Discrete Penalty Layers Admit Multisymplectic Integration

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1 Introduction

The good energy behavior of AVIs was studied in Lew et al. 2003 [5], wherein it is conjectured that this behavior is due to the integrator possessing the geometric property of multisymplecticity. In the proof that AVIs are multisymplectic, the paper assumes that the asynchronous potentials act on distinct triangles in a spatial triangulation of the system. This assumption would seem to preclude incorporation of nested penalty layers for collision response: since for every (vertex, face) or (edge, edge) pair, potentials depend on that pair, no required spatial triangulation exists. In this report we show that multisymplecticity holds even for AVIs whose potentials do not respect a spatial triangulation.

2 Variational Integrators

Let $\gamma(t)$ be a piecewise-regular trajectory through configuration space $\mathbf{Q}$, and $\dot{\gamma}(t) = \frac{d}{dt}\gamma(t)$ be the configurational velocity at time t. For simplicity we shall assume that the kinetic energy of the system T depends only on configurational velocity, and that the potential energy V depends only on configurational position, so that we may write the Lagrangian L at time t as

$$L(q, \dot{q}) = T(\dot{q}) - V(q). \tag{1}$$

Then given the configuration of the system q_0 at time t_0 and q_f at t_f, Hamilton's principle [3] states that the trajectory of the system $\gamma(t)$ joining $\gamma(t_0) = q_0$ and $\gamma(t_f) = q_f$ is a stationary point of the action functional

$$S(\gamma) = \int_{t_0}^{t_f} L\left[\gamma(t), \dot{\gamma}(t)\right] dt$$

with respect to taking variations $\delta\gamma$ of γ which leave γ fixed at the endpoints t_0, t_f. In other words, γ satisfies

$$dS(\gamma) \cdot \delta\gamma = 0. \tag{2}$$

Integrating by parts, and using that $\delta\gamma$ vanishes at t_0 and t_1, we compute

$$\begin{aligned} dS(\gamma)\cdot\delta\gamma &= \int_{t_0}^{t_f}\left(\frac{\partial L}{\partial q}(\gamma,\dot\gamma)\cdot\delta\gamma+\frac{\partial L}{\partial\dot q}(\gamma,\dot\gamma)\cdot\delta\dot\gamma\right)dt \\ &= \int_{t_0}^{t_f}-\frac{\partial V}{\partial q}(\gamma)\cdot\delta\gamma\,dt+\int_{t_0}^{t_f}\frac{\partial T}{\partial\dot q}(\dot\gamma)\cdot\delta\dot\gamma\,dt \\ &= \int_{t_0}^{t_f}-\frac{\partial V}{\partial q}(\gamma)\cdot\delta\gamma\,dt+\frac{\partial T}{\partial\dot q}(\dot\gamma)\cdot\delta\gamma\Big|_{t_0}^{t_f}-\int_{t_0}^{t_f}\frac{d}{dt}\left[\frac{\partial T}{\partial\dot q}(\dot\gamma)\right]\cdot\delta\gamma\,dt \\ &= \int_{t_0}^{t_f}\left(-\frac{\partial V}{\partial q}(\gamma)-\frac{\partial^2 T}{\partial\dot q^2}(\dot\gamma)\ddot\gamma\right)\cdot\delta\gamma\,dt=0. \end{aligned}$$

Since this equality must hold for all variations $\delta\gamma$ that fix γ's endpoints, we must have

$$\frac{\partial V}{\partial q}(\gamma)+\frac{\partial^2 T}{\partial\dot q^2}(\dot\gamma)\ddot\gamma=0, \tag{3}$$

the *Euler-Lagrange equation* of the system. This equation is a second-order ordinary differential equation, and so has a unique solution γ given two initial values $\gamma(t_0)$ and $\dot\gamma(t_0)$.

2.1 Symplecticity

The flow $\Theta_s : [\gamma(t),\dot\gamma(t)]\mapsto[\gamma(t+s),\dot\gamma(t+s)]$ given by (3) has many structure-preserving properties; in particular it is momentum-preserving, energy-preserving, and symplectic [4]. To see this last property, for the remainder of this section we restrict the space of trajectories to those that satisfy the Euler-Lagrange equations. For such trajectories, and relaxing the requirement that $\delta\gamma$ fix the endpoints of γ, we have

$$dS(\gamma)\cdot\delta\gamma=\frac{\partial T}{\partial\dot q}\left[\pi_{\dot q}(q,\dot q)\right]\cdot\delta\gamma\Big|_{t_0}^{t_f}, \tag{4}$$

where $\pi_{\dot q}$ is projection onto the second factor.

