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# First LQCD Physics Runs with MILC and P4RHMC

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## Disclaimer

## First LQCD Physics Runs with MILC and P4RHMC
Initial set of finite temperature runs with milc and p4rhmc codes to
demonstrate feasibility of LQCD runs on BG/L.

# Background

An initial series of physics LQCD runs were submitted to the BG/L science
bank with the milc and p4rhmc. Both runs were for lattice dimensions of
$32^2x8$. The p4 calculation was performed with v2.0 QMP_MPI.X (semi-
optomized p4 code using qmp over mpi) and milc v7.2, also using RHMC,
but not specifically optimized for BlueGene. Calculations were performed
along lines of constant physics, with the light quark masses 2-3 times their
physics values and the strange quark mass set by $m_{ud} = 0.1m_s$.

Job submissions was performed using the standard milc and p4 scripts
provided provided on the ubgl cluster. Initial thermalized lattices for each
code were also provided in this way. The only modifications for running on
BG/L were to the directory names and the mT parameter which determines
job durations (24 hrs on BG/L vs. 4 hrs on ubgl). The milc scripts were set
to resubmit themselves 10 times, and the p4 scripts were submitted serially
using the "psub -d" job dependency option. The runp4rhmc.tcsh could
not be used to resubmit due to the 30m time limit imposed on interactive
jobs. Most jobs were submitted to the smallest, 512 node partitions, but
both codes could also run on the 1024 node partitions with a gain of only
30-50%.

The majority of jobs ran without error. Stalled jobs were often indicative
of a communication gap within a partition that LC was able to fix quickly.
On some occasion a zero-length lattice file was deleted to allow jobs to
restart successfully. Approximately 1000 trajectories were calculated for
each beta value, see Table . The analysis was performed with the standard
analysis scripts for each code, make_summary.pl for milc and analysis.tcsh
for p4rhmc. All lattices, log files, and job submission scripts have been
archived to permanent storage for subsequent analysis.

# MILC results

Results for the Polyakov loop and $<\bar{\psi}\psi>$ (see Fig. 1) show the expected be-
havior for a phase transition and moreover are quite consistent with previous

| milc $\beta$ | T | lattice range | partition | min./10 traj. |
|---|---|---|---|---|
| 6.458 | 139.8 | 115–1100 | 1024 | 54 |
| 6.50 | 148.3 | 125–1120 | 512 | 76 |
| 6.55 | 158.4 | 160–720 | 512/1024 | 80/52 |
| 6.60 | 169.1 | 145–1145 | 512 | 82 |
| 6.65 | 180.1 | 115–730 | 512/1024 | 86/54 |
| 6.70 | 191.2 | 269–1275 | 512 | 68 |
| 6.76 | 204.9 | 217–1215 | 512 | 88 |
| 6.80 | 213.9 | 205–950 | 1024 | 52 |
| 6.85 | 226.4 | 170–970 | 1024 | 40 |
| 6.90 | 238.3 | 115–1015 | 1024 | 38 |
| 6.95 | 251.4 | 100–1000 | 1024 | 34 |
| 7.00 | 264.3 | 130–1030 | 1024 | 34 |
| 7.08 | $\sim$284.4 | 120–1020 | 1024 | 34 |
| p4 $\beta$ | $T/T_c$ | lattice range | partition | min./10 traj. |
| 3.50 | $\sim$0.91 | 220–888 | 512 | 80 |
| 3.55 | $\sim$0.98 | 170–974 | 512 | 85 |
| 3.60 | $\sim$1.12 | 520–1499 | 512 | 46 |
| 3.65 | $\sim$1.21 | 410–1330 | 512 | 30 |

Table 1: Run statistics and times for BG/L. The temperature value for $\beta = 7.08$ is a linear interpolation for $\beta = 7.05, 7.10$. $T/T_c$ values for p4 are only a rough approximation.

calculations from the milc collaboration using a slightly different version of the code and a smaller lattice. Because the initial lattices were thermalized, the plotted values are a straightforward average of the lattice values, with an autocorrelation correction applied.

## P4RHMC results

Results for the $< \bar{\psi}\psi >$, wilson line, plaquette, and rectangle (the four values calculated by the analysis script are shown in Fig. 2. The susceptibilities for these values are given in the scanned printouts at the end of this document.
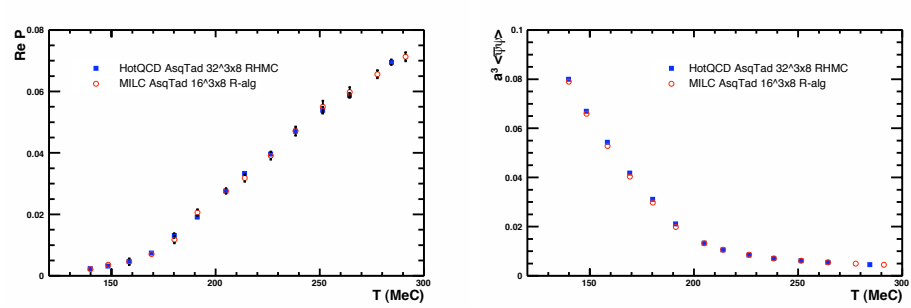
Figure 1: Polyakov loop and $< \bar{\psi}\psi >$ for hotQCD runs on BG/L with rhmc milc v7.2 code on $32^3 x 8$ lattice compared to previous runs with a $16^3 x 8$ lattice using the R-algorithm.



