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VARIATIONAL FORMULATION OF DISCONTINUOUS-GALERKIN TIME INTEGRATORS

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Abstract. *Variational integrators provide a way to design structure-preserving time integrators for problems presenting a Lagrangian structure. The basic idea consists in obtaining algorithms from a discrete analogue of Hamilton's variational principle. Then, the discrete trajectories are stationary points of a discrete analogue of the action functional. The resulting methods enjoy a number of remarkable properties: i) they exactly conserves the momenta associated to the symmetries of a discrete version of the Lagrangian, ii) they define a discrete symplectic flow on the phase space and iii) they show an error in the total energy that remains bounded for exponentially long periods of time. A particularly interesting family of such methods is given by the so called Galerkin variational integrators. Their construction is based on approximating the trajectory of the system by means of piecewise continuous polynomials and providing suitable quadrature rules to approximate the action functional. Then, increasing the order of the interpolating polynomials and the accuracy of the quadrature rules allow to obtain higher order time integrators. In this work we extend the Galerkin methods to the discontinuous case yielding to a family of discontinuous-Galerkin (dG)-methods. To this end, we resort to using two key ingredients: 1) the trajectory of the system is approximated by means of piecewise polynomials which may presents a finite number of discontinuities across time interval boundaries and 2) we approximate the velocity of the system by means of an appropriate dG-time-derivative of the trajectory following some ideas presented in [1, 2] for static problems in elasticity. The resulting algorithms corresponds to a family of discontinuous-symplectic Runge-Kutta methods.*

1 INTRODUCTION

The construction of integrators for which the trajectories preserve invariants of the original system is the realm of structured or geometric integration, see e.g. [3, 4, 5]. Variational integrators (VI) provide a way to design structure-preserving time integrators for problems whose dynamics is generated by a Hamiltonian. The basic idea behind these methods is to obtain the algorithm from discrete analog to Hamilton's variational principle. In this way, the computed discrete trajectories are stationary points of a discrete action functional, the discrete action sum. As a result, the discrete trajectories approximate the exact trajectories of the system, and nearly exactly preserve the exact energy of the system for long times [4, Ch. 9]. Moreover, if the discrete action sum is designed to respect symmetries of the original action functional, then by virtue of a discrete version of Noether's theorem, the discrete trajectories conserve the momenta conjugate to each one of these symmetries, see e.g. [6]. Finally, the resulting algorithms are symplectic by design. Nowadays it is possible to find a vast literature on VIs. Most of the basic theory and analytical results may be reviewed in [7, 8, 9, 6, 10, 11, 12].

These methods have been successfully applied in numerous fields, such as to the construction of asynchronous integration methods in solid mechanics [6, 10], to problems with constraints [11, 13], to problems with contact [14, 15, 16, 17], with oscillatory solutions [18], to Langevin and stochastic differential equations [19, 20], to problems where the evolution takes place over a nonlinear manifold [21, 22, 23], to thermoelasticity [24, 25, 26] and to incompressible fluids [27], to name some of the most relevant ones.

In this paper, we extend the standard methodology to constructuct (continuous) Galerkin time integrators to the discontinuous case. The basic idea consists in approximating the discrete Lagrangian by means of piecewise discontinuous polynomials. The corresponding discrete approximation to the velocity in the time interval is obtained by means of using the Discontinuous-Galerkin (DG) derivative [1, 2]. The resulting integrators provide a methodology for constructing discontinuous integrators which automatically have a number of properties: (i) they are symplectic, (ii) they exactly preserve the momenta associated to symmetries, (iii) and they have excellent longtime energy behavior (see [6, 10, 12, 28]). The proposed methodology is showcased through some examples.

2 Formulation of variational integrators

We consider a finite-dimensional mechanical system characterized by a Lagrangian function $L(\mathbf{q}, \dot{\mathbf{q}})$ with $\mathbf{q} = (\mathrm{q}^1, ..., \mathrm{q}^n)$ being generalized coordinates defined on a configuration space Q and $\dot{\mathbf{q}}$ the velocities corresponding to time-dependent curves on Q. The action functional over the time interval $[t_a, t_b]$ is formed integrating the Lagrangian function along $\mathbf{q}(t)$ as

$$S[\mathbf{q}(\cdot)] = \int_{t_a}^{t_b} L\left(\mathbf{q}(t), \dot{\mathbf{q}}(t)\right)\ dt. \tag{1}$$

