Unified Theory of Adaptive-Softened N-Body Dynamics

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Abstract

I formulate self-gravitating N-body dynamics in an *extended phase space* where the *global* Plummer softening length ϵ is itself a canonical coordinate. A harmonic spring drives ϵ toward a smooth, pair-distance–dependent target $\epsilon_\star(q)$, while a quartic wall prevents excursions outside $\left[\epsilon_{\min}, \epsilon_{\max}\right]$. A fixed-step, symmetric Strang splitting combines three *exact* sub-flows—kinetic drift, potential kick (Plummer + wall), and harmonic spring—into a second-order *symplectic, time-reversible* integrator. Linear and angular momentum are conserved to machine precision and a backward-error bound controls the long-time drift of a modified energy by $\mathcal{O}(h^2)$, independent of the run length. All benchmark and ML-training datasets shipped with this paper are generated by this `ham_soft` integrator in production mode.

0 Notation and Phase-Space Manifold

Symbol	Definition	Dimension
$q_i \in \mathbb{R}^d$	Cartesian position of body i	L
$p_i = m_i \dot{q}_i$	Canonical momentum	$\mathrm{M\,L\,T^{-1}}$
ϵ	Global Plummer softening	L
π	Momentum conjugate to ϵ	$\mathrm{M\,L\,T^{-1}}$
$\epsilon_\star(q)$	Target softening (smooth, ≥ 0)	L
$m_i > 0$	Mass of body i	M
G	Gravitational constant	$\mathrm{L^3\ M^{-1}\ T^{-2}}$
μ_{soft}	Oscillator "soft mass"	M
k_{soft}	Spring constant	$\mathrm{M\ T^{-2}}$
ω_{spr}	$\sqrt{k_{\mathrm{soft}}/\mu_{\mathrm{soft}}}$	$\mathrm{T^{-1}}$
$S_{\mathrm{bar}}(\epsilon)$	Quartic wall potential	$\mathrm{M\ L^2\ T^{-2}}$
α	Log-sum-exp smoothing scale	L
$\lambda > 1$	Log-sum-exp safety factor	—
$r_{ij} = \lvert q_i - q_j \rvert$	Pair distance	L
$r_{\max}$	$\max_{i<j} r_{ij}$ (block-max)	L
θ_{cap}	Spring phase cap (default 0.1 rad)	—
ϕ_{BH}	Barnes–Hut opening angle (default 0.5)	—

Extended phase-space $\Gamma = (q, p, \epsilon, \pi) \in \mathbb{R}^{2dN+2}$, symplectic form $\omega = \sum_{i=1}^{N} \mathrm{d}q_i \wedge \mathrm{d}p_i + \mathrm{d}\epsilon \wedge \mathrm{d}\pi$.

1 Extended Hamiltonian

$$\boxed{H_{\text{ext}} = \underbrace{\tfrac{1}{2}\sum_i \frac{\|p_i\|^2}{m_i}}_{T(p)} + \underbrace{V_{\text{grav}}(q,\epsilon) + S_{\text{bar}}(\epsilon)}_{V(q,\epsilon)} + \underbrace{\frac{\pi^2}{2\mu_{\text{soft}}} + \frac{k_{\text{soft}}}{2}\big(\epsilon - \epsilon_\star(q)\big)^2}_{S(\epsilon,\pi;q)}} \tag{1}$$

where $V_{\text{grav}} = -G\sum_{i<j} \dfrac{m_i m_j}{\sqrt{r_{ij}^2 + \epsilon^2}}$ and

$$S_{\text{bar}}(\epsilon) = \frac{k_{\text{wall}}}{4}\Big[(\epsilon - \epsilon_{\min})^{-4} + (\epsilon - \epsilon_{\max})^{-4}\Big].$$

1.1 Oscillator parameters (production mode)

$$\boxed{\mu_{\text{soft}} = \mu_{\text{soft}}^{\text{init}}, \quad k_{\text{soft}} = k_{\text{soft}}^{\text{init}}, \quad \omega_{\text{spr}} = \sqrt{k_{\text{soft}}/\mu_{\text{soft}}}}$$

Both parameters are frozen. A compile-time flag `HAM_SOFT_EXPERIMENTAL` re-enables time-varying heuristics; such runs are labelled *non-symplectic*.

