Self-tuning Hamiltonian Monte Carlo

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NEC Labs Europe, Heidelberg

November 2023

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Molecular Dynamics

- Discretization of Newton's equation $\Rightarrow$ effective shadow Hamiltonian and numeric errors
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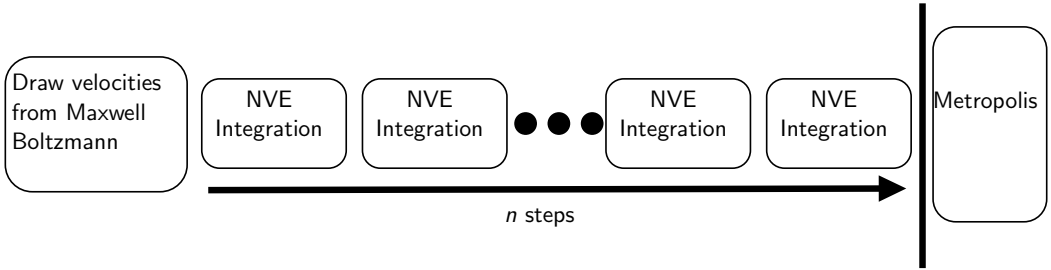
- What if we combine elements of both? Profit?
- Provides structured way to set-up moves based on microcanonical MD simulations
- Guaranteed to sample from the target distribution by Monte Carlo accept/reject

How does it work?



A priori, arbitrary integrator can be used. We restrict ourselves to velocity verlet.

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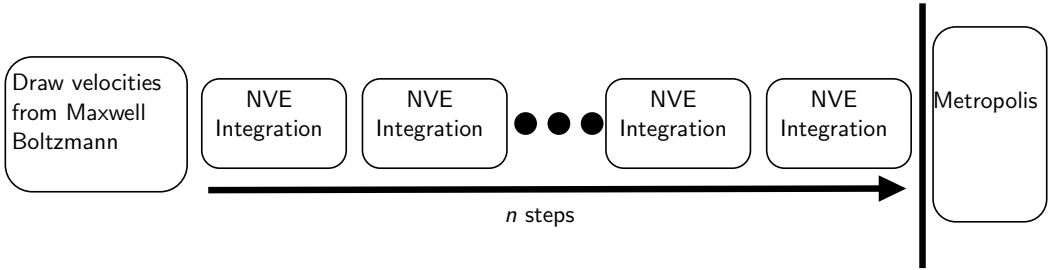

A priori, arbitrary integrator can be used. We restrict ourselves to velocity verlet. At least two free parameters: number of integrations steps n and timestep Δt of integrator $\rightarrow$ performance of HMC crucially depends on these parameters

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NVE Integrator (velocity verlet):

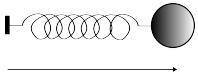
$$\boldsymbol{v}_i\left(t + \frac{1}{2}\Delta t_i\right) = \boldsymbol{v}_i(t) + \frac{1}{2}\boldsymbol{a}_i(t)\Delta t_i \quad (1a)$$

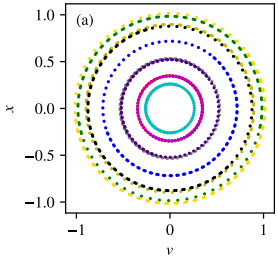
$$\boldsymbol{x}_i(t + \Delta t_i) = \boldsymbol{x}_i(t) + \boldsymbol{v}_i\left(t + \frac{1}{2}\Delta t_i\right)\Delta t_i \quad (1b)$$

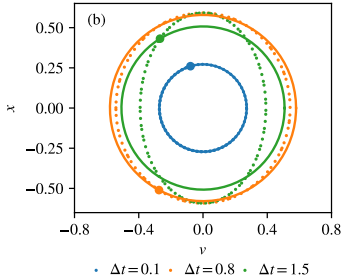
Recalculate $\boldsymbol{a}_i(t + \Delta t_i)$ from the new positions with $\boldsymbol{a}_i = -1/m\partial/\partial \boldsymbol{x}_i U(\boldsymbol{x})$ (1c)

$$\boldsymbol{v}_i(t + \Delta t_i) = \boldsymbol{v}_i\left(t + \frac{1}{2}\Delta t_i\right) + \frac{1}{2}\boldsymbol{a}_i(t + \Delta t_i)\Delta t_i \quad (1d)$$