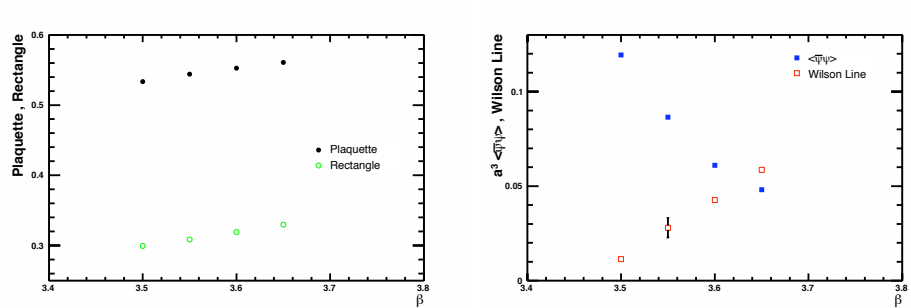Figure 2: $< \bar{\psi}\psi >$, wilson line, plaquette, and rectangle values for the hotQCD runs on BG/L using v2 of the qmp over mpi p4rhmc executable.

## Document Scans

The following pages contain scanned output from the milc and p4 analysis scripts.

```
Beta=3.50
################################################
#Acceptance
Accepted=529, Total=888, Rate=0.595720720720721, Expected=0.57953721088964,
<exp(-dH)> = 0.978768820077014, sqrt(<dH^2>) = 1.29463368392649
################################################
#Chiral Condensate (pbp)
#Total size of pbp.dat = 1760
#pbp block size = 50
#pbp_frequencey = 10
#pbp_hits_per_measurement = 10
#pbp_thermalization = 0
#Mass pbp error
2.7000000000000000e-02 0.119399965128281 0.000367232734501994
#Mass pbp_sus error
2.7000000000000000e-02 2.86294275008834e-06 6.65781897388574e-07
#Mass pbp error
2.7000000000000001e-03 0.0434017552825711 0.000639703862274105
#Mass pbp_sus error
2.7000000000000001e-03 8.41065186850181e-06 2.1681994061165e-06
################################################
################################################
#Plaquette
#Total size of plaq.dat = 888
#block size = 50
#thermalization = 0
#plaq error
0.533404654936936 5.19957187480285e-05
#plaq_sus error
1.06179313825851e-07 1.47964262039581e-08
################################################
################################################
#Rectangle
#Total size of rect.dat = 888
#block size = 50
#thermalization = 0
#rect error
0.295571561735221 7.47730622597145e-05
#rect_sus error
1.06179313825851e-07 1.47964262039581e-08
################################################
################################################
#Wilson line
#Total size of wline.dat = 3552
#block size = 50
#thermalization = 0
#wline error
0.0114463137677228 0.00064889729411625
#wline_sus error
9.22856866025235e-05 7.34306704847714e-06
################################################
```

```
Beta=3.55
##################################################
#Acceptance
Accepted=602, Total=974, Rate=0.618069815195072,
Expected=0.621124249127309, <exp(-dH)> = 1.44243795146652e+258,
sqrt(<dH^2>) = 19.8733367669342
##################################################
#Chiral Condensate (pbp)
#Total size of pbp.dat = 1940
#pbp block size = 50
#pbp_frequencey = 10
#pbp_hits_per_measurement = 10
#pbp_thermalization = 0
#Mass pbp error
2.3000000000000000e-02 0.0864284484282444 0.0010169066744434
#Mass pbp_sus error
2.3000000000000000e-02 2.49445484894626e-05 2.37061024204272e-05
#Mass pbp error
2.3000000000000000e-03 0.0179379823036629 0.000585045018885014
#Mass pbp_sus error
2.3000000000000000e-03 8.96500998048327e-06 5.60464451348084e-06
##################################################
##################################################
#Plaquette
#Total size of plaq.dat = 974
#block size = 50
#thermalization = 0
#plaq error
0.543919863278722 0.000508359068909031
#plaq_sus error
2.88762591772768e-05 2.87911985169822e-05
##################################################
##################################################
#Rectangle
#Total size of rect.dat = 974
#block size = 50
#thermalization = 0
#rect error
0.308699194882008 0.000731583419452446
#rect_sus error
2.88762591772768e-05 2.87911985169822e-05
##################################################
##################################################
#Wilson line
#Total size of wline.dat = 3896
#block size = 50
#thermalization = 0
#wline error
