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Visualization as a tool for understanding QCD evolution algorithms

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Abstract. In this paper we present a project of visualizing topological charge in Lattice QCD in order to understand its evolution under the Markov Chain Monte Carlo algorithms and how to maximize its equilibration. Lattice QCD is a very computationally expensive technology for computing properties of composite particles from a few fundamental parameters such as quark masses. Our research plays an important role in validating these computations by showing that the autocorrelation length is small and it can eventually lead to even more efficient algorithms.

1. Introduction and Motivations

The Standard Model of Particle Physics provides a strikingly successful description of the structure of the matter down to scales of 10^{-18}m. The basic degrees of freedom are elementary particles including quarks and leptons which interact with each other according to strong and electro-weak interactions. Quarks play a special role in this model because their interacting are mediated by the exchange of gluons; thus, they create bound states such as the proton, the neutron and the majority of particles that constitute the richness of structures that we observe in the physical world. The part of the Standard Model that describes quarks and gluons is called Quantum Chromo Dynamics (QCD). The ability to perform computations in QCD is of critical importance in Particle and Nuclear Physics. It enables us to determine fundamental parameters of the Standard Model from experiments, compare experimental results with model predictions, and eventually find discrepancies that can shed some light into yet unknown smaller structures and laws of physics at higher energy. It enables us to calculate the equation of state, transport coefficients, and other properties of hadronic matter and the quark gluon plasma explored in relativistic heavy ion collisions at RHIC the LHC. It also enables us to calculate the spectrum, structure, and interactions of mesons and baryons from first principles and lies at the heart of explorations at Jefferson Lab, RHIC spin, and a future electron-ion collider.

Since quarks are subject to strong interactions, standard perturbative techniques are inadequate to perform many interesting computations. For computing the spectrum of the model and computing the lifetime of composite particles, the purely numerical approach known as Lattice QCD that has been the most productive[2].

Lattice QCD consists of taking a small portion of space (a cube of $\sim 10^{-15}$m of size) for a brief time interval ($\sim 10^{-23}$secs), discretizing it on a four dimensional lattice, and simulating numerically the dynamics of QCD inside. The spatial fields do not evolve over time as in ordinary classical systems. Instead, the fields, that are defined on the four-dimensional Euclidean space-time, evolve over a fictitious MCMC time (τ). Lattice QCD computations consist of measuring correlation functions over the possible four dimensional configurations of the fields, each weighted by a number that encodes the dynamics of QCD[1]. Quantities like particles masses and lifetimes can be determined from these correlations.

In practice, the four dimensional configurations are created using Markov Chain Monte Carlo (MCMC) algorithms. Examples are the Molecular Dynamics algorithm or the Hybrid Monte Carlo algorithm. Each configuration is generated from the previous one using a transition in probability that encodes the laws of QCD dynamics.

In this paper, we describe how visualization techniques can be useful to provide information about these algorithms, about the data that is being generated.

The quark fields can be integrated out and, while they play a critical role in the inner workings of the algorithms, they are not part of the actual configurations. The latter only contain gauge degrees of freedom representing gluons, hence they are usually referred to as gauge configurations. Typical gauge configurations have sizes that range from 32×24^3 to 192×64^3 points; which correspond to a size ranging from 256 MBytes to 15 GBytes each (in single precision). A typical Lattice QCD computation generates and utilizes about 1000 of these gauge configurations, thus requiring multiple TBytes of storage. Algorithms are always parallel because of the size of the problem of Lattice QCD.

A typical problem consists in determining whether this small subset of the infinite space of all possible gauge configuration is sufficiently representative and whether the statistical uncertainty determined from the averages can be trusted. From a physical perspective the gauge configurations can be grouped into equivalence classes characterized by their topological charge density.

Our goal is to visualize this topological charge density and measure how fast/slow it evolved under the MCMC for different algorithms and different simulation parameters (the dynamic quark mass in particular). This would provide us with a proof that current Lattice QCD computation are adequately sampling the space of all possible configurations as opposed to getting stuck in one topological sector, and provide a effective tool for developing algorithms that maximize equilibration of the topological charge.

