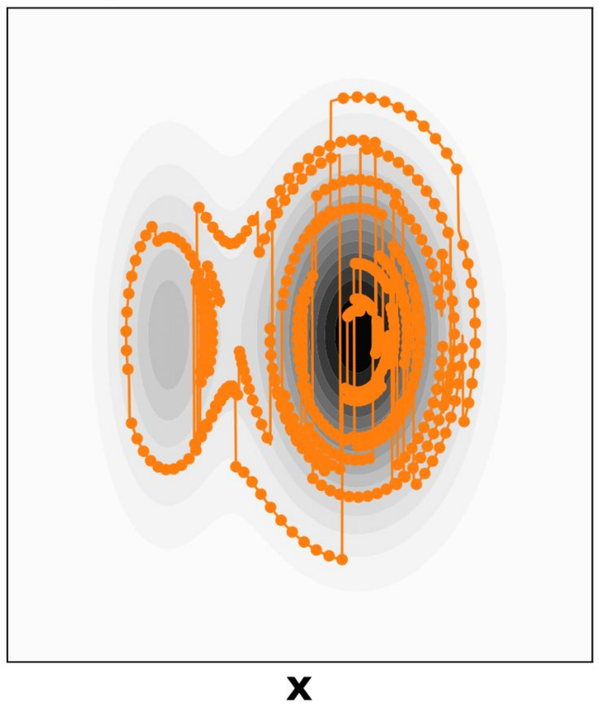
Problem: sample from a given differentiable distribution p(**x**)
Solution: add momentum and use the Hamiltonian dynamics to efficiently sample the high-dimensional constant-energy-surface,

Momentum resampling ensures canonical target

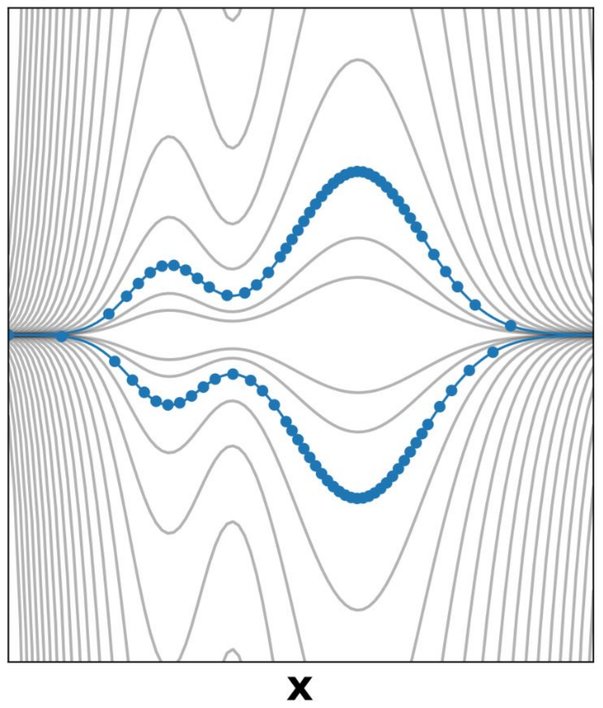
Canonical HMC

$p(\mathbf{x}, \mathbf{\Pi}) \propto e^{-H(\mathbf{x}, \mathbf{\Pi})}$



Microcanonical HMC

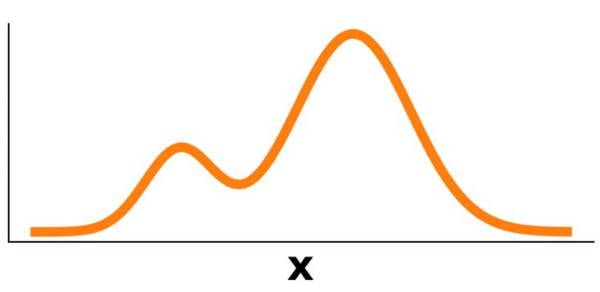
$p(\mathbf{x}, \mathbf{\Pi}) \propto \delta(H(\mathbf{x}, \mathbf{\Pi}) - E)$

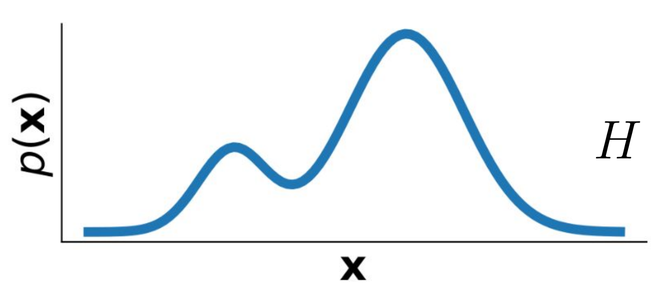


Momentum resampling preserves the Hamiltonian and is only used to boost ergodicity.

