Visual Study of Timeline and Collaborative Events of Ion Trajectories in Glass Structure

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ABSTRACT

Our perception of the ion trajectories has largely relied on numerical and statistical analysis of data from experimental dimension and computer simulation results (Funke, 1993; Ngai, 1993; Smith et al., 1995; Ngai et al., 1998; Ngai et al., 2002). In particular, we considered a simulated 3D time-varying model of ion trajectory and examined the temporal correlation among chaotic movement of the ions. Our goal is to contrive effective visual study to assist scientists, especially physicists, in ascertaining temporal correlation among intricate and apparently chaotic time-varying datasets. We proposed a hybrid application with combination of iconic techniques, global and local colour scale and opacity scheme for spatio-temporal depiction. We illustrated also few images that can offer an effective tool for visually mining 3D time-varying scientific datasets.

Key words :
system application, spatio-temporal visualisation, coding theory, colour scale, time-varying datasets, molecular dynamics, iconic representation

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 have proposed a variety of ionic conduction models, ranging from the correlated forward and backward hopping of single cations (Funke, 1993), to collaborative process involving the transport of many mobile cations (Ngai, 1993; Smith et al., 1995; Ngai et al., 1998).

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 (Greaves and Ngai, 1995; Ngai et al., 1998; Ngai et al., 2002). However, experimental data which measure macroscopic properties and lack in structural periodicity do not provide any description of the atomic structure and trajectories. Any detailed observation of spatio-temporal collaborative of ion trajectories is not possible at the moment. The glass structure and trajectories over the spatial and temporal scales relevant to the diffusion processes therefore remain undetermined by the experiments.

The advancement 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 (Oviedo and Sanz, 1998; Sunyer et al., 2002; Meyer et al., 2004) and identified both localized hopping and long-range collaborative jumps

(Habasaki and Hiwatari, 2002). Collaborative transport is less likely to occur at low temperature or at low alkali concentration and in mixed alkali compositions (Rao and Balasubramanian, 1995; Smith et al., 1995; Greaves, 1998). 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 (Maass et al., 1995). 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 $(Na_{(1-x)}K_x)_2 Si_2O_5$ have been calculated, using the Molecular Simulation Package. In these models (cclrc), Si , and 0 (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 (Vessal et al., 1989), 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 an angle formed by atoms i, j and k.

Simulations of the trajectories have been performed at the fixed temperature of 1800˚K and over duration of 20-100ps. They involve the integration of Newton's equations of motion for each time step and 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 (Habasaki and Hiwatari, 2002) and the analysis of time series events also conducted (Habasaki et al., 2005).

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.

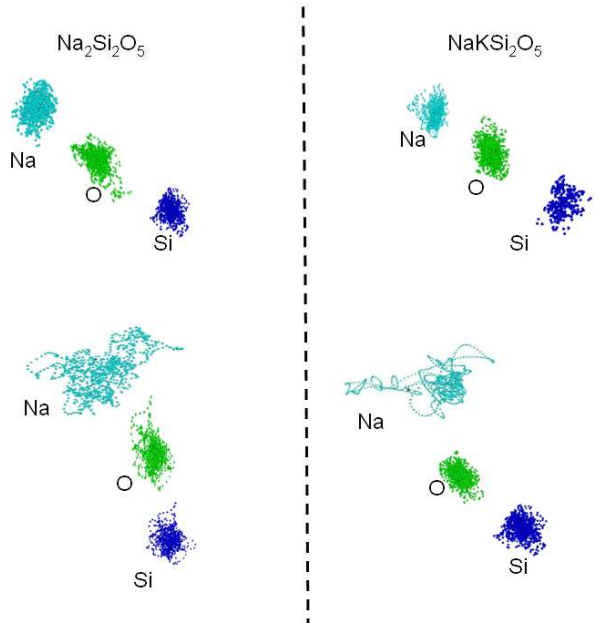


Figure 1. Attractors for neighbouring ions are shown for $Na_2Si_2O_5$ (left) and $NaKSi_2O_5$ (Kenwright and Lane) glasses. Sodium (Na) attractors appear to be more mobile than others, indicating their possible involvement in spatio-temporal collaboration

