Fourier acceleration, the HMC algorithm and renormalizability

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LatticeQCD Exascale Computing Project

EXASCALE COMPUTING PROJECT

Outline

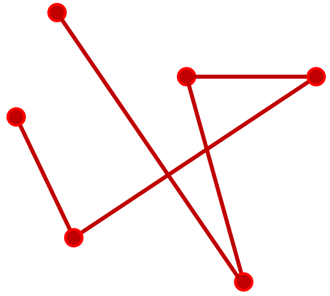
- Fourier acceleration:
  reduce critical slowing down
- Autocorrelations in field theory
  - Langevin
  - Hybrid Monte Carlo (HMC)
- Apply to Fourier acceleration
- Conclusion

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.

Rich Brower	Boston	Chulwoo Jung	BNL
Peter Boyle	Edinburgh	Robert Mawhinney	Columbia
Norman Christ	Columbia	Kostas Orginos	W&M
Guido Cossu	Edinburgh	James Osborn	ANL
Carleton Detar	Utah	Jiqun Tu	Columbia
Yong-Chull Jang	BNL	Evan Wickenden	Columbia
Xiao-Yong Jin	ANL	Yidi Zhao	Columbia

HMC Fourier acceleration



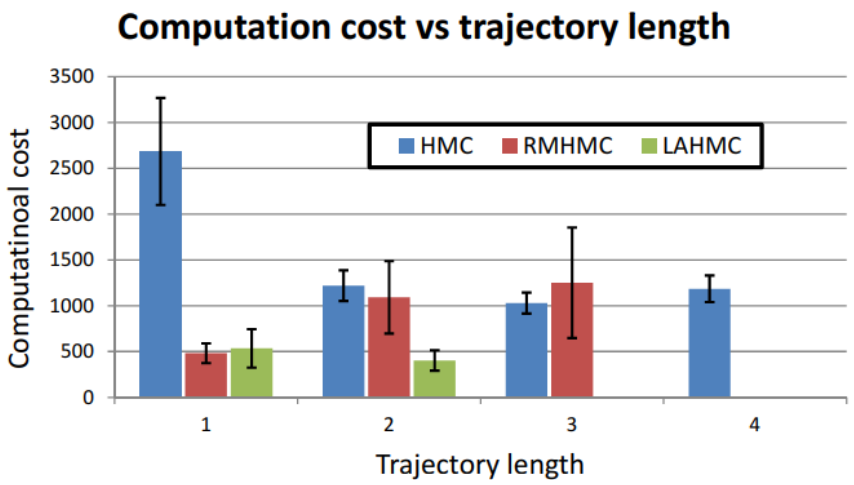
- HMC mixes classical ballistic motion with momentum randomization
- Introduce fifth simulation dimension with momenta π_l conjugate to each U_l:

$$\mathcal{H} = \sum_l \pi_l \frac{1}{2M} \pi_l + \mathcal{S}(U)$$

- Critical slowing down:
  - Length of classical trajectories ~ $1/\Lambda_{\text{QCD}}$
  - 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]: $M \to \nabla^2_{\text{lat}}$



- Gauge fixed HMC (GFHMC) [Yidi Zhao, next talk] $M \to \sum_\mu \sin^2(k_\mu^2/2)$
- 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 $a \rightarrow 0$?
- How well do we understand gauge evolution in the $a \rightarrow 0$ limit?
  - Langevin: renormalizable.
    [J. Zinn-Justin, Nucl Phys B275 (1986) 135]
  - HMC: non-local divergences.
    Luscher & Schaefer, JHEP 1104 (2011) 104, arXiv:1103.1810]
- 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.

