Comparison of Galerkin Methods applied to Classical Mechanics

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Abstract. In this paper we compare two Galerkin finite element methods in time which use continuous and discontinuous piecewise polynomials for trial and test functions. We apply both methods for approximating the solution of Hamilton's canonical equations. Considering natural systems, we investigate the algorithmic conservation properties of both methods for linear time finite elements applied to the one-body central force problem. In this context, we present quadrature rules leading to algorithmic total energy and angular momentum conservation, respectively.

Keywords. Galerkin method, finite element method, initial value problem, Hamilton's canonical equations, conservation laws, quadrature.

1 Introduction

In the present paper we compare the algorithmic conservation properties of the discontinuous Galerkin (dG) method with those of the continuous Galerkin (cG) method for natural mechanical systems.

In particular, we consider autonomous natural Hamiltonian systems and use the two different Galerkin methods for solving Hamilton's canonical equations pertaining to the one-body central force problem. Therefore, the conservation of total energy as well as total angular momentum is treated. The dG method can be traced back to Lasaint and Raviart [15], see also the book of Eriksson et al. [6]. For the cG method, usually accredited to Hulme [14], see also Eriksson et al. [6], the algorithmic conservation properties have been examined in Betsch and Steinmann [3, 4, 5].

Since the exact calculation of the time integrals appearing in the cG and dG method is rarely feasible, we investigate the influence of specific quadrature rules on the algorithmic conservation properties of both methods.

An outline of the paper is as follows. In Section 2, we begin by recalling the definition of a natural system and Hamilton's canonical equations. Subsequently, we give a review of the conservation laws prevailing in the systems we consider; see Arnold [1]. Firstly, we point out the total energy conservation in natural systems and thereafter, we review the law of conservation of total angular momentum pertaining to only one particle in accordance with Goldstein [8]. Section 3 contains the underlying initial value problem to be solved. Then, after we have presented the continuous as well as the discontinuous Galerkin finite element approximation of Hamilton's canonical equations, we point out that the continuous Galerkin finite element method inherently conserves an autonomous Hamiltonian after each time step (algorithmic conservation). Subsequently, we demonstrate a possibility to prove a decay of the algorithmic Hamiltonian determined by the discontinuous Galerkin finite element method provided that particular conditions hold. We conclude this section by demonstrating a relationship between both methods in the case of linear time finite elements. In Section 4, we investigate the algorithmic conservation properties of the continuous as well as the discontinuous Galerkin finite element method for motions of one particle in a three-dimensional central force field, where we restrict ourselves to linear time finite elements. Firstly, we consider solely Hooke's central force law and thereafter we let the central force law be arbitrary. In this connection, we point out for arbitrary central force laws how algorithmic conservation of total energy and total angular momentum can be obtained by applying specific quadrature rules. Conclusions are drawn in Section 5.

2 Hamilton's canonical equations and conservation laws

2.1 Definition of a natural system

Let $\{q_i\}_{i=1}^{n_{dof}}$ be a set of independent generalized coordinates of a Lagrangian dynamical system with n_{dof} degrees of freedom, which are arranged into the generalized coordinate vector $\boldsymbol{q} := (q_i)_{i=1}^{n_{dof}} \in \mathbb{R}^{n_{dof}}$. A *natural system* consists of a Lagrangian $L := T - V$, where the total kinetic energy $T = T(\boldsymbol{q}, \dot{\boldsymbol{q}})$ is a positive definite

quadratic form with respect to the generalized velocity vector $\dot{\boldsymbol{q}} = \mathrm{d}\boldsymbol{q}/\mathrm{d}t$. Furthermore, $V = V(\boldsymbol{q})$ denotes the total potential energy from which the set of conservative generalized forces $\{Q_i\}_{i=1}^{n_{dof}}$ are derived by $\boldsymbol{Q} = -\partial_{\boldsymbol{q}} V$, where $\boldsymbol{Q} := (Q_i)_{i=1}^{n_{dof}} \in \mathbb{R}^{n_{dof}}$ denotes the generalized force vector.

2.2 Hamilton's canonical equations

In the Hamiltonian approach of dynamics the motion of the system is described by $2n_{dof}$ independent variables. Thus the equations of motion are in terms of $2n_{dof}$ first-order differential equations; see Arnold [1].

Theorem 2.1 *Given a Lagrangian L being convex with respect to the generalized velocity vector $\dot{\boldsymbol{q}}$. Then, Lagrange's equation $\dot{\boldsymbol{p}} = \partial_{\boldsymbol{q}} L$, where $\boldsymbol{p} = \partial_{\dot{\boldsymbol{q}}} L$, is equivalent to Hamilton's canonical equations, given by*

$$\dot{\boldsymbol{q}} = \partial_{\boldsymbol{p}} H, \qquad \dot{\boldsymbol{p}} = -\partial_{\boldsymbol{q}} H\,, \tag{1}$$

where H is the Legendre transform of the Lagrangian L viewed as a function of $\dot{\boldsymbol{q}}$.

Proof. Owing to the convexity of the Lagrangian L, the Legendre transform of L with respect to $\dot{\boldsymbol{q}}$, given by

$$H(\boldsymbol{q}, \boldsymbol{p}) := \sup_{\dot{\boldsymbol{q}}} h(\boldsymbol{q}, \dot{\boldsymbol{q}}, \boldsymbol{p}), \tag{2}$$

where $h(\boldsymbol{q}, \dot{\boldsymbol{q}}, \boldsymbol{p}) := \boldsymbol{p} \cdot \dot{\boldsymbol{q}} - L(\boldsymbol{q}, \dot{\boldsymbol{q}})$, is unique. The new vector variable $\boldsymbol{p}$ is thus defined from the extremal condition $\partial_{\dot{\boldsymbol{q}}} h = \boldsymbol{0}$ as

$$\boldsymbol{p} := \partial_{\dot{\boldsymbol{q}}} L. \tag{3}$$

The total differential of the Hamiltonian $H = H(\boldsymbol{q}, \boldsymbol{p})$ is equal to the total differential of $h = h(\boldsymbol{q}, \dot{\boldsymbol{q}}, \boldsymbol{p})$ for $\boldsymbol{p} = \partial_{\dot{\boldsymbol{q}}} L$. Taking equation (3) into account, a comparison of the coefficients pertaining to the remaining differentials furnishes Hamilton's canonical equations (1). Therefore, Lagrange's equation and Hamilton's canonical equations are equivalent. ■

Remark 2.1 The scalar function $H(\boldsymbol{q}, \boldsymbol{p})$ is called the *Hamiltonian*. With regard to definition (3), one refers to the new vector variable $\boldsymbol{p}$ as the *generalized momentum vector*.

Remark 2.2 Hamilton's canonical equations describe the dynamics of the system which is therefore called *Hamiltonian system*.

Remark 2.3 The convexity of the Lagrangian L with respect to $\dot{\boldsymbol{q}}$ is generally fulfilled for natural systems owing to the positive definite quadratic form of the kinetic energy T.

2.3 Conservation of the total energy of natural systems

Theorem 2.2 *Given a natural Hamiltonian system. If the Hamiltonian H does not depend explicitly on time, that is, $\partial_t H = 0$, the total energy is conserved.*

We prove Theorem 2.2 by two preliminary results represented by the following lemmas; see Arnold [1, 2].

Lemma 2.1 *The Hamiltonian H of a natural system is the total energy of the system, that is, $H = T + V$.*

Proof. Owing to the quadratic form with respect to $\dot{\boldsymbol{q}}$, T is homogeneous of degree two. Therefore, Euler's theorem for homogeneous functions yields $\partial_{\dot{\boldsymbol{q}}} T \cdot \dot{\boldsymbol{q}} = 2\,T$. Since the potential energy $V = V(\boldsymbol{q})$ depends only on $\boldsymbol{q}$, one obtains $\partial_{\dot{\boldsymbol{q}}} L = \partial_{\dot{\boldsymbol{q}}} T$. Accordingly, with equation (3) the function h results in $h = 2\,T - (T - V) = T + V$ and thus the Hamiltonian reads $H = (T + V)|_{\dot{\boldsymbol{q}} \to \boldsymbol{p}}$. ■

Lemma 2.2 *Given an arbitrary Hamiltonian System. If the Hamiltonian H does not depend explicitly on time (autonomous Hamiltonian system), the Hamiltonian is conserved, that is, $H(\boldsymbol{q}, \boldsymbol{p}) = const.$*

Proof. For a system whose Hamiltonian does not depend explicitly on time, Hamilton's canonical equations lead to $\dot{H} = \partial_{\boldsymbol{p}} H \cdot (-\partial_{\boldsymbol{q}} H) + \partial_{\boldsymbol{q}} H \cdot \partial_{\boldsymbol{p}} H = 0$. Therefore, the Hamiltonian H remains constant. ■

Proof of Theorem 2.2 By Lemma 2.1 the total energy of a natural system is equal to its Hamiltonian H. According to Lemma 2.2, the Hamiltonian H of an autonomous Hamiltonian system is a constant of the motion. Hence it follows that the total energy of a natural autonomous Hamiltonian system is conserved. ■

2.4 Conservation of the total angular momentum of a particle

Consider the motion of a particle of mass m in the three-dimensional Euclidean space $\mathbb{E}^3$ relative to an inertial Cartesian coordinate system with the origin O.

We begin by recalling some definitions:

Definition 2.1 Let $\boldsymbol{P} := m\,\dot{\boldsymbol{r}}$ denote the *total linear momentum* of a particle of mass m, where $\boldsymbol{r}$ is the radius vector of the particle beginning at the origin O.

Remark 2.4 Notice that if q_i is not a Cartesian coordinate, the corresponding generalized momentum p_i does not necessarily have the dimension of the linear momentum P_i, $i = 1, 2, \ldots, n_{dof}$.

Notation 2.1 In the following, we use the briefer notation $1(1)n := 1, 2, \ldots, n$, where $n \in \mathbb{N}$.

Definition 2.2 The *total angular momentum* of a particle of mass m about O, denoted by $\boldsymbol{L}$, is defined as $\boldsymbol{L} := \boldsymbol{r} \times \boldsymbol{P}$.

Definition 2.3 The *total torque* $\boldsymbol{N}$ about O is the vector product $\boldsymbol{N} := \boldsymbol{r} \times \boldsymbol{F}$, where $\boldsymbol{F} = \dot{\boldsymbol{P}}$ is the total force.

Now let us formulate the law of conservation of total angular momentum as

Theorem 2.3 *If the total torque $\boldsymbol{N}$ about O vanishes, then the total angular momentum $\boldsymbol{L}$ about O is a constant of the motion.*

Proof. We may write the total torque as

$$\boldsymbol{N} = \boldsymbol{r} \times \frac{\mathrm{d}}{\mathrm{d}t}\,(m\,\dot{\boldsymbol{r}}) = \frac{\mathrm{d}}{\mathrm{d}t}\,(\boldsymbol{r} \times m\,\dot{\boldsymbol{r}}) - \dot{\boldsymbol{r}} \times m\,\dot{\boldsymbol{r}} = \dot{\boldsymbol{L}}, \tag{4}$$

where the product rule of differentiation was used. Hence, for a vanishing total torque $\boldsymbol{N}$ the total angular momentum $\boldsymbol{L}$ is preserved. ■

2.5 Compact formulation of the initial-value problem

For our ensuing considerations it proves convenient to rewrite Hamilton's canonical equations in a more compact form by introducing the new variable $\boldsymbol{z} := (\boldsymbol{q}, \boldsymbol{p}) \in \mathbb{R}^{2n_{dof}}$, known as *symplectic variable*; see Arnold [2]. On the vector space $\mathbb{R}^{2n_{dof}}$ a symplectic linear structure is given by a nondegenerate bilinear skew-symmetric 2-form in terms of the *skew-scalar product* $[\boldsymbol{u}, \boldsymbol{v}] = -[\boldsymbol{v}, \boldsymbol{u}]$, $\boldsymbol{u}, \boldsymbol{v} \in \mathbb{R}^{2n_{dof}}$; see Arnold [1, 2]. The vector space $\mathbb{R}^{2n_{dof}}$, together with the symplectic structure $[\bullet, \bullet]$, is called a *symplectic vector space*. The symplectic basis of $\mathbb{R}^{2n_{dof}}$, denoded by $\{\boldsymbol{e}_{q_i}, \boldsymbol{e}_{p_i}\}_{i=1}^{n_{dof}}$, is defined by $[\boldsymbol{e}_{p_i}, \boldsymbol{e}_{q_j}] = \delta_{ij}$ and $[\boldsymbol{e}_{q_i}, \boldsymbol{e}_{q_j}] = [\boldsymbol{e}_{p_i}, \boldsymbol{e}_{p_j}] = 0$, $i, j = 1(1)n_{dof}$. The skew-scalar product can be expressed in terms of a scalar product by $[\boldsymbol{u}, \boldsymbol{v}] := (\boldsymbol{J}\boldsymbol{u}, \boldsymbol{v})$. The matrix of the skew-symmetric operator $\boldsymbol{J}$ with respect to the symplectic basis assumes the form of a $2n_{dof} \times 2n_{dof}$ hypermatrix $\boldsymbol{J} \in \mathcal{M}_{2n_{dof}}(\mathbb{R})$ over $\mathbb{R}$, given by

$$\boldsymbol{J} := \begin{bmatrix} \boldsymbol{O} & \boldsymbol{I} \\ -\boldsymbol{I} & \boldsymbol{O} \end{bmatrix}, \tag{5}$$

where the matrices $\boldsymbol{O}, \boldsymbol{I} \in \mathcal{M}_{n_{dof}}(\mathbb{R})$ are the $n_{dof} \times n_{dof}$ zero and identity matrix, respectively. According to Arnold [2], the hypermatrix $\boldsymbol{J}$ is called the *symplectic unit matrix* .

