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STABILIZED INTEGRATION OF HAMILTONIAN SYSTEMS WITH HARD-SPHERE INEQUALITY CONSTRAINTS*

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Abstract. We consider numerical methods for resolving the dynamics of a Hamiltonian N-body problem subject to hard-sphere inequality constraints. The dynamics of these mixed systems consists of smooth flow of a Hamiltonian system between collisions with an impulsive momentum exchange at the points of collision. The inclusion of these impulses makes traditional backward error analysis inappropriate since the flow is discontinuous and cannot be interpreted using a single modified smooth Hamiltonian system. We introduce two methods which respect the underlying modified smooth Hamiltonian system through the use of a modified map and collision operator at points of collision. In numerical experiments, these new methods show dramatically improved energy conservation over long time intervals.

Key words. collision Verlet, hard spheres, geometric integration, Hamiltonian systems, backward error analysis, inequality constraints, impact dynamics

AMS subject classifications. 65P10, 65L05, 82B80

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1. Introduction.

The dynamics of a collection of rigid spherical bodies interacting in a smooth potential field can be described by a collisional Hamiltonian system. The dynamics is characterized by smooth Hamiltonian flow between contacts, with impulsive forces acting at the points of collision. Due to the inclusion of these impulsive forces, traditional methods for smooth N-body systems can be applied only between collisions. At points of contact, the momenta of the colliding spheres are exchanged in the normal direction, which introduces a discontinuity in the trajectory in phase-space. This type of model setting arises in molecular and polymer dynamics studies [4, 16, 19]. Related problems arise in development of computer gaming ("physics engines") and in a variety of modeling applications in materials science.

The dynamics of pure hard-sphere systems, in the absence of a smooth potential, can be resolved efficiently using a traditional event-driven algorithm [1]. This method follows the exact linear trajectories of each sphere between collisions, updating the momenta of each pair of colliding spheres at each collision. Once additional smooth forces are introduced, this algorithm can no longer be applied since the trajectories between collisions are not linear (and cannot be resolved exactly).

A number of hybrid methods for approximating the dynamics of collisional Hamiltonian systems have been proposed in the literature [5, 9, 10, 14, 17, 18]. In all of these methods the traditional Störmer–Verlet algorithm [21] is used to resolve the trajectory between collisions. Points of collision are detected by either checking for overlap at the end of the step [14] or during the step [9, 17, 18] or by formally solving for the time to the next collision [5, 10], and collisions are then resolved by momentum exchange between the colliding spheres using the energy/momentum balance of an

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elastic collision. Depending on the algorithm, the strength of the impulsive forces is selected to conserve the "true energy" from the smooth Hamiltonian [10] or a "discrete energy" corresponding to a discrete variational principle [5].

The principle advantage of symplectic integrators, when applied with a fixed stepsize to a smooth Hamiltonian system, is the enhanced stability, which can be understood through backward error analysis. A Hamiltonian perturbation series may be developed in such a way that the numerical method can be viewed as equivalent (up to a minor discrepancy) to the exact dynamics of the modified continuous system [3, 7, 15]. This implies a stability result for the underlying symplectic integrator which can be used to explain the lack of secular energy drift over very long time intervals.

The challenge in understanding hybrid numerical methods using backward error analysis is twofold. First, near points of collision the algorithm is effectively applying a symplectic integrator with a variable stepsize. Hence, we cannot view the numerical trajectory as the product of a single modified Hamiltonian. Second, the trajectory is not continuously differentiable since the exact solution is only piecewise smooth (i.e., smooth between collisions with discontinuities at the collision times).

The objective of this paper is to develop hybrid algorithms which can be understood using backward error analysis. We will do this by respecting the underlying modified Hamiltonian of the smooth numerical method through points of collision. We hypothesize a reference Hamiltonian expansion associated to a fixed timestep map, and propagation within a collisional step is then designed to preserve this modified Hamiltonian to a certain accuracy. At the point of impact, a modified collision operator is developed which likewise preserves the reference Hamiltonian. The result is a scheme with superb long-term stability properties relative to the existing alternatives, albeit at an increased per-timestep cost. In the molecular setting, where impacts are usually frequent, our scheme can be used to compute accurate benchmark solutions.

In section 2, we introduce collisional dynamics for Hamiltonian systems, defining both the collision time and the collision operator. In the subsections, we review the primitive splitting algorithm [18], collision Verlet algorithm [10], and variational collision integrator [5]. In section 3, we discuss backward error analysis for symplectic integrators applied to smooth Hamiltonian systems and provide the first two terms of the modified Hamiltonian for the Verlet method. In section 3.1, we derive the time-reversible modified collision Verlet algorithm (MCVA), based on a modified collision operator and higher-order integration of the modified flow in pre- and postcollision steps. In section 3.2, we introduce a projected collision Verlet algorithm (PCVA) which uses a non–time-reversible modified energy projection to stabilize the collision Verlet algorithm (CVA). In section 4, we present results from numerical experiments highlighting the potential improvements afforded the modified (MCVA) and projected (PCVA) methods. Finally, our conclusions are given in section 5.

