Silvano Simula

INFN - Roma Tre

INFN meeting on
Large Scale Computing at INFN
Physics Department, University of Rome *La Sapienza*
February 13th, 2017

IS LQCD123

Participants of Italian Institutions (14 people):

RM1: G. Martinelli
RM2: P. Dimopoulos, G. de Divitiis, R. Frezzotti, G.C. Rossi, N. Tantalo
RM3: D. Giusti, V. Lubicz, L. Riggio, G. Salerno, F. Sanfilippo, S. Simula, C. Tarantino,
SISSA: P. Labus

Collaborators from non-italian Institutions (16 people):

DESY: K. Jansen
University of Bern: G. Bergner, U. Wenger
University of Bonn: P. Ferenc, B. Kostrezwa, M. Petschlies, F. Pittler, M. Ueding, C. Urbach
University of Cyprus & Wuppertal: S. Bacchio, J. Finkenrath, H. Panagopoulos
University of Edinburg: M. Garofalo
University of Frankfurt: S. Capitani
University of Grenoble: M. Mangin-Brinet

main research topics of LQCD123

1. production of QCD gauge ensembles at the physical point with $N_f = 2+1+1$ dynamical quarks, production of QCD+QED gauge ensembles with $N_f = 1+1+1$ and C* boundary conditions

2. QED corrections to hadron observables for flavor physics studies

3. leptonic and semileptonic decays of mesons, neutral meson oscillations

4. non-perturbative fermion mass generation

past computing resources

* from PRACE and ISCRA projects (2012-2016): ~ 140 Mcore-hours (BG/Q equivalent)
* from INFN-Cineca agreement (2014-2016): ~ 110 Mcore-hours (BG/Q equivalent)

during the years 2014-2016 the computing time has been acknowledged in:

8 peer-reviewed publications (with ~ 160 citations on HEP-INSPIRE)
16 proceedings (with ~ 100 citations on HEP-INSPIRE)

Production of QCD gauge ensembles at the physical point with N_f = 2+1+1 dynamical quarks

The European Twisted-Mass Collaboration is currently simulating QCD with N_f=2+1+1 flavors of maximally twisted clover Wilson quarks with light quarks close to the physical pion point.

The multi-year plan is to generate gauge ensembles with the following setups:

- lattice spacing of ~0.1 fm and pion masses of ~170, ~220 and ~280 MeV with lattice volumes of 32^3*64 and 48^3*96;

- lattice spacing of ~0.08 fm and pion masses of ~135 and ~220 MeV with lattice volumes of 48^3*96 and 64^3*128;

- lattice spacing of ~0.06 fm and pion masses of ~135 and ~220 MeV with lattice volumes of 64^3*128 and 96^3*192.

The software package is the tmLQCD one developed by ETMC with highly optimized solvers of the Dirac equation
(we assume an improvement factor of ~ 2 due to the future implementation of QphiX libraries)