Hamilton's canonical equations are now equivalent to *Hamilton's equation*, given by

$$\dot{\boldsymbol{z}} = \boldsymbol{J} DH(\boldsymbol{z}). \tag{6}$$

Remark 2.5 Using the fact that $\mathcal{M}_{2n_{dof}}(\mathbb{R})$ is homeomorphic to $\mathbb{R}^{(2n_{dof})^2}$, in the subsequent discussion we also regard the symplectic variable $\boldsymbol{z}$ and Hamilton's equation (6) as matrix and system of generally nonlinear equations, respectively. Then, $DH(\boldsymbol{z})$ is the *Jacobian* of the Hamiltonian H with respect to $\boldsymbol{z}$.

Supplemented with the initial condition $\boldsymbol{z}(t_0) = \boldsymbol{z}_{t_0}$, the equation (6) gives rise to the following *initial-value problem*: find $\boldsymbol{z} : I_t \to \mathbb{R}^{2n_{dof}}$ such that

$$\left\{ \begin{array}{ll} \dot{\boldsymbol{z}}(t) & = \boldsymbol{J} DH(\boldsymbol{z}(t)) \quad \text{for} \quad t_0 < t \leq T, \\ \boldsymbol{z}(t_0) & = \boldsymbol{z}_{t_0}, \end{array} \right. \tag{7}$$

where $I_t := [t_0, t_0 + T]$ is the time interval of interest.

To obtain a numerical solution of the initial-value problem (7) on the time interval I_t, we perform a discretization in time. Therefore, for the given interval I_t we let $t_0 < t_1 < \ldots < t_N$ be a partition into subintervals $I_n := [t_{n-1}, t_n]$ of length $h_n := t_n - t_{n-1}$, $n = 1(1)N$. We further introduce a transformation T_n to a master element $I_\alpha := [0, 1]$, defined by

$$T_n : t \mapsto \alpha(t) := \frac{t - t_{n-1}}{t_n - t_{n-1}} = \frac{t - t_{n-1}}{h_n}. \tag{8}$$

In other words, we substitute the variable α and the differential operator $\mathrm{d}/\mathrm{d}\alpha$ for the time t and the differential operator $\mathrm{d}/\mathrm{d}t = h_n^{-1}\, \mathrm{d}/\mathrm{d}\alpha$, respectively.

In view of the finite element formulations treated next, we consider the following alternative statement of the initial value problem: find $\boldsymbol{z} : I_\alpha \to \mathbb{R}^{2n_{dof}}$ such that

$$\left\{ \begin{array}{ll} \boldsymbol{z}'(\alpha) & = h_n \boldsymbol{J} DH(\boldsymbol{z}(\alpha)) \quad \text{for} \quad 0 < \alpha \leq 1, \\ \boldsymbol{z}(0) & = \boldsymbol{z}_0, \end{array} \right. \tag{9}$$

where the prime indicates differentiation with respect to α, that is, $(\bullet)' = \mathrm{d}(\bullet)/\mathrm{d}\alpha$.

3 Galerkin finite element formulations

We focus next on two alternative finite element formulations for the numerical solution of the initial value problem (9). In particular, the two formulations are based upon the continuous and discontinuous Galerkin method.

3.1 The continuous Galerkin cG(k) method

Let $\mathcal{P}^k(0,1)^{2n_{dof}}$ denote the space of $2n_{dof}$-dimensional polynomials of degree k on the interval I_α. The continuous Galerkin approximation of the inital value problem (9) is formulated by: find a trial function $\boldsymbol{z}^h \in \mathcal{P}^k(0,1)^{2n_{dof}}$ such that for all test functions $\delta \boldsymbol{z}^h \in \mathcal{P}^{k-1}(0,1)^{2n_{dof}}$,

$$\int_0^1 \boldsymbol{J} \delta \boldsymbol{z}^h \cdot \left[\left(\boldsymbol{z}^h \right)' - h_n \boldsymbol{J} DH(\boldsymbol{z}^h) \right] d\alpha = 0. \tag{10}$$

We refer to the weighted residual statement (10) as the *weak form* of the initial-value problem (9); see Betsch and Steinmann [3, 4, 5].

Remark 3.1 Concerning Hamilton's equation (6), the coefficients of the trial and test functions are vectors of the symplectic vector space $\mathbb{R}^{2n_{dof}}$ with the structure $[\bullet, \bullet]$. Therefore the skew-orthogonality of two vectors $\boldsymbol{u}, \boldsymbol{v} \in \mathbb{R}^{2n_{dof}}$ is defined by $[\boldsymbol{u}, \boldsymbol{v}] = \boldsymbol{J}\boldsymbol{u} \cdot \boldsymbol{v} = 0$. Accordingly, the Galerkin orthogonality is given by the weighted residual statement (10).

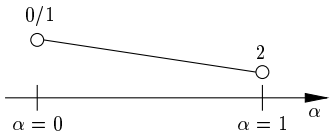

Figure 3.1 Continuous polynomial approximation ($k=1$) on the master element I_α.

As basis of $\mathcal{P}^k(0,1)^{2n_{dof}}$ we use the Lagrange basis $\{M_I(\alpha)\}_{I=1}^{k+1}$ associated to the distinct $k+1$ nodes $\alpha_1<\alpha_2<\ldots<\alpha_{k+1}$ in I_α, which is determined by the requirement that $M_I(\alpha_J)=\delta_{IJ}$, the Kronecker delta. The explicit expression for the basis function $M_I(\alpha)$ is

$$M_I(\alpha) = \prod_{\substack{J=1 \\ J\neq I}}^{k+1} \frac{\alpha-\alpha_J}{\alpha_I-\alpha_J}, \quad I=1(1)k+1. \tag{11}$$

Remark 3.2 By definition $\prod_{J\in\emptyset}=1$. Therefore, for the case $k=0$ we obtain from equation (11) the nodal shape function $M_1=1$.

Remark 3.3 We refer to Table 3.1 for the Lagrange basis functions $\{M_I(\alpha)\}_{I=1}^{k+1}$ of polynomial degree $k=0(1)2$.

Satisfying $\boldsymbol{z}_I := \boldsymbol{z}^h(\alpha_I)$ at the nodes $\{\alpha_I\}_{I=1}^{k+1}$, the polynomial $\boldsymbol{z}^h(\alpha)\in\mathcal{P}^k(0,1)^{2n_{dof}}$ may be expressed in terms of the corresponding Lagrange basis as

$$\boldsymbol{z}^h(\alpha) = \sum_{I=1}^{k+1} M_I(\alpha)\,\boldsymbol{z}_I, \tag{12}$$

so that the values $\{\boldsymbol{z}^h(\alpha_I)\}_{I=1}^{k+1}$ are the coefficients of $\boldsymbol{z}^h(\alpha)$ with respect to the Lagrange basis.

For global continuity of the trial functions we have to state the following continuity condition at the beginning of each time step (compare with Figure 3.1 and equation (9)):

$$\boldsymbol{z}_1 = \boldsymbol{z}_0. \tag{13}$$

Notation 3.1 We also refer to the Lagrange basis and the Lagrange basis functions as the *nodal basis* and the *nodal shape functions*, respectively.

The test function $\delta\boldsymbol{z}^h$ is an element of the space $\mathcal{P}^{k-1}(0,1)^{2n_{dof}}$ such that it takes the form, given by

$$\delta\boldsymbol{z}^h(\alpha) = \sum_{I=1}^{k} \tilde{M}_I(\alpha)\,\delta\boldsymbol{z}_I, \tag{14}$$

where $\tilde{M}_I$ indicates reduced shape functions defined by the relation

$$\left(\boldsymbol{z}^h\right)'(\alpha) = \sum_{I=1}^{k+1} M_I'(\alpha)\,\boldsymbol{z}_I =: \sum_{I=1}^{k} \tilde{M}_I(\alpha)\,\tilde{\boldsymbol{z}}_I. \tag{15}$$

$k=0$	$M_1 = 1$
$k=1$	$M_1 = 1-\alpha$
	$M_2 = \alpha$
$k=2$	$M_1 = (2\alpha-1)(\alpha-1)$
	$M_2 = -4\alpha(\alpha-1)$
	$M_3 = \alpha(2\alpha-1)$

Table 3.1 Lagrange basis functions $M_I(\alpha)$ of polynomial degree $k=0(1)2$.

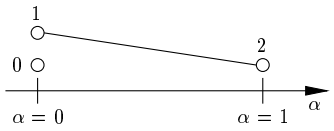

Figure 3.2 Discontinuous polynomial approximation ($k=1$) on the master element.

Remark 3.4 Note that the test function (14) leads to possible discontinuities across the element boundaries.

Remark 3.5 We refer to Table 3.2 for the reduced shape functions $\{\tilde{M}_I(\alpha)\}_{I=1}^k$ and the associated quantities $\{\tilde{\boldsymbol{z}}_I\}_{I=1}^k$ of polynomial degree $k=1(1)2$.

Notation 3.2 Following the terminology of Eriksson et al. [6], we refer to the continuous Galerkin finite element method just defined briefly as the continuous Galerkin *cG(k) method*.

Inserting equations (14) and (15) into the weak form (10), owing to the arbitrariness of the $\{\delta\boldsymbol{z}_I\}_{I=1}^k$ on each subinterval I_n one obtains the following set of equations (*general cG(k) method*):

$$\sum_{J=1}^{k}\int_0^1 \tilde{M}_I\tilde{M}_J d\alpha\,\tilde{\boldsymbol{z}}_J - h_n\int_0^1 \tilde{M}_I\boldsymbol{J}DH(\boldsymbol{z}^h)d\alpha = \boldsymbol{0}, \tag{16}$$

for $I=1(1)k$, where $\boldsymbol{0}$ indicates the zero vector.

The k equations (16) represent a family of implicit multi-level one-step schemes of which a specific member is obtained by selecting the polynomial degree k as well as a specific quadrature rule for computing the integrals of the generally nonlinear Jacobian DH.

3.2 The discontinuous Galerkin dG(k) method

Secondly, we use a Galerkin finite element method for which the trial as well as the test functions are discontinuous piecewise polynomials of degree k. This method is known as the discontinuous Galerkin *dG(k) method*; see Eriksson et al. [6]. Owing to the degree k of the test functions, the number of the algebraic equations is increased by one in contrast to the continuous Galerkin cG(k) method.

Let the trial space as well as the test space be given by $\mathcal{P}^k(0,1)^{2n_{dof}}$. Further, let the trial function $\boldsymbol{z}^h(\alpha)$ have the same form as in the continuous Galerkin cG(k) method, that is, the form given by equation (12). However, let the test function have the form

$$\delta\boldsymbol{z}^h(\alpha) = \sum_{I=1}^{k+1} M_I(\alpha)\,\delta\boldsymbol{z}_I. \tag{17}$$

To prevent that the nodal values $\{\boldsymbol{z}_I\}_{I=1}^{k+1}$ of the trial function are over-determined, one gives up the continuity condition (13). For that reason, one generally gets a jump $[\![\boldsymbol{z}^h]\!] := \boldsymbol{z}_1 - \boldsymbol{z}_0 \neq \boldsymbol{0}$ (discontinuity) in the master element I_α; see Figure 3.2.

The weak form of the discontinuous Galerkin method for solving the initial-value problem (9) approximately is as follows:

$$\int_0^1 \boldsymbol{J}\delta\boldsymbol{z}^h\cdot\Big[\big(\boldsymbol{z}^h\big)' - h_n\boldsymbol{J}DH(\boldsymbol{z}^h)\Big]\,d\alpha + \boldsymbol{J}\delta\boldsymbol{z}_1\cdot[\![\boldsymbol{z}^h]\!] = 0. \tag{18}$$

$k=1$	$\tilde{M}_1 = 1$	$\tilde{\boldsymbol{z}}_1 = \boldsymbol{z}_2 - \boldsymbol{z}_1$
$k=2$	$\tilde{M}_1 = 1-\alpha$	$\tilde{\boldsymbol{z}}_1 = -3\boldsymbol{z}_1 + 4\boldsymbol{z}_2 - \boldsymbol{z}_3$
	$\tilde{M}_2 = \alpha$	$\tilde{\boldsymbol{z}}_2 = \boldsymbol{z}_1 - 4\boldsymbol{z}_2 + 3\boldsymbol{z}_3$

Table 3.2 Reduced shape functions $\tilde{M}_I(\alpha)$ and associated quantities $\tilde{\boldsymbol{z}}_I$ for polynomial degree $k=1(1)2$.

Because of the presence of the term $\boldsymbol{J}\,\delta\boldsymbol{z}_1 \cdot [\![\boldsymbol{z}^h]\!]$, the initial condition is satisfied weakly.

Taking into account the finite element approximations (12) and (17), the weak form (18) furnishes the following system of equations (*general dG(k) method*):

$$\sum_{J=1}^{k+1} \int_0^1 M_I M_J' d\alpha\, \boldsymbol{z}_J - h_n \int_0^1 M_I \boldsymbol{J} DH(\boldsymbol{z}^h) d\alpha + \delta_{1I} [\![\boldsymbol{z}^h]\!] = \boldsymbol{0}, \tag{19}$$

for $I=1(1)k+1$, where we introduced the Kronecker delta δ_{1I} to express the identity $\delta\boldsymbol{z}_1 = \delta_{1I}\delta\boldsymbol{z}_I$.

