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Full QCD on APE100 Machines.

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Abstract

We present the first tests and results from a study of QCD with two flavours of dynamical Wilson fermions using the Hybrid Monte Carlo Algorithm (HMCA) on APE100 machines.

Initially we have tested the algorithm without fermions to produce SU(3) pure gauge configurations. The simulations have been performed on a 6^4 lattice at $\beta = 5.7$ and $\beta = 6.0$.

Then we started with the full QCD simulations. The HMCA parameters have been tuned using a wide class of tests performed on a 8^4 and on $12^3 \times 32$ lattices. First results for the mesons correlations functions on $12^3 \times 32$ lattice are obtained at $\beta = 5.3$.

In this paper we are briefly facing some technical aspects: we discuss about the inversion algorithm for the fermionic operator, we underline the methods used to overcome the problems arising using a 32 bits machine and we discuss the implementation of a new random number generator for APE100 machines.

Finally we propose different scenarios for the simulation of physical observables, with respect to the memory capacity and speed of different APE100 configurations.

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1 Introduction.

Numerical simulations of Quantum Field Theories on the lattice by means of Monte Carlo methods have become an important tool to understand and predict non-perturbative phenomena in particle physics. The quantitative study of some aspects of quantum field theories, for example the determination of the hadronic mass spectrum of QCD, requires non-perturbative approach as such as the lattice one.

Up to now most of the numerical simulations in lattice QCD have been performed in the quenched approximation and results on large lattices with high statistics have been obtained[1]. In this drastic and uncontrolled approximation the QCD calculations are performed neglecting the contribution of the sea quarks. The only way to estimate the quenched systematic error is to repeat the calculations with dynamical sea quarks, but these simulations require one or two orders of magnitude more CPU time than the quenched ones.

In the last years some groups have started the simulations of full QCD using the Hybrid Monte Carlo algorithm[2] both for staggered and for Wilson dynamical fermions[3]. In the case of the simulations of QCD with two degenerate flavours of Wilson fermions the mass spectrum and decay constants calculations[4] are restricted to 16^3 spatial lattice size, with $\beta = 5.3 - 5.6$ and up to $(\frac{m_\pi}{m_\rho})^2 \sim 0.3$. There are no results about the glueballs mass spectrum for Wilson dynamical fermions.

In these full QCD calculations the main sources of errors have been found to be the correlations between different molecular dynamics trajectories[5][6] and finite size effects[7]. There are preliminary studies on the correlations for Wilson dynamical fermions, while the finite size effects have been studied, up to now, only for staggered fermions.

In order to control all possible systematic and statistical errors in a realistic full QCD simulation, a great amount of CPU time and a large memory capacity are required. These are the problems that caused the development of QCD-dedicated parallel supercomputers[8]. The APE100 parallel machines[9] promise to be a good tool to face the problem of unquenched QCD simulations.

APE100 is a synchronous SIMD machine, composed of a 3-dimensional cubic mesh of processors, with periodic boundary conditions. Each node contains a floating point processor (MAD)[10], a memory bank of 1M 32-bit words and a network interface device. The main advantage of this simple structure is modularity: the mesh can be enlarged to obtain more processing power. A scalar CPU takes care of the program flow and of all integer operations that essentially amount to address computation and do-loop book-keeping. The MAD processor operates on IEEE 32-bit floating point number (single precision).

The results presented in this paper are obtained using the single board configuration (8 nodes disposed on a $2 \times 2 \times 2$ cube), with a peak speed of 400 Mflops and the "tube" configuration (128 nodes disposed on a $2 \times 2 \times 32$ lattice) with a peak speed of 6.4 Gflops. The next available APE100 configurations will be the 25 Gflops "tower" (512 nodes in a $8 \times 8 \times 8$ lattice) and the full 100 Gflop APE100 with 2048 nodes arranged on a $16 \times 16 \times 8$ lattice.

In this paper we present the implementation of the HMCA on the APE100 machines, the tests performed and the QCD results obtained up to now. In section 2. we review the basic formalism of unquenched QCD, then in section 3. we present the Hybrid Monte Carlo algorithm implemented on APE100 and we underline the parameters' tuning required and the tests which can be performed. A short technical discussion about the single precision aspects, the inversion algorithms and the random number generator used will be found in section 6. A detailed analysis of the technical aspects of the implementation of the HMCA on the APE100 machines and of the performances obtained will be presented separately[11].

In section 4. we present the tests and the results obtained using the HMCA in the quenched approximation on 6^4 lattices at $\beta = 5.7$ and $\beta = 6.0$, while in section 5. we present the results for the full QCD case. The latter have been obtained on 8^4 and on $12^3 \times 32$ lattices at $\beta = 5.3$, with values of Wilson hopping parameter k_{sea} lower than that corresponding to the strange one. Finally in section 7. we report our conclusions and discuss the full QCD simulations that can be faced with the different APE100 machines configurations.

