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Summary of working group activities in non-perturbative quantum chromodynamics (lattice gauge theory)

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Abstract. We summarize the activities of the lattice gauge theory section of the working group activities in non-perturbative QCD.

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1. Introduction

The lattice gauge theory subgroup of the working group in non-perturbative QCD consisted of Mridupavan Deka, Sourendu Gupta, N D Hari Dass, Rajarshi Roy, Sayantan Sharma and Pushan Majumdar.

The problems that were identified for discussion and possible further pursuit were

(i) deflating QCD (low mode projection),
(ii) fixed topology calculation of Green functions with the overlap operator,
(iii) computing on the graphical processing unit.

We summarize the status of activities in each of the topics in turn.

2. Deflation

The most time-consuming part of lattice gauge theory simulations is computing the quark propagator which requires an inversion of the Dirac operator on a source vector. The inversion time is proportional to the condition number (ratio of the highest to lowest eigenvalues) of the matrix which represents the Dirac operator. This keeps on increasing as one goes towards the chiral regime (realistic pion masses) and the smallest eigenvalue becomes several orders of magnitude smaller than the largest eigenvalue. Small eigenvalues create another problem, viz. they generate large forces in the molecular dynamics evolution. They therefore have to be handled by drastically reducing the time step of the evolution so that the system does not stray too far from the equilibrium energy surface.

As the number of small eigenvalues is itself small, a promising solution to this problem is to project out the small eigenvalues of the Dirac operator and treat them separately and exactly. This procedure goes under the name 'Deflation'. The problem with deflation is that ususal textbook methods scale as V^2, where V is the lattice volume and that is too expensive to be of practical use. The simulation algorithm itself scales as $V^{5/4}$. Thus deflation would slow down the whole process too much.

In this workshop we have discussed two papers by Martin Lüscher [1,2] which discuss efficient deflation techniques, with the idea of incorporating them into our own simulation programs.

3. Issues with chiral symmetry on the lattice

On the lattice, one can prove the theorem [3] (Nielsen–Ninomiya theorem) which states that a Dirac operator which is local, has the correct continuum limit, has no spurious poles and has continuum chiral properties does not exist.

The most naive acceptable Dirac operator was proposed by Wilson and is known as the Wilson–Dirac operator which is denoted as D_{W}. However, this Dirac operator breaks chiral symmetry explicitly.

Till date the best that can be done is to write down a Dirac operator with a lattice chiral symmetry. This symmetry transformation is slightly different from the continuum transformation (but reduces to the continuum transformation in the limit of the lattice spacing a going to zero) and is given by [4] $\psi \to \psi + i\epsilon\delta\psi$ and $\bar{\psi} \to \bar{\psi} + i\epsilon\delta\bar{\psi}$ with $\delta\psi = \gamma_5(1 - \frac{1}{2}aD)\psi$ and $\delta\bar{\psi} = \bar{\psi}(1 - \frac{1}{2}aD)\gamma_5$. The corresponding operator, called the overlap operator [5], can be written as

$$D_{\mathrm{OV}} = 1 + \frac{1 - D_{\mathrm{W}}}{\sqrt{(1 - D_{\mathrm{W}})^{\dagger}(1 - D_{\mathrm{W}})}}. \tag{1}$$

A problem in simulations with this Dirac operator is that it sometimes produces a very small eigenvalue. Since the force used in the evolution equations is proportional to the derivative of the inverse of the Dirac operator, a small eigenvalue can generate a large force and move the system far away from the equilibrium energy surface. This is related to the appearance of zero modes of the Dirac operator (i.e. topology change).

There are two options to handle this situation: either one has to very carefully handle the large force [6], or one can simulate using a fixed topology action [7]. It is strongly suspected that the former method yields an algorithm which scales as $\mathcal{O}(V^2)$ and is therefore difficult to use at larger volumes. We discuss the second possibility here.

