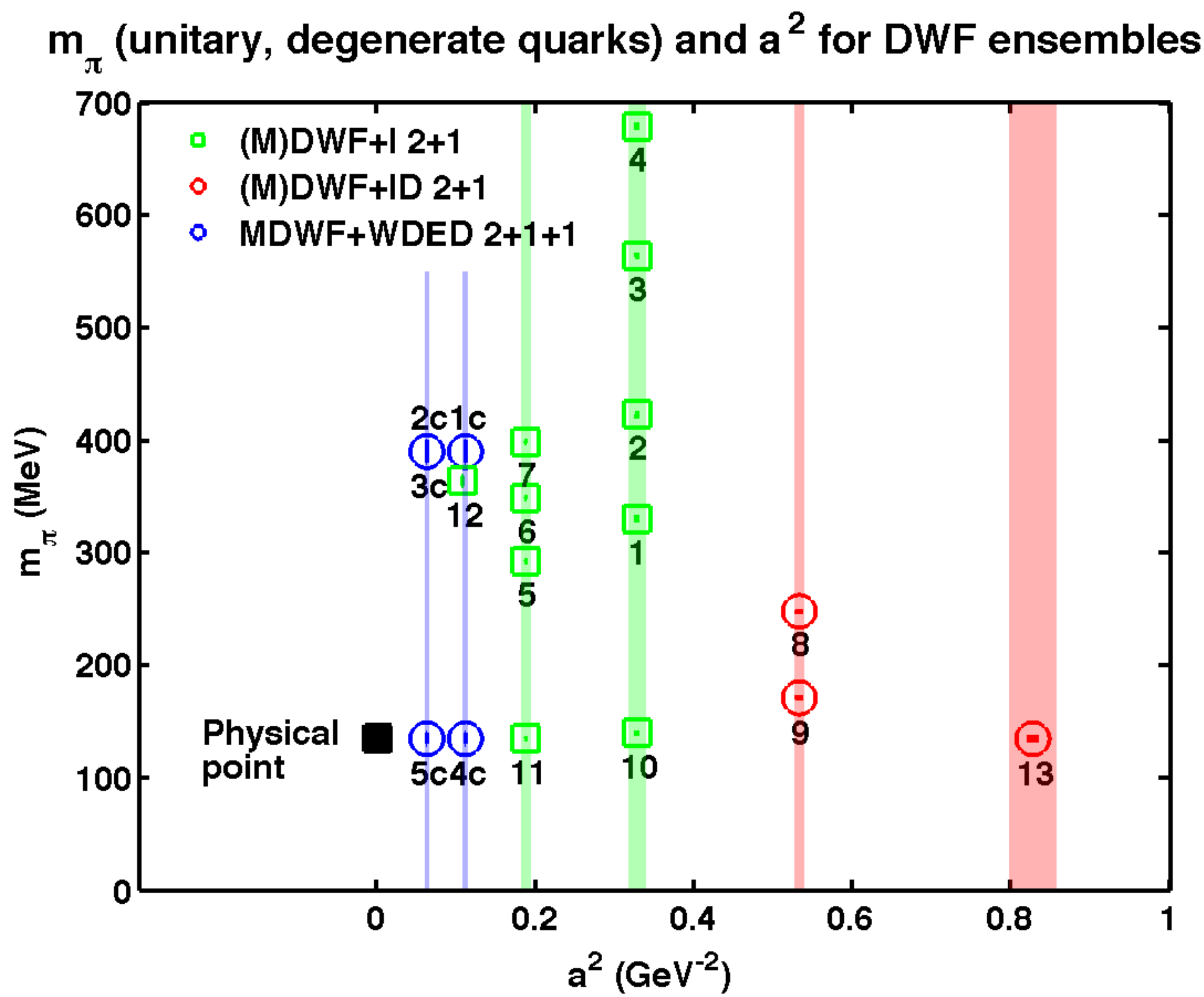
Generating 2+1+1 flavor Mobius Domain Wall Fermion Configurations