<u>multi-year computing resources (shared with ETMC)</u>

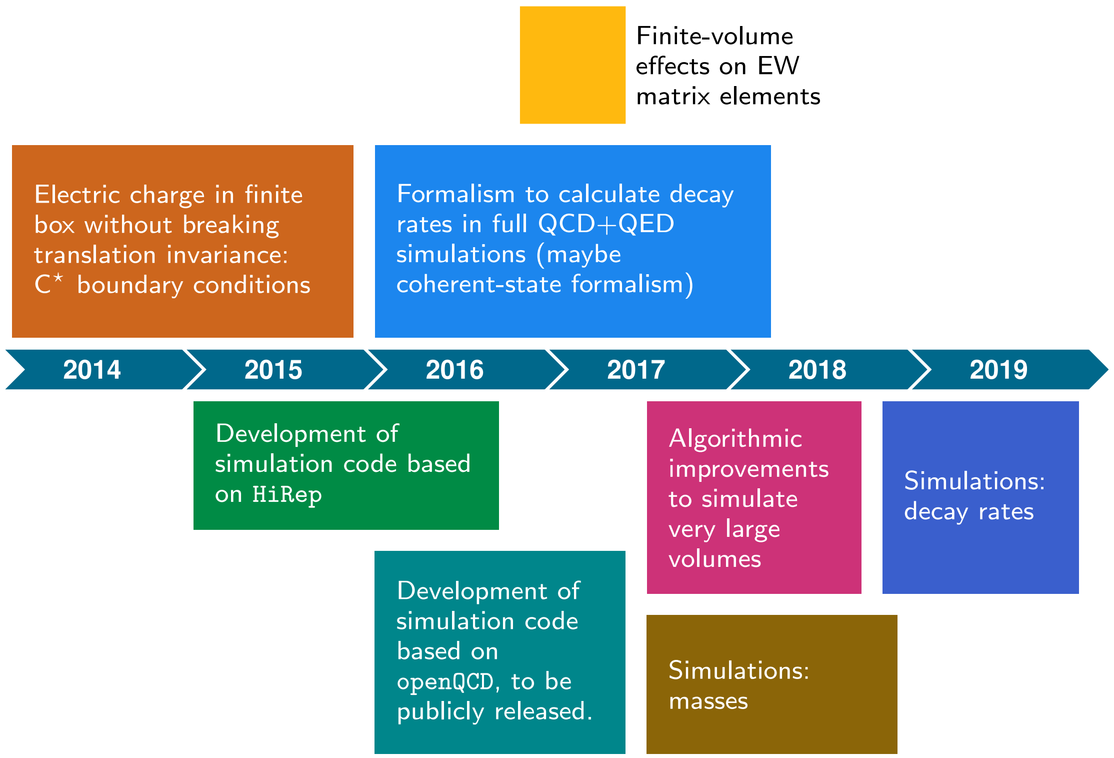
~ 4000 trajectories per gauge ensemble, ~ 3 out of 7 gauge ensembles

our estimate is ~ **200 Mcore-hours on Marconi KNL** (~ 600 Mcore-hours BG/Q equivalent)

Lucini et al. JHEP 1602 (2016) 076

- QED_C is a *local* formulation of QED on the finite volume, a theoretically sound setup
- by enforcing charge conjugation boundary conditions one can study charged states without having to fix the gauge
- the finite volume regularizes infrared divergences without the need of additional (non-local) prescriptions

$$A_\mu(x + \boldsymbol{i}L) = -A_\mu(x)$$



- we are starting a new initiative focused on QCD+QED_C simulations (CERN, Dublin, Odense, Madrid, Rome, ?)
- currently we have a code based on `HiRep`, very flexible but not particularly efficient

$$n_f = 1+1+1\ , \quad m_\pi \sim 420\ \text{MeV}\ , \quad m_\pi L \sim 5\ , \quad a = 0.065\ \text{fm} \qquad \longmapsto \qquad 18\ \text{Mcore-hours}$$

  but we are working on a new efficient code based on `openQCD`, the code will be publicly available by the end of the year

- in the medium/long term we plan to perform simulations on volumes as large as 8 fm at nearly physical values of the pion mass: a realistic estimate of the cost of a typical simulation will be available in a few months
- access to INFN computing resources will boost significantly this new initiative, particularly at these early stages!

QED corrections to hadron observables for flavor physics studies

Precision flavour physics is particularly powerful for exploring the limits of the Standard Model and in searching for inconsistencies which would signal new physics.

The main goal of large-scale simulations using the lattice formulation of QCD is the ab-initio evaluation of the non-perturbative QCD effects in physical processes.

The recent, impressive improvement in lattice computations has led to a precision approaching O(1%) for a number of quantities and therefore in order to make further progress electromagnetic effects and other isospin-breaking contributions have to be considered.

For many relevant physical quantities, as in the case of leptonic and semileptonic decays of hadrons, the presence of infrared divergences in the intermediate steps of the calculation, cancelled by the Block-Nordsieck mechanism, require a new, dedicated strategy, which has been developed [PRD91 (2015)] and successfully applied to the case of $\pi_{\ell 2}$ and $K_{\ell 2}$ decays [Lat '16]

The main open issue is the removal of the quenched approximation of QED (in which sea quark charges are neglected). To this end we need to calculate (fermionic) disconnected diagrams, which arise from the sea quarks or from the sea and valence quarks. For the computation of disconnected quark loops an unbiased stochastic estimate of all-to-all propagators is required. This involves typically the use of a non-negligible number of stochastic sources per QCD gauge configuration.

