Unified Theory of Adaptive-Softened N-Body Dynamics
(rigorized production manuscript, vWORKS)

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Abstract

I formulate self-gravitating N-body dynamics in an extended phase space where a single global Plummer softening length ϵ is a canonical coordinate with conjugate momentum π. A harmonic spring couples ϵ to a smooth, permutation-invariant target $\epsilon_\star(q)$ and a quartic barrier $S_{\mathrm{bar}}(\epsilon)$ confines ϵ to $(\epsilon_{\min}, \epsilon_{\max})$. I prove that the exact sub-flows for the drift (T), potential ($V = V_{\mathrm{grav}} + S_{\mathrm{bar}}$) and spring ($S$) compose into a second-order, self-adjoint, symplectic Strang map. Linear momentum and angular momentum are conserved exactly in the continuous system and by each exact sub-flow, hence by the fixed-step composition up to roundoff. I establish a barrier lemma that yields a closed-form distance of $\epsilon(t)$ from the singular endpoints on all energy sublevels, and I give a backward-error result: on any compact analytic domain the method preserves a modified Hamiltonian $H_h = H_{\mathrm{ext}} + h^2 C_3 + O(h^4)$ and the physical-energy drift is $O(h^2)$ for exponentially long times. I also discuss when Barnes–Hut accelerations are conservative and how a truncated-pairs proxy recovers symplecticity when the cutoff mask is fixed in a neighborhood.

0. Notation and phase space

Let $d \in \{2, 3\}$ and $q = (q_1, \ldots, q_N) \in (\mathbb{R}^d)^N$, $p = (p_1, \ldots, p_N)$ with $p_i = m_i \dot{q}_i$. I extend the phase space by the pair $(\epsilon, \pi) \in \mathbb{R}^2$. The canonical one-form and symplectic two-form are

$$\theta = \sum_{i=1}^{N} p_i \cdot \mathrm{d}q_i + \pi\ \mathrm{d}\epsilon, \qquad \omega = \mathrm{d}\theta = \sum_{i=1}^{N} \mathrm{d}q_i \wedge \mathrm{d}p_i + \mathrm{d}\epsilon \wedge \mathrm{d}\pi.$$

I use $r_{ij} = \|q_i - q_j\|$, $\rho_{ij} = \sqrt{r_{ij}^2 + \epsilon^2}$, total mass $M_{\mathrm{tot}} = \sum_i m_i$, and $\epsilon_{\mathrm{gap}} := \min(\epsilon - \epsilon_{\min}, \epsilon_{\max} - \epsilon)$.

Symbol	Definition	Units
$V_{\mathrm{grav}}(q, \epsilon)$	$-G \sum_{i<j} \dfrac{m_i m_j}{\rho_{ij}}$	energy
$S_{\mathrm{bar}}(\epsilon)$	$\dfrac{k_{\mathrm{wall}}}{4} \left[(\epsilon - \epsilon_{\min})^{-4} + (\epsilon - \epsilon_{\max})^{-4}\right]$	energy
$T(p)$	$\frac{1}{2} \sum_i \dfrac{\|p_i\|^2}{m_i}$	energy
$S(\epsilon, \pi; q)$	$\dfrac{\pi^2}{2\mu_{\mathrm{soft}}} + \dfrac{k_{\mathrm{soft}}}{2} \left(\epsilon - \epsilon_\star(q)\right)^2$	energy
ω_{spr}	$\sqrt{k_{\mathrm{soft}}/\mu_{\mathrm{soft}}}$	T^{-1}

The barrier stiffness obeys $[k_{\mathrm{wall}}] = M L^6 T^{-2}$, consistent with $S_{\mathrm{bar}} \sim k_{\mathrm{wall}}\, \epsilon^{-4}$.

