

On converting any one-step method to a variational integrator of the same order

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Abstract

In the formalism of constrained mechanics, such as that which underlies the SHAKE and RATTLE methods of molecular dynamics, we present an algorithm to convert any one-step integration method to a variational integrator of the same order. The one-step method is arbitrary, and the conversion can be automated, resulting in a powerful and flexible approach to the generation of novel variational integrators with arbitrary order.

1 Introduction

Consider a Lagrangian system defined by configuration space $\hat{\mathcal{Q}} \equiv \{q\} \equiv \mathbb{R}^N$, velocity phase space $\mathbf{T}\hat{\mathcal{Q}} = \{(q, v)\} = \mathbb{R}^{2N}$, and Lagrangian $L: \hat{\mathcal{Q}} \rightarrow \mathbb{R}$. Assume there is a holonomic constraint $g(q) = 0$, $g: \hat{\mathcal{Q}} \rightarrow \mathbb{R}^d$, suppose g has full rank, and let $\mathcal{Q} = g^{-1}(0)$. The system evolves along curves $q(t) \in \mathcal{Q}$ that are critical points of the action

$$S \equiv \int_a^b L(q(t), v(t)) dt \quad (1.1)$$

subject to the fixed endpoint constraints $q(a), q(b)$ constant, and the first order constraint $v(t) = q'(t)$. This variational principle is equivalent to the Euler–Lagrange equations

$$\frac{dq^i}{dt} = v^i, \quad \frac{dv^i}{dt} = A^i(q, v), \quad (1.2)$$

where $A(q, v)$ is found by solving the linear (Lagrange multiplier) problem (implicit sum on repeated indices)

$$\begin{aligned} \frac{\partial^2 L}{\partial v^i \partial v^j} A^j - \lambda_a \frac{\partial g^a}{\partial q^i} &= -\frac{\partial^2 L}{\partial v^i \partial q^j} v^j + \frac{\partial L}{\partial q^i}, \\ -\frac{\partial g^a}{\partial q^i} A^i &= \frac{\partial^2 g^a}{\partial q^i \partial q^j} v^i v^j. \end{aligned} \quad (1.3)$$

These are the general Lagrangian systems. For example, they specialize to the Euler equations for the motion of a rigid body [1, 12] by taking $\hat{\mathcal{Q}}$ to be the 3×3 matrices $\{A\}$ and g^a to be the the upper triangular

entries of $AA^T - \mathbf{1}$. And they specialize to the Kirchhoff approximations for the motion of an underwater vehicle [9, 15]. The same explicitly constrained formalism is exploited in the molecular dynamics algorithms SHAKE and RATTLE [2, 7, 8, 16].

The objective here is symplectic and momentum-preserving simulation of (1.2). Such simulations may be systematically generated by discretizing the defining variational principles, as in [11, 13, 17], and particularly [10], which is specific to the constrained formalism.

The theory of variational integrators is elaborated in [3, 4], based on geometric discretizations of the velocity phase space $\mathbf{T}\mathcal{Q}$, i.e., based on

1. certain assignments of *curve segments* to each $(q, v) \in \mathbf{T}\hat{\mathcal{Q}}$, where (q, v) is tangent to \mathcal{Q} ; and
2. a *discrete Lagrangian* L_h that approximates S_t for $t = h$; S_t is defined to be the classical action (1.1) with $a = 0$, $b = t$ subject to (1.2), and satisfies

$$\frac{dS_t}{dt} = L(q^i, v^i). \quad (1.4)$$

The discrete variational principle is a finite-dimensional constrained optimization problem, in which the objective function is a sum of the discrete Lagrangian on sequences in $\mathbf{T}\mathcal{Q}$. If the curve segments associated with the elements of the sequence agree to order r with the exact evolution of the Lagrangian system and the discrete Lagrangian agrees to order r with the exact classical action, then the variational integrator is order r accurate [14].

By definition, any one-step numerical integration method of order r gives order r accurate solutions to Equations (1.2) and (1.4). Any such method can be used to provide the curve segments and discrete Lagrangian that are required to construct a variational integrator as outlined above. In this article we derive the variational integrator from the corresponding discrete Euler–Lagrange equations in terms of a one-step integrator of (1.2) and (1.4).

2 Basic Algorithm

Given a Lagrangian L , a constraint g , and a one-step numerical integrator of order r , which we call the *standard layer*, for the initial-value problem

$$\begin{aligned} \frac{dq^i}{dt} &= v^i, & \frac{dv^i}{dt} &= A^i(q, v), & \frac{dS_t}{dt} &= L(q, v), \\ q(0) &= q, & v(0) &= v, & S_t(0) &= 0, \end{aligned}$$

the aim is to generate a symplectic integrator of the same order. Let the standard layer be represented by

$$(q, v) \mapsto R_t(q, v) = (R_t^q(q, v), R_t^v(q, v), R_t^S(q, v)).$$

Assume that the standard layer exactly preserves the constraint; this restriction will be lifted later. By differentiating $g(q) = 0$, the space of vectors tangent to $\mathcal{Q} = g^{-1}(0)$ is

$$\mathbf{T}\mathcal{Q} \equiv \{w \equiv (q, v) : \mathbf{D}g(q)v = 0\}.$$

Differentiating again,

$$\left. \frac{d}{d\epsilon} \right|_{\epsilon=0} \mathbf{D}g(q + \epsilon \delta q)(v + \epsilon \delta v) = v^T \mathbf{D}^2g(q) \delta q + \mathbf{D}g(q) \delta v, \quad (2.1)$$

and so

$$\mathbf{TTQ} \equiv \{ \delta w \equiv ((q, v), (\delta q, \delta v)) : \mathbf{D}g(q) \delta q = 0, v^T \mathbf{D}^2g(q) \delta q + \mathbf{D}g(q) \delta v = 0 \}.$$