2. Collisional dynamics. We consider the dynamics of a system of N hard spheres interacting under a conservative potential $V(q)$:

$$\begin{aligned} H(q,p) &= \frac{1}{2}p^t M^{-1} p + V(q), \\ d(q_i,q_j) &\geq r_i + r_j \quad \forall i \neq j, \quad i,j \in 1 \cdots N. \end{aligned} \tag{2.1}$$

In this notation, the ith sphere has radius r_i, and the distance between two spheres is given by the standard Euclidean metric, $d(q_i,q_j) = \|q_i - q_j\|_2$.

Given the flow map, Ψ, for the contact-free system, H, we can describe the flow map for the hard-sphere system, Φ_t, as a sequence of smooth steps separated by

collisions. Assuming n_c collisions within the interval $[0, t]$, we have

$$\Phi_t = \Psi_{\Delta\tau_{n_c}} \circ R \circ \cdots \circ \Psi_{\Delta\tau_1} \circ R \circ \Psi_{\Delta\tau_0}. \tag{2.2}$$

The time of each collision is denoted by τ_i, and the time increment between τ_i and τ_{i+1} by $\Delta\tau_i$. The endpoints of the interval are assigned to $\tau_0 = 0$ and $\tau_{n_c+1} = t$. The map R is the collision operator which exchanges momenta between the two colliding spheres,

$$R\,(q, p) = (q, p + \alpha\,\vec{u}_{col})\,,$$

where $\vec{u}^{col}$ is a vector normal to the inequality constraint surface and α is a nonzero Lagrange multiplier selected to enforce conservation of energy,

$$H \circ R = H.$$

The resulting trajectory is piecewise smooth on the restricted phase-space

$$\Omega_{\text{HS}} = \{(q, p) \in \Gamma \mid d\,(q_i, q_j) \geq r_i + r_j \quad \forall i \neq j, \quad i, j \in 1 \cdots N\}\,,$$

where Γ is the phase-space for the contact-free problem.

2.1. Splitting methods. One technique for handling the inclusion of smooth forces in hard-sphere simulations is to use a splitting method. To derive a numerical method, one may start by decomposing the full Hamiltonian into terms, H_a and H_b, which contain the kinetic and potential energy, respectively:

$$\begin{aligned} &H_a\,(q, p) = \frac{1}{2} p^t M^{-1} p, \quad H_b\,(q, p) = V\,(q)\,, \\ &d\,(q_i, q_j) \geq r_i + r_j \quad \forall i \neq j, \quad i, j \in 1 \cdots N. \end{aligned}$$

The flow of the H_a system is pure hard-sphere motion which can be solved exactly with a standard event driven algorithm. The H_b system applies the force to the momenta, leaving the particles fixed. Composing a full timestep of the flow of H_a with two half-timesteps of H_b results in a hard-sphere analogue to the Verlet method, first proposed by Suh et al. [18] in an equivalent form. Denoting the t-flow of the hard-sphere system by the map Ψ_t^{HS}, we can write this splitting algorithm as follows:

Primitive splitting algorithm (PSA):

$$\begin{aligned} &p_-^{n+1/2} = p^n - \tfrac{\Delta t}{2} \nabla V\,(q^n), \\ &\left(q^{n+1}, p_+^{n+1/2}\right) = \Psi_{\Delta t}^{\text{HS}}\left(q^n, p_-^{n+1/2}\right), \\ &p^{n+1} = p_+^{n+1/2} - \tfrac{\Delta t}{2} \nabla V\left(q^{n+1}\right). \end{aligned}$$

As illustrated in [10] using a one-dimensional model problem, the energy is (in general) only conserved to first order if there is a collision within the step. The reason is that although the operator splitting is symmetric, the collisions do not necessarily occur symmetrically within the step. To understand this better, we consider a general two-body problem in $\mathbb{R}^3$, with one body fixed at the origin, and a sphere diameter l:

$$H\,(q, p) = \frac{1}{2\,m} \|p\|^2 + V\,(q) \quad \text{with} \quad \|q\| \geq l.$$

