Analysis of parameter for Local Colour Scale in Ion Trajectories

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Abstract

Spatio-temporal dataset is a collection of datasets where data is vary in both space and time. Theoretically, such a datasets can be considered as a continuous and discrete. For example, specification of the function, $F : E^d \times T \to R^n$, where E^d denotes d-dimensional Euclidean space, $T = R^* \cap \{\infty\}$ the domain of time and R^n an n-dimensional scalar field. Examples, of such data sets include time-varying simulation results, films and videos, time-varying medical datasets, geometry models with motion or deformation, meteorological measurements and many more. It is therefore highly desirable to use visualisation to summarize meaningful information in higher dimensional spatio-temporal data sets. In physics, ion trajectories has totally relied on statistical analysis from experimental and computer simulation results [1-5]. To help the physicists to identify and trigger the timeline and collaborative events in ion trajectory, we need the codes to distinguish the events according to timeline-based events. In coding theory, we need such a code that can represent each of the events in timeline series. Moreover, the code itself must help in identifying and trigger the events if there is a collaborative event among chaotic movements of ion trajectories. In particular, we propose a Colour Number Coding Scheme for depicting the time series of ion trajectories [6]. We discuss the method of depicting the time series in relation to the encoding series of timeline events in ion trajectories. We also point out some of the advantages of this method in terms of accuracy according to human observer.

Keywords: coding theory, spatio-temporal, ion dynamics, streamline, colour scale, visual representation

1. INTRODUCTION

The transport of ions within aperiodic glass structures has remained an enigma for many years, the resolution of which will be critical for explaining the huge versatility of glass in technology, including its homogeneity, and its electrical, mechanical and chemical characteristics. Physicists has proposed a variety of ionic conduction models, ranging from the correlated forward and backward hopping of single cations [7], to collaborative process involving the transport of many mobile cations [8-10].

Experimentally, the collaborative character of ion trajectories in glasses can be inferred from dielectric and ion transport properties. The existence of such collaborative phenomena was suggested by examining ionic conductivity data, tracer diffusion measurements and dielectric data collected from experiments [10-12]. However experimental data, which measures macroscopic properties and lacks in structural periodicity, does not provide any description of the atomic structure and trajectories. Any detailed observation of spatio-temporal collaborative in ion trajectories is not possible at moment. The glass structure and trajectories over the spatial and temporal scales relevant to the diffusion processes therefore remain undetermined at large from the experiments.

With the advance of computational science, large scale simulations of molecular trajectories, followed by statistical analysis, have resulted in better comprehension of ion trajectories in glasses. These approaches have established the clustering of alkalis [1, 3, 4], and identified both localized hopping and long-range collaborative jumps [13]. Collaborative transport is less likely at low temperature or at low alkali concentration, and in mixed alkali compositions [8, 14, 15]. This latter phenomenon is known as the mixed-alkali effect and has been interpreted by involving an energy penalty, which inhibits hops to sites previously occupied by a different alkali type [16]. Many of these ideas beg the question of visualisation to clarify the relationship between glass structure and ion trajectories at the local level.

In a comprehensive study of single and mixed alkali glasses, 1080 atom models of composition $(Na_{(1-x)}K_x)_2Si_2O_5$ have been calculated using the Molecular Simulation Package. In these models [17], Si (silicon) and O (oxygen) atoms form the silicate network, which hosts alkali Na (sodium) and K (potassium) ions in a number of suitable spatial domains. The short-range Van der Waals interactions are modelled by the Buckingham potential :

$$U(r_{i,j}) = A\exp\left(-\frac{r_{i,j}}{\rho}\right) - \frac{C}{r_i^6,_j}$$

where U and $r_{i,j}$ denote the energy and the interatomic distance for the pair of atoms i and j respectively. The long-range Coulomb interactions are handled via the standard Ewald sum.

In order to form the silicate network, the model potential for the 0-0, 0-Si interactions is based on that of [18], and three-body components are used to control the 0-Si-O and Si-O-Si angular distributions $U(\theta_{i,j,k})$ where $\theta_{i,j,k}$, is angle formed by atoms i, j and k.

