
Enhanced Drift Sampling: Rare-Event Free-Energy Estimation with Tilted Drift Targets

Francesco Alesiani
NEC Laboratories Europe
francesco.alesiani@neclab.eu

Gerrit Gerhartz
NEC Laboratories Europe
gerrit.gerhartz@neclab.eu

Henrik Christiansen
NEC Laboratories Europe
henrik.christiansen@neclab.eu

Mathias Niepert
University of Stuttgart
mathias.niepert@ki.uni-stuttgart.de

Abstract

Rare-state free-energy estimation remains exponentially expensive under direct equilibrium sampling, even when generative models provide approximately independent configurations. Enhanced Diffusion Sampling addresses this problem by steering pretrained diffusion models toward biased ensembles, but requires multistep reverse-SDE integration and Feynman–Kac correction weights. We introduce *Enhanced Drift Sampling* (ENDS), which transfers biasing and reweighting to one-step drifting generators by tilting a reference bank with $w \propto e^{-b}$. We develop steering, adaptation, and multi-step refinement variants for umbrella, metadynamics, and linear biases. Exact thermodynamic reweighting requires exact biased windows; approximate drifted windows additionally require adequate bank coverage and proposal overlap. On a double well, an exact-tilt oracle reduces generated-sample requirements, whereas the tested finite-step protocol fails from a collapsed initialization. Umbrella variants reconstruct toy and alanine potentials of mean force, and tilted BioEmu ensembles reduce finite-sample error for the emulator’s own rare-state probability, but do not remove its discrepancy from molecular-dynamics references.

1 Introduction

Free-energy calculations are central to the in-silico validation of materials and drug candidates. They require adequate sampling of the relevant equilibrium states; transition regions are additionally important for kinetics, pathway questions, and some collective-variable methods. Estimating equilibrium observables of complex molecular systems is limited by two complementary bottlenecks [1]: (i) slow mixing of Markovian dynamics across metastable states, and (ii) undersampling of rare states even with independent draws from $p(x)$. For states A and B , define $\Delta G_{B-A} = G_B - G_A = -k_B T \log[P(B)/P(A)]$ and $\Delta g_{B-A} = \beta \Delta G_{B-A}$, where $\beta = (k_B T)^{-1}$. Estimating the minority-state probability to fixed relative precision by direct sampling then requires $O(e^{|\Delta g_{B-A}|})$ samples in the rare-event regime. Generative equilibrium samplers—Boltzmann generators [2], diffusion models [3, 4], and emulators such as BioEmu [5]—primarily attack (i) by producing (approximately) i.i.d. samples. They do not remove (ii): direct estimation of a folding free energy to fixed precision still requires exponentially many equilibrium samples as the reduced minority-state gap grows [1].

Classical enhanced sampling [6, 7] attacks (ii) by sampling biased ensembles $q \propto p e^{-b}$ and reweighting [8]. Throughout, $u = \beta U$ and $b = \beta B$ denote dimensionless reduced physical and bias potentials,

respectively; all toy-system free energies are reported in units of $k_B T$. EDS [1] transfers this paradigm to pretrained diffusion samplers through Feynman–Kac Corrector (FKC) steering and associated path weights [9], yielding UmbrellaDiff, MetaDiff, and ΔG -Diff. The remaining cost is multi-step reverse SDE integration per steered sample.

Unlike diffusion models that rely on multi-step reverse SDE integration [3, 4], *drifting generative models* [10] learn a deterministic, one-step pushforward map $f_\theta : \mathcal{N}(0, I) \rightarrow q_\theta$. Under Gaussian smoothing σ , the population drift field toward a target density p is $V_{p,q}^{(\sigma)}(x) = \sigma^2 \nabla_x \log[p_\sigma(x)/q_\sigma(x)]$, which reflects a difference of smoothed scores [11, 12].

Enhanced Diffusion Sampling (EDS) [1] enables rare-event estimation by steering diffusion models via Feynman–Kac Correctors (FKC) [9], but incurs high costs from multi-step score evaluations and path-weight tracking. Transferring this paradigm to one-step drifting generators cuts sampling cost to a single function evaluation (1-NFE), enabling rapid generation from tilted targets while offloading thermodynamic unbiasing to static importance weighting or MBAR [8].

We transfer the EDS bias-and-reweight approach to drifting generators and propose **Enhanced Drift Sampling (ENDS)**. We represent $p^{(b)} \propto p e^{-b}$ either with exact target samples or, approximately, by weighting reference affinities with $w \propto e^{-b}$. Standard e^b reweighting and MBAR are exact for samples from $p^{(b)}$; approximate drifted windows retain proposal bias [8]. This yields UMBRELLADRIFT, METADRIFT, and ΔG -DRIFT.

Our contributions are: (i) a biased-score identity and consistency results for the associated estimators (Sec. 4); (ii) the ENDS-STEER, ENDS-ADAPT, and ENDS-REFINE variants, together with umbrella, metadynamics, and linear-tilt protocols; and (iii) experiments that isolate practical bank coverage and proposal overlap, compare amortized one-step generation with multistep baselines, and evaluate the approach on alanine and frozen BioEmu ensembles.

2 Related work

Umbrella sampling [6], metadynamics [7], and multistate reweighting [8] are standard for free energies when suitable collective variables (CVs) exist. EDS [1] combines these ideas with diffusion steering; related work biases energy-based diffusion samplers along CVs [13]. Flows [2], adjoint matching [14], and proximal neural samplers [15] learn samplers from energies or data. ENDS targets the EDS *emulator* setting: it operates on pretrained pushforwards, does not require evaluable energies at inference time, and remains compatible with energy-based reference buffers. Without proposal densities or path weights, its reweighting guarantee is limited to exact biased windows. Deng et al. [10] introduce training-time drift fields for one-step generation. Turan et al. [11] and Lai et al. [12] establish the connection between Gaussian drift and score differences and analyze the effect of kernel choice. Franz et al. [16] recover conservative fields through sharp normalization, and He et al. [17] connect drifting to Sinkhorn divergences. Drift Flow Matching [18] motivates our optional multi-step refinement (ENDS-REFINE) when a one-pass generator has low effective sample size (ESS) after tilting.

