Fourier acceleration, the HMC algorithm and renormalizability

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LatticeQCD Exascale Computing Project
Outline

• Fourier acceleration: reduce critical slowing down
• Autocorrelations in field theory
  – Langevin
  – Hybrid Monte Carlo (HMC)
• Apply to Fourier acceleration
• Conclusion
Reduce Critical slowing down

- The DOE-funded Exascale Computing Project is supporting exascale-targeted lattice QCD research in the US.
- This includes efforts to accelerate the generation of gauge ensembles.

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HMC Fourier acceleration

- HMC mixes classical ballistic motion with momentum randomization
- Introduce fifth simulation dimension with momenta $\pi_i$ conjugate to each $U_i$:
  \[ \mathcal{H} = \sum_i \frac{1}{2M} \pi_i \pi_i + S(U) \]
- Critical slowing down:
  - Length of classical trajectories $\sim 1/\Lambda_{QCD}$
  - Integration step size must be $\sim a$
  - Number of steps grows as $1/a$
- Change $M$ so higher frequency modes have a larger mass and a smaller velocity
HMC Fourier acceleration

- Riemannian Manifold HMC (RMHMC) [Guido Cossu, Lattice 2017]: $M \rightarrow \nabla^2_{\text{lat}}$

- Gauge fixed HMC (GFHMC) [Yidi Zhao, next talk] $M \rightarrow \sum_{\mu} \sin^2(\frac{k_{\mu}^2}{2})$

- Hyperplane accelerated HMC [Kostas Orginos]
- Quasi-Newton HMC [Xiao-Yong Jin, this session]
Fourier acceleration and asymptotic freedom

- For uncoupled harmonic oscillators perfect Fourier acceleration is possible.
- Perhaps works for lattice QCD too – keep physical integration step size fixed as $a \to 0$?
- How well do we understand gauge evolution in the $a \to 0$ limit?
- How are these conclusions affected by Fourier acceleration?
Langevin evolution

- Formulate a continuum version of the evolution (the Langevin equation)

\[
\dot{\phi}(x, t) = -\frac{\delta}{\delta \phi(x, t)} S[\phi] + \eta(x, t) \\
= -(\partial_{\mu} \partial_{\mu} + m^2)\phi - \frac{\lambda}{3!} \phi(x, t)^3 + \eta(x, t)
\]

\[\langle \eta(x, t)\eta(y, s) \rangle = 2\delta(x - y)\delta(t - s)\]

- Construct a generating function for the 5-D correlation functions.

\[
\mathcal{Z}[J] = \int d[\eta] \delta \left( \dot{\phi}(x, t) + \frac{\delta}{\delta \phi(x, t)} S[\phi] - \eta \right) e^{-\int dxdt \{\eta(x,t)^2 - J(x,t)\phi(x,t)\}}
\]

\[
= \int d[\phi] \det \left[ \frac{d}{dt} + \frac{\delta^2 S}{\delta \phi \delta \phi} \right] e^{-\int dxdt \left\{ \left( \phi(x,t) + \frac{\delta}{\delta \phi(x,t)} S[\phi] \right)^2 - J(x,t)\phi(x,t) \right\}}
\]
Langevin evolution [Zinn-Justin]

- $\mathcal{Z}[J]$ defines an unusual, 5-D theory with
  - gauge-theory-like BRS symmetry
  - Ward – Takahashi identities

$$\mathcal{Z}[J] = \int d[\phi] \det \left[ \frac{d}{dt} + \frac{\delta^2 S}{\delta \phi \delta \phi} \right] e^{-\int dx dt \left\{ \left( \frac{\delta}{\delta \phi(x,t)} S[\phi] \right)^2 - J(x,t) \phi(x,t) \right\}}$$

- Only counter terms that rescale parameters are allowed.
- However, Langevin method is a random walk with steps of size $a$ and critical exponent of 2.
Hybrid Monte Carlo
[Luscher & Schaefer]