0.027998448826372 0.00511237921358849
#wline_sus error
0.00126323411701561 0.00117248357605506
##################################################
```

```
Beta=3.60
##################################################
#Acceptance
Accepted=976, Total=1499, Rate=0.651100733822548,
Expected=0.662290960633756, <exp(-dH)> = 1.04178328815545, sqrt(<dH^2>) =
0.975668561352681
##################################################
#Chiral Condensate (pbp)
#Total size of pbp.dat = 2980
#pbp block size = 50
#pbp_frequencey = 10
#pbp_hits_per_measurement = 10
#pbp_thermalization = 0
#Mass pbp error
1.9000000000000000e-02 0.0610334546566235 0.0001148030116974431
#Mass pbp_sus error
1.9000000000000000e-02 7.69943665976901e-07 1.64708242555334e-07
#Mass pbp error
1.9000000000000000e-03 0.00724866160710683 8.01416814748782e-05
#Mass pbp_sus error
1.9000000000000000e-03 3.56966743712924e-07 6.15938483773753e-08
##################################################
##################################################
#Plaquette
#Total size of plaq.dat = 1499
#block size = 50
#thermalization = 0
#plaq error
0.552496068520259 2.69686744044083e-05
#plaq_sus error
8.03147972794349e-08 7.5234029740991e-09
##################################################
##################################################
#Rectangle
#Total size of rect.dat = 1499
#block size = 50
#thermalization = 0
#rect error
0.319275096295671 4.04361561747931e-05
#rect_sus error
8.03147972794349e-08 7.5234029740991e-09
##################################################
##################################################
#Wilson line
#Total size of wline.dat = 5996
#block size = 50
#thermalization = 0
#wline error
0.0426372960039281 0.000656094355427005
#wline_sus error
0.000101727972404155 5.46618788153355e-06
##################################################
```

```
Beta=3.65
################################################
#Acceptance
Accepted=1330, Total=1330, Rate=1, Expected=1, <exp(-dH)> =
1.18280553932348, sqrt(<dH^2>) = 0.911269556979087
################################################
#Chiral Condensate (pbp)
#Total size of pbp.dat = 2641
#pbp block size = 50
#pbp_frequencey = 10
#pbp_hits_per_measurement = 10
#pbp_thermalization = 0
#Mass pbp error
1.7000000000000001e-02 0.0480606950987239 9.07932752620176e-05
#Mass pbp_sus error
1.7000000000000001e-02 2.80102369882062e-07 5.49556109699087e-08
#Mass pbp error
1.6999999999999999e-03 0.00501251792378543 2.29210544538443e-05
#Mass pbp_sus error
1.6999999999999999e-03 1.79841657623586e-07 1.49056172255761e-07
################################################
################################################
#Plaquette
#Total size of plaq.dat = 1330
#block size = 50
#thermalization = 0
#plaq error
0.560855647595524 1.92442024723551e-05
#plaq_sus error
7.07497811714687e-08 3.62045769595841e-09
################################################
################################################
#Rectangle
#Total size of rect.dat = 1330
#block size = 50
#thermalization = 0
#rect error
0.329693188694171 3.00506256505537e-05
#rect_sus error
7.07497811714687e-08 3.62045769595841e-09
################################################
################################################
#Wilson line
#Total size of wline.dat = 5320
#block size = 50
#thermalization = 0
#wline error
0.0586068380618468 0.000787393578630855
#wline_sus error
0.000115403715888074 4.18906249435554e-06
################################################
```