Simulations of the trajectories have been performed at the fixed temperature of 1800K and over duration of 20-100ps. They involve the integration of Newton's equations of motion for each time step an each atom, which allows the calculation of the individual atomic trajectories over time. At this temperature, a fraction of the alkali Na and K ions can be mobile, travelling through a comparatively frozen silicate network.

Studying the complicated events that result in ion migration from statistical functions, however, has proved elusive in the past. Most ions stay close to the same position over time, but some can move a considerable distance, typically within about 10^{-11} seconds. The latter events have been interpreted as collaborative [13] and the analysis of time series events also conducted [5].

Using visualisation, it becomes possible for us to probe these complex compositional dependent processes by looking at the choreography of neighbouring ions. The distinction of different mobility of ions can be clearly seen in Figure 1 which shows the movements of neighbouring Na (blue), 0 (cyan) and Si (green) ions in disilicate glasses. Ion tracks are reduced to attractors using the Ruelle-Taken formalism. These are mainly roughly spherical in shape, ion motion being contained within a short distance $(< 10_{10} m)$, but the mobile Na ions in the lower half clearly travel much further.

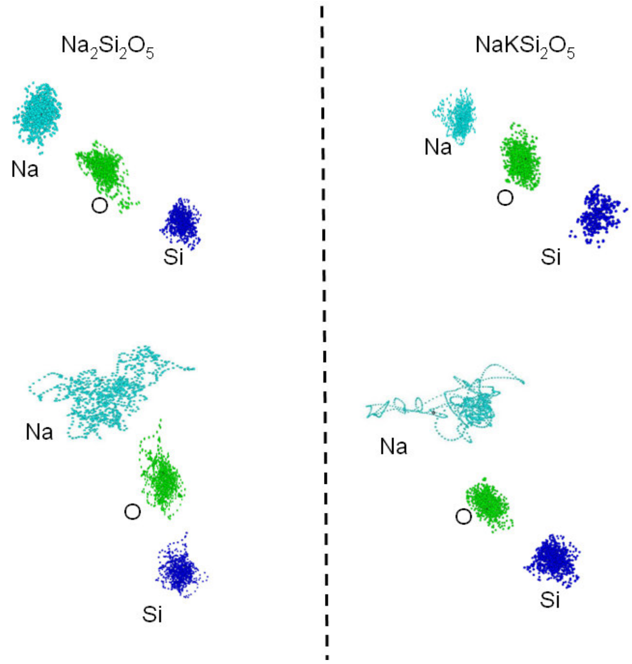


FIGURE 1 : Attractors for neighbouring ions are shown for Na2Si2O5 (left) and NaKSi2O5 (right) glasses. Sodium (Na) attractors appear to be more mobile than others, indicating their possible involvement in spatio-temporal collaboration.

The simulation results include various thermodynamic properties of the simulated ensemble average, the positions of the bonds between atoms and the trajectories of ions as time-varying series of 3D points, which can be forwarded to the visualisation process. In this work, we are particularly interested in the identification of time series event and collaborative activities from a given collection of such trajectories for ions a,b,….:

$$P_{a,0},\ P_{a,1},\ \dots,\ P_{a,n};$$
$$P_{b,0},\ P_{b,1},\ \dots,\ P_{b,n};$$
$$\dots\dots$$

The paper is organized as follows. Firsts, we discuss existing and relevant codes which is available in time-varying visualisation in Section 2 and followed with Section 3 for spatial orientation topic. In Section 4, we divided the explanation into two concrete situations. We introduced our method that's called Global and Local Colour Scale. In Section 6, we highlight the issue of timeline events which is before collaboration takes place. In this section, we enumerate various parameters which are important in perceiving the accuracy of timeline events. We discuss the pros and cons of using those parameters in our visual representation with the same input datasets. Finally, in Section 7 we concluded our study

2. RELATED WORK

Since the late 1990's, researchers in coding theory have been searching for developing, improving, applying or generating a codes. Several applications have been developed, including error controlling system [19], fault tolerant or fault diagnosis/monitoring [20], analysis model [21], developing framework [22] and communication system [23]. Some of the effort combined with another field of research such as complexity theory [24], system theory [25] and test pattern generators [26]. Some researchers borrowed a technique from coding theory concept to solve some research problem such as in testing problems [27], cryptography [28], optical flow [29], adaptive radar [30], algorithm [31] and neural network [32].