Hamilton's principle states that the system evolves following trajectories that are a stationary point of $S[\mathbf{q}(\cdot)]$ under arbitrary variations in the set of all smooth enough trajectories that leave the end-points fixed. This condition yields the so called *Euler-Lagrange* (E-L) equations, namely

$$\frac{\partial L}{\partial \mathrm{q}^i}(\mathbf{q}(t), \dot{\mathbf{q}}(t)) - \frac{d}{dt}\left(\frac{\partial}{\partial L\dot{\mathrm{q}}^i}(\mathbf{q}(t), \dot{\mathbf{q}}(t))\right) = 0, \qquad i = 1, ..., n. \tag{2}$$

Moreover, Noether's theorem states that there exists a correspondence between the quantities conserved along solution trajectories and the symmetries of the Lagrangian [29].

The Hamiltonian function $\mathsf{H} : \mathsf{T}^*Q \to \mathbb{R}$ is obtained as the *Legendre transformation* of the Lagrangian function in the velocity variables as

$$H(\mathbf{q}, \mathbf{p}) = \mathbf{p} \cdot \dot{\mathbf{q}} - L(\mathbf{q}, \dot{\mathbf{q}}), \tag{3}$$

which considers the change of variables $(\mathbf{q}, \dot{\mathbf{q}}) \to (\mathbf{q}, \mathbf{p})$ after the introduction of the conjugated (mechanical) momenta,

$$\mathbf{p} = \frac{\partial L}{\partial \dot{\mathbf{q}}}(\mathbf{q}, \dot{\mathbf{q}}). \tag{4}$$

Then, taking the time derivative of (3) it is possible to see that the equations of motion (2) may be rephrased in the following completely equivalent (Hamiltonian) form,

$$\dot{\mathbf{z}} = \mathbf{J}\frac{\partial H}{\partial \mathbf{z}}(\mathbf{z}), \qquad \mathbf{z}(t^0) = \mathbf{z}^0, \tag{5}$$

where $\mathbf{z} = (\mathbf{q}, \mathbf{p})$ and

$$\mathbf{J} = \begin{pmatrix} \mathbf{0}_{n\times n} & \mathbf{I}_{n\times n} \\ -\mathbf{I}_{n\times n} & \mathbf{0}_{n\times n} \end{pmatrix}$$

is a cannonical symplectic matrix [29]. Moreover, $\mathbf{0}_{n\times n}$ and $\mathbf{I}_{n\times n}$ are $n-$dimensional zero and identity matrices.

Two significant characteristics of time continuous (autonomous) Hamiltonian systems are:

- The Hamiltonian function H is along solution trajectories of the system (5).
- They define symplectic flows over the phase space (cotangent bundle) T^*Q as explained in [4, Ch. 6] or [30, Ch. 4].

2.1 General discretization procedure

The basic idea behind the formulation of variational integrators consists in a constructing discrete approximations of the action sum instead of developing methods based on the discretization of the Euler-Lagrange equations. A complete review of the methods may be found for example in [31, 6, 10]. Then, we begin by partitioning the time interval of interest into equally spaced intervals of length $h = (t_b - t_a)/N_t$, and set $t^k = t_a + kh$ for $k = 0, \ldots, N_t$. The discrete Lagrangian $L_d : Q \times Q \times \mathbb{R} \to \mathbb{R}$ is constructed to approximate the action integral over a time step $[0, h]$ as

$$L_d(\mathbf{q}^0, \mathbf{q}^1, h) \approx \int_0^h L(\mathbf{q}(t), \dot{\mathbf{q}}(t))\, dt, \tag{6}$$

where $\mathbf{q}(t) : [0, h] \to Q$ is the solution of equations (2) subjected to $\mathbf{q}(0) = \mathbf{q}^0$ and $\mathbf{q}(h) = \mathbf{q}^h$ [11]. Then, the discrete action sum is constructed as

$$S_d(\mathbf{q}^0, ..., \mathbf{q}^{N_t}, h) = \sum_{k=0}^{N_t-1} \mathsf{L}_d(\mathbf{q}^k, \mathbf{q}^{k+1}, h), \tag{7}$$

and a discrete version of Hamilton's principle allows to deduce the discrete Euler-Lagrange equations (DEL) as