Lattice 2014
Columbia University
June 24, 2014

Robert Mawhinney
Columbia University
RBC and UKQCD Collaborations

RBC/UKQCD Dynamical (M)DWF Ensembles



2+1 Flavor Ensembles

Ens.	Action	$1/a$	Lattice	m_l	m_s	m_{res}	m_π	Size
	(F+G)	(GeV)	volume		(in lattice units)		(MeV)	(fm)
1	DWF+I	1.75(3)	$24^3\times64\times16$	0.005	0.04	0.00308	330	2.7
2	DWF+I	1.75(3)	$24^3\times64\times16$	0.01	0.04	0.00308	420	2.7
3	DWF+I	1.75(3)	$24^3\times64\times16$	0.02	0.04	0.00308	560	2.7
4	DWF+I	1.75(3)	$24^3\times64\times16$	0.03	0.04	0.00308	670	2.7
5	DWF+I	2.31(4)	$32^3\times64\times16$	0.004	0.03	0.000664	310	2.6
6	DWF+I	2.31(4)	$32^3\times64\times16$	0.006	0.03	0.000664	370	2.6
7	DWF+I	2.31(4)	$32^3\times64\times16$	0.008	0.03	0.000664	420	2.6
8	DWF+ID	1.37(1)	$32^3\times64\times32$	0.0042	0.046	0.00184	250	4.5
9	DWF+ID	1.37(1)	$32^3\times64\times32$	0.001	0.046	0.00184	180	4.5
10	MDWF+I	1.75(3)	$48^3\times96\times24$	0.00078	0.0362	0.000614	138	5.5
11	MDWF+I	2.31(4)	$64^3\times128\times12$	0.000678	0.02661	0.000314	139	5.5
12	DWF+I	3.06(6)	$32^3\times64\times12$	0.0047	0.0186	0.00060	380	2.0
13	MDWF+ID	1.12(4)	$32^3\times64\times24$	0.00022	0.05960	0.0021	135	5.8

2+1+1 Flavor Ensembles

Ens.	$1/a$	Lattice	m_l	m_s	m_c	m_{res}	m_π	Size
	(GeV)	volume		(in lattice units)		(MeV)	(fm)	
1c	3.0	$32^3\times64\times12$	0.0047	0.0186	0.243	0.0018	~ 400	2.1
2c	4.0	$32^3\times64\times12$	0.0041	0.0146	0.183	0.0002	~ 400	1.6
3c	4.0	$48^3\times96\times12$	0.0041	0.0146	0.183	0.0002	~ 400	2.4
4c	3.0	$80^2\times96\times192\times24$	0.0002	0.0186	0.243	0.0005	140	5.3-6.4
5c	4.0	$128^3\times256\times12$	0.0003	0.0146	0.183	0.0002	140	6.4

Why 2+1+1 Flavors with 1/a = 3 GeV?

Natural next step, having completed two 2+1 flavor ensembles with physical pions and (5.5 fm)^3 volume. (ESP time at ANL and 5-10× faster measurement package.)

* B_K statistical error reduced from 1% to ~0.2%. Essentially no chiral extrapolation error. Now reduce 4% pert. matching error, with NPR across m_c on finer lattices.

* K_{l3} $f_+(0)$ statistical error 0.15-0.2%. Analysis almost finalized.

2+1+1 flavor ensembles with physical quark masses, (5.5 fm)^3 volume and full continuum symmetries provide a platform for measurements of many observables. RBC and UKQCD have many members interested in many topics.