2. Visualization

Typical production gauge configurations appear to be separated by enough MCMC steps and there is no visible continuity in the topological charge. In order to measure autocorrelation in the topological charge we generated *ad hoc* gauge configurations with small trajectories for two different algorithms and different dynamical quark masses.

- **Wilson** Two sets of $24^3 \times 32$ dynamical Wilson gauge configurations with $\beta = 5.6$ and quark masses of $m_1 = 66$MeV and $m_2 = 33$MeV respectively. Each set consists of 1000 trajectories with a 0.1 molecular dynamics time units, saved every 2 time units ($dt = 0.2$). To integrate Hamilton's equations a multi-step 2nd order symmetric symplectic integrator was used (Omelyan) [3].
- **DWF**: One set of $24^3 \times 64$ dynamical gauge configurations generated with Domain Wall Fermions (two degenerate light ones, $m_u = 14$MeV, and one strange, $m_s = 74$MeV) and Iwasaki gauge action at $\beta = 2.13$, saved every 1/6 of a trajectory ($dt = 0.1\bar{6}$). Further details can be found in [4] and the references therein.

Each gauge configuration consists of a set of $SU(3)$ matrices $U_{x,y}$ for every pair of neighbor sites x, y on the lattice. Given a quark field q_y, the $U_{x,y}$ matrix represent the change in the quark field under parallel transport from $y \to x$, *i.e.*, $q_y \to q_x = U_{x,y} q_y$. Therefore $U_{y,x} = U^H_{x,y}$.

The topological charge is computed in three steps according to the definition:

- The gauge field was smoothed by n-iterations of a "cooling step"
$$U_{x,y} \to U_{x,y} = P_{SU(3)}(\alpha U_{x,y} + (1-\alpha) S_{x,y}) \tag{1}$$
where $P_{SU(3)}$ is a projection operator into SU(3) and $S_{x,y}$ is the average of all products of three consecutive links connecting x with y.
- We computed the chromo-electro-magnetic field defined by
$$F_{x,\mu,\nu} = \frac{1}{2}\mathrm{Re}(A_{x,\mu,\nu} - A^H_{x,\mu,\nu}) \tag{2}$$
where $A_{x,\mu,\nu}$ is the average of the product of four consecutive links in the μ, ν plane starting and ending at point x.
- We computed the topological charge density, defined by
$$Q_x = \frac{1}{32\pi^2} \sum_{\mu\nu\rho\sigma} \epsilon_{\mu\nu\rho\sigma} \mathrm{Tr}(F_{x,\mu,\nu} F_{x,\rho,\sigma}) \tag{3}$$

In fig. 1 we show three images of iso-surfaces of topological charge density for one gauge configuration for different numbers of cooling steps (0,10,15). In fig. 2 we show three images of iso-surfaces of topological charge density for the same number of cooling steps (20) for different consecutive gauge configurations separated by 6 trajectories.

3. Autocorrelation and Hurst Exponent

In addition to the visualization of the topological charge density we also computed the average autocorreleation $R(\tau)$ and average Hurst exponent H for each independent Markov Chain. First we computed the autocorrelation and the Hurst exponent over the MCMC time (τ) for each lattice point, then we averaged the results over all lattice points. The Hurst exponent is computed using the standard R/S technique described in ref. [5]. In fractal geometry, the Hurst exponent is also known as "index of dependence", it measures the relative tendency of a time series to either strongly regress to the mean or cluster in a direction. H is 0.5 for white noise. H is related to the auto-correlation length via $R(\tau) \simeq \tau^{2H-2}$ and $2-H$ is known as the "fractal dimension" of the problem.

Our results are summarized in the following table.

Action	quark masses	H
Wilson	66MeV	0.966
Wilson	33MeV	0.973
DWF	69,17MeV	0.908

The autocorrelation is plotted is fig. 3

Notice how the autocorrelation becomes negative at around 100 MCMC steps. This may indicates an alternating pattern in the data, but a larger MCMC chain will be required to validate this hypothesis.