Applying the PSA to this system, on an interval with a single collision, results in

$$p_-^{1/2} = p^0 - \tfrac{1}{2}\Delta t\,\nabla V\left(q^0\right), \qquad q_c = q^0 + \Delta t_c\, p_-^{1/2}/m,$$

$$\vec{u}_{col} = q_c, \qquad p_+^{1/2} = p_-^{1/2} + \alpha\,\vec{u}_{col},$$

$$q^1 = q_c + (\Delta t - \Delta t_c)\, p_+^{1/2}/m, \qquad p^1 = p_+^{1/2} - \tfrac{1}{2}\Delta t\,\nabla V\left(q^1\right),$$

where Δt_c and q_c are the time and position of the collision, respectively. The nonzero Lagrange multiplier, α, is selected under the constraint that the energy is conserved during the collision:

$$\alpha = -2\,\frac{\vec{u}_{col}\cdot p_-^{1/2}}{\vec{u}_{col}\cdot\vec{u}_{col}}.$$

To find the change in energy over one step, we insert the expressions for q^1 and p^1 into the Hamiltonian and expand about the point of collision, $q = q_c$:

$$\begin{aligned}\Delta H &:= H\left(q^1,p^1\right) - H\left(q^0,p^0\right)\\ &= -\frac{(\Delta t - 2\Delta t_c)}{m}\,\frac{q_c^T p_-^{1/2}}{q_c^T q_c}\,q_c^T\nabla V\left(q_c\right) + O\left[\Delta t^2\right].\end{aligned}$$

The conservation of energy is only first order through a collision, unless one of three properties holds: (1) the collision happens at the exact middle of the timestep, (2) the directional derivative of the potential is zero along the vector q_c, or (3) the momentum vector at the point of collision is orthogonal to q_c. Assuming a finite number of collisions on any fixed time interval, it can be shown that the primitive algorithm is only first-order accurate [10].

2.2. Collision Verlet algorithm. To correct the order-reduction in the primitive algorithm, an improved method called "collision Verlet" was proposed in [10]. The idea is to approximate the smooth maps in the exact flow, as written in (2.2), by the Verlet map, $\Psi_{\Delta t}$:

$$\begin{aligned}q^{n+1} &= q^n + \Delta t M^{-1}p^n - \frac{\Delta t^2}{2}\nabla V\left(q^n\right),\\ p^{n+1} &= p^n - \frac{\Delta t}{2}\nabla V\left(q^n\right) - \frac{\Delta t}{2}\nabla V\left(q^{n+1}\right).\end{aligned}$$

This results in a method that steps between collisions with Verlet and applies the (impulse) momentum exchange map, R, at each collision. The time to the next collision is defined as the smallest positive stepsize that results in collision (i.e., violates the inequality constraints):

$$\text{CollisionTime}\left[\Psi,q,p\right] := \min\left\{t>0 \mid \Psi_t\left(q,p\right)\in\partial\Omega_{\text{HS}}\right\}.$$

By stepping between collisions with Verlet, the collisions occur only between Verlet steps and there is no order-reduction in the local conservation of energy. To maintain stability and reversibility, a fixed outer timestep is imposed. The resulting algorithm follows.

COLLISION VERLET ALGORITHM (CVA).

$\left(\hat{q}^0, \hat{p}^0\right) = (q^n, p^n)$

$\tau_{max} = \Delta t$ and $k = 0$

while $(\tau_{max} > 0)$

$\Delta\tau_k = \min\left\{\tau_{max}, \text{CollisionTime}\left[\Psi, \hat{q}^k, \hat{p}^k\right]\right\}$

$(\hat{q}^c, \hat{p}^c) = \Psi_{\Delta\tau_k}\left(\hat{q}^k, \hat{p}^k\right)$

if "collision" then

$\left(\hat{q}^{k+1}, \hat{p}^{k+1}\right) = R\left(\hat{q}^c, \hat{p}^c\right)$

else

$\left(\hat{q}^{k+1}, \hat{p}^{k+1}\right) = \left(\hat{q}^c, \hat{p}^c\right)$

end-if

$\tau_{max} = \tau_{max} - \Delta\tau_k$ and $k = k + 1$

end-while

$\left(q^{n+1}, p^{n+1}\right) = \left(\hat{q}^k, \hat{p}^k\right)$

This method can be generalized by replacing the base numerical map, Ψ, with another symplectic time-reversible method. However, this could significantly complicate the computation of the collision time. For the standard N-body problem with Verlet as the base map, collision times are determined by finding the smallest positive root of a sequence of quartic polynomials for each pair of particles. This can be performed relatively efficiently through the use of hash-tables, neighbor-lists, and root bracket techniques (see [10]). Most important is that solving for the collision time does not require implicit iteration of the smooth forces.

