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Computer simulations of the theory of strong interactions

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Summary. — This talk gives a very fast overview of the algorithms commonly used to perform computer simulations of the theory of Strong Interactions (QCD) for scientists working on problems arising in different scientific fields whose solution requires numerical simulations of many interacting degrees of freedom.

PACS 11.15.Ha – Lattice gauge theory.
PACS 12.38.Gc – Lattice QCD calculations.

1. – Introduction

The quantum field theory of the Strong Interactions, called Quantum Chromo Dynamics (QCD), is formulated in terms of fundamental degrees of freedom. These are the quarks, *i.e.* six particles of different gravitational mass (of different flavor) carrying twelve internal quantum numbers (three color and four spinor indexes) and the gluons, *i.e.* eight particles playing for the strong interactions the role played from the photon for electromagnetism, represented as a traceless hermitian matrix acting in color space.

The peculiarity of QCD with respect to the theories of the other known interactions, all built on the principle of gauge invariance, is that the strong coupling constant is not (always) small. More precisely, the strong force is small when the quarks are "glued" together to form a bound state, generically called hadron, and gets stronger and stronger when one tries to pull apart one of the quarks. At some point the energy accumulated into the system gets sufficiently big to create a quark-antiquark pair and the original system rearranges into two or more new hadrons. This mechanism is known as asymptotic freedom [1, 2] and it is believed to be responsible for the so-called confinement of the quarks inside the hadrons. The consequences of confinement for theorists making phenomenological predictions starting from QCD is that we cannot set up a perturbative expansion in powers of the strong coupling constant and we cannot use the concept of "test charge", tools that have been both proved extremely useful in the study of the other fundamental interactions. As an example one can think of a proton, a bound state of three (valence) quarks whose mass is almost enterally due to their binding energy,

the three quarks being almost massless: that is very different from what happens for an electromagnetically bound state, a hydrogen atom say, and that is why a nuclear bomb is much more dangerous than a firecracker.

Quarks interact also weakly and electromagnetically. The most beautiful and interesting phenomenology shown by hadronic systems is indeed due to weak interactions among bound states containing quarks of different flavor. Though perturbative tools can be used when studying electroweak interactions of leptons (electrons, neutrinos and their heavier "copies") these techniques are not useful when applied to confined quarks. The only known theoretical tool that we have in our hands to study QCD by starting from its formulation in terms of fundamental degrees of freedom are computer simulations.

2. – Feynmann to Wilson: "go on a lattice!"

QCD can be studied on a computer by introducing a finite volume, by discretizing the four space-time dimensions and by defining the theory on the resulting "lattice" [3]. The formulation of the discrete theory is not unique because of the freedom to modify the interactions by terms that vanish in the continuum and/or infinite volume limits (*i.e.* by sending the lattice spacing a to zero and the number of points in each direction N_i to infinity). The scope of this talk is to give a flavor of the complexity of lattice QCD (LQCD) calculations so I will briefly sketch how a typical simulation goes on without entering too much into the details.

In order to make predictions from the theory we have to calculate the expectation values of observables according to

$$\langle \mathcal{O} \rangle = \mathcal{N} \int \delta U \; e^{-S_g[U]} \det \left\{ (M^\dagger[U] + m)(M[U] + m) \right\} \; \mathcal{O}\left[\frac{1}{M[U] + m} \right], \tag{1}$$