1.2 Target softening $\epsilon_\star(q)$

Definition.

$$\epsilon_\star(q) = \frac{\alpha}{\lambda}\,\text{softplus}\big(-\lambda L(q)\big), \qquad L(q) := \log\sum_{i<j} e^{-r_{ij}/\alpha}. \tag{2}$$

Gradient (complete).

$$\boxed{\frac{\partial \epsilon_\star}{\partial q_i} = \sigma_\star \sum_{j\neq i} w_{ij}\frac{q_i - q_j}{r_{ij}}, \qquad \sigma_\star := \big(1 + e^{\lambda L}\big)^{-1}} \tag{3}$$

with symmetrised weights

$$w_{ij} = \frac{\exp[-(r_{ij} - r_{\max})/\alpha]}{\sum_{k<l}\exp[-(r_{kl} - r_{\max})/\alpha]}, \qquad w_{ij} = w_{ji}.$$

Note. Patch G1 corrects the exponent in the logistic prefactor $\sigma_\star$. Earlier drafts erroneously used $1+e^{4\lambda L/\alpha}$; the proper factor is $\big(1+e^{\lambda L}\big)^{-1}$, which restores the force amplitude and preserves torque cancellation.

2 Canonical Equations of Motion

$$
\begin{aligned}
\dot q_i &= \frac{p_i}{m_i},\\
\dot p_i &= -\nabla_{q_i} V + k_{\text{soft}}(\epsilon-\epsilon_\star)\nabla_{q_i}\epsilon_\star,\\
\dot\epsilon &= \frac{\pi}{\mu_{\text{soft}}},\\
\dot\pi &= -\partial_\epsilon V - k_{\text{soft}}(\epsilon-\epsilon_\star),
\end{aligned}
\qquad -\partial_\epsilon V = -G\sum_{i<j}\frac{m_i m_j\,\epsilon}{(r_{ij}^2+\epsilon^2)^{3/2}} - \partial_\epsilon S_{\text{bar}}(\epsilon). \tag{4}
$$

3 Exact Spring Sub-Flow (S_{harm})

Freeze q and $\epsilon_\star^{\text{in}} := \epsilon_\star(q)$ for the entire sub-flow. Defining $\Delta = \epsilon - \epsilon_\star^{\text{in}}$, $\eta = \pi/(\mu_{\text{soft}}\omega_{\text{spr}})$, the flow over τ is

$$
\begin{bmatrix}\Delta(\tau)\\ \eta(\tau)\end{bmatrix} = R(\theta)\begin{bmatrix}\Delta(0)\\ \eta(0)\end{bmatrix}, \qquad R(\theta) = \begin{bmatrix}\cos\theta & \sin\theta\\ -\sin\theta & \cos\theta\end{bmatrix}, \qquad \theta = \omega_{\text{spr}}\tau,
$$

with momentum impulse $p_i \leftarrow p_i + k_{\text{soft}}\mathcal{I}(\tau)\,\nabla_{q_i}\epsilon_\star^{\text{in}}$, $\mathcal{I}(\tau) = \big[\Delta(0)\sin\theta + \eta(0)(1-\cos\theta)\big]/\omega_{\text{spr}}$.

4 Second-Order Fixed-Step Symplectic Integrator

$$
\boxed{\Phi^h = \varphi_S^{h/2}\circ\varphi_V^{h/2}\circ\varphi_T^{h}\circ\varphi_V^{h/2}\circ\varphi_S^{h/2}} \tag{5}
$$

Each $\varphi_V^{h/2}$ updates (p,π) while *holding* (q,ϵ) fixed:

$$
\begin{aligned}
p_i &\leftarrow p_i - \frac{h}{2}\nabla_{q_i}\Big[V_{\text{grav}} + S_{\text{bar}}\Big],\\
\pi &\leftarrow \pi - \frac{h}{2}\partial_\epsilon\Big[V_{\text{grav}} + S_{\text{bar}}\Big].
\end{aligned}
$$

Because h is constant, Φ^h is symmetric and symplectic.

5 Boundary Handling — Smooth Barrier

$S_{\text{bar}}(\epsilon)$ is part of the Hamiltonian and is integrated exactly by the φ_V half-kick. If $\epsilon > 0.9\,\epsilon_{\max}$ *and* $|\pi| > \pi_{\text{crit}} = 0.1\sqrt{2\mu_{\text{soft}}H_{\text{ext}}(0)}$, the run aborts; no non-canonical step-size adjustment is attempted.

6 Conserved and Monitored Invariants

6.1 Linear momentum

By translational symmetry of V_{grav} and the barrier's dependence on ϵ only, $\sum_i p_i$ is conserved up to roundoff in the fixed-step scheme.

6.2 Angular momentum

With gradient (3), pairwise antisymmetry gives $\sum_i q_i \times \nabla_{q_i} \epsilon_\star = 0$, so the total angular momentum is conserved up to roundoff.

