Studies of Gauge-fixed Fourier acceleration for SU(3) gauge theory

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Yikai Huo, Norman H. Christ, Rana Urek

Columbia University

RBC/UKQCD Collaborations

COLUMBIA UNIVERSITY

SciDAC 5

ECP EXASCALE COMPUTING PROJECT

The RBC & UKQCD collaborations

Boston University
Nobuyuki Matsumoto

BNL and BNL/RBRC
Peter Boyle
Taku Izubuchi
Christopher Kelly
Shigemi Ohta (KEK)
Amarji Soni
Masaaki Tomii
Xin-Yu Tuo
Shuhei Yamamoto

University of Cambridge
Nelson Lachini

CERN
Matteo Di Carlo
Felix Erben
Andreas Jüttner (Southampton)
Tobias Tsang

Columbia University
Norman Christ
Sarah Fields
Ceran Hu
Yikai Huo
Joseph Karpie (JLab)
Erik Lundstrum
Bob Mawhinney
Bigeng Wang (Kentucky)

University of Connecticut
Tom Blum
Jonas Hildebrand
Luchang Jin
Vaishakhi Moningi
Anton Shcherbakov
Douglas Stewart
Joshua Swaim

DESY Zeuthen
Raoul Hodgson

Edinburgh University
Luigi Del Debbio
Vera Gülpers
Maxwell T. Hansen
Nils Hermansson-Truedsson
Ryan Hill
Antonin Portelli
Azusa Yamaguchi

Johannes Gutenberg University of Mainz
Alessandro Barone

Liverpool Hope/Uni. of Liverpool
Nicolas Garron

LLNL
Aaron Meyer

Autonomous University of Madrid
Nikolai Husung

University of Milano Bicocca
Mattia Bruno

Nara Women's University
Hiroshi Ohki

Peking University
Xu Feng
Tian Lin

University of Regensburg
Andreas Hackl
Daniel Knüttel
Christoph Lehner
Sebastian Spiegel

RIKEN CCS
Yasumichi Aoki

University of Siegen
Matthew Black
Anastasia Boushmelev
Oliver Witzel

University of Southampton
Bipasha Chakraborty
Ahmed Elgaziari
Jonathan Flynn
Joe McKeon
Rajnandini Mukherjee
Callum Radley-Scott
Chris Sachrajda

Stony Brook University
Fangcheng He
Sergey Syritsyn (RBRC)

Outline

- Critical slowing down in Lattice QCD
- Examine softly gauge-fixed 4D SU(3) gauge theory
- Introduce naïve Fourier acceleration
- Study resulting acceleration for 16^4 volume at β=6, 7 and 10
- Conclusions

Contributors: Luchang Jin, Ahmed Sheta, Yidi Zhao

Critical slowing down in lattice QCD

- Molecular dynamics (MD) time separating independent samples grows as $a \rightarrow 0$:
  - Barriers between topological sectors become harder to penetrate. (tunneling)
  - Longer MD time (defined at the lattice scale) is needed to decorrelate at a physical distance which is a growing number of lattice units: $\tau \sim a^{-x}$. (critical slowing down)
- Tunneling: open boundary conditions
- Critical slowing down: Fourier acceleration

Critical slowing down in lattice QCD

- Molecular dynamics (MD) time separating independent samples grows as $a \rightarrow 0$:
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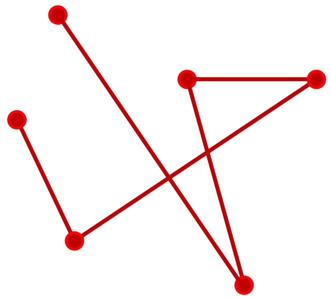
- Tunneling: open boundary conditions
- Critical slowing down: Fourier acceleration

Critical slowing down and HMC

- Introduce fifth simulation dimension with momenta π_l conjugate to each U_l :



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

- HMC executes ballistic motion (“trajectory”) between momentum randomizations
- At tree level expect: $\tau \sim N_{\text{steps}} \sim R\rho/a$ [Kennedy & Pendleton]
- Pure-gauge simulation:
  - $\tau \sim 1/a^2$ [Luscher & Schaefer]
  - Attributed to non-renormalizability of HMC