Analogous to the continuous Galerkin cG(k) method, a specific time-stepping scheme is defined by fixing k and choosing a specific quadrature rule for calculating the integrals of DH.

3.3 The algorithmic Hamiltonian of the continuous Galerkin cG(k) method

Notation 3.3 In the following we refer to $H_i := H(\boldsymbol{z}_i)$, $i=0(1)k+1$, as the *algorithmic Hamiltonian* or the *algorithmic total energy*, respectively, at the ith node of the master element I_α.

Theorem 3.1 *The continuous Galerkin cG(k) method conserves an autonomous Hamiltonian H algorithmically.*

Proof. Consider the weak form (10) of the continuous Galerkin cG(k) method. Due to the arbitrariness of the $\{\delta\boldsymbol{z}_I\}_{I=1}^k$, the test functions may be written as

$$\delta\boldsymbol{z}^h = (\boldsymbol{z}^h)'. \tag{20}$$

Employing equation (20) in equation (10), the weak form takes the form

$$\int_0^1 \boldsymbol{J}\left(\boldsymbol{z}^h\right)' \cdot \left(\boldsymbol{z}^h\right)' d\alpha - h_n \int_0^1 \boldsymbol{J}\left(\boldsymbol{z}^h\right)' \cdot \boldsymbol{J} DH(\boldsymbol{z}^h) d\alpha = 0. \tag{21}$$

Owing to the skew-symmetry of the symplectic unit matrix $\boldsymbol{J}$, the first term vanishes and moreover, utilizing the orthogonality of $\boldsymbol{J}$, one obtains

$$\int_0^1 DH(\boldsymbol{z}^h) \cdot \left(\boldsymbol{z}^h\right)' d\alpha = 0. \tag{22}$$

On the other hand, the Fundamental Theorem of Calculus states for an autonomous Hamiltonian H

$$\int_0^1 H'(\alpha)\, d\alpha = \int_0^1 DH(\boldsymbol{z}^h) \cdot \left(\boldsymbol{z}^h\right)' d\alpha = H_{k+1} - H_1, \tag{23}$$

Applying equation (23) to equation (22) implies that an autonomous Hamiltonian is conserved algorithmically, that is, $H_{k+1} = H_1$. ■

3.4 The algorithmic Hamiltonian of the discontinuous Galerkin dG(k) method

Proposition 3.1 *Let the Hamiltonian H be convex with respect to z and autonomous. Then, the discontinuous Galerkin dG(k) method yields a decay of the algorithmic Hamiltonian $H(\boldsymbol{z}^h)$ for (i) constant time finite elements, that is, $k = 0$, in conjunction with an arbitrary potential V, and for (ii) arbitrary k if $DH(\boldsymbol{z}^h) = \boldsymbol{H}\boldsymbol{z}^h$, with $\boldsymbol{H} \in \mathcal{M}_{2n_{dof}}(\mathbb{R})$ being constant.*

Proof. Consider the weak form (18). Owing to the arbitrariness of the $\{\delta\boldsymbol{z}_I\}_{I=1}^{k+1}$, the test space is such that the following relationship between the trial functions and the test functions hold for (i) and (ii):

$$\delta\boldsymbol{z}^h = \boldsymbol{J}^{-1} DH(\boldsymbol{z}^h). \tag{24}$$

In the present case the Fundamental Theorem of Calculus can be written as

$$\int_0^1 DH(\boldsymbol{z}^h) \cdot \left(\boldsymbol{z}^h\right)' d\alpha = H_{k+1} - H_1. \tag{25}$$

Then, substituting from equation (24) into the weak form (18) leads to

$$H_{k+1} - H_1 + DH(\boldsymbol{z}_1) \cdot [\![\boldsymbol{z}^h]\!] = 0, \tag{26}$$

where the skew-symmetry of the symplectic unit matrix $\boldsymbol{J}$ has been taken into account.

On the other hand, write the algorithmic Hamiltonian $H_0 = H(\boldsymbol{z}_1 - [\![\boldsymbol{z}^h]\!])$ by means of Taylor's theorem in the following form:

$$H_0 = H_1 - DH(\boldsymbol{z}_1) \cdot [\![\boldsymbol{z}^h]\!] + Q_\xi([\![\boldsymbol{z}^h]\!]), \tag{27}$$

where $Q_\xi([\![\boldsymbol{z}^h]\!]) := \frac{1}{2}\,\boldsymbol{\mathcal{H}}_\xi[\![\boldsymbol{z}^h]\!] \cdot [\![\boldsymbol{z}^h]\!]$. The matrix $\boldsymbol{\mathcal{H}}_\xi := D^2H(\boldsymbol{z}_\xi)$ is defined as the *Hessian* of the Hamiltonian H at $\boldsymbol{z}_\xi$ with $\boldsymbol{z}_\xi \in [\boldsymbol{z}_0, \boldsymbol{z}_1]$.

Finally, replacing H_1 in equation (27) with equation (26), one obtains

$$H_{k+1} - H_0 = -Q_\xi([\![\boldsymbol{z}^h]\!]). \tag{28}$$

A convex Hamiltonian implies a positive definite quadratic form $Q_\xi([\![\boldsymbol{z}^h]\!])$. Therefore, according to equation (28) a convex Hamiltonian leads to a decay of the algorithmic Hamiltonian $H(\boldsymbol{z}^h)$. ■

Remark 3.6 Obviously, the latter case is fulfilled by a quadratic potential V; also see Hulbert [12].

3.5 Derivation of cG(1) time-stepping schemes using the general dG(1) method

Notation 3.4 We refer to *quadrature* as the approximated integration of an arbitrary function $f(\alpha)$ over I_α, that is,

$$\int_0^1 f(\alpha) d\alpha \approx \sum_{l=1}^{N_q} f(\alpha_l)\, w_l, \tag{29}$$

where $\{w_l\}_{l=1}^{N_q} \in \mathbb{R}$ and $\{\alpha_l\}_{l=1}^{N_q} \in I_\alpha$ denote the weights and points of the quadrature, respectively.

Proposition 3.2 *The general cG(1) and dG(1) methods generate identical time-stepping schemes with a continuous solution if one quadrature point at $\alpha = 1/2$ is employed.*

Proof. Consider the general dG(1) method, which reads

$$\frac{1}{2}\,\boldsymbol{z}_2 + \frac{1}{2}\,\boldsymbol{z}_1 - \boldsymbol{z}_0 - h_n \int_0^1 M_1 \boldsymbol{J} DH(\boldsymbol{z}^h) d\alpha = \boldsymbol{0}, \tag{30}$$

$$\frac{1}{2}\,\boldsymbol{z}_2 - \frac{1}{2}\,\boldsymbol{z}_1 - h_n \int_0^1 M_2 \boldsymbol{J} DH(\boldsymbol{z}^h) d\alpha = \boldsymbol{0}. \tag{31}$$

Addition of equation (30) and equation (31) renders

$$\boldsymbol{z}_2 - \boldsymbol{z}_0 - h_n \int_0^1 (M_1 + M_2)\, \boldsymbol{J} DH(\boldsymbol{z}^h) d\alpha = \boldsymbol{0}, \tag{32}$$

and subtracting equations (30), (31), one obtains

$$\boldsymbol{z}_1 - \boldsymbol{z}_0 + h_n \int_0^1 (M_2 - M_1)\, \boldsymbol{J} DH(\boldsymbol{z}^h) d\alpha = \boldsymbol{0}. \tag{33}$$

With the nodal shape functions $M_1 = 1 - \alpha$ and $M_2 = \alpha$, we obtain $M_1 + M_2 = 1$ and $M_2 - M_1 = 2\,\alpha - 1$.

Applying quadrature with one point at $\alpha = 1/2$ to the integrals in equations (32) and (33) yields the dG(1) time-stepping scheme

$$\boldsymbol{z}_2 - \boldsymbol{z}_0 - h_n\, \boldsymbol{W} \boldsymbol{J} DH(\boldsymbol{z}^h(\frac{1}{2})) = \boldsymbol{0}, \tag{34}$$

$$\boldsymbol{z}_1 - \boldsymbol{z}_0 = \boldsymbol{0}, \tag{35}$$

where

$$\boldsymbol{W} = \begin{bmatrix} w_p \boldsymbol{I} & \boldsymbol{O} \\ \boldsymbol{O} & w_q \boldsymbol{I} \end{bmatrix}. \tag{36}$$

The weights w_p and w_q are associated to the quadrature of $\partial_{\boldsymbol{p}} H$ and $\partial_{\boldsymbol{q}} H$, respectively.

Equation (35) is identical with the continuity condition (13). Therefore, the solution obtained by one quadrature point at $\alpha = 1/2$ is continuous. Employing equation (35) in equation (34) leads to

$$\boldsymbol{z}_2 - \boldsymbol{z}_1 - h_n \boldsymbol{W} \boldsymbol{J} DH(\boldsymbol{z}^h(\frac{1}{2})) = \boldsymbol{0}. \tag{37}$$

On the other hand, the general cG(1) method is given by

$$\boldsymbol{z}_2 - \boldsymbol{z}_1 - h_n \int_0^1 \boldsymbol{J} DH(\boldsymbol{z}^h) d\alpha = \boldsymbol{0}. \tag{38}$$

The time-stepping scheme (37) is identical with the scheme emanating from the general cG(1) method (38) associated with one quadrature point at $\alpha = 1/2$ ■

Remark 3.7 Employing one quadrature point in the general dG(1) method may be interpreted as 'reduced integration'. This term stems from the finite element method in space; see Hughes [10].

4 The one-body central force problem and linear time finite elements

This section contains a detailed investigation of the algorithmic properties of the cG(1) and dG(1) method. In this connection we apply both methods to a representative Hamiltonian system, namely the one-body central force problem.

4.1 Hamiltonian formulation

Consider the motion of a particle of mass m in the ambient three-dimensional Euclidean space $\mathbb{E}^3$ relative to an inertial coordinate system. Apply the Cartesian coordinates $\{q_i\}_{i=1}^{n_{dof}}$ to describe the $n_{dof} = 3$ degrees of freedom. Accordingly, with respect to a Cartesian basis $\{\boldsymbol{e}_i\}_{i=1}^{n_{dof}}$ the position of the particle can be described by the radius vector $\boldsymbol{r}(\boldsymbol{q}) := \sum_{j=1}^{3} q_j \boldsymbol{e}_j$. Let an external conservative central force field

$$\boldsymbol{F} = -\partial_{\boldsymbol{r}} V = -\frac{\mathrm{d}V(r)}{\mathrm{d}r} \boldsymbol{u}_r =: f(r)\, \boldsymbol{u}_r \tag{39}$$

act on the particle. Here, $r := \|\boldsymbol{r}\|$ is the magnitude of the radius vector with respect to the Euclidean norm $\|\bullet\|$, so the vector $\boldsymbol{u}_r := \boldsymbol{r}/r$ denotes the unit vector in direction of the radius vector and the scalar function f represents the magnitude of the external force $\boldsymbol{F}$.

Remark 4.1 Since the external force $\boldsymbol{F}$ is collinear with the radius vector $\boldsymbol{r}$, the orbits of the particle lie in a plane; see Arnold [1].

The Lagrangian $L = T - V$ of the natural system at hand is given by

$$L(\boldsymbol{q}, \dot{\boldsymbol{q}}) = \frac{1}{2} m\, \dot{\boldsymbol{r}}(\boldsymbol{q})^2 - V(r(\boldsymbol{q})) = \frac{1}{2} m \left(\partial_{\boldsymbol{q}} \boldsymbol{r} \cdot \dot{\boldsymbol{q}}\right)^2 - V(r(\boldsymbol{q})) = \frac{1}{2} m\, \dot{\boldsymbol{q}} \cdot \dot{\boldsymbol{q}} - V(\sqrt{\boldsymbol{q} \cdot \boldsymbol{q}}), \tag{40}$$

Furthermore, in view of definition (3), the generalized momentum vector $\boldsymbol{p}$ reads

$$\boldsymbol{p} = \partial_{\dot{\boldsymbol{q}}} L = m\, \dot{\boldsymbol{q}}, \tag{41}$$

where the differentiation rule for quadratic forms was used.

Remark 4.2 Owing to the application of Cartesian coordinates, the spaces $\mathbb{R}^3$ and $\mathbb{E}^3$ are homeomorphic and hence the generalized coordinate vector $\boldsymbol{q} \in \mathbb{R}^3$ and the generalized momentum vector $\boldsymbol{p} \in \mathbb{R}^3$ have the dimensions of the radius vector $\boldsymbol{r} \in \mathbb{E}^3$ and the linear momentum vector $\boldsymbol{P} \in \mathbb{E}^3$, respectively.

Substituting the generalized velocity vector in the total kinetic energy T with the generalized momentum vector (41) gives the Hamiltonian

$$H(\boldsymbol{q}, \boldsymbol{p}) = \frac{1}{2\,m}\,\boldsymbol{p} \cdot \boldsymbol{p} + V(\sqrt{\boldsymbol{q} \cdot \boldsymbol{q}}). \tag{42}$$

Remark 4.3 Despite the simplicity of the considered model problem, the structure of its Hamiltonian (42) coincides with that of much more involved problems such as nonlinear elastodynamics in semi-discrete form; see Betsch and Steinmann [3].

