

# HAMILTONIAN MONTE CARLO (HMC) - COMPLETE FLOWCHART

Mathematical Foundation and Algorithmic Structure

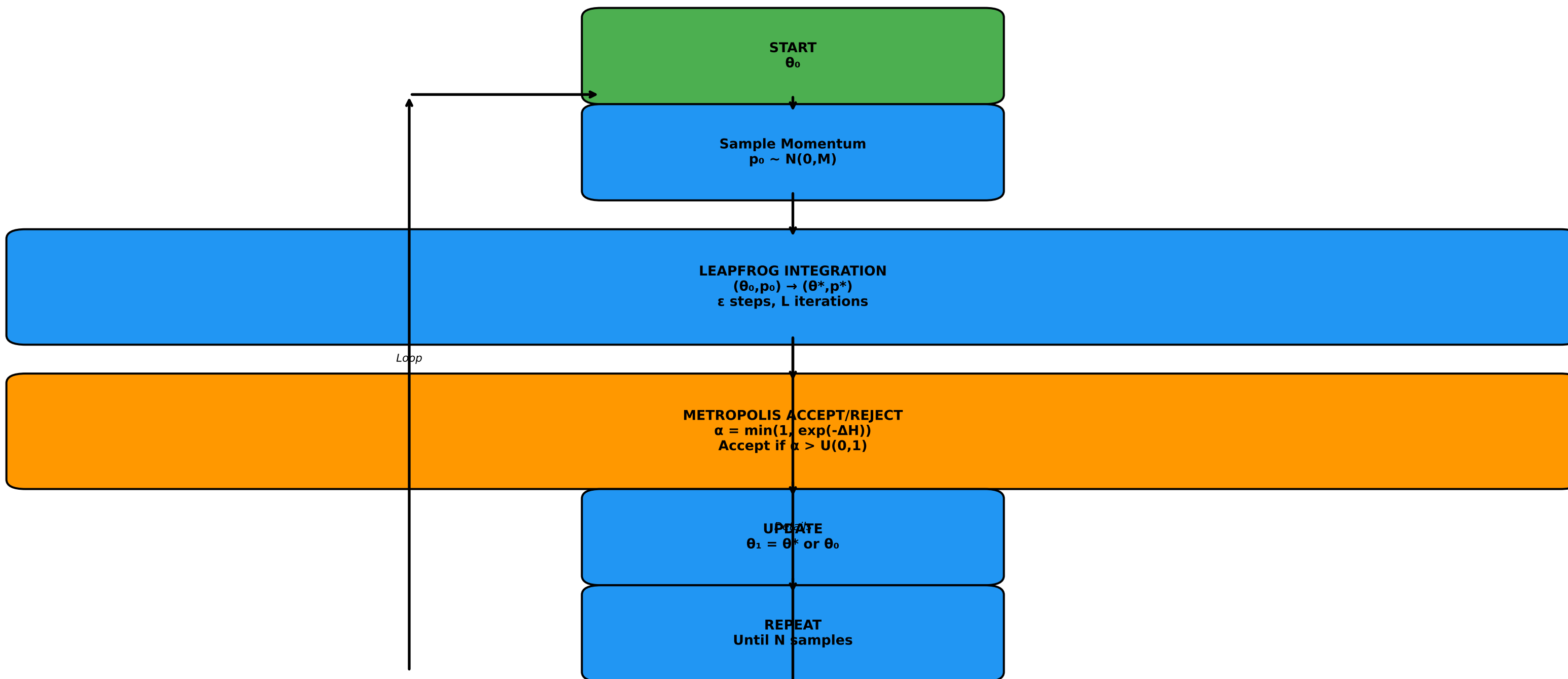
## 1. MATHEMATICAL FOUNDATION

Target Distribution  
 $\pi(\theta) \propto \exp(-U(\theta))$

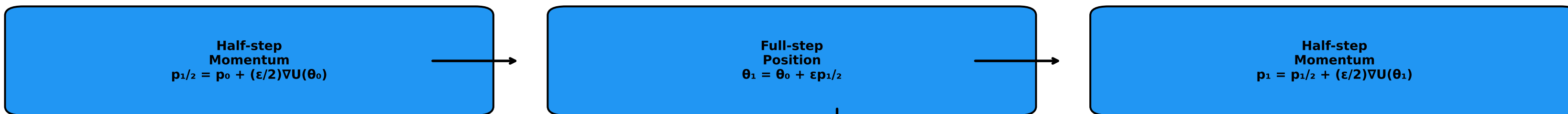
Hamiltonian Function  
 $H(\theta, p) = U(\theta) + \frac{1}{2}p^T M^{-1}p$

Canonical Equations:  $d\theta/dt = M^{-1}p$ ,  $dp/dt = -\nabla U(\theta)$

## 2. MAIN HMC ALGORITHM

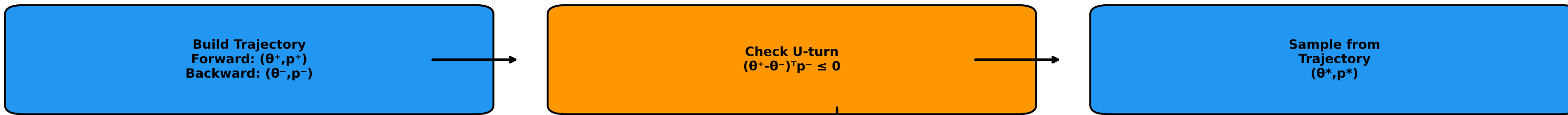


## 3. LEAPFROG INTEGRATION DETAILS

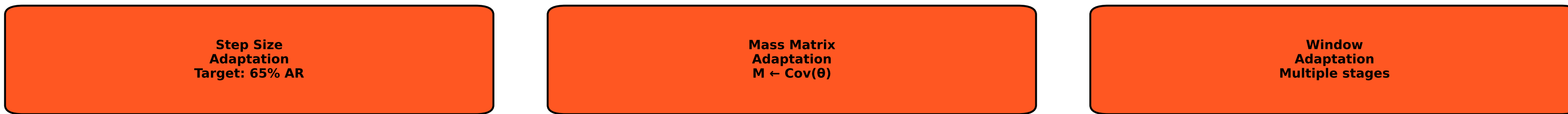


Properties: Reversible, Volume-preserving, Symplectic,  $O(\epsilon^2)$  accurate

## 4. NUTS (NO-U-TURN SAMPLER)



## 5. ADAPTATION MECHANISMS



## 6. KEY EQUATIONS

$H(\theta, p) = U(\theta) + \frac{1}{2}p^T M^{-1}p$

$d\theta/dt = M^{-1}p$ ,  $dp/dt = -\nabla U(\theta)$

$\alpha = \min(1, \exp(-\Delta H))$

$\pi(\theta)T(\theta \rightarrow \theta') = \pi(\theta')T(\theta' \rightarrow \theta)$