Fourier acceleration

- Recall for a system of simple harmonic oscillators:

$$H = \sum_{i=1}^{N} \left\{ \frac{p_i^2}{2M} + \frac{k_i}{2} q_i^2 \right\}$$

  - Arrange $j < i \rightarrow k_j < k_i$
  - Frequencies are $\omega_i^2 = k_i/M$
  - Time between independent samples determined by $1/\omega_1$ but integration step size determined by $1/\omega_N$
  - Number of steps ~ ω_N/ω_1 grows with the ratio of scales.
- Growth of effort with ω_N/ω_1 can be eliminated:
  - Make M mode-dependent: $M \rightarrow M_i = k_i$
  - Now $\omega_i^2 = k_i/M_i = 1$, removing the problem!

Fourier acceleration & lattice QCD

- "Fourier" acceleration is complicated by local gauge symmetry:
  - Fix the gauge *or*
  - Identify gauge-covariant "modes", *e.g*. those of gauge covariant Laplacian (RMHMC – talk of Sarah Fields)
- Soft gauge fixing:

$$Z = \int d[U] \frac{e^{-S_{\rm Wilson}[U]} \int d[g] e^{-S_{\rm GF}[U^g]}}{\int d[g'] e^{-S_{\rm GF}[U^{g'}]}}$$

$$= \int d[U] \frac{e^{-S_{\rm Wilson}[U] - S_{\rm GF}[U]}}{\int d[g'] e^{-S_{\rm GF}[U^{g'}]}}$$

1. Transform U → U^g
2. Drop $\int d[g]$

Soft gauge fixing

- Partition function:

$$Z = \int d[U] \frac{e^{-S_{\mathrm{Wilson}}[U]-S_{GF}[U]}}{\int d[g']e^{-S_{GF}[U^{g'}]}}$$

- Completely softly gauge-fixed action:

$$S[U] = S_{\mathrm{Wilson}}[U] + S_{GF}[U] + S_{FP}[U]$$

$$S_{FP}[U] = -\ln\left(\int d[g]e^{-S_{GF}[U^g]}\right)$$

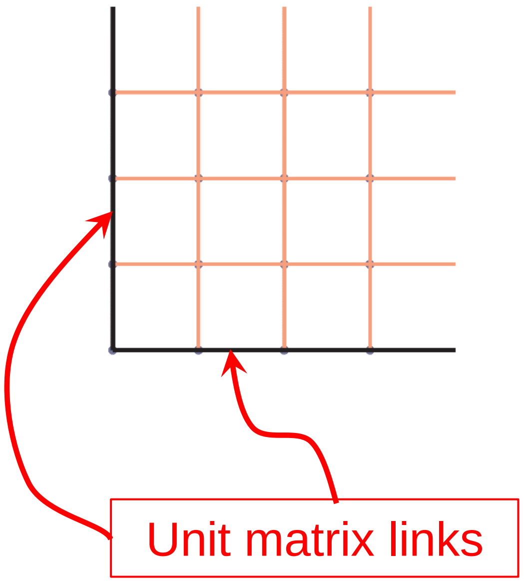
- For Landau gauge:

$$S_{GF}[U] = -\frac{\beta M}{3}\sum_{n,\mu}\mathrm{Tr}\left\{U_\mu(n)\right\}$$

- Introduced in 1990 to solve Gribov copy problem:
  - D. Zwanziger, Nuclear Physics B345 (1990) 461-471.
  - Parrinello andJona-Lasinio, Phys Lett B251 175-180.

Fourier acceleration

- Connect links as a torus but set boundary links to the unit matrix:
- Let $\{\phi_{n\mu}^{T}(k,i)\}_{1 \leq i \leq 3}$ and $\phi_{n\mu}^{L}(k)$ be the transverse and longitudinal free-field modes for unit boundaries.



