openQ*D simulation code for QCD+QED

Marina Krstić Marinković
CERN & Trinity College Dublin

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

Isabel Campos(UAM&CSIC), Patrick Fritzsch(CERN), Martin Hansen(CP3),
Agostino Patella(CERN&Plymouth), Alberto Ramos(CERN), Nazario Tantalo(Roma 2)

Lattice 2017 Granada, June 18-24 2017

QED in openQ*D code (with C* boundary conditions)

[see previous talk by A. Patella]

- Dirac operator for the O(a) improved Wilson fermions (SU(3)+U(1)):

$$D_W = m_0 + \sum_{\mu=0}^{3} \frac{1}{2}\{\gamma_\mu(\nabla_\mu + \nabla^*_\mu) - \nabla_\mu \nabla^*_\mu\} + \delta D_b + \underbrace{c_{sw,3} \sum_{\mu,\nu=0}^{3} \frac{i}{4}\sigma_{\mu\nu}\hat{F}_{\mu\nu}}_{SU(3)\ \text{SW-term}} + \underbrace{c_{sw,1} \sum_{\mu,\nu=0}^{3} \frac{i}{4}\sigma_{\mu\nu}\hat{A}_{\mu\nu}}_{U(1)\ \text{SW-term}}$$

- Auxiliary **U(3)** fields used for the construction of **D$_W$**:

$$W_\mu(x) = U_\mu(x) e^{i\hat{q}A_\mu(x)}$$
$$\nabla_\mu \psi(x) = W_\mu(x)\psi(x+\hat{\mu}) - \psi(x)$$
$$\nabla^*_\mu \psi(x) = \psi(x) - W^\dagger_\mu(x-\hat{\mu})\psi(x-\hat{\mu})$$

- $\hat{q} = q/q_{el}$ [cf. Lucini, Patella, Ramos, Tantalo: arXiv:1509.01636]

- $S_G^{QED} = \dfrac{1}{4\pi\alpha_{QED} q_{el}^2} \sum_P (1 - U_P)$

QED in openQ*D code

- U(1) gauge fields:
  - ➡ fundamental field: non-compact (A_μ)
  - ➡ compact field $z_\mu = e^{iA_\mu}$, derived from the non-compact (after each update of A_μ)
  - ➡ in order to have both compact and non-compact formulations of U(1) in `openQ*C`

- Current version of the `openQ*C` code [alpha-version, http://rcstar.web.cern.ch/]
  - ➡ supports only the U(1) compact action

- Stable release will include:
  - ➡ U(1) non-compact action
  - ➡ Fourier acceleration

[http://rcstar.web.cern.ch]

Sample QCD+QED run in openQ*D

- QED+QCD run with **openQ*C** [**HiRep** runs discussed in M. Hansen's talk, Thu. 17.50]
- Nf=2+1; periodic b.c. in time; C* b.c. in space
- L=16, T=32 (simulated volume 32x32x16x16 c.f. A. Patella's talk, Thu. 17.10)
- Starting point: CLS based 2+1 ensembles (H200, VOLUME —> VOLUME / 2^4)