2 Unquenched QCD

The greatest obstacle to the simulation of QCD on a lattice is the inclusion of dynamical fermions. Most of the simulations of lattice QCD have ignored the contributions of sea quarks by using the quenched (or "valence") approximation. The QCD Lagrangian is

$$L_{QCD} = L_{YM} + \sum_{f=1}^{N_f} \bar{\psi}_f(\not{D} + m)\psi_f \ , \tag{2.1}$$

where $L_{YM} = -\frac{1}{4}F^{\mu\nu a}F^{\mu\nu a}$, f is the flavour index and D is the usual covariant derivative. The Feynman path integral for the partition function Z is:

$$Z = \int \mathcal{D}A_\mu \mathcal{D}\bar{\psi}\mathcal{D}\psi e^{-\int d^4x L_{QCD}} \ . \tag{2.2}$$

The integration over the fermionic degrees of freedom gives

$$Z = \int \mathcal{D}A_\mu [det(\not{D} + m)]^{N_f} e^{-\int d^4x L_{YM}} \ . \tag{2.3}$$

In the quenched approximation the number of flavours, N_f is set to zero. Consequently, in terms of perturbative approach, in this approximation one does not consider sea quark contribution to physical observables, neglecting virtual quark loops and treating fermions as static degrees of freedom.

It will be interesting to study the effects of the sea quarks on all the QCD observables, and particularly on that ones that are supposed to present strong discrepancies with the quenched results, such as the σ-term of the nucleon[12],[13], or the the $(\pi - \eta')$ mass splitting. Of course, if one could reach the physical m_π/m_ρ value, the most interesting observable would be the branching ratio of the $\rho \to 2\pi$ decay. Up to now the numerical full QCD studies [3] are performed at high quark masses, with statistic not comparable with the quenched one.

In order to go beyond the quenched approximation, we need to calculate the non-local fermionic determinant. A standard way to compute a determinant requires[14] about $N \sim O(V)$ arithmetic operations so the use of standard Monte Carlo algorithms (like Metropolis, which requires the calculations of the fermionic determinant for the updating of each link) is practically impossible.

Taking into account the effects of the sea quarks one can write the fermionic determinant by the introduction of a path integral over the pseudofermionic fields ϕ. Let call $M = (\not{D} + m)$,

$$Z = \int \mathcal{D}A_\mu \left[detM\right]^{\dagger\frac{N_f}{2}} \left[detM\right]^{\frac{N_f}{2}} e^{-\int d^4x L_{YM}} \tag{2.4}$$

$$= \int \mathcal{D}A_\mu det\left[M^\dagger M\right]^{\frac{N_f}{2}} e^{-\int d^4x L_{YM}} \tag{2.5}$$

$$= \int \mathcal{D}A_\mu \; e^{-\int d^4x L_{YM}} \int \mathcal{D}\phi\mathcal{D}\phi^* e^{-\phi^*[M^\dagger M]^{-\frac{N_f}{2}}\phi} \; . \tag{2.6}$$

On the lattice the previous path integral becomes

$$Z = \int \mathcal{D}U \; \mathcal{D}\phi\mathcal{D}\phi^* \; e^{-S_G(U)-\phi[M^\dagger M]^{-\frac{N_f}{2}}\phi^*} \tag{2.7}$$

where $S_G(U)$ is the standard $SU(3)$ Wilson action for the gauge fields,

$$S_G(U) = \frac{\beta}{N_{col}} \sum_{\Box} tr(I - Re(U_\Box)) \tag{2.8}$$

and the sum is over the plaquettes

$$U_\Box = U_\mu(x)U_\nu(x+\mu)U^\dagger_\mu(x+\nu)U^\dagger_\nu(x) \; . \tag{2.9}$$

One observable which is generally calculated also in full QCD simulations is the plaquette $\sum_\Box tr(Re(U_\Box))$ that is related to the pure gauge energy as we can see from eq.(2.8).

We have used the following formulation of the fermionic operator M, that appears in the lattice action (2.7):

$$M(x,y) = \delta_{x,y} - k\sum_{\mu=1}^{4}\Big[(1+\gamma_\mu)U_\mu^\dagger(x)\delta_{x,y-\mu} + (1-\gamma_\mu)U_\mu(x-\mu)\delta_{x,y+\mu}\Big]\ . \quad (2.10)$$

In the next section we discuss the algorithm that we use to generate full QCD configurations of link fields $\{U_\mu(x)\}$ distributed according to the measure present in the path integral of eq.(2.7). Given a set of these $\{U_\mu(x)\}$ configurations one can perform a calculation of the quark propagator in order to study the hadronic mass spectrum and the meson decay constants.

For example to perform a study of the meson properties we have to compute the following correlation functions:

$$G_{55}(t) = \sum_{\vec{x}} < P_5(\vec{x},t)P_5^\dagger(\vec{0},0) > \quad (2.11)$$

for pseudoscalar meson and

$$G_{kk}(t) = \sum_{k=1,3}\sum_{\vec{x}} < V_k(\vec{x},t)V_k^\dagger(\vec{0},0) > \quad (2.12)$$

for vector mesons. P_5, V_k are the local pseudoscalar density and vector currents respectively:

$$P_5(\vec{x},t) = i\bar{\psi}(\vec{x},t)\gamma_5\psi(\vec{x},t) \quad (2.13)$$

$$V_k(\vec{x},t) = \bar{\psi}(\vec{x},t)\gamma_k\psi(\vec{x},t) \quad (2.14)$$

where ψ is the spinor corresponding to the quark with Wilson hopping parameter k, which we will call $k_{valence}$, which can be equal or different from the k_{sea} value. Usually it is interesting to extract the hadronic mass spectrum for different value of $k_{valence}$, at fixed k_{sea} in order to study the chiral limit.