2.3. Variational collision integrator. An alternative approach for deriving geometric integrators is to discretize the Lagrangian directly [11, 12, 13]. The resulting algorithms are typically two-step methods, but can be rewritten in one-step form using a Legendre transformation. For example, the standard second-order discrete Lagrangian,

$$L_d\left(q^n, q^{n+1}, \Delta t\right) := \frac{\Delta t}{2}\left(\frac{q^{n+1} - q^n}{\Delta t}\right)^T M\left(\frac{q^{n+1} - q^n}{\Delta t}\right) - \Delta t\,\frac{V\left(q^n\right) + V\left(q^{n+1}\right)}{2},$$

can be used to derive the well-known Störmer method

$$\frac{1}{\Delta t^2} M\left(q^{n+1} - 2q^n + q^{n-1}\right) = -\nabla V\left(q^n\right).$$

One can show that this is equivalent to the leapfrog/Verlet method with the half-step momenta defined by

$$p^{n+1/2} := \frac{1}{\Delta t}\left(q^{n+1} - q^n\right).$$

More recently, this approach has been applied to nonsmooth mechanics, which has allowed for the development of nonsmooth variational integrators for contact problems (see [5]). By considering variations in the trajectory and collision time, one can obtain

equations for both the smooth map between collisions and the impulses at points of collision. For the second-order discrete Lagrangian, the map between collisions is the Störmer/leapfrog/Verlet map. At points of collision, the standard collision map is applied,

$$R_\alpha (q,p) = (q, p + \alpha\, \vec{u}_{col}),$$

with the "strength of collision," $\alpha \neq 0$, selected to conserve the "discrete energy" function,

$$E_d\left(q^{n+1}, q^n, \Delta t\right) := \frac{1}{2}\frac{\left(q^{n+1}-q^n\right)^T}{\Delta t} M \frac{\left(q^{n+1}-q^n\right)}{\Delta t} + \frac{V\left(q^{n+1}\right) + V\left(q^n\right)}{2},$$

across each collision.

Comparing this method to the CVA, we find that they are identical up to the determination of the strength of collision, α. By conserving the discrete energy (as opposed to the exact energy), the discrete Lagrangian method is implicit in the forces due to the coupling between strength and time of collision.

3. Backward error analysis. In the context of collisional dynamical systems classical forward error analysis is impractical due to the conditioning of an individual trajectory. In particular, the flow corresponding to two nearly identical initial conditions diverges exponentially over a short time interval due to the intrinsic sensitivity of the flow to perturbation. This sensitivity is inherited by the numerical method, and bounds on the accuracy of the numerical trajectory must have a corresponding exponential growth.

In backward error analysis, the error induced by the numerical algorithm is expressed as a perturbation of the problem or vector field. This is especially appealing in areas such as molecular dynamics where statistical averages are used to compute properties of the system and it is assumed that these averages are independent of the initial conditions.

For smooth Hamiltonian systems the connection between a symplectic integrator and the existence of a modified Hamiltonian system has been investigated by several authors [3, 15]. A series can be developed by matching terms in the Taylor series expansions of the numerical method and the solution operator for the modified system.

For the Verlet algorithm,

$$\begin{aligned} p^{n+1/2} &= p^n - \frac{\Delta t}{2}\nabla_q V\left(q^n\right), \\ q^{n+1} &= q^n + \Delta t M^{-1} p^{n+1/2}, \\ p^{n+1} &= p^{n+1/2} - \frac{\Delta t}{2}\nabla_q V\left(q^{n+1}\right), \end{aligned}$$

the modified Hamiltonian can be written as

$$H^{\Delta t}_{[4,VV]}(q,p) = H(q,p) + \frac{\Delta t^2}{4!}H_2(q,p) + \frac{\Delta t^4}{6!}H_4(q,p) + O\left[\Delta t^6\right],$$

where H_2 and H_4 are defined by

$$H_2(q,p) := \frac{2\, p_i\, p_j}{m_i\, m_j} V_{q_i q_j}(q) + \frac{-1}{m_i} V_{q_i}(q)^2,$$

$$H_4(q,p) := \frac{-p_i\, p_j\, p_k\, p_l}{m_i\, m_j\, m_k\, m_l} V_{q_i q_j q_k q_l} + \frac{-3}{m_i\, m_j} V_{q_i q_j} V_{q_i} V_{q_j} + \frac{12\, p_j\, p_k}{m_i\, m_j\, m_k} V_{q_i q_j} V_{q_i q_k} + \frac{6\, p_j\, p_k}{m_i\, m_j\, m_k} V_{q_i q_j q_k} V_{q_i}.$$

Here we have employed Einstein notation with summation over all repeated indices. Subscripts of coordinates indicate partial derivatives with respect to that coordinate.

Note that this modified Hamiltonian is conserved by the Verlet method with sixth-order accuracy, compared to the original Hamiltonian which is conserved only to second-order. Since it is a higher-order invariant, it is reasonable to expect that preserving the modified Hamiltonian through collisions would stabilize the resulting numerical method.

3.1. Modified collisions. Unfortunately, there is no analogous modified Hamiltonian when symplectic integrators are naively applied to nonsmooth collisional systems. For the CVA, it is during the steps involving collisions that the traditional backward error analysis breaks down. To remedy this situation, we explore the reasons for this destabilization.