• Use continuum equation for Generalized HMC

\[ \partial_t \pi = -\frac{\delta S[\phi]}{\delta \phi(x,t)} - 2\mu_0 \pi + \eta(x,t) \quad \partial_t \phi(x,t) = \pi(x,t) \]

\[ \partial_t^2 \phi(x,t) = -2\mu_0 \partial_t \phi(x,t) - (-\partial_\mu \partial_\mu + m_0^2)\phi(x,t) - \frac{\lambda}{3!} \phi^3(x,t) + \eta(x,t) \]

\[ \langle \eta(x,t)\eta(y,s) \rangle = 4\mu_0 \delta(x-y)\delta(t-s) \]

• Solve for \( \phi(x,t)[\eta] \) as a power series in \( \lambda \) using the Green’s function:

\[ K(x,t) = \int \frac{d^4p}{(2\pi)^5} \frac{d\omega}{\omega^2 - i\mu_0\omega + p^2 + m_0^2} e^{i(p\cdot x - \omega t)} \]
Hybrid Monte Carlo
[Luscher & Schaefer]

- General HMC correlation function can be constructed from two components:

\[
\langle \phi(x_1, t_1)[\eta] \phi(x_2, t_2)[\eta] \ldots \phi(x_N, t_N)[\eta]\rangle_{\eta}
\]

\[
(x, t) \quad \equiv \quad \int d^4y ds K(x - y, t - s) \phi^3(y, s)
\]

\[
(x, t) \quad \equiv \quad \int d^4z dr K(x - z, t - r) K(x - z, s - r)
\]
Hybrid Monte Carlo
[Luscher & Schaefer]

- General HMC correlation function can be constructed from two components:

\[
\langle \phi(x_1, t_1)[\eta] \phi(x_2, t_2)[\eta] \cdots \phi(x_N, t_N)[\eta] \rangle_\eta \\
\equiv \int d^4 y d s K(x - y, t - s) \phi^3(y, s)
\]

\[
\langle x, t \rangle \equiv \int d^4 z d r K(x - z, t - r) K(x - z, s - r)
\]

\[
\frac{e^{-2\mu_0(t-s)}}{32\pi^3} \delta \left( (x - y)^2 - (t - s)^2 \right) \frac{1}{\epsilon}
\]
Hybrid Monte Carlo
[Luscher & Schaefer]

• General HMC correlation function can be constructed from two components:

\[ \langle \phi(x_1, t_1)[\eta] \phi(x_2, t_2)[\eta] \ldots \phi(x_N, t_N)[\eta] \rangle_{\eta} \]

\[ = \int d^4y ds K(x - y, t - s)\phi^3(y, s) \]

\[ = \int d^4z dr K(x - z, t - r)K(x - z, s - r) \]

Cannot be removed by a local counter term

\[ = \frac{e^{-2\mu_0(t-s)}}{32\pi^3} \delta \left( (x - y)^2 - (t - s)^2 \right) \frac{1}{\epsilon} \]

HMC not renormalizable
Add Fourier acceleration


\[
(-\partial_\mu \partial_\mu + \vec{m}^2) \partial_t \phi(x, t) = -\frac{\delta}{\delta \phi(x, t)} S[\phi] + \eta(x, t)
\]

\[
= -(\partial_\mu \partial_\mu + m^2)\phi - \frac{\lambda}{3!} \phi(x, t)^3 + \eta(x, t)
\]

\[
\langle \eta(x, t)\eta(y, s) \rangle = 2(-\partial_\mu \partial_\mu + \vec{m}^2)\delta(x - y)\delta(t - s)
\]

- **HMC**

\[
\partial_t \phi(x, t) = \frac{1}{(-\partial_\mu \partial_\mu + \vec{m}^2)} \pi(x, t) \quad \partial_t \pi = -\frac{\delta S[\phi]}{\delta \phi(x, t)} - 2\mu_0 \pi + \eta(x, t)
\]

\[
(-\partial_\mu \partial_\mu + \vec{m}^2) \partial_t^2 \phi(x, t) = -2\mu_0 (-\partial_\mu \partial_\mu + \vec{m}^2) \partial_t \phi(x, t)
\]

\[
-(-\partial_\mu \partial_\mu + m_0^2)\phi(x, t) - \frac{\lambda}{3!} \phi^3(x, t) + \eta(x, t)
\]

\[
\langle \eta(x, t)\eta(y, s) \rangle = 4\mu_0 (-\partial_\mu \partial_\mu + \vec{m}^2)\delta(x - y)\delta(t - s)
\]
Divide by \((-\partial_\mu \partial_\mu + \tilde{m}^2)\)