- Use Fourier-accelerating K.E. term in Hamiltonian:

$$H = \sum_{k,i} \tilde{\pi}_a^{T}(k,i) \frac{1}{2k^2} \tilde{\pi}_a^{T}(k,i) + \sum_{k} \tilde{\pi}_a^{L}(k) \frac{1}{2M^2} \tilde{\pi}_a^{L}(k) + S(U)$$

Where

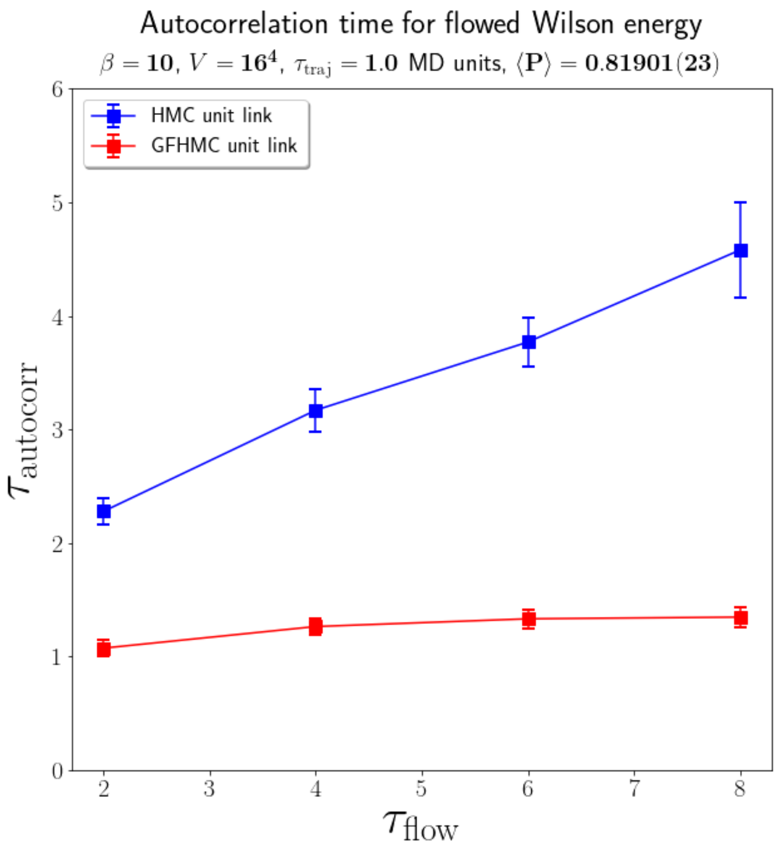
$$\pi_a(n,\mu) = \sum_{k,i} \tilde{\pi}_a^{T}(k,i) \phi_{n\mu}^{T}(k,i) + \sum_{k} \tilde{\pi}_a^{L}(k) \phi_{n\mu}^{L}(k)$$