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

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

Langevin evolution
[Zinn-Justin]

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

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

- 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
  [Horowitz, Nucl Phys B280, (1987) 510]

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

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

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

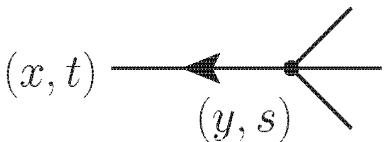
- Solve for $\phi(x,t)[\eta]$ as a power series in λ using the Green's function:

$$K(x,t) = \int \frac{d^4p\, d\omega}{(2\pi)^5} \frac{e^{i(p\cdot x - \omega t)}}{\omega^2 - i\mu_0\omega + p^2 + m_0^2}$$

Hybrid Monte Carlo
[Luscher & Schaefer]

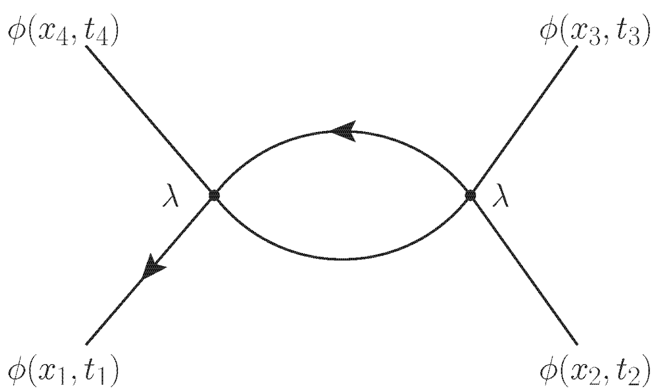
- General HMC correlation function can be constructed from two components:

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



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

$$\equiv \int d^4z\, dr\, K(x - z, t - r) K(x - z, s - r)$$



Hybrid Monte Carlo
[Luscher & Schaefer]

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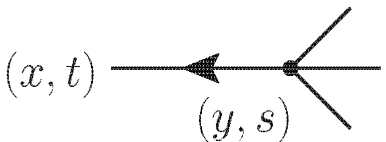
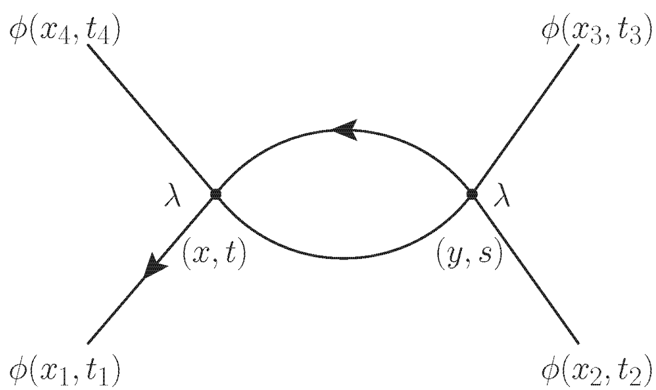


$$\equiv \int d^4y\,ds\,K(x-y,t-s)\phi^3(y,s)$$

$$\equiv \int d^4z\,dr\,K(x-z,t-r)K(x-z,s-r)$$

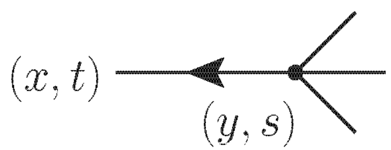


$$= \frac{e^{-2\mu_0(t-s)}}{32\pi^3}\,\delta\left((x-y)^2-(t-s)^2\right)\frac{1}{\epsilon}$$

Hybrid Monte Carlo
[Luscher & Schaefer]

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

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



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

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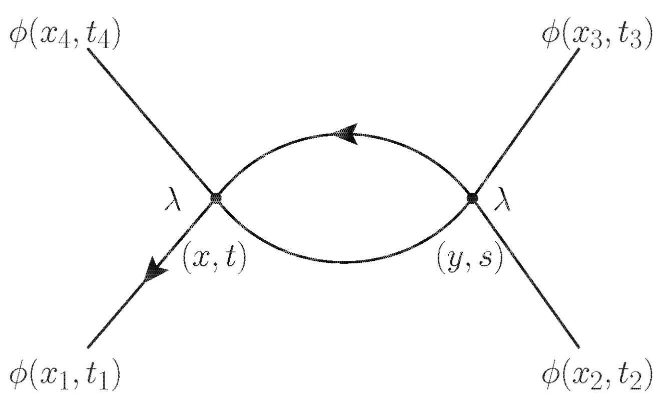


