QCDVis: a tool for the visualization of Lattice Quantum Chromodynamics data

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Abstract
This extended abstract describes an application currently in development to support visualization and analysis of Lattice Quantum Chromodynamics (LQCD) data. Core to our approach is the use of topology driven visualization to first segment the data and then to calculate properties of individual objects present on the lattice. LQCD simulations provide data that is periodic across four space-time dimensions, presenting challenges in analysis and visual interpretation.

Categories and Subject Descriptors (according to ACM CCS):
J.2 [Computer Applications]: Physical sciences and engineering—Physics

1. Introduction
Quantum chromodynamics, most commonly referred to as QCD, is a relativistic quantum field theory for the strong interaction between sub-atomic particles called quarks and gluons. The most systematic way of calculating the strong interactions of QCD is a computational approach known as lattice gauge theory or lattice QCD (LQCD). Space-time is discretised so that field variables are formulated on the sites and links of a four-dimensional hypercubic lattice (fig. 2). This technique allows the gluon field to be represented using $3 \times 3$ complex matrices in four space-time dimensions. Importance sampling techniques can then be employed to calculate physics observables as functions of the fields, averaged over a statistically-generated and suitably weighted ensemble of field configurations.

2. Background
The use of visualization in QCD is often limited to dimension independent forms such as line graphs to plot properties of simulations as part of a larger ensemble. Visualization of...
a space-time nature are less frequently observed but do occasionally occur in literature on the subject making use of established computer graphics techniques including isosurface extraction and direct volume rendering.

Surface plots were used in [Han90] to view 2D slices of data to give a basic understanding of energy distributions in a field. Application of visualization to QCD in higher dimensions first appear in the form of three dimensional plots [FMT97] of instantons showing their correlation to other lattice observables.

More detailed visualizations were performed by Leinweber [Lei00] as a way of conveying to the physics community that visualization of large data sets would help their understanding of QCD. More recently DiPierro et al. [DZS10a, DZS10b, Di 07, DCJ 09, Di 12] produced several visualizations as part of a larger project with the aim of unifying various active LQCD projects.

![Figure 2](image1.png)

**Figure 2:** Left: The data exists on a 4D hypercubic lattice. Right: each site on has links (λ, κ, μ, ν) representing four dimensional space-time (x, y, z, t).

### 3. Scalar heightfield generation

In Lattice QCD field strength variables are defined by navigating around the 4D lattice. Closed loops from a given origin are referred to as a plaquette, represented by a $C_2$ matrix. Topological charge density is a loop around all four dimensions from an origin point, meaning values are a multiplicative combination of three spatial plaquettes and three time-like plaquettes (fig. 3). For storage, visualization and processing purposes field variables are stored as either 3D volumes split across the time domain, or as 4D hyper-volumes. Values represent the field strength at a given point in 4D space by taking the Real part of the matrix trace.

### 4. QCDVis application

Use of the contour tree algorithm [TV98] allows the transition from simple isosurfaces to representation of distinct objects in the data. This has two benefits; first, optimized visualization techniques can be applied to the data. Second, properties can be calculated on distinct contours as opposed to the level set as a whole, allowing the calculation of physical measurements of objects existing in the data.

Each object is computed and rendered in parallel using a modified form of the algorithm proposed in [CP04] for a given isovalue. The output of the algorithm is a triangle mesh that continually varies with isovalue. It is possible to compute features of these meshes, including moments using techniques discussed in [ZC01].

At present it is possible to compute the surface area, volume and centre-of-mass of LQCD objects by performing a sum over each triangle in the mesh. In order to compute volume ($M_{000}$) a tetrahedron is formed for each triangle by placing an additional vertex at the origin (1). Centre of mass requires the calculation of three first order moments (2). Each triangle is evaluated to give a weighted average in the $x$, $y$ and $z$ planes, scaled by its contributing volume. The final centre of mass for the object is calculated as a positional vector that must be scaled by the entire objects volume (3).

$$M_{000} = \frac{1}{6} \left( -x_2y_2z_1 + x_2y_3z_1 + x_3y_1z_2 - x_1y_3z_2 - x_2y_1z_3 + x_1y_2z_3 \right)$$

where $<x_n, y_n, z_n>$ represent vertices of a triangle (1)

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\[ M_{100} = \frac{1}{4}(x_1 + x_2 + x_3)M_{000} \]
\[ M_{010} = \frac{1}{4}(y_1 + y_2 + y_3)M_{000} \]
\[ M_{001} = \frac{1}{4}(z_1 + z_2 + z_3)M_{000} \]  
\[ (2) \]

Centre of mass = \[
\begin{bmatrix}
M_{100} \\
M_{010} \\
M_{001} \\
M_{000}
\end{bmatrix}
\]  
\[ (3) \]

The moment of inertia requires the computation of the eigenvectors of the 2nd order tensor given in (4), requiring further statistical measures of the mesh. Eigenvalues and eigenvectors are computed using Schur decomposition through the use of the Eigen linear algebra library [GJO10]. The three normalised vectors returned are sorted in order of magnitude of their generating eigenvalue, with the largest being the principle component axis. This allows the vectors to be colour coded and visualized originating from the centre of mass as shown in fig. 4.

\[ \text{Inertia Tensor} = \begin{bmatrix}
M_{200} & M_{110} & M_{101} \\
M_{110} & M_{020} & M_{011} \\
M_{101} & M_{011} & M_{002}
\end{bmatrix} \]  
\[ (4) \]

Figure 4: The moment inertia is visualized as three vectors originating from the centre-of-mass of the objects.

5. Domain specialist feedback

The application has been developed with continued input from domain specialists as an iterative process. An initial set of features were requested by physicists, including proximity and shape of objects in the data, with functionality further dictated by user feedback. Data exploration has proved to be an important part of this process as the theoretical nature of the data means that questions are not always known in advance.

An example of this is the effect of the chemical potential parameter (\(\mu\)) on simulations. Upon viewing examples of the data at differing chemical potentials, physicists began to question if increasing this variable would distort the shape of objects uniformly. To determine if this happens we must work at the ensemble level, integrating properties across the isovalue range that relates to each object for all configurations. For this purpose parallel computation of meshes at differing isovvalues has been incorporated in to the program, these are cached and retrieved as required for rendering or querying of properties.

6. Future work

A feature of LQCD simulations that proves problematic is that the lattice is periodic in all four dimensions. Objects are permitted to exist across opposing boundaries; this results in the generation of open meshes (fig. 5) that are incompatible with calculations discussed in section 4.

Figure 5: The periodic nature of the data causes the generation of open meshes when an object is divided by a boundary.

Current work is focused on closing meshes using knowledge of the heightfield topology. Upon completion of this task it is necessary to evaluate situations where an object is separated into two or more parts. Individual sections can then be computed and summed, giving a robust method for evaluating any object within the data.

References


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