QCDOC and Dynamical Domain Wall Fermion Simulations

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RBC Collaboration

SCIDAC All-Hands Meeting
Jefferson National Laboratory
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1. Some DWF issues
2. Exact QCD algorithms
3. Choosing actions and parameters
4. Physics to do

RBRC-BNL-CU (RBC) Collaboration, May 2005

RBRC

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Recent Previous Members

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Noaki, Jun-Ichi
Orginos, Kostas
Yamada, Norikazu

Laiho, Jack

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UKQCD Collaborators on DWF Calculations, May 2005

UKQCD

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Boyle, P. A.

Clark, M. A.

Joo, B.

Kennedy, A. D.

Kenway, R. D.

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Tweedie, R. J.

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Domain Wall Fermion Operator

- Introduce extra dimension, labeled by s

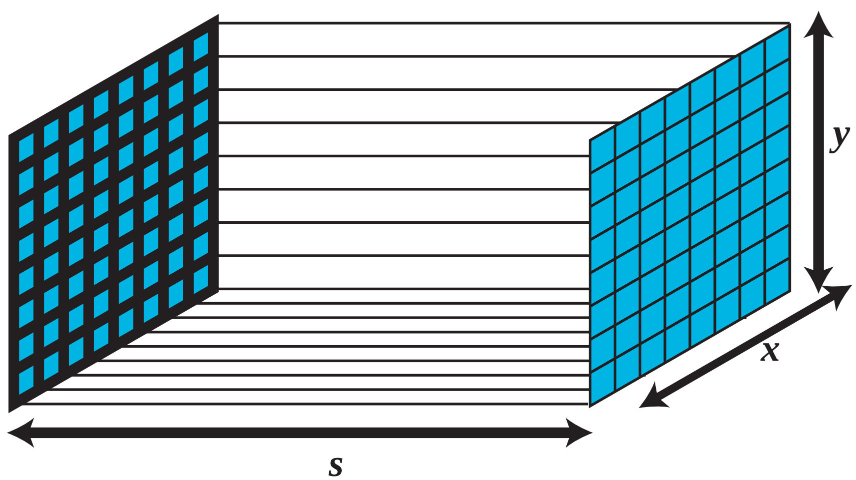
$$D_{x,s;x',s'} = \delta_{s,s'} D^{\parallel}_{x,x'} + \delta_{x,x'} D^{\perp}_{s,s'}$$

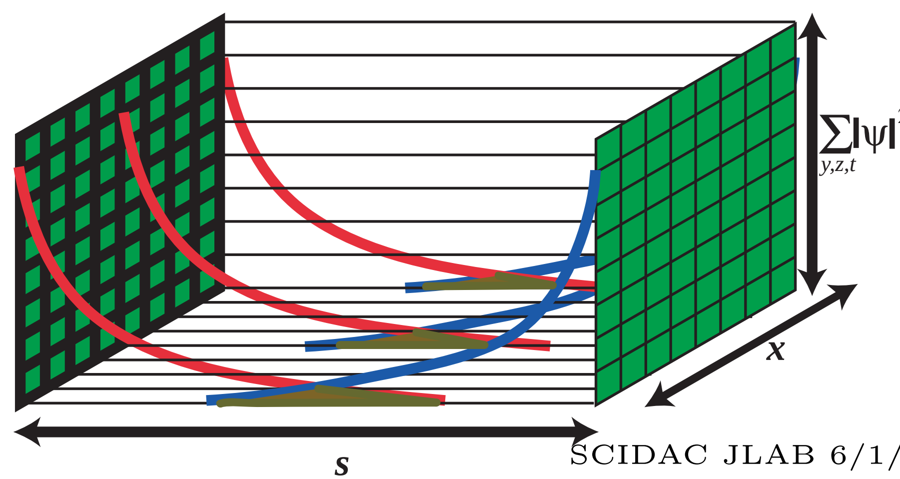
- $D^{\parallel}_{x,x'}$ is a Wilson Dirac operator with an opposite sign for the mass term.

$$D^{\parallel}_{x,x'} = \frac{1}{2}\sum_{\mu=1}^{4}\left[(1-\gamma_\mu)U_{x,\mu}\delta_{x+\hat{\mu},x'} + (1+\gamma_\mu)U^{\dagger}_{x',\mu}\delta_{x-\hat{\mu},x'}\right] + (M_5 - 4)\delta_{x,x'}$$

- $D^{\perp}_{s,s'}$ couples points in fifth dimension, distinguishing left and right handed fermions

$$\frac{1}{2}\left[(1-\gamma_5)\delta_{s+1,s'} + (1+\gamma_5)\delta_{s-1,s'} - 2\delta_{s,s'}\right] - \frac{m_f}{2}\left[(1-\gamma_5)\delta_{s,L_s-1}\delta_{0,s'} + (1+\gamma_5)\delta_{s,0}\delta_{L_s-1,s'}\right]$$





Residual Chiral Symmetry Breaking for DWF

- Consider introducing in action a $SU(N_f)$ matrix Ω through term at $l \equiv L_s/2$

$$-\sum_x \left\{ \overline{\Psi}_{x,l-1} P_L \left(\Omega^\dagger - 1\right) \Psi_{x,l} + \overline{\Psi}_{x,l} P_R \left(\Omega - 1\right) \Psi_{x,l-1} \right\} \qquad \Omega \to U_R \, \Omega \, U_L^\dagger$$

- Conventional DWF recovered by $\Omega \to 1$
- QCD chiral Lagrangian $\mathcal{L}^{(2)}_{\mathrm{QCD}}$, with $\Sigma \equiv \exp\left[2i\phi^a t^a / f\right]$ and mass matrix M is:

$$\frac{f^2}{8} \mathrm{Tr}\left(\partial_\mu \Sigma \partial^\mu \Sigma^\dagger\right) + v \, \mathrm{Tr}\left[M\Sigma + (M\Sigma)^\dagger\right] + v' \, \mathrm{Tr}\left[\Omega\Sigma + (\Omega\Sigma)^\dagger\right] + v'' \, \mathrm{Tr}\left[\Omega M^\dagger + \Omega^\dagger M\right]$$

- For modes bound to walls of fifth dimension, Ω enters Green's functions as

$$\Omega e^{-\alpha L_s} \quad \Rightarrow \quad v', v'' \sim e^{-\alpha L_s}$$

- Chiral condensate from differentiating w.r.t. mass, m_π^2 from expanding Σ

$$-\langle \overline{q} q \rangle (m_f = 0, L_s) \sim v + v'' \qquad v = \frac{f^2 m^2_{\pi^+}}{4(m_u + m_d + 2m_{\mathrm{res}})} \quad m_{\mathrm{res}} \equiv v'/v$$

Chiral Perturbation Theory Comparisons

- The chiral Lagrangian at the next order contains new low-energy constants for continuum QCD, denoted by L_i for $i = 1$ to 10.
- For m_π^2, 2 terms are needed

$$(2L_6 - L_4) \qquad\qquad (2L_8 - L_5)$$

- For DWF, at finite lattice spacing, the same terms are needed, although now one has $L_i(a) = L_i + \mathcal{O}(a^2)$.
- For DWF, to fit partially quenched data for $m_{\rm PS}^2$ and $f_{\rm PS}$ to NLO one needs 6 parameters and the known value for $m_{\rm res}$.
- For ASQTAD staggered, one needs 10 parameters. The additional 4 parameters come from lattice terms which break symmetries.
- Fewer parameters for DWF should give better control over the chiral limit.

