new class of energy-preserving numerical integration methods, J. Phys. A 41 (2008) 045206.
[18] J.L. Cieśliński, B. Ratkiewicz, Energy-preserving numerical schemes of high accuracy for one-dimensional Hamiltonian systems, J. Phys. A 44 (2011) 155206.
[19] A. Harten, P.D. Lax, B. van Leer, On upstream differencing and Godunov-type schemes for hyperbolic conservation laws, SIAM Rev. 25 (1983) 35–61.