The notation $\mathbf{T}_w\mathbf{TQ}$ denotes the vector space $\{ \delta w : (w, \delta w) \in \mathbf{TTQ} \}$. \mathbf{TQ} and \mathbf{TTQ} are of course the first and second tangent bundle of the constraint. The notation for $\mathbf{D}^2g(q)$ is problematic; it is a bilinear form with values in \mathbb{R}^d . The quantity $v^T \mathbf{D}^2g(q)$, where $v \in \mathbb{R}^N$, denotes the $d \times N$ matrix $v^i \partial^2 g^a / \partial q^i \partial q^j(q)$.

We now construct the *symplectic layer* by defining the following quantities.

1. *The bias*: a pair of numbers

$$-1 \leq \alpha^- \leq 0, \quad 0 \leq \alpha^+ \leq 1,$$

such that $\alpha^+ - \alpha^- = 1$.

2. *The time step*: a number $h > 0$.

3. *The maps ∂_h^\pm and the discrete Lagrangian L_h* : the required curve segments are associated with each element (q, v) by $t \mapsto R_t^q(q, v)$ and the discrete Lagrangian is obtained from $(q, v) \mapsto R_h^S(q, v)$. R_t^v is not used. The ends of the segments provide the maps

$$\partial_h^-(q, v) \equiv R_{h\alpha^-}^q(q, v), \quad \partial_h^+(q, v) \equiv R_{h\alpha^+}^q(q, v),$$

and the discrete Lagrangian

$$L_h(q, v) \equiv R_{h\alpha^+}^S(q, v) - R_{h\alpha^-}^S(q, v).$$

4. *The time step of the symplectic layer*: Given $w_1 = (q_1, v_1) \in \mathbf{TQ}$, solve the following *discrete Euler–Lagrange equations* [4] for $w_2 = (q_2, v_2) \in \mathbf{TQ}$:

$$\mathbf{D}L_h(w_1) \delta w_1 + \mathbf{D}L_h(w_2) \delta w_2 = 0,$$

$$\partial_h^+(w_1) = \partial_h^-(w_2),$$

for all $\delta w_1, \delta w_2$ satisfying

$$\mathbf{D}\partial_h^-(w_1) \delta w_1 = 0, \quad \mathbf{D}\partial_h^+(w_2) \delta w_2 = 0,$$

$$\mathbf{D}\partial_h^+(w_1) \delta w_1 = \mathbf{D}\partial_h^-(w_2) \delta w_2,$$

$$(w_1, \delta w_1) \in \mathbf{TTQ}, \quad (w_2, \delta w_2) \in \mathbf{TTQ}.$$

It is not necessary that the *same* standard layer provides both ∂_h^- and ∂_h^+ . For example, using any method to construct ∂_h^+ , the *adjoint* [6] of the same method to construct ∂_h^- , and the bias $\alpha^- = \alpha^+ = \frac{1}{2}$, one evidently obtains a self-adjoint symplectic layer. Self-adjoint methods respect time reversal in the sense that a negative time step exactly reverses the discrete evolution. Also, self-adjoint methods are necessarily of even order: an odd-order self-adjoint method in fact has the next higher (even) order of accuracy because its odd order truncation errors must equal their negatives.

The symplectic layer corresponds to the finite-dimensional discrete variational principle of finding the critical points of the *discrete action*

$$S_h(w, \tilde{w}) \equiv L_h(w) + L_h(\tilde{w})$$

subject to the constraints

$$\begin{aligned}\partial_h^-(w) &= \text{constant}, & \partial_h^+(\tilde{w}) &= \text{constant}, \\ \partial_h^+(w) &= \partial_h^-(\tilde{w}), \\ g(q, v) &= 0, & g(\tilde{q}, \tilde{v}) &= 0,\end{aligned}$$

as discussed in [4].

By the general theory, the maps $\partial_h^-, \partial_h^+$ split $\mathbf{TTQ} = \ker \mathbf{D}\partial_h^- \oplus \ker \mathbf{D}\partial_h^+$; i.e., $(w, \delta w)$ splits as

$$\begin{aligned}\delta w &= \delta w^+ + \delta w^-, \\ \delta w^+ &\in \ker \mathbf{D}\partial_h^-(w), & \delta w^- &\in \ker \mathbf{D}\partial_h^+(w).\end{aligned}$$

(In the second line, the presence of plus with minus is intentional and conforms to the notation of [4].) The *discrete Lagrange one-form* is defined by

$$\theta_{L_h}^-(w) \delta w \equiv -\mathbf{D}L_h(w) \delta w^-,$$

and the general theory assures that the symplectic layer is a symplectic integrator with respect to $\omega_{L_h} \equiv -d\theta_{L_h}^-$.