In order to extract the meson masses one can fit the two point correlation functions in the eqs.(2.11-2.12) to the expressions:

$$G_i(t) = \frac{Z_i}{M_i}e^{-M_i\frac{T}{2}}cosh(M_i(\frac{T}{2}-t)), \quad i = 55,\ kk \quad (2.15)$$

where T is the lattice size in time. The data for the mesonic correlation functions can be fitted to the previous functions, obtaining M_i. The time interval which should be used in the fit can be chosen by checking that the effective mass $m_{eff}(t) = log(G(t)/G(t+1))$ reaches a plateau value in the time interval considered which agrees with the result of the fit. Preliminary results for the mesons mass spectrum are reported in section 5.

In the next section we present the Hybrid Monte Carlo algorithm which is used to obtain full QCD configurations.

3 The Hybrid Monte Carlo Algorithm.

In this section we describe the HMCA that we are using for the full QCD simulation. The HMCA generates gauge configurations and pseudofermionic fields distributed according to the measure given in eq.(2.7). This is done at first suggesting a change to the whole lattice using the Φ algorithm[2], and then globally accepting or rejecting this change in the Metropolis step. These two steps are cyclically repeated.

In the first step, in order to obtain the proposal for the new configuration in the Φ algorithm, one introduces an Hamiltonian $\mathcal{H}(P,U)$ which depends on the link variables $P_\mu(x)$ and $U_\mu(x)$:

$$\mathcal{H}(P,U) = \frac{1}{2}tr(P^2) + S_G(U) + \phi^\dagger(M^\dagger M)^{-1}\phi \tag{3.1}$$

$U_\mu(x)$ are the standard gauge link variables, while $P_\mu(x)$ play the role of Hamiltonian conjugate momenta. The sum of the second and the third term in equation (3.1) is exactly the action that appears in the exponential of eq.(2.7). The physical observables are not affected by the new term depending on P, because it can be factored out becoming gaussian integral that only affects the normalization.

The Hamiltonian variables are initialized in the following way: to generate the pseudofermionic ϕ fields we extract random complex numbers η distributed as $P(\eta) \propto e^{(-\eta^\dagger\eta)}$. In this way $\phi = M^\dagger\eta$ is distributed according to the pseudofermionic measure of the partition function (2.7). The ϕ fields have no dynamic and thus there are no ϕ-conjugate momenta into the Hamiltonian.

In order to generate the $P_\mu(x)$ variables we extract real random numbers $g^a_\mu(x)$ which are drawn with probability distribution $P(g) \propto e^{(-g^2)}$, and then we construct:

$$P_\mu(x) = \sum_{a=1}^{8} g^a_\mu(x)\lambda_a \tag{3.2}$$

where λ^a are the Gell-Mann matrices. We want to note that both $P_\mu(x)$ and ϕ variables are generated randomly to ensure ergodicity.

The (P, U) configuration is evolved according to the Hamiltonian equations of motion, which in the QCD case can be obtained in the following way. In order for the matrix $U_\mu(x)$ to remain an element of $SU(3)$, if $P_\mu(x)$ momenta are traceless and hermitian operators, the equation of motion for $U_\mu(x)$ must be

$$\dot{U}_\mu(x) = iP_\mu(x)U_\mu(x) \ . \tag{3.3}$$

To obtain the evolution equation for the $P_\mu(x)$, we require the Hamiltonian to be a constant of the motion[2], $\dot{\mathcal{H}} = 0$. In this way we find

$$\dot{P}_\mu(x) = -\frac{\delta S(U)}{\delta U} + \phi^*(M^\dagger M)^{-1}\left[M^\dagger \frac{\delta M}{\delta U} + \frac{\delta M^\dagger}{\delta U}M\right](M^\dagger M)^{-1}\phi \ . \tag{3.4}$$

To obtain a "trajectory" we have to refresh the $P_\mu(x)$ and the $\phi(x)$ variables and then to evolve the (U, P) configuration for a fixed time τ. In the numerical integration of the Hamiltonian equations we introduce a finite time step dt. The number of molecular dynamics steps is N_{MD}, and the trajectory length is $\tau = dt \times N_{MD}$.

We have initially tested the implementation of this algorithm in the absence of fermionic fields. Under these conditions the algorithm is used to produce quenched pure gauge configurations. These configurations can be statistically compared with those ones obtained with well tested existing Metropolis program.

