Open Access and Peer Reviewed Journal ISSN 2394-2231 https://www.ijctjournal.org/

RESEARCH ARTICLE OPEN ACCESS

HKD-Water: Exact Incremental Reevaluation of Local Perturbations in a TIP4P/2005 Molecular Water Interaction Workload

Michael Yang

August 2026

Abstract

We present HKD-Water, a reproducible benchmark for exact incremental reevaluation of localized perturbations in a molecular-water interaction workload. The public artifact uses the rigid four-site TIP4P/2005 interaction model and compares a localized update against an independent full reevaluation after every perturbation. The scientific result is expressed in two deliberately separate metrics: measured wall-clock speedup and a machine-independent logical interaction cycle reduction. The released implementation is publication-safe: it contains the reference physics, benchmark construction, exactness test, timing harness, and cryptographic fingerprints, but no proprietary HKD indexing, persistence, dispatch, cache, or acceleration implementation. The benchmark is an interaction reevaluation experiment rather than a complete molecular-dynamics trajectory.

Keywords— TIP4P/2005; molecular water; incremental computation; localized perturbation; molecular simulation; exact computation.

1 Motivation

TIP4P/2005 is a widely used rigid four-site water model designed for condensed phases of water [1]. Recent molecular-dynamics work by Wang, Kuo, Zeng, Tang, and Wu examined water reorientation and hydrogen-bond-network effects under nanoconfinement, illustrating the continuing importance of computationally resolved water dynamics [2]. The broader molecular-simulation tradition demonstrates the value of computational experiments in which microscopic interactions are explicitly evaluated [3]. In many such computations, however, a small state change affects only a fraction of the total interaction workload. Incremental-computation research has established the general principle that outputs can sometimes be updated by reevaluating affected work rather than repeating an entire computation [4].

HKD-Water studies that principle in a narrowly defined molecular-water setting. The goal of this paper is not to disclose the proprietary HKD acceleration mechanism. Instead, it memorializes a falsifiable numerical invariant and provides a public reference artifact capable of validating that invariant.

2 Benchmark

The reference program constructs a periodic, liquid-density-like configuration of rigid TIP4P/2005 molecules. Oxygen–oxygen Lennard–Jones interactions and charge-site Coulomb interactions are evaluated for molecular pairs obtained from a periodic spatial neighbor search. The public implementation uses NumPy and SciPy, whose scientific-computing infrastructure is described by Virtanen et al. [5].

A candidate list is constructed at a cutoff plus a finite skin. Each benchmark update displaces one molecule by less than the skin width. The affected set is the set of candidate molecular pairs incident on the displaced molecule. The public artifact then performs two computations:

$$E_{\mathrm{inc}} = E_{\mathrm{old}} - E_{\mathrm{affected,old}} + E_{\mathrm{affected,new}}, \tag{1}$$

and, independently,

$$E_{\text{full}} = \sum_{p \in P} E_p(\mathbf{x}_{\text{new}}). \tag{2}$$

The principal correctness condition is

$$|E_{\text{inc}} - E_{\text{full}}| \leq 10^{-8} \text{ kcal mol}^{-1}. \tag{3}$$

The benchmark performs multiple deterministic perturbations and verifies the condition after every update.

3 Speed Metrics

Wall-clock speedup is measured directly:

$$S_{\text{wall}} = \frac{t_{\text{full}}}{t_{\text{affected}}}. \tag{4}$$

We separately report a logical interaction-cycle reduction:

$$S_{\text{logical}} = \frac{|P|}{|P_{\text{affected}}|}. \tag{5}$$

One logical interaction cycle is defined as one candidate molecular-pair evaluation by the reference interaction kernel. This definition is machine-independent and must not be confused with processor clock cycles. Consequently, the paper makes no inference from logical-cycle reduction to a particular hardware-cycle count.

4 Reproducibility and Disclosure Boundary

The released file `hkd_water_publication_safe.py` records the random seed, numerical parameters, software versions, exactness tolerance, measured timings, logical-cycle counts, and SHA-256 fingerprints of the initial and final position arrays. It deliberately contains no proprietary HKD module, private file format, active-state ABI, sparse-address representation, dependency encoding, cache policy, persistence protocol, or dispatcher.

This separation allows the numerical claim to be independently inspected while preserving the implementation boundary of the acceleration system. A licensed or private HKD implementation can be evaluated against exactly the same public reference condition without being embedded in the publication artifact.

5 Reference Run

A reference execution of the released artifact on the author's macOS Python 3.10 environment used 20,000 molecules, seven localized updates, seed 17, a 9.0 Å interaction cutoff, and a 1.0 Å neighbor skin. The resulting measurements are reported in Table 1. Wall-clock timings are environment-dependent measurements; the exactness criterion and logical-cycle definition are independent of processor clock rate.

The reference run reported the following state fingerprints. The initial position-array SHA-256 digest is

`2a1aa3b9c7d63ba19482c5d4c8c7d30bc6acb1482b89cfc8e6ea6ae6a6c0a924`

and the final position-array SHA-256 digest is

`37ec6ff34af2e2358cafdf8cfd5cf6e4d300c06ca6743804aa3961db2bc35dab`.

These hashes identify the numerical state of the reported execution without exposing proprietary HKD internals.

The SHA-256 digest of the released Python artifact used for this reference run is

`06a9a87cea7ce570ad865d694f484d50747654a212cb24c8b727f41823d255b5`.

This digest identifies the exact public benchmark implementation independently of any private HKD runtime.

Table 1: Reference execution of the publication-safe artifact.

Quantity	Result
Molecules	20,000
Candidate molecular pairs	1,499,093
Neighbor-list construction time	0.101975 s
Initial full evaluation time	0.644038 s
Maximum absolute energy error	2.910e-11 kcal/mol
Exactness tolerance	1.0e-08 kcal/mol
Median affected reevaluation time	0.000206000 s
Median full reevaluation time	0.694397583 s
Median measured wall speedup	3467.67×
Median logical-cycle reduction	9671.57×
Logical-cycle range	9428.26–15779.93×
Neighbor-skin certificate	PASS
Exactness certificate	PASS

6 Interpretation

The useful result is not that a complete molecular-dynamics simulation has been accelerated by the reported factor. The present artifact does not integrate equations of motion, compute a trajectory, thermostat an ensemble, or establish equilibrated thermodynamic observables. Its narrower claim is that, for a localized perturbation under the stated neighbor-list safety condition, exact pair-energy reevaluation can be validated by recomputing only the affected candidate-pair terms and comparing the resulting total with an independent full reevaluation.

This distinction also makes the performance statement stronger scientifically: the exactness criterion, measured wall-clock ratio, and logical work reduction are separately observable quantities rather than a single extrapolated claim.

7 Conclusion

HKD-Water establishes a compact, reproducible reference experiment for exact incremental molecular-water interaction reevaluation. The public artifact memorializes the scientific claim while maintaining a strict disclosure boundary around proprietary HKD acceleration machinery. Future work can extend the same validation discipline to force and torque evaluation, neighbor-list maintenance, time integration, ensemble control, and full molecular-dynamics trajectories.

References

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