Concerning the potential $V(\boldsymbol{q})$ in (42), our investigations focus next on two distinct applications. Firstly, we consider Hooke's central force law, and secondly, we deal with arbitrary central force laws.

4.2 Hooke's central force law

4.2.1 The Hamiltonian

Hooke's central force law, also known as isotropic harmonic oscillator, is a linear restoring force connected with each degree of freedom; see Goldstein [8]. The associated potential is given by the quadratic form $V = -\frac{1}{2}\,\boldsymbol{q}^T(c\,\boldsymbol{I})\,\boldsymbol{q}$, where $c < 0$, with respect to the generalized coordinate vector. In accordance with equation (42), one obtains the Hamiltonian

$$H(\boldsymbol{q}, \boldsymbol{p}) = \frac{1}{2\,m}\,\boldsymbol{p}^T\boldsymbol{I}\,\boldsymbol{p} - \frac{1}{2}\,c\,\boldsymbol{q}^T\boldsymbol{I}\,\boldsymbol{q}. \tag{43}$$

Using symplectic notation, equation (43) can be written in the form

$$H = \frac{1}{2}\,\boldsymbol{z}^T\boldsymbol{H}\,\boldsymbol{z}, \tag{44}$$

where $\boldsymbol{H} \in \mathcal{M}_{2n_{dof}}(\mathbb{R})$ is a 6×6 matrix of the form

$$\boldsymbol{H} = \begin{bmatrix} -c\,\boldsymbol{I} & \boldsymbol{O} \\ \boldsymbol{O} & \frac{1}{m}\,\boldsymbol{I} \end{bmatrix}. \tag{45}$$

Accordingly, the Jacobian is given by

$$DH(\boldsymbol{z}) = \boldsymbol{H}\,\boldsymbol{z}. \tag{46}$$

4.2.2 The algorithmic total energy

According to equation (44), the algorithmic total energy H_{k+1} at the last node of the master element is given by

$$H_{k+1} = \frac{1}{2}\,\boldsymbol{z}_{k+1}^T\,\boldsymbol{H}\,\boldsymbol{z}_{k+1}. \tag{47}$$

In the present case, a specific time-stepping scheme generated by the cG(k) or dG(k) method, respectively, can be cast in the form

$$\boldsymbol{z}_{k+1} = \boldsymbol{A}_k\,\boldsymbol{z}_0, \tag{48}$$

where for the cG(k) method the continuity condition (13) is to be included. The matrix $\boldsymbol{A}_k \in \mathcal{M}_{2n_{dof}}(\mathbb{R})$ denotes the so-called *amplification matrix*. According to Richtmyer and Morton [17], we refer to (48) as the two-level scheme of the cG(k) or dG(k) method, respectively. Furthermore, referring to Gantmacher [7], one is able to substitute the so-called Lagrange-Sylvester's interpolation polynomial of $\boldsymbol{A}_k$ for the matrix $\boldsymbol{A}_k$ itself.

Remark 4.4 The Lagrange-Sylvester's interpolation polynomial is attributed to Sylvester [20].

If the roots $\{\lambda_i\}_{i=1}^{N_m}$ of the minimal polynomial pertaining to $\boldsymbol{A}_k$ are distinct, one has

$$\boldsymbol{A}_k = \sum_{i=1}^{N_m} \boldsymbol{A}_{k,i}\, \lambda_i. \tag{49}$$

The matrices $\{\boldsymbol{A}_{k,i}\}_{i=1}^{N_m} \in \mathcal{M}_{2n_{dof}}(\mathbb{C})$ are called the *constituent matrices* of the Lagrange-Sylvester's interpolation polynomial of $\boldsymbol{A}_k$. For distinct roots $\{\lambda_i\}_{i=1}^{N_m}$, one has

$$\boldsymbol{A}_{k,i} = \prod_{\substack{j=1 \\ j\neq i}}^{N_m} \frac{\boldsymbol{A}_k - \lambda_j \boldsymbol{1}}{\lambda_i - \lambda_j}, \quad i = 1(1)N_m. \tag{50}$$

Remark 4.5 The representation of a square matrix with distinct roots of the corresponding minimal polynomial by the Lagrange-Sylvester's interpolation as above corresponds with the spectral representation of a symmetric second-order tensor in connection with the Serrin formula; see Morman [16].

Notation 4.1 Let us refer to *exact quadrature* as the exact integration of functions $f(\alpha)$ over I_α.

Proposition 4.1 *The cG(1) method associated with exact quadrature preserves the algorithmic total energy.*

We use the following lemmas for the proof.

Lemma 4.1 *The algorithmic total energy H_2 determined by the cG(1) method associated with exact quadrature is given by $H_2 = \rho^2 H_0$, where ρ denotes the spectral radius of the amplification matrix.*

Proof. Consider the general cG(1) method (38). Employ the Jacobian (46) and compute the integral by using exact quadrature. The amplification matrix of the arising time-stepping scheme takes the form

$$\boldsymbol{A}_1 = \frac{1}{1+\frac{\Omega^2}{4}} \begin{bmatrix} (1-\frac{\Omega^2}{4})\, \boldsymbol{I} & \frac{h_n}{m}\, \boldsymbol{I} \\ h_n\, c\, \boldsymbol{I} & (1-\frac{\Omega^2}{4})\, \boldsymbol{I} \end{bmatrix}, \tag{51}$$

where according to Hughes and Liu [11] $\Omega := h_n\, \omega$ is called the *sampling frequency* and $\omega := \sqrt{-c/m}$, $c<0$, denotes the eigenfrequency of the isotropic harmonic oscillator. The eigenvalues of the amplification matrix (51) are given by

$$\lambda_1 = \lambda_3 = \lambda_5 = \frac{4 - \Omega^2 + i\, 4\, \Omega}{4 + \Omega^2}, \qquad \lambda_2 = \lambda_4 = \lambda_6 = \overline{\lambda_1} = \overline{\lambda_3} = \overline{\lambda_5}, \tag{52}$$

where i denotes the imaginary unit and the overline indicates the complex conjugate. Accordingly, the amplification matrix (51) has multiple eigenvalues, that is, the characteristic polynomial

$$P_c(\lambda) = \prod_{i=1}^{6} (\lambda - \lambda_i) = ((\lambda - \lambda_1)\, (\lambda - \lambda_2))^3 \tag{53}$$

of $\boldsymbol{A}_1$ has multiple roots. According to the characteristic polynomial (53), the minimal polynomial $P_m(\lambda)$ is given by $P_m(\lambda) = (\lambda - \lambda_1)\, (\lambda - \lambda_2)$. Obviously, it is $N_m = \deg(P_m) = 2$, where $\deg(P_m)$ denotes the degree of the minimal polynomial. Determining the constituent matrices in view of equation (50) furnishes

$$\boldsymbol{A}_{1,1} = \frac{1}{2} \begin{bmatrix} \boldsymbol{I} & \frac{1}{i\,\omega\, m}\, \boldsymbol{I} \\ i\,\omega\, m\, \boldsymbol{I} & \boldsymbol{I} \end{bmatrix}, \qquad \boldsymbol{A}_{1,2} = \frac{1}{2} \begin{bmatrix} \boldsymbol{I} & \frac{-1}{i\,\omega\, m}\, \boldsymbol{I} \\ -i\,\omega\, m\, \boldsymbol{I} & \boldsymbol{I} \end{bmatrix}. \tag{54}$$

After employing equations (48) and (49) in equation (47), the algorithmic total energy H_2 is given by

$$H_2 = \frac{1}{2}\, \rho^2\, \boldsymbol{z}_0^T \left(\sum_{\substack{i,j=1 \\ j\neq i}}^{2} \boldsymbol{A}_{1,i}^T\, \boldsymbol{H}\, \boldsymbol{A}_{1,j} \right) \boldsymbol{z}_0 + \frac{1}{2}\, \boldsymbol{z}_0^T \left(\sum_{i=1}^{2} \lambda_i^2 \boldsymbol{A}_{1,i}^T\, \boldsymbol{H}\, \boldsymbol{A}_{1,i} \right) \boldsymbol{z}_0, \tag{55}$$

where ρ denotes the spectral radius $\rho(\boldsymbol{A}_k) := \max|\lambda_i| = \sqrt{\lambda_1 \lambda_2}$, $i = 1(1) N_m$, because the roots λ_1 and λ_2 are complex conjugate. The constituent matrices (54) satisfy the conditions

$$\sum_{\substack{i,j=1 \\ j \neq i}}^{2} \boldsymbol{A}_{1,i}^T \boldsymbol{H} \boldsymbol{A}_{1,j} = \boldsymbol{H}, \qquad \boldsymbol{A}_{1,i}^T \boldsymbol{H} \boldsymbol{A}_{1,i} = \boldsymbol{O}_2, \quad i = 1(1)2, \tag{56}$$

where $\boldsymbol{O}_2 \in \mathcal{M}_{2n_{dof}}(\mathbb{R})$ denotes the $2n_{dof} \times 2n_{dof}$ zero matrix. Employing the equations (56) in equation (55) leads for $k=1$ to $H_2 = \frac{1}{2} \rho^2 \boldsymbol{z}_0^T \boldsymbol{H} \boldsymbol{z}_0 = \rho^2 H_0$, so that for the cG(1) method $H_0 = H_1$ by the continuity condition (13). ■

Lemma 4.2 *The amplification matrix of the cG(1) method associated with exact quadrature has a squared spectral radius equal to one, that is,* $\rho^2 = 1$.

Proof. By the eigenvalues (52), the squared spectral radius $\rho^2 = \lambda_1 \lambda_2$ results in $\rho^2 = 1$. ■

Proof of Proposition 4.1 By Lemma 4.1 in conjunction with Lemma 4.2 the algorithmic total energy is preserved in the sense $H_2 = H_0$ (see Figure 4.1), as already pointed out in Subsection 3.3. ■

Definition 4.1 We say that the quadrature is *symmetric* if the quadrature points $\alpha_1 < \alpha_2 < \ldots < \alpha_{N_q}$ and the associated weights $w_1, \ldots, w_{N_q}$ satisfy $1 = \alpha_{N_q - i} + \alpha_{1+i}$ and $w_{N_q - i} = w_{1+i}$, $i = 0(1)\mathrm{int}([N_q - 1]/2)$, respectively. The function $\mathrm{int}(\bullet)$ gives the integer part of its argument.

Remark 4.6 The conditions in Definition 4.1 mean (i) that the quadrature points lie in pairs $(\alpha_{N_q - i}, \alpha_{1+i})$ symmetrical to the midpoint of I_α ($\alpha = 1/2$) and, additionally, a quadrature point exists at $\alpha = 1/2$ for an odd number of quadrature points and (ii) that the weights $(w_{N_q - i}, w_{1+i})$ of the quadrature points pertaining to such a pair $(\alpha_{N_q - i}, \alpha_{1+i})$ are identical.

Remark 4.7 For example, according to Schwarz [19], the Gaussian quadrature, whose quadrature points are identical to the zeros of the Legendre polynomials relating to I_α, is symmetric. Further, the trapezoidal rule with a quadrature point on each boundary of the master element I_α is also symmetric.

Remark 4.8 Note that the midpoint rule is identical to the Gaussian quadrature with one quadrature point.

Proposition 4.2 *The cG(1) method associated with symmetric quadrature conserves the algorithmic total energy.*

The proof rests upon the following lemmas.

Lemma 4.3 *The algorithmic total energy calculated by the cG(1) method associated with quadrature reads* $H_2 = \rho^2 H_0$, *where* ρ *denotes the spectral radius of the amplification matrix.*

Proof. Using quadrature to approximate the integral of the general cG(1) method (38), the amplification matrix of the arising time-stepping scheme is given by

$$\boldsymbol{A}_1 = \frac{1}{1 + \beta_2^2 \Omega^2} \begin{bmatrix} (1 + \beta_1 \beta_2 \Omega^2) \boldsymbol{I} & \frac{h_n}{m} (\beta_1 + \beta_2) \boldsymbol{I} \\ h_n c (\beta_1 + \beta_2) \boldsymbol{I} & (1 + \beta_1 \beta_2 \Omega^2) \boldsymbol{I} \end{bmatrix}, \tag{57}$$

where we have introduced

$$\beta_i := \sum_{l=1}^{N_q} M_i(\alpha_l) w_l, \quad i = 1(1)k+1. \tag{58}$$

Regarding the amplification matrix (57), the constituent matrices also take the form of the matrices (54), so that by Lemma 4.1 the algorithmic total energy reads $H_2 = \frac{1}{2} \rho^2 \boldsymbol{z}_0^T \boldsymbol{H} \boldsymbol{z}_0 = \rho^2 H_0$, whereby $H_0 = H_1$ for the cG(1) method owing to equation (13). ■

Lemma 4.4 *The amplification matrix of the cG(1) method associated with symmetric quadrature has a squared spectral radius equal to one, that is,* $\rho^2 = 1$.