The first possible explanation lies in the use of a variable stepsize to step to and from the point of collision. This variable stepsize means we can no longer view the numerical trajectory as being close to the exact dynamics of a single modified Hamiltonian system. Hence, the stability implied by this traditional backward error analysis for collision-free systems must be modified for the collisional case.

One way to remedy this problem is to use a higher-order integrator to solve for the dynamics of the modified Hamiltonian, $H^{\Delta t}_{[2,VV]}$, during these steps to and away from points of collision. As long as the collisions are relatively infrequent (e.g., high accuracy or low density), most of the steps will be propagated by the less expensive Verlet method, and the added cost of the more accurate integrator should not be prohibitive.

The second possible cause of the destabilization is that, while the collision operator conserves energy, it does not conserve the modified Hamiltonian. For the standard collision operator, the strength of collision is defined by requiring conservation of the unmodified energy:

$$H \circ R_\alpha(q,p) - H(q,p) = 0,$$

$$R_\alpha(q,p) := (q, p + \alpha\, \vec{u}_{col}).$$

This is a quadratic equation with one nontrivial root,

$$\alpha = -2\, \frac{\vec{u}_{col}^T M^{-1} p}{\vec{u}_{col}^T M^{-1} \vec{u}_{col}}.$$

If instead we required the collision map to conserve the second-order modified Hamiltonian, $H^{\Delta t}_{[2,VV]}$, we would obtain a different quadratic equation:

$$H^{\Delta t}_{[2,VV]} \circ R_{\hat{\alpha}}(q,p) - H^{\Delta t}_{[2,VV]}(q,p) = 0,$$

which (in general) has a different solution

$$\hat{\alpha} = -2\, \frac{\vec{u}_{col}^T \left(M^{-1} + \Delta t^2\, V''(q)/12\right) p}{\vec{u}_{col}^T \left(M^{-1} + \Delta t^2\, V''(q)/12\right) \vec{u}_{col}}.$$

Note: this technique could be extended to the $H^{\Delta t}_{[4,VV]}$ modified Hamiltonian, through solution of a quartic equation; indeed even higher-order approximations could be constructed in the same way, albeit at additional computational cost due to the need to compute higher derivatives of the potential V.

Based on these two observations, we propose the MCVA which respects the modified Hamiltonian through collisions. In what follows, Ψ is the Verlet algorithm, and $\Psi^{[*]}$ is the symplectic fourth-order Gauss method applied to the $H^{\Delta t}_{[2,VV]}$ modified Hamiltonian. The modified collision operator is denoted by $R^{[*]}_{\alpha}$, which uses the value of α that conserves the modified Hamiltonian, $H^{\Delta t}_{[2,VV]}$, when there is a collision (and is the identity otherwise).

Modified Collision Verlet Algorithm (MCVA).

$\left(\hat{q}^0, \hat{p}^0\right) = (q^n, p^n)$

$\tau_{max} = \Delta t$ and $k = 0$

while $(\tau_{max} > 0)$

  $\Delta\tau_k = \min\left\{\tau_{max}, \text{CollisionTime}\left[\Psi^{[*]}, \hat{q}^k, \hat{p}^k\right]\right\}$

  if $(\Delta\tau_k == \Delta t)$ then

    $\left(\hat{q}^{k+1}, \hat{p}^{k+1}\right) = \Psi_{\Delta\tau_k}\left(\hat{q}^k, \hat{p}^k\right)$

  else

    $(\hat{q}^c, \hat{p}^c) = \Psi^{[*]}_{\Delta\tau_k}\left(\hat{q}^k, \hat{p}^k\right)$

    if "collision" then

      $\left(\hat{q}^{k+1}, \hat{p}^{k+1}\right) = R^{[*]}_{\alpha}\left(\hat{q}^c, \hat{p}^c\right)$

    else

      $\left(\hat{q}^{k+1}, \hat{p}^{k+1}\right) = (\hat{q}^c, \hat{p}^c)$

    end-if

  end-if

  $\tau_{max} = \tau_{max} - \Delta\tau_k$ and $k = k + 1$

end-while

$\left(q^{n+1}, p^{n+1}\right) = \left(\hat{q}^k, \hat{p}^k\right)$

At each step in the process, this algorithm conserves the $H^{\Delta t}_{[2,VV]}$ modified Hamiltonian to fourth-order accuracy. When there is no collision, the method is simply the standard Verlet method, Ψ. Stepping both to and from collisions, a fourth-order geometric integrator, $\Psi^{[*]}$, is applied to the dynamics of the modified Hamiltonian, $H^{\Delta t}_{[2,VV]}$. We should note that it is necessary to use the higher-order method for both the pre- and postcollision steps, since these steps would otherwise not conserve the modified Hamiltonian. At the points of collision the modified collision operator, $R^{[*]}_{\alpha}$, preserves the $H^{\Delta t}_{[2,VV]}$ modified Hamiltonian exactly.