Cannot be removed by a local counter term

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

HMC not renormalizable

Add Fourier acceleration

- Langevin [G. Batrouni, *et al*. Phys Rev D32 2736 (1985)]

$$
\begin{aligned}
(-\partial_\mu\partial_\mu + \widetilde{m}^2)\partial_t\phi(x,t) &= -\frac{\delta}{\delta\phi(x,t)}S[\phi] + \eta(x,t) \\
&= -(\partial_\mu\partial_\mu + m^2)\phi - \frac{\lambda}{3!}\phi(x,t)^3 + \eta(x,t) \\
\langle\eta(x,t)\eta(y,s)\rangle &= 2(-\partial_\mu\partial_\mu + \widetilde{m}^2)\delta(x-y)\delta(t-s)
\end{aligned}
$$

- HMC

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

$$
\begin{aligned}
(-\partial_\mu\partial_\mu + \widetilde{m}^2)\partial_t^2\phi(x,t) &= -2\mu_0(-\partial_\mu\partial_\mu + \widetilde{m}^2)\partial_t\phi(x,t) \\
&\quad -(-\partial_\mu\partial_\mu + m_0^2)\phi(x,t) - \frac{\lambda}{3!}\phi^3(x,t) + \eta(x,t) \\
\langle\eta(x,t)\eta(y,s)\rangle &= 4\mu_0(-\partial_\mu\partial_\mu + \widetilde{m}^2)\delta(x-y)\delta(t-s)
\end{aligned}
$$

Divide by $(-\partial_\mu\partial_\mu + \widetilde{m}^2)$

- Langevin

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

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

- HMC

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

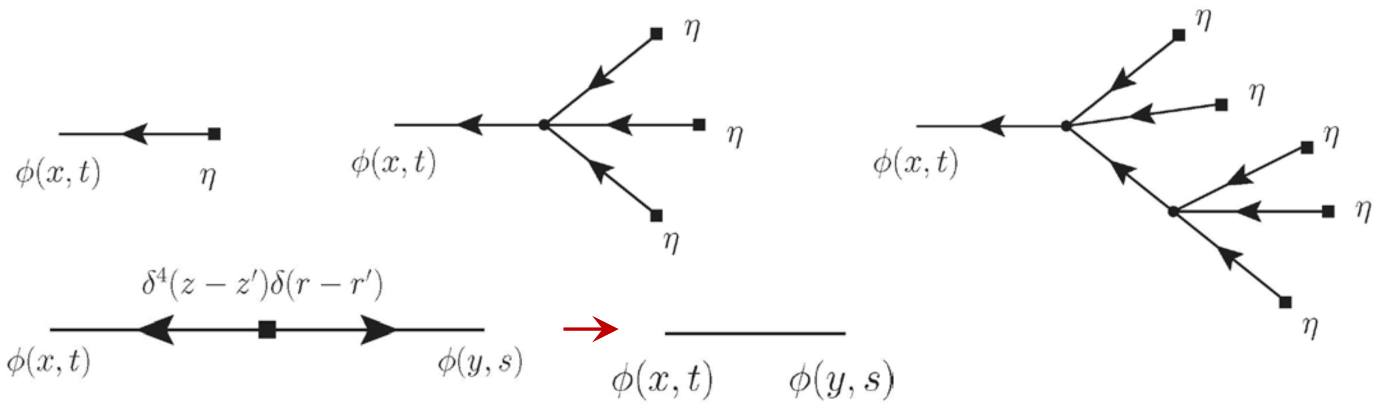
$$\langle \eta(x,t)\eta(y,s)\rangle \;=\; 4\mu_0\langle x|\frac{1}{(-\partial_\mu\partial_\mu + m^2)}|y\rangle\;\delta(t-s)$$

- Evolution time and space-time “factorize” !