Proof. The squared spectral radius ρ^2 corresponding to the amplification matrix (57) is given by

$$\rho^2 = \frac{1 + \beta_1^2 \Omega^2}{1 + \beta_2^2 \Omega^2}. \tag{59}$$

Accordingly, $\rho^2 = 1$ leads to the following restriction on the quadrature rules:

$$\beta_1^2 = \beta_2^2. \tag{60}$$

Considering the definition of the $\{\beta_i\}_{i=1}^2$ in equation (58), the restriction takes the form:

$$\sum_{l=1}^{N_q} (1 - 2\,\alpha_l) w_l = 0, \tag{61}$$

Taking into consideration Definition 4.1, one obtains

$$\sum_{l=1}^{N_q} (1 - 2\,\alpha_l) w_l = \sum_{l=0}^{\nu} 2\left(1 - \alpha_{1+l} - \alpha_{N_q - l}\right) w_{1+l} = 0, \tag{62}$$

where $\nu = \mathrm{int}(N_q/2)$. Consequently, for arbitrary weights the parentheses have to vanish separately, which is fulfilled by symmetric quadrature. Therefore, symmetric quadrature renders $\rho^2 = 1$. ■

Proof of Proposition 4.2 By Lemma 4.3 the algorithmic conservation condition is $\rho^2 = 1$. This condition is fulfilled by symmetric quadrature in view of Lemma 4.4. Consequently, symmetric quadrature conserves the total energy of the cG(1) method algorithmically. ■

Corollary 4.1 *The midpoint rule preserves the algorithmic total energy computed with the cG(1) method.*

Proof. The midpoint rule is according to Definition 4.1 a symmetric one-point quadrature rule. By Proposition 4.2 the algorithmic total energy determined by the cG(1) method is preserved for symmetric quadrature; see Figure 4.2. ■

Proposition 4.3 *The algorithmic total energy determined by the dG(1) method associated with exact quadrature decays, that is,* $H_2 < H_0$.

The proof relies on the following lemmas.

Lemma 4.5 *The algorithmic total energy* H_2 *determined by the dG(1) method associated with exact quadrature is given by* $H_2 = \rho^2 H_0$, *where* ρ *denotes the spectral radius of the amplification matrix.*

Proof. Consider the general dG(1) method (30), (31) in conjunction with the Jacobian (46) and exactly evaluated integrals. The elimination of the internal node $\boldsymbol{z}_1$ leads to a two-level scheme with the amplification matrix

$$\boldsymbol{A}_1 = \frac{-2}{\Omega^4 + 4\,\Omega^2 + 36} \begin{bmatrix} (7\,\Omega^2 - 18)\,\boldsymbol{I} & \frac{h_n}{m}\,(\Omega^2 - 18)\,\boldsymbol{I} \\ h_n\,c\,(\Omega^2 - 18)\,\boldsymbol{I} & (7\,\Omega^2 - 18)\,\boldsymbol{I} \end{bmatrix}. \tag{63}$$

The constituent matrices $\boldsymbol{A}_{1,1}$, $\boldsymbol{A}_{1,2}$ pertaining to the amplification matrix (63) and the matrices (54) of the cG(1) method are identical. Hence the algorithmic total energy at the node 2 is according to Lemma 4.1 given by $H_2 = \rho^2 H_0$. ■

Lemma 4.6 *The amplification matrix of the dG(1) method associated with exact quadrature has a squared spectral radius being less than one, that is,* $\rho^2 < 1$.

Proof. The eigenvalues of the amplification matrix (63) read

$$\lambda_1 = \lambda_3 = \lambda_5 = -2\,\frac{7\,\Omega^2 - 18 + i\,\Omega\,\left(\Omega^2 - 18\right)}{\Omega^4 + 4\,\Omega^2 + 36}, \qquad \lambda_2 = \lambda_4 = \lambda_6 = \overline{\lambda_1} = \overline{\lambda_3} = \overline{\lambda_5}, \tag{64}$$

where i denotes the imaginary unit; also see Hulbert [13] and Ruge [18]. Thus, the squared spectral radius $\rho^2 = \lambda_1 \lambda_2$ is given by

$$\rho^2 = \frac{4\,\Omega^2 + 36}{\Omega^4 + 4\,\Omega^2 + 36}. \tag{65}$$

Since the denominator is larger than the numerator for all sampling frequencies $\Omega \neq 0$, the squared spectral radius ρ^2 is less than one. ■

Proof of Proposition 4.3 By Lemma 4.6 the squared spectral radius is less than one, so that the algorithmic total energy decays in view of Lemma 4.5; see Figure 4.1. ■

Proposition 4.4 *Considering symmetric quadrature, only one quadrature point preserves the algorithmic total energy computed with the dG(1) method. In all other cases the algorithmic total energy decays.*

The proof rests upon the following lemmas.

Lemma 4.7 *The algorithmic total energy calculated by the dG(1) method associated with quadrature reads* $H_2 = \rho^2\,H_0$, *where* ρ *denotes the spectral radius of the amplification matrix.*

Proof. Consider the general dG(1) method (30), (31). Employing the Jacobian (46) and approximating the integral by using quadrature, one obtains

$$\left(\frac{1}{2}\mathbf{1} - \beta_{12} h_n \boldsymbol{J}\boldsymbol{H}\right) \boldsymbol{z}_2 + \left(\frac{1}{2}\mathbf{1} - \beta_{11} h_n \boldsymbol{J}\boldsymbol{H}\right) \boldsymbol{z}_1 - \boldsymbol{z}_0 = \mathbf{0}, \tag{66}$$

$$\left(\frac{1}{2}\mathbf{1} - \beta_{22} h_n \boldsymbol{J}\boldsymbol{H}\right) \boldsymbol{z}_2 - \left(\frac{1}{2}\mathbf{1} + \beta_{12} h_n \boldsymbol{J}\boldsymbol{H}\right) \boldsymbol{z}_1 = \mathbf{0}, \tag{67}$$

where

$$\beta_{ij} = \sum_{l=1}^{N_q} M_i(\alpha_l)\, M_j(\alpha_l)\, w_l, \quad i,j = 1(1)k{+}1. \tag{68}$$

Because of the complicated terms, we omit an explicit representation of the amplification matrix. The constituent matrices pertaining to the time-stepping scheme (66), (67) are identical with the matrices (54) of the cG(1) method. Therefore, the algorithmic total energy is, in view of Lemma 4.1, given by $H_2 = \rho^2\,H_0$. ■

Lemma 4.8 *Applying symmetric quadrature to the dG(1) method, only one quadrature point can lead to a squared spectral radius of the respective amplification matrix being equal to one, that is,* $\rho^2 = 1$. *In all other cases* $\rho^2 < 1$ *holds.*

Proof. The squared spectral radius corresponding to the time-stepping scheme (66), (67) reads

$$\rho^2 = \frac{1 + 4\beta_{12}^2\Omega^2}{1 + 4\beta_{12}^2\Omega^2 + \left(\beta_{22} - \beta_{11}\right)^2 \Omega^2 + 4\left(\beta_{12}^2 - \beta_{11}\beta_{22}\right)^2 \Omega^4}. \tag{69}$$

Consequently, for sampling frequencies $\Omega \neq 0$ the squared spectral radius is equal to one if

$$\beta_{11} = \beta_{22}, \tag{70}$$

$$\beta_{12}^2 = \beta_{22}^2. \tag{71}$$

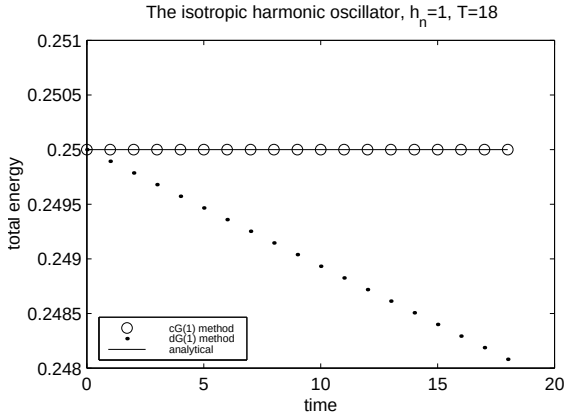

Figure 4.1 Total energy $H = H(t)$ of an isotropic harmonic oscillator with mass $m = 2$, total energy $H = 0.25$ and potential constant $c = -0.25$. Computed with the cG(1) and dG(1) method with $h_n = 1$.

Otherwise the squared spectral radius is less than one for $\Omega \neq 0$. The relation (70) is equivalent to equation (60), so that symmetric quadrature satisfies condition (70). Moreover, considering symmetric quadrature, equation (71) leads to

$$\sum_{l=0}^{N_q} \alpha_l \, (1 - 2\,\alpha_l) \, w_l = \sum_{l=0}^{\nu} \left(-1 + 4\,\alpha_{1+l} - 4\,\alpha_{1+l}^2\right) w_{1+l} = \sum_{l=0}^{\nu} (-4) \left(\frac{1}{2} - \alpha_{1+l}\right)^2 w_{1+l} = 0, \tag{72}$$

where $\nu = \mathrm{int}(N_q/2)$. To fulfill equation (72) for arbitrary weights the parentheses have to vanish separately. Therefore, one finds that solely one quadrature point at $\alpha = 1/2$ fulfills equation (70) as well as equation (71). ■

Proof of Proposition 4.4 According to Lemma 4.7, algorithmic total energy conservation demands $\rho^2 = 1$. Taking into account Lemma 4.8, the algorithmic total energy conservation is only given by applying symmetric one-point quadrature. ■

Corollary 4.2 *The midpoint rule preserves the algorithmic total energy computed with the dG(1) method.*

Proof. By Definition 4.1, the midpoint rule is a symmetric one-point quadrature rule. Hence, according to Proposition 4.4 the algorithmic total energy determined by the dG(1) method is preserved; see Figure 4.2. ■

Figure 4.3 demonstrates a comparison of the spectral radii pertaining to the dG(1) method associated with specific quadrature rules. We are able to see that the quadrature influences the frequency region in which the spectral radius ρ has a strong slope. Accordingly, the applied quadrature affects the frequency range of numerical dissipation.

4.2.3 The algorithmic total angular momentum

Consider the isotropic harmonic oscillator. This subsection deals with the total angular momentum $\boldsymbol{L}$ of a particle of mass m.

Referring to Subsection 2.4, the total angular momentum $\boldsymbol{L}$ is defined as $\boldsymbol{L} = \boldsymbol{r} \times \boldsymbol{P}$. By Remark 4.2, the use of Cartesian coordinates leads to the total angular momentum determined by $\boldsymbol{L} = \boldsymbol{q} \times \boldsymbol{p}$. However, within our computational setting, we are interested in the algorithmic total angular momentum $\boldsymbol{L}_{k+1}$, given by

$$\boldsymbol{L}_{k+1} = \boldsymbol{q}_{k+1} \times \boldsymbol{p}_{k+1}, \tag{73}$$

where the index indicates the value at the $k+1$ node of the master element I_α pertaining to our Galerkin finite element discretization.

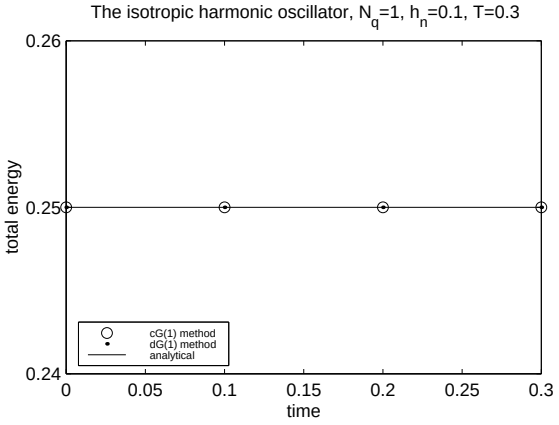

Figure 4.2 Total energy $H = H(t)$ of an isotropic harmonic oscillator with mass $m = 2$, total energy $H = 0.25$ and potential constant $c = -0.25$. Computed with the cG(1) and dG(1) method associated with the midpoint rule ($N_q = 1$) and with a time step size $h_n = 0.1$.

Remark 4.9 Owing to equation (13), $L_0 = L_1$ for the cG(k) method.

Proposition 4.5 *Considering exact quadrature or quadrature, the algorithmic total angular momentum $\boldsymbol{L}_2$ determined by the cG(1) or the dG(1) method is given by $\boldsymbol{L}_2 = \rho^2 \boldsymbol{L}_0$, where ρ denotes the spectral radius of the respective amplification matrix.*

Proof. To obtain the generalized coordinate vector $\boldsymbol{q}_{k+1}$ and the generalized momentum vector $\boldsymbol{p}_{k+1}$ in dependence of the initial values $\boldsymbol{q}_0$ and $\boldsymbol{p}_0$, we consider the two-level scheme (48) in conjunction with the amplification matrix (49). The minimal polynomial of the isotropic harmonic oscillator has two distinct roots ($N_m = 2$), so that we get the two-level scheme $\boldsymbol{z}_{k+1} = \sum_{i=1}^{2} \lambda_i \boldsymbol{A}_{k,i} \boldsymbol{z}_0$. However, the determination of the algorithmic total angular momentum requires leaving the symplectic notation:

$$\begin{bmatrix} \boldsymbol{q}_{k+1} \\ \boldsymbol{p}_{k+1} \end{bmatrix} = \sum_{i=1}^{2} \lambda_i \begin{bmatrix} \boldsymbol{A}_{k,i}^{(1,1)} & \boldsymbol{A}_{k,i}^{(1,2)} \\ \boldsymbol{A}_{k,i}^{(2,1)} & \boldsymbol{A}_{k,i}^{(2,2)} \end{bmatrix} \begin{bmatrix} \boldsymbol{q}_0 \\ \boldsymbol{p}_0 \end{bmatrix}, \tag{74}$$

where the matrices $\{\boldsymbol{A}_{k,i}^{(l,m)}\}_{l,m=1}^{2} \in \mathcal{M}_{n_{dof}}(\mathbb{C})$ denote the four $n_{dof} \times n_{dof}$ blocks of the constituent matrix $\boldsymbol{A}_{k,i} \in \mathcal{M}_{2n_{dof}}(\mathbb{C})$, $i = 1(1)2$.