Since the collision time is determined by the higher-order method, solving for the collision time will (in general) require solving an equation which is implicit in the smooth potential, V. To reduce this cost, we first compute the collision time using the lower-order Verlet method, Ψ. If a collision is detected, we recompute the

collision time with the higher-order Gauss method, $\Psi^{[*]}$. If the higher-order method does not find a collision within the time interval, then we assume that there is no collision, and the algorithm continues. A potential deficiency of this approach is that some "grazing" collisions may be missed when Δt is sufficiently large. However, such collisions are rare, and the cost reduction afforded by "prescreening" using the standard quartic polynomial-based collision detection is significant. For this reason, we use this variant in the numerical experiments in section 4.

3.2. Modified energy projection. A far less costly method for conserving the modified Hamiltonian through collisions is to use projections. There is a considerable amount of freedom in selecting the type of projection. For simplicity, we apply momenta rescaling after each collision and at the end of steps with collisions. For a step with n_c collisions, this results in the following algorithm.

PROJECTED COLLISION VERLET ALGORITHM (PCVA).
$\left(\hat{q}^0, \hat{p}^0\right) = (q^n, p^n)$
$\tau_{max} = \Delta t$ and $k = 0$
while $(\tau_{max} > 0)$
  $\Delta\tau_k = \min\left\{\tau_{max}, \text{CollisionTime}\left[\Psi, \hat{q}^k, \hat{p}^k\right]\right\}$
  $\left(\hat{q}^c, \hat{p}^c\right) = \Psi_{\Delta\tau_k}\left(\hat{q}^k, \hat{p}^k\right)$
  if "collision" then
    $\left(\hat{q}^{k+1}, \hat{p}^{k+1}\right) = R\left(\hat{q}^c, \hat{p}^c\right)$
  else
    $\left(\hat{q}^{k+1}, \hat{p}^{k+1}\right) = \left(\hat{q}^c, \hat{p}^c\right)$
  end-if
  if $(\Delta\tau_k \neq \Delta t)$ then
    Solve $H^{\Delta t}_{[2,VV]}\left(\hat{q}^{k+1}, \alpha\hat{p}^{k+1}\right) = H^{\Delta t}_{[2,VV]}\left(\hat{q}^k, \hat{p}^k\right)$
    Project $\hat{p}^{k+1} = \alpha\hat{p}^{k+1}$
  end-if
  $\tau_{max} = \tau_{max} - \Delta\tau_k$ and $k = k + 1$
end for
$\left(q^{n+1}, p^{n+1}\right) = \left(\hat{q}^k, \hat{p}^k\right)$

Since the modified Hamiltonian, $H^{\Delta t}_{[2,VV]}$, is quadratic in p, this method requires solving a scalar quadratic equation for α at each step. If there are no collisions during the previous step, then the step was propagated by the Verlet method, which conserves the $H^{\Delta t}_{[2,VV]}$ modified Hamiltonian to fourth-order accuracy. Hence, there is no need to perform the projection after full Verlet steps to obtain fourth-order "near conservation" of the modified energy. We should note that the inclusion of these projections destroys any reversibility in the underlying collisional algorithm. It is possible to use reversible projections [8]; however, this would involve including a prestep projection, which would make the resulting algorithm implicit.

4. Numerical experiment: Impact pendulum chain. As a numerical experiment, we compare the "primitive splitting algorithm" (PSA) [18] and "collision Verlet algorithm" (CVA) [10] with the new "modified collision Verlet algorithm" (MCVA) and "projected collision Verlet algorithm" (PCVA). As a test problem, we consider a chain of hard spheres in two dimensions connected by linear springs and attached to a hard wall (see Figure 4.1). Each spring has unit rest length, $r_0 = 1$, and spring constant, $k_s = 1$, resulting in a smooth potential of the form

$$V(\vec{q}_1, \ldots, \vec{q}_N) = \sum_{i=1}^{N-1} \frac{k_s}{2} \left(\|\vec{q}_{i+1} - \vec{q}_i\| - r_0 \right)^2 .$$

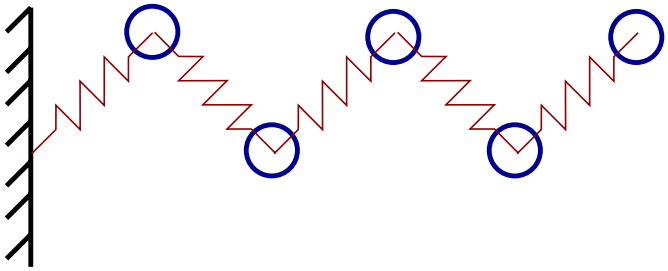

FIG. 4.1. *An impact pendulum chain: Hard spheres are connected with linear springs, each with the same spring constant and nonzero rest length. Collisions occur both between pairs of spheres and between spheres and the hard wall.*

The entire spring chain is attached to the origin, with a hard wall in the $x = 0$ plane. The diameter of each sphere is set to 0.9, just less than the spring rest length, to allow for a moderate collision frequency both between spheres and with the wall. For simplicity, it is assumed that each sphere has unit mass.