Lattice QCD Algorithms

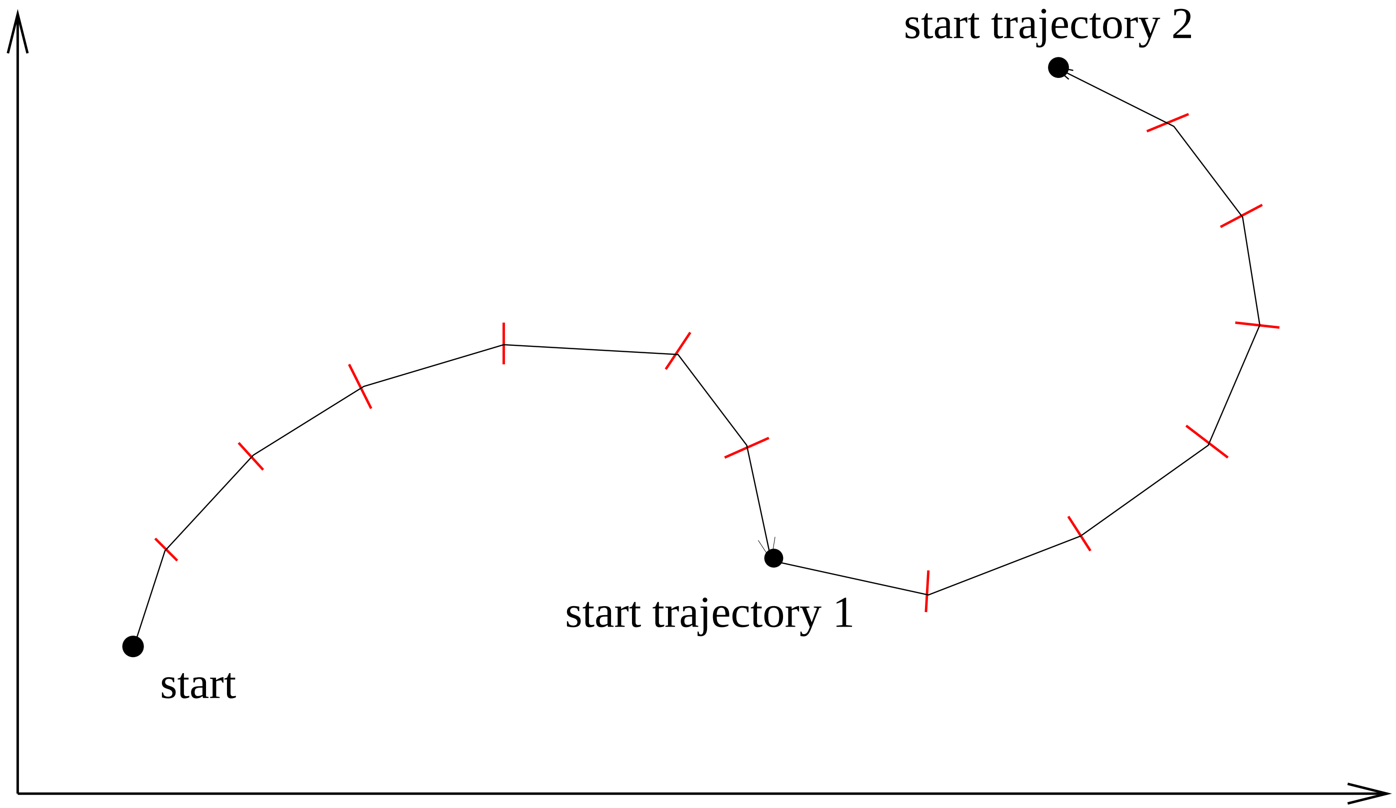
- Fermion determinant represented by "pseudo fermion" fields

$$Z = \int [dU]\,[d\psi]\,[d\bar\psi]\,\exp\{-\beta S_g + \bar\psi(\not{D}+m)\psi\} = \int [dU]\,\det(\not{D}+m)\exp\{-\beta S_g\}$$
$$= \int [dU]\,[d\phi^*][d\phi]\exp\{-\beta S_g + \phi^*(\not{D}+m)^{-1}\phi\}$$
$$= \int [dU]\,[d\Pi]\,[d\phi^*][d\phi]\exp\{-\Pi^2 - \beta S_g + \phi^*(\not{D}+m)^{-1}\phi\}$$
$$= \int [dU]\,[d\Pi]\,[d\phi^*][d\phi]\exp\left\{-\Pi^2 - \beta S_g + \phi^*[(\not{D}+m)(\not{D}^\dagger+m)]^{-1/2}\phi\right\}$$

- Since $\det(\not{D}+m)$ is positive definite, it equals $\det[(\not{D}+m)(\not{D}^\dagger+m)]^{-1/2}$.
- All eigenvalues of $(\not{D}+m)(\not{D}^\dagger+m)$ are positive, which yields a positive definite probability weight for a single quark flavor.
- The Rational Hybrid Monte Carlo algorithm of Clark and Kennedy (UKQCD) is an exact algorithm that utilizes the square root.
- Therefore, 2+1 flavor DWF QCD can be simulated with an exact algorithm.