Defining the staples

$$V_\mu(x) = \quad \sum_\nu \Big(U_\nu(x+\mu,t)U^\dagger_\mu(x+\nu,t)U^\dagger_\nu(x,t)$$

$$+U^\dagger_\nu(x+\mu-\nu,t)U^\dagger_\mu(x-\nu,t)U_\nu(x-\nu,t)\Big) \ , \tag{3.5}$$

the discrete evolution equations for the "quenched" case can be written as:

$$U_\mu(x,t+dt) = e^{iP_\mu(x,t)dt}U_\mu(x,t) \tag{3.6}$$

$$P_\mu(x,t+dt) = P_\mu(x,t) + \tfrac{i\beta}{N}dt\hat{T}\left[U_\mu(x,t)V_\mu(x)\right] \ , \tag{3.7}$$

where $\hat{T}$ is the traceless antihermitian projector:

$$\hat{T}(A) = (A - A^\dagger) - \frac{1}{N}\mathbf{I}\ Tr(A - A^\dagger) \ . \tag{3.8}$$

The discrete evolutions equations used in the full case are

$$U_\mu(x,t+dt) = e^{iP_\mu(x,t)dt}U_\mu(x,t) \tag{3.9}$$

$$P_\mu(x,t+dt) = P_\mu(x,t)$$

$$+\, idtT\left[\frac{\beta}{6}U_\mu(x,t)V_\mu(x) - k_{sea}\cdot tr_{Dirac}(U_\mu(x,t)F_\mu(x))\right] \tag{3.10}$$

where in the third term in eq.(2.21) the trace is over the Dirac indices and

$$F_\mu(x) = (1+\gamma_\mu)Y(x+\mu)\chi^\dagger(x) + (1-\gamma_\mu)\chi(x+\mu)Y^\dagger(x) \tag{3.11}$$

with

$$\chi(x) = \ \left(M^\dagger M\right)^{-1}\phi \tag{3.12}$$

$$Y(x) = \ M\left(M^\dagger M\right)^{-1}\phi \ . \tag{3.13}$$

In the previous equations we used an expansion of the exponential up to fourth order, which guarantees the time reversibility[1]. At each step of the molecular dynamics evolution we normalized the $SU(3)$ link matrices U_μ.

[1]We have also tried sixth order in the exponential expansion, without any significative difference in reversibility.

In the time integration of the Hamiltonian equation we use a leap-frog algorithm [2],[15], which is time reversible and area preserving in the phase space. The reversibility assures the validity of the principle of detailed balance. The leap-frog algorithm disentangles the update of U and P variables, that are no more evaluated at the same time: we perform an initial halfstep of size $dt/2$, and then a chain of $N_{MD}-1$ steps of size dt, alternatively in U and P. Eventually, a last halfstep for the P momenta produces the $U(\tau), P(\tau)$ configuration. The deterministically proposed configuration over the whole lattice (U', P') is then globally accepted or rejected with a probability

$$\varrho = \min\left(1, e^{-(\mathcal{H}(P',U')-\mathcal{H}(P,U))}\right) \ . \tag{3.14}$$

If we consider the usual Metropolis algorithm applied to full QCD we see that in a single sweep we need to make as many inversions of the fermionic operator as the number of the links we want to update, ($\mathcal{O}$(V)), while with a trajectory of the HMCA we obtain the probability distribution (2.7) with only $\mathcal{O}(1)$ inversions. The main difference between the two algorithms is that in the Metropolis case the links of the new configuration are chosen randomly and the accept/reject condition is imposed link by link (locally), while in the HMCA the new configuration is obtained by the previous deterministic equations (3.3,3.4) and the accept/reject condition is imposed over the whole configuration (globally).

A useful test for the implementation of the HMCA is the identity [16]:

$$< e^{-\delta\mathcal{H}} >= 1 \ . \tag{3.15}$$

where $\delta H = H(P', U') - H(P, U) = H' - H$. This identity follows from the validity of the Liouville theorem of the Hamiltonian evolution $\mathcal{D}U\mathcal{D}P = \mathcal{D}U'\mathcal{D}P'$ and becomes exact when the system has reached the equilibrium:

$$1 = \frac{Z}{Z} = \frac{1}{Z}\int \mathcal{D}U'\mathcal{D}P' e^{-\mathcal{H}'} = \frac{1}{Z}\int \mathcal{D}U\mathcal{D}P e^{-\mathcal{H}} e^{\mathcal{H}-\mathcal{H}'} \ . \tag{3.16}$$

The (3.16) is satisfied for every choice of the algorithm parameters and permits a fine control on the proposed configuration. This identity is not satisfied if the iterative inversion algorithm for the pseudofermionic operator

$M^\dagger M$ is not successfully completed, with a strong enough degree of convergence. Then we can check the validity of eq.(3.15) to test the thermalization of our configuration and to fix the value of the residue of the inversion. In the previous identity the average is taken over all the trajectories (accepted or not accepted). A consequence of equation (3.15) is that we expect[16] that

$$< \mathcal{H}^{'} - \mathcal{H} > \geq \ 0 \ . \tag{3.17}$$

We use periodic boundary condition on the gauge fields. On the fermionic field we use periodic boundary condition in the time direction and periodic or antiperiodic spatial boundary condition.

An important feature of the HMCA is the parameter's tuning. There are many parameters that have to be tuned: the free technical parameter are N_{MD}, the number of steps of a molecular dynamics (MD) trajectory and dt, the length of each step. The free physical ones are $\beta = \frac{6}{g^2}$ and the hopping parameter k_{sea} into the fermionic operator M related to the sea quark mass. The physical parameters appear both in the evolution equations (3.9-3.10) and in the accept/reject Hamiltonian of eq.(3.14), so a further possible tuning, which has not been explored in the present paper, is the usage[2] in the evolution equations of a β_{MD} and a k_{MD} different from the ones used in the accept/reject Hamiltonian.