Since initial conditions $(q,\dot q)$ are in bijection with trajectories satisfying the Euler-Lagrange equation, such trajectories γ can be uniquely parametrized by initial conditions $[\gamma(t_0),\dot\gamma(t_0)]$. For the remainder of this section we also restrict variations $\delta\gamma$ to those which preserve that γ satisfies the Euler-Lagrange equations; these are also parametrized by variations of the initial conditions, $(\delta q,\delta\dot q)$. For conciseness of notation, we will write $\nu(t)=(\gamma(t),\dot\gamma(t))$ and $\delta\nu(t)=[\delta\gamma(t),\delta\dot\gamma(t)]$; using this notation we write the above two facts as $\nu(t)=\Theta_{t-t_0}\nu(t_0)$ and $\delta\nu(t)=\Theta_{t-t_0*}\delta\nu(t_0)$. The action (1), a functional on trajectories γ, can also be rewritten as a function S_i of the intial conditions,

$$S_i(q,\dot q)=\int_0^{t_f-t_0}L\left[\Theta_t(q,\dot q)\right]dt,$$

so that

$$dS(\gamma)\cdot\delta\gamma=dS_i\left[\nu(t_0)\right]\cdot\delta\nu(t_0).$$

Substituting all of these expressions into (4), we get

$$
\begin{aligned}
dS_i\left[\nu(t_0)\right]\cdot\delta\nu(t_0) &= \left(\frac{\partial T}{\partial\dot{q}}\circ\pi_{\dot{q}}\right)\left[\Theta_{t-t_0}\nu(t_0)\right]\cdot\delta\gamma(t)\Big|_{t_0}^{t_f}\\
&= \left(\frac{\partial T}{\partial\dot{q}}\circ\pi_{\dot{q}}\right)\left[\Theta_{t-t_0}\nu(t_0)\right]dq\cdot\delta\nu(t)\Big|_{t_0}^{t_f}\\
&= \left(\frac{\partial T}{\partial\dot{q}}\circ\pi_{\dot{q}}\right)\left[\Theta_{t-t_0}\nu(t_0)\right]dq\cdot\Theta_{t-t_0*}\delta\nu(t_0)\Big|_{t_0}^{t_f}\\
&= \left(\frac{\partial T}{\partial\dot{q}}\circ\pi_{\dot{q}}\right)\left[\Theta_{t_f-t_0}\nu(t_0)\right]dq\cdot\Theta_{t_f-t_0*}\delta\nu(t_0)-\left(\frac{\partial T}{\partial\dot{q}}\circ\pi_{\dot{q}}\right)\left[\nu(t_0)\right]dq\cdot\delta\nu(t_0)\\
&= \left({\Theta_{t_f-t_0}}^*\theta_L-\theta_L\right)_{\nu(t_0)}\cdot\delta\nu(t_0),
\end{aligned}
$$

where θ_L is the one-form $\left(\frac{\partial T}{\partial\dot{q}}\circ\pi_{\dot{q}}\right)dq$. Since dS_i is exact,

$$d^2S_i=0={\Theta_{t_f-t_0}}^*d\theta_L-d\theta_L,$$

so since t_0 and t_f are arbitrary, $\Theta_s^*d\theta_L=d\theta_L$, and Θ preserves the so-called *symplectic form* $d\theta_L$.

2.2 Discretization

Following Hairer et al. [2], we now turn our attention to discretizing Hamilton's principle, and derive a numerical integrator that shares many of the structure-preserving properties of the continuous flow Θ_s. Consider a discretization of the trajectory $\gamma:[t_0,t_f]\to\mathbf{Q}$ by a piecewise linear trajectory interpolating n points $\mathbf{q}=\{q_0,q_1,\dots q_{n-1}\}$, with $q_0=\gamma(t_0)$ and $q_{n-1}=\gamma(t_f)$, where the discrete velocity $\dot{q}_{i+1/2}$ on the segment between q_i and q_{i+1} is

$$\dot{q}_{i+1/2}=\frac{q_{i+1}-q_i}{h},\quad h=\frac{t_f-t_0}{n}.$$

We seek an analogue of (3) in this discrete setting. To that end, we formulate a discrete Lagrangian

$$L_d(q_a,q_b)=T\left(\frac{q_b-q_a}{h}\right)-V(q_b)\tag{5}$$

and discrete action

$$S_d(\mathbf{q})=\sum_{i=0}^{n-2}hL_d(q_i,q_{i+1}).\tag{6}$$

Motivated by (2), we impose a discrete Hamilton's principle:

$$dS_d(\mathbf{q})\cdot\delta\mathbf{q}=0$$

for all variations $\delta\mathbf{q}=\{\delta q_0,\delta q_1,\dots,\delta q_{n-1}\}$ that fix $\mathbf{q}$ at its endpoints, i.e. , with $\delta q_0=\delta q_{n-1}=0$. For ease of notation, we define versions of the kinetic and potential energy terms in (5) that depend on (q_a,q_b) instead of $(q,\dot{q})$:

$$
\begin{aligned}
T_d(q_a,q_b) &= T\left(\frac{q_b-q_a}{h}\right)\\
T_d'(q_a,q_b) &= \frac{\partial T}{\partial\dot{q}}\left(\frac{q_b-q_a}{h}\right)\\
V_d(q_a,q_b) &= V(q_b)\\
V_d'(q_a,q_b) &= \frac{\partial V}{\partial q}(q_b).
\end{aligned}
$$