However, through the codes itself, many researcher were try to enhance the performance of the codes. For example, Kieffer was study the rate and performance of a sequence codes along a sample sequence of symbols generated by a stationary ergodic information source [33] but differently with Ishikawa, he used to improving the communication performance in hypercube multiprocessor with bus connection through coding theory concept [34]. Some researchers improve the codes in different way such as Vardy used to enhance the codes by minimum distance of the code [35]. Moreover, Garcia and Stichtenoth were shows an algebraic functions field as a useful tool for improving the codes by determine the number of rational places [36].

For Rains, they improved the codes by determine the bound through finding the minimum distance of the codes using the length [37]. In ions trajectory, to help the physicists to identify and trigger the timeline and collaboration events, we need the codes that can be identify the events according to timeline-based events. From the above review, we need such a codes that can represent each of the events in timeline series. Moreover, the code itself must help in identifying and trigger the events if there is a collaboration among the ion trajectories.

Many researchers have recently noted that there is a work for solving the problem in some research area with the help of coding theory concept such as in data security [28], optical flow [29], communication channel [30] and neural network [32]. One problem often overlooked when rendering time-varying data sets based on coding theory concept is to associate a particular event with a precise moment on the timeline. This is useful not only for determine the time of an event but also for identification corresponding parties involved in collaboration. Very few researchers has given their attention in literature on timeline encoding especially in codes.

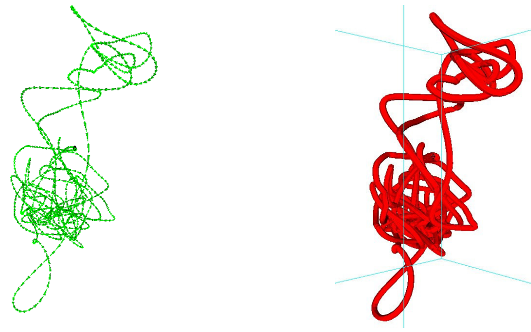
Location codes is a labelling technique that represented tetrahedral elements within a mesh. Lee et al. [38] used this technique for labelling triangular faces. There are also a few authors used this idea for their works such as Evans et al. [39] who use an array where the label of a node determines the node location in the array. Thus, Zhou et al. [40] used this strategy to addressing the children and parents in managing the multiresolution tetrahedral volume data. A similar data structure is used by Gerstner and Rumpf [41] for extracting isosurfaces at different levels of details. Location code also has been used in spatio-temporal database research for labeling purpose as well [42]. Since then, there is another labeling scheme has been introduce like LPT code [43]. It was extension from the location code itself. The origin idea for labeling codes has comes from Gargantini [44]. She was introduced the effective way for represented the quadtrees with her codes called gargantini codes. After that, quadcode has been published by Li and Loew [45] for representing geometric concepts in the coded images, such as location, distance and adjacency.

Designing efficient image representations and manipulations with bincodes has been proposed by Ouksel and Yaagoub [46]. This codes will represent a black rectangular sub-image in the image. The code is formed by interleaving the binary representations of the x- and y-coordinates of the subimage and its level in the corresponding bintree. Some enhancement had been made on the bincodes itself by Lin et al. [47]. There is few more codes had been introduce in image representation such as sarkar's code [48, 49], logicodes [50], restricted logicodes [50] and symbolic codes [51]. All those codes closely related to the image representation. Since there is no such a codes for time-varying datasets in ion trajectories. Here, we introduced our own codes that can be useful to visualise a series of timelines in ion trajectories [6] [52].

3. SPATIAL ORIENTATION

In this section, we will first examine the more challenging task for visualising temporal information in order to identify the series of events. We will discuss the use of glyph, colour and opacity in our visual representations and present the methods for constructing and rendering composite visualisation that convey a rich a collection of distinguishable visual features for assisting in a visually data mining processing

Given an ion trajectory as a series of n+1 points, $p_0, p_1, ..., p_n$, we have n consecutive vector segments, $v_0, v_1, ..., v_n$ where $v_i = (p_i - p_{i-1})$. One can visualise such a trajectory using streamlines or vector glyphs.