$$D_2L_d(\mathbf{q}^{k-1}, \mathbf{q}^k) + D_1L_d(\mathbf{q}^k, \mathbf{q}^{k+1}) = 0, \qquad k = 1, ..., N_t - 1, \tag{8}$$

where $D_i L_d$ denotes the partial derivative of L_d with respect the i[th] slot and the time step length h has been omitted in the arguments of L_d to alleviate the notation. The above system of equations defines an update map from $Q \times Q$ to itself known as the *discrete Lagrangian flow map* which takes a point $(\mathbf{q}^{k-1}, \mathbf{q}^k)$ to $(\mathbf{q}^k, \mathbf{q}^{k+1})$. The discrete counterpart of the momenta (4) are defined by means of a discrete Legendre transformation according to

$$\mathbf{\Pi}^k = -D_1 L_d(\mathbf{q}^k, \mathbf{q}^{k+1}), \tag{9a}$$

$$\mathbf{\Pi}^{k+1} = D_2 L_d(\mathbf{q}^k, \mathbf{q}^{k+1}). \tag{9b}$$

The above equations define the *discrete Hamiltonian flow map* wich takes a point $(\mathbf{q}^k, \mathbf{\Pi}^k)$ to $(\mathbf{q}^{k+1}, \mathbf{\Pi}^{k+1})$. This maps defines implicitly a time integrator expressed in the so called *position-momentum* form. The procedure consist in solving (9a) for $\mathbf{q}^{k+1}$ and then replacing it in Eq. (9b) to obtain $\mathbf{\Pi}^{k+1}$.

A convergence result on variational integrators in [11] states that if L_d is an $\mathcal{O}(h^{p+1})$ $(p > 1)$ approximation for the action on a time step and some standard smoothness conditions on L are satisfied, then (i) the discrete Hamiltonian flow maps is an $\mathcal{O}(h^{p+1})$ approximation of the exact flow of the system on T^*Q and (ii) the discrete Legendre transformation of L_d has error that decays at least as h^{p+1}. Therefore, higher-order approximations in (6) result in correspondingly higher-order integrators.

2.2 Continuous Galerkin VI

The basic idea behind the formulation of continuous Galerkin rules consist in extending tow order quadrature rule to higher order. To this end, we consider s control points $\{\mathbf{q}^0_\nu\}_{\nu=0,\dots,s}$ (with $\mathbf{q}^0_0 = \mathbf{q}^0$ and $\mathbf{q}^0_s = \mathbf{q}^1$) corresponding to the values of the trajectory at control times $\{d_\nu h\}_{\nu=0,\dots,s}$ with $0 = d_0 < d_1 < \dots < d_s = 1$. Moreover, we assume that the trajectory over $[0, h]$ is approximated by a unique $s-$degree polynomial $\mathbf{q}_p(t; \mathbf{q}^0_0, \dots, \mathbf{q}^0_s, h) \in \mathbb{P}^s([0, h])$ such that

$$\mathbf{q}_p(d_\nu h) = \mathbf{q}^0_\nu, \qquad \nu \in \{0, 1, \dots, s\}.$$

See Figure 1-a, c. Then, providing an appropriate quadrature rule, the discrete Lagrangian is obtained as

$$L_d(\mathbf{q}^0, \mathbf{q}^1, h) = \inf_{\substack{\mathbf{q}(t)\in\mathbb{P}^s([0,h]) \\ \mathbf{q}(0)=\mathbf{q}^0, \mathbf{q}(h)=\mathbf{q}^1}} \sum_{i=1}^{n_q} w_i L(\mathbf{q}_p(\xi^i), \dot{\mathbf{q}}_p(\xi_i)). \tag{10}$$

Thwn, we obtain that the discrete action sum will be of the form

$$S_d\left(\left\{\mathbf{q}^0_\nu\right\}_{\nu=0,\dots,s}, \dots, \left\{\mathbf{q}^N_\nu\right\}_{\nu=0,\dots,s}\right), \tag{11}$$

subjected to the continuity constraints

$$\mathbf{q}^i_s = \mathbf{q}^{i+1}_0, \qquad i \in \{1, \dots, N-1\}. \tag{12}$$

Enforcing the action sum to be stationary under arbitrary variations $\{\delta\mathbf{q}^0_\nu\}_{\nu=0,\dots,s}$ that held the endpoints of the trajectory fixed yields to the DEL equations (8) plus the following extra conditions

$$\frac{\partial S_d}{\partial \mathbf{q}^i_\nu}\left(\left\{\mathbf{q}^0_\nu\right\}_{\nu=0,\dots,s}, \dots, \left\{\mathbf{q}^N_\nu\right\}_{\nu=0,\dots,s}\right) = 0, \qquad \begin{array}{c} i = 1, \dots, N-1 \\ \nu = 1, \dots, s-1 \end{array}, \tag{13}$$

which ensures that the values of the trajectory at the control point fulfil the infimum condition (10).