In Lagrangian systems, the Noether theorem shows that the presence of continuous symmetry is equivalent to the presence of conserved momenta. For example, translational [rotational] symmetry implies conservation of linear [angular] momentum; see [1, 12] for the basic theory, some of which the discussion here must assume. The discrete Noether theorem provides the same symmetry-momentum equivalence for discrete Lagrangian systems: Suppose that a symmetry group \mathcal{G} acts on $\hat{\mathcal{Q}}$, such that

1. g is invariant;
2. $\partial_h^+, \partial_h^-$ intertwine the lift of the action to \mathbf{TQ} ; and
3. L_h is invariant.

Let \mathfrak{g} be the Lie algebra of \mathcal{G} , and let $\xi \in \mathfrak{g}$. Then the symplectic layer preserves the *discrete momentum* defined by

$$J_\xi(w) \equiv -\theta_{L_h}^-(w)\xi w,$$

where $\xi \in \mathfrak{g}$ and ξw is the infinitesimal generator of ξ at w . For example, \mathcal{G} could be a matrix Lie group that acts on \mathbb{R}^N by matrix multiplication, the exact Lagrangian L invariant, the constraint g invariant, and the standard layer an explicit Runge–Kutta method. Then the standard layer intertwines the action on \mathbf{TQ} , and L_h is invariant, and the symplectic layer will preserve the corresponding discrete momenta.

Neither the discrete symplectic form nor the discrete momentum equals in general the continuous counterpart. For example, if the system is rotationally invariant then the symplectic layer need not preserve some familiar mechanical angular momentum. The discrete Lagrangian system has its own version of angular momentum, which is near to the continuous one, but through its dependence on $\partial_h^-, \partial_h^+$, is in general a complicated function of (q, v) .

3 Constrained algorithm

We require the following standard lemma, which will justify the use of a variety of (Lagrange) multipliers.

Lemma 3.1. *Suppose that $A: \mathbb{E} \rightarrow \mathbb{F}$ and $\mu: \mathbb{E} \rightarrow \mathbb{G}$ are linear. Let μ be onto. Then $A(e) = 0$ for all e such that $\mu(e) = 0$ if and only if there is a $\lambda: \mathbb{G} \rightarrow \mathbb{F}$ such that $A = \lambda\mu$.*

Proof. Suppose A is zero on $\ker \mu$. Then A drops to $\bar{A}: \mathbb{E}/\ker \mu \rightarrow \mathbb{F}$. Also, μ drops to $\bar{\mu}: \mathbb{E}/\ker \mu \rightarrow \mathbb{G}$, and this is a linear isomorphism since μ is onto. Set $\lambda \equiv \bar{A}\bar{\mu}^{-1}$. Then, letting $\pi: \mathbb{E} \rightarrow \mathbb{E}/\ker \mu$ be the quotient map, $\lambda\mu(e) = \bar{A}\bar{\mu}^{-1}\mu(e) = \bar{A}\pi(e) = A(e)$. Conversely, if $A = \lambda\mu$ and $\mu(e) = 0$ then $A(e) = \lambda(\mu(e)) = \lambda(0) = 0$. \square

We develop the equations used in the algorithm incrementally in stages; see Figures 1 and 2. In the figures, the dimension counts for the equations and variables are at right. The stages are equivalent representations of the same algorithm, starting from the fundamental description of the algorithm in Stage 0. Only the equations appearing in Stage 4 are implemented and solved in practice. In going from Stage 0 to Stage 4, we increase the number of equations to be solved from $5(N-d)$ to $12N+5d$.

Stage 0: The fundamental algorithm, given directly on the constrained phase space, as in [4]. The fundamental algorithm is defined on $\mathcal{Q} = g^{-1}(0)$, regarded as a submanifold of $\hat{\mathcal{Q}}$. The constraints

$$\mathbf{D}\partial_h^-(w_1)\delta w_1 = 0, \quad \mathbf{D}\partial_h^+(w_2)\delta w_2 = 0,$$

are enforced with multipliers (in $\mathbf{T}\mathcal{Q}$) λ^- and λ^+ , both having dimension $\dim \mathcal{Q} = N-d$. The constraint

$$\mathbf{D}\partial_h^+(w_1)\delta w_1 = \mathbf{D}\partial_h^-(w_2)\delta w_2,$$

is enforced with a multiplier μ . Setting δw_1 and δw_2 alternately to zero gives the two equations (S0.2) and (S0.1), respectively. The *connecting constraint* $\partial_h^+(w_1) = \partial_h^-(w_2)$ translates unchanged to (S0.3).

Stage 1: Enforce the restriction $\delta w_i \in \mathbf{T}_{w_i}\mathbf{T}\mathcal{Q}$ by introducing multipliers. The restriction $(\delta q, \delta v) = \delta w \in \mathbf{T}_w\mathbf{T}\mathcal{Q}$ is

$$\mathbf{D}g(q)\delta q = 0, \quad v^T \mathbf{D}^2g(q)\delta q + \mathbf{D}g(q)\delta v = 0.$$

For each equation in (S0.1) and (S0.2), there are two corresponding multipliers ν_1, ν_2 , which are row vectors of length d .

Stage 2: Disambiguate $\lambda^-, \lambda^+, \mu$. The multipliers $\lambda^+, \lambda^-, \mu$ are ambiguous as row vectors in \mathbb{R}^N up to any vector orthogonal to the constraint. Specifying them into $\mathbf{T}\mathcal{Q}$ disambiguates them. Because $\mathcal{Q} = g^{-1}(0)$ and the rows of $\mathbf{D}g$ span the orthogonal complement to the tangent space of \mathcal{Q} , the multipliers should have zero dot product with the rows of $\mathbf{D}g$, e.g., $\lambda \mathbf{D}g(q)^T = 0$ for a multiplier λ at $q \in \mathcal{Q}$.

