## US site report

Oliver Witzel<br>Center for Computational Science

## BOSTON UNIVERSITY

21st International Lattice Data Grid Workshop
December 13, 2013

## US resources

| machine | architecture | CPU cores | accelerators |
| :--- | :--- | :---: | :---: |
| BNL USQCD 1/2 rack | BG/Q | 8192 | - |
| ALCF "Mira" | BG/Q | 786432 | - |
| OLCF "Titan" | Cray XK7 | 299088 | 18688 K 20 |
| TACC "Stampede" | Dell C8220 | 102400 | 6400 Phi |
| NCSA "Blue Waters" | Cray XE6 + XK7 | 396032 | 4224 K 20 |

- 3 BG/Q racks at BNL for exclusive use by RBC
- USQCD INCITE grants: 290 M hrs at ALCF and 140 M hrs at OLCF
- Individual science collaborations have access to Stampede and Blue Waters as well as other NSF founded facilities


## MILC: $\mathrm{HISQ} N_{f}=2+1+1$

- Strange and charm close to physical value
- Variable $u / d$-quark masses down to physical value $\left(0.04 m_{s}\right)$
- Box sizes greater than 3.2 pion Compton wavelengths
- Four lattice spacings with each three different $u / d$-quark masses: $(0.15 \mathrm{fm}, 0.12 \mathrm{fm}, 0.09 \mathrm{fm}, 0.06 \mathrm{fm}) \times\left(0.04 \mathrm{~m}_{s}, 0.1 \mathrm{~m}_{s}, 0.2 \mathrm{~m}_{s}\right)$
- Three volumes for use in finite-volume studies:
$a \approx 0.12 \mathrm{fm}$ and $m_{l}=0.1 m_{s}$ with box sizes $3.2,4.3$, and 5.4 pion Compton wavelengths
- Generation of $a \approx 0.045 \mathrm{fm}$ and $m_{l}=0.02 m_{s}$ started
- Once complete, lattices will be stored at NERSC and Fermilab, intended mark-up for the ILDG metadata catalog
- Resources: ALCF BG/Q, Blue Waters


## Hadron Spectrum Collaboration: anisotropic clover $N_{f}=2+1$

- $m_{\pi} \approx 230 \mathrm{MeV}$, anisotropy $\xi \approx 3.5\left(a_{s} \approx 0.125 \mathrm{fm}, a_{t} \approx 0.035 \mathrm{fm}\right)$
- $32^{3} \times 256$ : total: 11506 traj. (incl. thermalization) in two streams Resource: OLCF and ALCF BG/P, LLNL BG/P, NERSC (Hopper) Status: generation complete, analysis on-going
- $40^{3} \times 256$ : total: 6562 traj. (incl. thermalization) in five streams Resource: OLCF JaguarPF and Titan (a few traj. on Blue Waters) Last $O(3000)$ trajectories generated on Titan fully on GPUs using QDP-JIT+QUDA+Chroma


## JLabQCD: isotropic clover $N_{f}=2+1$

- Isotropic clover fermion action with one iteration stout-link smearing
- Tree-level tadpole-improved Symanzik gauge action
- Non-perturbatively tuned cSW
- $O(1000)$ to $O(10000)$ configurations per ensemble:

$$
\begin{array}{lll}
a \approx 0.13 \mathrm{fm} & M_{\pi}=300 \text { to } 800 \mathrm{MeV} & 48^{3} \times 96 \text { to } 16^{3} \times 48 \\
a \approx 0.10 \mathrm{fm} & M_{\pi}=800 \mathrm{MeV} & 48^{3} \times 64 \text { to } 16^{3} \times 48 \\
a \approx 0.09 \mathrm{fm} & M_{\pi}=800 \mathrm{MeV} & 16^{3} \times 48 \\
a \approx 0.08 \mathrm{fm} & M_{\pi}=450 \text { to } 800 \mathrm{MeV} & 32^{3} \times 96 \text { to } 16^{3} \times 48
\end{array}
$$