$$
\begin{aligned}
dS_d(\mathbf{q})\cdot\delta\mathbf{q} &= \sum_{i=0}^{n-2} h\left(D_1L_d(q_i,q_{i+1})\cdot\delta q_i + D_2L_d(q_i,q_{i+1})\cdot\delta q_{i+1}\right)\\
&= \sum_{i=0}^{n-2} h\left(-\frac{1}{h}T_d'(q_i,q_{i+1})\cdot\delta q_i + \frac{1}{h}T_d'(q_i,q_{i+1})\cdot\delta q_{i+1} - \frac{\partial V}{\partial q}(q_{i+1})\cdot\delta q_{i+1}\right)\\
&= \sum_{i=0}^{n-2} -T_d'(q_i,q_{i+1})\cdot\delta q_i + \sum_{i=1}^{n-1}\left(T_d'(q_{i-1},q_i)\cdot\delta q_i - h\frac{\partial V}{\partial q}(q_i)\cdot\delta q_i\right)\\
&= T_d'(q_{n-2},q_{n-1})\cdot\delta q_{n-1} - T_d'(q_0,q_1)\cdot\delta q_0 - h\frac{\partial V}{\partial q}(q_{n-1})\cdot\delta q_{n-1}\\
&\quad + \sum_{i=1}^{n-2}\left(T_d'(q_{i-1},q_i) - T_d'(q_i,q_{i+1}) - h\frac{\partial V}{\partial q}(q_i)\right)\cdot\delta q_i\\
&= \sum_{i=1}^{n-2}\left(T_d'(q_{i-1},q_i) - T_d'(q_i,q_{i+1}) - h\frac{\partial V}{\partial q}(q_i)\right)\cdot\delta q_i = 0.
\end{aligned}
$$

Since δq_i is unconstrained for $1 \le i \le n-2$, we must have

$$
\frac{\partial T}{\partial \dot{q}}(\dot{q}_{i+1/2}) - \frac{\partial T}{\partial \dot{q}}(\dot{q}_{i-1/2}) = -h\frac{\partial V}{\partial q}(q_i), \quad i = 1,\ldots,n-2, \tag{7}
$$

the *discrete Euler-Langrange equations* of the system.

Unlike in the continuous settings, the discrete Euler-Lagrange equations do not always have a unique solution given initial values q_0 and q_1. We therefore assume in all that follows that T_d and V_d are of a form so that (7) gives a unique q_{i+1} given q_i and q_{i-1} - this assumption always holds, for instance, in the typical case where T_d is quadratic in $\dot{q}$. Then the discrete Euler-Lagrange equations give a well-defined discrete flow

$$
F : (q_{i-1}, q_i) \mapsto (q_i, q_{i+1}),
$$

which recovers the entire trajectory from initial conditions, in perfect analogy to the continuous setting.

2.3 Symplecticity of the Discrete Flow

We now would like a symplectic form preserved by F, just as $d\theta_L$ is preserved by Θ. As in the continuous setting, we restrict trajectories $\mathbf{q}$ to those that satisfy the discrete Euler-Lagrange equations, and variations to first variations, yielding

$$
dS_d(\mathbf{q})\cdot\delta\mathbf{q} = T_d'(q_{n-2},q_{n-1})\cdot\delta q_{n-1} - T_d'(q_0,q_1)\cdot\delta q_0 - h\frac{\partial V}{\partial q}(q_{n-1})\cdot\delta q_{n-1}.
$$

We denote by F^k the discrete flow F composed with itself k times, or k "steps" of F. We remark again that all $\mathbf{q}$ satisfying (7) can be parametrized by initial conditions $\nu_0 = (q_0, q_1)$, and first variations by $\delta\nu_0 = (\delta q_0, \delta q_1)$, so that we can rewrite the discrete action as

$$
S_{id}(\nu_0) = \sum_{i=0}^{n-2} \Delta t L_d(F^i\nu_0).
$$

Putting together all of the pieces,

$$\begin{aligned}
dS_{id}(\nu_0)\cdot\delta\nu_0 &= dS_d(\mathbf{q})\cdot\delta\mathbf{q} \\
&= T_d'(q_{n-2},q_{n-1})\cdot\delta q_{n-1} - T_d'(q_0,q_1)\cdot\delta q_0 - h\frac{\partial V}{\partial q}(q_{n-1})\cdot\delta q_{n-1} \\
&= \left[T_d'(F^{n-2}\nu_0) - hV'(F^{n-2}\nu_0)\right]\cdot\delta q_{n-1} - T_d'(\nu_0)\cdot\delta q_0 \\
&= \left[T_d'(F^{n-2}\nu_0) - hV'(F^{n-2}\nu_0)\right] dq_b\cdot {F^{n-2}}_*\delta\nu_0 - T_d'(\nu_0)dq_a\cdot\delta\nu_0 \\
&= \theta^+_{F^{n-2}\nu_0}\cdot {F^{n-2}}_*\delta\nu_0 + \theta^-_{\nu_0}\cdot\delta\nu_0 \\
&= \left(F^{n-2^*}\theta^+\right)_{\nu_0}\cdot\delta\nu_0 + \theta^-_{\nu_0}\cdot\delta\nu_0.
\end{aligned}$$