3 Method

Preliminaries Let $p(x) \propto e^{-u(x)}$ be a probability density on $\Omega \subset \mathbb{R}^d$, with reduced potential $u = \beta U$, and assume $0 < \int p(x) e^{-b(x)} dx < \infty$. For exact samples $x \sim p^{(b)}$, and an observable o , we have that $\mathbb{E}_p[o] = \mathbb{E}_{p^{(b)}}[oe^b]/\mathbb{E}_{p^{(b)}}[e^b]$. If the generated distribution differs from $p^{(b)}$, this identity no longer removes the generator’s transport error. We call a set of reference samples $\mathcal{Y} = \{y_j\}$, with $y_j \sim p$, a *bank*. **EDS** targets $q \propto p e^{-b}$ with FKC-steered reverse SDEs and carries correction weights for imperfect steering [1]. A **drifting** generator f_θ induces the pushforward distribution $q_\theta = (f_\theta)_\# p_{\text{prior}}$, where p_{prior} is typically $\mathcal{N}(0, I)$. Under a Gaussian kernel,

$$V_{p,q}^{(\sigma)}(x) = \sigma^2 \nabla_x \log \frac{p_\sigma(x)}{q_\sigma(x)}, \quad (1)$$

where $p_\sigma(x) = (p * \phi_\sigma)(x)$, $q_\sigma(x) = (q * \phi_\sigma)(x)$ denote Gaussian-smoothed densities convolved with isotropic kernel $\phi_\sigma(z) = (2\pi\sigma^2)^{-d/2} \exp(-\|z\|_2^2/(2\sigma^2))$ [11, 12], with $(p * k)(x) = \int_{\mathbb{R}^d} p(y)k(x - y) dy$. Tilting $p \mapsto p^{(b)}$ is the drifting analogue of the ∇b control used by EDS.

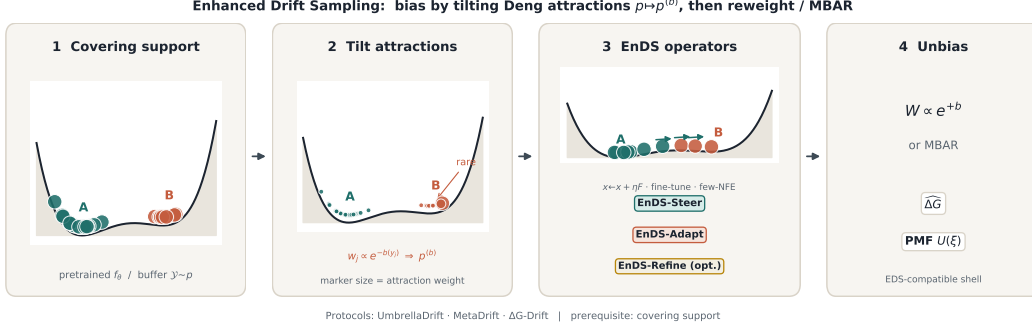


Figure 1: Enhanced Drift Sampling pipeline: tilt a state-covering reference bank toward $p^{(b)}$, apply a drift variant, and estimate equilibrium quantities by e^b reweighting or MBAR. Exact recovery requires exact biased windows or an additional valid proposal correction.

EnDS Figure 1 summarizes the ENDS pipeline. The two exponential factors in Fig. 1 serve different purposes: e^{-b} favors reference configurations in the desired biased ensemble, whereas e^b removes that bias during estimation. Following the affinity construction of Deng et al. [10], we approximate a tilted target by multiplying reference affinities by $w_j \propto \exp[-b(y_j)]$. Because these weights enter after the affinity softmaxes and also affect feature scaling, the resulting empirical drift is not an exact Monte Carlo discretization of the Gaussian population field. When the energy is available, we can instead draw reference samples directly from $p^{(b)}$ and assign unit weights; we refer to this idealized setting as *exact tilt*. For affinity scales $\mathcal{R}$ (e.g. $\{0.02, 0.05, 0.2\}$; see Section F), define

$$\hat{V}_{\mathcal{R},w}(x; \mathcal{Y}) := s \sum_{R \in \mathcal{R}} \hat{V}_R(x; \mathcal{Y}, w), \quad (2)$$

Each $\hat{V}_R$ compares local generated and reference neighborhoods, attracting particles toward regions emphasized by the tilted bank and counteracting generator overrepresentation. Multiple scales combine broad and local corrections without making the empirical weighting exact. In **ENDS-STEER**, we initialize $x = f_\theta(\epsilon)$ and apply inference-time updates $x \leftarrow x + \eta \hat{V}_{\mathcal{R},w}$, without modifying θ . With **ENDS-ADAPT**, we briefly fine-tune the generator using stop-gradient drift targets and weighted reference samples, after which generation requires one generator evaluation. In **ENDS-REFINE**, we apply a short sequence of annealed drift updates toward fixed samples from $p^{(b)}$, inspired by Drift Flow Matching [18]; see Appendix C for details. Section I provides a detailed comparison and algorithmic specifications for the three strategies.

Protocols. Bias potentials $b(y)$ target low-dimensional collective variables (CVs) $\xi(y) : \mathbb{R}^d \rightarrow \mathbb{R}^k$, yielding biased ensembles $p^{(b)}(y) \propto p(y)e^{-b(y)}$. The bias function $b(y)$ defines the protocol. **UMBRELLADRIFT** applies harmonic biases $b_k(y) = \frac{1}{2}\beta k_k(\xi(y) - \xi_0^{(k)})^2$ centered at window locations $\xi_0^{(k)}$ to a collective variable (CV) ξ and uses MBAR to estimate the potential of mean force (PMF) [6, 8]. **METADRIFT** deposits well-tempered hills $b(y, t) = \sum_{t' < t} W_0 \exp\left(-\frac{\beta V(y, t')}{\gamma - 1}\right) \exp\left(-\frac{(\xi(y) - \xi(t'))^2}{2\sigma_{\text{CV}}^2}\right)$ along ξ . Exact pooling across the changing biases requires a time-dependent normalization offset $c(t)$ [19, 20]; absent that correction and quasi-stationarity assumptions, our online curve is an exploratory diagnostic rather than a consistent equilibrium estimator. **ΔG-DRIFT** uses dimensionless linear tilts $b_a(y) = a \xi(y)$ (so a has reciprocal units of ξ) and a reweighted two-state estimator (Algorithm 1).

4 Theory

Proposition 1 (Biased score identity). Under a Gaussian kernel of bandwidth σ , $V_{p^{(b)},q}^{(\sigma)}(x) = \sigma^2 \nabla_x \log((pe^{-b})_\sigma(x)/q_\sigma(x))$. For the Gaussian population operator, $q = p^{(b)}$ implies that the field vanishes. Conversely, on connected $\mathbb{R}^d$, $V \equiv 0$ implies $q = p^{(b)}$ by injectivity of Gaussian convolution [11]. Separate identifiability results exist for sharp-normalized and fully converged

Sinkhorn operators under their respective assumptions [16, 17]; they do not establish identifiability of the weighted empirical drift used here.

Proposition 2 (Estimator consistency). If window k yields exact i.i.d. samples from $q_k \propto p e^{-b_k}$, then single-window importance reweighting recovers $\mathbb{E}_p[o]$ almost surely under the stated first-moment conditions. For MBAR, additionally let $N_k/N \rightarrow \lambda_k > 0$, assume evaluable reduced-potential differences and an irreducible population overlap matrix; then the free-energy offsets (up to a common constant) and target expectations are consistent [8, 1].