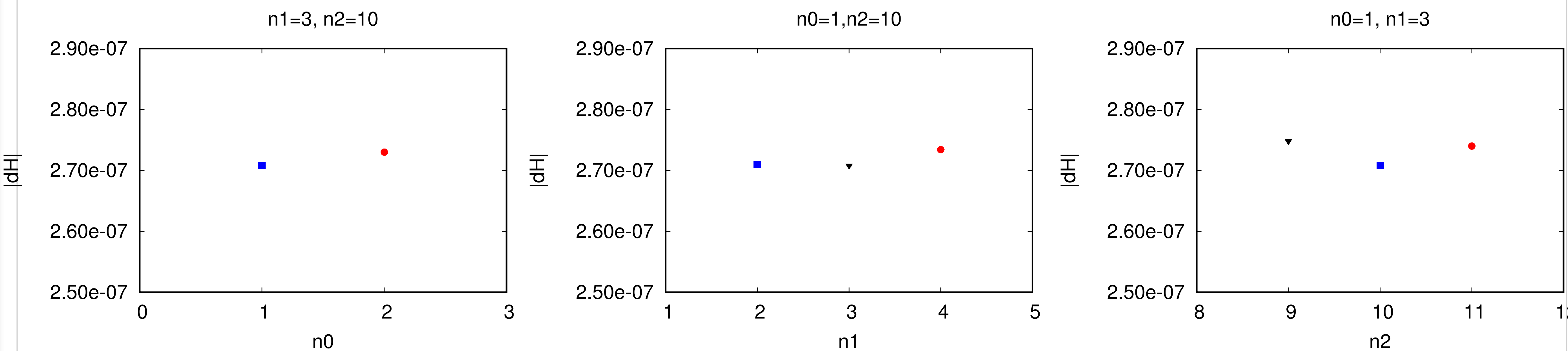
- Test run:
- U(1) parameters: $\alpha_{QED} = 0.05 \approx 7\alpha_{QED}^{phys}$ (Wilson action)
- SU(3) parameters: $\beta = 3.55 \quad \kappa = 0.137$ (Lüscher Weisz action)
- At $\alpha_{QED} = 0:$ $m_\pi \approx 420\mathrm{MeV}$
- Martin Hansen: **HiRep** and gauge-invariant interpolating operators for charged states

Reversibility and the conservation of the Hamiltonian

- Length of the MD trajectory: $\tau_{MD}=0.7$
- 4th order Omelyan-Mryglod-Folk integrator
- 3 MD integration levels

n0	n1	n2
U(1) frc.	SU(3) frc.	ferm. frc.
1	3	10

- Reversibility tests
- Different choices of time-steps at the three MD-integration levels:



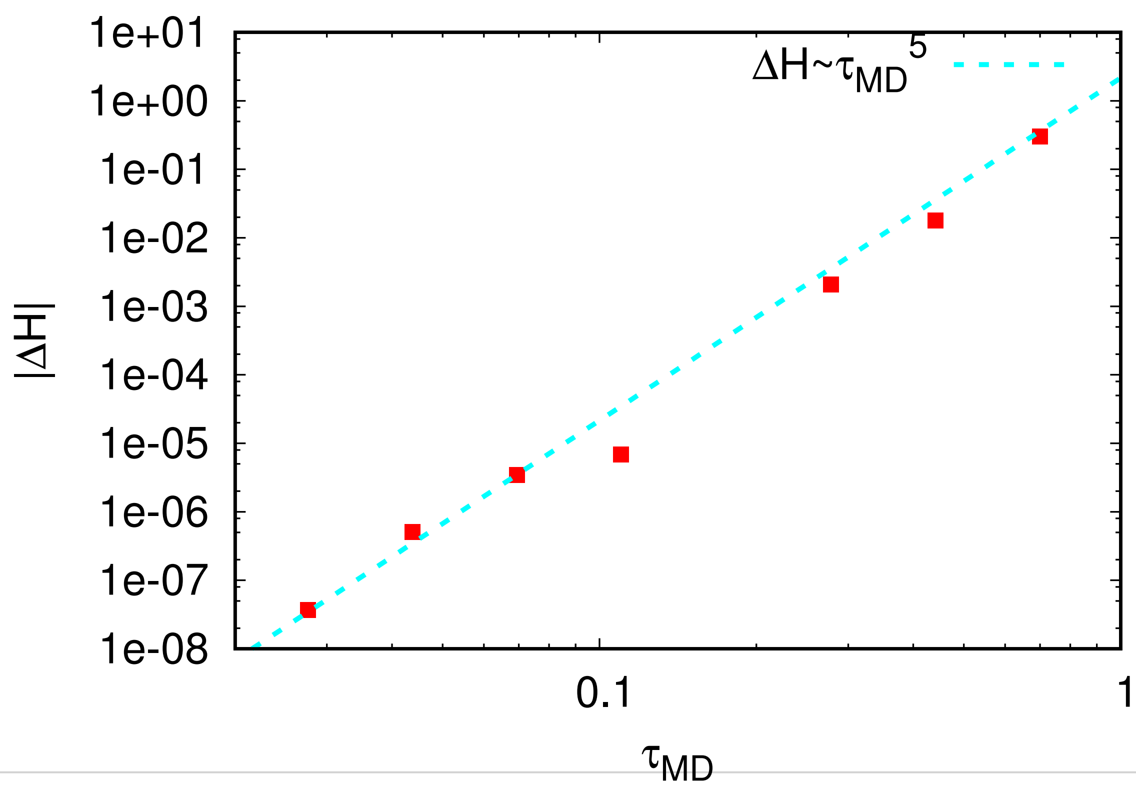
- Violation coming almost entirely from the solver precision ($10^{-10}/10^{-11}$: ferm. force/action)
- When increased to ($10^{-13}/10^{-13}$): |dH|=2.42e-09