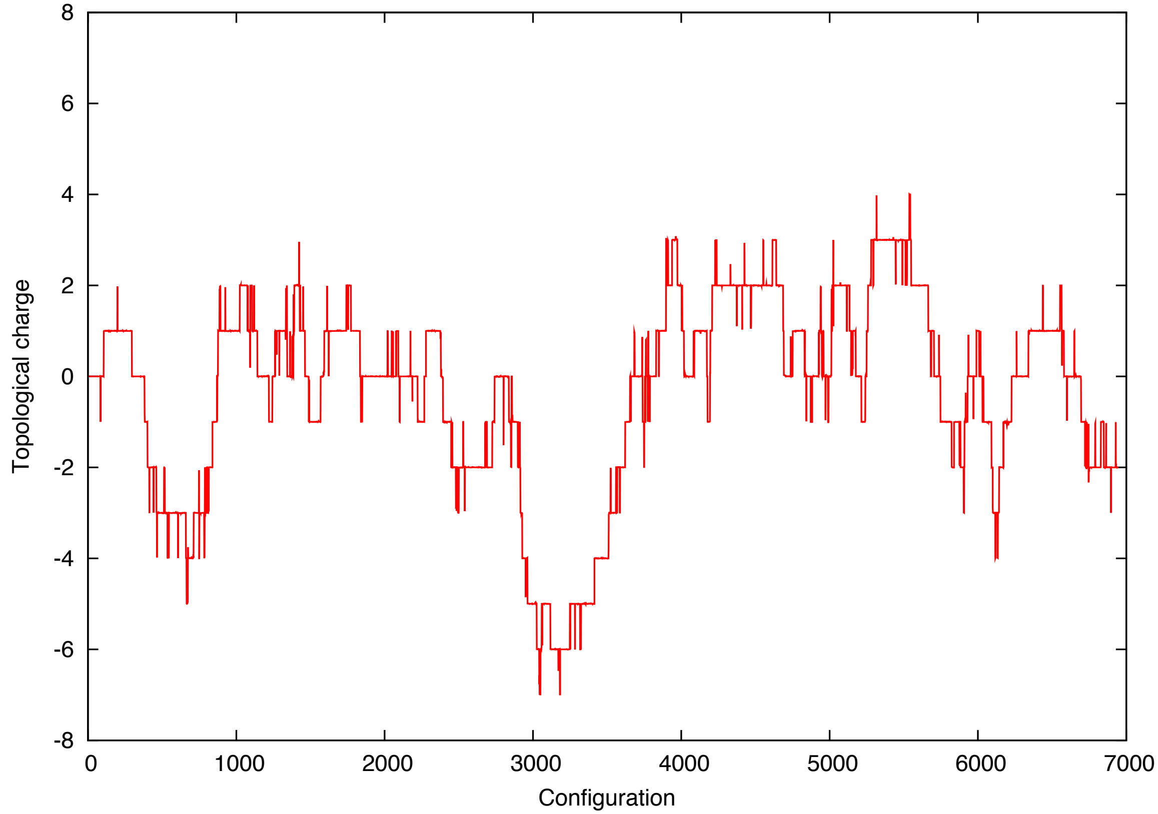
Want weaker coupling lattice to continue moving toward continuum limit

Many observables require charm quark besides obvious charm observables: K_L - K_S difference needs charm for GIM; previous kaon work being done in 3 flavor effective theory, adding charm removes reliance on integrating out charm in the continuum; precision ε'/ε likely requires 4 flavor theory.

Problem: topology moves very slowly for Iwasaki + DWF at 1/a = 3 GeV.

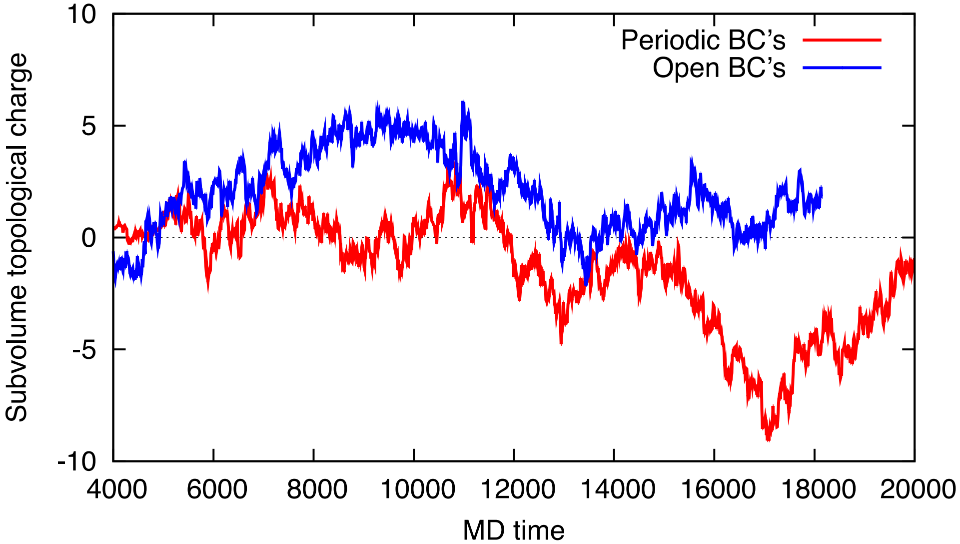
Toplogical Evolution: 2+1 flavors, Iwasaki +DWF