(a) glyph (b) tube

FIGURE 2 : Streamlines of trajectory sodium #169

In Figure 2(a) and (b), even though each image, which represents a vector segment, depict the instantaneous velocity at a given time interval with its length or the direction of the motion with its pointer but its does not much help to visualise a time series events in ion dynamics. Probably with this method the viewer might know which ion is moving or static as shown in the Figure 2. In the next section, we will highlight a method that can give more understand about time series events in ion dynamics.

4. TEMPORAL INFORMATION

When involving a sequence of timeline events, the complexity task is to reveal the time of an event and the classification corresponding parties which participate in collaboration. But the issues of cooperation or collaboration will not discuss at moment. At the same time, this task will turn into tremendously complicated if there are hundreds or thousands of collaborative events occur. Given an ion trajectory as a series of n+1 points, $p_0, p_1, ..., p_n$, we have n consecutive vector segments, $v_0, v_1, ..., v_n$, where v_i = $(p_i - p_{i-1})$.

4.1 Global Colour Scale

Through streamlines itself, it is difficult to differentiate between the top and bottom trajectories, even though they are presenting a motion in opposite directions. In complexity of movement, at the global level, the viewer should be able to observe a global time frame of the ion trajectory before we going into high degree of temporal information. As shown in Figure 3, the purpose of global colour scale had been used because it will help viewer to determine the global time frame for the events. Finally, we introduced our novel method that we called Global Key Colours [6].

FIGURE 3 : Seven Key Colour for Global Colour Scale

4.2 Local Colour Scale

In order to correlate each vector segment with the timeline more accurately and hence to improve the differentiation of different vector segments, we introduce a Colour Number Coding Scheme in our visualisation [6]. Given a small set of key colours, $c_1, c_2, ..., c_k\,(k > 1)$ and distinctive interval-colour (e.g., while, black or grey depending on the background colour), we code a group of consecutive m vectors as a k-nary number, terminated by a vector in the interval-colour. Given n as the total number of vectors and we always assign the interval-colour to the first vector, we need to find the smallest integer m that satisfies Equation 1 :

$$(m+1)k^m \geq n \text{ ....(1)}$$

For instance, when n = 1000, using two key colours, say red and green, we need in m = 7 colour digits. We have m = 5 for k = 3, m = 4 for k = 4, and m = 2 when k reaches 19. The selection of m and k needs to address the balance between a smaller number of colours or a smaller number of colour digits in each group of vectors. The former ensured more distinguishable colours in visualisation, and the alteration reduces the deductive effort for determine the temporal position of each vector. Figure 4 shows a quaternary colour coding scheme for ion tracks with 1000 vectors.

FIGURE 4 : Quaternary Colour Coding Scheme for trajectory of sodium #169

As mentioned previously, global colour scale would be able to visualise global time frame only instead of local time frame. In Figure 5 we show a comparison between global and local colour time scale. In this paper we choose quaternary colour coding scheme for local colour scale which is k=4 for our comparison result with global colour scale. According to our result that shown in Figure 5, we understand local colour scale will help the viewer to distinguish each timeline events in ion trajectories and the purpose of global colour scale is to summarise all the timeline events or the global time frame in ion trajectories.

