Interactive Spatiotemporal Visualization of Phase Space Particle Trajectories using Distance Plots

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ABSTRACT
The distance plot (or unthresholded recurrence plot) has been shown to be a useful tool for analyzing spatiotemporal patterns in high-dimensional phase space trajectories. We incorporate this technique into an interactive visualization with multiple linked phase plots, and extend the distance plot to also visualize marker particle weights from particle-in-cell (PIC) simulations together with the phase space trajectories. By linking the distance plot with phase plots, one can more easily investigate the spatiotemporal patterns, and by extending the plot to visualize particle weights in conjunction with the phase space trajectories, the visualization better supports the needs of domain experts studying particle-in-cell simulations. We demonstrate our resulting visualization design using particles from an XGC Tokamak fusion simulation.

Index Terms: Human-centered computing—Visualization—Visualization application domains—Scientific visualization

1 INTRODUCTION
Distance plots and recurrence plots [7] are useful for highlighting recurrent patterns and dynamical transitions in phase space trajectories from multidimensional complex systems. Despite an embrace by communities in domain sciences and applied mathematics, the visualization community has yet to robustly investigate their use as an interactive tool for qualitative visualization. Specifically, in many-particle systems (especially PIC simulations where particles commonly carry time varying weights), there are several issues that should be addressed if one wishes to utilize these techniques. Standard procedures for applying recurrence quantification analysis (RQA) are error prone and tedious even for simpler single component systems. The significance of a single component (e.g. particle) in a many-component system such as a PIC Tokamak simulation, the overall complexity of the entire system and its boundary conditions, and the complex meaning of a trajectory that carries a weight, makes the setting highly non-trivial. A typical application of RQA to these kinds of particle trajectories would be problematic. Despite these limitations, it is clear that recurrence plots, and especially the distance plot, can be useful for understanding the spatiotemporal patterns of these trajectories. In this paper, we show how this can be done through the combination of a novel distance plot visualization, and linked phase space views.

Our main contribution is the extension of the plot to also visualize the weights of marker particles in PIC simulations. This is important for researchers studying Tokamak fusion simulations, since the particles often carry time varying weights which identify each particle’s contribution to the overall particle distribution. While interactive recurrence plots have been used for information visualization [1] [2], linking them with phase plots for studying scientific simulation data appears to be novel in application. A small additional novelty to our visualization is the incorporation of marks on the distance plot to indicate occurrences of events. We apply these methods to study phase space trajectories of particles from the XGC Tokamak fusion simulation [5]. Our preliminary results show interesting patterns related to little understood dynamical interactions between the phase space trajectories and evolution of particle weights, and correlations between the weights and trajectories in terms of their (quasi) periodicity.

2 BACKGROUND

The phase space of a dynamical system includes those variables which are necessary to uniquely describe the systems state. A trajectory of a dynamical system therefore represents an evolution of the systems state over time from a particular initial condition. A single particle in a many-particle system can be viewed as a component (or subsystem) of the overall system, that follows its own phase space trajectory.

In practice, it is common to refer to a plot in which time is a parameter rather than an axis as a phase plot, regardless of whether each axis is technically one of the actual phase space variables of the system.

2.1 Distance and Recurrence plots
A recurrence plot is a symmetric binary matrix where the columns/rows represent time steps, and the cells (i,j) represent the mapping R(i,j) = 1 if ||xi – xj|| < ε else 0, where xi is phase...
space vector of the system at time \( t \). Similarly, the unthresholded recurrence plot (or distance matrix) is the matrix with each cells \((i, j)\) representing the distances \(|x_i - x_j|\). Figure 1 demonstrates visually how the recurrence plot is computed and what it represents.