ensure the correct marginal **x**-distribution by tuning the Hamiltonian.

$$H = \frac{1}{2}|\mathbf{\Pi}|^2 - \log p(\boldsymbol{x})$$

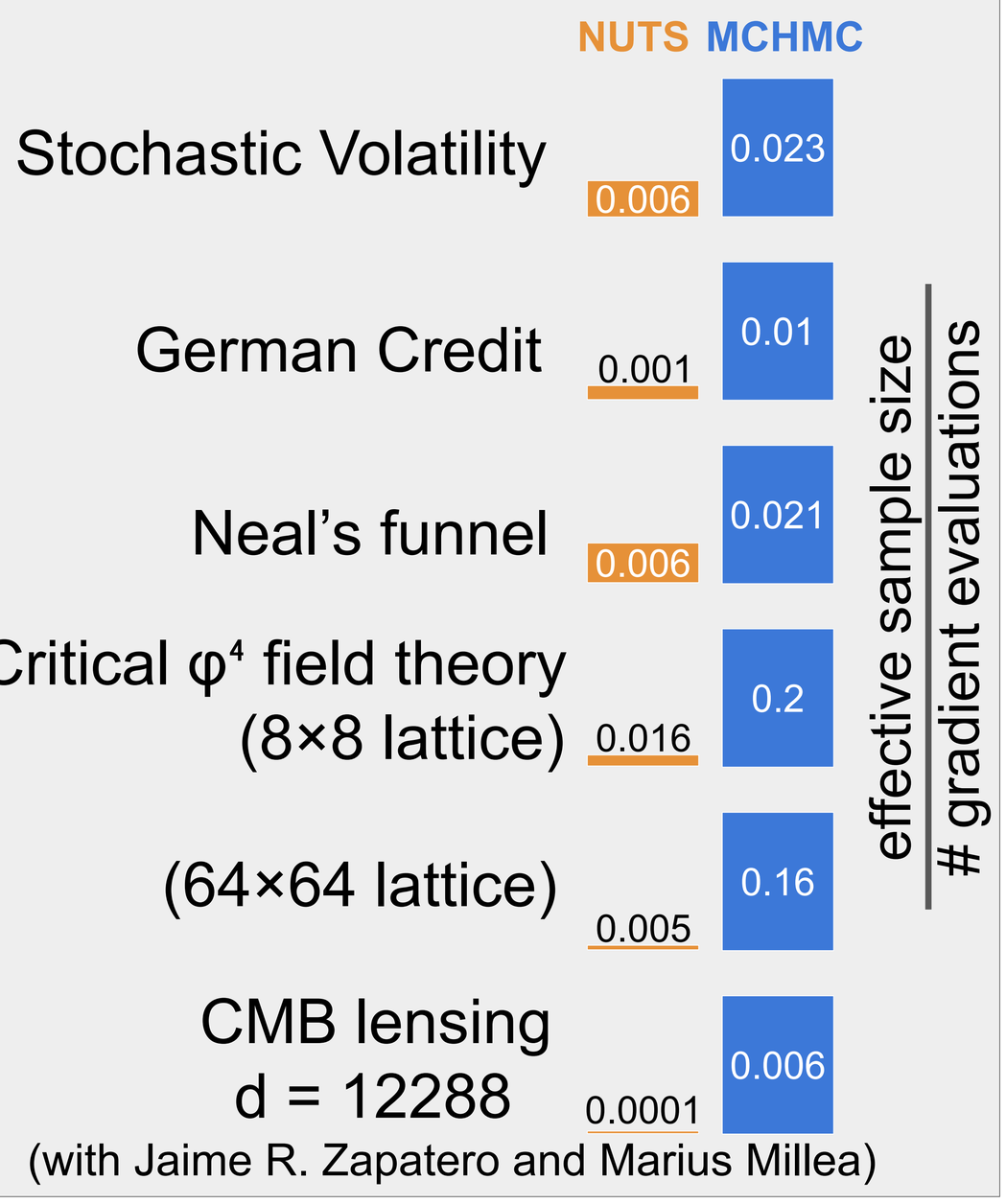




$$H = \frac{d}{2}\log\frac{|\mathbf{\Pi}|^2}{d} - \log p(\boldsymbol{x})$$

- Severalfold faster sampling in low dimensions
- **Orders of magnitude** faster sampling in **high dimensions**
- Automatic **hyperparameter tuning**
- Extremely **fast burn-in**
- Provable convergence
- Python (JAX), Julia and C++ implementations

Experiments



(with Jaime R. Zapatero and Marius Millea)