for the indicated two-forms θ^+ and θ^-. Since $d(hL_d) = \theta^+ + \theta^-$, $d^2(hL_d) = 0 = d\theta^+ + d\theta^-$. Moreover ν_0 is arbitrary, hence

$$d^2S_{id} = 0 = F^{n-2^*}d\theta^+ + d\theta^- = -F^{n-2^*}d\theta^- + d\theta^-,$$

so

$$d\theta^- = F^{n-2^*}d\theta^-.$$

Since n is arbitrary, we conclude that the discrete flow F preserves the symplectic form $d\theta^-$. Using backwards error analysis, it can be shown that this geometric property guarantees that integrating with F introduces no energy drift for a number of steps exponential in Δt [2], a highly desirable property when simulating molecular dynamic or other Hamiltonian systems whose qualitative behavior is substantially affected by errors in energy.

3 Asynchronous Variational Integrators

In section 2.2 we formulated an action functional (6) as the integration of a single discrete Lagrangian over a single time step size h. Such a construction is cumbersome when modeling multiple potentials of varying stiffnesses acting on different parts of the system: to prevent instability we are forced to integrate the entire system at the resolution of the stiffest force. Given a spacial triangulation $\mathcal{T} = \{T_i\}$ of the system, asynchronous variational integrators (AVIs), as described in Lew et al. 2003 [5], are a family of numerical integrators, derived from a discrete Hamilton's principle, that support integrating potentials on different triangles at different time steps.

Instead of a global discrete Lagrangian, we instead imbue each triangle T_i with a local discrete Lagragian

$$L_d^i(q_a^i, q_b^i) = \int_{t_a}^{t_b} T^i\left[\dot{q}^i(t)\right]dt - h^iV^i(q_b^i),$$

where T^i and V^i are the elemental kinetic and potential energies on T_i, respectively, $h^i = t_b - t_a$ is the elemental time step, and $\dot{q}^i(t)$, the elemental velocity at time t, is left imprecise for the moment. We no longer assume that velocity is constant between times t_a and t_b—a potential on another triangle that shares a vertex with T_i might change T_i's velocity—so unlike for the discrete Lagrangian (5), here we cannot explicitly integrate the kinetic energy term. For this reason we now write the Lagrangian as an integrated quantity, instead of deferring the integration to inside the action.

We have that each triangle is only concerned with certains moments in time - namely, integer multiples of h^i - and that these moments are inconsistent across triangles. We therefore subdivide time in a way compatible with all triangles: for a τ-length interval of time, we define

$$\Xi(\tau) = \bigcup_{T_i\in\mathcal{T}}\bigcup_{j=0}^{\lfloor\tau/h^i\rfloor} jh^i.$$

That is, $\Xi(\tau)$ is the set of all integer multiples less than τ of all elemental time steps. Ξ can be ordered, and in particular we let $\xi(i)$ be the $(i+1)$-st least element of Ξ. If n is the cardinality Ξ, we then discretize a trajectory of duration τ by linearly interpolating intermediate configurations $q_0, q_1, \ldots, q_{n-1}$, where q_i is the configuration of the system at time $\xi(i)$. We discretize velocity as $\dot{q}_{k+1/2} = \frac{q_{k+1}-q_k}{\xi(k+1)-\xi(k)}$ on the segment of the trajectory between q_k and q_{k+1}. We now need to write a global action functional of these trajectories that sums the above elemental Lagrangians, which we do in the natural way:

$$S_{AVI}(\mathbf{q}) = \sum_{T_i \in \mathcal{T}} \sum_{j=0}^{\lfloor \tau/h^i \rfloor} L_d^i \left(q_j^i, q_{j+1}^i\right). \tag{8}$$

As before, we consider variations $\delta\mathbf{q} = \{\delta q_0, \ldots, \delta q_{n-1}\}$ with $\delta q_0 = \delta q_{n-1} = 0$, and impose Hamilton's principle,

$$dS_{AVI}(\mathbf{q}) \cdot \delta\mathbf{q} = 0.$$

To avoid becoming bogged down in notation, we let $\omega^i(j) = \xi^{-1}(jh^i)$–that is, ω maps local time indices for T^i to global indices into Ξ–and will write q_j interchangeably for $\pi_i q_j$, the restriction of the (global) configuration q_j to an elemental configuration on T_i. Then