In QCD, the topological charge Q and the vacuum angle θ are conjugate variables. Assuming G_Q to be the Green function at a fixed topological charge Q, one can write, at finite volume, $G_Q = G_\theta + \mathcal{O}\left(\frac{1}{V}\right)$, where G_θ is the Green function at a fixed value of θ. The partition function in this case is given by

$$\begin{aligned} Z_Q &= \frac{1}{2\pi}\int_{-\pi}^{\pi} \mathrm{d}\theta\, \mathrm{e}^{iQ\theta} Z_\theta = \frac{1}{2\pi}\int_{-\pi}^{\pi} \mathrm{d}\theta\, \mathrm{e}^{iQ\theta - VE(\theta)} \\ &= \frac{1}{2\pi}\int_{-\pi}^{\pi} \mathrm{d}\theta\, \mathrm{e}^{-VF(\theta)}. \end{aligned} \tag{2}$$

Defining the topological susceptibility, χ_t, as

$$\chi_t = \frac{\langle 0|Q^2|0\rangle}{V} = \left.\frac{\mathrm{d}^2 E(\theta)}{\mathrm{d}\theta^2}\right|_{\theta=0}, \tag{3}$$

we can perform a saddle point evaluation of Z_Q at $\theta = \theta_c = iQ/V\chi_t$. This gives

$$Z_Q = \frac{\mathrm{e}^{-Q^2/2\chi_t V}}{\sqrt{2\pi\chi_t V}}\left[1 - \frac{c_4}{8\chi_t^2 V} + \mathcal{O}\left(\frac{1}{V^2}\right)\right], \tag{4}$$

where c_4 is the coefficient of θ^4 in the expansion of $E(\theta)$. Similarly, one obtains the Green functions (for large volume) as

$$\begin{aligned} G_Q \;=\; & G(\theta=0) + G^{(2)}(0)\frac{1}{2\chi_t V}\left[1 - \frac{Q^2}{\chi_t V} - \frac{c_4}{2\chi_t^2 V}\right] + G^{(4)}(0)\frac{1}{8\chi_t^2 V} \\ & + G^{(1)}(0)\frac{iQ}{\chi_t V}\left[1 - \frac{c_4}{2\chi_t^2 V}\right] + G^{(3)}(0)\frac{iQ}{2\chi_t^2 V^2} + \mathcal{O}\left(\frac{1}{V^3}\right). \end{aligned} \tag{5}$$

In this scheme of calculations, χ_t and c_4 are obtained from lattice simulations using axial ward identities.

4. Computing with the graphical processing unit (GPU)

With the advent of the GPU [8] it is possible to get a Teraflop of computing power on a desktop (using, say, four Fermi cards). This results in huge savings both in cost and power consumption. The main problem still remains is that it is not very easy to harness this computing power for running one's own program. Usually the program has to be rewritten for efficient running on GPUs. The lay-out of the data needs to be changed keeping in mind the architecture of the card where the program is going to run. Currently, almost all programming for the GPU has to be done through CUDA [9], a C-like language. This too is a big barrier in a community where most people use FORTRAN as their programming language. Portland group now has a FORTRAN compiler that includes GPU support [10] but it is still in its early stages.

5. Conclusion

We are currently trying to choose an appropriate Dirac operator using which we can construct the overlap operator. Our strategy is to study the spectra for different variations of the Wilson operator and then choose one with an optimal spread of eigenvalues. Once this is done, we can work earnestly with the deflation methods and incorporate them in our programs.

We are very strongly pursuing development of programs in CUDA to be run on the GPUs. We have also procured two GPU cards on which we are testing the programs and in the near future we hope to be able to run our entire simulation on the GPUs.

References

[1] M Lüscher, *J. High Energy Phys.* **7**, 81 (2007)
[2] M Lüscher, *J. High Energy Phys.* **12**, 11 (2007)
[3] H B Nielsen and M Ninomiya, *Phys. Lett.* **B105**, 219 (1981); *Nucl. Phys.* **B185**, 20 (1981); *Nucl. Phys.* **B193**, 173 (1981)
[4] M Lüscher, *Phys. Lett.* **B428**, 342 (1998)
[5] H Neuberger, *Phys. Lett.* **B427**, 353 (1998)
[6] Z Fodor, S D Katz and K K Szabo, *J. High Energy Phys.* **3**, 408 (2004)
T A DeGrand and S Schaefer, *Phys. Rev.* **D71**, 034507 (2005)
[7] JLQCD Collaboration: S Hashimoto *et al*, *Proc. Sci.* (Lattice 2006) 052
S Aoki, H Fukaya, S Hashimoto and T Onogi, *Phys. Rev.* **D76**, 054508 (2007); *Proc. Sci.* (Lattice 2007) 080
[8] See the talk by N D Hari Dass (this meeting) for an introduction to GPU computing
[9] http://www.nvidia.com/object/cuda_home.html
[10] http://www.pgroup.com/resources/accel.htm