For the cG(1) method as well as for the dG(1) method, one obtains the constituent matrices (54) by applying exact quadrature as well as quadrature, so that the blocks of the constituent matrices have the form $\boldsymbol{A}_{1,i}^{(l,m)} = a_{1,i}^{(l,m)} \boldsymbol{I}$. Thus expansion of the matrices on the right side and introduction of an explicit representation leads to the following two equations:

$$\begin{aligned} \boldsymbol{q}_2 &= \textstyle\sum_{i=1}^{2} \lambda_i \, a_{1,i}^{(1,1)} \, \boldsymbol{q}_0 + \sum_{i=1}^{2} \lambda_i \, a_{1,i}^{(1,2)} \, \boldsymbol{p}_0, \\ \boldsymbol{p}_2 &= \textstyle\sum_{i=1}^{2} \lambda_i \, a_{1,i}^{(2,1)} \, \boldsymbol{q}_0 + \sum_{i=1}^{2} \lambda_i \, a_{1,i}^{(2,2)} \, \boldsymbol{p}_0. \end{aligned} \tag{75}$$

We employ the equations (75) in the equation (73) and obtain after a simplification

$$\boldsymbol{L}_2 = \sum_{i,j=1}^{2} \lambda_i \, \lambda_j \left(a_{1,i}^{(1,1)} \, a_{1,j}^{(2,2)} - a_{1,i}^{(1,2)} \, a_{1,j}^{(2,1)} \right) \boldsymbol{L}_0. \tag{76}$$

The coefficients of the constituent matrices (54) pertaining to the main diagonal blocks are identical one half, that is, $a_{1,i}^{(l,l)} = 1/2$, $l = 1(1)2$, and the coefficients pertaining to the off-diagonal blocks satisfy the identities $a_{1,i}^{(1,2)} \, a_{1,j \neq i}^{(2,1)} = -1/4$ and $a_{1,i}^{(1,2)} \, a_{1,j=i}^{(2,1)} = 1/4$, so that $\boldsymbol{L}_2 = \rho^2 \boldsymbol{L}_0$, where $\rho^2 = \lambda_1 \, \lambda_2$ denotes the squared spectral radius. ■

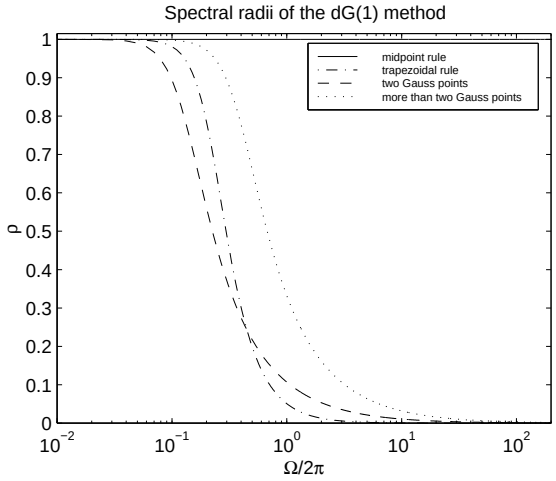

Figure 4.3 Spectral radii of the dG(1) method associated with specific symmetric quadratures.

Corollary 4.3 *The algorithmic total angular momentum calculated with the cG(1) method associated with exact quadrature is preserved.*

Proof. According to Lemma 4.2, the squared spectral radius of the cG(1) method associated with exact quadrature is equal to one. Accordingly, by Proposition 4.5 the algorithmic total angular momentum is preserved in the sense that $\boldsymbol{L}_2 = \boldsymbol{L}_0 = \boldsymbol{L}_1$; see Figure 4.4. ■

Corollary 4.4 *The algorithmic total angular momentum calculated with the cG(1) method associated with symmetric quadrature is preserved.*

Proof. By Lemma 4.4 the squared spectral radius of the amplification matrix pertaining to the cG(1) method associated with symmetric quadrature is given by $\rho^2 = 1$. According to Proposition 4.5, $\rho^2 = 1$ implies algorithmic total angular momentum conservation. ■

Corollary 4.5 *The algorithmic total angular momentum determined by the dG(1) method associated with exact quadrature decays, that is,* $\boldsymbol{L}_2 < \boldsymbol{L}_0$.

Proof. In view of Lemma 4.6, applying exact quadrature to the dG(1) method furnishes a squared spectral radius being less than one, so that according to Proposition 4.5 the algorithmic total angular momentum decays; see Figure 4.4. ■

Corollary 4.6 *Considering the dG(1) method associated with symmetric quadrature, solely one quadrature point preserves the algorithmic total angular momentum. In all other cases the algorithmic total angular momentum decays.*

Proof. With regard to Proposition 4.5, the algorithmic total angular momentum decays if the squared spectral radius ρ^2 is less than one and is preserved if $\rho^2 = 1$ is fulfilled. By Lemma 4.8 only one symmetric quadrature point satisfying $\rho^2 = 1$, in all other cases $\rho^2 < 1$ holds, so that the algorithmic total angular momentum decays. ■

Corollary 4.7 *The cG(1) method associated with the midpoint rule preserves the algorithmic total angular momentum.*

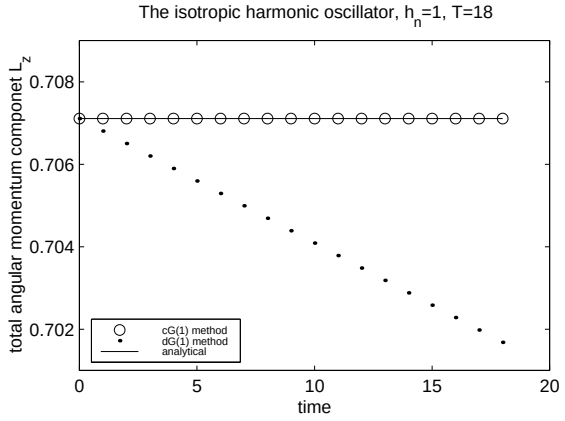

Figure 4.4 The nonvanishing total angular momentum component $L_\zeta = L_\zeta(t)$, where the ζ-axis is perpendicular to the plane of motion, of an isotropic harmonic oscillator with mass $m=2$, total energy $H=0.25$ and potential constant $c=-0.25$. Computed with the cG(1) and dG(1) method with a time step size $h_n=1$.

Proof. The midpoint rule is according to Definition 4.1 a symmetric one-point quadrature rule. Therefore, by Corollar 4.4 the cG(1) method preserves the total angular momentum; see Figure 4.5. ■

Corollary 4.8 *The dG(1) method associated with the midpoint rule preserves the algorithmic total angular momentum.*

Proof. By Definition 4.1, the midpoint rule is a symmetric one-point quadrature rule. Therefore, according to Corollar 4.6 the total angular momentum determined by the dG(1) method is preserved; see Figure 4.5. ■

4.3 Arbitrary central force laws

4.3.1 The Hamiltonian

Owing to equation (42), the Hamiltonian of the one-body central force problem reads

$$H(\boldsymbol{q},\boldsymbol{p}) = \frac{1}{2\,m}\,\boldsymbol{p}^T\boldsymbol{I}\,\boldsymbol{p} + V(r), \tag{77}$$

where $r = \sqrt{\boldsymbol{q}^T\boldsymbol{I}\,\boldsymbol{q}}$ denotes the magnitude of the radius vector $\boldsymbol{r}$. Consequently, the Jacobian $DH(\boldsymbol{z})$ takes the form

$$DH = \begin{bmatrix} \partial_{\boldsymbol{q}} V \\ \frac{1}{m}\,\boldsymbol{I}\,\boldsymbol{p} \end{bmatrix} = \begin{bmatrix} -f(r)\,\partial_{\boldsymbol{q}} r \\ \frac{1}{m}\,\boldsymbol{I}\,\boldsymbol{p} \end{bmatrix} = \begin{bmatrix} -\frac{f(r)}{r}\,\boldsymbol{I}\,\boldsymbol{q} \\ \frac{1}{m}\,\boldsymbol{I}\,\boldsymbol{p} \end{bmatrix}, \tag{78}$$

where $f(r) = -dV(r)/dr$ indicates the magnitude of the conservative central force according to equation (39). Hence it follows that the Jacobian matrix $DH(\boldsymbol{z})$ can be written as

$$DH(\boldsymbol{z}) = \boldsymbol{H}(\boldsymbol{z})\,\boldsymbol{z}, \tag{79}$$

where

$$\boldsymbol{H}(\boldsymbol{z}) = \begin{bmatrix} -\frac{f(r)}{r}\,\boldsymbol{I} & \boldsymbol{O} \\ \boldsymbol{O} & \frac{1}{m}\,\boldsymbol{I} \end{bmatrix}. \tag{80}$$

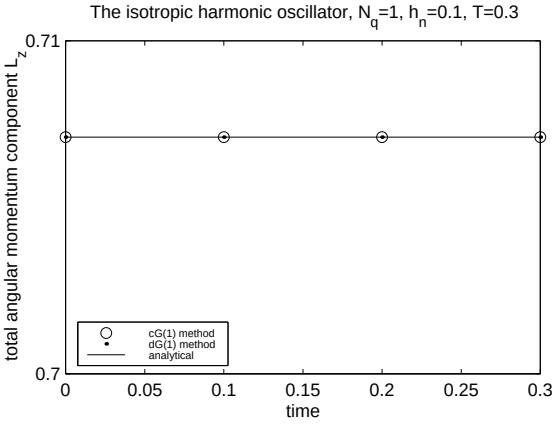

Figure 4.5 The nonvanishing total angular momentum component $L_\zeta = L_\zeta(t)$, where the ζ-axis is perpendicular to the plane of motion, of an isotropic harmonic oscillator with mass $m=2$, total energy $H=0.25$ and potential constant $c=-0.25$. Computed with the cG(1) and dG(1) method associated with the midpoint rule ($N_q=1$) and with a time step size $h_n=0.1$.

4.3.2 The algorithmic total energy conservation

Proposition 4.6 *The cG(1) method associated with symmetric one-point quadrature only conserves the algorithmic total energy by employing particular weights.*

Proof. According to Section 3.3 we achieve algorithmic total energy conserving time-stepping schemes by the general cG(k) method if the quadrature satisfies the Fundamental Theorem of Calculus, that is, the applied quadrature has to fulfill equation (23) which is equivalent to

$$\int_0^1 \left(\partial_{\boldsymbol{q}} H \cdot \boldsymbol{q}' + \partial_{\boldsymbol{p}} H \cdot \boldsymbol{p}'\right) d\alpha = H(\alpha)|_{\alpha=0}^{\alpha=1}. \tag{81}$$

We consider natural systems, therefore equation (81) can be written as

$$\int_0^1 \partial_{\boldsymbol{q}} V \cdot \boldsymbol{q}' d\alpha - V(\alpha)|_{\alpha=0}^{\alpha=1} = T(\alpha)|_{\alpha=0}^{\alpha=1} - \int_0^1 \partial_{\boldsymbol{p}} T \cdot \boldsymbol{p}' d\alpha. \tag{82}$$

Now if the Fundamental Theorem of Calculus is satisfied for the potential energy V as well as for the kinetic energy T, both sides of equation (82) vanish and therefore equation (81) is identically fulfilled. By exact quadrature the Fundamental Theorem of Calculus is always fulfilled, however, quadrature does not fulfill the Fundamental Theorem of Calculus in general.

Let us consider the cG(1) time-stepping scheme (37) emanating from symmetric quadrature with one quadrature point. We employ the Jacobian (79) and quit the symplectic notation. Ultimately, we obtain

$$\boldsymbol{q}_2 - \boldsymbol{q}_1 - \frac{h_n}{m} w_p \boldsymbol{p}^h(\frac{1}{2}) = \boldsymbol{0}, \tag{83}$$

$$\boldsymbol{p}_2 - \boldsymbol{p}_1 - h_n w_q \frac{f(r^h(1/2))}{r^h(1/2)} \boldsymbol{q}^h(\frac{1}{2}) = \boldsymbol{0}. \tag{84}$$

As aforementioned, the condition for algorithmic total energy conservation is the fulfillment of the Fundamental Theorem of Calculus for the potential energy V as well as for the kinetic energy T. Therefore, the weights w_q and w_p are determined such that this conditions hold; see Betsch and Steinmann [4].

With regard to the Jacobian (79), the conditions read

$$T_2 - T_1 = \int_0^1 \frac{1}{m} \boldsymbol{p}^h \cdot \left(\boldsymbol{p}^h\right)' d\alpha, \tag{85}$$

$$V_2 - V_1 = -\int_0^1 \frac{f(r^h)}{r^h} \boldsymbol{q}^h \cdot \left(\boldsymbol{q}^h\right)' d\alpha. \tag{86}$$

Considering linear time finite elements, employing the trial function $\boldsymbol{p}^h = \sum_{i=1}^2 M_i\, \boldsymbol{p}_i$, where $M_1 = 1-\alpha$ and $M_2 = \alpha$ are the nodal shape functions, in equation (85) and applying symmetric one-point quadrature, one obtains after expanding

$$T_2 - T_1 = w_p \left(\frac{1}{2\,m}\, \boldsymbol{p}_2^T \boldsymbol{p}_2 - \frac{1}{2\,m}\, \boldsymbol{p}_1^T \boldsymbol{p}_1 \right). \tag{87}$$

On account of the identity $H = T + V$ in conjunction with equation (77), equation (87) can be written as $T_2 - T_1 = w_p\ (T_2 - T_1)$. Therefore, the Fundamental Theorem of Calculus for the kinetic energy T is fulfilled by $w_p = 1$, that is, the midpoint rule.