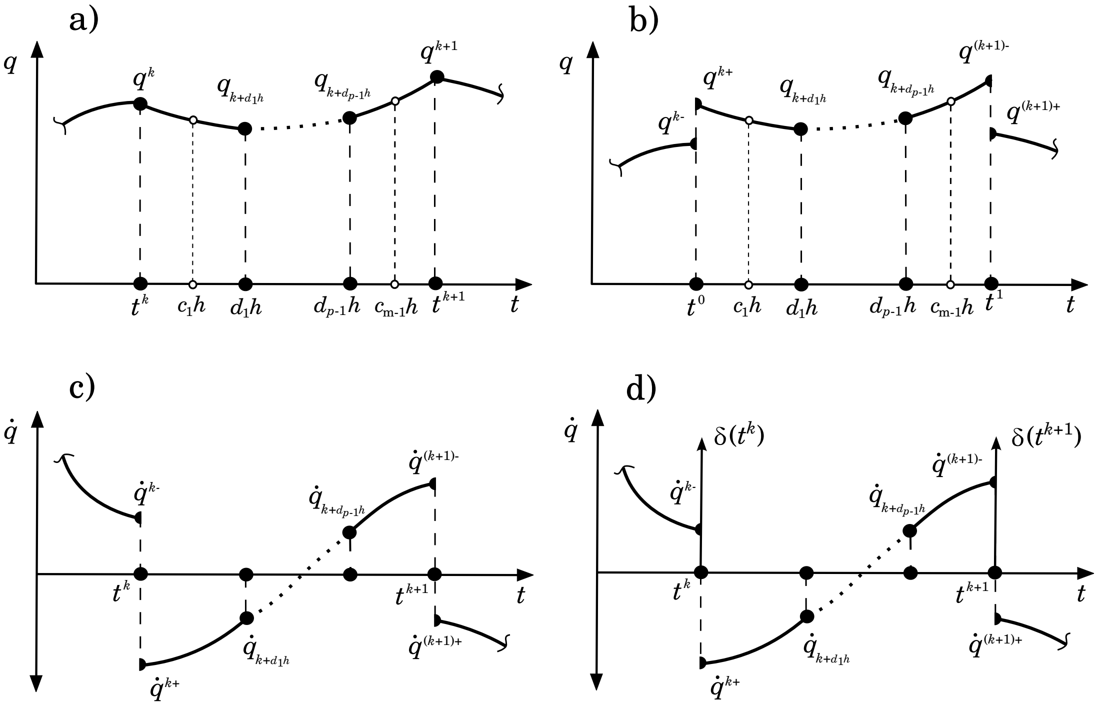

Figure 1: $a)$ Schematic representation of a piecewise-continuous polynonial used to interpolate $\mathbf{q}(t)$ in echa time step. $b)$ Piecewise-discontinuous polynomial. $c)$ Velocity profile obtained for the case $a)$. $d)$ Velocity profile for the case $b)$.

3 Formulation of discontinuous Galerkin VI

In this case we we allow to $\mathbf{q}^p(t; \mathbf{q}_0^0, ..., \mathbf{q}_s^0, h)$ to be discontinuous across time interval boundaries. Thus, relaxing the constraint (12). See figure (1-b). Then, we have that

$$\mathbf{q}^{k+} = \lim_{\epsilon \to 0^+} \mathbf{q}_p(t^k + \epsilon) \neq \lim_{\epsilon \to 0^-} \mathbf{q}_p(t^k + \epsilon) = \mathbf{q}^{k-}. \tag{14}$$