Stage 3: Lift the restriction that the standard layer preserves the constraint. A numerical integrator of order r used in the standard layer will in general preserve the constraint g only to accuracy order r . We posit a map $\iota: \mathbb{R}^N \times \mathbb{R}^d \rightarrow \mathbb{R}^N$ such that

1. $\iota(q, 0) = q$; and
2. if $g(q) = 0$, then $\text{Im } \mathbf{D}_\theta \iota(q, 0)$ is a complement of $\ker \mathbf{D}g$; i.e., $\text{Im } \mathbf{D}_\theta \iota(q, 0) \oplus \ker \mathbf{D}g(q) = \mathbb{R}^N$ for all $q \in \mathcal{Q}$.

Stage 0: Given $w_1 = (q_1, v_1) \in \mathbf{TQ}$ solve, for $w_2 = (q_2, v_2) \in \mathbf{TQ}$, the equations		
(S0.1)	$(\mathbf{D}L_h(w_1) = \lambda^- \mathbf{D}\hat{\partial}_h^-(w_1) + \mu \mathbf{D}\hat{\partial}_h^+(w_1))\delta w_1 \quad \forall \delta w_1 \in \mathbf{T}_{w_1} \mathbf{TQ}$	$2(N-d)$
(S0.2)	$(\mathbf{D}L_h(w_2) = \lambda^+ \mathbf{D}\hat{\partial}_h^+(w_2) - \mu \mathbf{D}\hat{\partial}_h^-(w_2))\delta w_2 \quad \forall \delta w_2 \in \mathbf{T}_{w_2} \mathbf{TQ}$	$2(N-d)$
(S0.3)	$\hat{\partial}_h^+(w_1) = \hat{\partial}_h^-(w_2)$	$N-d$
		$5N-5d$
	Lagrange multipliers $\lambda^-, \lambda^+, \mu$	$3(N-d)$
	time advanced state $(q_2, v_2) \in \mathbf{TQ}$	$2(N-d)$
		$5N-5d$
Stage 1:		
(S1.1)	$\mathbf{D}L_h(w_1) = \lambda^- \mathbf{D}\hat{\partial}_h^-(w_1) + \mu \mathbf{D}\hat{\partial}_h^+(w_1) + \nu_1^- [\mathbf{D}g(q_1), 0] + \nu_2^- [v_1^T \mathbf{D}^2 g(q_1), \mathbf{D}g(q_1)]$	$2N$
(S1.2)	$\mathbf{D}L_h(w_2) = \lambda^+ \mathbf{D}\hat{\partial}_h^+(w_2) - \mu \mathbf{D}\hat{\partial}_h^-(w_2) + \nu_1^+ [\mathbf{D}g(q_2), 0] + \nu_2^+ [v_2^T \mathbf{D}^2 g(q_2), \mathbf{D}g(q_2)]$	$2N$
(S1.3)	$\hat{\partial}_h^+(w_1) = \hat{\partial}_h^-(w_2)$	$N-d$
		$5N-d$
	Lagrange multipliers $\lambda^-, \lambda^+, \mu$	$3(N-d)$
	Lagrange multipliers $\nu_1^+, \nu_2^+, \nu_1^-, \nu_2^-$	$4d$
	time advanced state $(q_2, v_2) \in \mathbf{TQ}$	$2(N-d)$
		$5N-d$
Stage 2:		
(S2.1)	$\mathbf{D}L_h(w_1) = \lambda^- \mathbf{D}\hat{\partial}_h^-(w_1) + \mu \mathbf{D}\hat{\partial}_h^+(w_1) + \nu_1^- [\mathbf{D}g(q_1), 0] + \nu_2^- [v_1^T \mathbf{D}^2 g(q_1), \mathbf{D}g(q_1)]$	$2N$