Next we employ the trial function $\boldsymbol{q}^h = \sum_{i=1}^2 M_i\, \boldsymbol{q}_i$ in equation (86) and get after using symmetric one-point quadrature

$$V_2 - V_1 = -w_q\, \frac{f(r^h(1/2))}{2\, r^h(1/2)}\ \left(r_2^2 - r_1^2\right), \tag{88}$$

where $r^2 = \boldsymbol{q} \cdot \boldsymbol{q}$ has been taken into account. Hence it follows that we obtain the weight

$$w_q = -\frac{V_2 - V_1}{r_2^2 - r_1^2}\, \frac{2\, r^h(1/2)}{f(r^h(1/2))}. \tag{89}$$

The determined weights w_p and w_q yield the following time-stepping scheme:

$$\boldsymbol{q}_2 - \boldsymbol{q}_1 - \frac{h_n}{2\,m}\ (\boldsymbol{p}_1 + \boldsymbol{p}_2) = \boldsymbol{0}, \tag{90}$$

$$\boldsymbol{p}_2 - \boldsymbol{p}_1 + h_n\, \frac{V_2 - V_1}{r_2^2 - r_1^2}\ (\boldsymbol{q}_1 + \boldsymbol{q}_2) = \boldsymbol{0}. \tag{91}$$

Notation 4.2 According to Betsch and Steinmann [4], we refer to the symmetric one-point quadrature with the weights $w_p = 1$ and w_q from equation (89) as the *modified midpoint rule*.

Now consider the time-stepping scheme (90), (91). First we scalar multiply equation (91) with $(\boldsymbol{q}_2 - \boldsymbol{q}_1)$. Then, taking into account the identity $r^2 = \boldsymbol{q} \cdot \boldsymbol{q}$, one obtains

$$(\boldsymbol{p}_2 - \boldsymbol{p}_1) \cdot (\boldsymbol{q}_2 - \boldsymbol{q}_1) + h_n\ (V_2 - V_1) = 0. \tag{92}$$

Next, we employ equation (90) in equation (92) and convert the result such that

$$h_n \left(\frac{1}{2\,m}\, \boldsymbol{p}_2^T \boldsymbol{p}_2 - \frac{1}{2\,m}\, \boldsymbol{p}_1^T \boldsymbol{p}_1 \right) + h_n\ (V_2 - V_1) = 0. \tag{93}$$

With regard to equation (87), where $w_p = 1$, for a nonvanishing time step size h_n the equation (93) leads to $H_2 = H_1$, that is, algorithmic total energy conservation of the cG(1) method; see Figure 4.6. ■

Corollary 4.9 *The algorithmic total energy determined by the dG(1) method associated with the modified midpoint rule is conserved.*

Proof. With regard to Proposition 3.2 the general dG(1) method leads to a cG(1) time-stepping scheme by using one quadrature point at $\alpha = 1/2$, that is, applying a symmetric one-point quadrature (see Remark 4.6). By Proposition 4.6 the modified midpoint rule preserves the algorithmic total energy of the cG(1) method; see Figure 4.6. ■

4.3.3 The algorithmic total angular momentum conservation

With regard to equation (73) the algorithmic total angular momentum for linear time finite elements is given by

$$\boldsymbol{L}_2 = \boldsymbol{q}_2 \times \boldsymbol{p}_2. \tag{94}$$

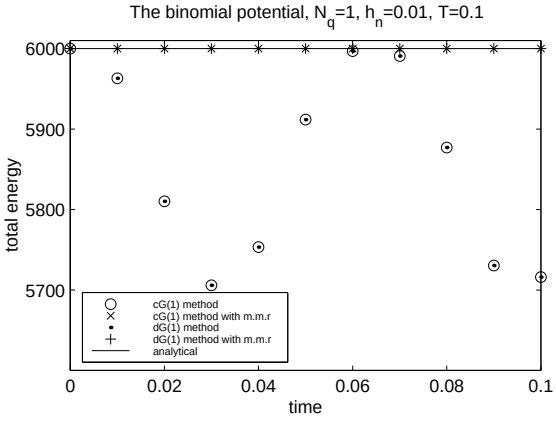

Figure 4.6 Total energy $H = H(t)$ of the potential $V = \frac{1}{2}\, c\left(r^2 - 1\right)^2$ with mass $m = 2$, total energy $H = 6000$ and potential constant $c = 1000$. Computed with the cG(1) and dG(1) method associated with midpoint rule as well as modified midpoint rule (m.m.r). That is, $N_q = 1$. The time step size h_n is 0.01.

Proposition 4.7 *Considering the cG(1) method associated with symmetric quadrature, only a symmetric one-point quadrature preserves the total angular momentum of the cG(1) method algorithmically, that is,* $\boldsymbol{L}_{\alpha=0} = \boldsymbol{L}_{\alpha=1}$*, for all central force laws* $f(r)$*.*

We prove Proposition 4.7 by the following lemma.

Lemma 4.9 *The algorithmic total angular momentum calculated with the cG(1) method associated with quadrature can be written as* $\boldsymbol{L}_2 = \boldsymbol{L}_1 + h_n\, \boldsymbol{N}_2$*, where* h_n *denotes the time step size and* $\boldsymbol{N}_2$ *a vector.*

Proof. Consider the general cG(1) method (38). Taking the Jacobian (79) in account and leaving the symplectic notation, one obtains

$$\boldsymbol{q}_2 - \boldsymbol{q}_1 - \frac{h_n}{m} \int_0^1 \boldsymbol{p}^h \, d\alpha = \boldsymbol{0}, \tag{95}$$

$$\boldsymbol{p}_2 - \boldsymbol{p}_1 - h_n \int_0^1 \frac{f(r^h)}{r^h}\, \boldsymbol{q}^h \, d\alpha = \boldsymbol{0}. \tag{96}$$

Employing the linear trial functions and introducing simultaneously quadrature, one obtains $\int_0^1 \boldsymbol{p}^h \, d\alpha \approx \sum_{i=1}^2 \beta_i\, \boldsymbol{p}_i$ and $\int_0^1 \frac{f(r^h)}{r^h}\, \boldsymbol{q}^h \, d\alpha \approx \sum_{i=1}^2 \eta_i\, \boldsymbol{q}_i$, respectively, where

$$\eta_i := -\sum_{l=1}^{N_q} M_i(\alpha_l)\, \frac{f(r^h(\alpha_l))}{r^h(\alpha_l)}\, w_l, \quad i = 1(1)k{+}1. \tag{97}$$

Accordingly, one obtains the following time-stepping scheme:

$$\boldsymbol{q}_2 - \boldsymbol{q}_1 - \frac{h_n}{m}\left(\beta_1\, \boldsymbol{p}_1 + \beta_2\, \boldsymbol{p}_2\right) = \boldsymbol{0} \tag{98}$$

$$\boldsymbol{p}_2 - \boldsymbol{p}_1 + h_n\left(\eta_1\, \boldsymbol{q}_1 + \eta_2\, \boldsymbol{q}_2\right) = \boldsymbol{0} \tag{99}$$

At first we take the cross product with $\boldsymbol{p}_2$ from the right on both sides of equation (98). The consideration of equation (94) renders the following algorithmic total angular momentum:

$$\boldsymbol{L}_2 = \boldsymbol{q}_1 \times \boldsymbol{p}_2 + \frac{h_n}{m}\, \beta_1\, \boldsymbol{p}_1 \times \boldsymbol{p}_2. \tag{100}$$

Next, vector multiplication from the left of both sides of equation (99) with $\boldsymbol{q}_1$ furnishes

$$\boldsymbol{q}_1 \times \boldsymbol{p}_2 = \boldsymbol{L}_1 - h_n\, \eta_2\, \boldsymbol{q}_1 \times \boldsymbol{q}_2, \tag{101}$$

where the identity $\boldsymbol{L}_1 = \boldsymbol{q}_1 \times \boldsymbol{p}_1$ has been used. Now an elimination of $\boldsymbol{p}_2$ in the time-stepping scheme (98), (99) and a subsequently vector multiplication of the resulting equation with $\boldsymbol{p}_2$ leads to

$$\frac{h_n}{m} \boldsymbol{p}_1 \times \boldsymbol{p}_2 = h_n \frac{\eta_1 + \eta_2}{\beta_1 + \beta_2} \boldsymbol{q}_1 \times \boldsymbol{q}_2. \tag{102}$$

Finally, employing the equations (101) and (102), equation (100) yields the following relation for the algorithmic total angular momentum:

$$\boldsymbol{L}_2 = \boldsymbol{L}_1 + h_n \, \boldsymbol{N}_2, \tag{103}$$

where

$$\boldsymbol{N}_2 = \frac{\beta_1 \, \eta_1 - \beta_2 \, \eta_2}{\beta_1 + \beta_2} \, \boldsymbol{q}_1 \times \boldsymbol{q}_2. \tag{104}$$

■

Remark 4.10 Equation (103) can be related to the rate of change (4) of the total angular momentum. One obtains $\boldsymbol{\Delta}^{(1)} = \boldsymbol{N}_2$, where $\boldsymbol{\Delta}^{(1)} = \frac{1}{h_n} (\boldsymbol{L}_2 - \boldsymbol{L}_0)$ denotes the first divided forward difference of the total angular momentum $\boldsymbol{L}(\alpha)$ of the master element I_α; see Hildebrand [9]. Thus we may interprete $\boldsymbol{\Delta}^{(1)} = \boldsymbol{N}_2$ as the algorithmic counterpart of the rate of change (4) of the total angular momentum.

Notation 4.3 Due to Remark 4.10, we generally refer to $\boldsymbol{N}_{k+1}$ as the *algorithmic total torque* of the cG(k) and dG(k) method, respectively.

Proof of Proposition 4.7 By Lemma 4.9, the condition for the conservation of the algorithmic total angular momentum $\boldsymbol{L}_2$, in the sense that $\boldsymbol{L}_2 = \boldsymbol{L}_1$, is $\boldsymbol{N}_2 = \boldsymbol{0}$. Because of the integrals in the algorithmic total torque $\boldsymbol{N}_2$, which are approximated by quadrature, we may interprete the condition $\boldsymbol{N}_2 = \boldsymbol{0}$ as a restriction on the positions of the quadrature points $\{\alpha_i\}_{i=1}^{N_q}$.

By equation (104) the conservation condition reads $(\beta_1 \, \eta_1 - \beta_2 \, \eta_2) \, \boldsymbol{q}_1 \times \boldsymbol{q}_2 = \boldsymbol{0}$. If the central force vanishes ($f(r) = 0$) then (i) the $\{\eta_1\}_{i=1}^2$ are vanishing and (ii) the orbit is a line which implies $\boldsymbol{q}_2 = a \, \boldsymbol{q}_1$, $a \in \mathbb{R}$, so that the cross product $\boldsymbol{q}_1 \times \boldsymbol{q}_2$ vanishes. For $f(r) \neq 0$ the cross product $\boldsymbol{q}_1 \times \boldsymbol{q}_2$ is not vanishing in general. Therefore, the conservation condition is reduced to $(\beta_1 \, \eta_1 - \beta_2 \, \eta_2) = 0$.

Taking into account the definitions (58) and (97) of the coefficients $\{\beta_i\}_{i=1}^{k+1}$ and $\{\eta_i\}_{i=1}^{k+1}$, respectively, and the nodal shape functions (11), we obtain the following condition for algorithmic total angular momentum conservation:

$$\sum_{\substack{l,L=1 \\ l \neq L}}^{N_q} (1 - \alpha_l - \alpha_L) \, \frac{f(r^h(\alpha_L))}{r^h(\alpha_L)} \, w_l \, w_L + \sum_{l=1}^{N_q} (1 - 2 \, \alpha_l) \, \frac{f(r^h(\alpha_l))}{r^h(\alpha_l)} \, w_l^2 = 0. \tag{105}$$

Considering symmetric quadrature, by the relations $M_1(\alpha_{N_q - i}) = M_2(\alpha_{1+i})$ and $M_2(\alpha_{N_q - i}) = M_1(\alpha_{1+i})$, $i = 0(1)\mathrm{int}([N_q - 1]/2)$, only the parentheses of the pairs $(\alpha_{N_q - i}, \alpha_{1+i})$ vanish. Consequently, for an arbitrary central force law $f(r)$ as well as for arbitrary weights, equation (105) is fulfilled if $\alpha_1 = \alpha_2 = \ldots = \alpha_{N_q} = 1/2$. Therefore, only one quadrature point at $\alpha = 1/2$, that is, symmetric one-point quadrature, leads to algorithmic total angular momentum conservation; see Betsch and Steinmann [4]. ■

Remark 4.11 A symmetric one-point quadrature satisfies the auxiliary condition $\beta_1 + \beta_2 \neq 0$.

Corollary 4.10 *The algorithmic total angular momentum determined by the cG(1) method associated with the midpoint rule or the modified midpoint rule is conserved.*

Proof. The symmetric one-point quadrature includes the midpoint rule as well as the modified midpoint rule. Accordingly, the cG(1) method associated with the midpoint rule or the modified midpoint rule conserves the algorithmic total angular momentum in view of Proposition 4.7; see Figure 4.7. ■

Proposition 4.8 *Considering the dG(1) method associated with symmetric quadrature, solely one quadrature point preserves the algorithmic total angular momentum of the dG(1) method for all central force laws $f(r)$.*

To prove Proposition 4.8 we use the following lemma.