$$\begin{aligned}
S_{AVI}(\mathbf{q}) &= \sum_{T_i \in \mathcal{T}} \left(\sum_{j=0}^{\lfloor \tau/h^i \rfloor - 1} L_d^i \left(q_j^i, q_{j+1}^i\right) + \int_{j=\lfloor \tau/h^i \rfloor h^i}^{T} T^i \left[\dot{q}^i(t)\right] dt \right) \\
&= \sum_{T_i \in \mathcal{T}} \left(\sum_{j=0}^{\lfloor \tau/h^i \rfloor - 1} L_d^i \left(q_{\omega^i(j)}, q_{\omega^i(j+1)}\right) + \int_{j=\lfloor \tau/h^i \rfloor h^i}^{\tau} T^i \left[\dot{q}^i(t)\right] dt \right) \\
&= \sum_{T_i \in \mathcal{T}} \left(\sum_{j=0}^{\lfloor \tau/h^i \rfloor - 1} \left(\int_{jh^i}^{(j+1)h^i} T^i \left[\dot{q}^i(t)\right] dt - h^i V^i(q_{\omega^i(j+1)}) \right) + \int_{j=\lfloor \tau/h^i \rfloor h^i}^{\tau} T^i \left[\dot{q}^i(t)\right] dt \right) \\
&= \sum_{T_i \in \mathcal{T}} \left(\sum_{k=0}^{n-2} \left[\xi(k+1) - \xi(k)\right] T^i \left(\frac{q_{k+1} - q_k}{\xi(k+1) - \xi(k)} \right) - \sum_{j=0}^{\lfloor \tau/h^i \rfloor - 1} h^i V^i(q_{\omega^i(j+1)}) \right).
\end{aligned}$$

Thus, writing

$$\begin{aligned}
T_d^i(q_a, q_b, t_a, t_b) &= T^i \left(\frac{q_b - q_a}{t_b - t_a} \right) \\
T_d^{i\prime}(q_a, q_b, t_a, t_b) &= \frac{\partial T^i}{\partial \dot{q}} \left(\frac{q_b - q_a}{t_b - t_a} \right) \\
V_d^i(q_a, q_b, t_a, t_b) &= V^i(q_b) \\
V_d^{i\prime}(q_a, q_b, t_a, t_b) &= \frac{\partial V^i}{\partial q}(q_b),
\end{aligned}$$

$$
\begin{aligned}
dS_{AVI}(\mathbf{q}) \cdot \delta\mathbf{q} &= \sum_{T_i \in \mathcal{T}} \left(\sum_{k=0}^{n-2} T_d^{i\prime}\left[q_k, q_{k+1}, \xi(k), \xi(k+1)\right] \cdot \delta q_{k+1} - \sum_{k=0}^{n-2} T_d^{i\prime}\left[q_k, q_{k+1}, \xi(k), \xi(k+1)\right] \cdot \delta q_k \right) \\
&\quad - \sum_{T_i \in \mathcal{T}} \sum_{j=1}^{\lfloor \tau/h^i \rfloor} h^i \frac{\partial V^i}{\partial q^i}(q_{\omega^i(j)}) \cdot \delta q_{\omega^i(j)} \\
&= \sum_{T_i \in \mathcal{T}} \left(T_d^{i\prime}\left[q_{n-2}, q_{n-1}, \xi(n-2), \xi(n-1)\right] \cdot \delta q_n - T_d^{i\prime}\left[q_0, q_1, \xi(0), \xi(1)\right] \cdot \delta q_0 \right) \\
&\quad + \sum_{T_i \in \mathcal{T}} \sum_{k=1}^{n-2} \left(T_d^{i\prime}\left[q_{k-1}, q_k, \xi(k-1), \xi(k)\right] - T_d^{i\prime}\left[q_k, q_{k+1}, \xi(k), \xi(k+1)\right] \right) \cdot \delta q_k \\
&\quad - \sum_{T_i \in \mathcal{T}} \sum_{j=1}^{\lfloor \tau/h^i \rfloor} h^i \frac{\partial V^i}{\partial q^i}(q_{\omega^i(j)}) \cdot \delta q_{\omega^i(j)} \\
&= \sum_{T_i \in \mathcal{T}} \sum_{k=1}^{n-2} \left(T_d^{i\prime}\left[q_{k-1}, q_k, \xi(k-1), \xi(k)\right] - T_d^{i\prime}\left[q_k, q_{k+1}, \xi(k), \xi(k+1)\right] \right) \cdot \delta qk \\
&\quad - \sum_{k=0}^{n-2} \sum_{h^i | \xi(k)} h^i \frac{\partial V^i}{\partial q^i}(q_{k+1}) \cdot \delta q_{k+1} \\
&= \sum_{k=1}^{n-2} \sum_{T_i \in \mathcal{T}} \left(T_d^{i\prime}\left[q_{k-1}, q_k, \xi(k-1), \xi(k)\right] - T_d^{i\prime}\left[q_k, q_{k+1}, \xi(k), \xi(k+1)\right] \right) \cdot \delta q_k \\
&\quad - \sum_{k=1}^{n-2} \sum_{h^i | \xi(k)} h^i \frac{\partial V^i}{\partial q^i}(q_k) \cdot \delta q_k,
\end{aligned}
$$

where we abuse the notation $h^i | m$ to mean, "all elemental time steps h^i which evenly divide m." Writing the total kinetic energy of the system $\sum_{T_i \in \mathcal{T}} T^i$ as T_{tot}, for AVIs we recover the discrete Euler-Lagrange equations

$$
\frac{\partial T_{tot}}{\partial \dot{q}}(\dot{q}_{k+1/2}) - \frac{\partial T_{tot}}{\partial \dot{q}}(\dot{q}_{k-1/2}) = - \sum_{h^i | \xi(k)} h^i \frac{\partial V^i}{\partial q^i}(q_k). \tag{9}
$$