One Dimensional Harmonic Oscillator







- Hamiltonian (in $d = 1$ with $m = k = 1$)

$$\mathcal{H} = U(x) + T(v) = 0.5(x^2 + v^2),$$

simulated at constant temperature $T = 0.5$

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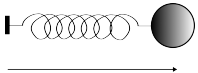

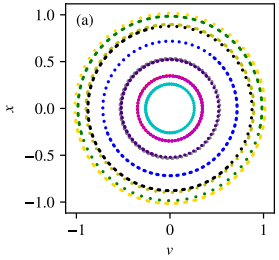

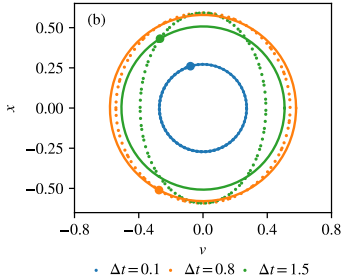

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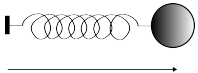

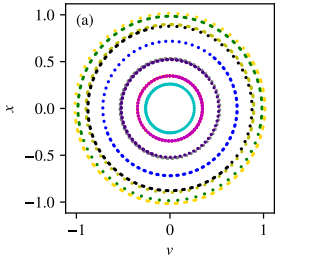

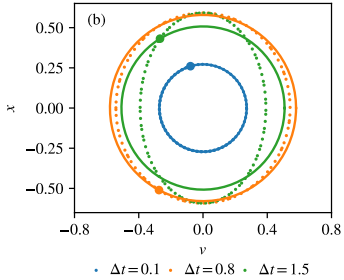

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- Every new proposal is obtained by setting a different total energy level via the picking of velocities from Maxwell-Boltzmann, as shown in (a).
- Using different Δt has major effect on simulated system ("shadow" Hamiltonian), see (b) $\rightarrow$ reflected in acceptance rate of MH.

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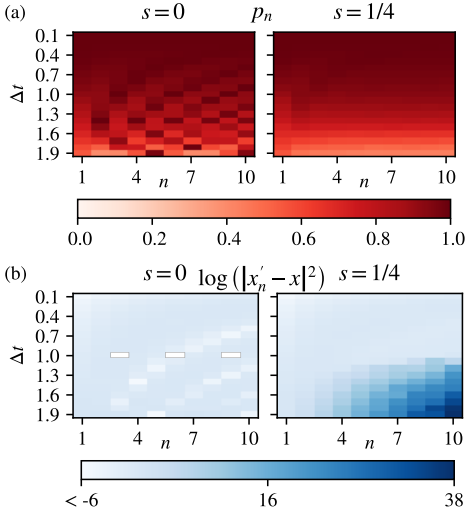
- This loss multiplies the acceptance rate p_n times the movement in spatial space $|\boldsymbol{x}'_n - \boldsymbol{x}_0|$ to some power b
  - b controls how important large jumps are compared to small ones

Jitter vs no-jitter



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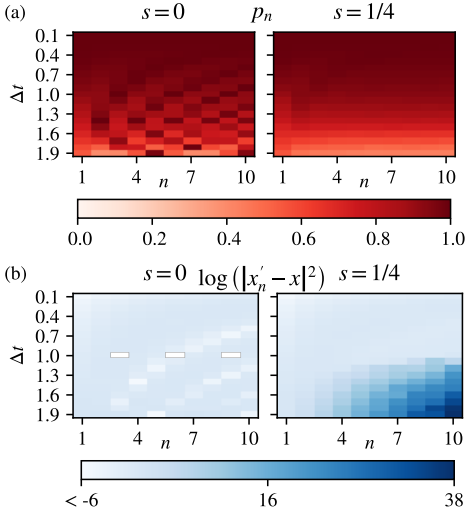