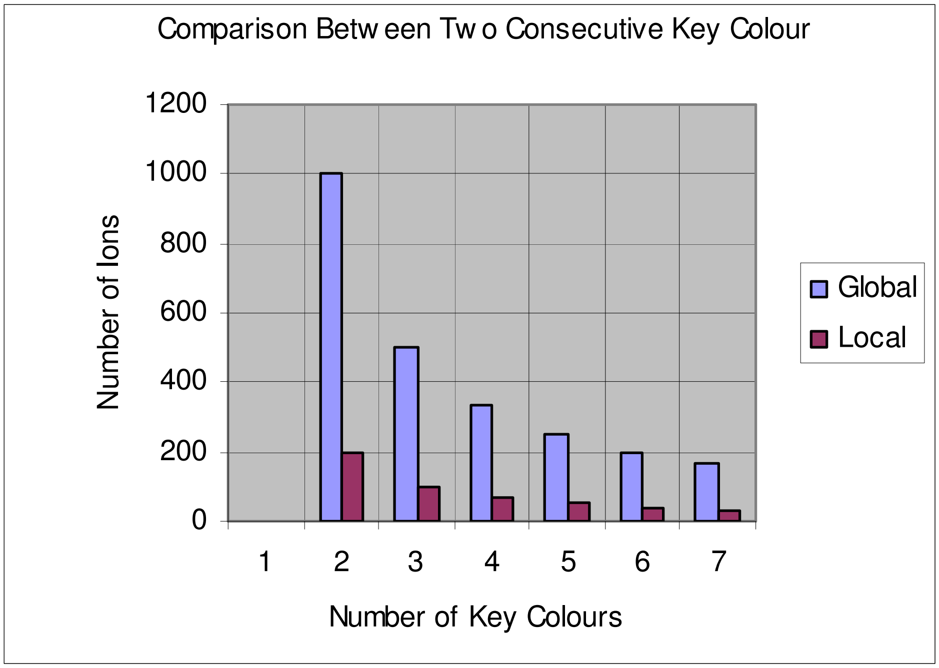


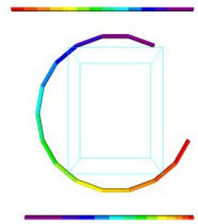
FIGURE 5 : Comparison between global and local colour scale

In the following section, the composition of local colour scale will be elaborated in details. The main concern of this particular section will show the visual representation of local time scale to help the viewer in analysing the collaborative events in future. Moreover it will be a tool for scientists as well in analysing any scientific datasets especially in time-varying datasets.

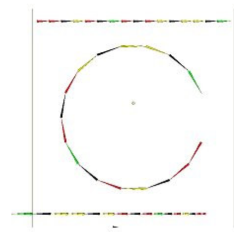
5. COMPOSITING RENDERING

Through composition of above-mentioned colour scales together, we provided an effective visual representation for visualising spatio-temporal of ion trajectories. To simplify the clarification about colour scale we constructed testing trajectories as shown in Figure 6. The top trajectory represents an object travelling from left to right at a constant velocity, the center one travelling in a circle at a constant speed and the bottom one travelling from right to left at a steadily increasing speed.

In Figure 6(a), streamline had been coloured by Global Colour Scale. Even though, it can differentiated between the top and bottom trajectories and representing the motion in opposite direction at different speed but this is for global scale viewing only.



(a) Global Colour Scale – *n* key colours



(b) Local Colour Scale – *colour number coding scheme*

FIGURE 6: Time Coding Colour Scale

Figure 6(b) shows each conical glyph, which represents a vector segment with Local Colour Scale, depict instantaneous velocity at a given time interval with its length and the direction of the motion with its pointer. The combination of method in Figure 6(a) and 6(b) are shown in Figure 7.

Initially, the viewers can visualise the global scale only. To let the viewers can see the local scale, the viewers must move closely to the trajectory and they will see the local scale inside the global scale. Figure 7 shows the local colour scale when the viewers come close to the ion trajectories.