1 Extended Hamiltonian and equations of motion

I study the Hamiltonian

$$\boxed{H_{\text{ext}}(q,p,\epsilon,\pi) = T(p) + V_{\text{grav}}(q,\epsilon) + S_{\text{bar}}(\epsilon) + \frac{\pi^2}{2\mu_{\text{soft}}} + \frac{k_{\text{soft}}}{2}\big(\epsilon - \epsilon_\star(q)\big)^2} \tag{1}$$

with fixed positive parameters $\mu_{\text{soft}}, k_{\text{soft}}, k_{\text{wall}}, \epsilon_{\min}, \epsilon_{\max}$ and a smooth target $\epsilon_\star$ to be specified below. Hamilton's equations are

$$\begin{aligned} \dot{q}_i &= \frac{p_i}{m_i}, \\ \dot{p}_i &= -\nabla_{q_i} V_{\text{grav}}(q,\epsilon) + k_{\text{soft}}\big(\epsilon - \epsilon_\star(q)\big)\,\nabla_{q_i}\epsilon_\star(q), \\ \dot{\epsilon} &= \frac{\pi}{\mu_{\text{soft}}}, \\ \dot{\pi} &= -\partial_\epsilon V_{\text{grav}}(q,\epsilon) - \partial_\epsilon S_{\text{bar}}(\epsilon) - k_{\text{soft}}\big(\epsilon - \epsilon_\star(q)\big), \end{aligned} \tag{2}$$

with

$$\partial_\epsilon V_{\text{grav}}(q,\epsilon) = G\epsilon \sum_{i<j} \frac{m_i m_j}{\rho_{ij}^3}, \qquad \partial_\epsilon S_{\text{bar}}(\epsilon) = -k_{\text{wall}}\Big[(\epsilon-\epsilon_{\min})^{-5} + (\epsilon-\epsilon_{\max})^{-5}\Big].$$

2 The target $\epsilon_\star(q)$: definition, smoothness, and gradient

I only require that $\epsilon_\star(q)$ be a smooth, permutation-invariant function of the pair distances r_{ij}. For a concrete, production-ready choice I use the log-sum-exp "soft-min" over pair distances:

$$\epsilon_\star(q) = \frac{\alpha}{\lambda}\,\text{softplus}\big(-\lambda L(q)\big), \qquad L(q) := \log \sum_{i<j} e^{-r_{ij}/\alpha}, \tag{3}$$

with $\alpha > 0$ and $\lambda > 1$; $\text{softplus}(z) = \log(1+e^z)$. On the collision-free domain $\{q : r_{ij} > 0\ \forall i \neq j\}$ the map $q \mapsto r_{ij}$ is analytic, hence L and $\epsilon_\star$ are real-analytic. The gradient is

$$\boxed{\nabla_{q_i}\epsilon_\star(q) = \sigma_\star(q)\sum_{j\neq i} w_{ij}(q)\,\frac{q_i - q_j}{r_{ij}}, \quad \sigma_\star(q) = \frac{1}{1+e^{\lambda L(q)}}, \quad w_{ij} = \frac{e^{-r_{ij}/\alpha}}{\sum_{k<\ell} e^{-r_{k\ell}/\alpha}}\,,} \tag{4}$$

so $w_{ij} = w_{ji}$ and $\sum_{i<j} w_{ij} = 1$. This symmetry immediately implies

$$\sum_{i=1}^{N} \nabla_{q_i}\epsilon_\star(q) = 0, \qquad \sum_{i=1}^{N} q_i \times \nabla_{q_i}\epsilon_\star(q) = 0 \quad (d=3). \tag{5}$$

3 Exact sub-flows and the Strang composition

Split $H_{\text{ext}} = T + V + S$ with $V := V_{\text{grav}} + S_{\text{bar}}$. Denote the exact flows by φ_T^τ, φ_V^τ, φ_S^τ.

Drift (T). φ_T^τ advances q affinely at fixed p,ϵ,π: $q_i \mapsto q_i + \tau\, p_i/m_i$, p,ϵ,π unchanged.

Potential half-kick (V). φ_V^τ holds (q,ϵ) fixed and updates (p,π) by constant right-hand sides:

$$p_i \mapsto p_i - \tau\,\nabla_{q_i}\big(V_{\rm grav}(q,\epsilon) + S_{\rm bar}(\epsilon)\big), \qquad \pi \mapsto \pi - \tau\,\partial_\epsilon\big(V_{\rm grav}(q,\epsilon) + S_{\rm bar}(\epsilon)\big).$$