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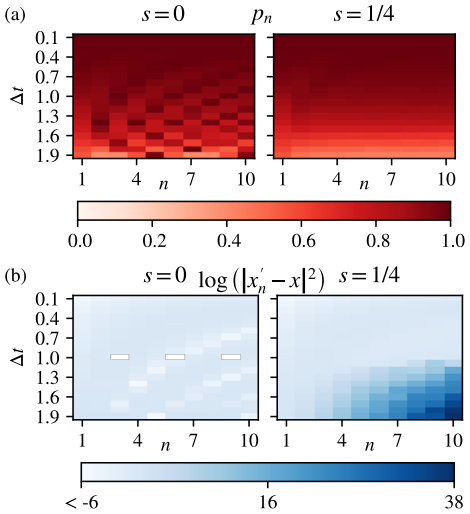
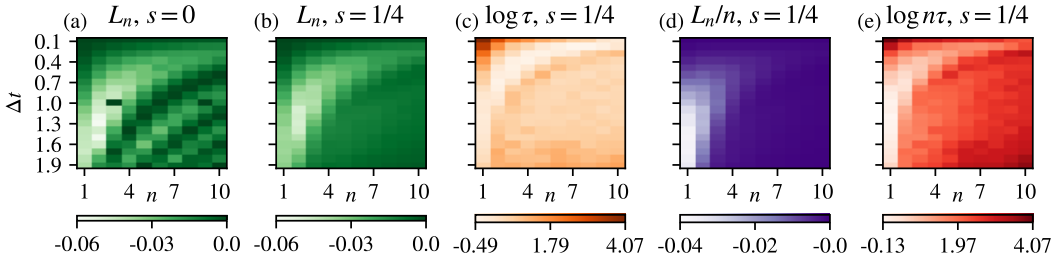


- Several minima/maxima in the acceptance rate and jump distance.
- Unsuited as "loss" since we would just run into the next local minima.
- Solution: Introduce "jittering" of Δt, i.e., pick for every iteration the timestep from a normal distribution

$$\Delta t' \sim \mathcal{N}(\Delta t, s\Delta t),$$

with relative variance s.

Loss definition



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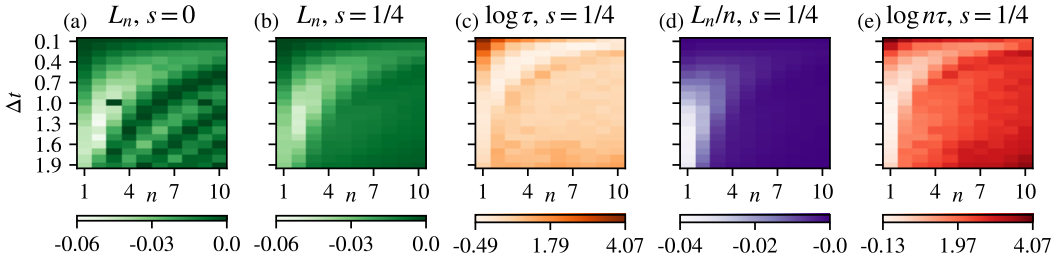

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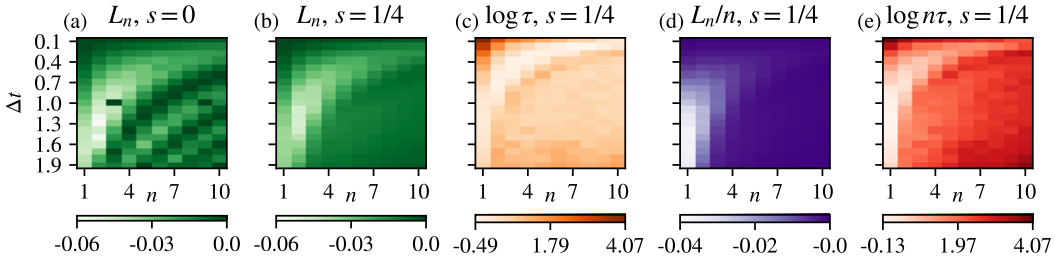