These equations are similar to those we derived for synchronous vartional integrators (7), except that only a subset of potentials V_d^i contribute during each time step. As in the synchronous case, if, as is typical, T_{tot} is quadratic in $\dot{q}$, (9) give rise to an explicit numerical integrator that is particularly easy to implement in practice.

3.1 Multisymplecticity

The right hand side of (9) depends on $\xi(k)$, and so unlike (7), the Euler-Lagrange equations for AVIs are time dependent, and do not give rise to a uniform update rule $F(q_{i-1}, q_i) \mapsto (q_i, q_{i+1})$. Instead, we consider the total, time-dependent flow $\hat{F}^k(q_0, q_i) \mapsto (q_{k-1}, q_k)$. Once again, we parametrize trajectories satisfying (9) by $\nu_0 = (q_0, q_1)$, and first variations by $\delta\nu_0 = (\delta q_0, \delta q_1)$. Restricting ourselves to such trajectories and variations, we rewrite the action (8) as

$$
S_{iAVI} = \sum_{T_i \in \mathcal{T}} \left(\sum_{k=0}^{n-2} \left[\xi(k+1) - \xi(k)\right] T_d^i \left(\hat{F}^k(\nu_0), \xi(k), \xi(k+1) \right) - \sum_{j=0}^{\lfloor \tau/h^i \rfloor - 1} h^i V_d^i(\hat{F}^{\omega^i(j+1)}(\nu_0), 0, 0) \right).
$$

Then

```
loop
    (E, V, h, t) ← Q.pop                                   // Pop event E with potential V, time step h,
                                                           // and scheduled time t, from time-ordered queue Q
    ξ := stencil(E)                                        // global indices of the local stencil
    for i ∈ ξ do
        x_i ← x_i + (t − t_i) ẋ_i                          // advance vertex to current time (see §3)
        t_i ← t                                            // update vertex's clock
    end for
    if E is a (external, internal, contact) force event then
        q̇_ξ ← q̇_ξ − h M_ξ^{-1} ∂V/∂q_ξ                     // local impulses, local mass (see §3)
        Q.push(E, V, h, t + h)                             // Return the event to the queue, with new time
                  i∈ξ
        for j ∈ ⋃ contingent(i) do
                i
            s ← failureTime(E_j)                           // compute new event time (see §5.1)
            Q.update(E_j, s)                               // reschedule the contingent event (see §5.2)
        end for
    else if E is certificate failure then
        update KDS certificate, reschedule in Q            // see §5.1 and §5.3
        (de)activate penalty forces                        // see §4
    end if
end loop
```

$$
\begin{aligned}
dS_{iAVI}(\nu)\cdot\delta\nu &= dS_{AVI}(\mathbf{q})\cdot\delta\mathbf{q} \\
&= \sum_{T_i\in\mathcal{T}}\left(T_d^{i\prime}\left[q_{n-2},q_{n-1},\xi(n-2),\xi(n-1)\right]\cdot\delta q_{n-1} - T_d^{i\prime}\left[q_0,q_1,\xi(0),\xi(1)\right]\cdot\delta q_0\right) \\
&\quad - \sum_{h^i|\xi(n-1)} h^i\frac{\partial V^i}{\partial q^i}(q_{n-1})\cdot\delta q_{n-1} \\
&= \sum_{T_i\in\mathcal{T}}\left(T_d^{i\prime}\left[\hat{F}^{n-2}(\nu_0),\xi(n-2),\xi(n-1)\right]\cdot\delta q_{n-1} - T_d^{i\prime}\left[\nu_0,0,\xi(1)\right]\cdot\delta q_0\right) \\
&\quad - \sum_{h^i|\xi(n-1)} h^i V_d^{i\prime}\left[\hat{F}^{n-1}(\nu_0),0,0\right]\cdot\delta q_{n-1} \\
&= \left(-\sum_{T_i\in\mathcal{T}} T_d^{i\prime}\left[\nu_0,0,\xi(1)\right]\right)dq_a\cdot\delta\nu_0 \\
&\quad + \left(\sum_{T_i\in\mathcal{T}} T_d^{i\prime}\left[\hat{F}^{n-2}(\nu_0),\xi(n-2),\xi(n-1)\right] - \sum_{h^i|\xi(n-1)} h^i V_d^{i\prime}\left[\hat{F}^{n-2}(\nu_0),0,0\right]\right)dq_b \\
&\quad \cdot\hat{F}_*^{n-2}\delta\nu_0 \\
&= \theta^-_{\nu_0}\cdot\delta\nu_0 + \theta^+_{\hat{F}^{n-2}\nu_0}\cdot\hat{F}^{n-2}{}_*\delta\nu_0 \\
&= \left(\theta^- + \hat{F}^{n-2*}\theta^+\right)_{\nu_0}\cdot\delta\nu_0
\end{aligned}
$$