Spring block (S). With q frozen, set $\epsilon_\star^{\rm in} = \epsilon_\star(q)$ and write $\Delta := \epsilon - \epsilon_\star^{\rm in}$, $\zeta := \pi/(\mu_{\rm soft}\,\omega_{\rm spr})$. Over τ the pair (Δ,ζ) rotates by angle $\theta = \omega_{\rm spr}\tau$:

$$\begin{bmatrix}\Delta(\tau)\\ \zeta(\tau)\end{bmatrix} = \begin{bmatrix}\cos\theta & \sin\theta\\ -\sin\theta & \cos\theta\end{bmatrix}\begin{bmatrix}\Delta(0)\\ \zeta(0)\end{bmatrix},$$

so $\epsilon \mapsto \epsilon_\star^{\rm in} + \Delta(\tau)$ and

$$p_i \mapsto p_i + k_{\rm soft}\,\mathcal{I}(\tau)\,\nabla_{q_i}\epsilon_\star(q), \qquad \mathcal{I}(\tau) = \frac{\Delta(0)\sin\theta + \zeta(0)(1-\cos\theta)}{\omega_{\rm spr}}.$$

Strang map. For a fixed step $h > 0$ I define

$$\boxed{\Phi^h = \varphi_S^{h/2}\circ\varphi_V^{h/2}\circ\varphi_T^{h}\circ\varphi_V^{h/2}\circ\varphi_S^{h/2}\,.} \tag{6}$$

4 Symplecticity and time-reversibility (self-adjointness)

Proposition 1. *Each exact sub-flow is symplectic on (Γ,ω), hence the Strang map Φ^h in (6) is symplectic. Moreover, with the canonical involution $R(q,p,\epsilon,\pi) = (q,-p,\epsilon,-\pi)$ I have $R\circ\Phi^h\circ R = (\Phi^h)^{-1}$, i.e. Φ^h is time-reversible (self-adjoint).*

Proof. For any Hamiltonian H, the vector field X_H satisfies $\iota_{X_H}\omega = \mathrm{d}H$, so $\mathcal{L}_{X_H}\omega = \mathrm{d}(\iota_{X_H}\omega) = \mathrm{d}^2H = 0$ and the exact flow φ_H^τ preserves ω. Composition preserves symplecticity, so Φ^h is symplectic. Each of T,V,S is invariant under R (even in p or π, or independent of them), hence $R\circ\varphi_H^\tau\circ R = \varphi_H^{-\tau}$ and the palindromic product yields $R\circ\Phi^h\circ R = (\Phi^h)^{-1}$. □

5 Linear and angular momentum conservation

Proposition 2 (linear momentum). *With (2) the total momentum $P := \sum_i p_i$ satisfies $\dot P = 0$. Each exact sub-flow preserves P, hence the fixed-step map Φ^h preserves P in exact arithmetic.*

Proof. $\sum_i -\nabla_{q_i}V_{\rm grav} = 0$ by pairwise antisymmetry; $\nabla_{q_i}S_{\rm bar} \equiv 0$; and by (5), $\sum_i \nabla_{q_i}\epsilon_\star = 0$. The same cancellations hold blockwise. □

Proposition 3 (angular momentum). *Let $L := \sum_i q_i\times p_i$ in $d=3$ (or the bivector $L = \sum_i q_i\wedge p_i$ in general d). Then $\dot L = 0$ under (2). Each exact sub-flow preserves L, hence Φ^h preserves L in exact arithmetic.*

Proof. The gravitational force is central, $S_{\rm bar}$ has no q-gradient, and (5) yields $\sum_i q_i\times\nabla_{q_i}\epsilon_\star = 0$. Blockwise conservation follows. □

6 Barrier well-posedness of ϵ

Lemma 4 (energy sublevel confinement). *Let* $E_0 = H_{\mathrm{ext}}(q(0), p(0), \epsilon(0), \pi(0)) < \infty$ *with* $\epsilon(0) \in (\epsilon_{\min}, \epsilon_{\max})$. *Then for all* t *the solution satisfies*

$$\epsilon(t) \in \big[\epsilon_{\min} + \delta_E,\ \epsilon_{\max} - \delta_E\big], \qquad \delta_E := \min\left\{ \left(\frac{k_{\mathrm{wall}}}{4(E_0 + C_g)} \right)^{1/4},\ \frac{\epsilon_{\max} - \epsilon_{\min}}{2} \right\},$$

where $C_g := G \sum_{i<j} \dfrac{m_i m_j}{\epsilon_{\min}}$.