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- "Real objective": Autocorrelation time in units of computational effort $n\tau$, so consider "loss" per computational effort L_n/n

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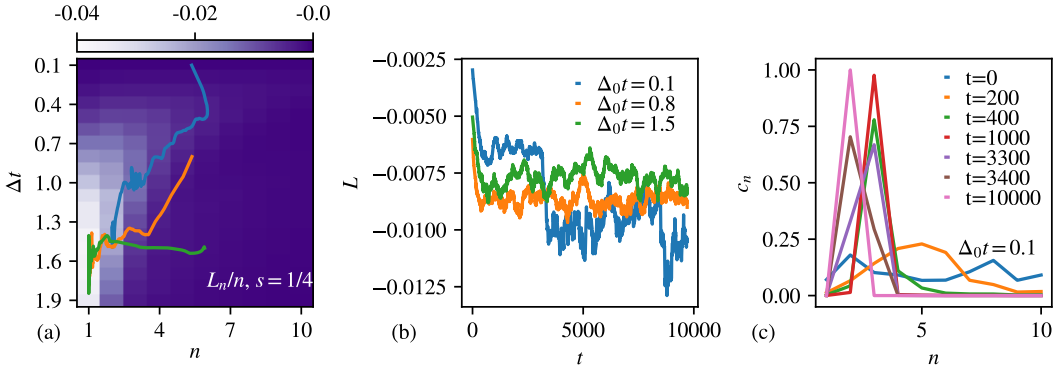
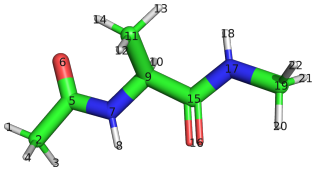
- The c_n are in practice obtained as softmax of unrestricted parameters C_n, i.e.,

$$c_n = \sigma(W_n) = \frac{e^{C_n}}{\sum_{n=1}^{N} e^{C_n}}$$

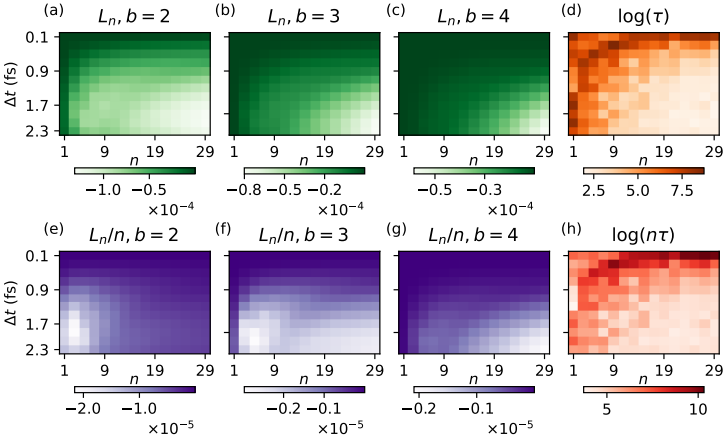
Learning Trajectories for the Harmonic Oscillator