Reversibility and the conservation of the Hamiltonian

- Length of the MD trajectory: τ_{MD}=0.7
- 4th order Omelyan-Mryglod-Folk integrator
- 3 MD integration levels

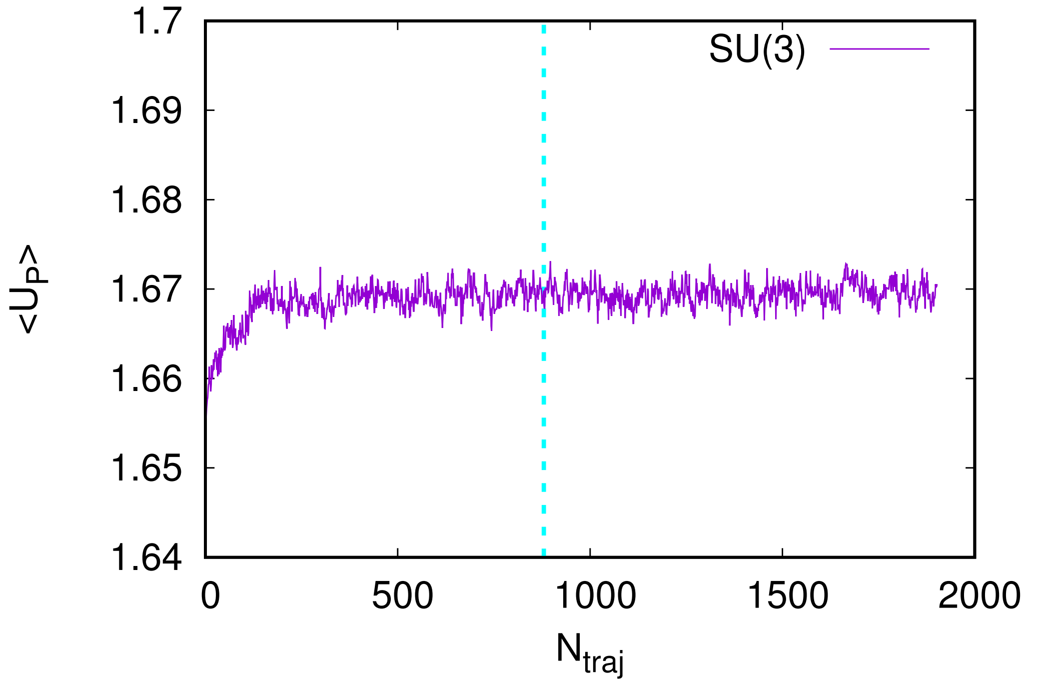
n0	n1	n2
U(1) frc.	SU(3) frc.	ferm. frc.
1	3	10

- Dependence of the energy violation on the MD trajectory length
- Number of steps in the integrator is kept fixed