Moreover, we define

$$\begin{aligned} [\![\mathbf{q}]\!]^k &:= \mathbf{q}^{k-} - \mathbf{q}^{k+}, && \text{(jump operator)} \\ \{\mathbf{q}\}^k &:= \frac{1}{2}(\mathbf{q}^{k-} + \mathbf{q}^{k+}), && \text{(average operator)}. \end{aligned}$$

and following [1, 2] we define the Discontinuous-Galerkin approximation to the time derivative (DG-derivative) of $\mathbf{q}_p(t)$ as

$$D_{DG}\mathbf{q}_p := \dot{\mathbf{q}}_p - r([\![\hat{\mathbf{q}} - \mathbf{q}]\!]) - l(\{\hat{\mathbf{q}} - \mathbf{q}\}),$$

where $\dot{\mathbf{q}}_p$ means derivation in each time interval, $\hat{\mathbf{q}}$ is a numerical flux (to be given bellow) and the right and left lifting operators $r(\cdot)$ and $l(\cdot)$ are defined as

$$\begin{aligned} \int_0^T r(\varphi)\tau \, dt &:= -\sum_{k=0}^{N} \varphi^k \{\tau\}^k, \\ \int_0^T l(\varphi)\tau \, dt &:= -\sum_{k=1}^{N-1} \varphi^k [\![\tau]\!]^k, \end{aligned}$$

for all $\tau \in V_h^{n'} := \{v \in L_2(0;T) \ : \ v|_{(t^k,t^{k+1})} \in P^{n'}(t^k;t^{k+1}\}$ with $n' \geq n-1$ and $\mathbf{q}_p \in V_h^n$.

Considering the *Bassi-Rebay* [2] approximation for the flux, $\hat{\mathbf{q}} = \{\mathbf{q}\}$, we obtain that

$$L_d(\mathbf{q}_p, D_{DG}\mathbf{q}_p, h) = \sum_{i=1}^{n_g} w_i L(\mathbf{q}_p(\xi_i), D_{DG}\mathbf{q}_p(\xi_i)) \approx \int_{t^k}^{t^{k+1}} L(\mathbf{q}, \dot{\mathbf{q}})\ dt,$$

where $\{\xi_i, w_i\}_{i=1,\ldots,n_g}$ is a set of quadrature points and the corresponding weights used to approximate the action over $[t^k, t^{k+1}]$.

4 Examples

In the following examples we consider separable Lagrangian functions of the form

$$L(\mathbf{q}, \dot{\mathbf{q}}) = \mathbf{M}\dot{\mathbf{q}} \cdot \dot{\mathbf{q}} - V(\mathbf{q}).$$

4.1 Bassi-Rebay

We consider a discontinuous piecewise linear approximation for $\mathbf{q} \in [t^k, t^{k+1}]$. In this case we always have $p^{k-} = p^{(k+1)+}$.

The discrete Lagrangian is

$$\begin{aligned} &L_d\left(q^{k-}, q^{k+}, q^{(k+1)-}, q^{(k+1)+}, \Delta t\right) \\ &= M\frac{\left(-q^{k-} - q^{k+} + q^{(k+1)-} + q^{(k+1)+}\right)^2}{8\Delta t} - \int_{t_k}^{t_{k+1}} V(q)\ dt \end{aligned}$$

The algorithm in position-momentum form thus reads

$$\begin{aligned} p^{k-} &= M\frac{\left(-q^{k-} - q^{k+} + q^{(k+1)-} + q^{(k+1)+}\right)}{4\Delta t}, \\ p^{k+} &= M\frac{\left(-q^{k-} - q^{k+} + q^{(k+1)-} + q^{(k+1)+}\right)}{4\Delta t} + \frac{\partial}{\partial q^{k+}} \int_{t_k}^{t_{k+1}} V(q)\ dt, \\ p^{(k+1)-} &= M\frac{\left(-q^{k-} - q^{k+} + q^{(k+1)-} + q^{(k+1)+}\right)}{4\Delta t} - \frac{\partial}{\partial q^{(k+1)-}} \int_{t_k}^{t_{k+1}} V(q)\ dt, \\ p^{(k+1)+} &= M\frac{\left(-q^{k-} - q^{k+} + q^{(k+1)-} + q^{(k+1)+}\right)}{4\Delta t}. \end{aligned}$$

