HMC using Nambu generalized mechanics

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Outline

- HMC
- Extended phase space and Nambu mechanics
- Discretization of Nambu mechanics for QCD
- Preliminary test results

HMC

We can add fictitious variables to the theory without changing its physical content

$$\int [dU] O(U) \exp\big(-S(U)\big) = \text{const.} \int [d\pi][dU]\, O(U) \exp\big(-S(U) - f(\pi)\big).$$

Accept/rejecting with H(U, π) = $S(U) + f(\pi)$ will produce the correct probability distribution provided sample generation

- Preserves the measure $[d\pi][dU]$
- Satisfies detailed balance
- Ergodic
- (Preferably) Good preservation of H(U, π) for high acceptance rate

HMC cont.

Interpret H(U, π) = $S(U) + f(\pi)$ as the Hamiltonian of a mechanical system and evolve with Hamilton's equations

- Preserves phase space measure
- Exact reversibility (detailed balance)
- Frequent momenta refreshments (Ergodicity)
- Conserves (approx.) H(U, π)

Additional fictitious variables

Add additional variables provided the required properties are satisfied

$$\int [dU] O(U) \exp\big(-S(U)\big) = \text{const.} \int [d\rho][d\pi][dU] O(U) \exp\big(-S(U) - f(\pi) - l(\rho)\big)$$

- Preserves the measure $[d\rho]\ [d\pi][dU]$
- Satisfies detailed balance
- Ergodic
- (Preferably) Good preservation of H(U, π , ρ)= $S(U) + f(\pi) + l(\rho)$ for high acceptance rate

These are all satisfied by Nambu's generalized Hamiltonian dynamics

Nambu's generalized mechanics

In the minimal extension of Hamiltonian mechanics (n=3) (Phys. Rev. D 7, 2405)

- Let the three real variables (p,q,r) be a triplet of dynamical variables in a 3D phase space
- Generalization of the usual canonical pair (p,q)
- Introduce two 'Hamiltonians' H(p,q,r) and G(p,q,r) which determine the dynamics

Nambu postulated the following equations of motion

$$\frac{dq}{dt} = \frac{\partial H}{\partial p}\frac{\partial G}{\partial r} - \frac{\partial H}{\partial r}\frac{\partial G}{\partial p}, \qquad \frac{dp}{dt} = \frac{\partial H}{\partial r}\frac{\partial G}{\partial q} - \frac{\partial H}{\partial q}\frac{\partial G}{\partial r}, \qquad \frac{dr}{dt} = \frac{\partial H}{\partial q}\frac{\partial G}{\partial p} - \frac{\partial H}{\partial p}\frac{\partial G}{\partial r}.$$

Introduce the vector notation $\vec{x} = (q, p, r)$

$$\frac{d\vec{x}}{dt} = \vec{\nabla} H \times \vec{\nabla} G.$$

Nambu Mechanics (NM) cont.

$$\frac{d\vec{x}}{dt} = \vec{\nabla}H \times \vec{\nabla}G.$$

- The velocity field has zero divergence

$$\vec{\nabla} \cdot \left(\vec{\nabla}H \times \vec{\nabla}G\right) = 0$$

Thus, Nambu equations of motion are incompressible flows in phase space

- Equations of motion can be expressed as a generalized Poisson bracket called Nambu bracket

$$\dot{F} = [F, H, G] = \vec{\nabla}F \cdot \left(\vec{\nabla}H \times \vec{\nabla}G\right)$$

- This implies the separate conservation of H and G

$$[H, H, G] = [G, H, G] = 0$$

Many-body NM

- Write

$$\dot{F} = [F, H, G] = \frac{(F, H, G)}{(q, p, r)}$$

- Extend phase space to 3N dimensions $\vec{x}_i$ (i=1,...,N)

$$\dot{F} = [F, H, G] = \sum_{i=1}^{N} \frac{(F, H, G)}{(q_i, p_i, r_i)}$$

Many body NM and Lie groups

- For SU(3) gauge links $U(x,\mu)$ we can associate a q_i with each direction in the Lie algebra with derivatives of functions $f(U)$ evaluated as

$$\partial_{q(i,x,\mu)} f(U) = \frac{d}{dt} f(U_t)\bigg|_{t=0}, U_t = e^{-tT^i} U(x,\mu)$$

- For each q_i introduce a Nambu canonical triplet (q_i, p_i, r_i)
- Therefore 8 p_i and 8 r_i live at each (x, μ)