- If resources available, extension to physical pions
- Currently ILDG mark-up not intended
- Resources: NERSC, Kraken, ALCF BG/P, OLCF


## RBC-UKQCD: (M)DWF $N_{f}=2+1$

- BNL lattice archive moved to Columbia University (new website in progress; files are accessible via scp and globus online)
- Existing ensembles will be marked-up/made publicly available on ILDG

$$
\begin{array}{lll}
24^{3} \times 64 \times 16 & a \approx 0.11 \mathrm{fm} & \text { DWF+I } \\
32^{3} \times 64 \times 16 & a \approx 0.08 \mathrm{fm} & \text { DWF+I } \\
32^{3} \times 64 \times 32 & a \approx 0.14 \mathrm{fm} & \text { DWF+ID }
\end{array}
$$

- Currently generated ensembles
$48^{3} \times 96 \times 24 \quad a \approx 0.11 \mathrm{fm}$ MDWF+I physical $M_{\pi}, 1300$ therm. MDTU $64^{3} \times 128 \times 12 \quad a \approx 0.08 \mathrm{fm}$ MDWF+I physical $M_{\pi}, 1400$ therm. MDTU $32^{3} \times 64 \times 24 \quad a \approx 0.18 \mathrm{fm}$ MDWF+ID physical $M_{\pi}$ $32^{3} \times 64 \times 12 \quad a \approx 0.06 \mathrm{fm}$ DWF $+\mathrm{I} \quad M_{\pi} \approx 380 \mathrm{MeV}$
- Resources: ALCF BG/Q and BG/Qs at UoE and BNL


## USBSM: $\operatorname{SU}(3)$ gauge group and $N_{f}=8$ staggered

- Staggered fermions improved with one step nHyp link-smearing
- Adjoint plaquette action at $\beta_{F}=5.0$ and $\beta_{A}=-\beta_{F} / 4$
- Truncate at least 300 MDTU for thermalization
- Resource: ALCF BG/P, evolution now performed in FUEL (qhmc)

| masses | $64^{3} \times 128$ | $48^{3} \times 96$ | $32^{3} \times 64$ | $24^{3} \times 48$ | $16^{3} \times 32$ |
| :---: | :---: | :---: | :---: | :---: | :---: |
| 0.002 | 70 |  |  |  |  |
| 0.003 | 185 |  |  |  |  |
| 0.004 | 252 | 1152 |  |  |  |
| 0.006 |  | 1170 |  |  |  |
| 0.008 |  | 1755 | 3024 |  |  |
| 0.010 |  | 2250 | 6792 | 3012 |  |
| 0.015 |  |  | 3018 | 10074 |  |
| 0.020 |  |  |  | 10074 | 3000 |
| 0.030 |  |  |  |  | 3000 |
| 0.040 |  |  |  |  | 3000 |
| 0.050 |  |  |  |  | 3000 |

## LSD: $\operatorname{SU}(3)$ gauge group with domain-wall fermions

- Iwasaki gauge action
- $L_{s}=16, M_{5}=1.8$

| $N_{f}$ | $\left(\frac{L}{a}\right)^{3} \times \frac{T}{a}$ | $\beta$ | $m_{f}$ |
| :---: | :---: | :---: | :---: |
| 2 | $24^{3} \times 48$ | 2.7 | $[0.01: 0.005: 0.03]$ |
|  | $32^{3} \times 64$ | 2.7 | $[0.005: 0.005: 0.03]$ |
| 6 | $16^{3} \times 32$ | 2.1 | $[0.01: 0.005: 0.045]$ |
|  | $32^{3} \times 64$ | 2.1 | $[0.005: 0.005: 0.03]$ |
| 8 | $16^{3} \times 32$ | 1.95 | $[0.015: 0.005: 0.05]$ |
|  | $32^{3} \times 64$ | 1.95 | $[0.01: 0.005: 0.03]$ |
| 10 | $16^{3} \times 32$ | 1.95 | $[0.01: 0.005: 0.06]$ |
|  | $32^{3} \times 64$ | 1.95 | $[0.005: 0.005: 0.03]$ |