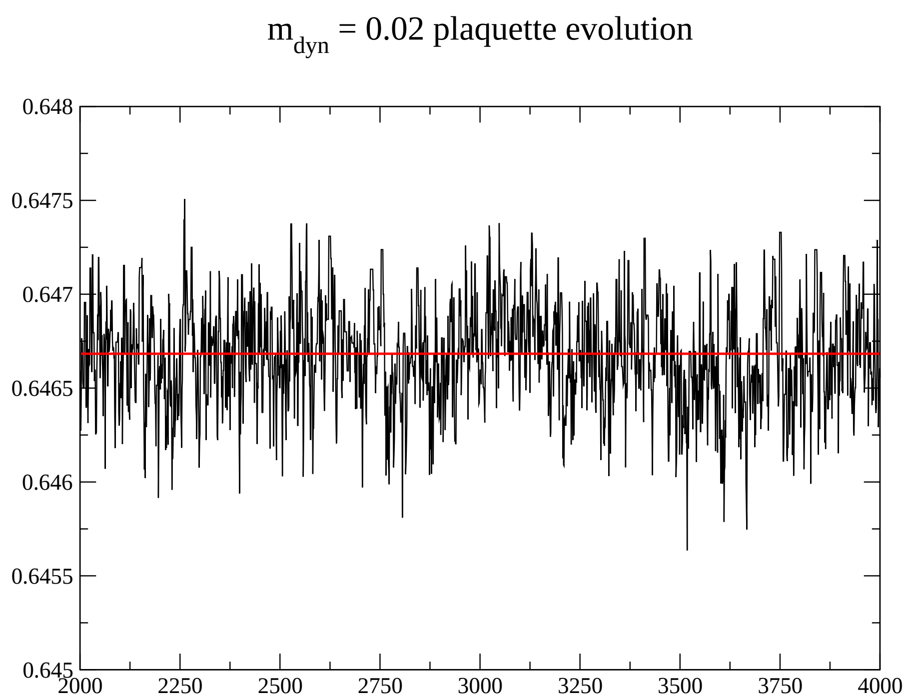
Moving Through the Phase Space of QCD

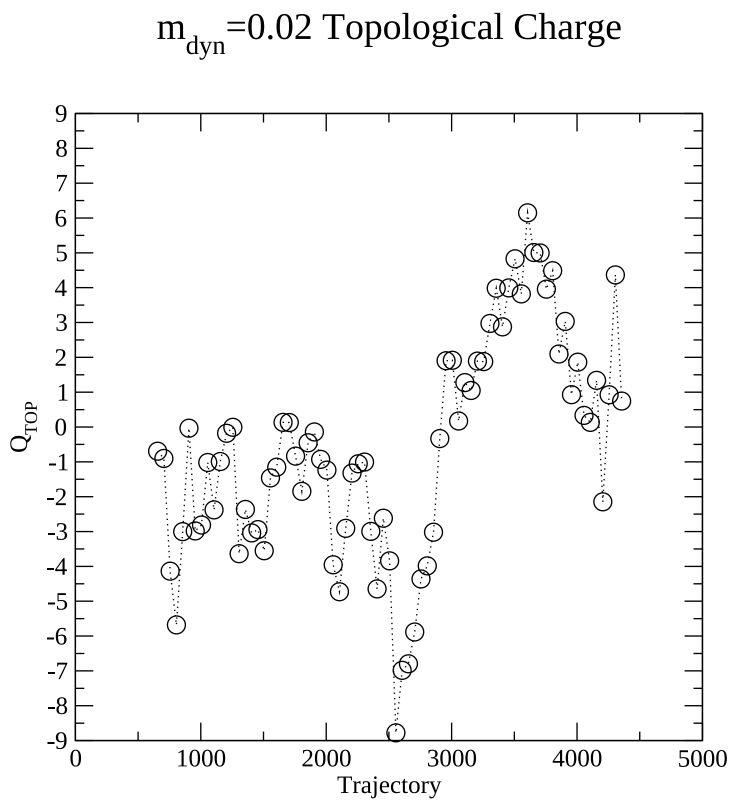
- RHMC implemented in CPS software for QCDOC
- Motion through phase space occurs in small steps
- What is efficiency for decorrelating gluon configurations?



Evolution of $N_f = 2$ Lattices with $m_{\text{dyn}} \approx m_{\text{strange}}/2$

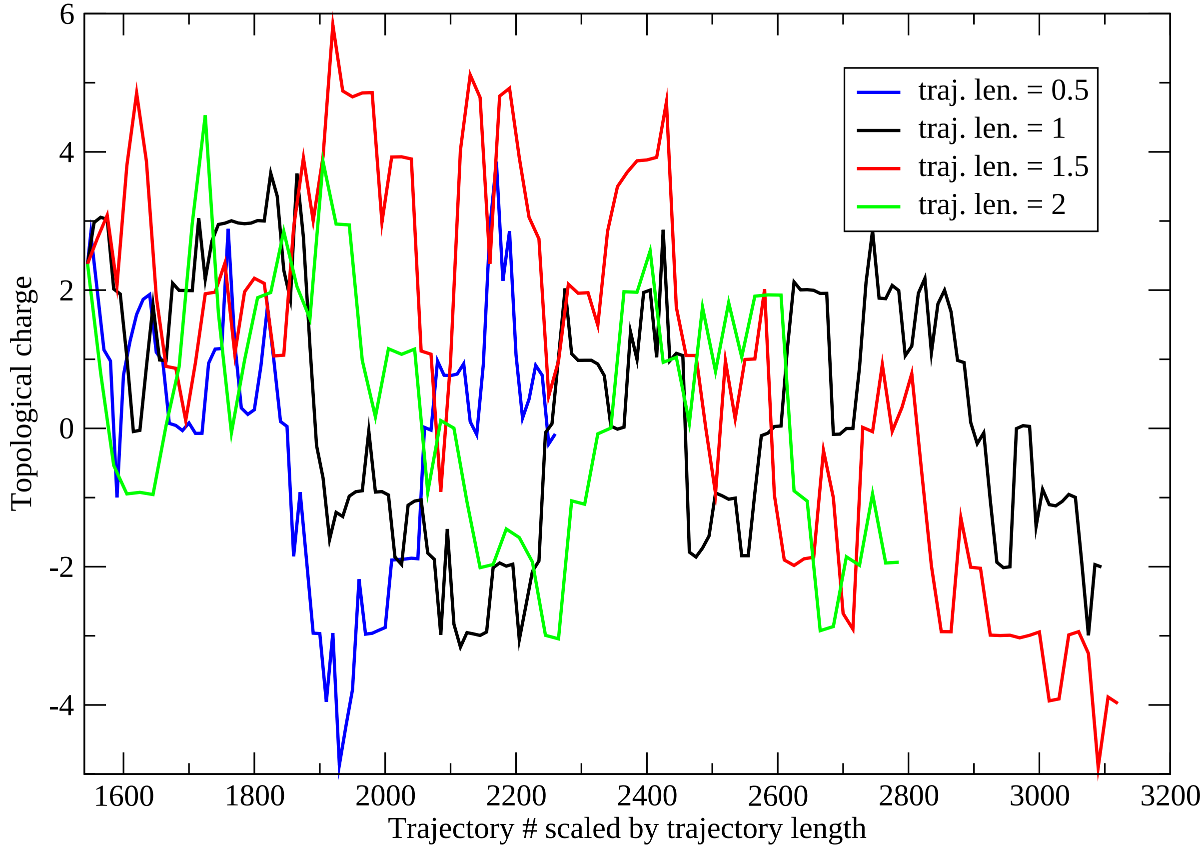
- Long autocorrelation times can yield underestimation of errors
- Topological fluctuations correctly weighted for DWF, if evolutions are long enough to sample phase space.