![Figure 1: A depiction of the Tokamak fusion device. Left) A cross section depicting the poloidal plane, and two important types of particle modes, trapped (blue), and passing (red).](image)

**2.2 Tokamak Simulations**

Tokamak devices are being investigated for harnessing fusion as a clean and vast energy source. These devices work by confining hydrogen plasmas within toroidal magnetic fields, while heating them up to the extreme temperatures required for fusion reactions to occur. For the XGC Tokamak simulations, each particle lives in a 5D phase space, that includes 3 physical dimensions and 2 velocity dimensions (perpendicular and parallel to the local surface of its toroidal magnetic field). Figure 2 depicts the Tokamak device as well as the two important types of particle trajectories (trapped and passing) that are featured in our analysis. The particles in XGC additionally each carry time varying weights that represent their contribution to the overall phase space particle distribution.

**2.3 Requirements**

Our design is motivated by three primary challenges. First, the trajectories of interest are typically at least 5D. One approach is the use of multiple linked views to visualize different sub-spaces. However, we wish to identify patterns in the higher dimensional space since they are meaningful for domain scientists to understand the systems dynamics. Distance plots are useful for finding high dimensional patterns in dynamical systems, yet they lack spatial context. Second, physicists who develop and study XGC stress the importance of analyzing the particle weights in conjunction with the phase space trajectories. Third, we would like to support the study of a phenomena of interest. These factors motivated our design which includes an extended distance plot that also shows the particle weights, markers indicating occurrences of discrete events that cue specific phenomena, and includes multiple linked 2D phase plot views.

**3 RELATED WORK**

The more general problem of how to visualize multivariate temporal scientific data has been studied extensively. Some approaches include dimensionality reduction, linked and coordinate views, glyphs, and 2D or 3D plots or volume visualizations with additional variables mapped through color [4]. Other techniques, specifically for analyzing multidimensional trajectories or pathlines, include similarity analysis [14], clustering [6], and flow feature based pathline attributes [15]. The problem with these methods that we address with this work, is the difficulty of exploring recurrent patterns in high dimensional spaces.

Distance plots and recurrence plots have been proven useful for these purposes [7]. Extensions of the recurrence plot include fuzzy recurrence plots [11], which use cluster centers as an alternative to discrete states, as well as cross recurrence plots [3] and joint recurrence plots [9], which can be used in limited circumstances to analyze separate trajectories together. Additionally, Poincaré plots and Poincaré maps are also used to study recurrence in dynamical systems. Sanderson et al. used them to study recurrent patterns in toroidal magnetic fields [12], and Tricoche et al. applied these methods within a more general study of topological features in area preserving maps [16].

In terms of interactive visualization, and domain specific extensions, a “conceptual recurrence plot” was proposed by Agus et al. for finding patterns in human discourse [1]. Additionally, Demiralp et al. applied recurrence plots within an interactive system for studying eye movements associated with visual-cognitive tasks [2]. However, existing recurrence plots do not support visualizing the combination of particle weights along with the phase space trajectories, and interactive use to compliment multiple coordinated phase space views has not been explored. Previous work addressed visualization of Tokamak particle distributions through weighted, spatially organized velocity histograms [10]. While useful for visualizing local changes in the particle distribution over time, they lacked in the ability to analyze patterns in the particle trajectories.

**4 METHODS**

**4.1 Linking Distance Plots with phase space Plots**

Since distance plots primarily show temporal patterns, and trajectory plots primarily show spatial patterns, we use an interactive linking between them to enable a more intuitive and detailed analysis of the phase space trajectories. By hovering the mouse over cells within the distance plots, the associated pairs of time steps are selected and their corresponding points are then plotted in each of the phase plots, as in Figure 3.

One procedure that one could apply to analyze the recurrence patterns in this manner, is to first select an interesting time step (e.g.
Figure 4: A group of linked phase plots together with our custom distance plot. The left plot represents the poloidal plane, the lower middle plot represents velocity space, the upper middle plot represents the two angles of rotation (toroidal and poloidal), and the upper right plot represents the particle weight and magnetic radius. The background of each of these phase plots shows a heatmap based aggregation of all of the particles weights, while the specific trajectory being singled out is shown in bright green. This trajectories distance plot is shown in the lower right corner. The analyst has selected a cell in the distance plot and the states corresponding to this pair of time steps are plotted in each of the phase plots (black point with white border and white point with black border).