In our first experiment, we start with a chain of five spheres aligned along the x-axis with unit spacing. The second and fourth spheres are given random initial velocity of unit length, and we follow the dynamics for 5000 units of time. This results in approximately 12000 collisions over the time interval. We apply each of the numerical methods with a decreasing sequence of time stepsizes ranging from 0.3 to 0.001. A method is considered unstable if the energy deviates by more than 100% over the course of the simulation.

Figure 4.2 shows the conservation of energy as a function of stepsize. As expected the PSA is only first-order accurate, while the other methods are second-order. The CVA conserves energy far better than the PSA, but about an order of magnitude worse than the MCVA and PCVA. It is interesting that the MCVA and PCVA do so well since they were designed to conserve $H^{\Delta t}_{[2,VV]}$ (as opposed to H) and only in steps with collisions. The PSA has such severe energy drift that it was stable only for the smallest stepsizes.

In Figure 4.3, the conservation of the modified Hamiltonian, $H^{\Delta t}_{[2,VV]}$, is shown as a function of stepsize. Recall that the Verlet method with a fixed stepsize conserves $H^{\Delta t}_{[2,VV]}$ with fourth-order accuracy. As expected, only the PCVA and MCVA retain $H^{\Delta t}_{[2,VV]}$ as a higher-order invariant. The CVA and PSA conserve $H^{\Delta t}_{[2,VV]}$ about as well as they conserve the unmodified energy, H.

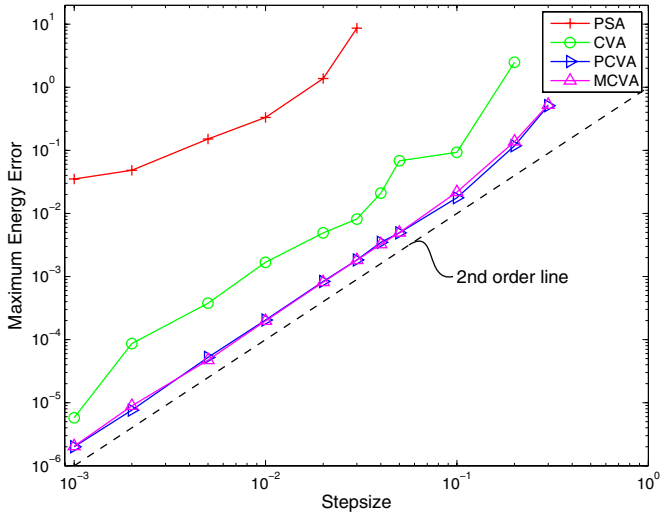

FIG. 4.2. *Maximum absolute energy error as a function of time stepsize.*

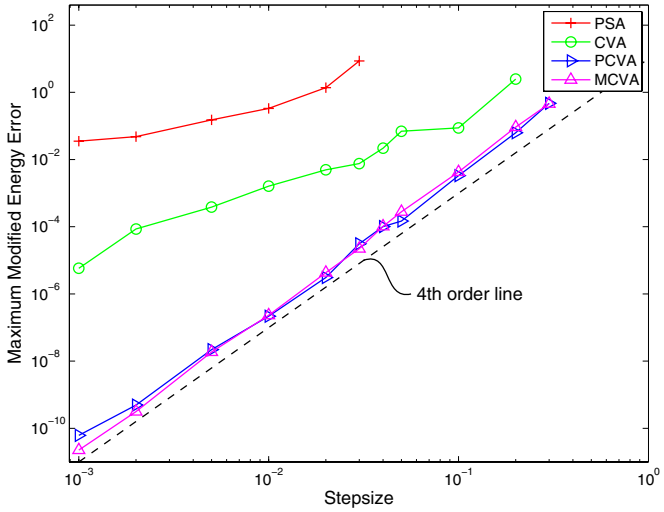

FIG. 4.3. *Maximum absolute "modified" energy error as a function of time stepsize.*

To investigate the energy drift, in Figure 4.4 we show the absolute deviation in energy as a function of time for a moderate stepsize of 0.02. The collisions have destabilized the PSA, and energy is severely drifting. Energy is drifting for the CVA as well, although not as severely as for the PSA. The PCVA and MCVA are remarkably stable with no visible sign of energy drift over a relatively long time interval with more than 10 000 collisions. We stress that the method approximates the modified Hamiltonian only to fourth-order accuracy, and no rigorous claim is made regarding the long-term stability of either the PCVA or MCVA method on long time intervals. However, the example given here nonetheless demonstrates a remarkable numerical stability, suggesting a practical stability enhancement. The situation is reminiscent of enhanced stability seen in "pseudosymplectic" numerical methods [2] which admit partial modified Hamiltonians of a given order of accuracy greater than the classical method order.