Proofs appear in Appendix A. Weighted empirical affinities provide a finite-sample, multi- R approximation to attraction toward $p^{(b)}$; Proposition 1 identifies the Gaussian population target, not the practical update rule. Consequently, Proposition 2 does not make finite-step ENDS-STEER, ENDS-ADAPT, or ENDS-REFINE estimates unbiased. Bank coverage supplies states to the empirical target, whereas proposal overlap controls reweighting stability. Increasing the sample count reduces variance only after both are adequate.

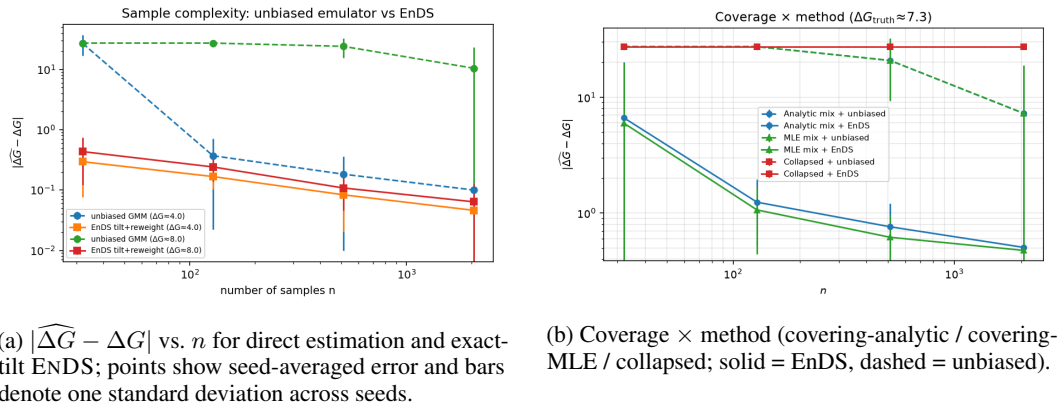
5 Experiments

Exact-tilt oracle. When the reduced potential u is evaluable, *exact tilt* draws $x_i \sim p^{(b)} \propto p e^{-b}$ (analytic / grid / MCMC under $u+b$) with unit reference weights, then estimates observables by $W_i \propto e^{b(x_i)}$ (or MBAR). This is a **calibration oracle**: it isolates EDS-style reweighting from generator transport error. It is **not** an amortized claim about a pretrained f_θ alone; acquiring $p^{(b)}$ samples (and any training on them) requires energy access and is excluded from 1-NFE / wall-clock comparisons unless stated. Approximate ENDS (weighted p -bank and/or finite-step Steer/Adapt/Refine) may retain transport bias after nominal e^b reweighting.

Sample complexity and coverage. We first study an asymmetric one-dimensional double well using eight random seeds and a two-component Gaussian mixture model (GMM) with non-negligible mass in both wells. We call an initialization *collapsed* when its proposal places negligible mass in the minority well; in that case, weighting existing samples cannot by itself create the missing support. At the reduced toy-potential parameter $\Delta G_{\text{param}}=8$, direct estimation frequently observes no minority-state samples for $n \leq 512$, whereas exact-tilt ENDS with e^b reweighting attains $|\text{err}| \approx 0.43 k_B T$ at $n=32$ and $\approx 0.06 k_B T$ at $n=2048$ (Fig. 2; detailed values in Appendix B, Table 1). Appendix B also defines the state estimator and zero-count handling. Exact-tilt ENDS improves with n when the proposal has useful overlap with both wells; the tested finite-step procedure does not achieve useful overlap from the collapsed initialization. An estimated mixture with maximum-likelihood weights performs similarly to the analytic mixture (Appendix B). Variant comparisons (ENDS-STEER, ENDS-ADAPT, ENDS-REFINE) against direct sampling and multistep baselines are reported in Sections B and C. ENDS-ADAPT is strongest in amortized 1-NFE settings with adequate overlap, ENDS-STEER is cheapest but overlap-sensitive, and ENDS-REFINE helps low-overlap cases at higher inference cost.

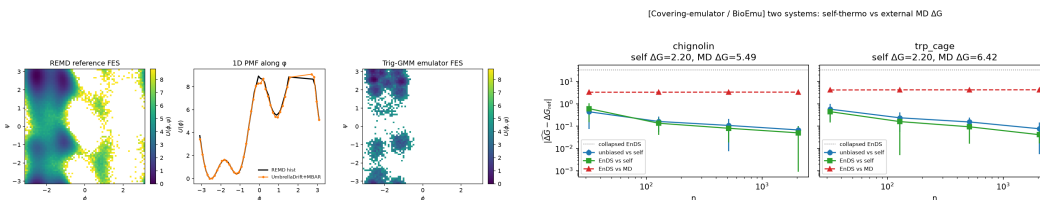
Uncertainty and variance. Error bars in Figures 2 and 10, and Table 1 are one standard deviation across seeds (8 seeds for primary double-well/refine analyses; 5 for the hybrid MCMC annex in Fig. 9 and Table 2). Variance is highest in low-overlap regimes because rare-state hit/miss events are seed dependent and reweighting ESS is low.

Oracle cost and molecular experiments. In the oracle comparison, the trained exact-tilt generator reaches $|\text{err}| \approx 0.20 k_B T$ in one forward pass; FKC-EDS and Langevin require substantially more evaluations for comparable accuracy (Appendix B, Table 1, Fig. 4). These counts are not equivalent costs, and the generator result excludes target generation and training. Buffer-based UMBRELLADRIFT with MBAR reconstructs the reduced one-dimensional alanine PMF $\beta F(\phi) = -\log p(\phi) + C$ (aligned RMSE ≈ 0.17 over evaluated bins) using 300 K REMD targets [21, 22]; the trained structure-level drifting estimator is less accurate. For frozen BioEmu [5], tilted ensembles reduce finite-sample error for the emulator’s own rare-state probability relative to unbiased draws. They do not correct the approximately 3–4 $k_B T$ discrepancy from the long-MD references in these experiments. Figure 3 reports molecular evaluations with Alanine-dipeptide, Chignolin, and Trp-Cage.



(a) $|\widehat{\Delta G} - \Delta G|$ vs. n for direct estimation and exact-tilt ENDS; points show seed-averaged error and bars denote one standard deviation across seeds. (b) Coverage $\times$ method (covering-analytic / covering-MLE / collapsed; solid = ENDS, dashed = unbiased).

Figure 2: **Left:** generated-sample scaling of direct estimation and the exact-tilt ENDS oracle for $\Delta G_{\text{param}}=8$. **Right:** covering cases (analytic and MLE) show the expected ordering, while collapsed coverage fails under both unbiased and ENDS curves. Zero-hit direct estimates use the implementation’s finite display regularization and should be interpreted as failures rather than calibrated errors.



(a) Alanine REMD benchmark: buffer-based UMBREL-LADRIFT + MBAR reconstructs the one-dimensional reduced PMF $\beta F(\phi)$ (aligned RMSE ≈ 0.17 over evaluated bins). (b) Frozen BioEmu benchmark: ENDS tilt improves finite-sample estimation for the emulator distribution, while the separate BioEmu-to-MD discrepancy remains.