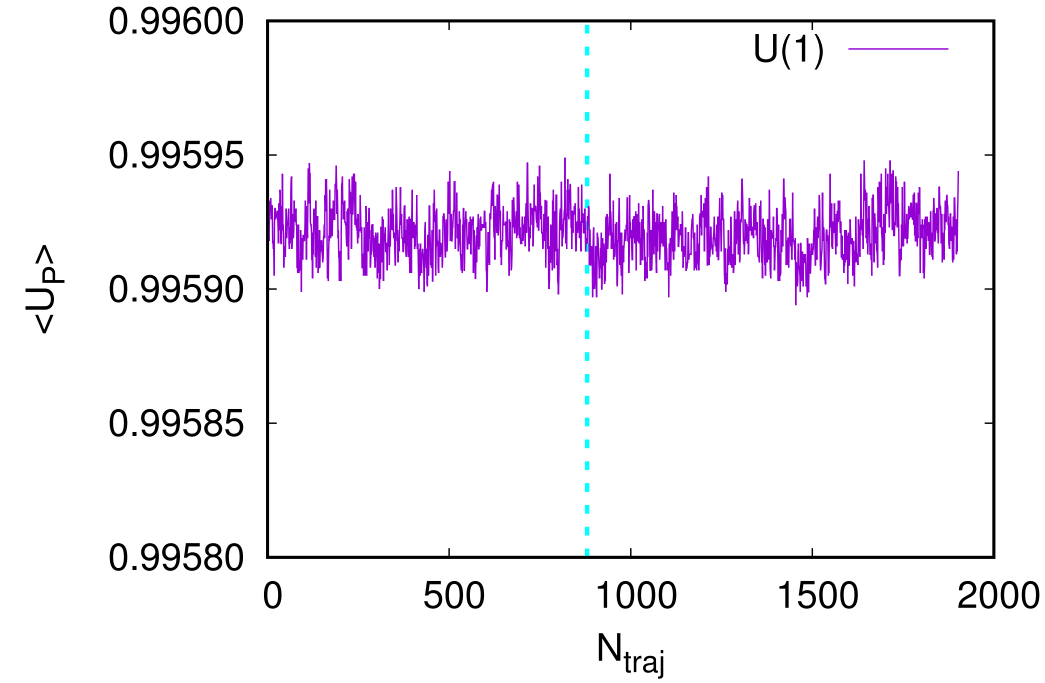


SU(3) and U(1) Plaquette

- SU(3) Plaquette



- U(1) Plaquette

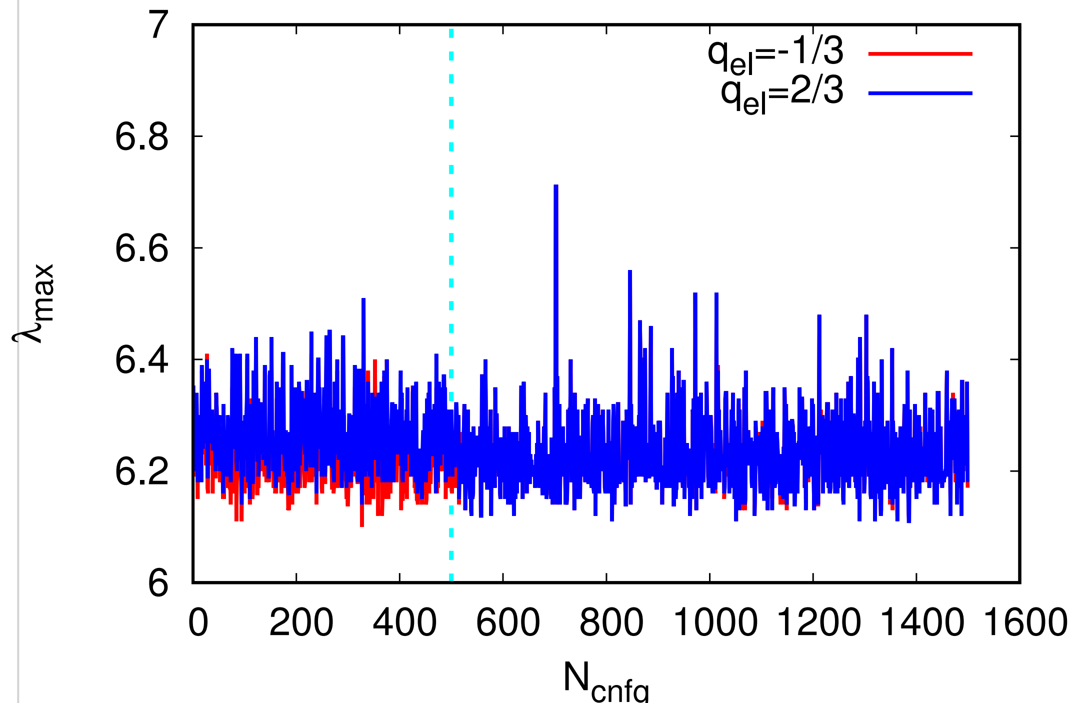