for one-forms θ^- and θ^+. Once again we have that

$$0 = d^2S = d\theta^- + \hat{F}^{n-2*}d\theta^+, \tag{10}$$

but unlike when our action was a sum of Lagrangians, from the *multisymplectic form formula* (10) we have no way of relating $d\theta^-$ to $d\theta^+$, and thus do not recover symplectic structure preservation. Nevertheless, Lew et al. [5] conjecture that this multisymplectic structure leads to the good energy behavior observed for AVIs.

4 Triangulation-Free AVIs

The above formulation of AVIs assumed a spatial triangulation over which we defined distinct, local Lagrangians. We now present a simple extension that supports potentials with arbitrary, possibly nondisjoint spatial stencil.

Let $\{V_i\}$ be potentials with time steps h^i. As in AVIs, for trajectories of duration τ we define the set of times

$$\Xi(\tau) = \bigcup_{V_i} \bigcup_{j=0}^{\lfloor \tau/h^i \rfloor} jh^i,$$

the smallest set of times compatible with the time steps of all of the potentials. Again, let Ξ have cardinality n, $\xi(i)$ be the $(i+1)$-th least element of Ξ, and $\omega^i(j) = \xi^{-1}(j\Delta t^i)$. Then, for $T(\dot{q})$ the kinetic energy of the entire configuration, $T_d(q_a, q_b, t_a, t_b) = T\left(\frac{q_b - q_a}{t_b - t_a}\right)$, and $T_d'(q_a, q_b, t_a, t_b) = \frac{\partial T}{\partial \dot{q}}\left(\frac{q_b - q_a}{t_b - t_a}\right)$, we write the action

$$S_g(\mathbf{q}) = \sum_{j=0}^{n-2} \left[\xi(j+1) - \xi(j)\right] T_d\left[q_j, q_{j+1}, \xi(j), \xi(j+1)\right] - \sum_{V_i} \sum_{j=1}^{\lfloor \tau/h^i \rfloor} h^i V_i(q_{\omega^i(j)}).$$

We have made no attempt to define a Lagrangian pairing the kinetic and potential energy terms; we will see that an action defined this way still leads to a multisymplectic numeric integrator.

To that end we impose $dS_g(\mathbf{q}) \cdot \delta\mathbf{q} = 0$ for variations with $\delta q_0 = \delta q_{n-1} = 0$. Then we rewrite S_g as

$$S_g(\mathbf{q}) = \sum_{j=0}^{n-2} \left[\xi(j+1) - \xi(j)\right] T_d\left[q_j, q_{j+1}, \xi(j), \xi(j+1)\right] - \sum_{j=1}^{n-1} \sum_{h^i | \xi(j)} h^i V_i(q_j)$$

so that

$$\begin{aligned}
dS_g(\mathbf{q}) \cdot \delta\mathbf{q} &= \sum_{j=0}^{n-2} \left(T_d'\left[q_j, q_{j+1}, \xi(j), \xi(j+1)\right] \cdot \delta q_{j+1} - T_d'\left[q_j, q_{j+1}, \xi(j), \xi(j+1]\right) \cdot \delta q_j\right) \\
&\quad - \sum_{j=1}^{n-1} \sum_{h^i | \xi(j)} h^i \frac{\partial V_i}{\partial q}(q_j) \cdot \delta q_j \\
&= T_d'\left[q_{n-2}, q_{n-1}, \xi(n-2), \xi(n-1)\right] \cdot \delta q_{n-1} - T_d'\left[q_0, q_1, \xi(0), \xi(1)\right] \cdot \delta q_0 \\
&\quad - \sum_{h^i | \xi(n-1)} h^i \frac{\partial V^i}{\partial q}(q_{n-1}) \cdot \delta q_{n-1} \\
&\quad + \sum_{j=1}^{n-2} \left(T_d'\left[q_{j-1}, q_j, \xi(j-1), \xi(j)\right] - T_d'\left[q_j, q_{j+1}, \xi(j), \xi(j+1)\right] - \sum_{h^i | \xi(j)} h^i \frac{\partial V^i}{\partial q}(q_j) \right) \cdot \delta q_j \\
&= \sum_{j=1}^{n-2} \left(T_d'\left[q_{j-1}, q_j, \xi(j-1), \xi(j)\right] - T_d'\left[q_j, q_{j+1}, \xi(j), \xi(j+1)\right] - \sum_{h^i | \xi(j)} h^i \frac{\partial V^i}{\partial q}(q_j) \right) \cdot \delta q_j.
\end{aligned}$$

The Euler-Lagrange equations are then

$$\frac{\partial T}{\partial \dot{q}}(\dot{q}_{k+1/2}) - \frac{\partial T}{\partial \dot{q}}(\dot{q}_{k-1/2}) = - \sum_{h^i | \xi(k)} h^i \frac{\partial V^i}{\partial q^i}(q_k), \tag{11}$$

exactly the same as the Euler-Lagrange equations (9) for ordinary AVIs. Triangulation-free AVIs can thus be integrated in exactly the same manner as ordinary AVIs, for instance, by using Algorithm 3.