Evolution of $N_f = 3$ Lattices with $m_{\rm dyn} \approx m_{\rm strange}$

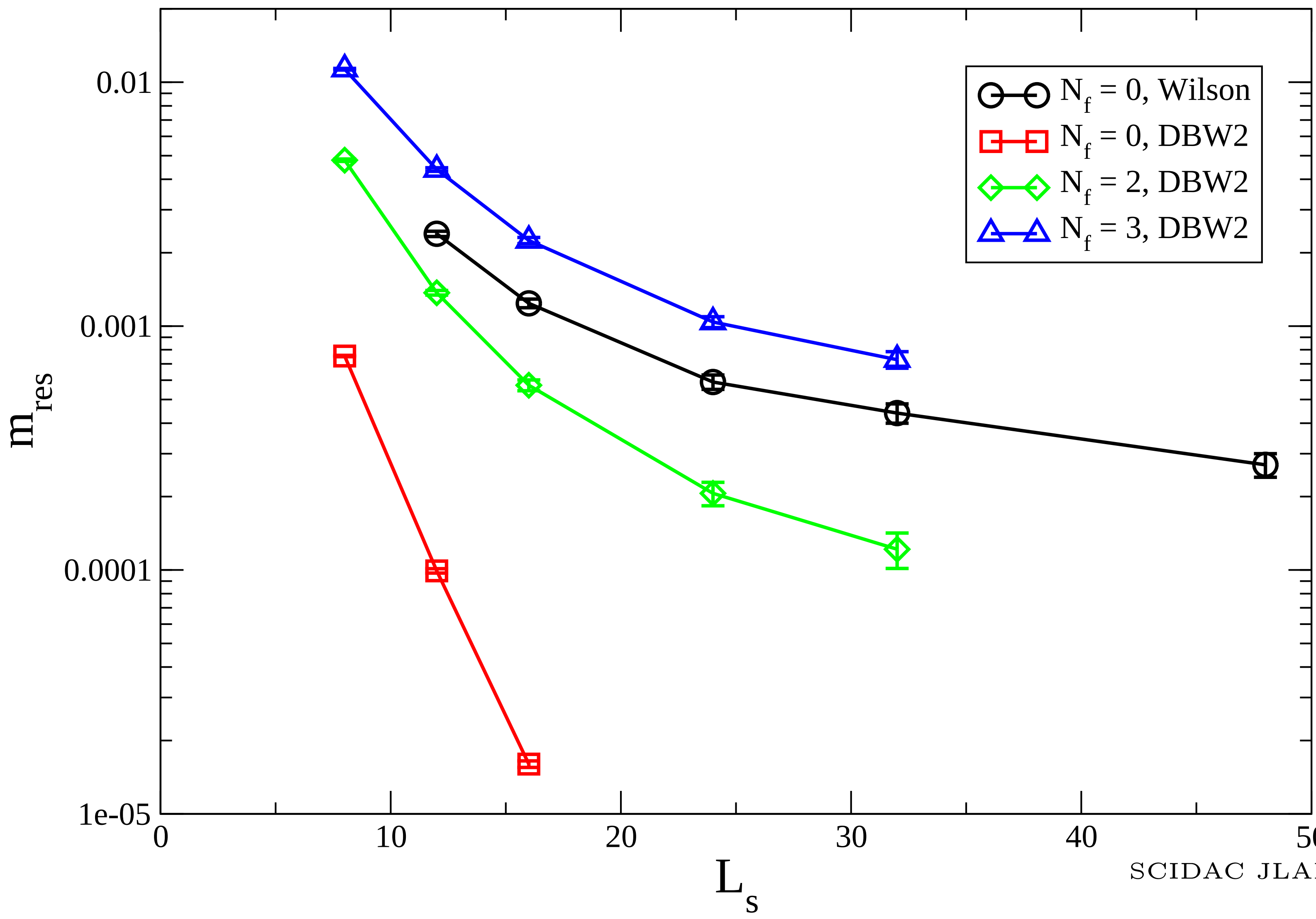
- Check correlation time versus length of trajectory with RHMC.



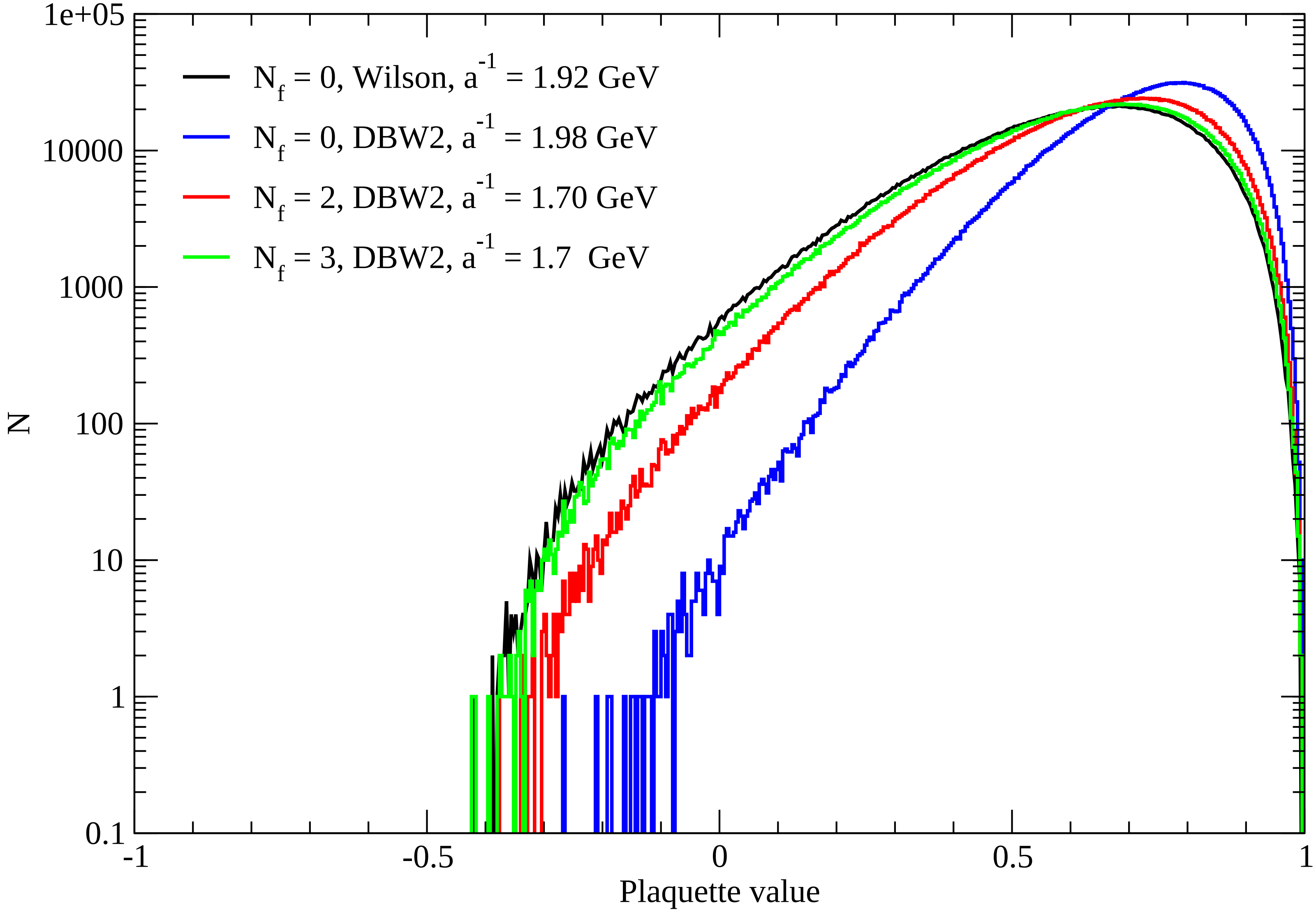
m_{res} versus L_s for $N_f = 0, 2$ and 3