Figure 3: Molecular experiments with ENDS: alanine PMF reconstruction and BioEmu rare-state estimation.

6 Discussion and conclusion

ENDS reweights exact biased windows via EDS-style estimators or MBAR; approximate windows retain transport bias without proposal or path corrections. We treat exact-tilt as a theoretical upper bound under ideal target distributions. Our experiments show that reference banks must cover relevant target states and that final proposals require non-negligible support overlap. The failure of our collapsed initialization reflects a limitation of the finite-step protocol rather than a fundamental transport map constraint. In higher dimensions, finite-step degradation occurs when step budgets are exceeded, local kernels underresolve anisotropic modes, or transition-region bank coverage is sparse—causing overlap loss and ESS collapse. When overlap is adequate, including for frozen BioEmu ensembles, ENDS reduces finite-sample error relative to direct emulator sampling. For surrogate samplers (e.g., BioEmu or Boltzmann generators), we distinguish *surrogate-consistent* variance reduction from *physical ground-truth* recovery: improving surrogate sampling is useful, but physical claims require direct MD validation (PMFs, state occupancies, free energies). In our evaluations, exact-tilt, ENDS-ADAPT, and multi-window umbrella sampling prove more reliable than ENDS-STEER. Given suitable targets, ENDS enables efficient post-training 1-NFE generation, though end-to-end costs still include target acquisition and network training.

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A Theory proofs

Lemma 1 (Gaussian convolution identity). *For a Gaussian kernel φ_σ , the mean-shift field of a density ρ satisfies $\sigma^2 \nabla \log \rho_\sigma(x) = \int (y - x) \varphi_\sigma(x - y) \rho(y) dy / \rho_\sigma(x)$. This is the classical Gaussian mean-shift (Tweedie) identity; it appears as the attractive (respectively, repulsive) building block in Turan et al. [11] (App. A.1) and Lai et al. [12].*

Proof of Proposition 1. Differentiate under the integral to obtain Lemma 1: $\partial_{x_i} \rho_\sigma = \int \partial_{x_i} \varphi_\sigma \rho$ with $\partial_{x_i} \varphi_\sigma(x - y) = -(x_i - y_i) \varphi_\sigma / \sigma^2$, hence $\sigma^2 \nabla \log \rho_\sigma$ equals the Gaussian mean-shift field of ρ . Apply this to $\rho = p e^{-b}$ and $\rho = q$ and subtract:

$$V_{p^{(b)}, q}^{(\sigma)}(x) = \sigma^2 \nabla \log \frac{(p e^{-b})_\sigma(x)}{q_\sigma(x)}.$$

If $q = p^{(b)} = Z^{-1} p e^{-b}$, then $(p e^{-b})_\sigma = Z q_\sigma$, so $V \equiv 0$. Conversely, if $V \equiv 0$, then $\log[(p e^{-b})_\sigma / q_\sigma]$ is constant on connected $\mathbb{R}^d$. Normalization therefore gives $(p^{(b)})_\sigma = q_\sigma$. The Fourier transform of the Gaussian is strictly positive, so Gaussian convolution is injective on finite probability measures and $q = p^{(b)}$ [11]. Sharp-normalized and Sinkhorn identifiability concern different operators and assumptions [16, 17]. $\square$

Proof of Proposition 2. Single window. If $x_i \sim q \propto p e^{-b}$ i.i.d., then $W_i \propto e^{b(x_i)}$ are importance weights for p , and the usual LLN / SLLN for IS recovers $\mathbb{E}_p[o]$ whenever $\mathbb{E}_q[W|o] < \infty$ and $\mathbb{E}_q[W] < \infty$. **Multi-window.** With exact samples from $\{q_k \propto p e^{-b_k}\}$, $N_k/N \rightarrow \lambda_k > 0$, evaluable reduced-potential differences, and an irreducible population overlap matrix, MBAR recovers free-energy offsets (up to a common additive constant) and target expectations under the regularity conditions of Shirts and Chodera [8]. ENDS changes how proposals are generated, not the algebra, but approximate windows violate the premise unless supplied with an additional valid correction [1]. $\square$

The Kish effective sample size (ESS) of weights $\{w_i\}$ is

$$\text{ESS}(w) = \frac{(\sum_i w_i)^2}{\sum_i w_i^2}.$$

For positive finite weights, the finite-sample ESS is always between 1 and N and is not a consistency condition. The first-moment assumptions above suffice for the SLLN; if $\mathbb{E}_q[W^2] < \infty$, then $\text{ESS}/N \rightarrow \mathbb{E}_q[W]^2 / \mathbb{E}_q[W^2]$ and standard finite-asymptotic-variance results may apply.

B Algorithm and additional figures

Algorithm 1 Single-tilt ΔG -DRIFT (exact-tilt oracle / approximate ENDS-STEER; not amortized f_θ alone)

- 1: **Input:** pretrained f_θ , bias b , buffer $\mathcal{Y}$, affinity scales $\mathcal{R}$, steps S , step size η
 - 2: Sample $x \leftarrow f_\theta(\epsilon)$; set $w(y) \propto e^{-b(y)}$ (or $\mathcal{Y} \sim p^{(b)}$)
 - 3: **for** $s = 1, \dots, S$ **do**
 - 4: $x \leftarrow x + \eta \hat{V}_{\mathcal{R}, w}(x; \mathcal{Y})$
 - 5: **end for**
 - 6: If x_i are exact $p^{(b)}$ samples, set $W_i \propto e^{b(x_i)}$ and return $\widehat{\Delta G}$; otherwise report that the estimate remains subject to transport bias
-

For disjoint state sets A and B , we use

$$\hat{P}_s = \frac{\sum_i W_i \mathbf{1}\{x_i \in s\}}{\sum_i W_i}, \quad \widehat{\Delta G}_{B-A} = -k_B T \log \frac{\hat{P}_B}{\hat{P}_A}.$$

The toy-system basin boundary is $x = 0$, with $A = \{x < 0\}$ and $B = \{x \geq 0\}$. Runs with $\hat{P}_A = 0$ or $\hat{P}_B = 0$ are zero-hit failures for which the unregularized estimator is infinite. Plots use finite clipped values for these failures; they are not finite thermodynamic estimates, and the code release must state the clipping threshold. Reported ESS percentages mean $100 \text{ ESS}/N$ after final reweighting.

B.1 Detailed sample-scaling and oracle comparison

Table 1 supplies the numerical values summarized in the main text. Its left half shows that direct sampling remains dominated by zero-hit failures as n grows, whereas the exact-tilt oracle error decreases from approximately 0.43 to $0.06 k_B T$ with an ESS fraction near one third. The right half and Fig. 4 compare amortized generation with FKC-EDS and Langevin. They show a forward-pass advantage after training, but not an end-to-end advantage: the ENDS row excludes exact-target acquisition and training, and the three evaluation types have different costs.