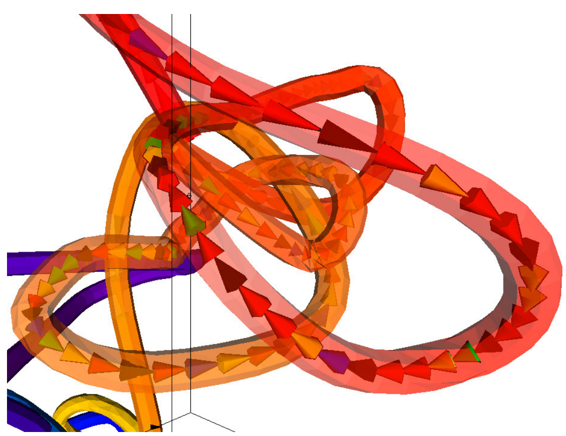


FIGURE 7 : Zooming effect when viewer come closer

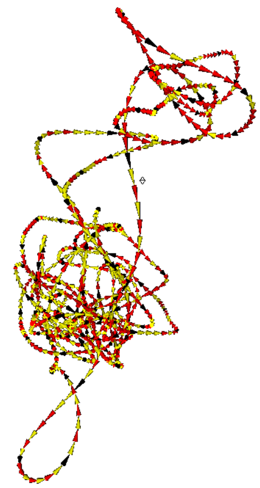
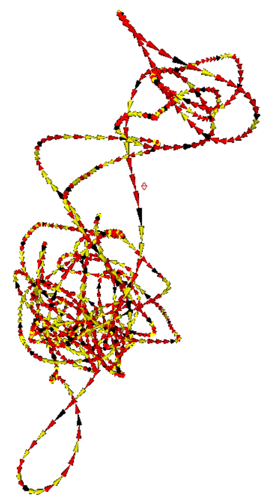
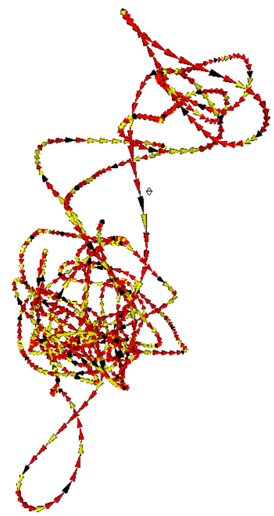
6. OPTIMUM PARAMETER SETTING FOR LOCAL COLOUR SCALE

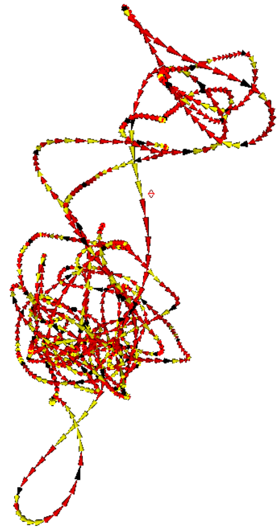
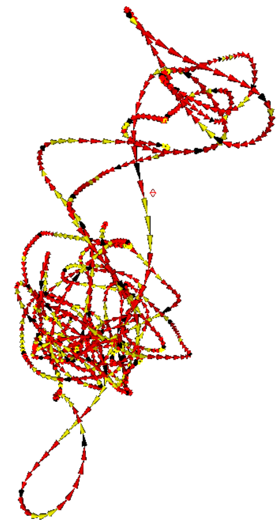
Without this section, we could not complete yet our visual representation. This is another issue that we think we should included in this part because it will support our objective. Initially, we want to show the effectiveness of the local colour scale scheme which is used in our study. Let begin the discussion for visualising time series events in ion trajectories.

In this section, we consider the selection of **m** and **k** parameter will become main factor in our local colour scale. According to Equation 1, we will shows all possibility of parameter **m** and **k** that have been applied on local colour scale. Our goal is to improve the correlation of each vector segment with the timeline event. That is why we introduced a Colour Number Coding Scheme in our visualisation.

6.1 Optimum Setting for m's

In Equation 1, when **k**=2, the minimum value for parameter m is 7 for n=1000. We can increase the value of parameter **m** until it reaches 1000 which is the maximum number of vector segment. This comparison is illustrated in Table 8. This table shows that when we increase the value of **m** until 1000, it will loss the accuracy of local scale timeline because it does not give any meaning to the viewers.

