LATTICE 2017
Granada

openQ*D simulation code for QCD+QED

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on behalf of the software-development team of the *RC* collaboration*:

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QCD+QED with C* boundary conditions

http://rcstar.web.cern.ch

- Long-term physics goal: calculate isospin breaking corrections to hadronic observables (e.g. masses, decay rates).
- C* boundary conditions provide a local and gauge-invariant setup to describe charged hadrons.
- Is it better to expand in α_{em} or to simulate QCD+QED? Agnostic point of view: go for a setup in which you can do both consistently, compare, and choose depending on the observable.
- Two independent simulation codes
  - `openQ*D`, which is an extension of `openQCD`, publicly available
    Marina Marinković talk @17.30
  - an extension of `HiRep`
    Martin Hansen talk @17.50
- Highlight of Martin's talk: charged-meson two-point functions can be calculated in a gauge-invariant way without loss of precision.

openQ*D main features

http://rcstar.web.cern.ch

- Extension of the openQCD-1.6 simulation code for QCD
  http://luscher.web.cern.ch/luscher/openQCD
- QCD, QCD+QED, very inefficient QED
- Compact QED, with Wilson and planar-double plaquette action
- $O(a)$ improved Wilson fermions
- Open, SF, open-SF, periodic boundary conditions in time
- Periodic, C* boundary conditions in space
- RHMC/HMC algorithm
- Hierarchical MD integrator; leap-frog, OMF-2, OMF-4 integrators
- Pole-splitting for RHMC, twisted-mass Hasenbusch for HMC
- Deflation-accelerated solver
- SSE/AVX acceleration
- RANLUX random-number generator

Features to be added in the stable release

- Non-compact QED
- Fourier acceleration for U(1) field

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openQ*D **tests**

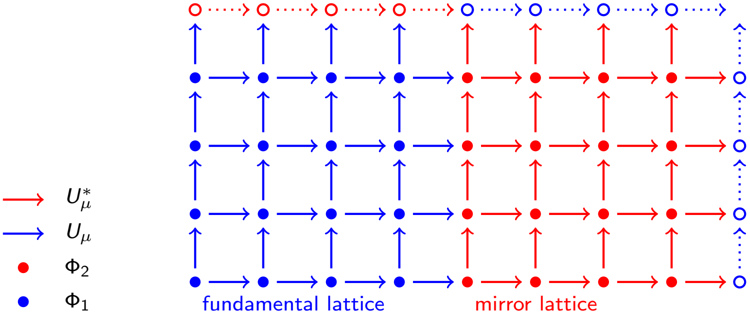
http://rcstar.web.cern.ch

- Modular code, each module has its own testing programs
- Typically gauge-covariance, translation-covariance are checked
- When possible, comparison with analytical calculations with abelian gauge fields
- Force = derivative of the action
- Reversibility of MD
- Approximate conservation of Hamiltonian along MD
- Comparison with `HiRep`
- ...

C^* b.c.s via orbifolding

$$\left|\mathrm{Pf}\; KCD[U \oplus U^*]\right| \propto \int [\mathrm{d}\Phi]\,[\mathrm{d}\Phi^\dagger]\;\exp\left\{-\Phi^\dagger (D^\dagger D[U \oplus U^*])^{-1/4}\Phi\right\}$$

$$\Phi(x + L\hat{k}) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \Phi \equiv K\Phi$$



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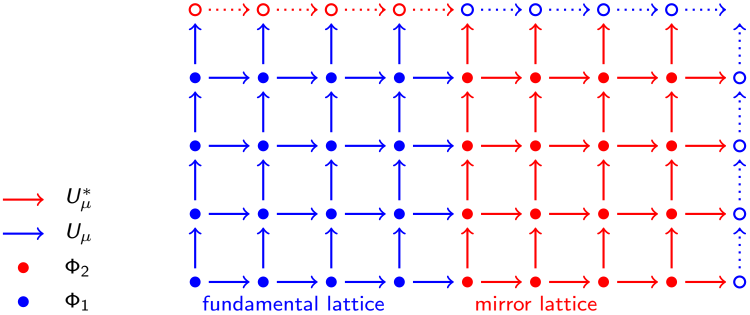
1 C* boundary conditions ⇒ Periodic boundary conditions