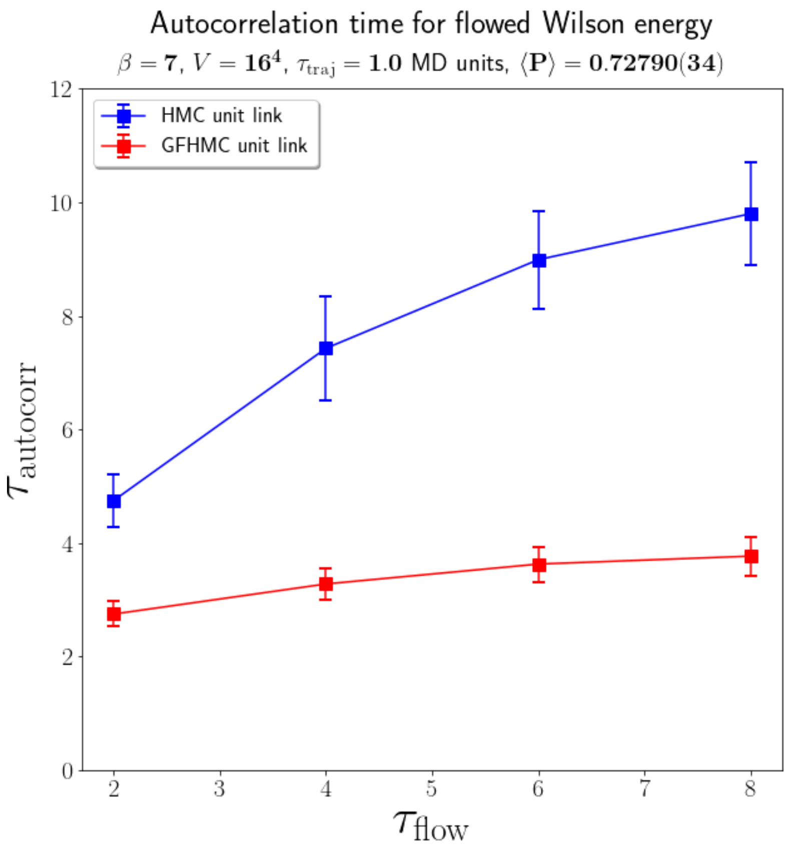
Computational Details

- SU(3) gauge theory, Wilson action
- 16^4 volume, $\beta = 6, 7, 10$ and ~~100~~
- Between 5K and 10K (GF)HMC trajectories
- Trajectory lengths of 0.6, 1.0 and 2.0 MD time units
- Soft gauge fixing
  - M = 3 for gauge fixed case
  - 200 heatbath sweeps for inner Monte Carlo
  - Small $\Delta t = 0.0125$, average plaquette is accurate at 1/1000
- Boundary conditions:
  - **Unit link**: see previous slide
  - **Frozen**: equilibrate configuration with periodic BCs, then leave links on boundary fixed.
- Study flowed Wilson energy, varying flow time.