(S2.2)	$\mathbf{D}L_h(w_2) = \lambda^+ \mathbf{D}\hat{\partial}_h^+(w_2) - \mu \mathbf{D}\hat{\partial}_h^-(w_2) + \nu_1^+ [\mathbf{D}g(q_2), 0] + \nu_2^+ [v_2^T \mathbf{D}^2 g(q_2), \mathbf{D}g(q_2)]$	$2N$
(S2.3)	$\hat{\partial}_h^+(w_1) = \hat{\partial}_h^-(w_2)$	$N-d$
(S2.4)	$\lambda^- \mathbf{D}g(\hat{\partial}_h^-(w_1))^T = 0, \quad \mu \mathbf{D}g(\bar{q})^T = 0, \quad \lambda^+ \mathbf{D}g(\hat{\partial}_h^+(w_2))^T = 0$	$3d$
		$5N+2d$
	Lagrange multipliers $\lambda^-, \lambda^+, \mu$	$3N$
	Lagrange multipliers $\nu_1^+, \nu_2^+, \nu_1^-, \nu_2^-$	$4d$
	time advanced state $(q_2, v_2) \in \mathbf{TQ}$	$2(N-d)$
		$5N+2d$
Stage 3:		
(S3.1)	$\mathbf{D}L_h(w_1) = \hat{\lambda}^- \mathbf{D}\hat{\partial}_h^-(w_1) + \hat{\mu}_1 \mathbf{D}\hat{\partial}_h^+(w_1) + \nu_1^- [\mathbf{D}g(q_1), 0] + \nu_2^- [v_1^T \mathbf{D}^2 g(q_1), \mathbf{D}g(q_1)]$	$2N$
(S3.2)	$\mathbf{D}L_h(w_2) = \hat{\lambda}^+ \mathbf{D}\hat{\partial}_h^+(w_2) - \hat{\mu}_2 \mathbf{D}\hat{\partial}_h^-(w_2) + \nu_1^+ [\mathbf{D}g(q_2), 0] + \nu_2^+ [v_2^T \mathbf{D}^2 g(q_2), \mathbf{D}g(q_2)]$	$2N$
(S3.3)	$(\hat{\lambda}^-)^T = \mathbf{D}\mathbb{P}(\hat{\partial}_h^-(w_1))^T (\lambda^-)^T, \quad (\hat{\lambda}^+)^T = \mathbf{D}\mathbb{P}(\hat{\partial}_h^+(w_2))^T (\lambda^+)^T$	$2N$
(S3.4)	$\hat{\mu}_1^T = \mathbf{D}\mathbb{P}(\hat{\partial}_h^+(w_1))^T \mu, \quad \hat{\mu}_2^T = \mathbf{D}\mathbb{P}(\hat{\partial}_h^-(w_2))^T \mu$	$2N$
(S3.5)	$\bar{q} = \mathbb{P}\hat{\partial}^+(w_1), \quad \hat{\partial}_h^-(w_2) = \iota(\bar{q}, \theta^+)$	$2N$
(S3.6)	$q_1^- = \mathbb{P}\hat{\partial}_h^-(w_1), \quad q_2^+ = \mathbb{P}\hat{\partial}_h^+(w_2)$	$2N$
(S3.7)	$g(q_2) = 0, \quad \mathbf{D}g(q_2)v_2 = 0$	$2d$
(S3.8)	$\lambda^- \mathbf{D}g(q_1^-)^T = 0, \quad \mu \mathbf{D}g(\bar{q})^T = 0, \quad \lambda^+ \mathbf{D}g(q_2^+)^T = 0$	$3d$
		$12N+5d$
	Lagrange multipliers $\lambda^-, \lambda^+, \mu, \hat{\lambda}^-, \hat{\lambda}^+, \hat{\mu}_1, \hat{\mu}_2$	$7N$
	Lagrange multipliers $\nu_1^+, \nu_2^+, \nu_1^-, \nu_2^-$	$4d$
	variables q_1^-, \bar{q}, q_2^+	$3N$
	variable θ^+	d
	time advanced state $(q_2, v_2) \in \mathbf{TQ}$	$2N$
		$12N+5d$