Nambu mechanics for HMC

- Now we can do the HMC with molecular dynamics steps replaced by Nambu mechanics
- Phase space $\{U(x, \mu), p_i(x, \mu), r_i(x, \mu)\}$ (i = 1,…,8)
- For target action $S_W(U)$ choose the following to be used in an accept/reject step

$$H = \frac{p^2}{2} + \frac{r^2}{2} + S_W(U)$$

$$p^2 = \sum_{x,\mu,i} p(i,x,\mu)p(i,x,\mu) \qquad r^2 = \sum_{x,\mu,i} r(i,x,\mu)r(i,x,\mu)$$

- Generate p and r according to $exp\left(-\frac{1}{2}z^2\right)$ and frequently refresh for ergodicity
- Function G(U,p,r) remains to be chosen

Nambu mechanics for HMC (cont.)

A safe choice for G is the general form

$$G = \alpha\frac{p^2}{2} + \gamma\frac{r^2}{2} + \kappa f(U).$$

- Where $f(U)$ can be *any arbitrary function of the gauge fields*, including non-local ones
- Forces from non-local objects enter molecular dynamics
- Recover the appropriate distribution by making accept/reject steps on H

Discretization for QCD

- Treat two variables as fixed while evolving the third
- Each update is a continuum Nambu-Hamiltonian flow with different (H’, G’)
- Alternating application approximates continuum evolution with target H and G
- Few additional force evaluations

$$p_i^{n+1/2} = p_i^n + \frac{\tau}{2}[p_i, H, G]\Big|_{(U^n, r^n)}$$

$$r_i^{n+1/2} = r_i^n + \frac{\tau}{2}[r_i, H, G]\Big|_{(U^n, p^{n+1/2})}$$

$$U^{n+1} = \exp\left(-\tau \sum_i [q_i, H, G] T^i\right)\Big|_{(r^{n+1/2}, p^{n+1/2})} U^n$$

$$r_i^{n+1} = r_i^n + \frac{\tau}{2}[r_i, H, G]\Big|_{(U^{n+1}, p^{n+1/2})}$$

$$p_i^{n+1} = p_i^n + \frac{\tau}{2}[p_i, H, G]\Big|_{(U^{n+1}, r^{n+1})}$$

$$[p_i, H, G] = \frac{\partial H}{\partial r_i}\frac{\partial G}{\partial q_i} - \frac{\partial H}{\partial q_i}\frac{\partial G}{\partial r_i}$$

$$[r_i, H, G] = \frac{\partial H}{\partial q_i}\frac{\partial G}{\partial p_i} - \frac{\partial H}{\partial p_i}\frac{\partial G}{\partial r_i}$$

$$[q_i, H, G] = \frac{\partial H}{\partial p_i}\frac{\partial G}{\partial r_i} - \frac{\partial H}{\partial r_i}\frac{\partial G}{\partial p_i}$$

Numerical experiments confirm these are reversible and display good conservation of H and G

Preliminary tests: 4D pure SU(3) gauge theory

Parameters

$$G = \alpha\frac{p^2}{2} + \gamma\frac{r^2}{2} + \kappa f(U),$$

$$\alpha = 0.0, \qquad \gamma = -\kappa = 0.5$$

$$f(U) = \mathrm{Re}(\sum \text{Polyakov loops}),$$

Equations of motion

$$\dot{U}(x,\mu)U(x,\mu)^{-1} = -\sum_i p_i r_i(\alpha-\gamma)T^i$$

$$\dot{p}_i(x,\mu) = r_i(x,\mu)\left(\gamma\beta\partial_{q(i,x,\mu)}S(U) - \kappa\partial_{q(i,x,\mu)}f(U)\right)$$