Table 1: Left: clipped $|\widehat{\Delta G} - \Delta G|$ over eight seeds with an overlapping GMM; zero-hit runs are failures. Right: trained exact-tilt generator compared with FKC-EDS and Langevin ($n=256$), excluding target acquisition and training.

$\Delta G_{\text{param}}/(k_B T)$	n	Direct error	ENDS error	ESS/ n
8	32	27.3	0.43	34%
8	512	24.1	0.11	34%
8	2048	10.4	0.06	32%
Method		evaluations	$ \text{err} /(k_B T)$	
ENDS exact tilt		1	0.20	
FKC-EDS		200	0.14	
Langevin		4000	0.13	

C Refine

When a one-pass generator places very little mass in the rare well, a short ENDS-STEER run may not move samples far enough. Our annealed refinement applies several Euler updates toward fixed $p^{(b)}$ targets, following the intuition of Drift Flow Matching without reproducing its training procedure [18]. On the overlapping GMM with $\Delta G_{\text{param}}=8$, it reduces the empirical error by an order of magnitude relative to direct generation, although it remains less accurate than exact tilt and does not produce a guaranteed exact biased window (Fig. 8).

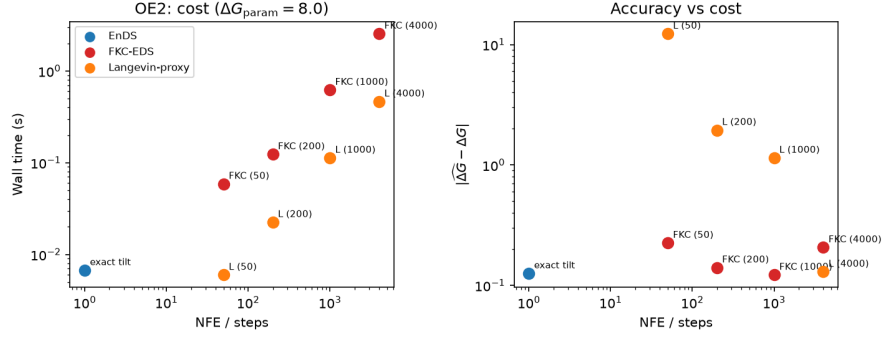


Figure 4: Method-specific evaluation count and wall-time comparison ($n=256$). The amortized one-step ENDS generator uses exact-tilt targets; FK-EDS uses exact biased VP scores; and Langevin evolves under $U + B$. Generator, score-network, and force evaluations are not equivalent costs. The oracle ENDS timing excludes exact-target acquisition and training. In this setup FK-EDS reaches the reported accuracy at roughly 200 score evaluations, whereas Langevin requires roughly 4000 force steps.

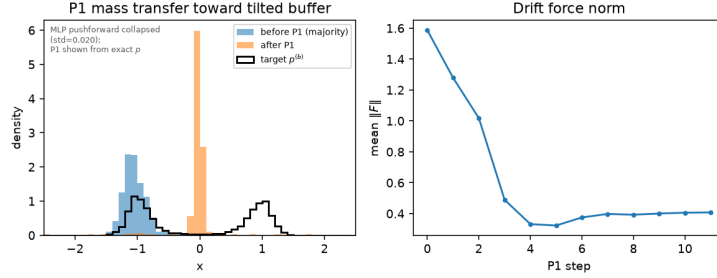


Figure 5: ENDS-STEER mass transfer toward a tilted buffer ($\Delta G_{\text{param}}=8$).

D Reproducibility

The reported figures use the experimental configurations specified by the affinity scales $\mathcal{R}$, tilt schedules, MBAR windows, and BioEmu filtering criteria. A reproducible release must additionally specify state boundaries, free-energy sign and units, zero-hit handling, PMF alignment and masking, metadynamics $c(t)$, train/reference splits, random seeds, hardware, and the reduction axes and numerical floors in the empirical drift. Toy double-well and overlapping-GMM experiments complete within minutes on a single GPU; the alanine buffer-based UMBRELLADRIFT and frozen BioEmu evaluations reuse published REMD data and BioEmu checkpoints. Alanine REMD data: Zenodo record 6993124 [22]. An anonymous code archive will accompany the submission.

E Unsmoothed score split vs. kernel drifting

A natural question is whether the classical identity

$$\nabla_x \log(p(x) e^{-b(x)}) = \nabla_x \log p(x) - \nabla_x b(x) \quad (3)$$

lets one implement biased drifting by taking an *unbiased* empirical kernel field and subtracting ∇b . We record when (3) applies and why it does *not* separate inside the Gaussian (or sharp) drifting operator.

Step 1 (unsmoothed Boltzmann). If $p \propto e^{-U}$, then (3) is immediate:

$$\nabla \log(pe^{-b}) = -\nabla U - \nabla b.$$

Continuous overdamped Langevin under the dimensional tilted potential $U + B$ has $p^{(b)} \propto pe^{-b}$ as its invariant law. A finite-step unadjusted discretization has step-size bias; HMC is exact only with a

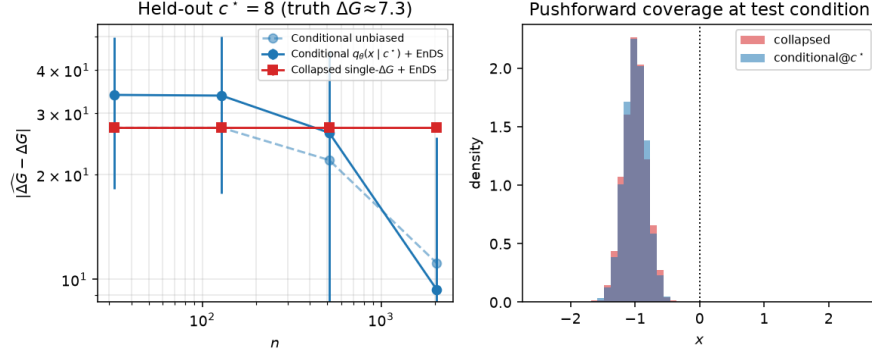


Figure 6: Conditional multi- ΔG GMM retains mass in both wells from $c \in \{2, 4, 6\}$ to the held-out value $c^*=8$.

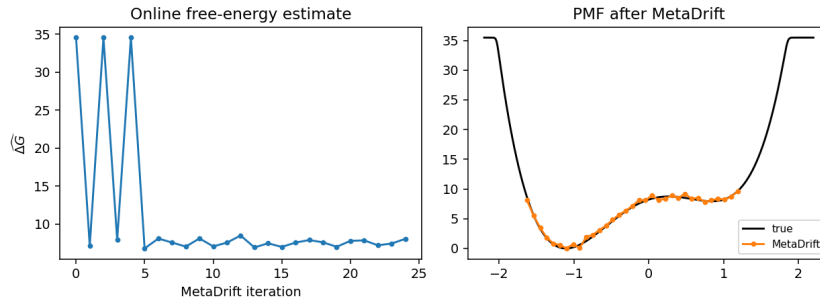


Figure 7: METADrift on the double well ($\Delta G_{\text{param}}=8$) using well-tempered hills and nominal online reweighting. Exact pooled reweighting would require weights proportional to $\exp[b_t(x_t) - c(t)]$ and appropriate quasi-stationarity assumptions [19, 20]; the displayed curve is therefore an exploratory diagnostic. **Left:** online ΔG by outer iteration; the horizontal line denotes the true value. **Right:** final reweighted PMF and the analytic reference.