6.3 Center of mass

The center-of-mass position and velocity follow free drift when forces are internal; monitor drift as part of CI.

6.4 Modified energy

A symmetric second-order method preserves a *modified Hamiltonian*

$$H_{\mathrm{mod}} = H_{\mathrm{ext}} + h^2 C_3 + O(h^4),$$

with the coefficient bounded by

$$\boxed{\|C_3\| \le \frac{G\, M_{\mathrm{tot}}^2}{\epsilon_{\mathrm{min}}} + \frac{k_{\mathrm{soft}}\epsilon_{\mathrm{max}}^3}{2\epsilon_{\mathrm{min}}} + \frac{k_{\mathrm{soft}}\epsilon_{\mathrm{max}}^3}{\epsilon_{\mathrm{min}}}\|\nabla\epsilon_\star\|_\infty + \frac{k_{\mathrm{wall}}}{4\epsilon_{\mathrm{gap}}^4}}$$

where $M_{\mathrm{tot}} = \sum_i m_i$ and

$$\epsilon_{\mathrm{gap}} = \min\bigl(\epsilon - \epsilon_{\mathrm{min}},\ \epsilon_{\mathrm{max}} - \epsilon\bigr).$$

For fixed h,

$$\bigl|H_{\mathrm{mod}}(t) - H_{\mathrm{mod}}(0)\bigr| \le C_3\, h^2, \qquad 0 \le t \lesssim c\, e^{\kappa/h}.$$

7 Fixed Sub-Step Schedule (production)

Let

$$h_{\mathrm{sub}} = \min\Bigl(\chi\tau_{\mathrm{grav}},\ \theta_{\mathrm{cap}}/\omega_{\mathrm{spr}},\ \chi_\epsilon\, \epsilon_{\mathrm{safe}}/|\dot\epsilon|\Bigr), \tag{7.1}$$

with $\tau_{\mathrm{grav}} = \min_{i<j} \dfrac{r_{ij}^{3/2}}{\sqrt{G(m_i + m_j)}}$, $\epsilon_{\mathrm{safe}} = 0.1(\epsilon_{\mathrm{max}} - \epsilon_{\mathrm{min}})$, $\chi = \chi_\epsilon = 0.9$. Set $n_{\mathrm{sub}} = \lceil h_{\mathrm{user}}/h_{\mathrm{sub}} \rceil$ at $t = 0$ and keep h_{sub} fixed.

8 Implementation Diagnostics & CI Thresholds

Check	Criterion
Jacobian symplecticity (finite diff)	$\|J^\top \omega J - \omega\|_F < 10^{-11}\sqrt{N}\max(1, \|J\|_F)$
Time-reversibility (round-trip)	$\|\Phi^h_{0\to T} \circ \Phi^h_{T\to 0}(x_0) - x_0\| < 10^{-12}\,(1 + \|x_0\|)$
Linear momentum conservation (FP64)	$\left\|\sum_i p_i(t) - \sum_i p_i(0)\right\| < 10^{-12}T$
Angular momentum conservation (FP64)	$\|L(t) - L(0)\| < 10^{-12}T$
Center-of-mass drift	$\|R_{\mathrm{CM}}(t) - R_{\mathrm{CM}}(0)\| < 10^{-10}T$
Modified-energy defect (FP64)	$< 10^{-7}\,h^2$
Modified-energy defect (FP32)	$< 5 \times 10^{-6}\,h^2$ Spring phase cap monitor
$\max\|\theta\| \le \theta_{\mathrm{cap}}$ (abort if violated)	
Barrier proximity monitor	$\epsilon_{\mathrm{gap}} \ge 0.05(\epsilon_{\max} - \epsilon_{\min})$
Performance budget	ns/step $\le$ baseline $\times$ 1.10

9 Heuristics

Barnes–Hut cache uses opening angle ϕ_{BH} (renamed from θ_{BH} to avoid collision with θ_{cap}).

A Experimental Adaptive Step Size (non-symplectic)

$$\omega_{ij} = \sqrt{\frac{G(m_i + m_j)}{(r_{ij}^2 + \epsilon^2)^{3/2}}}, \qquad h_{\mathrm{sub}} \le \chi \min_{i<j} \omega_{ij}^{-1}.$$

B Patch Ledger

P-15 Logistic factor in $\nabla\epsilon_\star$.

P-16 Barrier potential added to Hamiltonian and EOM.

P-17 Barrier term in C_3 bound.

P-18 V-kick updates (p, π); explicit algorithm line.

P-19 Distinct symbols: θ_{cap} vs ϕ_{BH}.