Figure 1: Stages 0–3.

Stage 4: Given $w_1 = (q_1, v_1) \in \mathcal{TQ}$ solve, for $w_2 = (q_2, v_2) \in \mathcal{TQ}$, the equations		
(S4.1)	$q_1^- = \mathbb{P}\hat{\delta}_h^-(w_1)$	N
(S4.2)	$\bar{q} = \mathbb{P}\hat{\delta}_h^+(w_1)$	N
(S4.3a)	$\hat{\lambda}^- \mathbf{D}_q \hat{\delta}_h^-(w_1) + \nu_1^- \mathbf{D}g(q_1) + \hat{\mu}_1 \mathbf{D}_q \hat{\delta}_h^+(w_1) + \nu_2^- v_1^T \mathbf{D}^2 g(q_1) - \mathbf{D}_q L_h(w_1) = 0$	N
(S4.3b)	$\lambda^- \mathbf{D}g(q_1^-)^T = 0$	d
(S4.3c)	$(\hat{\lambda}^-)^T = \mathbf{D}\mathbb{P}(\hat{\delta}_h^-(w_1))^T (\lambda^-)^T$	N
(S4.4a)	$\hat{\mu}_1 \mathbf{D}_v \hat{\delta}_h^+(w_1) + \nu_2^- \mathbf{D}g(q_1) + \hat{\lambda}^- \mathbf{D}_v \hat{\delta}_h^-(w_1) - \mathbf{D}_v L_h(w_1) = 0$	N
(S4.4b)	$\mu \mathbf{D}g(\bar{q})^T = 0$	d
(S4.4c)	$\hat{\mu}_1^T = \mathbf{D}\mathbb{P}(\hat{\delta}_h^+(w_1))^T \mu$	N
(S4.5a)	$\hat{\lambda}^+ \mathbf{D}_q \hat{\delta}_h^+(w_2) + \nu_1^+ \mathbf{D}g(q_2) - \hat{\mu}_2 \mathbf{D}_q \hat{\delta}_h^-(w_2) + \nu_2^+ v_2^T \mathbf{D}^2 g(q_2) - \mathbf{D}_q L_h(w_2) = 0$	N
(S4.5b)	$\lambda^+ \mathbf{D}g(q_2^+)^T = 0$	d
(S4.5c)	$(\hat{\lambda}^+)^T = \mathbf{D}\mathbb{P}(\hat{\delta}_h^+(w_2))^T (\lambda^+)^T$	N
(S4.6a)	$\mathbf{D}_v L_h(w_2) - \nu_2^+ \mathbf{D}g(q_2) - \hat{\lambda}^+ \mathbf{D}_v \hat{\delta}_h^+(w_2) + \hat{\mu}_2 \mathbf{D}\hat{\delta}_h^-(w_2) = 0$	N
(S4.6b)	$\mathbf{D}g(q_2)v_2 = 0$	d
(S4.6c)	$\hat{\mu}_2^T = \mathbf{D}\mathbb{P}(\hat{\delta}_h^-(w_2))^T \mu$	N
(S4.7a)	$\hat{\delta}_h^-(w_2) = \iota(\bar{q}, \theta^+)$	N
(S4.7b)	$g(q_2) = 0,$	d
(S4.8)	$q_2^+ = \mathbb{P}\hat{\delta}_h^+(w_2)$	N
		<hr/>
		$12N + 5d$
	Lagrange multipliers $\lambda^-, \lambda^+, \mu, \hat{\lambda}^+, \hat{\lambda}^-, \hat{\mu}_1, \hat{\mu}_2$	$7N$
	Lagrange multipliers $\nu_1^+, \nu_2^+, \nu_1^-, \nu_2^-$	$4d$
	variables q_1^-, \bar{q}, q_2^+	$3N$
	variable θ^+	$2d$
	time advanced state $(q_2, v_2) \in \mathcal{TQ}$	$2N$
		<hr/>
		$12N + 5d$
(S4.3a')	$(\lambda^- + \mu) + \nu_1^- G_0 + \nu_2^- v_1^T \mathbf{D}^2 g(q_1) - h \mathbf{D}_q L(q_1, v_1) = 0$	
(S4.3b')	$\lambda^- G_0^T = 0$	
(S4.4a')	$(h\alpha^- \lambda^- + h\alpha^+ \mu) + \nu_2^- G_0 - h v_1^T M_0 - h a_0 = 0$	
(S4.4b')	$\mu G_0^T = 0$	
(S4.5a')	$(\lambda^+ - \mu) + \nu_1^+ G_0 + \nu_2^+ v_1^T \mathbf{D}^2 g(q_1) - h \mathbf{D}_q L(q_1, v_1) = 0$	
(S4.5b')	$\lambda^+ G_0^T = 0$	
(S4.6a')	$h v_2^T M_0 - \nu_2^+ G_0 + h\alpha_0 - \lambda^+ + \mu = 0$	
(S4.6b')	$G_0 v_2 = 0$	
(S4.7a')	$(q_2 - \bar{q}) - \mathbf{D}g(q_1)^T \bar{\theta}^+ + h\alpha^+ v_2 = 0$	
(S4.7b')	$G_0(q_2 - \bar{q}) = 0$	

Figure 2: Stage 4: the derivatives in stage 3 are split into partial derivatives with respect to q and v , and the equations are reorganized. the approximates are correspondingly the bottom primed equations.

4 Implementation

We present here a strategy for the Stage 4 computation.

4.1 The vector field and its derivatives.

We now specialize to Lagrangians of the form

$$L \equiv \frac{1}{2} m_{ij}(q) v^i v^j + a_j(q) v^j - V(q). \quad (4.1)$$

This is the most general quadratic Lagrangian with configuration-dependent coefficients. As is easily verified, Equation (1.3) becomes

$$\begin{aligned} m_{ij} A^j - \lambda_a \frac{\partial g^a}{\partial q^i} &= -\Gamma_{ikl} v^k v^l - b_{ij} v^j - \frac{\partial V}{\partial q^i}, \\ -\frac{\partial g^a}{\partial q^i} A^i &= \frac{\partial^2 g^a}{\partial q^i \partial q^j} v^i v^j, \\ \Gamma_{ikl} &\equiv \frac{1}{2} \left(\frac{\partial m_{il}}{\partial q^k} + \frac{\partial m_{ik}}{\partial q^l} - \frac{\partial m_{kl}}{\partial q^i} \right), \\ b_{ij} &\equiv \frac{\partial a_i}{\partial q^j} - \frac{\partial a_j}{\partial q^i}. \end{aligned} \quad (4.2)$$

These are all linear equations for A and λ with coefficient matrix of the form

$$\begin{bmatrix} M(q) & -\mathbf{D}g(q)^T \\ -\mathbf{D}g(q) & 0 \end{bmatrix}, \quad M(q) \equiv [m_{ij}(q)]. \quad (4.3)$$

The algorithm requires the derivatives of the maps ∂_h^- and ∂_h^+ as well as the derivative of L_h . Automatic differentiation [5] can be used to compute these by computing the derivative of the one-step method in the standard layer that defines them. Alternatively, by Lemma 4.1 of [6], the derivative of the standard layer R_t that uses a Runge–Kutta method may be computed as the same Runge–Kutta method applied to the equations of first variation. In this case, it is only required to determine the derivative of the vector field.

