QCDVis: a tool for the visualisation of Quantum Chromodynamics (QCD) Data

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Quantum chromodynamics (QCD)

The strong interaction force
Quantum chromodynamics is the theory of the strong nuclear force.

Subnuclear matter
Studies the binding of hadronic matter, such as protons and neutrons.

Particles
Quarks are bound together by exchanging massless gluon particles.

QCD operates at the subnuclear scale on quarks and gluons.
Kenneth Wilson suggested that a discrete lattice could be used to model QCD systems [1].

Lattice is four-dimensional in Euclidean space-time, with space and time treated as equivalent. Data set in this study is relatively small (i.e. $12^3 \times 24$ sites), but current state-of-the-art lattice QCD uses lattices of up to $16^3 \times 128$.

All points on the lattice are treated equally using translational invariance. This means all boundaries including the time axis are periodic in nature.
Ensemble data

Ensemble sampling
Due to the quantum nature of lattice QCD, observables are computed as ensemble averages or expectation values.

Generation process
Each ensemble emerges from a Markov chain using an algorithm such as Hybrid Monte Carlo.

Research goals
Varying ensemble parameters allows physicists to model a phase diagram of lattice QCD. This is a long established field of study in lattice QCD.
Lattice fields

Computations
Various fields exist on the lattice. Each is computed as a closed loop from an origin point, or site, as a product of multiple complex matrices.

Properties
Although each of these computations result in a SU(2) complex matrix these can be reduced to a scalar value by taking the real part of the trace.

Output
Sweeping across the lattice enables construction of multiple scalar fields. The structures present in each field relate to different physical observables.
Cooling process

**Algorithm description**

Cooling is a technique that iteratively removes noise by varying the values of link variables. The output of the algorithm at each stage is a unique lattice configuration.

**Minimising the impact of cooling**

Whilst a largely accepted part of the lattice QCD process, physicists are reluctant to throw away information.

**Over cooling**

Over cooling occurs when the algorithm starts to erode or remove the intended lattice observables. Established techniques exist in lattice QCD to predict optimal levels of cooling.
Existing software

Histograms and surface plots are used frequently in domain literature.

Derek Leinweber used animated isosurfaces to demonstrate the visualisation of lattice QCD to the physics community [3].

More recently DiPierro et al. [4] used isosurfaces and direct volume rendering techniques to present a variety of lattice observables using VisIt and Paraview.

Visuals generated by Leinweber [3]

Visuals generated by DiPierro et al. [4]
Topological visualisation techniques

Contour tree [5]
Captures the connectivity in the sublevel and superlevel sets as the isovalue is varied.

A simple data set displayed with its contour tree at various isovalue. The rendered contours are generated using the flexible isosurface algorithm.
Topological visualisation techniques

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A generalisation of the contour tree where data can be defined on a non-simply connected domain, such as a torus.

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Flexible isosurfaces [7]
This algorithm uses path seeds extracted from the contour tree to generate connected contours.
Research questions

Existing lattice QCD software is static in design and doesn’t take advantage of topological visualisation techniques. We therefore ask the following questions:

- Is it possible to learn more about lattice QCD by applying topological visualisation techniques to the data?
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- How can topology support visual analysis to gain additional insights into lattice QCD data by dynamic interaction?
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- How can topology support visual analysis to gain additional insights into lattice QCD data by dynamic interaction?
- What happens to the structure of objects on the lattice as thermodynamic control parameters are varied?
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- Is it possible to learn more about lattice QCD by applying topological visualisation techniques to the data?
- How can topology support visual analysis to gain additional insights into lattice QCD data by dynamic interaction?
- What happens to the structure of objects on the lattice as thermodynamic control parameters are varied?
- Is it possible to extract quantitative data from the lattice using topology and surfaces of the data?
Data origin

Lattice QCD data sets are generated as part of large lattice collaborations. DiRAC includes multiple UK universities.
Framework overview

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Design
The QCDVis framework mainly consists of two modules:

- *The ensemble module* allows the user to generate various lattice fields.
- *The visualisation module* displays the lattice fields using topological visualisation techniques.
**Workflow**

**External Database**
- Ensemble simulations
- FORTRAN generated
- 4D lattice structure

**Data Set**
- Configurations
- Cooling slices
- Field variables
- Action (Wilson action)
- Topological charge density

**Data Selection**
- Field interactions, effects of cooling

**Field Generation**
- Validation
- 3D scalar fields
- Polyakov loop
- 4D scalar fields
- Plaquette fields
- Average Plaquette
- Difference Plaquette
- Topological charge density

**Visualisations**
- Seeded contours
- Tree / Graph Visualizations
- Infovis techniques
- Interaction
- selection / manipulation

**Statistical analysis**
- Extract overview of topology
- Reeb Graph
- Contour Tree
- Joint contour net
- Volumetric properties

**Topology**
- Compute
  - Contour Trees
  - Reeb Graphs
  - Joint contour net

**Hypervolume Slicing**
- 4D > 3D slices
- xyz, xyt, yzt, xzt

**Ensemble module**

**Visualisation module**

**User refactoring**

Boundaries and interaction between the two core modules of QCDVis.
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Boundaries and interaction between the two core modules of QCDVis.
The ensemble interface allows the user to generate various lattice fields.
Stability of the lattice under cooling is important in the configuration selection process.