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,….*:

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

The objective of this work is to develop an effective visual study and visualisation techniques to help scientists extract meaningful spatial and temporal information from spatio-temporal datasets. In this paper, we propose a hybrid scheme that uses streamline for orientation, global and local colour scale for depicting a timeline events and zooming effect with transparency scheme for probability of collaboration. With a collection of visual study, we demonstrate that this scheme can offer an effective tool for visually mining 3D time-varying datasets. We show that the visualisation not only confirm the presence of collaborative phenomena in ion dynamics but also help identify the dynamic patterns and trigger events of such movements. This enables scientists involved to develop more elegant and comprehensive hypotheses about scientific datasets.

The ability to convey temporal as well as spatial information is critical in our particular application, where the scientists need a visual representation that can effectively highlight the correlation between different ions in their motions among seemingly-chaotic trajectories, especially in collaborative events. This particular challenging requirement provided this work with the principal motivation.

In the rest of this paper, we will describe the application concerned and scientific background in Section 2. In this section, we will first examine the methods that can convey orientation information to

viewers. We will devote most of our focus to the visualisation of temporal information in order to confirm and identify the time series activities in the data sets. In Section 3, we will present some results of visual data mining process on glassy ion trajectories if there is a collaboration events, which will be followed by our concluding remarks in Section 4.

MATERIAL AND METHODS

Visualising Timeline Events

In this section, we will first examine the more challenging task for visualising temporal information in order to identify the series of events and collaborative 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 indistinguishable visual features for assisting in a visual data mining process.

A. Orientation

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.

In Figure 1, even though each conical glyph, which represents a vector segment, depicts the instantaneous velocity at a given time interval with its length and the direction of the motion with its pointer but it does not much help to visualise a time-series events and collaborative issues in ion dynamic without the combination of colour scale. In the next section, we will show the colour scale which should give more understanding about time-series events in ion dynamics.

Figure 1 : A trajectory of sodium #169

B. Temporal Information

When using visualisation to summarize a series of events along a timeline, perhaps the most difficult task is to associate a particular event with a precise moment on the timeline. This is useful not only to determine the time of an event but also for the identification of corresponding parties involved in collaborative events, but collaborative events are not included at the moment.

1) Global Colour Scale - In order to show the global timeline of events on streamline, we introduced Global Key Colours Scale. In this scheme, we used a small set of colour, $c_1, c_2, ..., c_k; (k > 1)$, then we assigned the colours to specific vector in the vector series :

$$\begin{array}{ccccccc} v_1 & v_u & \ldots & v_v & \ldots & v_n \\ c_1 & c_2 & \ldots & c_i & \ldots & c_k \end{array}$$

where indices such as u and v are pre-determined. For each vector that has not been assigned a colour, we obtain a colour by interpolating the two nearest neighbors with the specified key colours in each direction. This scheme allows a viewer to determine a time frame at a global scale with the help of key colours. In Figure 2, we choose seven key colours which form rainbow colour to visualise global scale of time series. At local level, the interpolation can make different vector segments indistinguishable. Moreover, it is possible to have the same or similar interpolated colours between different sets of consecutive key colours.

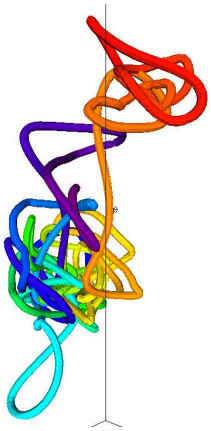


Figure 2 : Seven Key Colours for trajectory of sodium #169

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. 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.

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

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 ensures more distinguishable colours in visualisation, and the latter reduces the deductive effort for determining the temporal position of each vector. Figure 3 shows a quaternary colour coding scheme for ion tracks with 1000 vectors.