No	***M***	***k***	***Image***
1.	**7**	**2**	
2.	**8**	**2**	
3.	**9**	**2**	

4.	**2**	**10**	
5.	**2**	**11**	
6.	**2**	**22**	

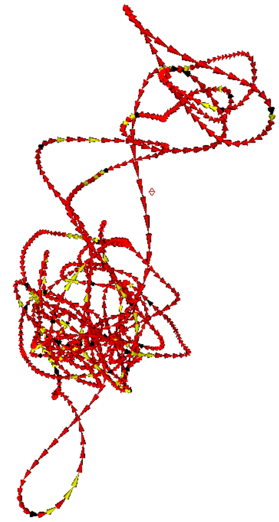
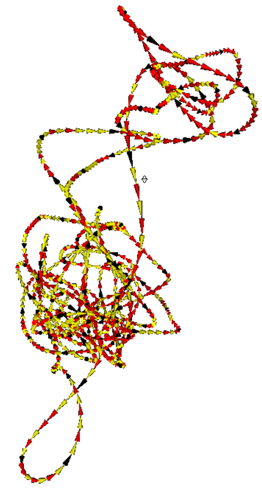
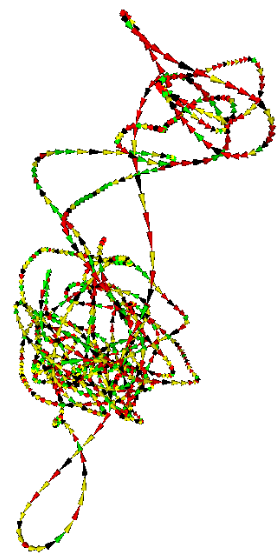
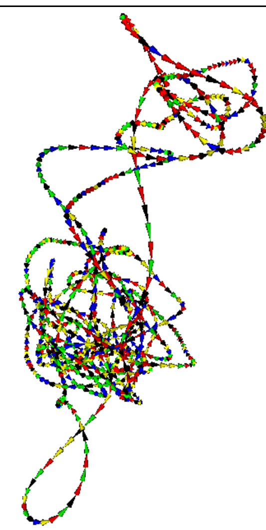
7.	**2**	**25**	
8.	**2**	**1000**	

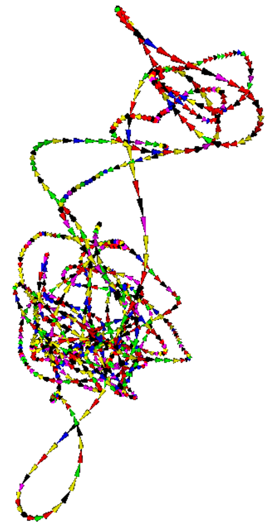
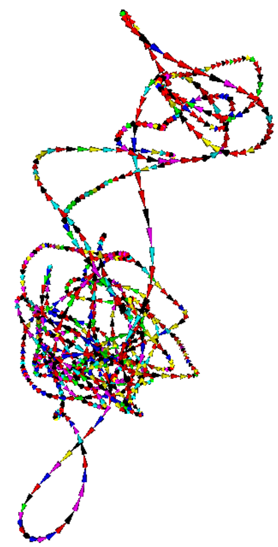
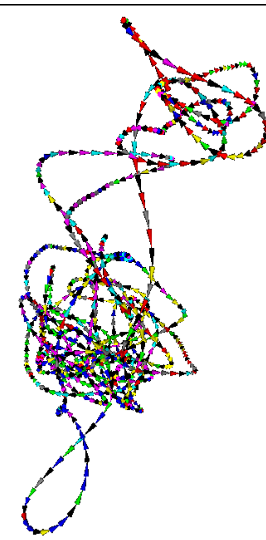
TABLE 8 : Experimental images for satisfying **m** parameter

6.2 Optimum Setting for k's

Our next experiment is to satisfy the value of parameter **k**. In Equation 1, a **k** will represent the total of colours that will be used. Same with the previous experiment, we can increase the colour, **k** up to 1000 colours, **k**=1000. Compare the results that we obtained from Table 9, those images rendered with small value of **k** are visually distinguishable than the images rendered with the high value of **k**.

No	m	K	Image

1.	**7**	**2**	
2.	**5**	**3**	
3.	**4**	**4**	

4.	**4**	**5**	
5.	**4**	**6**	
6.	**3**	**7**	

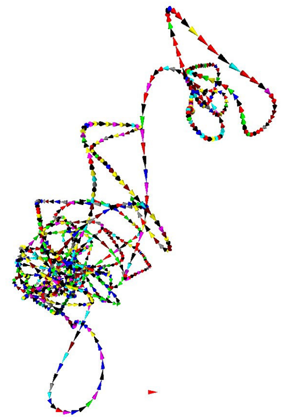
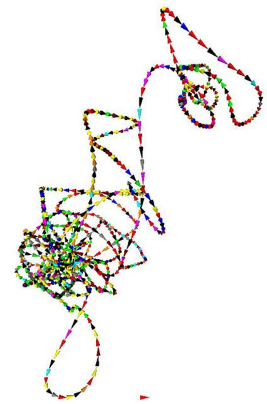
7.	**3**	**8**	
8.	**3**	**9**	
9.	**2**	**256**	