In our simulations we have fixed $\beta_{MD} = \beta$, $k_{MD} = k_{sea}$ and the value of $\tau = dt \times N_{MD}$, and we have studied the behaviour of the acceptance as a function of dt. We check that in an exact algorithm like the HMCA the value of the plaquette is independent from dt.

In the full HMCA evolution equations (3.9,3.10), we need the quantities reported in eqs.(3.12,3.13). To obtain $\chi(x)$ and then $Y(x)$ we have to perform the inversion of the fermionic operator $M^\dagger M$.

$$M^\dagger M \chi = \phi \ . \tag{3.18}$$

This is the most time-consuming part of the algorithm and must be repeated N_{MD} times for each trajectory. To solve eq.(3.18) we use the Conjugate Gradient algorithm described in section 6. We stop the iterative algorithm when

$$\frac{((M^\dagger M\chi - \phi), (M^\dagger M\chi - \phi))}{(\chi, \chi)} \;\le\; R \tag{3.19}$$

is lower than a fixed R value[18].

4 Quenched Results

In this section we summarize our results obtained using both the Hybrid Monte Carlo and Hybrid Molecular Dynamics algorithm[2] in the pure gauge case. We call Hybrid Molecular Dynamics algorithm an HMCA without the acceptance step. While the HMCA is an exact algorithm, the observables measured on configurations produced with HMD depend on the step size dt of the trajectory.

In order to test our HMCA we performed numerical simulations with only the pure gauge part of the action. This means that the proposed configuration is obtained using the Hamiltonian equations without pseudofermions degrees of freedom, see eqs.(3.6-3.7).

The simplest test we performed is the following: we check that the HMC pure gauge algorithm reproduces the same value of the plaquette as the Metropolis algorithm in a quenched simulation. Then we analyze the behaviour of the acceptance as a function of the step size dt and finally we verify that the identity (3.15) is satisfied for all our HMC simulations.

We perform numerical simulation on a 6^4 lattice at two different value of β, $\beta = 5.7$ and $\beta = 6.0$. For each value of β we studied the HMCA behaviour changing the free parameter dt. We choose the number of steps N_{MD} in order to maintain a fixed trajectory length, $\tau = dt \times N_{MD} \sim 0.5$. The results for the acceptance rates, for the plaquette values and for $< e^{-\delta\mathcal{H}} >$ are reported in Table 1.

We remark that the value of the plaquette is compatible with the quenched Metropolis result: for example, on a 6^4 lattice, from 4000 sweeps of the Metropolis algorithm after 1000 sweeps of thermalization we obtain $P(\beta = 6.0) = 0.5946(4)$, in agreement with the HMCA pure gauge result $P(\beta = 6.0) = 0.5951(2)$. Analogously at $\beta = 5.7$ the Metropolis data is $P(\beta = 5.7) = 0.5484(7)$ and the HMCA result is $0.5487(6)$.

β	dt	N_{MD}	N_{traj}	Accep.	Plaq.	$< e^{-\delta\mathcal{H}} >$
5.7	0.075	6	16000	16.5%	0.552(2)	1.2(3)
5.7	0.050	10	2000	56.7%	0.5491(6)	1.07(6)
5.7	0.025	20	4000	89.5%	0.5487(6)	1.002(3)
6.0	0.075	6	8000	13.0%	0.5950(3)	0.7(1)
6.0	0.050	10	2000	54.4%	0.5947(2)	0.99(3)
6.0	0.025	20	2000	87.4%	0.5951(2)	1.000(6)

Table 1: Hybrid Monte Carlo pure gauge simulations. All the simulations have been performed on a 6^4 lattice.

We note, as expected for an exact algorithm like HMCA, that within the errors the value of the plaquette does not depend on dt.

The errors quoted on the plaquette values have been obtained using the jacknife method: decreasing the number of the bins we analyze the behaviour of the error and we take the plateau value. In figure 1 we report the $\beta = 6.0$ plaquette as a function of the number of trajectories. We observe the presence of correlations on different scales. This is a well note problem of the HMCA and looking at this figure we can conclude that our errors may be underestimated. For this reason usually people prefer to use the Metropolis algorithm rather than HMCA to produce quenched uncorrelated configurations.

Looking at the data of Table 1 we note a sharp variation of the acceptance as a function of dt. An increase in the acceptance needs a decrement of the value of dt. In order to maintain a given acceptance the step size dt must be reduced when going to larger lattices, as we have found in some test simulations performed on $18^3 \times 32$ lattices[16][20].

As we underline in section 3, we checked, following ref.[16], that our HMCA simulations satisfy the identity (3.15). In this way we are sure that the thermalization has been done correctly and all the properties of the Hamiltonian equations are conserved in the implementation. In the pure gauge simulations we obtain the good results reported in the seventh column of Table 1.

