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QCD+QED with C* boundary conditions

RC*OC collaboration

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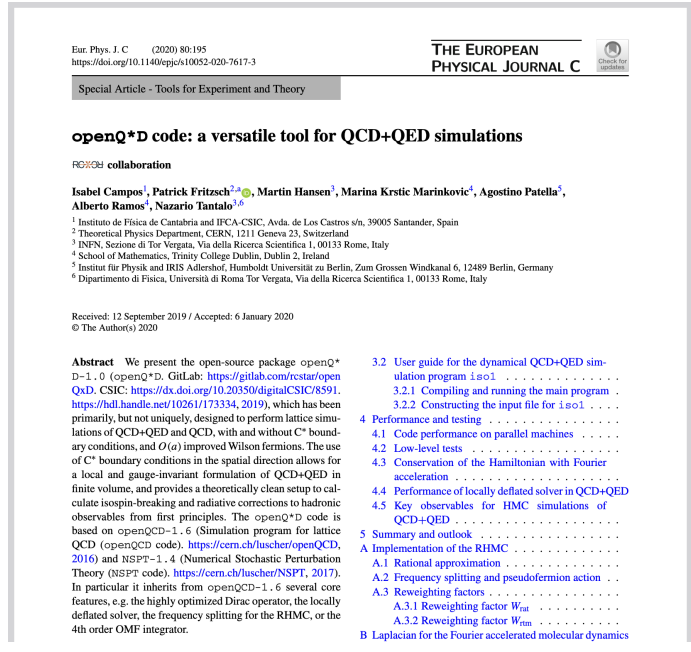

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Special Article - Tools for Experiment and Theory

openQ*D code: a versatile tool for QCD+QED simulations

RC*OR collaboration

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Abstract We present the open-source package `openQ*D-1.0` (`openQ*D`. GitLab: https://gitlab.com/rcstar/openQxD. CSIC: https://dx.doi.org/10.20350/digitalCSIC/8591. https://hdl.handle.net/10261/173334, 2019), which has been primarily, but not uniquely, designed to perform lattice simulations of QCD+QED and QCD, with and without C* boundary conditions, and $O(a)$ improved Wilson fermions. The use of C* boundary conditions in the spatial direction allows for a local and gauge-invariant formulation of QCD+QED in finite volume, and provides a theoretically clean setup to calculate isospin-breaking and radiative corrections to hadronic observables from first principles. The `openQ*D` code is based on `openQCD-1.6` (Simulation program for lattice QCD (`openQCD` code). https://cern.ch/luscher/openQCD, 2016) and `NSPT-1.4` (Numerical Stochastic Perturbation Theory (`NSPT` code). https://cern.ch/luscher/NSPT, 2017). In particular it inherits from `openQCD-1.6` several core features, e.g. the highly optimized Dirac operator, the locally deflated solver, the frequency splitting for the RHMC, or the 4th order OMF integrator.

3.2 User guide for the dynamical QCD+QED simulation program `iso1`
3.2.1 Compiling and running the main program
3.2.2 Constructing the input file for `iso1`
4 Performance and testing
4.1 Code performance on parallel machines
4.2 Low-level tests
4.3 Conservation of the Hamiltonian with Fourier acceleration
4.4 Performance of locally deflated solver in QCD+QED
4.5 Key observables for HMC simulations of QCD+QED
5 Summary and outlook
A Implementation of the RHMC
A.1 Rational approximation
A.2 Frequency splitting and pseudofermion action
A.3 Reweighting factors
A.3.1 Reweighting factor $W_{\rm rat}$
A.3.2 Reweighting factor $W_{\rm rm}$
B Laplacian for the Fourier accelerated molecular dynamics

Ensembles

ensemble	lattice	n.cnfg.	a [fm]	α	M_π [MeV]	$M_\pi L$	MDU dist
A450a07b324	64×32^3	2000	0.05	0.007299	400	3.2	2
A380a07b324	64×32^3	2000	0.05	0.007299	380	3	2
A400a07b324	64×32^3	2000	0.05	0.02	400	3.2	2
A500a50b324	64×32^3	2000	0.05	0.05	500	4	2
A360a50b324	64×32^3	2000	0.05	0.05	360	2.9	2
C380a50b324	96×48^3	600	0.05	0.05	380	4.6	2

Table: QCD+QED ensembles with C* boundary conditions and u+d+s+c sea quarks.

ensemble	lattice	n.cnfg.	sea quarks	a [fm]	M_π [MeV]	$M_\pi L$	MDU dist
A400a00b324	64×32^3	2000	u+d+s+c	0.054	400	3.5	2
B400a00b324	80×48^3	1084	u+d+s+c	0.054	400	5.3	2
C420a00b370	64×32^3	2000	u+d+s	0.049	420	3.3	2
B420a00b346	48×24^3	2000	u+d+s	0.075	420	3.8	2
D270a00b346	96×48^3	500	u+d+s	0.075	270	4.9	2
A420a00b334	32×16^3	2000	u+d+s	0.098	420	3.3	2
B420a00b334	48×24^3	2000	u+d+s	0.098	420	5.0	2
C420a00b334	64×32^3	2000	u+d+s	0.098	420	6.7	2

Table: QCD ensembles with C* boundary conditions.

Ensembles

- Lüscher–Weisz action for SU(3) gauge field
- Wilson action for U(1) field (no gauge fixing)
- $O(a)$-improved Wilson fermions with SU(3) and U(1) clover terms
- Periodic b.c. in time and C* boundary conditions in space
- `openQ*D-1.1` code, publicly available at `https://gitlab.com/rcstar/openQxD`
- HMC + fixed order rational approximation + reweighting factor
- Fourier acceleration for U(1) field
- Multilevel integrator, 2nd and 4th order integrators

Questionnaire

- Disk-space (only cnfg): 60 Tb within one year, more to come
- Data management plan: work in progress.
- Collected metadata
  - Detailed provenance: no
  - Physics and algorithm parameters: yes, input files
  - Plaquette value: yes
  - Checksum config files: no
- Ensembles are publicly available upon request
  - When: after publication on peer-review journal
  - Under which conditions: to be determined
  - Contact person for access: Agostino Patella
  - Format: binary, double precision, custom format
  - We will share also RHMC reweighting factors
  - We plan to upload to ILDG
  - For now configs are available as long as computing centers allow us to keep them
- ILDG
  - Do you have experience with ILDG? Little to none.
  - Do you expect/need any support/advice for uploading to ILDG? I think we will need it.
  - Are you or your collaborators interested in contributing to ILDG developments? Yes (metadata, data lakes).