1/a = 3 GeV and $m_\pi \approx 400$.



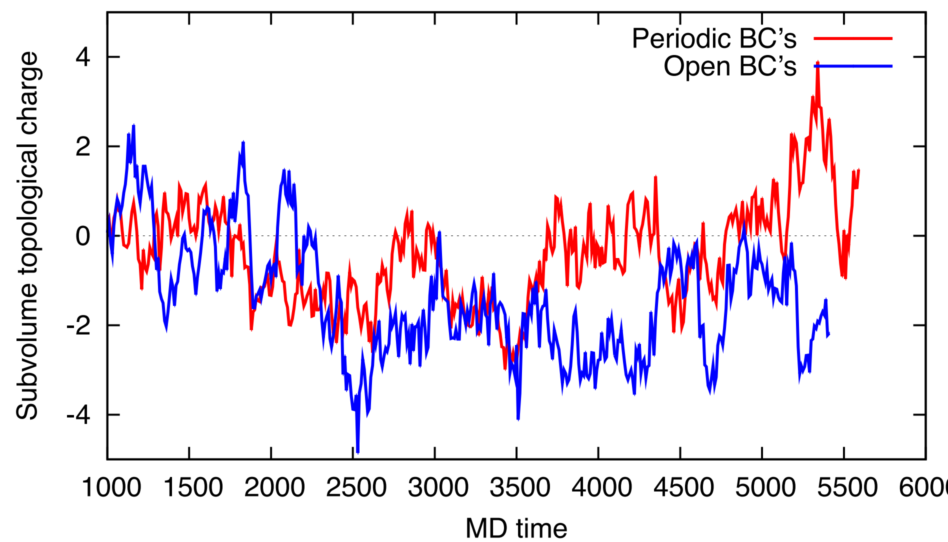
Thousands of MD time units

Open Boundary Conditions



(a) Iwasaki, $\beta = 2.9$

quenched, 1/a ~ 3 GeV



(b) Wilson, $\beta = 6.42$

quenched, 1/a ~ 4 GeV

Observe topological charge in central half-volume (T/4,3T/4)

No obvious difference in these 5k to 20k MD time unit runs.

5k MD trajectories is difficult for large volume, physical pion dynamical simulations.

Why aren't open boundary conditions helping very much, if at all?

Diffusion of Topological Charge in QCD Simulations

Compare open and closed boundary conditions on quenched DBW2 ensembles with volume $(1.6\ \mathrm{fm})^3 \times 3.2$ fm lattices and 1/a = 1 to 2 GeV using HMC algorithm.

Measure topology on all time slices. Find temporal correlations in Euclidean space and in Monte Carlo time fit well by simple diffusion equation with two free parameters: diffusion coefficient D, tunneling time τ_{tunn}. For DBW2, τ_{tunn} large