4.1.1 Piecewise linear $r_k(q)$

In this case, let ψ_k denote the standard $P^1([0,h])$ shape function of node k in time. Then,

$$r_k(1) = \begin{cases} h_{k-1}^{-1}(\psi_{k-1}(t) - 2\psi_k(t)), & t_{k-1} < t < t_k, \\ h_k^{-1}(-2\psi_k(t) + \psi_{k+1}(t)), & t_k < t < t_{k+1}, \\ 0, & \text{otherwise}. \end{cases}$$

As a result, with a constant $h_k = \Delta t$,

$$\begin{aligned} D_{DG}q|_{(t_k,t_{k+1})} &= \frac{q^{(k+1)-} - q^{k+}}{\Delta t} + r_k\left(q^{k-} - q^{k+}\right)(t) + r_{k+1}\left(q^{(k+1)-} - q^{(k+1)+}\right)(t) \\ &= \frac{q^{(k+1)-} - q^{k+}}{\Delta t} + \frac{1}{\Delta t}\left(q^{k-} - q^{k+}\right)\left(-2\psi_k(t) + \psi_{k+1}(t)\right) \\ &\quad + \frac{1}{\Delta t}\left(q^{(k+1)-} - q^{(k+1)+}\right)\left(\psi_k(t) - 2\psi_{k+1}(t)\right). \end{aligned}$$

We can use Simpson's rule (Lobatto quadrature rule with 3 points) to exactly integrate $M(D_{DG}q)^2$. Doing so yields

$$\begin{aligned}
&\int_{t_k}^{t_{k+1}} M(D_{DG}q)^2\, dt \\
&= \frac{M\Delta t}{6}\left[\frac{q^{(k+1)-}-q^{k+}}{\Delta t} - \frac{2}{\Delta t}\left(q^{k-}-q^{k+}\right) + \frac{1}{\Delta t}\left(q^{(k+1)-}-q^{(k+1)+}\right)\right]^2 \\
&\quad + \frac{2M\Delta t}{3}\left[\frac{q^{(k+1)-}-q^{k+}}{\Delta t} - \frac{1}{2\Delta t}\left(q^{k-}-q^{k+}\right) - \frac{1}{2\Delta t}\left(q^{(k+1)-}-q^{(k+1)+}\right)\right]^2 \\
&\quad + \frac{M\Delta t}{6}\left[\frac{q^{(k+1)-}-q^{k+}}{\Delta t} + \frac{1}{\Delta t}\left(q^{k-}-q^{k+}\right) - \frac{2}{\Delta t}\left(q^{(k+1)-}-q^{(k+1)+}\right)\right]^2 \\
&= \frac{M}{6\Delta t}\Big\{\left[-2q^{k-}+q^{k+}+2q^{(k+1)-}-q^{(k+1)+}\right]^2 + \left[-q^{k-}-q^{k+}+q^{(k+1)-}+q^{(k+1)+}\right]^2 \\
&\quad + \left[q^{k-}-2q^{k+}-q^{(k+1)-}+2q^{(k+1)+}\right]^2\Big\}
\end{aligned}$$

Thus

$$\begin{aligned}
&L_d\left(q^{k-}, q^{k+}, q^{(k+1)-}, q^{(k+1)+}, \Delta t\right) \\
&= \frac{M}{12\Delta t}\Big\{\left[-2q^{k-}+q^{k+}+2q^{(k+1)-}-q^{(k+1)+}\right]^2 + \left[-q^{k-}-q^{k+}+q^{(k+1)-}+q^{(k+1)+}\right]^2 \\
&\quad + \left[q^{k-}-2q^{k+}-q^{(k+1)-}+2q^{(k+1)+}\right]^2\Big\} - \int_{t_k}^{t_{k+1}} V(q)\, dt
\end{aligned}$$

The algorithm reads

$$\begin{aligned}
p^{k-} &= \frac{M}{2\Delta t}\left[-2q^{k-}+q^{k+}+2q^{(k+1)-}-q^{(k+1)+}\right], \\
p^{k+} &= \frac{M}{2\Delta t}\left[q^{k-}-2q^{k+}-q^{(k+1)-}+2q^{(k+1)+}\right] + \frac{\partial}{\partial q^{k+}}\int_{t_k}^{t_{k+1}} V(q)\, dt, \\
p^{(k+1)-} &= \frac{M}{2\Delta t}\left[-2q^{k-}+q^{k+}+2q^{(k+1)-}-q^{(k+1)+}\right] - \frac{\partial}{\partial q^{(k+1)-}}\int_{t_k}^{t_{k+1}} V(q)\, dt, \\
p^{(k+1)+} &= \frac{M}{2\Delta t}\left[q^{k-}-2q^{k+}-q^{(k+1)-}+2q^{(k+1)+}\right].
\end{aligned}$$