Metropolis correction and after equilibration. This is the invariant-distribution setting approximated by our evaluation-count/wall-clock proxy (biased Langevin) and by classical umbrella / metadynamics MD.

Step 2 (EDS-style reverse SDEs). Diffusion / FKC steering likewise acts on an instantaneous score $\nabla \log p_t$ along a noising path. Adding a control built from ∇b_t is the path-space analogue of (3) [1]. That construction assumes access to (approximate) scores of the *unsmoothed* tilted dynamics at each noise level—not a single frozen kernel field on equilibrium samples.

Step 3 (Gaussian / sharp drifting does not split). Drifting theory identifies the population field with a difference of *smoothed* scores (Lemma 1, Proposition 1):

$$V_{p^{(b)}, q}^{(\sigma)}(x) = \sigma^2 \nabla \log(p e^{-b})_\sigma(x) - \sigma^2 \nabla \log q_\sigma(x).$$

Convolution and log do not commute with the pointwise factor e^{-b} , so in general

$$\nabla \log(p e^{-b})_\sigma(x) \neq \nabla \log p_\sigma(x) - \nabla b(x). \quad (4)$$

Consequently one *cannot* form the biased Gaussian mean-shift field by computing the unbiased field $V_{p, q}^{(\sigma)}$ and subtracting ∇b . The same obstruction applies to empirical affinities: the desired population change is to the reference measure, implemented exactly by reference samples drawn from $p^{(b)}$ and only heuristically here by post-softmax $w_j \propto e^{-b(y_j)}$; subtracting ∇b from an unbiased kernel drift is not valid.

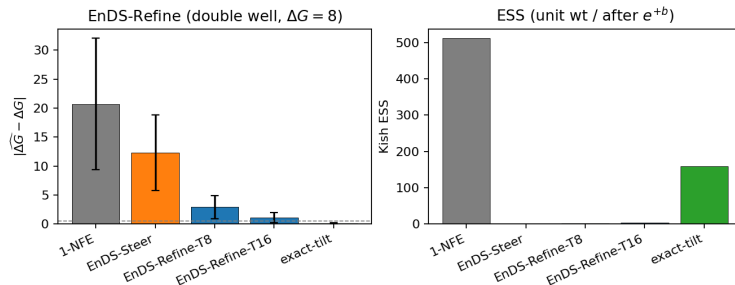


Figure 8: ENDS-REFINE with several drift updates compared with one-pass generation and exact tilt on the overlapping GMM.

Step 4 (when energies *are* available). If U (hence $\nabla \log p$) and b are evaluable, prefer one of:

1. **Exact tilt:** sample from $p^{(b)}$ (grid / MCMC / analytic) and use unit reference weights—as in our Tier 1 ΔG sweeps;
2. **Force-based dynamics:** run appropriately equilibrated Langevin / Metropolized HMC under $U + B$, then reweight with $W \propto e^{+b}$ or MBAR—as approximated in the evaluation-count proxy;
3. **Optional hybrid:** use (3) only inside energy-based correctors, while the drifting generator itself remains measure-tilted via (5); see Appendix G for Langevin / HMC alone vs. ENDS→MCMC refine.

In the emulator / REMD-buffer setting (energies unavailable at bias time), empirical measure tilting (5) remains available, but e^b /MBAR is exact only if the resulting windows equal the claimed biased ensembles or carry another valid proposal correction.

With the weights defined from the bank $\{y_j\}$

$$w_j \propto \exp(-b(y_j)) \quad (5)$$

Step 5 (limits where (4) softens). As $\sigma \rightarrow 0$, $\nabla \log \rho_\sigma \rightarrow \nabla \log \rho$ under standard regularity, so (3) is recovered asymptotically. For special pairs (e.g. linear b and Gaussian p) the smoothed score may again admit an exact closed form involving ∇b , but this is not true for general molecular biases (umbrellas, metadynamics hills) or nonparametric empirical affinities. We therefore treat (3) as the energy-based companion identity, and Proposition 1 as the kernel-drifting identity.

F Definition of the weighted empirical drift

We spell out the operator used in Algorithm 1 and (2), following the affinity construction of Deng et al. [10].

Targets and scaling. Write particles as features in $\mathbb{R}^S$. In our notation, the reference bank is $\mathcal{Y} = \{y_j\}$ and $\mathcal{R}$ is the list of affinity scales in (2). Given current generator particles $X = \{x_i\}_{i=1}^{C_g}$, optional auxiliary model samples N (often empty), and reference samples $\mathcal{Y}$, concatenate $T = [X \mid N \mid \mathcal{Y}]$ with column weights $w = [w_X \mid w_N \mid w_Y]$ (ENDS: w_Y as in (5), others typically 1). Let $D_{ij} = \|x_i - t_j\|_2$ and $\bar{D} = (\sum_{ij} D_{ij} w_j) / (C_g \sum_j w_j)$, with the corresponding global average over batch axes in the released implementation. Scale features by $s = \max(\bar{D} / \sqrt{S}, 10^{-3})$ and distances by $\bar{D}$, and mask self-distances among the C_g generators (add a large constant on the diagonal block) so generators do not attract themselves.

Per-scale drift. For each $R \in \mathcal{R}$, set logits $\ell_{ij} = -D_{ij}^{\text{norm}} / R$ and

$$A_{ij} = \sqrt{\max\{\text{softmax}_j(\ell)_{ij} \text{softmax}_i(\ell)_{ij}, 10^{-6}\}} w_j.$$

Split $A = [A^{\text{model}} | A^{\text{ref}}]$ at the model-sample versus reference-sample cut. Partial two-sided coefficients

$$C^{\text{model}} = -A^{\text{model}} \odot (\sum A^{\text{ref}}), \quad C^{\text{ref}} = A^{\text{ref}} \odot (\sum A^{\text{model}})$$

yield a raw field $\tilde{V}_R(x; \mathcal{Y}, w) = \sum_j C_{ij} t_j^{(\text{scaled})} - (\sum_j C_{ij}) x_i^{(\text{scaled})}$. Normalize $\hat{V}_R(x; \mathcal{Y}, w) = \tilde{V}_R / \sqrt{\max\{\text{mean}(\tilde{V}_R^2), 10^{-8}\}}$ and sum over R as in (2); the mean is over the released implementation's batch, generator, and feature axes. The weighted empirical drift in the original coordinates is $\hat{V}_{\mathcal{R}, w}(x; \mathcal{Y}) = s \cdot \sum_{R \in \mathcal{R}} \hat{V}_R(x; \mathcal{Y}, w)$ (equivalently $\text{goal} - x$ after unscaling the stop-gradient target). For numerical fidelity, squared distances are floored at 10^{-8} before taking square roots, and normalized self-distances receive the released finite mask constant 100. These safeguards, affinity floors, and RMS floors are part of the implemented operator.