Diffusion coefficient scales as $1/a^2$ and τ_{tunn} scales like $1/a^6$

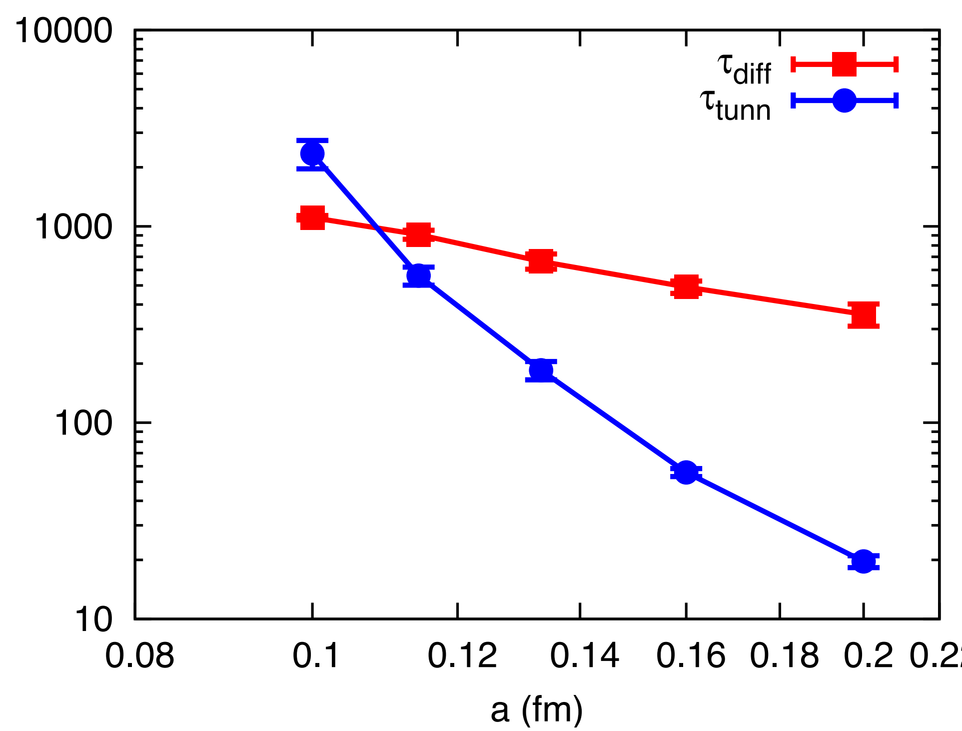
Topology diffuses in from the boundaries, but slowly. Worse for large T

Open boundary conditions do help for small enough a, but when they do, the integrated autocorreltion times are large and perhaps impractical for dynamical simulations

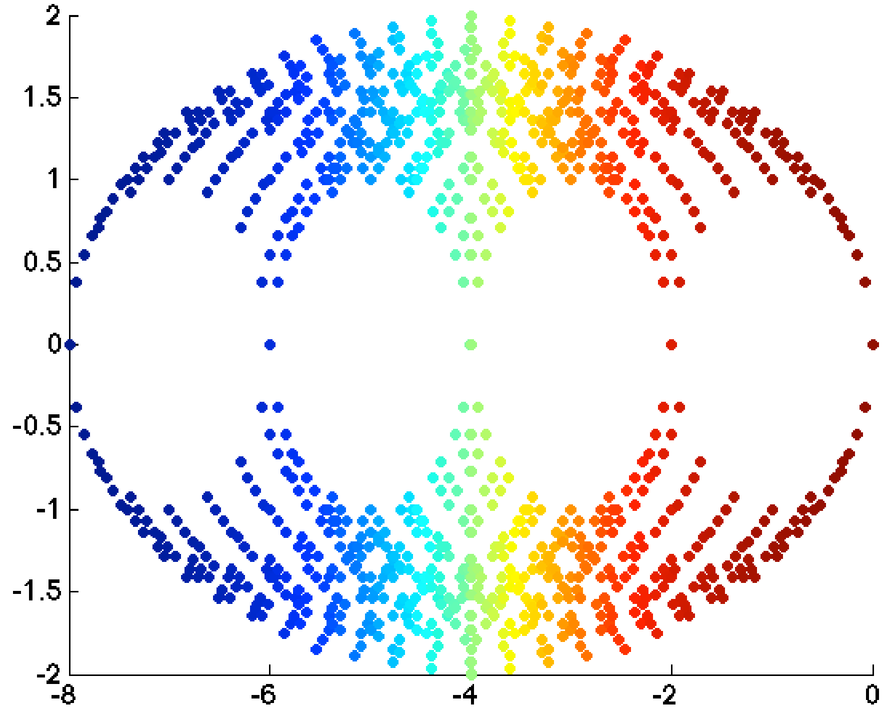
More in talk at Lattice 2014 by Greg Mc-Glynn

Paper posted: arXiv:1406.4551 [hep-lat]

Better algorithm needed!