Figure 5: The design of our distance plot based visualization incorporating events and particle weights. the upper left portion of the matrix represents the phase space distance plot, while the lower left represents the particle weights distance plot. Different color maps are used for each to distinguish them. In each case, lighter means smaller distances. The red/blue bands along the axis show the values of the weights over time with red indicating positive weight and blue negative weight. The points along the diagonal represent the events.

4.2 Incorporating Events

Scientists are commonly able to define meaningful events that may occur within their system of study. By incorporating these events into an interactive visualization, one can more easily investigate particular aspects of the data they are currently interested in. We incorporate events in our visualizations for both visual context, and selection. For visual context, points in time are recorded when the event of interest has occurred. The state of the system during these recorded events, are marked as points, and rendered over each of the linked phase space visualizations, as well as along the diagonals of the distance plots (where \( t = i = j \), corresponds to an event occurrence at time \( t \)). For selection, the analyst can directly select groups of events based on state through interactions on the phase plots, and then explore the associated trajectories and their correlations with the events.

The particular event we use in our analysis is the change of direction of rotation about the center of the poloidal plane. This is an indication of trapped particle modes. Passing particles are defined as particles which rotate fully about the center of the poloidal plane without turning around. Figure 2 illustrates these two types of trajectories. Research in this topic is ongoing and important for designing more stable Tokamak devices.

4.3 Incorporating Particle Weights

Since our collaborating physicists wish to analyze the particle weights in conjunction with the trajectories, we split the otherwise symmetric phase space distance plot into two halves, one for showing recurrent patterns in the phase space trajectory, and the other for...
showing recurring patterns of the particle weights. Second, we plot
the time series of the weights along the axis of the distance plot to
give addition context for gaining insight into the patterns. Figure 5
illustrates the design of the resulting distance plot, as well as the
placement of event based markings.

Figure 4 shows a group of phase plots together with the custom
distance plot. The phase plots show one selected trajectory (bright
green) with a weight based aggregation of all of the particles beneath
if for context. Read the caption of the figure for more details.

5 PERFORMANCE

The distance plot requires \( N^2 \) pairwise distance calculations on
vectors in \( \mathbb{R}^M \) where \( N \) is the number of time steps and \( M \) is the
dimension of the trajectory. The computation is embarrassingly
parallel and can be easily mapped to the GPU. Our implementation
performs the calculation on the CPU with thread level parallelism
using OpenMP which we found sufficient for our application. We
tested the performance on an Intel(R) Core(TM) i7-5930K CPU @
3.50GHz. Results for a range of time series lengths and dimensionli-
ties are shown in Figure 6, and demonstrate sufficient efficiency for
interactive visualization.

6 RESULTS

Figure 7 shows some examples of the distance plots for different
particles. An interesting pattern is an apparent correlation between
the quasi-periodicity of each of these aspects of the particle. That
is, it seems that the weights tend to oscillate with the orbits of the
particles in phase space. While this seems to be a tendency, it is not
a strict rule, and variations of interesting sub-patterns seem to occur
which may loosely or tightly follows this trend. While the presented
images only depict a few of many trajectories, the finding seems to
be consistent with the larger set of trajectories as well (based on a
visual inspection of a large sample). A more robust investigation in
close collaboration with expert physicists will be done in the future
to uncover the greater significance of these insights.