The destruction of lattice features can be further investigated using the visualisation module.
The visualisation module uses topological visualisation techniques to present the lattice fields.
Periodic objects in lattice QCD are correctly captured in the Reeb graph but not the contour tree.
Case study: Locate and visualise an instanton

Objective
Use the ensemble tool to locate an (anti-)instanton and examine its structure using the visualisation tool.

Work flow: ensemble module

1. Use statistics from the cooling process to estimate the position of the object in space-time.
2. Consult the lattice cooling graphs to find an optimal configuration to visualise.
3. Use the tool to generate the topological charge density field data.

From 15 cools the configuration \textit{conp0015} becomes stable. Note: the graph predicts a bias of 1 instanton.
**Case study: Locate and visualise an instanton**

**Work flow: visualisation module**

1. Visualise the object using temporal slicing.
2. Explore the effect of slicing along each spatial axis.
3. Vary the isovalue to understand the link between contours and topology graphs.
4. Examine related plaquette fields to understand structural similarity.

**(Anti)-instantons can be examined in isolation by selection in the contour tree.**
Case study: Inspect a cooling process event

Objective
An irregularity has been spotted in the cooling process — use QCDVis to examine what is happening.

Work flow: ensemble module

1. Examine the lattice cooling graphs to locate a drop in the Wilson action.
2. Use the statistics window to witness a global maxima become a minima in successive cooling iterations.
3. Generate scalar fields for the relevant cooling iterations.

A sudden drop in the Wilson action can relate to an instanton-anti-instanton annihilation or an object falling through the lattice.
Case study: Inspect a cooling process event

Work flow: visualisation module

1. Load multiple cooling slices into the visualisation module.
2. Locate the instanton object by setting a high isovalue.
3. Step through the cooling steps.
4. Witness the irregularity in the topological graphs and surfaces.
5. Change the isovalue selection to visualise the ‘new’ object.

Maxima at 36 cools.
Maxima at 37 cools.
Minima at 37 cools.

The instanton present at 36 cools appears to split into an instanton-anti-instanton pair at 37 cools.
QCDVis is a *dynamic* system for exploratory visualisation of lattice QCD data.
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Insights gained whilst using QCDVis have lead to new questions being asked of lattice QCD data.
Existing study is performed on data from a single source. There are many more lattice QCD projects in operation worldwide.

We are in the process of analysing entire lattice QCD ensembles using topological persistence measures from the Reeb graph.

We are investigating the interaction between different lattice fields using multivariate topological structures such as the Joint Contour Net [8].
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Plaquette fields

**Physical meaning**
Space-like plaquettes represent the magnetic field potential on the lattice and time-like plaquettes represent the electric field.

**Lattice computation**
The average of path ordered products of link variables in 2D planes from a site $U(X)$.

**Properties**
Scalar field in $\mathbb{R}^4$, with range $[-1.0, +1.0]$. 

Plaquettes are closed loops on the lattice. Top: the 3 space-like plaquettes; bottom: the 3 time-like plaquettes.
Topological charge density is computed by looping in all four space-time dimensions from a lattice site $U(X)$.

Physical meaning
Global minima and maxima in the topological charge density field relate to pseudo-particles called (anti-)instantons.

Lattice computation
A periodic path ordered product of link variables in all four space-time directions from a site $U(X)$.

Properties
Scalar field in $\mathbb{R}^4$, with range $\approx [-45.0, +45.0]$. 
Polyakov loop

**Physical meaning**

Used as a method of identifying the breaking of symmetry on the lattice. A good way of identifying transitions to a de-confined state.

**Lattice computation**

Periodic path ordered product of link variables in the time direction from a site $U(X)$.

$$f(X) = \frac{1}{2} \Re \left( Tr \left( \prod_{n=1}^{L_t} U_\mu (X + n \hat{t}) \right) \right)$$

where $\mu = 0$, $X \in \mathbb{Z}^3$

The Polyakov loop reduces the 4D lattice to a 3D scalar field.

**Properties**

Scalar field in $\mathbb{R}^3$, with range $[-1.0, +1.0]$. 
Case study 2

Maxima at 36 cools.

Maxima at 37 cools.

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