Complex Eigenvalues of Wilson Dirac Operator



Topology change in an approximately continuous algorithm (like HMC) requires that eigenvalues move through the center of the "holes" above, as the gauge field changes
- a gauge field with a dislocation

At strong coupling, DSDR term suppresses these dislocations

$$\frac{\det\left[D_W(-M+i\varepsilon_f\gamma^5)^\dagger D_W(-M+i\varepsilon_f\gamma^5)\right]}{\det\left[D_W(-M+i\varepsilon_b\gamma^5)^\dagger D_W(-M+i\varepsilon_b\gamma^5)\right]} = \prod_i \frac{\lambda_i^2+\varepsilon_f^2}{\lambda_i^2+\varepsilon_b^2}$$

Dislocation Enhancing Determinant (DED)

For DSDR, ε_f is small and ε_b is large, to suppress small eigenvalues of the twisted Wilson Dirac operator with large bare mass.

Get the opposite effect of DSDR by making ε_f is large and ε_b is small (~DSDR^{-1})

However, DSDR^{-1} gives a large positive β shift, needing more DSDR^{-1}, etc.

DED term is like DSDR^{-1} except we have used a function which primarily effects modes of the Wilson Dirac operator which are zero when a lattice dislocation occurs.

If we let λ be $\det[f(D^\dagger_{PC} D_{PC})]$ (where D is the preconditioned Wilson Dirac operator) with a mass of, say -1.5. The DED term is

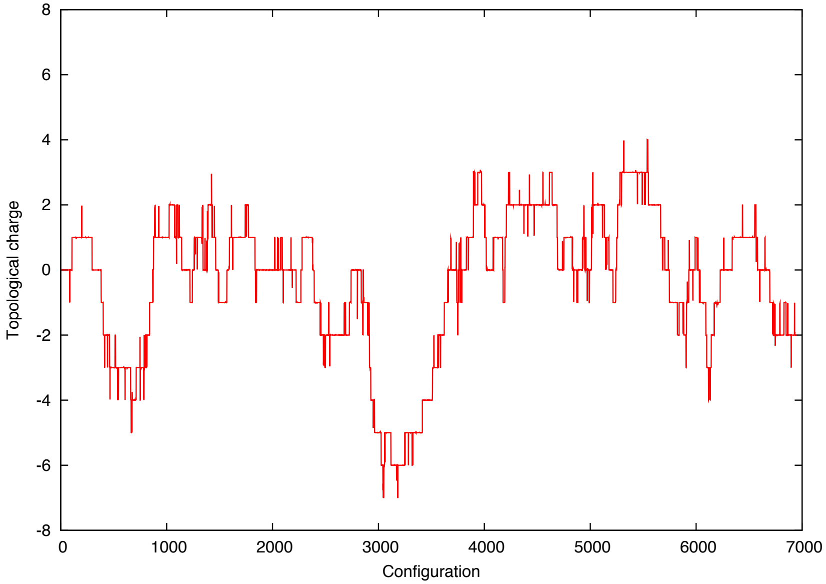
$$f(\lambda) = \left(1 - \frac{a}{\lambda^2 + b_1} + \frac{a}{\lambda^2 + b_2}\right)^{-2}$$