Compare gauge actions composed of plaquette and rectangle terms.

$$S_g = (\beta/3)\left\{(1 - 8c_1)\sum \mathrm{Re}(\mathrm{Tr}U_P) + c_1 \sum \mathrm{Re}(\mathrm{Tr}U_R)\right\}$$

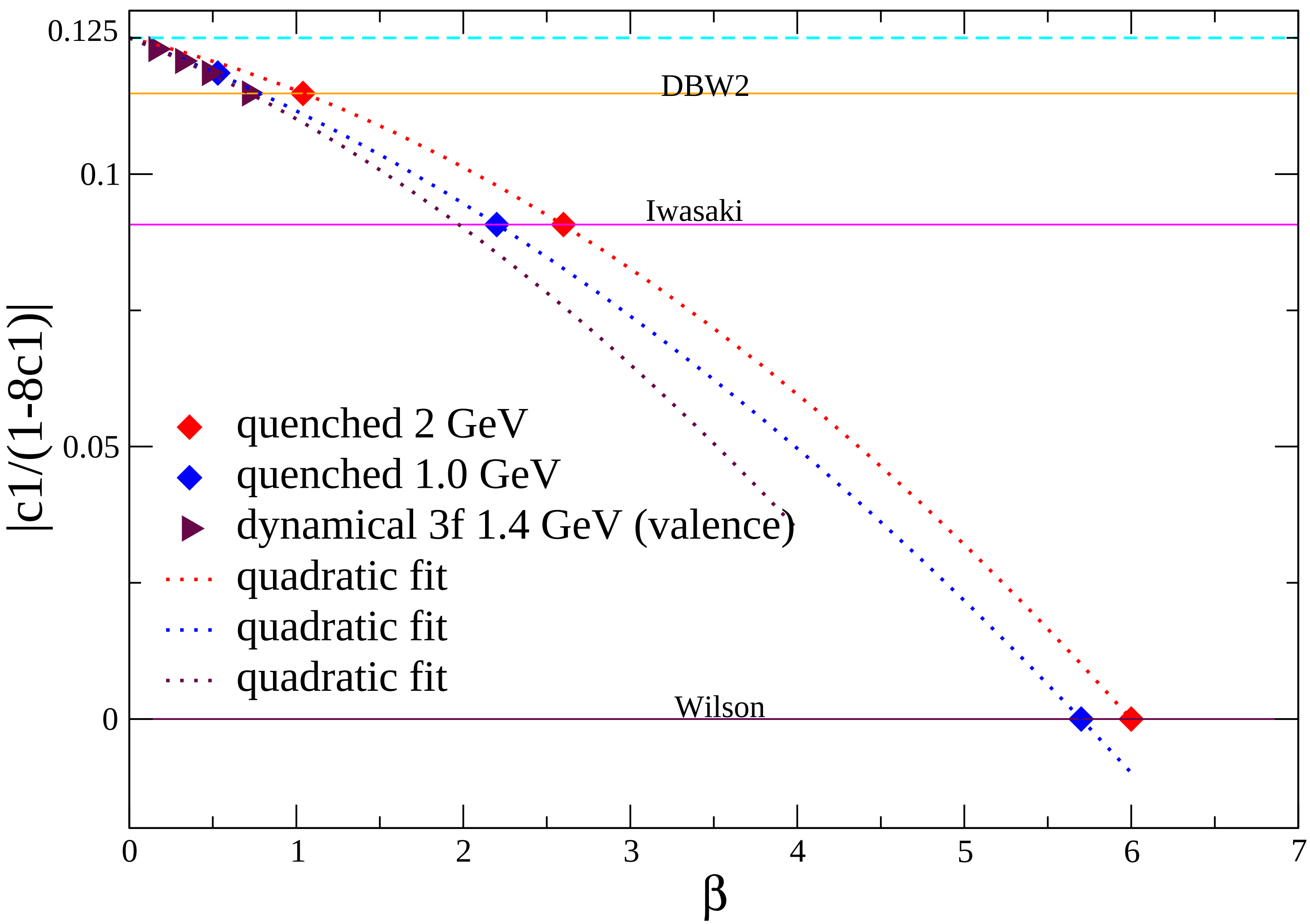


Plaquette Distributions at $a^{-1} \approx 2$ GeV

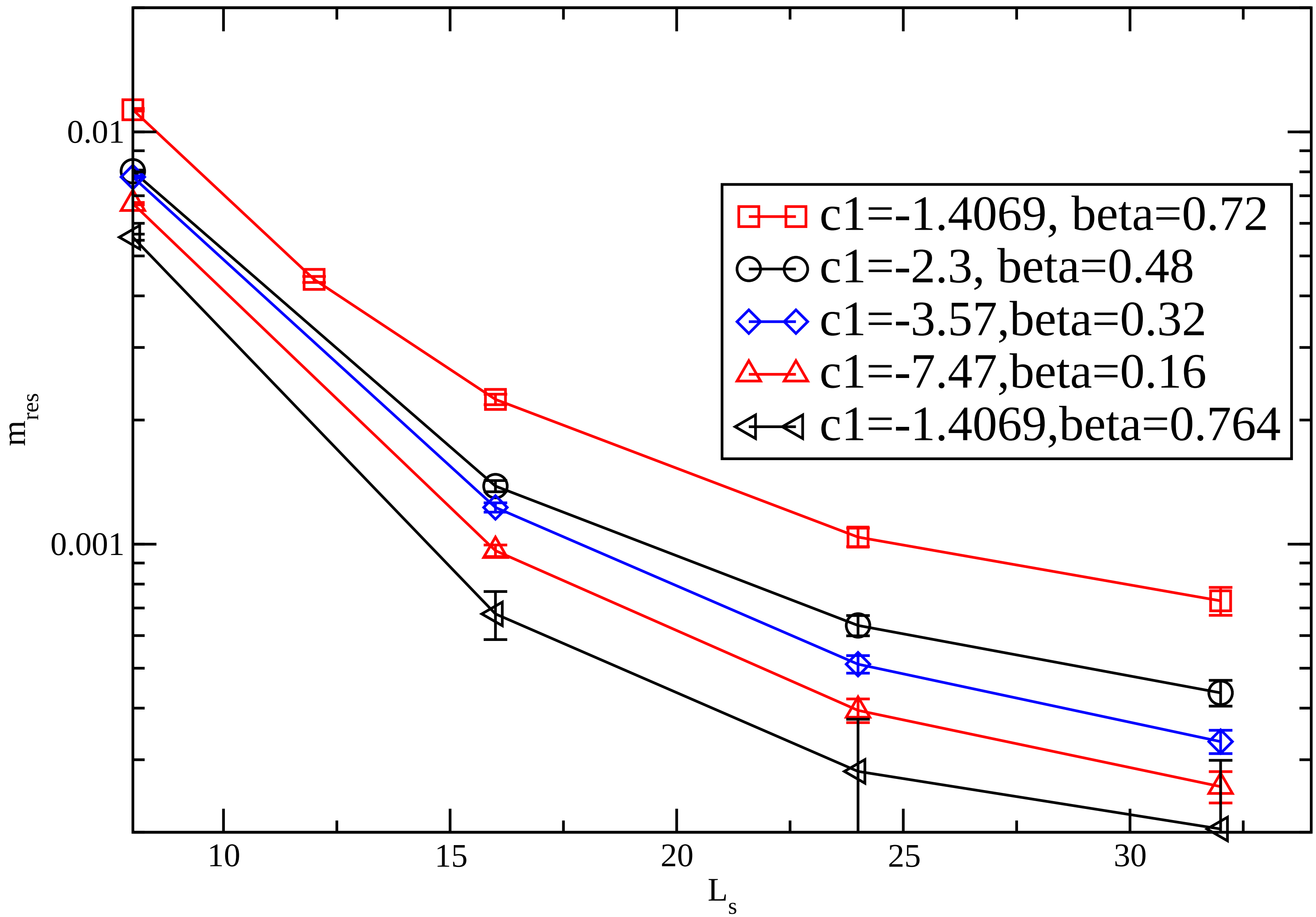