We also perform simulations using the HMDA, on a 6^4 lattice at $\beta = 5.7$ and $\beta = 6.0$. The results are summarized in Table 2. From the data of Table 2 we note, as expected, that the value of the plaquette obtained with a HMD

β	dt	N_{MD}	N_{traj}	Plaq.
5.7	0.100	5	1000	0.5315(15)
5.7	0.075	6	1000	0.5383(13)
5.7	0.050	10	1000	0.5438(11)
5.7	0.025	20	1000	0.5500(10)
6.0	0.100	5	1000	0.5803(5)
6.0	0.075	6	1000	0.5865(5)
6.0	0.050	10	1000	0.5917(4)
6.0	0.025	20	1000	0.5945(5)

Table 2: Hybrid Molecular Dynamics pure gauge simulations. All the simulations have been performed on a 6^4 lattice.

algorithm depends on dt. In fact the plaquette approaches from lower values the quenched result obtained using an HMCA, as noted in ref.[20].

5 Unquenched Results

In this section we present our tests and first results obtained using the APE100 machine for full QCD simulation.

All the simulations have been performed at $\beta = 5.3$ and $k_{sea} = 0.158$ on 8^4 and on $12^3 \times 32$ lattices. On 8^4 we use different values of dt and N_{MD}. In all the simulations we use periodic boundary conditions on the fermionic degrees of freedom, while for $dt = 0.02$, $N_{MD} = 25$ we use both periodic and antiperiodic spatial boundary conditions on the fermions.

Our tests consist in the calculation of the average value of the three different contributions at the Hamiltonian. We check that the P_μ link variables initialized according to eq.(3.2) at the begin of each trajectory, are distributed according to eq.(3.2) also at the end of each trajectories and that $< \frac{1}{2}\frac{1}{N_{link}}\sum_{x,\mu} tr(P_\mu^2(x)) >= 4.0$. We check that the pseudofermionic contribution to the action has an average equals to 12.0 and that the plaquette values are statistically comparable with the ones presented in the literature[18][5].

To invert the pseudofermionic operator $M^\dagger M$ we use a Conjugate Gra-

dt	N_{MD}	Ac.	$< \delta\mathcal{H} >$	$< e^{-\delta\mathcal{H}} >$	$< \phi^\dagger (M^\dagger M)^{-1} \phi >$	$< \frac{1}{2} tr(P^2) >$	Plaq.
0.04	13	54%	0.81(5)	1.03(6)	12.005(2)	3.995(1)	0.489(1)
0.02	25	88%	0.06(1)	1.00(2)	12.001(2)	3.999(1)	0.4894(8)
0.01	50	98%	0.003(4)	1.001(4)	12.002(2)	3.9991(7)	0.489(1)
0.02	25	89%	0.05(1)	1.01(1)	12.002(2)	3.9998(5)	0.490(1)

Table 3: Hybrid Monte Carlo full QCD simulations on 8^4 lattice, $\beta = 5.3$, $k_{sea} = 0.158$. The data in the first three rows are obtained using periodic boundary conditions on the fermionic degrees of freedom, while the last row contains data obtained using spatial antiperiodic and temporal periodic boundary conditions on the fermions. The number of trajectories for these simulations are 890, 678, 640, 967 from the top to the bottom of the Table respectively.

dient algorithm (see section 6.). We decrease the value of R (see eq.(3.19)) to obtain a variation in $\delta\mathcal{H}$ of the order of one percent. In the simulation reported in this paper we obtain this result for $R \leq 10^{-13}$. For example for a given $12^3 \times 32$ configuration (of the set used for the results in Table 4),varying the value of R in the stop condition of the CG algorithm we have found the δH results reported in Table 5. We note that 1% accuracy in $\delta\mathcal{H}$ requires $R \leq 10^{-13}$.

In these initial test we start our run from random U_μ configuration. Indeed starting from a configuration with a critical value of the hopping parameter k_c^{init} we want to reach the final thermalized configuration with $k_c = k_c(\beta)$. If in the thermalization we don't want to pass through a configuration with k_c equals to the value of k_{sea} of our unquenched simulation we have to start from a configuration warmer than the one we want to reach after the thermalization. This means that we can start our full QCD run also from a configuration just a little warmer than the final one, for example a pure gauge configuration with these properties. Indeed following the studies of ref.[18], for a given unquenched configuration we can estimate the equivalent gauge coupling for the quenched theory which has the same lattice scale.

The second and the fourth rows of Table 3 contain the data obtained using periodic and antiperiodic spatial boundary condition respectively. In this case the results are statistically comparable but if we look at figure 2. the behaviour of the plaquette versus the number of trajectories seems to be

dt	N_{MD}	Ac.	$< \delta\mathcal{H} >$	$< e^{-\delta\mathcal{H}} >$	$< \phi^\dagger(M^\dagger M)^{-1}\phi >$	$< \frac{1}{2}tr(P^2) >$	Plaq.
0.01	60	92%	0.04(1)	1.01(1)	12.0003(4)	4.0001(2)	0.4904(2)

Table 4: Hybrid Monte Carlo full QCD simulations on $12^3 \times 32$ lattice, $\beta = 5.3$, $k_{sea} = 0.158$, with periodic boundary conditions on the fermionic degrees of freedom.

different.