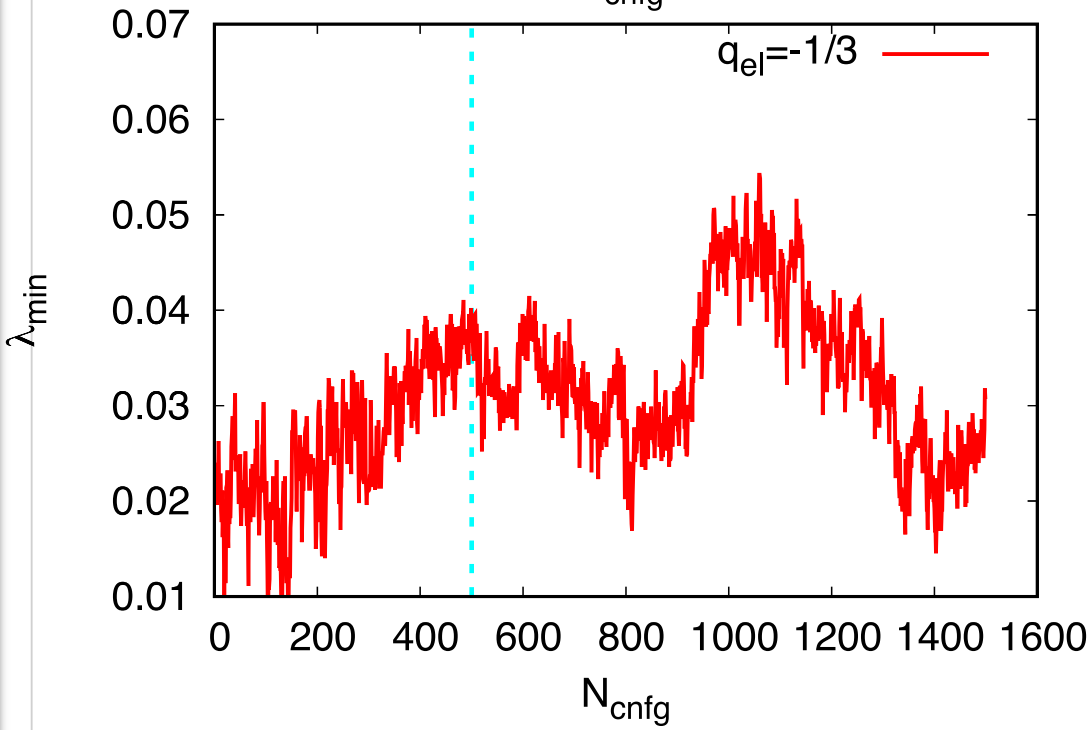
- In order to compare `openQ*D` with `HiRep`

  —> difference in the precision of the used rat. approximation has to be taken into account