To compute the derivative of A^j with respect to q^m and v^m , we differentiate the first equation in (4.2):

$$\begin{aligned} m_{ij} \frac{\partial A^j}{\partial q^m} - \frac{\partial \lambda_a}{\partial q^m} \frac{\partial g^a}{\partial q^i} &= -\frac{\partial \Gamma_{ikl}}{\partial q^m} v^k v^l - \frac{\partial b_{ij}}{\partial q^m} v^j - \frac{\partial^2 V}{\partial q^i \partial q^m} - \frac{\partial m_{ij}}{\partial q^m} A^j - \frac{\partial^2 g^a}{\partial q^i \partial q^m} \lambda_a, \\ m_{ij} \frac{\partial A^j}{\partial v^m} - \frac{\partial \lambda_a}{\partial v^m} \frac{\partial g^a}{\partial q^i} &= -2\Gamma_{ikm} v^k \end{aligned}$$

and for the constraints

$$\begin{aligned} -\frac{\partial g^a}{\partial q^i} \frac{\partial A^i}{\partial q^m} &= \frac{\partial^3 g^a}{\partial q^i \partial q^j \partial q^m} v^i v^j - \frac{\partial^2 g^a}{\partial q^i \partial q^m} A^i, \\ -\frac{\partial g^a}{\partial q^i} \frac{\partial A^i}{\partial v^m} &= 2 \frac{\partial^2 g^a}{\partial q^i \partial q^m} v^i. \end{aligned}$$

These resulting equations are linear in the required derivatives with coefficient matrix (4.3).

4.2 Fixed-point iteration

A possible approach for solving the Stage 4 (implicit) equations is by a fixed-point iteration. To find solutions to a generic equation $f(x) = 0$, split $f = f_0 - \Delta f$ such that, for all b , an explicit solution to the equation $f_0(x) = b$ is available. We call f_0 an *approximate*. If Δf is sufficiently small, then in a suitable neighbourhood of the solution, the iteration $x_{i+1} = f_0^{-1}(\Delta f(x_i))$ converges to a solution of $f(x) = 0$:

$$f_0(x) = \Delta f(x) = f_0(x) - f(x) \quad \Leftrightarrow \quad f(x) = 0.$$

The iteration is, given an initial iterate x_0 ,

$$r_{i+1} = f_0(x_i) - f(x_i), \quad \text{solve } f_0(x_{i+1}) = r_{i+1},$$

or equivalently, after substituting $f_0(x_i) = r_i$,

$$\begin{aligned} r_0 &= f_0(x_0), \\ r_{i+1} &= r_i - f(x_i), \\ \text{solve } f_0(x_{i+1}) &= r_{i+1}. \end{aligned} \tag{4.4}$$

This approach is useful for the Stage 4 equations because they are nonlinear and a good choice for f_0 is generally available. In this way, the Stage 4 computation may be organized into its equations and corresponding approximates. The required solution is obtained by iteratively evaluating the equations themselves and then solving for the approximates using (4.4).

4.3 Stage 4 approximates

Because the time step is small, the various configurations q_1, \bar{q}, q_2 , etc., are all close. Let G_0, M_0 , and a_0 , be approximations to $\mathbf{D}g(q)$, $M(q)$, and $a(q)$ respectively, obtained by evaluation at some such configuration; e.g., the configuration q_1 is a likely candidate.

Equations (S4.1), (S4.2), and (S4.8) are of the form of Equations (3.2), which, for sufficiently small h , can be effectively approximated by Taylor expansion of $g(q) = 0$ at $q = \hat{q}$:

$$\begin{aligned} (\hat{q} - q) - G_0^T \theta &= 0, \\ -G_0(\hat{q} - q) - g(\hat{q}) &= 0. \end{aligned}$$

Equations (S4.3c), (S4.4c), (S4.5c), and (S4.6c) involve the derivative of \mathbb{P} in expressions such as

$$\hat{\lambda}^T = \mathbf{D}\mathbb{P}(q)\lambda^T. \tag{4.5}$$

Differentiating equations (3.2) gives

$$\begin{aligned} \delta \hat{q} &= \delta q + \mathbf{D}g(q)^T \delta \theta + \mathbf{D}^2(\theta^T g)(q) \delta q, \\ \delta g &= \mathbf{D}g(q) \delta q. \end{aligned} \tag{4.6}$$

The matrix $\mathbf{D}\mathbb{P}(q)$ is obtained by discarding $\delta \theta$ after the inverse of (4.6), with $\delta g = 0$, i.e.,

$$\mathbf{D}\mathbb{P}(q) = \begin{bmatrix} \mathbf{1} & 0 \end{bmatrix} \begin{bmatrix} \mathbf{1} + \mathbf{D}^2(\theta^T g)(q) & \mathbf{D}g(q)^T \\ \mathbf{D}g(q) & 0 \end{bmatrix}^{-1} \begin{bmatrix} \mathbf{1} & 0 \\ 0 & 0 \end{bmatrix},$$

and Equation (4.5) becomes

$$\begin{bmatrix} \hat{\lambda}^r \\ 0 \end{bmatrix} = \begin{bmatrix} \mathbf{1} & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} \mathbf{1} + \mathbf{D}^2(\theta^r g)(q) & \mathbf{D}g(q)^T \\ \mathbf{D}g(q) & 0 \end{bmatrix}^{-1} \begin{bmatrix} \lambda^r \\ 0 \end{bmatrix}.$$

If we define a variable z and put it in place of the zero in the matrix at left, then we can put a unit matrix in the (2,2) slot of the first matrix on the right side, and invert. The result is the linear equation

$$\begin{bmatrix} \mathbf{1} + \mathbf{D}^2(\theta^r g)(q) & \mathbf{D}g(q)^T \\ \mathbf{D}g(q) & 0 \end{bmatrix} \begin{bmatrix} \hat{\lambda}^r \\ z \end{bmatrix} = \begin{bmatrix} \lambda^r \\ 0 \end{bmatrix}. \quad (4.7)$$