where the U's are unitary 3×3 complex matrices with $\det U = 1$ and we have four of them per lattice point (typical lattice sizes simulated nowadays have about $N_0 N_1 N_2 N_3 = 64 \times 32^3$ lattice points). The matrix $M[U]$ is the lattice Dirac operator and acts on a complex vector space of dimension $12 \times N_0 N_1 N_2 N_3$. In the previous expression we have neglected the determinants of four out of the six quarks (since they are heavier than the two retained, the up and down) and made the very good approximation that the up and down quarks have the same mass. Equation (1) is the link between quantum field theory and statistical physics. What changes from one statistical system to the other are the number and nature of the degrees of freedom (here $x = U$), their partition function (here $\exp[-V(x)] = \det\{(M^\dagger[U] + m)(M[U] + m)\} \exp[-S_g[U]]$) and the observable of interest but the algorithms used to calculate the partition function are very similar. Lattice QCD calculations are particularly difficult and expensive from the numerical point of view because of the determinant appearing in eq. (1) and of the peculiar functional dependence of $\mathcal{O}[(M[U] + m)^{-1}]$ that arise after the exact formal integration of the quark's degrees of freedom.

The problem can be attached by enlarging the phase space through the introduction of the conjugate momenta of the U's, the Π's, and complex bosonic variables ϕ and $\phi^\dagger$ that live in the vector space acted upon from the Dirac operator. In this space it is possible to set up an algorithm that generates a sequence of configurations distributed

according to the probability density

$$P[\Pi, U, \phi] \propto \exp\left[-\Pi^2/2 - S_g[U] - \phi^\dagger \frac{1}{(M^\dagger[U]+m)(M[U]+m)}\phi\right]. \tag{2}$$

Having such a sequence, a given observable can be calculated as the average over the subset of statistically independent gauge configurations so generated

$$\langle \mathcal{O} \rangle = \lim_{N\to\infty} \frac{1}{N} \sum_{i=1}^{N} \mathcal{O}\left[\frac{1}{M[U_i]+m}\right]. \tag{3}$$

The algorithms used to generate the sequence of gauge configurations are all variants of the exact Hybrid Monte Carlo (HMC) algorithm introduced in ref. [4]. The first step of the algorithm consists in extracting the Π's distributed according to $P[\Pi] \propto \exp[-\Pi^2/2]$ and the vectors χ and $\chi^\dagger$ distributed according to $P[\chi, \chi^\dagger] \propto \exp[-\chi^\dagger\chi/2]$ in order to obtain the vector $\phi = (M[U]+m)\chi$ and its conjugate. Subsequently one starts a Molecular Dynamics in the (Π, U) space at fixed ϕ according to the Hamiltonian $H[\Pi, U, \phi] = -\log P[\Pi, U, \phi]$. After an MD trajectory of length τ, the new configuration is accepted or rejected with probability

$$P_{\rm acc}[U] = \min(r, \exp[H[\Pi_0, U_0, \phi_0] - H[\Pi_\tau, U_\tau, \phi_\tau]]), \tag{4}$$

where $0 \leq r \leq 1$ is a random number extracted from a flat distribution and a new iteration is started with the new U's. On the one hand, the accept/reject step corrects for the errors due to the numerical integration of the MD equations and makes the algorithm exact. On the other hand, the time-step in the numerical integration of the MD equations must be chosen sufficiently small to get a good acceptance rate (say bigger than 80%). At each step of the MD evolution one needs to evaluate the "fermion force",

$$F_f[U, \phi] \propto \phi^\dagger \frac{1}{M[U]} \frac{\delta M[U]}{\delta U} \frac{1}{M[U]}\phi, \tag{5}$$

where we have defined $M[U] = (M^\dagger[U]+m)(M[U]+m)$. This requires the inversion of a huge matrix that gets worse and worse conditioned when the quark mass m is lowered toward its physical value.

3. – The Berlin wall and its fall

In 2001 the annual lattice conference was held in Berlin where it has been discussed the scaling of the HMC algorithm with the quark mass. The plot in the left panel of fig. 1 shows the scaling of the HMC algorithm as a function of the quark mass as obtained by the Japanese group [5]: the black curve exhibits a critical slowing down of the algorithm that goes a m^{-6} and the lattice community immediately realized that it would have been impossible to approach the physical point (marked by the red vertical line) without an improvement in simulation algorithms. This was the Berlin Wall (there are many other "walls" in lattice QCD simulations because of the very different thermalization times of the short-and long-distance collective variables and, in particular, of the topological ones [7]).