Lemma 4.10 *The algorithmic total angular momentum $\boldsymbol{L}_2$ computed with the dG(1) method associated with quadrature is given by $\boldsymbol{L}_2 = \boldsymbol{L}_0 + h_n \boldsymbol{N}_2$, where h_n denotes the time step size and $\boldsymbol{N}_2$ the algorithmic total torque.*

Proof. Consider the general dG(1) method (30), (31). The determination of the algorithmic total angular momentum demands the explicit representation of the general dG(1) method:

$$\frac{1}{2}\,\boldsymbol{q}_2 + \frac{1}{2}\,\boldsymbol{q}_1 - \boldsymbol{q}_0 - h_n \int_0^1 M_1(\alpha)\,\partial_{\boldsymbol{p}} H(\alpha) d\alpha = \boldsymbol{0}, \tag{106}$$

$$\frac{1}{2}\,\boldsymbol{p}_2 + \frac{1}{2}\,\boldsymbol{p}_1 - \boldsymbol{p}_0 + h_n \int_0^1 M_1(\alpha)\,\partial_{\boldsymbol{q}} H(\alpha) d\alpha = \boldsymbol{0}, \tag{107}$$

$$\frac{1}{2}\,\boldsymbol{q}_2 - \frac{1}{2}\,\boldsymbol{q}_1 - h_n \int_0^1 M_2(\alpha)\,\partial_{\boldsymbol{p}} H(\alpha) d\alpha = \boldsymbol{0}, \tag{108}$$

$$\frac{1}{2}\,\boldsymbol{p}_2 - \frac{1}{2}\,\boldsymbol{p}_1 + h_n \int_0^1 M_2(\alpha)\,\partial_{\boldsymbol{q}} H(\alpha) d\alpha = \boldsymbol{0}. \tag{109}$$

Taking the trial functions $\boldsymbol{p}^h(\alpha) = \sum_{j=1}^2 M_j(\alpha)\,\boldsymbol{p}_j$ and $\boldsymbol{q}^h(\alpha) = \sum_{j=1}^2 M_j(\alpha)\,\boldsymbol{q}_j$ as well as quadrature into consideration, one obtains the following time-stepping scheme:

$$\frac{1}{2}\,\boldsymbol{q}_2 + \frac{1}{2}\,\boldsymbol{q}_1 - \boldsymbol{q}_0 - \frac{h_n}{m} \sum_{j=1}^2 \beta_{1j}\,\boldsymbol{p}_j = \boldsymbol{0}, \tag{110}$$

$$\frac{1}{2}\,\boldsymbol{p}_2 + \frac{1}{2}\,\boldsymbol{p}_1 - \boldsymbol{p}_0 + h_n \sum_{j=1}^2 \eta_{1j}\,\boldsymbol{q}_j = \boldsymbol{0}, \tag{111}$$

$$\frac{1}{2}\,\boldsymbol{q}_2 - \frac{1}{2}\,\boldsymbol{q}_1 - \frac{h_n}{m} \sum_{j=1}^2 \beta_{j2}\,\boldsymbol{p}_j = \boldsymbol{0}, \tag{112}$$

$$\frac{1}{2}\,\boldsymbol{p}_2 - \frac{1}{2}\,\boldsymbol{p}_1 + h_n \sum_{j=1}^2 \eta_{j2}\,\boldsymbol{q}_j = \boldsymbol{0}, \tag{113}$$

where

$$\eta_{ij} := -\sum_{l=1}^{N_q} M_i(\alpha_l)\,M_j(\alpha_l)\,\frac{f(r^h(\alpha_l))}{r^h(\alpha_l)}\,w_l, \quad i = 1(1)k{+}1. \tag{114}$$

With regard to the definition (114), the coefficients η_{ij} are symmetric, that is, $\eta_{ij} = \eta_{ji}$. According to the definition (68), the coefficients β_{ij} are also symmetric. This symmetry has been taken into account in the equations (112) and (113).

Firstly, add equation (110) and equation (112) and use the identity $\beta_i = \beta_{i1} + \beta_{i2}$, where β_i is defined by equation (58), in accordance with the relation $M_1 + M_2 = 1$ of the nodal shape functions. On the other hand, add the equations (111) and (113) and use the relation $\eta_i = \eta_{i1} + \eta_{i2}$, also due to $M_1 + M_2 = 1$. The $\{\eta_i\}_{i=1}^{k+1}$ are defined by equation (97).

One obtains the algorithmic total angular momentum $\boldsymbol{L}_2$ by employing both relations just determined in equation (94):

$$\boldsymbol{L}_2 = \boldsymbol{L}_0 + \frac{h_n}{m}\beta_1 \boldsymbol{p}_1 \times \boldsymbol{p}_0 - h_n \left(\boldsymbol{q}_0 + \frac{h_n}{m}\beta_1 \boldsymbol{p}_1\right) \times \sum_{j=1}^2 \boldsymbol{\eta}_j\,\boldsymbol{q}_j, \tag{115}$$

where use has been made of the identity $\boldsymbol{L}_0 = \boldsymbol{q}_0 \times \boldsymbol{p}_0$.

Employing the difference of equation (113) and equation (111) in the middle term of equation (115), leads to

$$\boldsymbol{L}_2 = \boldsymbol{L}_0 - h_n\, \boldsymbol{q}_0 \times \sum_{j=1}^{2} \eta_j\, \boldsymbol{q}_j - \frac{2\, h_n^2}{m} \beta_1\, \boldsymbol{p}_1 \times \sum_{j=1}^{2} \eta_{j2}\, \boldsymbol{q}_j. \tag{116}$$

The generalized momentum vector $\boldsymbol{p}_1$ in the last term of equation (116) can be replaced by the combination of equation (113) with the sum of the equations (110) and (112). Ultimately, the algorithmic total angular momentum is given by

$$\boldsymbol{L}_2 = \boldsymbol{L}_0 + h_n\, \boldsymbol{N}_2, \tag{117}$$

where

$$\boldsymbol{N}_2 = \frac{\beta_1 - \beta_2}{\beta_1 + \beta_2} \left(\eta_{12}\, (\boldsymbol{q}_0 - \boldsymbol{q}_2) \times \boldsymbol{q}_1 + \eta_{22}\, \boldsymbol{q}_0 \times \boldsymbol{q}_2\right) + \eta_{12}\, (\boldsymbol{q}_1 - \boldsymbol{q}_0) \times \boldsymbol{q}_2 + \eta_{11}\, \boldsymbol{q}_1 \times \boldsymbol{q}_0. \tag{118}$$

■

Proof of Proposition 4.8 By Lemma 4.10 the conservation condition is the vanishing algorithmic total torque $\boldsymbol{N}_2$. Accordingly, we have to find quadrature points $\{\alpha_l\}_{i=1}^{N_q}$ satisfying the equation $\boldsymbol{N}_2 = \boldsymbol{0}$. The first term vanishes for an arbitrary central force law only if $\beta_1 = \beta_2$. Taking into consideration the nodal shape functions and symmetric quadrature, one obtains

$$\sum_{l=1}^{N_q} (1 - 2\,\alpha_l) w_l = \sum_{l=0}^{\nu} 2\left(1 - \alpha_{1+l} - \alpha_{N_q - l}\right) w_{1+l} = 0, \tag{119}$$

where $\nu = \mathrm{int}(N_q/2)$. Consequently, for arbitrary weights the parentheses have to vanish separately, which is fulfilled by symmetric quadrature.

The last two terms vanish for an arbitrary central force law only if $\boldsymbol{q}_0 = \boldsymbol{q}_1$, that is, a vanishing jump $[\![\boldsymbol{q}^h]\!]$. By the difference of the equation (110) and (112) the jump vanishes solely if $\beta_{i2} = \beta_{i1}$, $i = 1(1)2$. Taking symmetric quadrature and the nodal shape functions into account, both conditions lead to

$$\sum_{l=0}^{\nu} \left(\frac{1}{2} - \alpha_{1+l}\right)^2 w_{1+l} = 0, \tag{120}$$

where $\nu = \mathrm{int}(N_q/2)$. For arbitrary weights the parentheses have to vanish, so that $\alpha_1 = \alpha_2 = \ldots = \alpha_{N_q} = 1/2$ is the solution. Therefore, only a symmetric one-point quadrature preserves the algorithmic total angular momentum for an arbitrary central force law. ■

Corollary 4.11 *The algorithmic total angular momentum determined by the dG(1) method associated with the midpoint rule or the modified midpoint rule is conserved.*

Proof. Since the symmetric one-point quadrature includes the midpoint rule as well as the modified midpoint rule, the algorithmic total angular momentum determined by the dG(1) method associated with the midpoint rule or the modified midpoint rule is conserved according to Proposition 4.8; see Figure 4.7. ■

Corollary 4.12 *Considering the dG(1) method associated with symmetric quadrature, only a continuous solution, that is, $[\![z^h]\!] = 0$, preserves the algorithmic total angular momentum for all central force laws $f(r)$.*

Proof. According to Proposition 4.8, only a symmetric one-point quadrature preserves the total angular momentum algorithmically. Furthermore, owing to Proposition 3.2 a symmetric one-point quadrature applied to the general dG(1) method furnishes a cG(1) time-stepping scheme with a continuous solution, that is, $\boldsymbol{z}_0 = \boldsymbol{z}_1$. Consequently, only a continuous solution leads to algorithmic total angular momentum conservation for an arbitrary central force law in the sense that $\boldsymbol{L}_{\alpha=0} = \boldsymbol{L}_{\alpha=1}$. ■

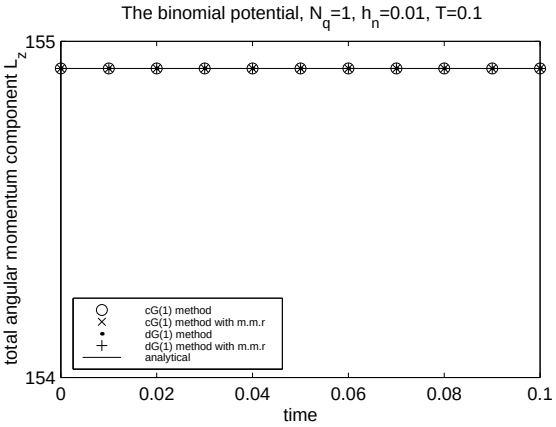

Figure 4.7 The nonvanishing total angular momentum component $L_\zeta = L_\zeta(t)$, where the ζ-axis is perpendicular to the plane of motion, of the potential $V = \frac{1}{2}\, c\left(r^2 - 1\right)^2$ with mass $m = 2$, total energy $H = 6000$ and potential constant $c = 1000$. Computed with the cG(1) and dG(1) method associated with midpoint rule as well as modified midpoint rule (m.m.r). That is, $N_q = 1$. The time step size h_n is 0.01.

5 Conclusions

The continuous Galerkin cG(k) method for holonomic mechanical systems, investigated by Betsch and Steinmann [3, 4, 5], was compared to the discontinuous Galerkin dG(k) method. In contrast to the inherent energy conservation of the cG(k) method, the dG(k) method achieves energy nonconservation in general. Energy dissipation of the dG(k) method has been shown for (i) $k = 0$ in conjunction with arbitrary potentials V and (ii) arbitrary k in the case of quadratic potentials V. Furthermore, we have shown that cG(1) time-stepping schemes can be derived from the dG(1) method by applying one quadrature point at the midpoint of the master element (reduced integration).

Considering quadratic potentials V, a relationship between the algorithmic conservation properties and the spectral radius of the amplification matrix pertaining to the cG(1) and dG(1) time-stepping schemes, respectively, emanating from exact as well as numerical quadrature, was derived. This relationship demonstrates the influence of numerical quadrature on the algorithmic conservation properties.

For arbitrary potentials V a quadrature rule, namely the modified midpoint rule, was presented which preserves the algorithmic total energy and angular momentum of the dG(1) method. Accordingly, algorithmic conservation is only possible for continuous approximations, that is, when the dG(1) method degenerates to the cG(1) method by employing one quadrature point at the midpoint of the master element.

We refer to Tables 5.1 for an overview of the numerous results.

cG(1)	Hooke's potential			Arbitrary potentials	
	exact	sym. quadrature		sym. quadrature	
		$N_q = 1$	$1 < N_q < \infty$	$N_q = 1$	$1 < N_q < \infty$
H	C	C	C	C*	
	exact	sym. quadrature		sym. quadrature	
		$N_q = 1$	$1 < N_q < \infty$	$N_q = 1$	$1 < N_q < \infty$
$\boldsymbol{L}$	C	C	C	C	NC

dG(1)	Hooke's potential			Arbitrary potentials	
	exact	sym. quadrature		sym. quadrature	
		$N_q = 1$	$1 < N_q < \infty$	$N_q = 1$	$1 < N_q < \infty$
H	D	C	D	C*	
	exact	sym. quadrature		sym. quadrature	
		$N_q = 1$	$1 < N_q < \infty$	$N_q = 1$	$1 < N_q < \infty$
$\boldsymbol{L}$	D	C	D	C	NC

Table 5.1 On the left and right, the algorithmic conservation properties of the cG(1) and dG(1) method, respectively, are depicted. 'C' denotes conservation, 'D' denotes decay, 'C*' denotes conservation only with modified midpoint rule and 'NC' denotes nonconservation. An empty box signifies the absence of a corresponding evidence or counterevidence.

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