It can be checked that when $V \equiv 0$, starting with $q^{0-} = q^{0+} = 0$ and $p^{0-} = p^{0+} = M/(2\Delta t)$, we get

$$p^{k-} = p^{k+} = M/(2\Delta t), \quad q^{k-} = q^{k+} = k.$$

4.2 Higher order methods

The lifting operator in terms of Legendre polynomials:

$$r_k(1) = \begin{cases} -(2h_{k-1})^{-1}\sum_{l=0}^{n}(2l+1)P_l(\xi(t)), & t_{k-1} < t < t_k, \\ -(2h_k)^{-1}\sum_{l=0}^{n}(-1)^l(2l+1)P_l(\xi(t)), & t_k < t < t_{k+1}, \\ 0, & \text{otherwise}. \end{cases}$$

The first few Legendre polynomials read

$$P_0(\xi) = 1, \quad P_1(\xi) = \xi, \quad P_2(\xi) = \frac{1}{2}\left(3\xi^2 - 1\right).$$

With $n = 0$ and 1 we recover the expressions of $r_k(1)$ above. With $n = 2$,

$$r_k(1) = \begin{cases} -(4h_{k-1})^{-1}\left(1 + 6\xi + 3\xi^2\right), & t_{k-1} < t < t_k, \\ -(4h_k)^{-1}\left(1 - 6\xi + 3\xi^2\right), & t_k < t < t_{k+1}, \\ 0, & \text{otherwise}. \end{cases}$$

The DG derivative with degrees of freedom q^{k+}, $q^{k+1/2}$, and $q^{(k+1)-}$ reads

$$\begin{aligned} & D_{DG}q|_{(t_k,t_{k+1})} \\ &= \frac{1}{\Delta t}\left[(2\xi - 1)\, q^{k+} - 4\xi q^{k+1/2} + (2\xi + 1)\, q^{(k+1)+}\right] \\ &\quad + r_k\left(q^{k-} - q^{k+}\right)(t) + r_{k+1}\left(q^{(k+1)-} - q^{(k+1)+}\right)(t) \\ &= \frac{1}{\Delta t}\left[(2\xi - 1)\, q^{k+} - 4\xi q^{k+1/2} + (2\xi + 1)\, q^{(k+1)+}\right] \\ &\quad - \frac{4}{\Delta t}\left(q^{k-} - q^{k+}\right)\left(1 - 6\xi + 3\xi^2\right) + \frac{4}{\Delta t}\left(q^{(k+1)-} - q^{(k+1)+}\right)\left(1 + 6\xi + 3\xi^2\right) \end{aligned}$$

The discrete Lagrangian reads

$$L_d\left(q^{k-}, q^{k+}, q^{k+1/2}, q^{(k+1)-}, q^{(k+1)+}, \Delta t\right) = \int_{t_k}^{t_{k+1}} \left(\frac{1}{2} M D_{DG} q^2 - V(q)\right) dt$$

The algorithm reads

$$\begin{aligned} p^{k-} &= -D_1 L_d\left(q^{k-}, q^{k+}, q^{k+1/2}, q^{(k+1)-}, q^{(k+1)+}, \Delta t\right), \\ p^{k+} &= -D_2 L_d\left(q^{k-}, q^{k+}, q^{k+1/2}, q^{(k+1)-}, q^{(k+1)+}, \Delta t\right), \\ 0 &= D_3 L_d\left(q^{k-}, q^{k+}, q^{k+1/2}, q^{(k+1)-}, q^{(k+1)+}, \Delta t\right), \\ p^{(k+1)-} &= D_4 L_d\left(q^{k-}, q^{k+}, q^{k+1/2}, q^{(k+1)-}, q^{(k+1)+}, \Delta t\right), \\ p^{(k+1)+} &= D_5 L_d\left(q^{k-}, q^{k+}, q^{k+1/2}, q^{(k+1)-}, q^{(k+1)+}, \Delta t\right). \end{aligned}$$

The Gauss quadrature rule with three points or the Lobatto rule with four points is sufficient to integrate the kinetic energy exactly.

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