- **Langevin**

\[
(\partial_t + 1) \phi(x, t) = -\frac{1}{(-\partial_\mu \partial_\mu + m^2)^3} \frac{\lambda}{3!} \phi(x, t)^3 + \eta(x, t)
\]

\[
\langle \eta(x, t) \eta(y, s) \rangle = 2 \langle x | \frac{1}{(-\partial_\mu \partial_\mu + m^2)^3} | y \rangle \delta(t - s)
\]

- **HMC**

\[
(\partial_t^2 + 2\mu_0 + 1) \partial_t \phi(x, t) = -\frac{1}{(-\partial_\mu \partial_\mu + m_0^2)^3} \frac{\lambda}{3!} \phi^3(x, t) + \eta(x, t)
\]

\[
\langle \eta(x, t) \eta(y, s) \rangle = 4\mu_0 \langle x | \frac{1}{(-\partial_\mu \partial_\mu + m^2)^3} | y \rangle \delta(t - s)
\]

- **Evolution time and space-time “factorize”!**
Separation of evolution time and space-time

• Recall graphical Langevin solution:

\[
\dot{\phi}(x, t) = -\left(\partial_\mu \partial_\mu + m^2\right)\phi - \frac{\lambda}{3!}\phi(x, t)^3 + \eta(x, t)
\]

\[
\delta^4(z - z')\delta(r - r')
\]

\[
K(p, t) = \theta(t)e^{-t} \cdot \frac{1}{p^2 + m^2}
\]

\[
G(p, t) = e^{-|t|} \cdot \frac{1}{p^2 + m^2}
\]
Separation of evolution time and space-time

• To arbitrary order in perturbation theory:

\[
\left\langle \phi(x_1, t_1)[\eta] \phi(x_2, t_2)[\eta] \cdots \phi(x_N, t_N)[\eta] \right\rangle_{\eta} = \sum_{\{\Gamma_5\}} I_{\Gamma_5}(t_1, t_2, \ldots, t_N) G_{\Gamma_4(\Gamma_5)}(x_1, x_2 \ldots, x_N)
\]

Depends only on evolution time

Usual 4-dim Green’s function for graph \( \Gamma_4 \)

– Sum over all 5-dim graphs \( \Gamma_5 \)

– 4-D Feynman graph for \( \Gamma_5 \) is \( \Gamma_4 (\Gamma_5) \)

– 4-D results guaranteed if: \( \sum_{\Gamma_5} I_{\Gamma_5}(t, t, \ldots, t) = 1 \)

• Dangerous Luscher-Schaefer structure cannot appear:

\[
\frac{e^{-2\mu_0(t-s)}}{32\pi^3} \delta \left( (x - y)^2 - (t - s)^2 \right) \frac{1}{\epsilon}
\]
Separation spoils renormalization

- **Langevin evolution, $\phi^3$ theory at order $\lambda^2$:**

\[
(\partial_t + 1) \phi(x, t) = -\frac{1}{(-\partial_\mu \partial_\mu + m^2)} \frac{\lambda}{2} \phi(x, t)^2 + \eta(x, t)
\]

\[\begin{align*}
\frac{1}{6} e^{-|t-s|} & \left[ 2 - e^{-|t-s|} \right] + \\
\frac{1}{6} e^{-|t-s|} & \left[ 1 + (t-s)\Theta(t-s) \right] + \\
\frac{1}{6} e^{-|t-s|} & \left[ 1 + (s-t)\Theta(s-t) \right]
\end{align*}\]

Equal only when $t = s$
Conclusion

- After Fourier acceleration, evolution time dependence has only the scale of the lattice spacing.
- The familiar cancelation between “divergences” and counter terms holds only at equal evolution times, even for the Langevin case.
- The objective of Fourier acceleration has been met: All auto-correlations on a physical time scale have been removed!
- Still a work in progress. What happens if $\bar{m} \neq m_0$? Evolution time and space-time weakly coupled.