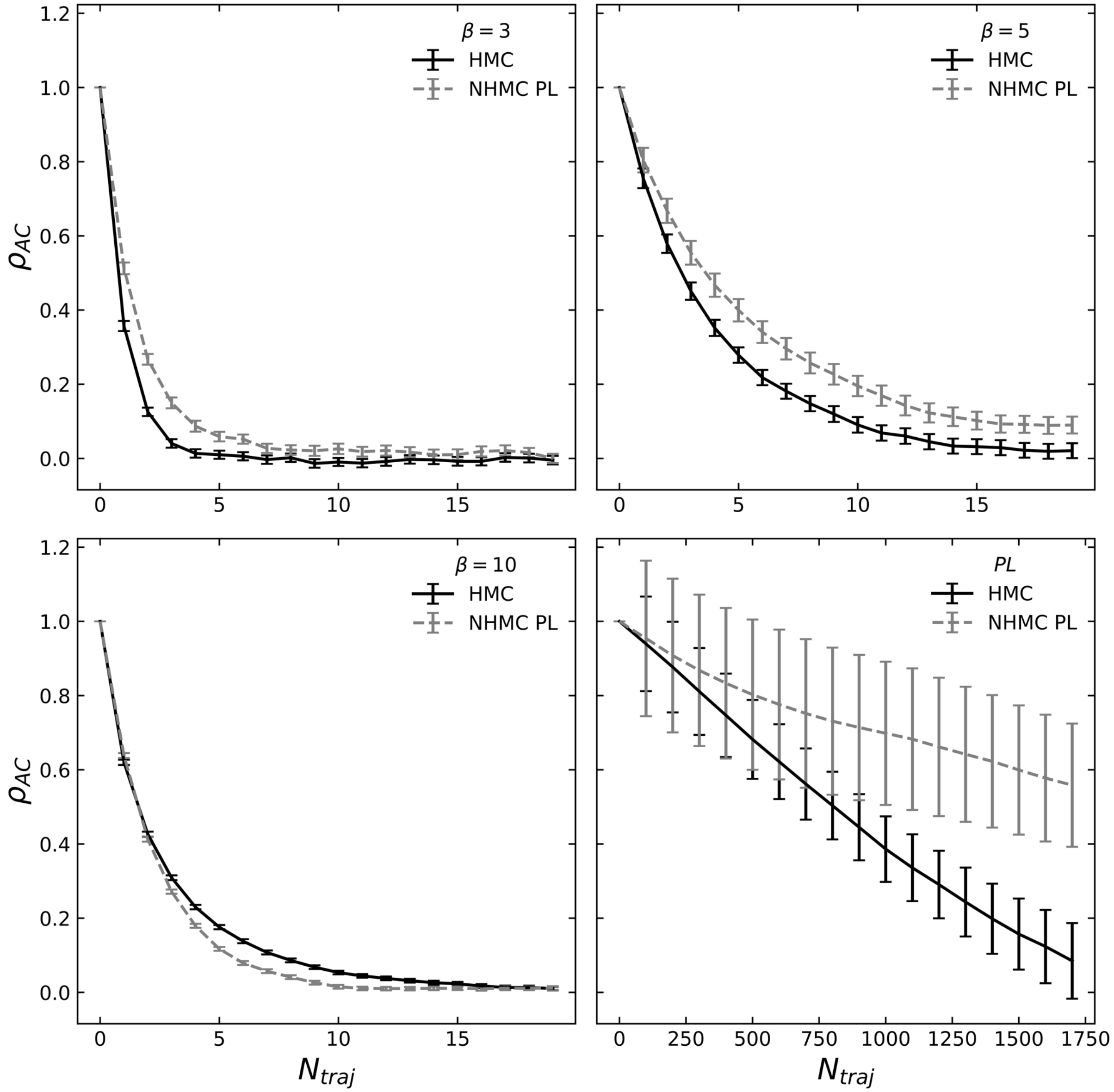
$$\dot{r}_i(x,\mu) = -p_i(x,\mu)\left(\alpha\beta\partial_{q(i,x,\mu)}S(U) - \kappa\partial_{q(i,x,\mu)}f(U)\right)$$

NHMC PL Plaquette values (8^4)				
β	plaquette	MD steps	accpt. rate	trajs
1.0	0.939857(73)	10	0.70	2k
3.0	0.794987(32)	25	0.80	10k
5.6	0.475512(75)	45	0.84	100k
7.0	0.328344(23)	50	0.79	20k
10.0	0.216650(17)	65	0.80	20k

HMC Plaquette values (8^4)				
β	plaquette	MD steps	accpt. rate	trajs
1.0	0.939913(55)	25	0.79	2k
3.0	0.794994(30)	45	0.80	10k
5.6	0.475446(72)	60	0.80	100k
7.0	0.328291(48)	80	0.77	20k
10.0	0.216656(16)	100	0.77	20k

Plaquette and Polyakov loop autocorrelations 8^4 lattice

- Adjust timestep τ until 0.80-0.85 acceptance ratio
- Run trajectory for 26 Wilson force evaluations
- HMC uses leapfrog algorithm
- Accept/reject step
- Refresh momenta