Full QCD with Plaquette plus Rectangle Actions

- Find lines with constant lattice spacing, a.
- Compare residual mass at fixed a.

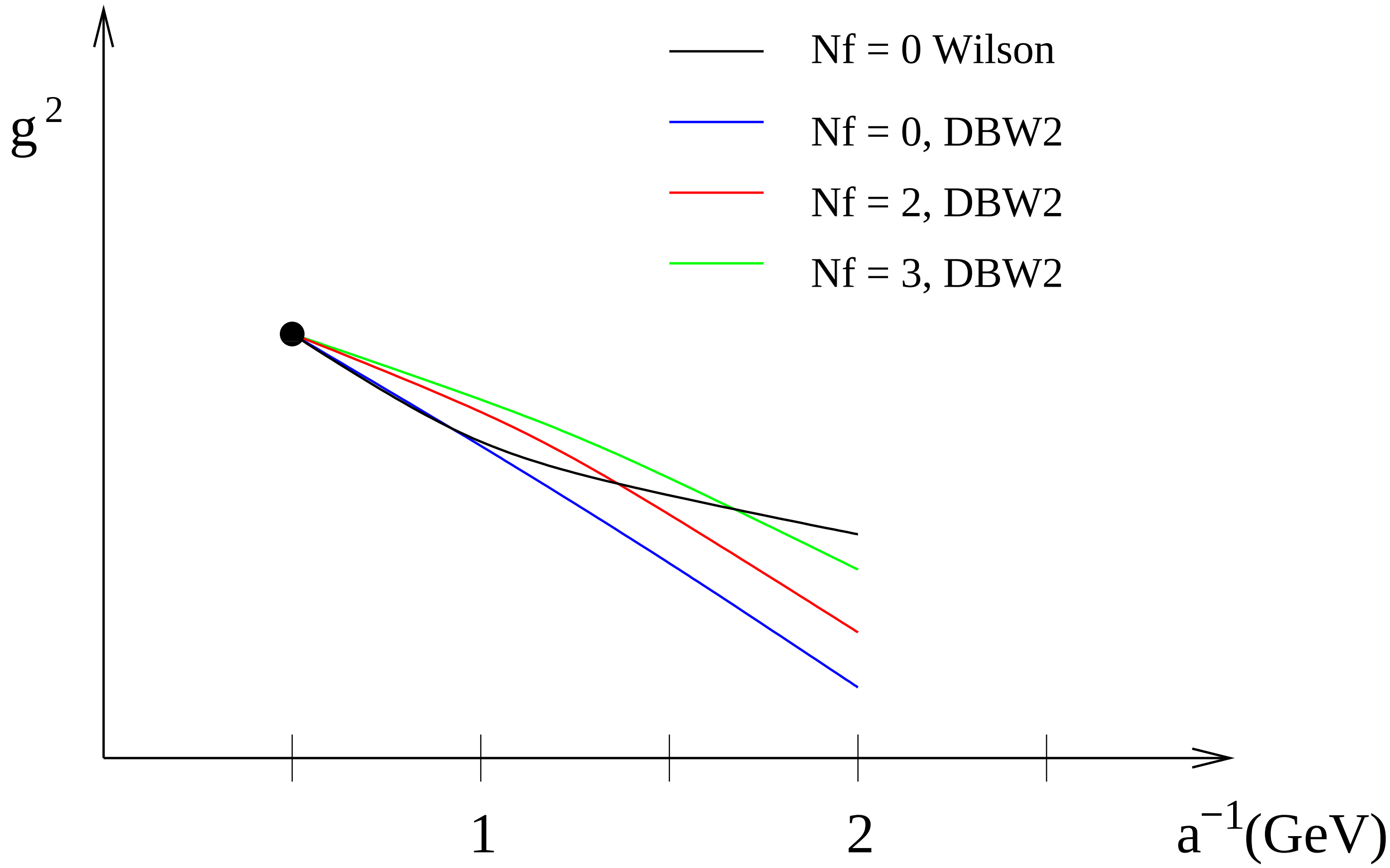


$m_{\rm res}$ for Plaquette plus Rectangle Actions



RG Evolution

- DBW2 action changes RG flow, so effective coupling strength at lattice scale is weaker.



