Using Nonequilibrium Fluctuation Theorems to Understand and Correct Errors in Equilibrium and Nonequilibrium Simulations of Discrete Langevin Dynamics

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I. INTRODUCTION

[illegible] L[illegible] [1],

$$dr = v\,dt,$$

$$dv = \frac{f(t)}{m}\,dt - \gamma v\,dt + \sqrt{\frac{2\gamma}{\beta m}}\,d\mathsf{W}(t),$$

[illegible] $\mathcal{H}(t)$. [illegible] r [illegible] v [illegible], m [illegible], f [illegible], $\beta = 1/k_B T$, k_B [illegible] B[illegible], T [illegible], γ [illegible] ([illegible]), [illegible] $\mathsf{W}(t)$ [illegible]. T[illegible], $f \equiv -\partial\mathcal{H}/\partial r$. F[illegible], r, v, f, [illegible] $d\mathsf{W}$ [illegible], [illegible] m [illegible].

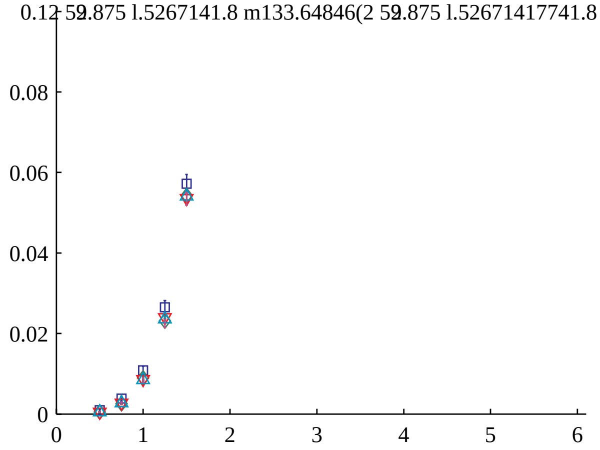
[illegible] L[illegible] [2]. H[illegible], [illegible]: E[illegible] H[illegible], [illegible] $\mathcal{H}$ [illegible]. (B[illegible]

$$v\left(n + \frac{1}{2}\right) = v(n) + \frac{t}{2}\frac{f(n)}{m},$$

$$r(n+1) = r(n) + t\,v\left(n + \tfrac{1}{2}\right),$$

$$v(n+1) = v\left(n + \frac{1}{2}\right) + \frac{t}{2}\frac{f(n+1)}{m}.$$

0.12 59.875 l.5267141.8 m133.64846(2 59.875 l.52671417741.8 m133910 l1253.879624.601 m125.4789627263 l135.478964.911653.879624.601 7 l1487.48 673



$F_e = 11.4 \pm 0.2 k_B T$ … $t = 1$ … F … F_e … $t \approx 5$ … 6 … 2 …

(F_e) … t (Fig. 2) …

$$F_e / N_{H_2O} k_B T \approx a \; t^4, \qquad (7)$$

… a … Fig. 2. T … M … 36 … H … $p_e(x) \propto$ e [$-\beta \mathcal{H}(x)$], … S. VI … E … L …

V. MULTIVARIATE FLUCTUATION THEOREM

… (…) … (… H …). … Eq. (4) … F … T … R … Eq. (4) … W_1, W_2 …

$$P[X|\;] = P[X|\;] e^{\beta\{W_1[X,\;] + W_2[X,\;] - F_e[\;]\}}. \qquad (8)$$

M … $\delta(W_1[X,\;] - W)\delta(W_2[X,\;] - W_{s\,had})$, … :

$$\frac{P(W, W_{s\,had})}{P(-W, -W_{s\,had})} = e^{\beta(W + W_{s\,had} - F_e)}. \qquad (9)$$

T … G … -G … [37,38]. Eq. (9) … $W + W_{s\,had} - F_e$ …

Eq. (9) … I … [22] … S … Eq. (9) … F … S. VI, … Eq. (12) … S. VII, … (ITFT) Eq. (15).

VI. RECOVERING EQUILIBRIUM STATISTICS FROM NONEQUILIBRIUM SIMULATIONS

N … L …

A 0

M C 42,43 ,

B

, e {$-\beta W_{s\ \mathrm{had}}$}

$$\frac{P(W < 0)}{P(W > 0)} \Big/ \langle e^{-\beta W} \rangle_{W > 0}, \quad (15)$$

Eq. (15) ... Sec. VI, ... $(\times)$ ... $\langle e^{-\beta W}\rangle_{W>0}/\langle e^{-\beta W}\rangle_{W>0}$ ... ITFT ... 32 ... 48).

VIII. EPILOGUE

NPT 1 298 K M C (GHMC [16,35] 0.5 . M C [58,59]. A 250 000 , 10 000 GHMC L E0. (3) 9.1/ s . 4096 0.25 7 2293 642.4 2^n ($n = 0, 1, \ldots, 12$). T 4096 ; 2 6 .

T E0. (6), 0 L , M , M :

$$F_{e} = \tfrac{1}{2}[\langle W_{0\to M}\rangle_{\mathrm{GHMC}} - \langle W_{M\to 2M}\rangle_{\mathrm{GHMC}}]. \qquad \text{(A1)}$$

H , $\langle\cdot\rangle_{\mathrm{GHMC}}$ L GHMC- . T $M = 2^n$ 0

$$\delta^2(\ F_{\mathrm{e}}) = [\ \mathrm{a}(W_{0\to M}) + \ \mathrm{a}(W_{M\to 2M}) - 2\mathrm{c}(W_{0\to M}, W_{M\to 2M})]/(4N_{\mathrm{eff}}), \quad \text{(A2)}$$

a(x) c(x, y) [illegible] , N_{eff} [illegible] 0 [illegible] .
(S S . 2.4 R . 60 .)