4. Conclusion

Our analysis demonstrates that the autocorrelation length of a topological charge is very small compared with the trajectory length of typical production grade Lattice QCD computations. Our work is still in progress and, as more data is analyzed, we hope to derive an empirical interpolating formula for the autocorrelation length as function of the simulation parameters.

Acknowledgments

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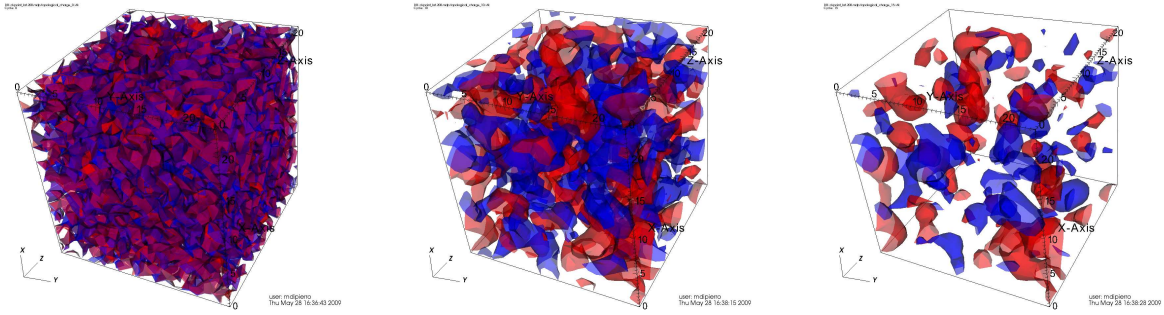

Figure 1. Iso-surfaces for a 3D slice of a topological charge density for one gauge configuration for different numbers of cooling steps (0,10, 15).

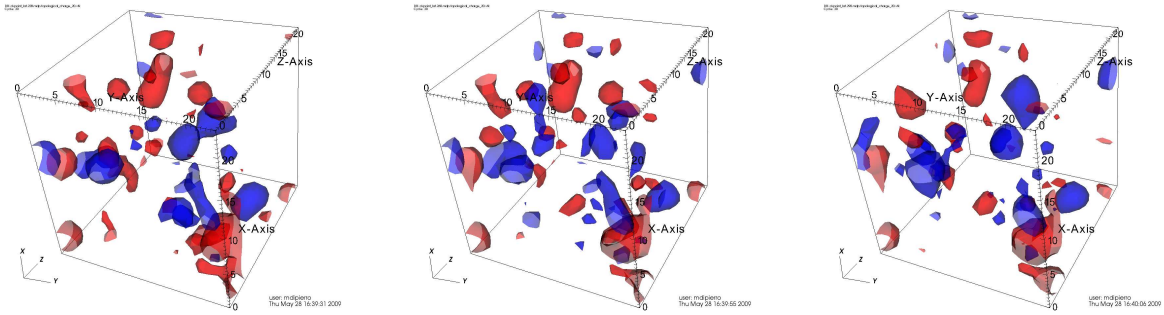

Figure 2. Iso-surfaces for a 3D slice of topological charge density for the same number of cooling steps (20) for different consecutive gauge configurations separated by 6 trajectories.

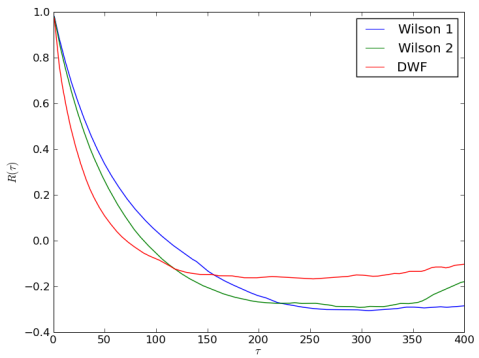

Figure 3. Autocorrelation length for the three sets of gauge configurations considered in the paper.