This replaces (S4.3c), (S4.4c), (S4.5c), and (S4.6c), and one can use the approximate

$$\begin{bmatrix} \mathbf{1} & G_0^T \\ G_0 & 0 \end{bmatrix} \begin{bmatrix} \hat{\lambda}^r \\ z \end{bmatrix} = \begin{bmatrix} \lambda^r \\ 0 \end{bmatrix}, \quad (4.8)$$

which is computationally equivalent to

$$\begin{bmatrix} \mathbf{1} & -G_0^T \\ -G_0 & 0 \end{bmatrix} \begin{bmatrix} -\hat{\lambda}^r \\ z \end{bmatrix} = \begin{bmatrix} -\lambda^r \\ 0 \end{bmatrix}.$$

The remaining approximates are driven by the basic data of the variational principle:

$$\begin{aligned} \mathbf{D}_q L_h &\approx h \mathbf{D}_q L, & \mathbf{D}_v L_h &\approx h v^T M_0 + h a_0, \\ \hat{\partial}_h^+(q, v) &\approx q + h \alpha^+ v, & \hat{\partial}_h^-(q, v) &\approx q + h \alpha^- v. \end{aligned} \quad (4.9)$$

In order, the approximates for Equations (4.3a,b) obtained from (4.9), $\hat{\lambda}^- \approx \lambda^-$, and $\hat{\mu} \approx \mu$ are as follows:

$$\begin{aligned} \mathbf{D}_q \partial_h^-(w_1) &\approx \mathbf{1}, & \hat{\lambda}^- \mathbf{D}_q \partial_h^-(w_1) &\approx \lambda^-, \\ \mathbf{D}_q \partial_h^+(w_1) &\approx \mathbf{1}, & \hat{\mu}_1 \mathbf{D}_q \partial_h^+(w_1) &\approx \mu, \\ \nu_1^- \mathbf{D}g(q_1) &\approx \nu_1^- G_0 = 0, \end{aligned}$$

resulting in

$$\begin{aligned} \lambda^- + \mu + \nu_1^- G_0 + \nu_2^- v_1^T \mathbf{D}^2 g(q_1) - h \mathbf{D}_q L(q_1, v_1) &= 0, \\ \lambda^- G_0^T &= 0. \end{aligned}$$

These are equations (S4.3a') and (S4.3b'). Similarly one obtains the approximates (S4.4a'b')–(S4.6a'b'), noting however that in (S4.5a') there are the further approximations

$$\nu_2^+ v_1^T \mathbf{D}^2 g(q_1) \approx \nu_2^- v_1^T \mathbf{D}^2 g(q_1), \quad \mathbf{D}_q L(q_2, v_2) \approx \mathbf{D}_q L(q_1, v_1).$$

Equations (S4.7a) and (S4.7b) are

$$\hat{\partial}_h^-(w_2) - \mathbf{D}g(\bar{q})^T \theta^+ = \bar{q}, \quad g(q_2) = 0,$$

which have to be solved for q_2 and θ^+ . Taylor expanding the second equation at \bar{q} , and using $g(\bar{q}) = 0$, gives the approximate

$$\begin{aligned} q_2 - \bar{q} - \mathbf{D}g(q_1)^T \theta^+ + h \alpha^+ v_2 &= 0, \\ G_0(q_2 - \bar{q}) &= 0, \end{aligned}$$

which are Equations (S4.7a'b').

4.4 Stage 4 solution

The approximates (S4.3a'b') through (S4.5a'b') are solvable for the multipliers

$$\lambda^-, \mu, \lambda^+, \nu_1^-, \nu_2^-, \nu_1^+,$$

and the linear equations are all of the form (4.8). Indeed, one adds α^- times (S4.3b') and α^+ times (S4.4b'), and then that together with (S4.4a') can be solved for $\alpha^- \lambda^- + \alpha^+ \mu$ and ν_2^- . Then, and similarly, (S4.3a'b') can be solved for $\lambda^- + \mu$ and ν_1^- . Together these give $\lambda^-, \mu, \nu_1^-, \nu_2^-$. Because μ is then known, (S4.5a') with (S4.5b') minus (S4.4b') provide λ^+ and ν_1^+ . In the same way (S4.6a'b') may be used to update ν_2^+ and v_2 . Finally, (S4.7a'b') are solved for q_2 and

$$\hat{\lambda}^-, \hat{\mu}_1, \hat{\mu}_2, \hat{\lambda}^+$$

occurring in (S4.3c), (S4.4c), (S4.5c), and (S4.6c'), may all be updated using appropriate versions of (4.7) and its approximates. The entire procedure can then be iterated until the variables q_2 and v_2 are at a predetermined accuracy.

It should be noted that the multipliers that impose the constraints g , i.e., $\nu_1^-, \nu_2^-, \nu_1^+, \nu_2^+$ are not unique. For example, doubling g results in halving these multipliers. Such multipliers are nonphysical, and convergence of the iteration of Stage 4 should not be bound to the convergence of the multipliers themselves. Rather, the degree of convergence can be determined from products such as $\nu_2^- \mathbf{D}g(q_1)$, which generally have the physical meaning of *force of constraint*; i.e., they are added directly in the equations to quantities with a physical interpretation.

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