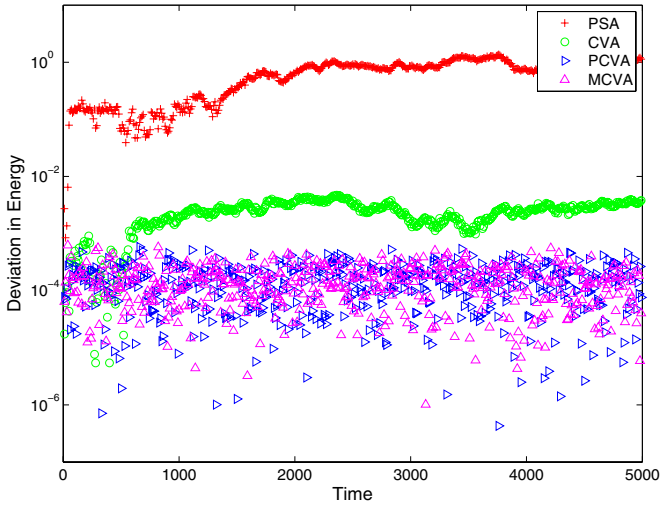

FIG. 4.4. *Absolute deviation in energy as a function of time.*

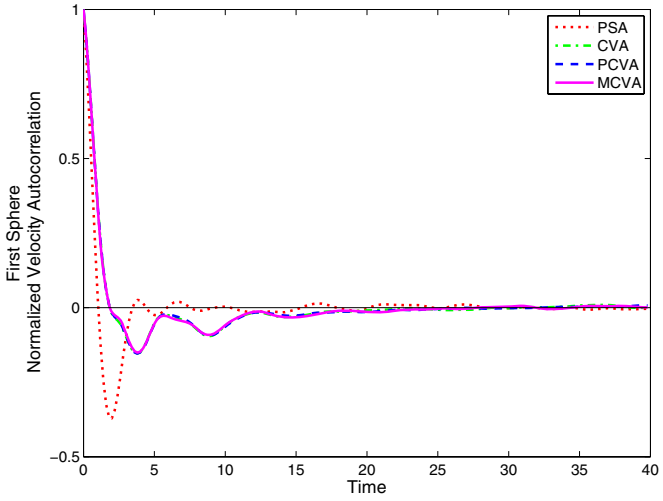

FIG. 4.5. *Velocity auto-correlation function for the first sphere in the chain.*

As pointed out by Tupper [20], projection-based methods may perform badly in terms of statistics. Good conservation of energy (by methods which do not explicitly conserve energy) typically suggests good equilibrium statistics, but the litmus test for evaluating the performance of molecular dynamics algorithms for statistical mechanics is the computation of the normalized velocity autocorrelation function [6],

$$A(t_k) := \frac{\langle v(t+t_k) \cdot v(t) \rangle}{\langle v(t) \cdot v(t) \rangle}.$$

The average, $\langle \cdot \rangle$, is taken over all time-origins t. To test the performance of our method for statistics, we increased the length of the simulation 10 times, and computed the velocity autocorrelation function for the first sphere in the chain using a stepsize of 0.02 as shown in Figure 4.5. The CVA, PCVA, and MCVA all produce similar velocity autocorrelation curves, while the curve produced by the PSA is clearly different.

5. Conclusion. We have investigated numerical methods for simulating the Hamiltonian N-body problem subject to hard-sphere inequality constraints. The dynamics of these mixed systems is characterized by smooth flow between collisions with impulsive forces at points of collision. The inclusion of these impulses makes traditional backward error analysis inappropriate since the flow is discontinuous and cannot be interpreted using a single modified smooth Hamiltonian system. We have derived two new methods which respect the underlying modified Hamiltonian of the numerical method (Verlet) used for the smooth system.

The first method, the MCVA, applies a higher-order symplectic integrator to the flow of the modified system in steps with collisions. At points of collision, the MCVA uses a modified collision operator which exactly conserves the modified Hamiltonian of the smooth system. In steps without collisions, the method reduces to the standard Verlet map. The second method, the PCVA, uses velocity rescaling to exactly conserve the modified Hamiltonian during steps with collisions. Like MCVA, this method also reduces to the standard Verlet map in steps without collisions.

In numerical experiments, we have compared the two new methods with the PSA and CVA. When applied to a long time simulation of a hard-sphere chain, the new methods have demonstrated dramatically improved energy conservation with very little drift. The additional computational cost of the MCVA and PCVA should not be prohibitive if collisions are relatively infrequent.

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