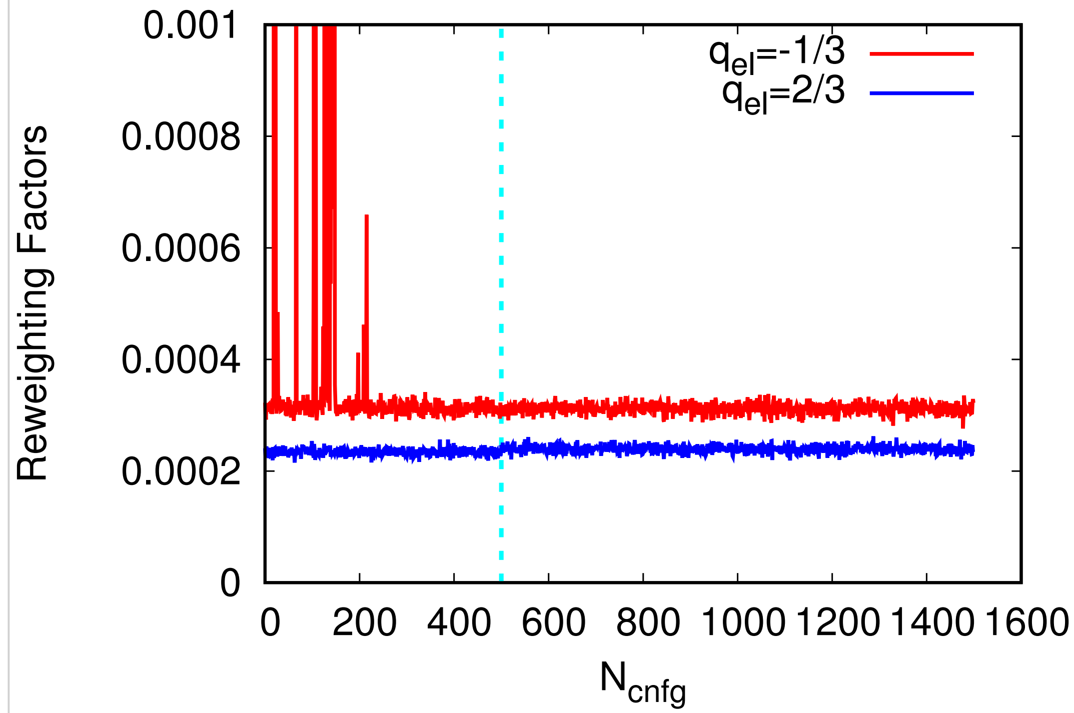
Spectral range of the Dirac operators

- Spectral range:





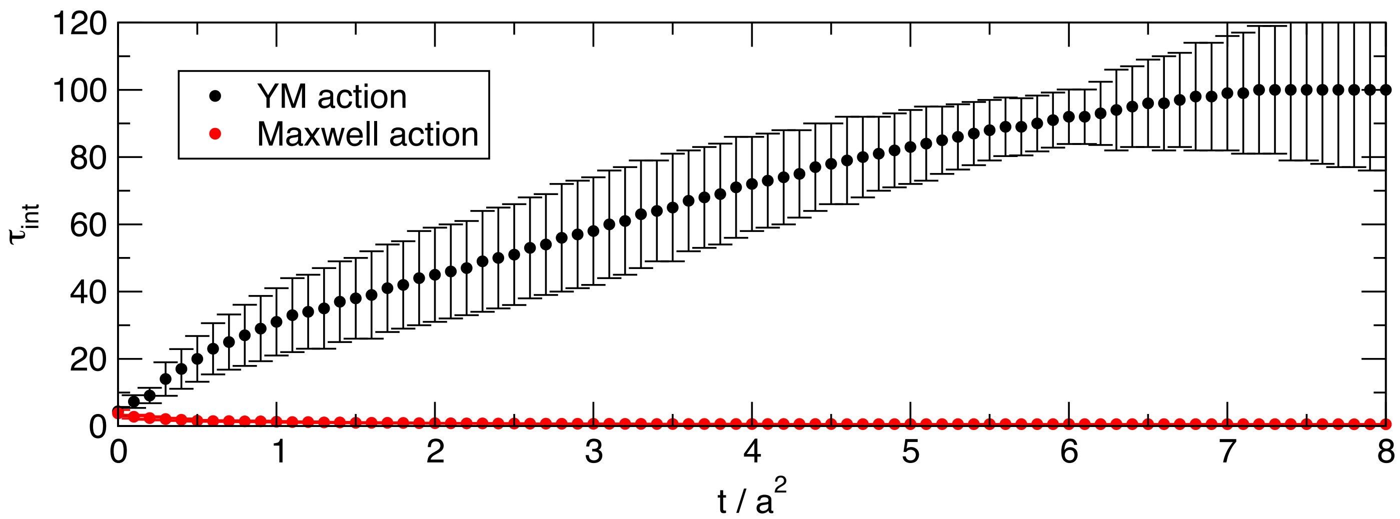
- In the rational approximation: [0.02,7.2]