Nt=8  (m_{u,d} = 0.1ms)

```
beta mu,d   ms   u0  ns nt   ReP  dReP chi_L dchi_L cgiter dcgiter pbp_ud dpbp_ud pbp_s dpbp_s
plaq dplaq  rect  drect pgm dpgm pb_dmdu_p_ud dpb_dmdu_p_ud pb_dmdu_p_s dpb_dmdu_p_s dS1 ddS1
dt accept N logfile
6.4580 0.00500 0.0500 0.8549 32
8 0.0024 0.0002 0.061 0.004 0.0 0.0 0.07995 0.00018 0.1940 0.0001 1.60249
0.00008 0.84230 0.00011 0.86229 0.00013 -4.89294 0.00025
-4.83945 0.00023 0.01430 0.00e+00 0.00e+00 0.00   880 o328f21b6458m00820m0820r.00115_01100
6.5000 0.00500 0.0500 0.8569 32
8 0.0032 0.0003 0.063 0.003 0.0 0.0 0.06690 0.00021 0.1755 0.0002 1.61820
0.00016 0.86239 0.00020 0.88358 0.00020 -4.88984 0.00036
-4.84416 0.00044 0.01430 0.00e+00 0.00e+00 0.00   900 o328f21b650m00765m0765r.00125_01120
6.5500 0.00500 0.0500 0.8594 32
8 0.0047 0.0005 0.074 0.006 0.0 0.0 0.05430 0.00023 0.1561 0.0002 1.63616
0.00014 0.88538 0.00019 0.90795 0.00022 -4.88030 0.00042
-4.84275 0.00045 0.01430 0.00e+00 0.00e+00 0.00   495 o328f21b655m00705m0705r.00160_00720
6.6000 0.00500 0.0500 0.8616 32
8 0.0074 0.0005 0.068 0.004 0.0 0.0 0.04182 0.00018 0.1377 0.0001 1.65320
0.00007 0.90737 0.00010 0.93115 0.00011 -4.87391 0.00018
-4.84310 0.00019 0.01430 0.00e+00 0.00e+00 0.00   925 o328f21b660m00650m0650r.00145_01145
6.6500 0.00500 0.0500 0.8636 32
8 0.0131 0.0008 0.075 0.007 0.0 0.0 0.03116 0.00052 0.1215 0.0003 1.66904
0.00010 0.92786 0.00014 0.95274 0.00020 -4.86806 0.00028
-4.84283 0.00040 0.01430 0.00e+00 0.00e+00 0.00   510 o328f21b665m00599m0599r.00115_00730
6.7000 0.00500 0.0500 0.8657 32
8 0.0191 0.0007 0.073 0.004 0.0 0.0 0.02109 0.00066 0.1062 0.0003 1.68470
0.00006 0.94827 0.00008 0.97417 0.00010 -4.85880 0.00023
-4.83838 0.00029 0.01250 0.00e+00 0.00e+00 0.00 1006 o328f21b670m00552m0552r.00269_01275
6.7600 0.00500 0.0500 0.8678 32
8 0.0276 0.0003 0.077 0.005 0.0 0.0 0.01332 0.00018 0.0905 0.0001 1.70190
0.00005 0.97067 0.00008 0.99759 0.00009 -4.85147 0.00015
-4.83587 0.00017 0.01250 0.00e+00 0.00e+00 0.00   995 o328f21b676m005m05r.00217_01215
6.8000 0.00500 0.0500 0.8692 32
8 0.0333 0.0005 0.085 0.012 0.0 0.0 0.01051 0.00018 0.0820 0.0002 1.71298
0.00007 0.98516 0.00009 1.01276 0.00009 -4.84532 0.00015
-4.83190 0.00014 0.01250 0.00e+00 0.00e+00 0.00   725 o328f21b680m00471m0471r.00205_00950
6.8500 0.00500 0.0500 0.8709 32
8 0.0396 0.0006 0.086 0.007 0.0 0.0 0.00842 0.00011 0.0727 0.0001 1.72655
0.00006 1.00295 0.00007 1.03123 0.00008 -4.83754 0.00014
-4.82664 0.00012 0.01250 0.00e+00 0.00e+00 0.00   750 o328f21b685m00437m0437r.00170_00970
6.9000 0.00500 0.0500 0.8726 32      ⊽⊍
8 0.0471 0.0006 0.090 0.007 0.0 0.0 0.00710 0.00007 0.0651 0.0001 1.73936
0.00006 1.01972 0.00008 1.04869 0.00010 -4.82857 0.00018
-4.81950 0.00019 0.01250 0.00e+00 0.00e+00 0.00   795 o328f21b690m00407m0407r.00115_01015
6.9500 0.00500 0.0500 0.8741 32
8 0.0539 0.0011 0.099 0.012 0.0 0.0 0.00617 0.00004 0.0586 0.0001 1.75185
0.00007 1.03624 0.00010 1.06578 0.00008 -4.82111 0.00013
-4.81347 0.00013 0.01250 0.00e+00 0.00e+00 0.00   780 o328f21b695m0038m038r.00100_01000
7.0000 0.00500 0.0500 0.8756 32
8 0.0587 0.0008 0.106 0.007 0.0 0.0 0.00551 0.00002 0.0531 0.0001 1.76394
0.00007 1.05223 0.00010 1.08235 0.00011 -4.81355 0.00011
-4.80699 0.00012 0.01250 0.00e+00 0.00e+00 0.00   805 o328f21b700m00355m0355r.00130_01030
7.0800 0.00500 0.0500 0.8779 32
8 0.0695 0.0009 0.115 0.010 0.0 0.0 0.00453 0.00002 0.0444 0.0001 1.78260
0.00006 1.07699 0.00008 1.10804 0.00010 -4.80141 0.00013
-4.79672 0.00013 0.01250 0.00e+00 0.00e+00 0.00   900 o328f21b708m0031m031r.00120_01120
```