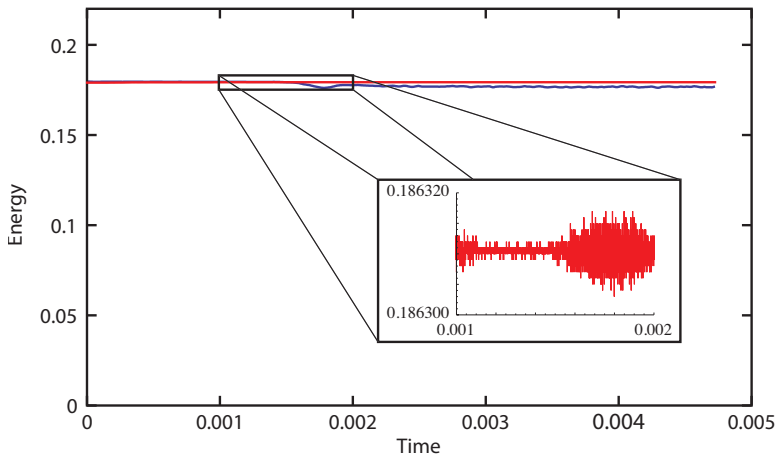

Figure 1: Total energy over time of a thin sphere colliding against a thin plate, simulated using our method (red) and decomposition contact response (dark blue).

4.1 Multisymplecticity

To show that triangulation-free AVIs still satisfy the multisymplectic form formula (10), we follow the derivation for multisymplecticity of ordinary AVIs. Replacing $\sum_{T_i \in \mathcal{T}} T_d^i$ with T_d in Section 3.1, an identical calculation shows triangulation-free AVIs satisfy (10).

5 Choice of Layer Distribution Function

The nested penalty layer construction described in the paper has as an algorithmic parameter the layer distribution function $\eta(l)$. The choice of this function has performance ramifications.

The total potential energy V of the nested penalty layers as a pair of colliding elements are about to enter layer n is given by

$$V(n) = \sum_{l=1}^{n-1} V^r_{\eta(l)}(\eta(n)) \approx \int_1^n V^r_{\eta(l)}(\eta(n))dl. \tag{12}$$

Assuming that penalty forces are integrated continuously, energy is exactly conserved, and no other forces act on the two elements, (12) can be used to continuously relate, for different η, the pre-collision kinetic energy of the elements (and thus their pre-collision relative velocities) to the approximate deepest penalty layer that needs to be activated to resolve the collision.

For simulations that tend to have primitives approaching each other at low velocities, a quickly-shrinking η is more efficient. Such an η bunches penalty layers nearer $g(\mathbf{q}) = 0$, and away from thickness $g(\mathbf{q}) = \eta(1)$, so that $\mathbf{q}$ will activate only a few low-stiffness penalty layers before being rebuffed. A collision is then averted without resorting to deeper layers and smaller time steps.

On the other hand, for simulations where primitives tend to approach at high velicities, a slowly-shrinking η is more efficient. Such a distribution function activates penalty layers earlier, so that each can exert a force over a greater distance. Stopping the collision then avoids needing to activate deep penalty layers of high stiffness and small time step.

Accordingly, we've found that $\eta(l) = \eta(1)l^{-1}$ works well for simulations with a lot of contact and low velocities, and $\eta(l) = \eta(1)l^{-1/4}$ works better for simulations with high-velocity impact. We note that this choice affects performance, but both choices guarantee safety, correctness, and progress for all scenarios.

6 Sphere-plate Impact

As an experimental test of the good energy behavior expected of our multisympletic approach, we simulated the impact of a spherical shell with a thin plate, as described in Cirak and West's article on Decomposition Contact Response [1]. A sphere of radius 0.125 approaches a plate of radius 0.35 with relative velocity 100. Both the sphere and the plate have thickness 0.0035. The time steps of our material forces (stretching and bending) are 10^{-7} (the same as those chosen by Cirak and West.)

Figure 1 compares energy over time when this simulation is run using both our method and DCR. Although both methods exhibit reasonably good energy behavior, under DCR the simulation slowly loses energy, whereas under our method there is no noticeable long-term drift. Closely examining the energy data produced by our method reveals the high-frequency, low-amplitude, qualitatively-negligible oscillations characteristic of symplectic integrators.

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