<u>multi-year computing resources needed</u>

~ 100 sources per gauge configuration, ~ 4000 gauge configurations (ETMC ensembles up to 64^3 * 128 lattices)

using efficient multigrid solvers our estimate is ~ **75 Mcore-hours on Marconi KNL** (~ 225 Mcore-hours BG/Q equivalent)

Leptonic and semileptonic decays of mesons, neutral meson oscillations

The past decade has seen a remarkable progress in the study of flavor and CP violation physics.

The extraction from experiments of useful phenomenological information on the Standard Model and/or New Physics fundamental parameters requires an accurate knowledge of the relevant hadronic matrix elements of the effective weak Hamiltonian.

Using large-scale QCD simulations on the lattice with the ETMC gauge ensembles we aim at an accurate determination of various quantities of utmost importance to constrain CKM matrix elements and, possibly, New Physics parameters, like e.g.

- the leptonic decay constants of K-, D- and B-mesons: e.g. $B_s \to \mu^+\mu^-$
- the vector and scalar form factors of the semileptonic decays of K-, D- and B-mesons: $K \to \pi \ell \nu_\ell, (D,B) \to (\pi, K, \rho, K^*) \ell \nu_\ell$
- the hadronic form factors relevant for the rare decays of the B-meson: $B \to (K, K^*) \ell^+ \ell^-$
- the bag parameters describing the CP-violating oscillations in neutral K-, D- and B-mesons

Two important features:

light, strange and charm quarks can be simulated dynamically on present lattices, while to reach the b-quark we will make use of the ETMC ratio method [JHEP 04 (2010)], which requires a series of simulated heavy-quark masses from m_c to ~$3m_c$.

the momentum dependence of the hadronic form factors require the use of non-periodic boundary conditions to inject arbitrary momenta on the lattice.

<u>multi-year computing resources needed</u>

~ 2 sources per gauge configuration, ~ 4000 gauge configurations (ETMC ensembles up to 64^3 * 128 lattices)
~ 10 values of injected momentum, ~ 10 values of quark masses from ~m_{ud} to ~$3m_c$

our estimate is ~ **150 Mcore-hours on Marconi KNL** (~ 450 Mcore-hours BG/Q equivalent)

Dynamical generation of natural fermion mass in a lattice model with gluons, quarks and scalars

INFN RM123 @ Tor Vergata

G. de Divitiis, R. Frezzotti and G. Rossi – in collaboration with

B. Kostrzewa, F. Pittler, C. Urbach @ Bonn Univ. – Physics Dept.

M. Garofalo @ Edinburgh Univ. – Physics and Astronomy Dept.

P. Dimopoulos @ Centro Studi e Ricerche Enrico Fermi – Roma

S. Capitani @ Frankfurt Univ. – Theoretical Physic Inst.

References: Frezzotti & Rossi Phys. Rev. D92 (2015) 054505,
Frezzotti, Garofalo & Rossi Phys. Rev. D93 (2016) 105030,
Capitani et al. arXiv:1611.03997, to appear in PoS LATTICE2016

In a $d = 4$ model with hard UV cutoff $(\sim 1/b)$ where

a Dirac fermion doublet is coupled to a SU(3) gauge field and
via Yukawa and “irrelevant” Wilson-like terms to a scalar (Φ)

$$L = L_{kin}(Q, A, \phi; g_0^2) + V(\Phi; m_0^2, \lambda_0) + \left[\left(\frac{b^2}{2}\rho \bar{Q}_L \overleftarrow{D} \Phi D Q_R + \eta \bar{Q}_L \Phi Q_R \right) + h.c. \right]$$

$\exists$ exact global chiral symmetry $(\chi_L \times \chi_R)$ acting on fermions and Φ
$\exists$ fermionic chiral symmetries broken by “irrelevant” Wilson-like terms

at a critical point fermion chirality is restored up to UV-cutoff effects

$\Rightarrow$ confinement & no fermion chiral-SSB in the Wigner phase of χ

$\Rightarrow$ fermion chiral-SSB and dynamical mass in the NG phase of χ

$$m_{ferm}^{dyn} = C_1 \Lambda_s = \mathrm{O}(\alpha_S^2)\Lambda_s \,,$$

unrelated to $\langle \Phi \rangle \gg \Lambda_s$ or UV-cutoff $\quad \leftrightarrow \quad$ *naturalness*