First results for the mass spectrum on $12^3 \times 32$ lattice are obtained at $\beta = 5.3$. The value of the HMCA parameter are those reported in Table 4. In this case we have 1180 preliminary trajectories. APE100 is currently running [21] at higher value of k_{sea}.

In figure 3. we report the behaviour of the plaquette, of $\phi^\dagger(M^\dagger M)^{-1}\phi$, of $-\delta\mathcal{H}$ and of $\frac{1}{2}\frac{1}{N_{link}}\sum_{x,\mu} tr(P_\mu^2(x))$ for the $12^3 \times 32$ simulation as functions of the trajectory number. As can be seen from table 4 the results for the testing variables are in good agreement with theoretical predictions and with the plaquette results reported in literature[18] . In figure 4 we report the average of the correlation functions for the pseudoscalar and for the vector mesons at $k_{valence} = k_{sea} = 0.158$. In figure 5 we report the behaviour of the effective mass for these particles.

In figure 6 we report the time history of pseudoscalar and vectorial correlation at euclidean time separation 11. From this figure we observe the presence of autocorrelation on different scales[5][6].

We start the run with 30 HMD trajectories, then we perform 180 thermalization HMC trajectories. At this point we invert the fermionic operator to obtain a propagator for a given $k_{valence}$ every 5 trajectories.

In this paper we report a preliminary analysis of the pseudoscalar and vectorial correlation functions (see eq (2.11-2.12)) obtained on this ensemble of unquenched configurations (see figure 4, 5, 6).

6 Technical Aspects.

In the implementation of the algorithm on the APE100 machine, some care must be devoted to possible problems due to the single-precision of the floating point units. With the lattices used in the actual full QCD simulations,

R	$\delta\mathcal{H}$
1.0e-06	-0.8375
1.0e-07	-0.6997
1.0e-08	0.1123
1.0e-09	0.1842
1.0e-10	0.1878
1.0e-12	0.1712
5.0e-13	0.1747
1.0e-13	0.1763
7.0e-14	0.1767

Table 5: The value of $\delta\mathcal{H}$ as a function of the precision R (see equation 3.19) of the inversion for a fixed configuration in the set described in Table 4.

this type of problems are not so important in iterative algorithms with stable solution, where, if convergence occurs, the fixed point solution is reached anyway, eventually with a larger number of iterations. The difference between single and double precision has to be paied in CPU time. However some improvements can be obtained taking care in the implementation of the inversion algorithm.

To solve the equation

$$\mathbf{M}^{\dagger}\mathbf{M}\chi = \phi \tag{6.1}$$

defining the residue at the n iterative step

$$R_n = \mathbf{M}^{\dagger}\mathbf{M}\chi_n - \phi \tag{6.2}$$

the Conjugate Gradient (CG) iterative equations are:

$$\chi_0 = 0 \ , \quad P_0 = R_0 \tag{6.3}$$

$$a_n = \frac{(R_n, R_n)}{(MP_n, MP_n)} \tag{6.4}$$

$$\chi_{n+1} = \chi_n + a_n P_n \tag{6.5}$$

$$R_{n+1} = R_n - a_n (M^{\dagger}M)\ P_n \tag{6.6}$$

$$b_n = \frac{(R_{n+1}, R_{n+1})}{(R_n, R_n)} \tag{6.7}$$

$$P_{n+1} = R_{n+1} + b_n P_n \tag{6.8}$$

where χ_n is the solution after n steps.

To compute the CG equations (6.4) and (6.7), we need to perform a global sum. On APE100 we use a tree algorithm. While a standard algorithm adds the items sequentially in a variable, our tree algorithm consists in summing the items in pair and in iterating this operation until the total sum is reached. Thus the tree algorithm is designed to sum only numbers of the same magnitude reducing the rounding errors.

We are also checking on APE100 machines a new algorithm proposed by Valerio Parisi[17] to correct for rounding errors in summation. This iterative algorithm uses a variable to dynamically backing up the informations lost in the sum.

More details of these algorithms will be presented in ref.[11].

While in the inversion algorithm the rounding errors can reduce the convergence velocity, in the calculations of $\delta\mathcal{H}$ they can cause systematic errors, because $\delta\mathcal{H}$ is used in the accept/reject condition.

Another technical aspect that we faced is the random number generation. In the HMCA simulation we need to initialize the P_μ and the ϕ variables at the start of each new trajectory. With large lattice for a single thermalized configuration we have to generate $\mathcal{O}(10^{10})$ random numbers. Although on the APE100 machines a random number generator is available and used in the quenched simulations since several years, we have been lead to create a new generator of real random number with different period, correlation and speed properties, in order to check the possible effects on the physical results.

The problem with APE100 is that the machine only works with 32 bits real numbers and allows a limited amount of mixed operations between real and integer numbers, while most of the tested random generators use integers in the algorithm and then convert the result into real numbers. We have designed[2] a new generator[19] combining three different algorithms, taking care that the rounding error effects do not ruin the statistical and long period properties. The mixing of the three generators can produce numbers that are more independent than those produced by each algorithm. In order to

[2]We thank G. Parisi for all the long and useful discussion we had with him about this subject.

test the implementation of the evolution equations (3.9, 3.10) and the good properties of the new random number generator we have checked that, during the whole evolution, the P_μ variables follow a gaussian distribution.