Figure 8 shows another finding. In this use case, the transition
from magnetic confinement to escape and subsequent absorption
by the Tokamak’s heat load diverter is studied. The focus is on
the relationships between weight fluctuation and the phase space
transitions from confinement to loss. This use case is interesting
since particle flux near the outer portion of the toroidal device is
strongly associated with particle loss, and a major driving force for
weight evolution as the simulation progresses. Understanding this

![Figure 6: Computation times for a distance plot from trajectories of
different dimensions and number of time steps.](image)

![Figure 7: Four examples of the dual phase space, particle weight
distance plots. The left two plots are from passing particle trajectories,
while the two on the right are from trapped particle trajectories, and
include marks representing the direction change events.](image)

![Figure 8: A particle on its transition from magnetic confinement to
escape and absorption by the heat load diverter. The arrow shows
that point along the trajectory in the upper view (in the poloidal plane),
corresponds to the time step where an anomalous change in the
evolution of the particle's weight occurred. It appears this marks an
onset of the transition, before the subsequent loss of confinement.](image)
process can help to design better simulation techniques in addition to the physics. Our finding highlights instances in which sudden anomalous weight changes are observed before it is obvious (based on the trajectory) that the particle is escaping. In the figure, the anomaly in the distance plot is pointed to by the black arrow, as the dark vertical band (representing a narrow spike in the particle’s weight). A linked phase plot of the poloidal plane is shown above the distance plot, and the point at which the anomaly occurred is pointed out as well. The direction change events plotted on the recurrence plot correspond to the point where the particle impacts the heat load diverter.

7 Discussion

This work stands as a good starting point for a line of new research for advanced interactive visualization of complex many-particle dynamical systems such as PIC Tokamak simulations with particle weights. Still, there are several challenges, limitations, and areas for further improvement and future work.

While applicable in many cases, distance plots are not always useful. For example, some systems have recurrence rates that are so far apart that analyzing them is impractical. Additionally, we apply distance plots as linked visualizations to deeper analyze phase space trajectories, yet in many cases they are used to study 1D observational time series data and the underlying phase space and associated trajectories are not available. In these cases recurrence is studied by first “reconstructing” a phase space through time-delay embedding. This workflow requires special stages in which one must be careful to properly reconstruct the phase space, and attempt to extract dynamical features without direct knowledge of the actual phase space of the system or its trajectories. Marwan provided a guide to avoiding common pitfalls in recurrence quantification analysis [8]. Note that in our application, we do not attempt recurrence quantification analysis since it would be problematic in our setting, but instead utilize the distance plot (unthresholded recurrence plot) for qualitative analysis. While thresholding is primarily used to support the process of RQA, in the setting where RQA is not the goal, the distance plot is considered a valuable representation for qualitative analysis. Still, thresholding has value in this setting, since it allows to clarify which states are the most recurrent (have the closest pairwise distances).

While a single recurrence plot only shows a single trajectory, once could explore a large set of trajectories by using the patterns within the recurrence plot as a basis for trajectory comparison and clustering as well as feature extraction and search. One possible direction is to use deep learning, for example neural networks/auto-encoders to learn latent features that are invariant to subtle, or uninteresting differences such as in phase alignment, or small differences in frequency.

We leave it as future work to robustly investigate the potential for these ideas. One additional challenge is scalability if distance plots for each separate trajectory need to be computed and stored at once. The strait-forward implementation will be computationally expensive in both time and space when dealing with a very large number of trajectories. To store each of the plots alone would require \( N \times T^2 \), where \( N \) is the number of trajectories, and \( T \) is the number of time steps. This is too much space to use in the case of large scale simulation data which can include thousands of time steps and hundreds of thousands to billions of particles. For this reason, the distance matrices will likely need to be computed on the fly and used as needed.

The main near term goal for our future work is to explore more use cases and to more robustly evaluate the technique through more formal experimentation and verification of results.

8 Conclusion

We present a combined phase plot and distance plot based approach for analyzing particle trajectories from many-particle simulations. An interactive linking between the distance plot and the phase plots allows to better see the spatiotemporal patterns of the trajectories. By also incorporating events into the visualization, we can gain even more context and investigate specific phenomena more easily, and by splitting the plot we can better correlate particle weight dynamics with phase space trajectories. The preliminary findings from our PIC Tokamak simulation application are interesting and demand further investigation. We will continue to advance this line of work, and hope that others will be inspired as well.

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References