2,3 C* boundary conditions ⇒ Periodic b.c. in 1 + Shifted b.c. in 2,3



Orbifold construction

- Double the lattice in direction 1, and use shifted boundary conditions in directions 2 and 3 if necessary.
- Initialize the gauge field such that $U_\mu(x + L_1\hat{1}) = U_\mu(x)^*$.
- Draw the momenta such that $\pi_\mu(x + L_1\hat{1}) = \pi_\mu(x)^*$.
- Replace the MD evolution equation for the momenta with

$$\pi'_\mu(x) = \pi_\mu(x) + \epsilon[F_\mu(x) + F_\mu(x + L_1\hat{1})^*]$$

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How much do we lose in performace by doubling the lattice?

- The gauge field and momenta get updated twice (in the fundamental and mirror lattice). We lose a factor 2x here.
- In the momentum update, the whole mirror lattice has to be copied into the fundamental lattice.
- The Dirac operator acts on a single flavour defined on the double lattice, instead than on two flavours defined on the fundamental lattice. The performance is unaffected.

In simulations that are heavily dominated by the inversion of the Dirac operator, the effect of the orbifold construction should be moderate.

Some tests – QCD with C*

Test case (CLS-2):

- QCD $N_f = 2$
- Wilson action $\beta = 5.2$ ($a \simeq 0.08$fm)
- Non-perturbatively $O(a)$ improved Wilson fermions
- Physical lattice 64×32^3
- $m_\pi \simeq 380$MeV; $m_\pi L \simeq 4.7$

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Overhead of orbifold construction $\lesssim$ 1% (expected to get better at lower masses)

- $S_f = \sum_{i=1}^{N_{\rm pf}} \phi_i^\dagger (D^\dagger D)^{-1/4} \phi_i$
- Rational approximation of order $(14, 14)$ with twisted-mass reweighting $\mu = 0.001$
- 3-level integrator (6 poles / 8 poles / gauge)
- Deflation-accelerated solver for lighter poles
- Acceptance 90–95%

Space b.c.s	Global lattice	Local lattice	$N_{\rm pf}$	Time MD traj
Periodic	$64 \times 32 \times 32 \times 32$	$8 \times 8 \times 8 \times 8$	4	3890s
3 C^*	$64 \times 64 \times 32 \times 32$	$8 \times 16 \times 8 \times 8$	2	3920s

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MSCG / Deflation $\simeq$ 3.5 (deflation expected to perform better at lower masses)

- $S_f = \sum_{i=1}^{N_{\rm pf}} \phi_i^\dagger (D^\dagger D)^{-1/4} \phi_i$
- Rational approximation of order $(14, 14)$ with twisted-mass reweighting $\mu = 0.001$
- 2-level integrator (fermion / gauge), acceptance not tuned
- C* boundary conditions

Solver	Time MD traj
Multi-shift CG	18500s
MSCG for heavy poles + Deflation for light poles	5210s

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RHMC / HMC $\simeq$ 5.5 (more work is needed for tuning)

- 3-level integrator (fermion / fermion / gauge)
- Acceptance 90–95%

Algorithm	Space b.c.s	Time MD traj
HMC + Twisted-mass Hasenbusch precond.	Periodic	$\sim$ 700s
RHMC-1/4	3C*	3920s

Partial conclusions

- `openQ*D-0.9a1` is publicly available
  `http://rcstar.web.cern.ch`
- This is an alpha version: some features are still missing and testing is not complete!!!
- Extension of `openQCD-1.6`
- QCD and QCD+QED
- C* boundary conditions
- Marina Marinković: QED
- Martin Hansen: `HiRep` and gauge-invariant interpolating operators for charged states