Separation of evolution time and space-time

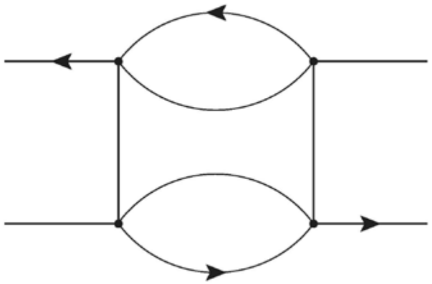
- Recall graphical Langevin solution:

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




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

→ $G(p,t) = e^{-|t|} \cdot \frac{1}{p^2+m^2}$



Separation of evolution time and space-time

- To arbitrary order in perturbation theory:

$$\Big\langle \phi(x_1,t_1)[\eta]\,\phi(x_2,t_2)[\eta]\dots\phi(x_N,t_N)[\eta]\Big\rangle_\eta$$

$$= \sum_{\{\Gamma_5\}} \underbrace{I_{\Gamma_5}(t_1,t_2,\dots,t_N)}_{\text{Depends only on evolution time}}\,\underbrace{G_{\Gamma_4(\Gamma_5)}(x_1,x_2\dots,x_N)}_{\text{Usual 4-dim Green's function for graph } \Gamma_4}$$

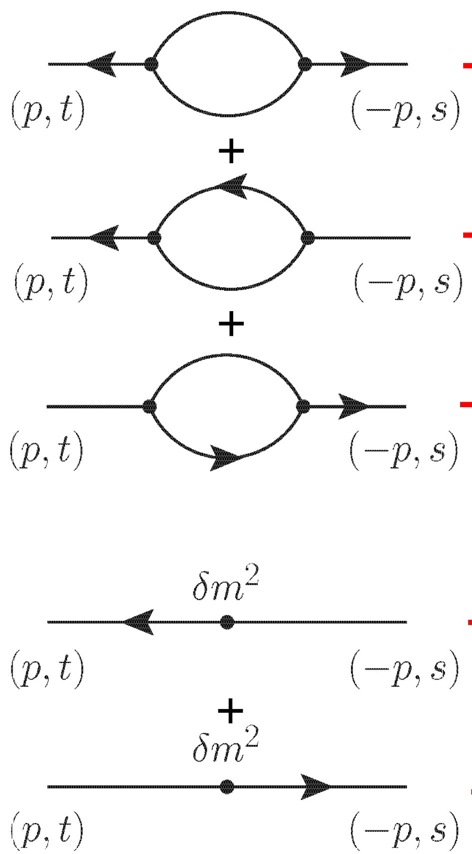
  - Sum over all 5-dim graphs Γ_5
  - 4-D Feynman graph for Γ_5 is $\Gamma_4\,(\Gamma_5)$
  - 4-D results guaranteed if: $\sum_{\substack{\Gamma_5 \\ \Gamma_4(\Gamma_5)=\Gamma_4}} I_{\Gamma_5}(t,t,\dots,t) = 1$

- 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, ϕ^3 theory at order λ^2 :

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



$$\left.\begin{array}{c} \frac{1}{6}e^{-|t-s|}\left[2 - e^{-|t-s|}\right] \\ + \\ \frac{1}{6}e^{-|t-s|}\left[1 + (t-s)\theta(t-s)\right] \\ + \\ \frac{1}{6}e^{-|t-s|}\left[1 + (s-t)\theta(s-t)\right] \end{array}\right\} \times \frac{1}{(p^2+m^2)^2}\int \frac{d^4k}{(2\pi)^4} \cdot \frac{1}{((k+p)^2+m^2)(k^2+m^2)}$$

Equal only when $t = s$

$$\left.\begin{array}{c} e^{-|t-s|}\left[\frac{1}{2} + (t-s)\theta(t-s)\right] \\ + \\ e^{-|t-s|}\left[\frac{1}{2} + (s-t)\theta(s-t)\right] \end{array}\right\} \times \frac{\delta m^2}{(p^2+m^2)^2}$$

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 $\widetilde{m} \neq m_0$? Evolution time and space-time weakly coupled.