Proof. $T \geq 0$ and $S \geq 0$, while $V_{\mathrm{grav}} \geq -C_g$ on $\epsilon \geq \epsilon_{\min}$. Hence $S_{\mathrm{bar}}(\epsilon(t)) \leq E_0 + C_g =: B$. Each summand in S_{bar} is nonnegative, so $(\epsilon - \epsilon_{\min})^{-4} \leq 4B/k_{\mathrm{wall}}$ and $(\epsilon_{\max} - \epsilon)^{-4} \leq 4B/k_{\mathrm{wall}}$. Take fourth roots. □

7 Backward error and modified energy

Fix $\rho > 0$ and $\delta > 0$ and define the open analytic domain

$$U_{\rho,\delta} = \{(q, p, \epsilon, \pi) :\ \min_{i<j} r_{ij} \geq \rho,\ \epsilon \in (\epsilon_{\min} + \delta, \epsilon_{\max} - \delta)\}.$$

On $U_{\rho,\delta}$, the vector field of H_{ext} and all iterated Poisson brackets built from T, V, S are analytic and bounded.

Proposition 5 (modified Hamiltonian and drift bound). *There exist* $h_0, \kappa, c > 0$ *such that for all* $0 < h \leq h_0$ *the Strang map* (6) *admits an analytic modified Hamiltonian*

$$H_h = H_{\mathrm{ext}} + h^2 C_3 + h^4 C_5 + \cdots$$

with only even powers, and

$$\Phi^h = \exp\big[h\, L_{H_h}\big] + O(e^{-\kappa/h}) \quad \text{on } U_{\rho,\delta}.$$

Along the discrete trajectory $x_n = \Phi^{nh}(x_0)$,

$$\big|H_{\mathrm{ext}}(x_n) - H_{\mathrm{ext}}(x_0)\big| \leq \|C_3\|_{\infty, U_{\rho,\delta}}\, h^2 + O(h^4) + O(e^{-\kappa/h}), \qquad 0 \leq nh \lesssim c\, e^{\kappa/h}.$$

Proof (sketch). Apply Baker–Campbell–Hausdorff to the palindromic product and use self-adjointness to remove even powers in $\log \Phi^h$. Analyticity on $U_{\rho,\delta}$ yields the exponentially accurate modified flow and the stated $O(h^2)$ drift for H_{ext}. □

A coarse, unit-consistent envelope for $\|C_3\|_{\infty, U_{\rho,\delta}}$ follows by bounding triple Poisson brackets of T, V, S:

$$\|C_3\|_{\infty, U_{\rho,\delta}} \lesssim \frac{G\, M_{\mathrm{tot}}^2}{\epsilon_{\min}} + \frac{k_{\mathrm{soft}}\, \epsilon_{\max}^3}{2\, \epsilon_{\min}} + \frac{k_{\mathrm{soft}}\, \epsilon_{\max}^3}{\epsilon_{\min}} \big\|\nabla \epsilon_\star\big\|_{\infty, U_{\rho,\delta}} + \frac{k_{\mathrm{wall}}}{4\, \epsilon_{\mathrm{gap}}^4}. \tag{7}$$

Any fixed choice of h that keeps the trajectory in $U_{\rho,\delta}$—e.g. by a spring-angle cap $|\omega_{\mathrm{spr}}|\, \frac{h}{2} \leq \theta_{\mathrm{cap}} < \pi$ and a gravitational limiter based on $\min_{i<j} \rho_{ij}/\sqrt{G(m_i + m_j)}$—is admissible.

8 Self-adjointness $\Rightarrow$ error parity

Lemma 6. *For the self-adjoint map Φ^h I have $\Phi^{-h} = (\Phi^h)^* = (\Phi^h)^{-1}$ and the formal Lie series $\log \Phi^h = \sum_{k\geq 1} h^k A_k$ contains only odd powers ($A_{2\ell} = 0$). Equivalently, the modified Hamiltonian H_h contains only even powers and the one-step local defect contains only odd powers.*

Proof. Self-adjointness gives $\Phi^{-h} = (\Phi^h)^{-1}$; comparing $\log \Phi^{-h}$ with $-\log \Phi^h$ forces $A_{2\ell} = 0$. ☐

9 Barnes–Hut accelerations and conservative truncations

A single V-kick is a Hamiltonian sub-flow iff the force derives from a potential evaluated consistently in both half-kicks. If I replace ∇V_{grav} with a Barnes–Hut force that is not the gradient of a single approximate potential (e.g. one-sided acceptances), symplecticity and exact momentum conservation need not hold, although time-reversibility may remain good in practice due to the palindromic structure.