Results

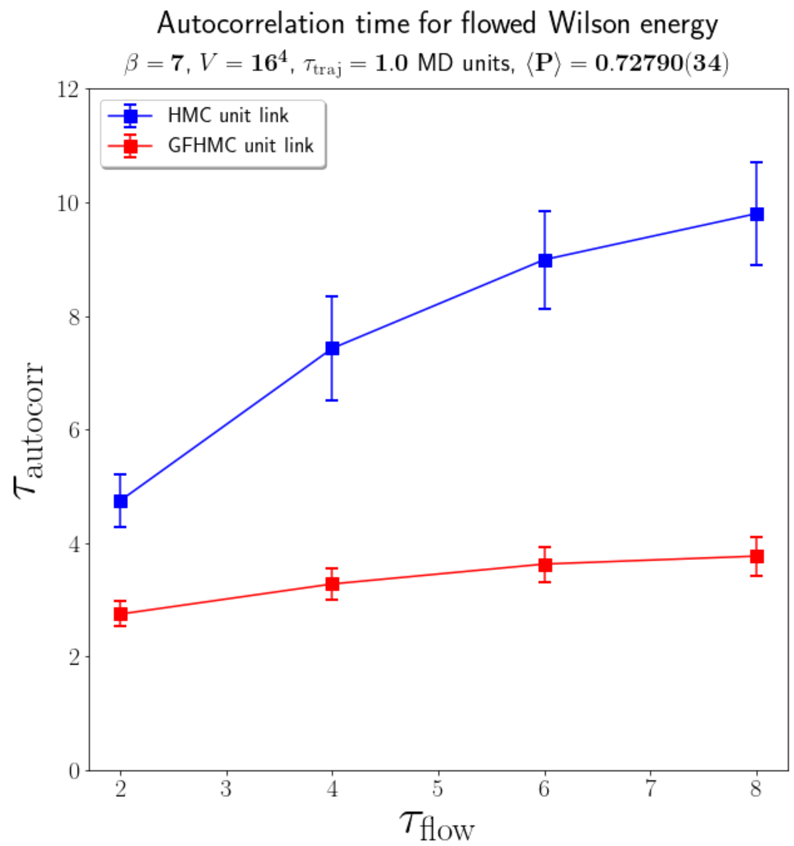
- Compare β = 10 and 7

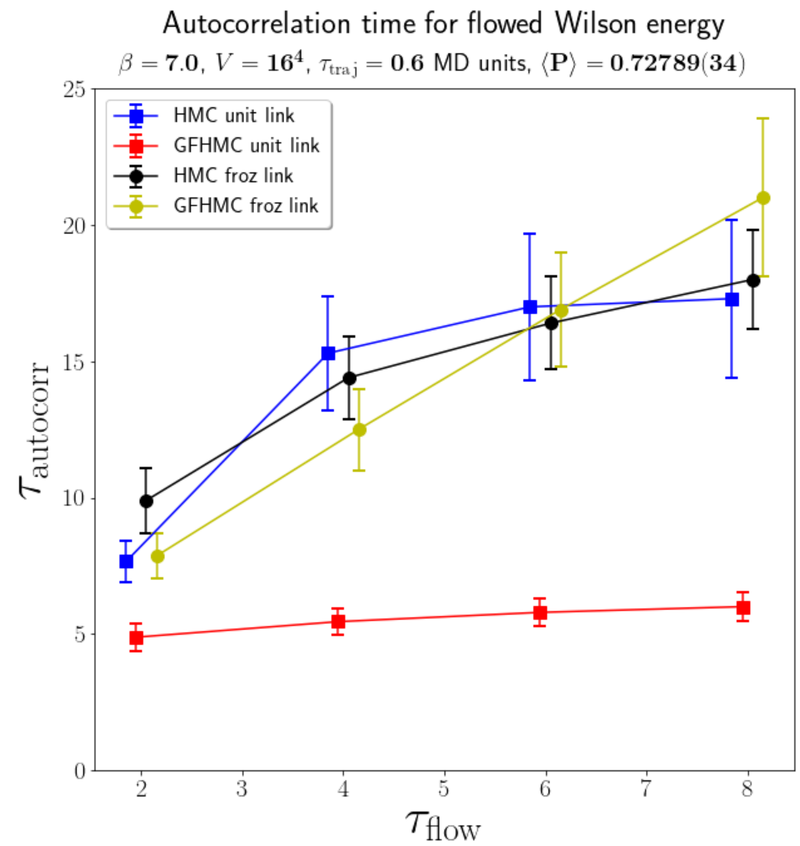




Results

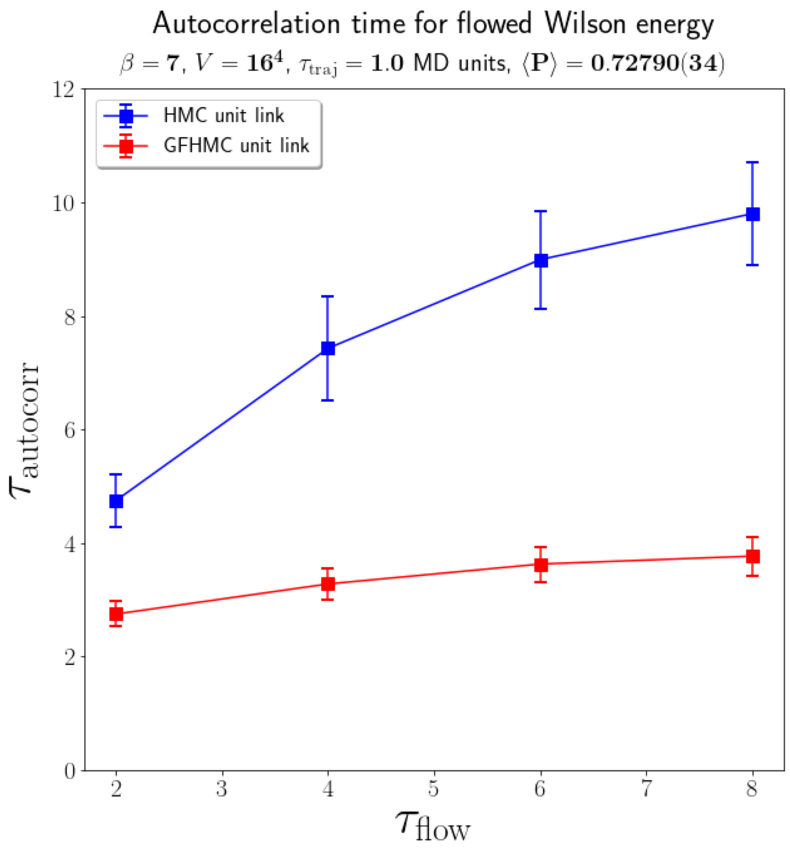
- At β = 7.0 compare two trajectory lengths: 1.0 and 0.6 MD units:

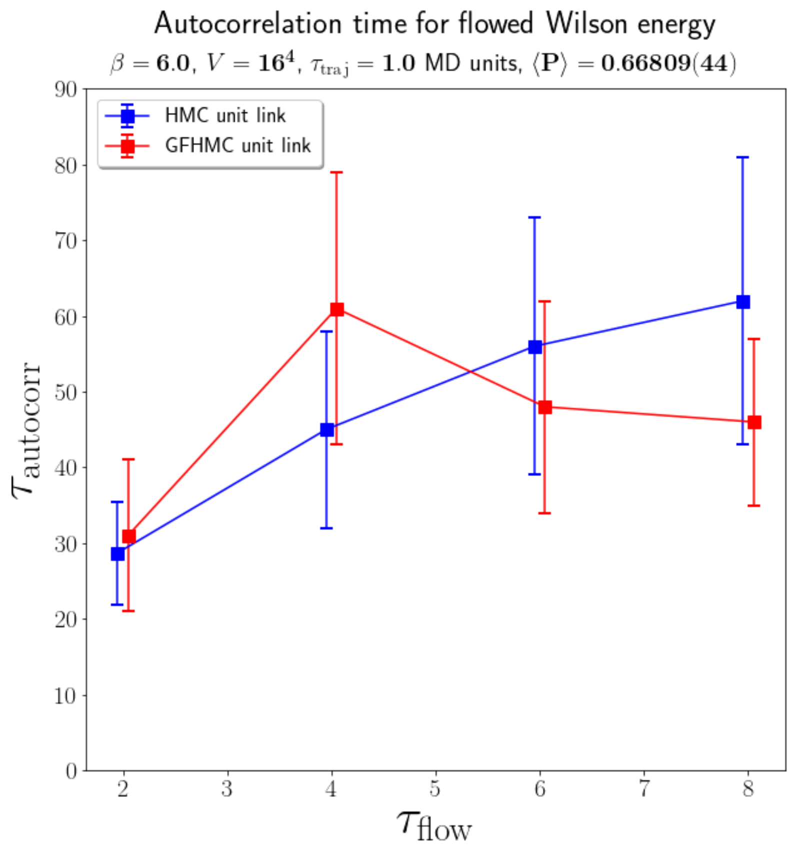




Results

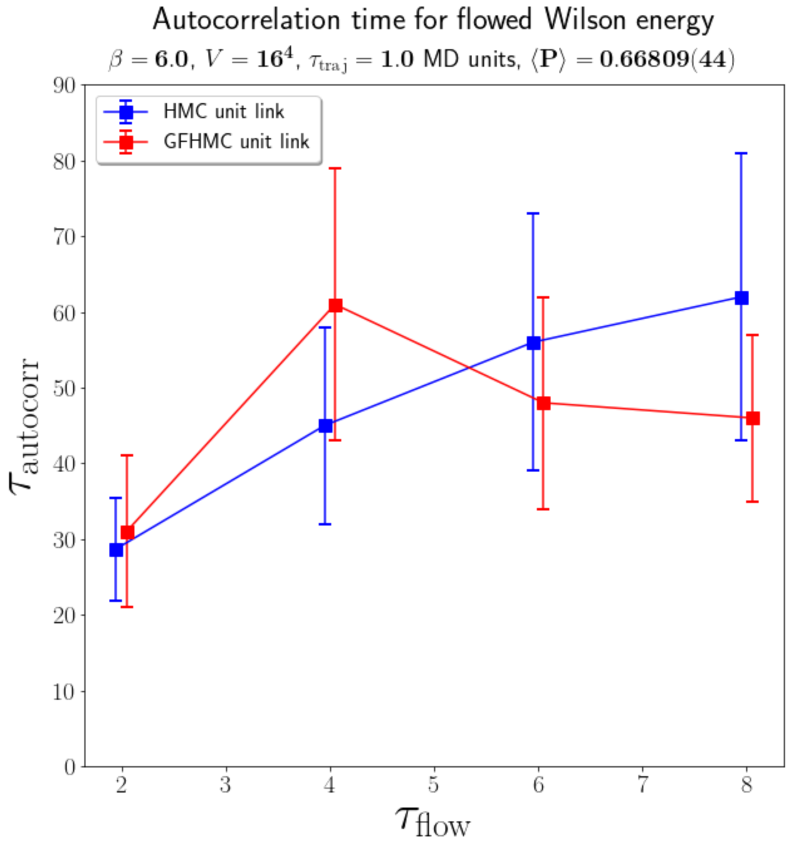
- Compare β = 7.0 and 6.0, trajectory length 1.0 MD units, unit link BC:

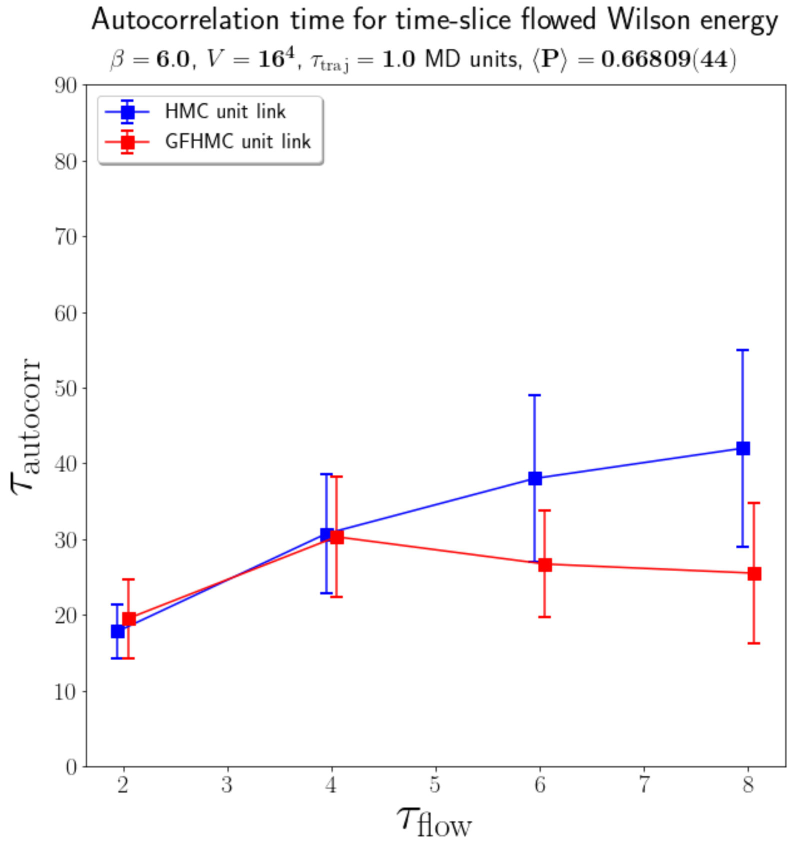




Results

- Compare b=6.0 4-volume versus time-slice averaged:





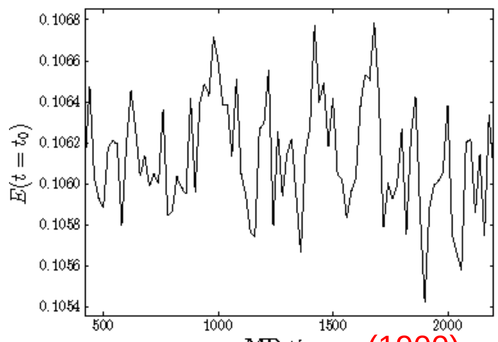
Conclusions

- Gauge-fixed Fourier acceleration reduces autocorrelation 3x at β = 7.0 for SU(3) Yang-Mills
- Using free-field modes appears to be important
- Acceleration of volume-averaged, flowed Wilson energy disappears at β = 6.0 (confined)
- Some acceleration may remain at β = 6.0 for time-slice averages?
- See presentations of Erik Lundstrum (Nambu HMC) and Sarah Fields (RMHMC) tomorrow at 2:15 and 2:35 in LT2.