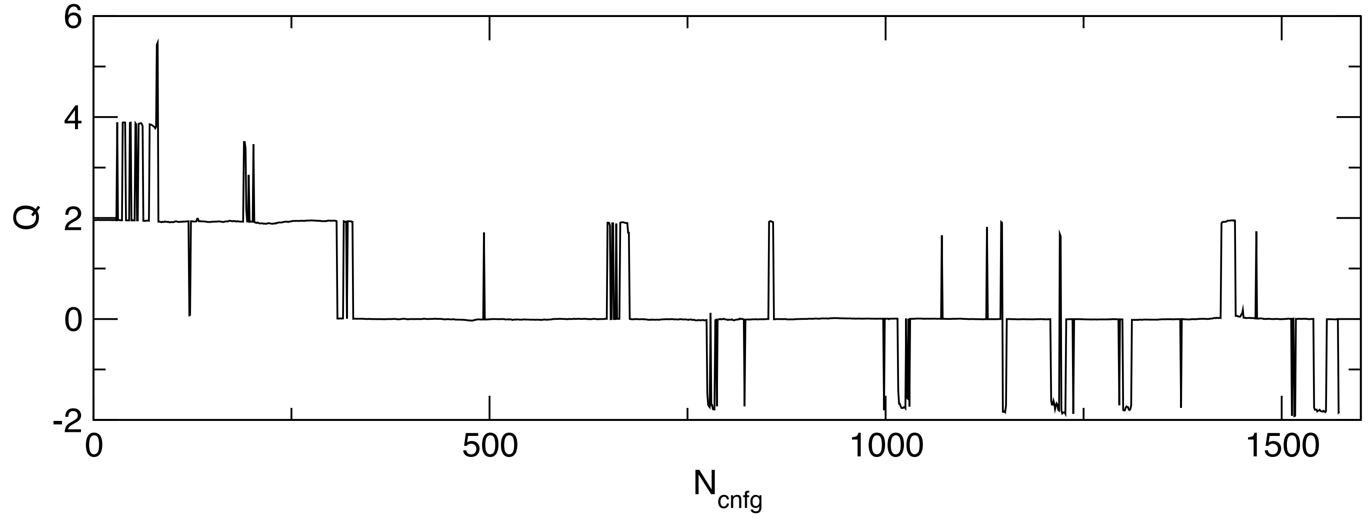


- q_{el}=-1/3: square root (u,s)
- q_{el}=2/3: fourth root (d)
- **openQ*D**: same order in the MD and accept/reject step; rel.err. ~10^{-8} (in the obs. 10^{-4})
- correct with the reweighting factor
- underestimated spectral range

Autocorrelations of SU(3) and U(1) gauge observables

- SU(3) autocorrelations grow with the flow time
- U(1) autocorrelations seem to be O(1) at all scales
- Tunnelling of Q_{top} slower than expected: careful error analysis required





Summary & Outlook

- `openQ*D:` open source code for QCD+QED [alpha-version, http://rcstar.web.cern.ch/]
- Based on openQCD: inherits the highly scalable DFL solver [http://luscher.web.cern.ch/luscher/openQCD/]
- Wide choice of bc's: periodic, C* in space; periodic, open, SF, open-SF in time.
- O(a) improved Wilson fermions (SW-terms for SU(3) and U(1))
- QED implemented for compact action; short-term plans: Fourier acceleration, non-compact U(1)
- Algorithm behaving as expected: stable, thermalised and rat. approx. working
- Quite large autocorrelations for the analysed SU(3) observables
- More tests in progress: more detailed comparison with `HiRep`

Thanks!

- CERN, CERN IT & Lattice Group@TH for managing and providing the computer cluster
- This work was supported by a grant from the Swiss National Supercomputing Centre (CSCS) under project s642
- We thank the University of Cantabria (Spain) for the access to the Altamira Supercomputer
- This work was supported by TCHPC (Research IT, Trinity College Dublin)
- CLS for the starting point run parameters
- Members of the RC* for enjoyable collaboration!