7 Full QCD on APE100 Machines.

As we said in the Introduction, the APE100 machines are parallel supercomputers with modular building blocks. At present we are using the "tube" configuration, which is composed by 128 processors (nodes, arranged on a $2 \times 2 \times 32$ three-dimensional structure) and has a peak speed of 6.4 Gflop. In the next future the "tower" configuration will be available, which is composed of 512 nodes, arranged in a $8 \times 8 \times 8$ configuration with a peak speed of 25.6 Gflop. Each node has a memory capacity of 4 Mbytes (10^6 real 32-bit words). With this amount of memory the maximum lattice size we can use in the case of a full QCD simulation on the "tube" is $20^3 \times 32$ while on the "tower" is 32^4.

The code as it is implemented can achieve a performance of 60 % of the peak speed on the most time consuming part (the inversion of the pseudofermionic $M^\dagger M$ operator and the staple calculations). We are implementing a more efficient code using the features of the next APE100 compiler.

In the $12^3 \times 32$ simulations reported in Section 5. we obtain an high acceptance (92%). From the studies on the 8^4 lattice we see that a good value of the acceptance can be reach going from $dt = 0.01, N_{MD} = 60$ to $dt = 0.03, N_{MD} = 20$. In this way we gain a factor three in the CPU time and we expect to obtain with a "tube" something like 1000 full QCD trajectories in 8 days on a $12^3 \times 32$ lattice with a quark mass in the strange quark region. Taking into account the autocorrelation modes we can generate $5 \div 10$ independent configurations in 8 days.

Looking at all the results of full QCD spectroscopy[3], we note that the more realistic simulations with two flavour Wilson fermions have been performed on $16^3 \times 32$ lattices with low statistics (see for example Table 1 of ref. [3]). Looking for example at the results of ref.[6], we note the large correlations that affect the time history of the pion propagator of fig.2. This is the same situation of fig.2.a of ref.[5].

This means that, more long runs have to be performed to deeply understanding the long scale correlations before obtaining realistic results. This is the first goal that we want to reach.

With a "tube" we are running on a $12^3 \times 32$ lattice at $\beta = 5.3$ and we are performing measures on the hadronic and glueballs mass spectrum. With a "tower" or with the full 100 Gflop, 2048 nodes machine, we can simulate full QCD on large lattices, comparable with those used today for staggered fermions. Large lattices are needed to control the errors coming from finite size effects. The study of this systematic error in the full QCD simulations will be another point to be understood.

With these powerful machines will be possible to repeat the calculations with dynamical see quarks of all the physical quantities (mass spectrum, decay constant, matrix elements, etc.) obtaining eventually the correct full QCD results.

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FIGURE CAPTIONS

Figure 1 The plaquette in a quenched (HMC) simulation as a function of the number of trajectories on a 6^4 lattice for the simulation at $\beta = 6.0$, $dt = 0.025$, $N_{MD} = 20$.

Figure 2.a The plaquette in a full (HMC) simulation with periodic boundary conditions as a function of the number of trajectories on a 8^4 lattice for the simulation at $\beta = 5.3$, $dt = 0.02$, $N_{MD} = 25$ $k_{sea} = 0.158$.

Figure 2.b Same as fig. 2a for anti periodic spatial boundary conditions as a function of the number of trajectories on a 8^4 lattice for the simulation at $\beta = 5.3$, $dt = 0.02$, $N_{MD} = 25$ $k_{sea} = 0.158$.

Figure 3 The plaquette (a), the $\phi^\dagger(M^\dagger M)^{-1}\phi$ (b), the $-\delta\mathcal{H}$ (c), and the $\frac{1}{2}\frac{1}{N_{link}}\sum_{x,mu} tr(P_\mu^2(x))$ (d) in a full (HMC) simulation with periodic boundary condition as a function of the number of trajectories on a $12^3 \times 32$ lattice for the simulation at $\beta = 5.3$, $dt = 0.01$, $N_{MD} = 60$ $k_{sea} = 0.158$.

Figure 4 The $G_{55}(t)$ correlation function of eq.(2.11) (a),and the $G_{kk}(t)$ correlation function of eq.(2.12) (b) in a full (HMC) simulation with periodic boundary conditions on a $12^3 \times 32$ lattice for the simulation at $\beta = 5.3$, $dt = 0.01$, $N_{MD} = 60$ $k_{sea} = 0.158$.

Figure 5 The pseudoscalar effective mass (a), and vectorial effective mass (b) in a full (HMC) simulation with periodic boundary conditions on a $12^3 \times 32$ lattice for the simulation at $\beta = 5.3$, $dt = 0.01$, $N_{MD} = 60$ $k_{sea} = 0.158$.

Figure 6 The $G_{55}(t)$ correlation function (a) and the $G_{kk}(t)$ correlation function (b) as a function of trajectories number for euclidean time separation 11 in a full (HMC) simulation with periodic boundary conditions on a $12^3 \times 32$ lattice for the simulation at $\beta = 5.3$, $dt = 0.01$, $N_{MD} = 60$ $k_{sea} = 0.158$.

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