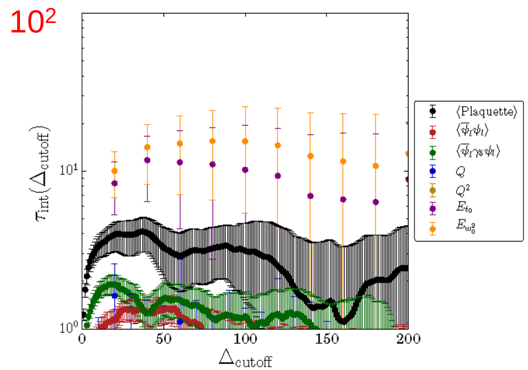
Backup

Physical DWF ensembles

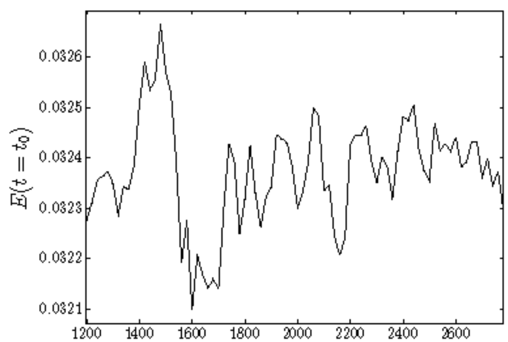
$E(t_0)$



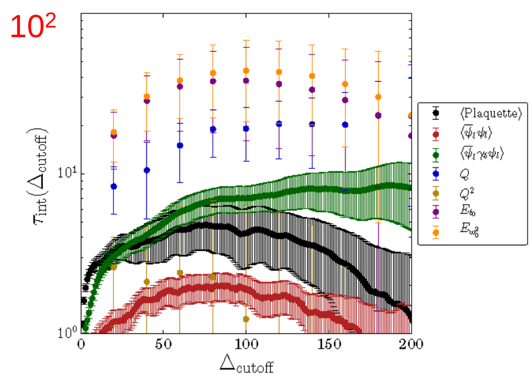
(1900)



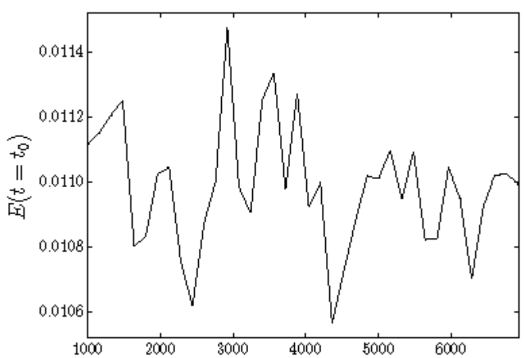
$1/a$ = 1.73 GeV, 48^3 x 96, m_π = 139 MeV



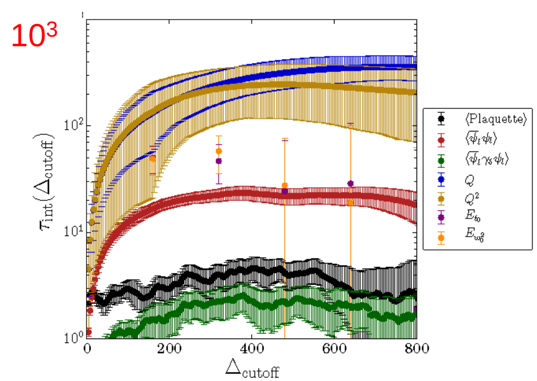
(1600)



$1/a$ = 2.36 GeV, 64^3 x 128, m_π = 139 MeV



(6000)



$1/a$ = 3.15 GeV, 32^3x64, m_π = 371 MeV