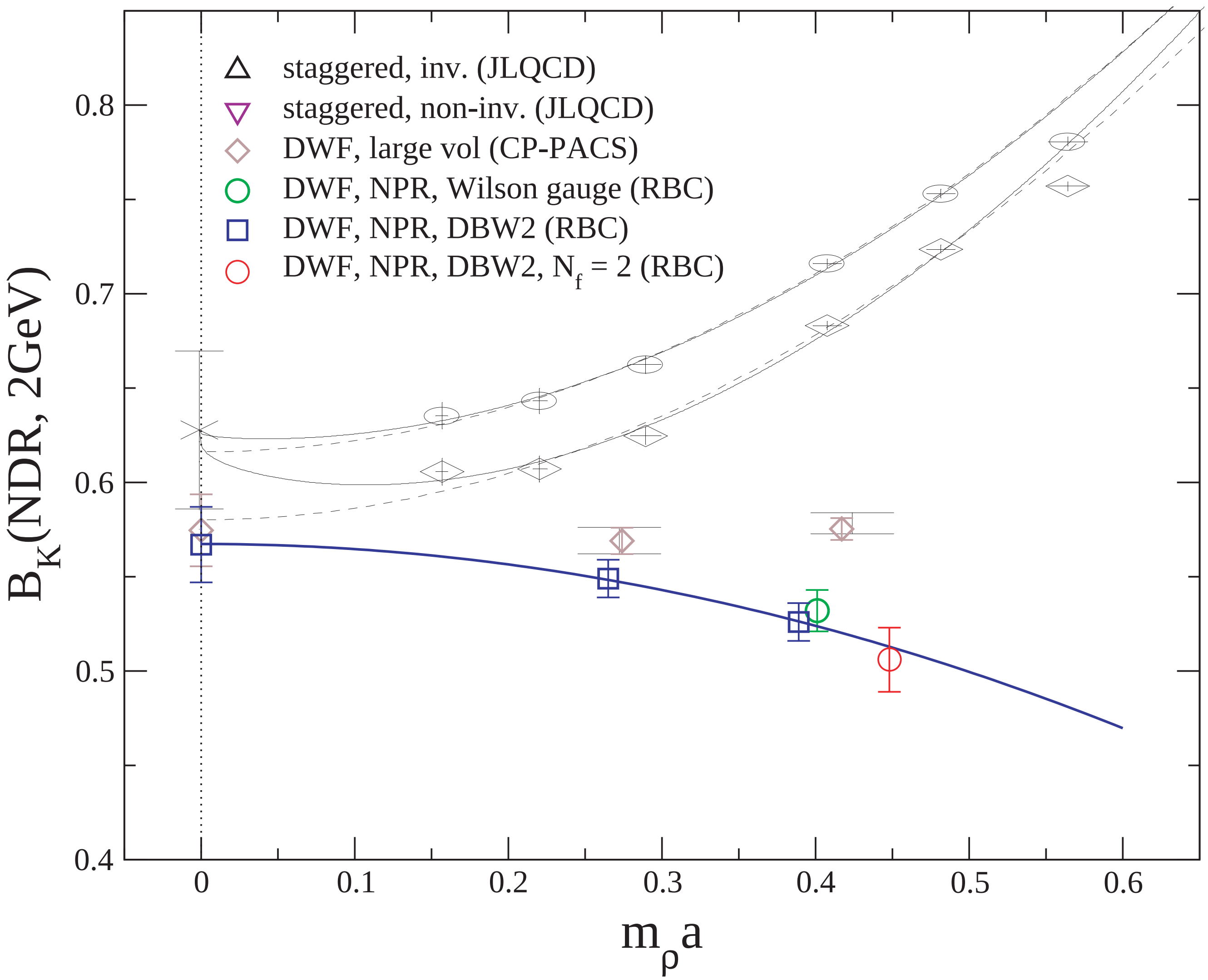
Physics Program -Two Primary Calculations

- 2+1 flavor $T = 0$ DWF using Rational HMC (RHMC) (≈ 0.6 of QCDOC)
  - Rectangle tests on $16^3 \times 32 \times 12$ - completed with $L_s = 8$
    - ≈ 1 month, done mostly during bring-up. 2 months
    - Can m_{res} be small for $a^{-1} \approx 1.3$ GeV? Yes.
  - If so, run with $16^3 \times 64 \times 16$, $a^{-1} \approx 1.3$ GeV. 2.5 fermi physical volume.
  - Follow with $24^3 \times 64 \times 16$ with $a^{-1} \approx 1.8$ GeV. 2.6 fm box. Ready to start
  - 10,000 trajectories on $24^3 \times 64 \times 16$ $m_u = m_d \approx m_s/5$ takes 1/2 year on 10k nodes. ($2\times$ uncertainty)
  - Studies above done with UKQCD collaboration. Are collaborating on lattice generation and physics.

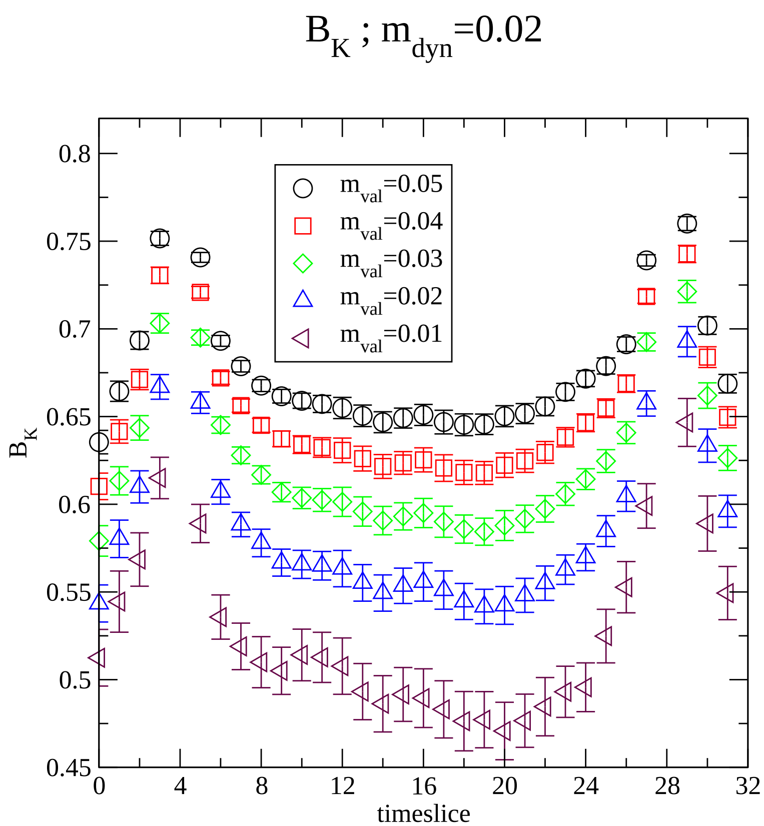
- 2+1 flavor thermo - staggered (P4 or ASQTAD). (≈ 0.3 of QCDOC)
  - P4 has better approach to Stefan-Boltzman limit (Heller, Karsch).
  - Zero temperature scaling study of P4 needed.
  - Do state of art determination of T_c with P4.
  - Continue to investigate thermodynamics with DWF.