Can expand this determinant

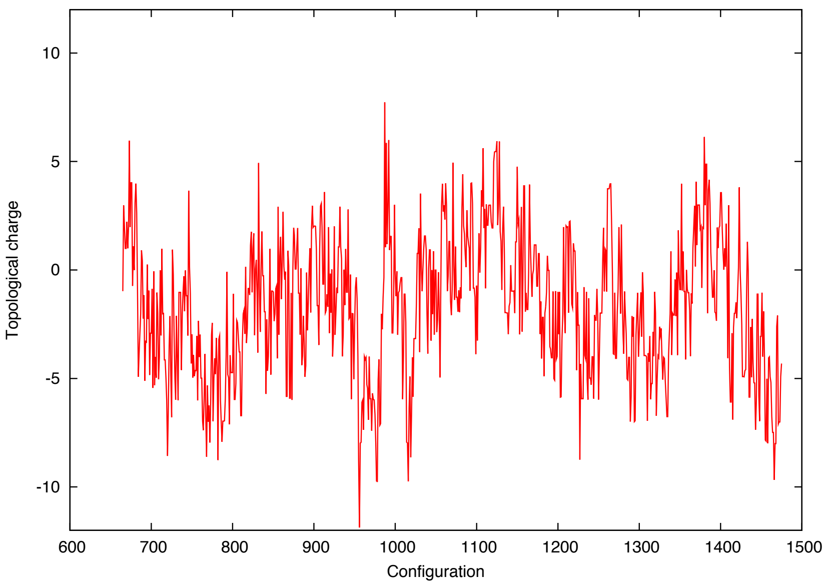
$$\begin{aligned}
\det\left[f\left(x\right)\right] &= \exp\left[\mathrm{Tr}\ln f\left(x\right)\right] \\
&= \exp\left[-2\mathrm{Tr}\ln\left(1 - \frac{a}{x + b_1} + \frac{a}{x + b_2}\right)\right] \\
&= \exp\left[-2\mathrm{Tr}\ln\left(\frac{\left(x + b_1\right)\left(x + b_2\right) + a\left(b_1 - b_2\right)}{\left(x + b_1\right)\left(x + b_2\right)}\right)\right] \\
&= \exp\left[2\mathrm{Tr}\ln\left\{\left(x + b_1\right)\left(x + b_2\right)\right\} - 2\mathrm{Tr}\ln\left\{\left(x + b_1\right)\left(x + b_2\right) + a(b_1 - b_2)\right\}\right]
\end{aligned}$$

Dislocation Enhancing Determinant

Iwasaki 2+1f, 7000 MD time units



WDED 2+1+1f, 900 MD time units



Graph compares topolgical evolution for 2+1 flavor Iwasaki ensemble to 2+1+1 flavor Wilson+DED ensemble. Both have 1/a = 3 GeV and $m_\pi \approx 400$.

Choose a set of DED parameters and tune to get tunneling at both 1/a = 3 and 4 GeV.

Have found an acceptable set, but tunneling is gone for 1/a = 5 GeV.

Basically shifting the tunneling mechanism that works well between 1.5 and 2.5 GeV to 3 and 4 GeV.

Ensemble Evolution

Smaller volume 2+1+1f ensembles being generated on RBC and UKQCD BGQ's.

Larger volume thermalization ($80^2 \times 96 \times 192 \times 16$) underway at ANL with large Mobius scale factor.

$L_S = 24$ and Mobius scale factor of 2 will get $m_{res} < m_{light}$.

DED term increases topological tunneling and dislocations and these increase m_{res}.

More aggressive Modius scaling parameters decrease L_s and increase CG iterations.

Estimate 1-1.5 M BGQ core hours per trajectory with current algorithm tuning, given 0.5 M BGQ core hours/traj. seeing currently during thermalization with smaller L_S.

Evolution algorithm is state-of-the art, using 5 Hasenbush intermediate masses, a multiple time step HMC/RHMC and the force gradient integrator.

Anticipate some speed up from algorithm tuning. Done after initial thermalization.

Force gradient 2× faster than Omelyan on $48^3 \times 96 \times 16$. Should produce an even larger speed-up here, given the much larger volume.

CPS evolution code uses Boyle's BAGEL solver.

Using state-of-the-art evolution algorithms, but are looking for improvements.

Summary

The new 2+1+1 flavor ensembles are a natural next step in approaching the continuum limit and removing systematic errors.

These are useful for any type of observables, because they are QCD with full vector and axial symmetries of the continuum at finite lattice spacing.

RBC and UKQCD focused on continuing kaon physics and adding charm physics.

Ideal platform for new measurements, such as K_L-K_S mass difference where charm loops are vital.