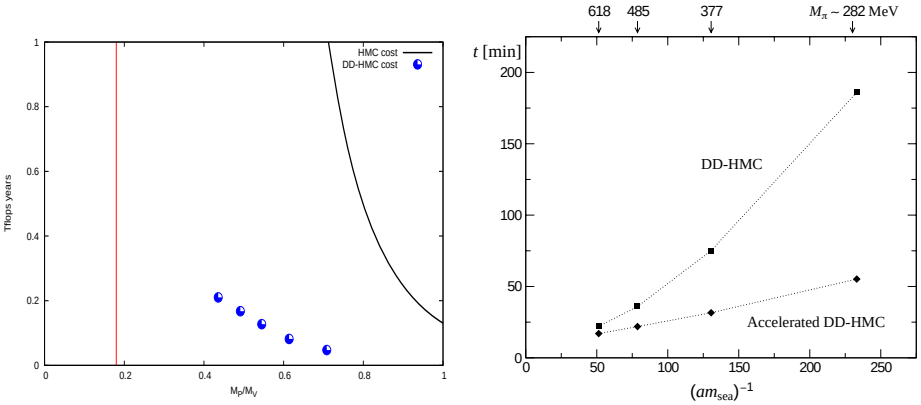

Fig. 1. – (Colour on-line) Left panel: cost of lattice QCD simulation in Teraflops per year as a function of the quark mass; the red vertical line marks the physical point while the black curve is the scaling of the HMC algorithm as discussed in ref. [5]; the blue points show the scaling of the DD-HMC algorithm. Right panel: time required to perform DD-HMC simulations of lattice QCD (in minutes) as a function of the inverse quark mass (the physical point is at $M_\pi = 140\,\mathrm{MeV}$); data are from ref. [6].

In ref. [8] M. Lüscher proposed a new algorithm of the HMC type based on domain decomposition. The whole lattice is divided into small blocks and the Dirac operator is factorized into the product of the operators acting within the blocks (short-distance physics) times the resulting Schur complement (long-distance physics). By factorizing the Dirac operator one can introduce a different vector ϕ_k for each factor and the resulting MD fermion force is the sum of several contributions:

$$M[U] = M_1[U]\; M_2[U] \dots \tag{6}$$

$$F_f[U,\phi] \propto \phi_1^\dagger \frac{1}{M_1[U]} \frac{\delta M_1[U]}{\delta U} \frac{1}{M_1[U]} \phi_1 + \phi_2^\dagger \frac{1}{M_2[U]} \frac{\delta M_2[U]}{\delta U} \frac{1}{M_2[U]} \phi_1 + \dots$$

If the different contributions to the MD have different magnitudes one can use a multiple time step integrator [9] in such a way that $\epsilon_1|F_1| \sim \epsilon_2|F_2| \sim \dots$, where the ϵ_i's are the different time steps. A big gain with respect to the unfactorized algorithm is obtained when the proposed factorization is such that the computationally demanding contributions to the force are the ones that have to be evaluated less frequently. The so-called DD-HMC algorithm of refs. [8, 6] achieves this goal by exploiting asymptotic freedom of the strong interactions. A systematic study of the scaling of the DD-HMC algorithm has been carried out in refs. [10-12] where a scaling with the first power of the inverse quark mass has been found, as shown by the blue points of fig. 1. Similar performances have been obtained by using similar ideas and by introducing different factorizations of the Dirac operator [13, 14].

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In this talk I have tried to give an idea of the complexity of lattice QCD calculations by sketching the algorithms that are commonly used to carry out these simulations but without describing the details of the theory and without even discussing any particular problem that would require the knowledge of strong interactions phenomenology.

Exhaustive recent reviews on the status of lattice QCD simulations can be found in refs. [15,16] while the details on the formulation of the theory on the lattice can be found in standard textbooks on the subject.

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