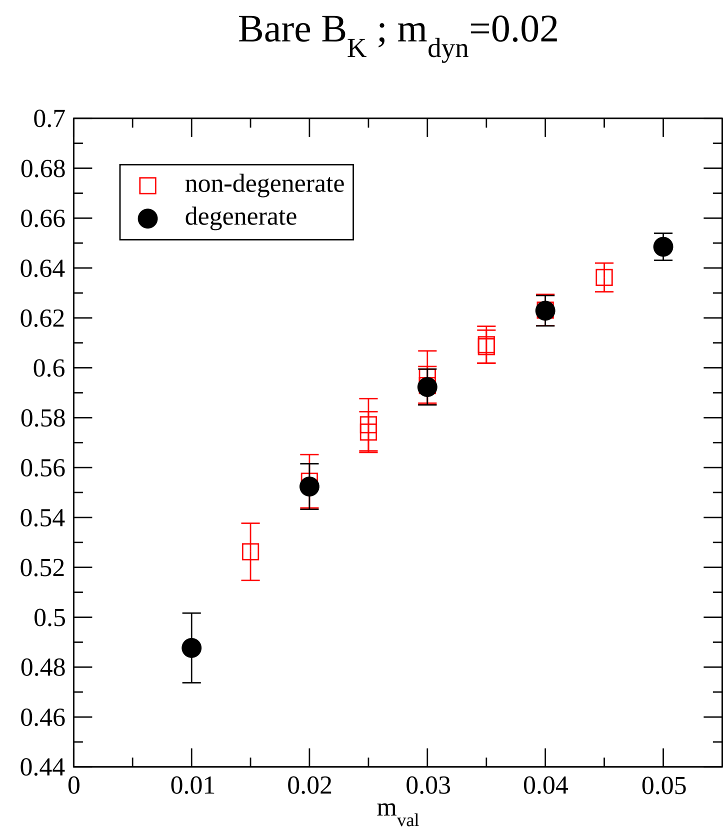
The Kaon B Parameter, $B_K^{\overline{\mathrm{MS}}}(\mu = 2\ \mathrm{GeV})$

	quenched $a \to 0$			dyn. $a^{-1} = 1.7$ GeV
PDG	JLQCD (stag)	CP-PACS (DWF)	RBC (DWF)	RBC (2f DWF)
0.65 ± 0.15	0.628 ± 0.042	0.575 ± 0.019	0.570 ± 0.020	0.492 ± 0.018



Improving B_K Determinations - Matrix Element Plateaus

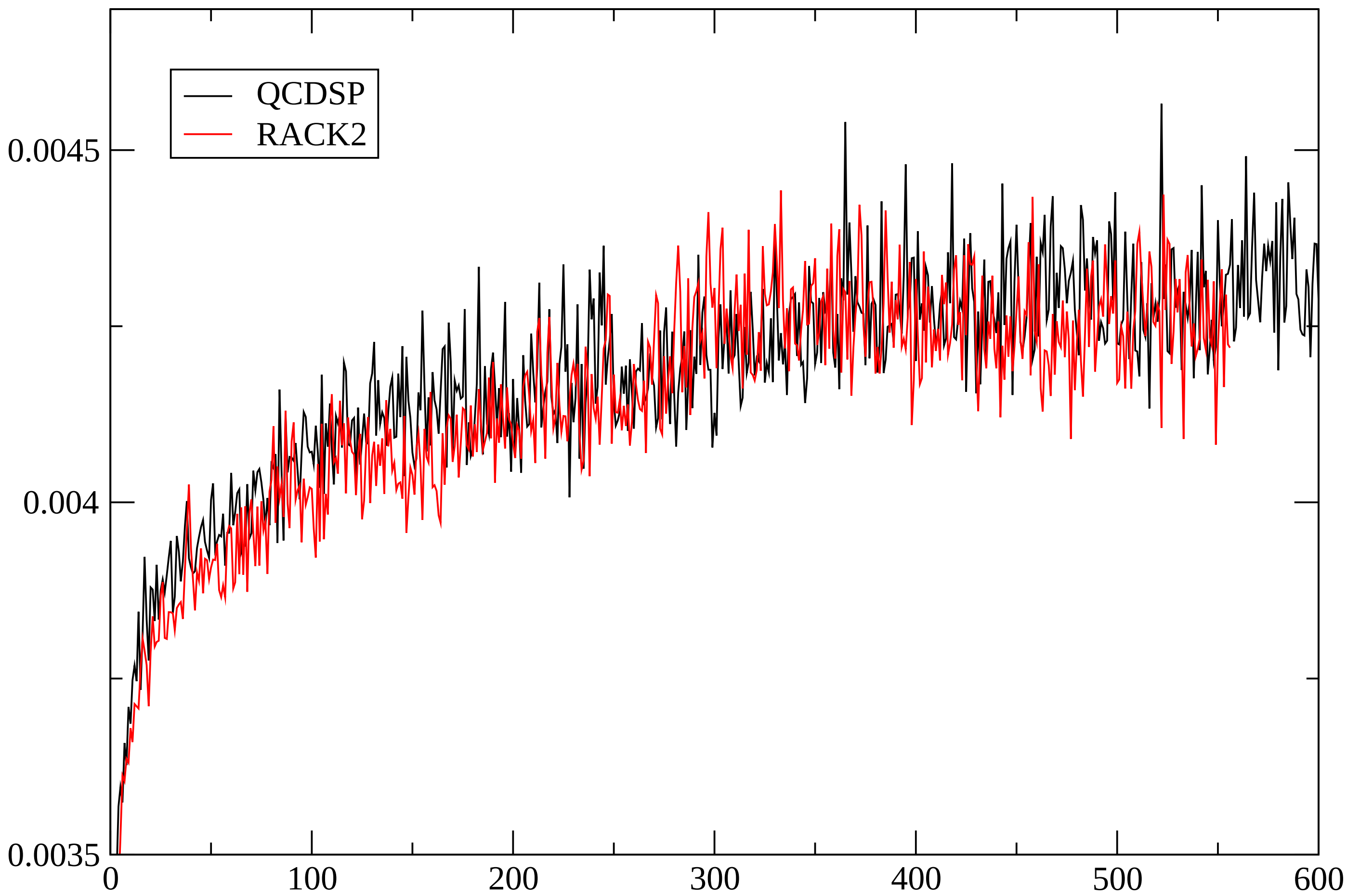




$m_{\text{dyn}} = 0.02$. The left-hand graph shows the plateau quality (degrades with decreasing valence quark mass). The right-hand graph shows the extracted bare B_K for all the combinations of masses.

$N_f = 2$ DWF on QCDOC

- 40 trajectories/day on 2048 node QCDSP
- 160 trajectories/day on 1024 node QCDOC
- QCDOC: $\sim 3\times$ operation count (old force term and no forecasting).



Conclusions and Outlook

- QCDOC provides powerful resource for Lattice QCD.
- 2 and 3 flavor dynamical DWF simulations on QCDSP show DWF working.
- 2+1 flavor DWF lattices allow calculations of weak matrix elements, nucleon properties and heavy quark physics.
- For B_K, no open theoretical issues. Precision requires careful control of systematics and good statistics.
- Lattices generated in next 6 months provide platform for nucleon, heavy quark, and kaon physics.
- Thermodynamics with improved staggered quarks now.
- Some QCDOC time for new ideas!