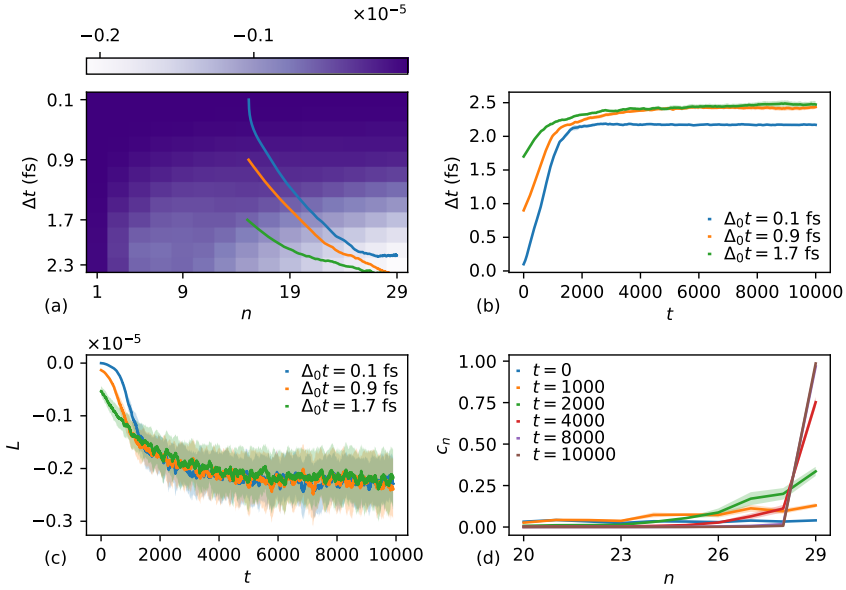
Alanine dipeptide loss surface and autocorrelation



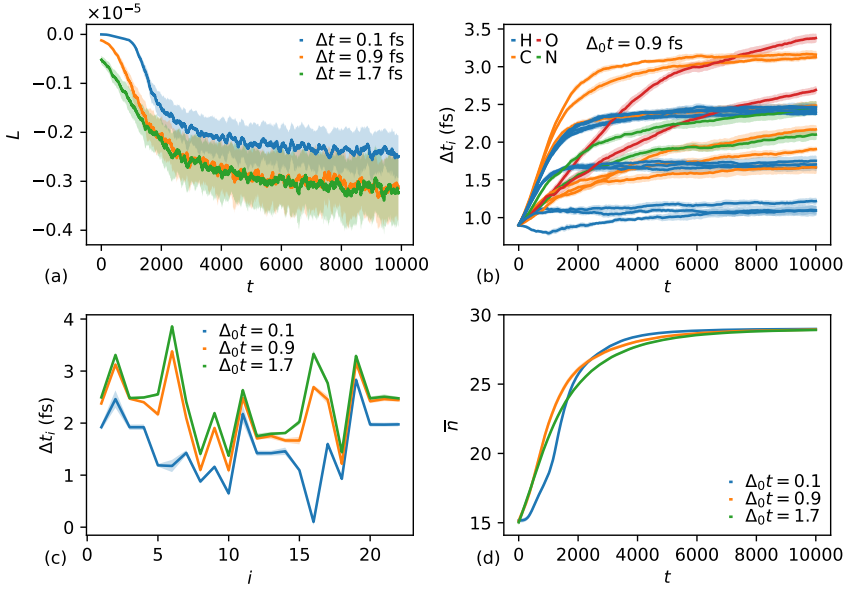
- Small peptide with 22 atoms.
- Common test system for novel methods.
- Simulated at $T = 300$ K.



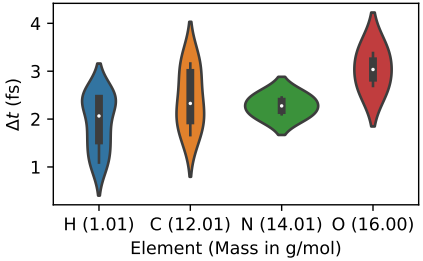
Learning for alanine dipeptide



Atom dependent timestep



Timesteps and Performance



$\Delta_0 t$	0.1 fs	0.9 fs	1.7 fs
τ for atom based Δt	12.7(2.6)	7.5(9)	7.5(1)
τ for global Δt	12.1(1.8)	10.0(1.0)	9.9(1.3)

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- Extended to atom-based timesteps – heuristic optimizers would have a hard time
- Atom-based timesteps provide speed-up of simulation – without additional runtime penalty at time of "production"

H. Christiansen, F. Errica, F. Alesiani, J. Chem. Phys. **159**, 234109 (2023)


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