Proposition 7 (conservative truncated-pairs proxy). *Fix $R_{\text{cut}} > 0$ and define the truncated potential*

$$\widetilde{V}(q, \epsilon) := -G \sum_{i<j,\ r_{ij} \leq R_{\text{cut}}} \frac{m_i m_j}{\rho_{ij}}.$$

If the cutoff mask $\{(i,j) : r_{ij} \leq R_{\text{cut}}\}$ is constant on an open neighborhood of a configuration (no pair lies at the threshold), then $\widetilde{V}$ is C^∞ in that neighborhood, the corresponding V-kick is an exact Hamiltonian sub-flow, and momentum and symplecticity hold exactly.

Proof. With a fixed mask the sum is finite and smooth in (q, ϵ); pairwise antisymmetry is preserved since the sum runs over unordered pairs. ☐

10 Fixed-step production schedule (sufficient conditions)

In production I choose and *hold fixed* a sub-step h_{sub} for the entire run by

$$h_{\text{sub}} = \min\Big\{\chi\, \tau_{\text{grav}},\ \theta_{\text{cap}}/\omega_{\text{spr}}\Big\}, \qquad \tau_{\text{grav}} := \min_{i<j} \sqrt{\frac{\rho_{ij}^3}{G(m_i + m_j)}}, \quad \chi = 0.9,$$

and set the macro step to an integer multiple of h_{sub}. The angle cap $|\theta| = \omega_{\text{spr}} h_{\text{sub}} \leq \theta_{\text{cap}} < \pi$ controls the spring rotation per sub-flow; together with the barrier lemma it keeps the trajectory inside a compact analytic subset of $U_{\rho,\delta}$ on practical time horizons, which is sufficient for the backward-error result.

Conclusion

By embedding the global softening length as a canonical coordinate and coupling it to a smooth, permutation-invariant target through a harmonic spring and a quartic barrier, I obtain a Hamiltonian system that admits three exact, easily composable sub-flows. Their palindromic Strang composition is symplectic and time-reversible, preserves linear and angular momentum by construction, keeps ϵ

a finite distance away from the singular endpoints on all energy sublevels, and admits a standard analytic backward-error analysis with $O(h^2)$ energy drift on exponentially long times. When hierarchical force evaluations are used, I either require a conservative approximation or I adopt a truncated-pairs proxy with a fixed mask in a neighborhood to retain exact symplecticity.

A Explicit Jacobian checks (optional)

For completeness I record the Jacobians of the drift/kick blocks in canonical coordinates (q, p, ϵ, π).

$$J_T = \begin{bmatrix} I & hM^{-1} & 0 & 0 \\ 0 & I & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}, \qquad J_V = \begin{bmatrix} I & 0 & 0 & 0 \\ -\frac{h}{2}V_{qq} & I & -\frac{h}{2}V_{q\epsilon} & 0 \\ 0 & 0 & 1 & 0 \\ -\frac{h}{2}V_{\epsilon q} & 0 & -\frac{h}{2}V_{\epsilon\epsilon} & 1 \end{bmatrix},$$

with symmetric Hessians. One checks $J^\top \Omega J = \Omega$, consistent with the Liouville-form proof. The spring block is a direct product of a rotation in (ϵ, π) with a momentum shear $p \mapsto p + \mathrm{const} \cdot \nabla\epsilon_\star(q)$, both symplectic.

B Units

$[V_{\text{grav}}] = [S_{\text{bar}}] = [T] = [\text{energy}] = ML^2T^{-2}$, $[\partial_\epsilon S_{\text{bar}}] = MLT^{-2}$, $[k_{\text{soft}}] = MT^{-2}$, $[\mu_{\text{soft}}] = M$, $[\omega_{\text{spr}}] = T^{-1}$, $[k_{\text{wall}}] = ML^6T^{-2}$.

C Alternative targets for $\epsilon_\star$ (implementation note)

The theory only needs $\epsilon_\star$ to be smooth and permutation-invariant in $\{r_{ij}\}$. In applications I may prefer a density-consistent construction that aggregates per-particle smoothing lengths h_i obtained from a kernel density estimator; any C^2 compact kernel and the usual implicit correction factors yield an explicit $\nabla\epsilon_\star$ with the same symmetry properties as (4). The conservation proofs are unaffected as they use only symmetry and smoothness.