Technically m_{ferm}^{dyn} stems from non-perturbative (NP) operator mixing:

$$\Gamma^{NG}_{\rm eff,loc} = {\rm Kin.\ terms} + V(\Phi) + \Big[(\eta-\eta_{cr})\zeta_0 \bar{Q}_L \phi Q_R + C_1 \Lambda_s \bar{Q}_L U Q_R + h.c.\Big]$$

a conjecture suggested by $m_{cr} = \frac{c_0}{a} + c_1 \Lambda_{QCD}$ in Wilson lattice QCD;
no analytic proof feasible – no renormalization theorems at NP level:

the NP mechanism can be (dis)proved only by numerical simulation !

Key feature of NP QFT + big potential for Beyond-SM model building:

assuming hyper-strong interactions with RGI scale $\Lambda_T \sim$ few TeV $\Rightarrow$

$\exists$ critical point where the same NP mechanism gives in *natural* way

$$m_{top}^{dyn} = {\rm O}(\alpha_s^2 \Lambda_T), \ \dots\ , \qquad m_{\mathcal{T}}^{dyn} = {\rm O}(\alpha_Y^2 \Lambda_T), \ \dots\ ,$$

weak boson masses $\quad (m_W^{dyn})^2 \sim g_W^2 \alpha_T^2 \Lambda_T^2 \times [2\ {\rm loop\ factor} \ll 1]$

& hyper-strongly interacting fermions $\Rightarrow$ WW bound state $\leftrightarrow$ Higgs

First NP lattice study of SU(3) gauge model with fermions + scalars

$L^{lat} = L_{kin}(U,\Phi;g_0^2) + V(\Phi;m_0^2,\lambda_0) + \bar\Psi D_{lat}(U,\Phi;\eta,\rho)\Psi\ , \quad \Psi = (u,d)^T$

$D_{lat}\Psi = \gamma\widetilde\nabla\Psi + \eta F\Psi - \rho\frac{b^2}{2}(F\widetilde\nabla\widetilde\nabla\Psi + \partial F\widetilde\nabla\Psi\text{−terms})\ , \quad F = \phi_0 1\!\!1 + i\gamma_5\phi_j\tau^j$

Started in quenched approximation & with naive lattice fermions

- (u,d) $\times$ 16 doublers even as $b \to 0$ [because W-like term has $d = 6$]
- exact $\chi_L \times \chi_R$, purely fermionic chiral symm. restored at η_{cr} up to O(b^2)
- use $D_{lat} + i\gamma_5\tau^3\mu_0$ to avoid exceptional (U,Φ)-conf. & then $\mu_0 \to 0$

Wigner phase: η_{cr}; NG phase: check presence of $m^{dyn}_{ferm} \sim C_1\Lambda_s$

- by studying WTI of fermionic chiral symmetry and $M^2_{PS} \sim m^{dyn}_{ferm}$ at η_{cr}
- using 3 lattice spacings (0.12 to 0.08 fm) & two volumes ($L \sim$ 2 and 3 fm)

Quenched study estimates (@Marconi-A2): $\sim$ 13 + 21 + 31 = 65 Mcoreh

Unquenching with DW fermions: new algorithm + feasibility $\sim$ 30 Mcoreh

multi-year computing resources for LQCD123

research topic	Mcore-hours on Marconi KNL
production of QCD gauge ensembles at the physical point with $N_f = 2+1+1$ dynamical quarks	200
production of QCD+QED gauge ensembles with $N_f = 1+1+1$ and C* boundary conditions	20
QED corrections to hadron observables for flavor physics studies	75
leptonic and semileptonic decays of mesons, neutral meson oscillations	150
non-perturbative fermion mass generation	95

	540

in the years 2017-2019 we expect from PRACE projects and INFN-Cineca agreement: ~180 Mcore-hours (~1/3 of the total)