Training loss. ENDS-ADAPT and the original drifting-model training procedure regress the scaled generator output onto the stop-gradient target $\text{goal} = x^{(\text{scaled})} + \sum_{R \in \mathcal{R}} \hat{V}_R(x; \mathcal{Y}, w)$ using an MSE loss (the JKO-style frozen field of 10). Multiplying w_j after the softmaxes is a heuristic empirical tilt; no result here proves that its finite-batch equilibrium is exactly $p^{(b)}$.

G ENDS proposals + Langevin / HMC refinement

When the energy U is available, biased sampling under $U+B$ is standard (Langevin, HMC), subject to discretization, equilibration, and acceptance diagnostics. ENDS remains useful as a *proposal*: exact-tilt samples, or approximate drifted samples with useful overlap, can place mass in the rare well, so a short energy-based refinement may match longer MCMC initialized in the majority well at lower force cost in this toy setup. Figure 9 and Table 2 report a controlled double-well comparison ($\Delta G_{\text{param}}=8$, $n=256$, $a=a^*$, unbiased $W \propto e^{+b}$, 5 seeds).

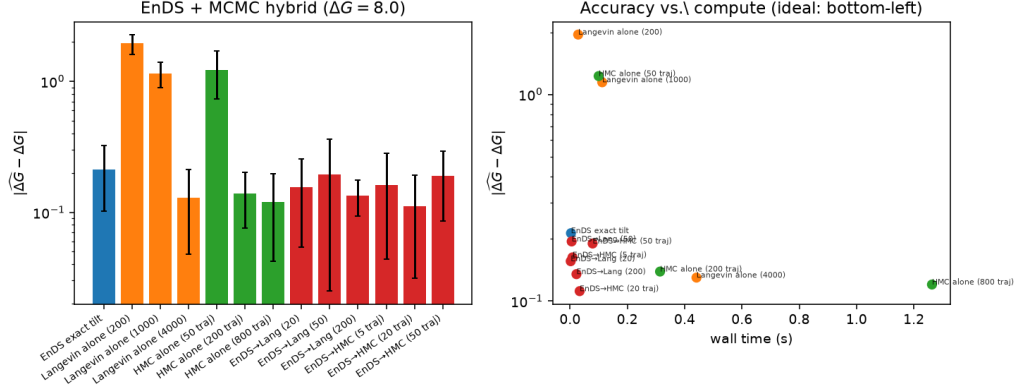


Figure 9: ENDS with MCMC refinement compared with Langevin and HMC alone on the double well ($\Delta G_{\text{param}}=8$). We evaluate exact-tilt ENDS and ENDS followed by short Langevin or HMC refinement against dynamics initialized at $x = -1$ under $U + B$. **Left:** $|\hat{\Delta G} - \Delta G|$ on a logarithmic scale. **Right:** error versus wall time. Long MCMC runs in this setup eventually match the exact-tilt oracle's accuracy, whereas short runs initialized in the majority well do not.

Takeaway. With U available, converged Langevin / Metropolized HMC under $U+B$ is a valid baseline; ENDS (or ENDS→short MCMC) is complementary when useful proposals are cheap relative to mixing from the majority well. Without U at bias time, empirical measure-tilted drifting remains applicable as a transport heuristic; exact e^b reweighting or MBAR still requires exact biased windows or another valid correction.

Table 2: Selected rows from the hybrid MCMC annex ($\Delta G_{\text{param}}=8$, $n=256$, mean $\pm$ std over 5 seeds). The evaluation count for HMC counts leapfrog force evaluations (≈ 10 per trajectory).

Method	evaluations	time (s)	$ \widehat{\Delta G} - \Delta G /(k_B T)$	frac. $x \geq 0$
ENDS exact tilt	1	0.003	0.21 ± 0.11	0.49
Langevin alone (200)	200	0.028	1.95 ± 0.33	0.05
Langevin alone (4000)	4000	0.44	0.13 ± 0.08	0.45
HMC alone (50 traj)	500	0.10	1.23 ± 0.49	0.19
HMC alone (200 traj)	2000	0.31	0.14 ± 0.06	0.43
ENDS $\rightarrow$ Lang (20)	21	0.002	0.16 ± 0.10	0.50
ENDS $\rightarrow$ HMC (20 traj)	201	0.034	0.11 ± 0.08	0.50

H EnDS-Refine: multi-step drift correction

ENDS-REFINE is an optional DFM-inspired corrector [18]. Starting from one-pass samples $x \sim q_\theta$, it follows the empirical drift toward fixed $p^{(b)}$ targets for T Euler steps while geometrically annealing the bandwidth from σ_0 to σ_1 . There is no learned two-time flow-matching network; refinement consists only of Euler updates of the empirical drift. Figure 10 reports results on the overlapping GMM for the double well ($\Delta G_{\text{param}}=8$, $n=512$, eight seeds). One-pass sampling produces almost no rare-well samples, and short ENDS-STEER ($T=3$) does not move them far enough. After nominal e^b reweighting, ENDS-REFINE with $T \in \{8, 16\}$ reduces the empirical error to approximately $1\text{--}2 k_B T$, compared with approximately $20 k_B T$ for direct generation and $11 k_B T$ for ENDS-STEER; exact tilt remains the calibrated oracle at approximately $0.12 k_B T$. Kish ESS after nominal e^b weighting stays low for drifted clouds that overshoot the balancing mixture. Because the refined law is approximate, this ESS does not diagnose or remove transport bias; ENDS-REFINE is a mass-transport heuristic, not a replacement for exact tilt or a valid proposal correction.

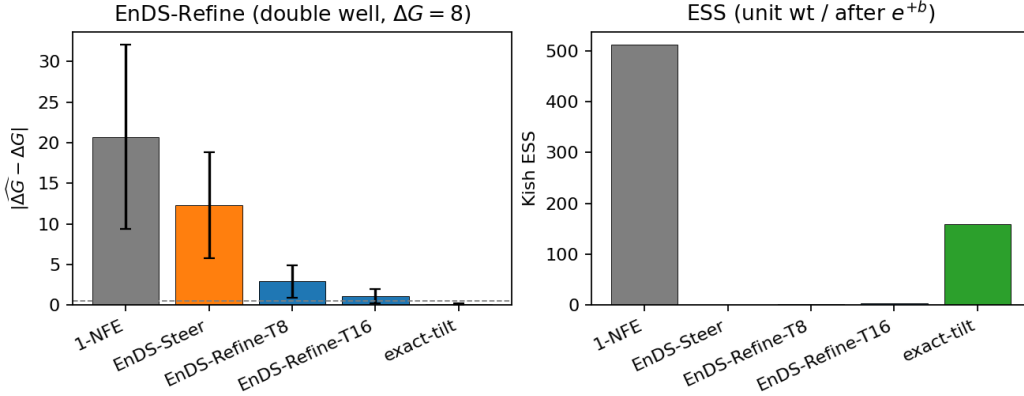


Figure 10: ENDS-REFINE using DFM-inspired Euler updates of the empirical drift (overlapping GMM, $\Delta G_{\text{param}}=8$, $n=512$). **Left:** mean $|\widehat{\Delta G} - \Delta G|$ with standard deviation over eight seeds. **Right:** Kish ESS. We compare one-pass generation, short ENDS-STEER ($T=3$), annealed ENDS-REFINE ($T \in \{8, 16\}$), and exact tilt. ENDS-REFINE improves mass transport but retains low ESS and uncontrolled transport bias after overshooting, whereas exact tilt remains the calibrated oracle.