<u>Parameters</u>

$$G = \alpha\frac{p^2}{2} + \gamma\frac{r^2}{2} + \kappa f(U),$$

$$\gamma = -\alpha = 0.1$$

$$\kappa = -0.5$$

Plaquette and Polyakov loop autocorrelations 8^4 lattice

- Adjust timestep τ until 0.80-0.85 acceptance ratio
- Run trajectory for 26 Wilson force evaluations
- HMC uses leapfrog algorithm
- Accept/reject step
- Refresh momenta

Parameters

$$G = \gamma \sum_{i,x,\mu} r(x,\mu,i) \quad + \kappa f(U)$$

$$\gamma = 0.8$$

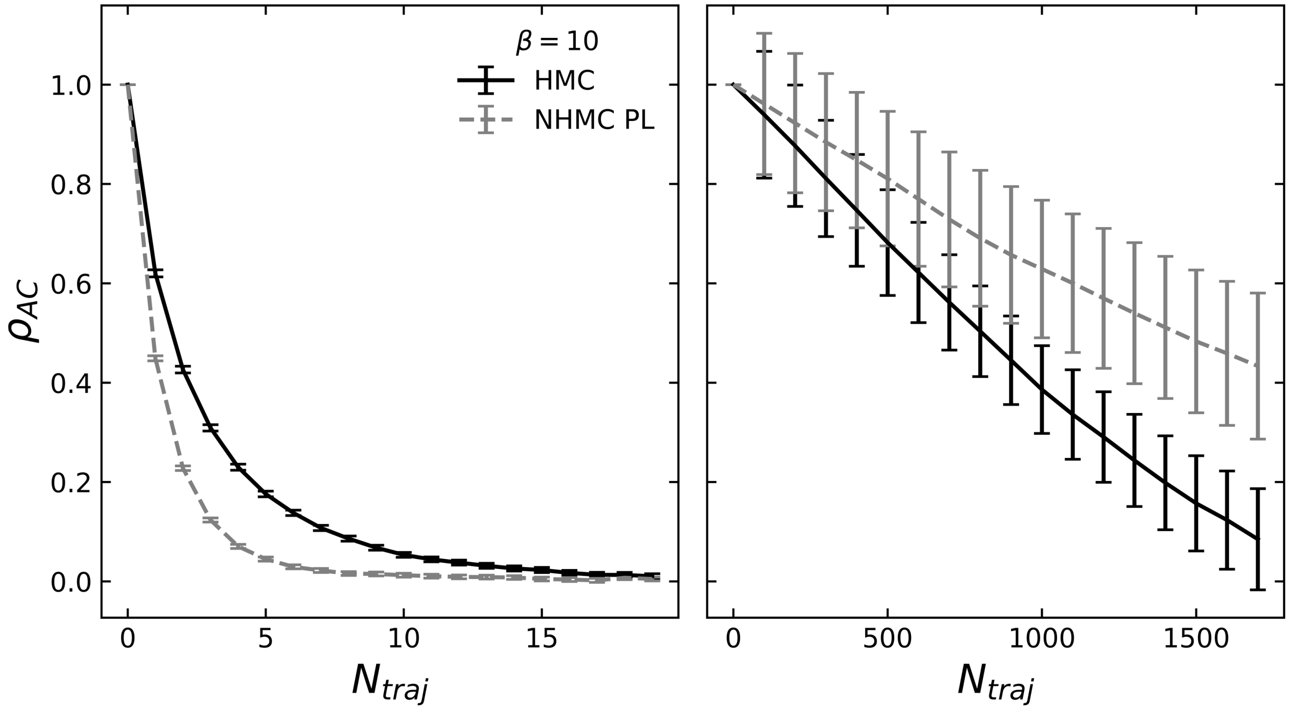
$$\kappa = 30.0$$

Equations of motion

$$\dot{U}(x,\mu)U(x,\mu)^{-1} = \sum_i \gamma\, p_i T^i$$

$$\dot{p}_i(x,\mu) = \left(\gamma\beta\partial^i_{q,\mu}S(U) - \kappa\, r_i(x,\mu)\, \partial^i_{q,\mu} f(U)\right)$$

$$\dot{r}_i(x,\mu) = p_i(x,\mu)\left(\kappa\partial^i_{q,\mu} f(U)\right)$$



Summary

- Successfully constructed a version of the HMC using Nambu mechanics for LQCD
- Molecular dynamics includes forces from non-local objects
- These forces exert an influence on the long-distance behavior of the gauge field

Next steps

- Identify non-local forces which have utility in fighting CSD
- Test with fermions and larger lattices