TABLE 9: Experimental Images for satisfying **k** parameter

6.3 Analysis of the images

In local colour scale, we used quaternary colour scale which **m**=4 and **k**=4. A **k** represent how many colour in one interval. The size of interval determine by **m** value. Among the interval of group of colours we put separator which is in black colours. When we found where is t=0 at global scale, we will applied transparency scheme to look into local colour scale. In Figure 7, we can see some sort of local colour scale which is started with four red cone, separator, yellow followed by three red cone and so on. This sort of colours represent the series of timeline.

If we look into number theory, quaternary number is the sort of **k**-nary number scheme like binary, tri-nary and etc. Here, we choose four colours which is red, yellow, green and blue. Each colour represent a code such as red = 0, yellow = 1, green = 2 and blue = 3. What are the quaternary number ? Quaternary number consists 0,1,2 and 3. In terms of codes, we want to develop a codes of k-nary number. With m=4 and k=4, we will produce some sort of codes like this : 0000, 0001,0002, 0003, 0010, 0014, … , 4443, 4444. These codes will represent a series of timeline that we will explain later in more challenging task when the cooperation events takes place. For the time being, its just enough to analysis t=0. According to Figure 7, from the portion of t=0 at the global scale, we can see there is sort of red cones and followed by black separator at the beginning of the trajectories. According to our calculation, red cones will represent a 0 value so it is become 0000. If we want to know what is the timeline, we have to simply convert those codeword which from quaternary based number to decimal based number [53-55]. Given the series of the codeword, $c_1, c_2, \ldots, c_k \ (k > 1)$. Below we show the way how to find the timeline using our codeword.

	separator	c_{k-1}	….	c_i	….	c_1	c_0
Total	=	$k^{k-1} \times c_{k-1}$	….	$k^i \times c_i$	….	$k^1 \times c_i$	$k^0 \times c_0$

$$t = (m+1) \times \text{total}$$

thus

separator	c_{k-1}	….	c_i	….	c_1	c_0
T_{t+k}	$T_{t+(k-1)}$	….	T_{t+i}	….	T_{t+1}	T_{t+0}

Let say, 0000 is the codeword while m and k are assigned to 4. Here, we show how to use the above method to get the timeline.

	separator	0_3	0_2	0_3	0_0
Total	=	$(4^3 \times 0_3)$	$(4^2 \times 0_2)$	$(4^1 \times 0_1)$	$(4^0 \times 0_0)$

$$t = (4+1) \times 0$$

thus

separator	0_3	0_2	0_1	0_0
T_{t+4}	T_{t+3}	T_{t+2}	T_{t+1}	T_{t+0}
T_{0+4}	T_{0+3}	T_{0+2}	T_{0+1}	T_{0+0}
T_4	T_3	T_2	T_1	T_0

Thus, we understand each of the codeword will help the viewers to determine a local time scale in ion trajectories.

It is clear that as the **k** or m are increased then the accuracy of local colour scale will loss as well. Thus, we need a balance selection between **k** and **m** that will satisfied our local colour scale. As a result, we choose **m**=4 and **k**=4 for n=1000 that we called quaternary colour coding scheme as shown in Figure 4.

7. CONCLUSION

The results show that our colour number coding scheme can be used to allow viewer to determine a time frame at low level in ion trajectories. Traditionally for lower dimensional spatio-temporal datasets are investigated using line graph, bar charts or other pictorial representation of a similar nature and animation, all of which require time-consuming and resources-consuming processes. However, our results indicates that Global and Local Time Scale may be used to visualise a timeline events without line graph, bar charts etc thus enabling the real time imaging of ion dynamics. Our work also can convey temporal information in a high degree of certainty and effective deployment of visualisation in complex spatio-temporal datasets. This enable us to form the basis of visually mining tools for collaborative ion dynamics in future.

8. REFERENCES

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