I Detailed Formalization of ENDS Operator Variants

To accommodate different computational budgets, target generation constraints, and sample-coverage regimes, ENDS provides three operational variants for transferring tilted reference fields to the target ensemble: **ENDS-STEER**, **ENDS-ADAPT**, and **ENDS-REFINE**. Table 3 summarizes their core mechanics, mathematical assumptions, and recommended use cases. Below, we provide formal algorithmic specifications for each variant.

Table 3: Comparison of ENDS operator variants.

Variant	Mechanics & Updates	Core Assumptions	Primary Use Case
ENDS-STEER	Inference-time Euler drift steps applied directly to pushforward samples $x_0 \sim (f_\theta)_{\#} p_{\text{prior}}$.	Local initial coverage of target features; small transport distances.	Fast inference without network retraining.
ENDS-ADAPT	Short parameter fine-tuning of f_θ using MSE loss against stop-gradient drift targets.	Representative weighted reference bank $\mathcal{Y}$; gradient access to f_θ .	Fully amortized 1-NFE generation across repeated bias sweeps.
ENDS-REFINE	Multi-step annealed drift Euler updates toward fixed $p^{(b)}$ targets.	Access to target $p^{(b)}$ buffer or high-density target samples.	Bridging low proposal overlap and severe mass-transport gaps.

I.1 ENDS-STEER: Inference-Time Particle Steering

ENDS-STEER leaves the pretrained generator parameters θ unchanged [10]. It draws initial samples $x_0 = f_\theta(\epsilon)$ and iteratively updates them in data space along the weighted empirical drift field $\hat{V}_{\mathcal{R},w}(x; \mathcal{Y})$ [10].

Algorithm 2 ENDS-STEER (Inference-Time Particle Steering)

- 1: **Input:** Pretrained generator f_θ , bias function $b(y)$, reference bank $\mathcal{Y} = \{y_j\}_{j=1}^{N_r}$, affinity scales $\mathcal{R}$, step count S , step size η .
 - 2: Draw initial batch $x_0 \leftarrow f_\theta(\epsilon)$ where $\epsilon \sim \mathcal{N}(0, I)$.
 - 3: Compute positive reference weights $w(y_j) \propto e^{-b(y_j)}$ (normalization arbitrary up to scale).
 - 4: **for** $s = 1, \dots, S$ **do**
 - 5: Compute Deng force $\hat{F}_{\mathcal{R},w}(x_{s-1}; \mathcal{Y})$ (attractive field toward weighted $\mathcal{Y}$ with implicit self-repulsion and per- R force normalization).
 - 6: Update particles: $x_s \leftarrow x_{s-1} + \eta \hat{F}_{\mathcal{R},w}(x_{s-1}; \mathcal{Y})$.
 - 7: **end for**
 - 8: **Output:** Steered samples x_S . Compute thermodynamic observables via $W_i \propto e^{b(x_S, i)}$ or MBAR.
-

I.2 ENDS-ADAPT: Amortized Generator Adaptation

ENDS-ADAPT fine-tunes the network parameters $\theta \rightarrow \theta^*$ over a few gradient steps using a stop-gradient regression objective [10, 11]. Once adapted, f_{θ^*} generates samples directly in $p^{(b)}$ in a single forward pass (1-NFE) [1].

Algorithm 3 ENDS-ADAPT (Amortized Generator Fine-Tuning)

- 1: **Input:** Pretrained generator f_θ , bias $b(y)$, reference bank $\mathcal{Y}$, affinity scales $\mathcal{R}$, adaptation steps K , learning rate γ .
 - 2: Compute positive reference weights $w(y_j) \propto e^{-b(y_j)}$.
 - 3: **for** $k = 1, \dots, K$ **do**
 - 4: Sample latent noise $\epsilon \sim \mathcal{N}(0, I)$ and generate batch $x = f_\theta(\epsilon)$.
 - 5: Construct stop-gradient target g from Deng force aggregation over $R \in \mathcal{R}$, where generated samples act as implicit negatives.
 - 6: Compute adaptation loss: $\mathcal{L}(\theta) = \frac{1}{|x|} \|x^{\text{scaled}} - g\|_2^2$.
 - 7: Update generator parameters: $\theta \leftarrow \theta - \gamma \nabla_\theta \mathcal{L}(\theta)$.
 - 8: **end for**
 - 9: **Output:** Adapted generator f_{θ^*} capable of 1-NFE sampling $x \sim q_{\theta^*}$.
-

I.3 ENDS-REFINE: Multi-Step Annealed Drift Correction

When the generator proposal q_θ has poor support overlap with $p^{(b)}$, single-pass sampling or short steering updates may fail to bridge the mode gap [9]. ENDS-REFINE performs an annealed sequence of Euler updates toward target $p^{(b)}$ reference samples while geometrically decaying the bandwidth σ [12].

Algorithm 4 ENDS-REFINE (Multi-Step Annealed Drift Refinement)

- 1: **Input:** Initial samples $x_0 \sim (f_\theta)_{\#} p_{\text{prior}}$, target buffer $\mathcal{Y} \sim p^{(b)}$, refinement steps T , initial bandwidth σ_0 , final bandwidth σ_1 , step size η .
 - 2: **for** $t = 1, \dots, T$ **do**
 - 3: Interpolate bandwidth geometrically: $\sigma_t = \sigma_0 \left(\frac{\sigma_1}{\sigma_0} \right)^{\frac{t-1}{T-1}}$.
 - 4: Set one-step scale list $\mathcal{R}_t \leftarrow (\sigma_t)$ (or use fixed multi-scale $\mathcal{R}$ without annealing).
 - 5: Compute Deng force $\hat{F}_{\mathcal{R}_t, w}(x_{t-1}; \mathcal{Y})$ toward fixed $\mathcal{Y}$ [10, 12].
 - 6: Update sample positions: $x_t \leftarrow x_{t-1} + \eta \hat{F}_{\mathcal{R}_t, w}(x_{t-1}; \mathcal{Y})$ [10, 11].
 - 7: **end for**
 - 8: **Output:** Refined samples x_T (subject to residual transport bias if target overlap is incomplete).
-