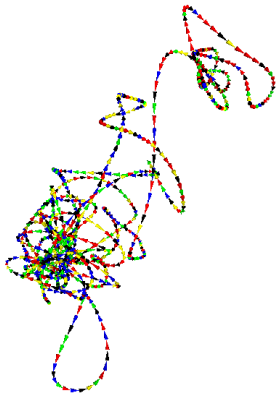


Figure 3 : Quaternary Colour Coding Scheme on sodium #169 trajectory

Visualising Collaborative Events

When collaborative events is take place between ions in the simulation results, then the possible method that we could use is opacity scheme. However, the details of this scheme, implementation and result will become the future work of this study. Even in this paper, we are not focusing on collaborative events but we extended a brief regarding transfer function that could be possible in our application. By combining all the above methods, we provide an effective visual representation for visualising collaborative ion dynamic. Figure 4 shows the example of collaborative events in ion dynamics.

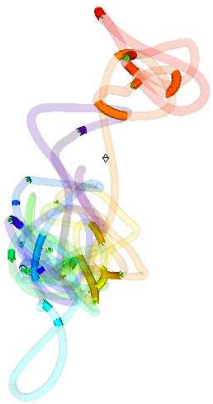


Figure 4 : Combination of collaborative visualisation ion dynamics

The main objective of this task is to discover if collaboration is exhibited between ions in the simulation results. As described previously, there is not well-defined description about collaboration events, although experiments suggested the existence of collaboration phenomena. We, including the physicists involved, did not know in what form a collaborative event may display, in what way ions may cooperate with each others or what event may cause ions entering in or disengaging from collaboration. Therefore, we have introduced a variable, ψ representing the probability of collaboration. Given a set of m hypothesized criteria of collaboration, we have :

$$\psi = \omega_1\psi_1 + \omega_2\psi_2 + ... + \omega_m\psi_m \qquad (2)$$

where ω_i is the weight of criterion i, and $\psi_1 + \psi_2 + ... + \psi_m = 1$. In this work, we have considered three such criteria, namely (1) the ability for two or more ions to maintain similar orientation, (2) the ability for two or more ions to maintain similar velocity, and (3) the ability for two or more ions to maintain constant gap between them. Given two corresponding vector segments, $v_{a,i}$ and $v_{b,i}$, belonging to two different ion trajectories, we have:

$$\psi_1 = \left(\frac{1}{2} \left(\frac{v_{a,i} \bullet v_{b,i}}{|v_{a,i}||v_{b,i}|} \right) \right)^{D_1} \tag{3}$$

where $D_1 \geq 0$ is de-highlighting factor. The larger the D_1 is, the less probable a vector is considered being involved in collaboration. With ψ_1, $v_{a,i}$ and $v_{b,i}$ are considered to be in collaboration, if they follow a similar direction.

As the velocity of an ion at particular time is reflected in the length of the corresponding vector segment, we define ψ_2 as:

$$\psi_2 = \left(1 - \frac{abs(|v_{a,i}| - |v_{b,i}|)}{|v_{a,i}| - |v_{b,i}|} \right)^{D_2}$$

where D_2 is similar to D_1 for ψ_1. With ψ_2, $v_{a,i}$ and $v_{b,i}$ are considered to be in collaboration, if they are of a similar length.

Let $p_{a,i-1}$ and $p_{a,i}$ be the two end points of v_a, and $p_{b,i-1}$ and $p_{b,i}$ be the two end points of v_{b_i}. It was suggested that ions may try to maintain an equispaced gap between them during their motion from time step *i-1* to *i*. Although one may consider to use a formula similar to ψ_2, it is not effective in measuring such criteria as the distance between $p_{a,i-1}$ and $p_{b,i-1}$ is normally much greater than that between $p_{a,i-1}$ and $p_{a,i}$. We thereby employ a standard indicator based on a small window of ion positions around v_{a_i} and v_{b_i}. Let the window size be *2w* and $w \geq 1$, we compute the distance between each pair of ion positions within the windows of two trajectories as:

$$d_j = |p_{a,j} - p_{b,j}|, \; j = i - w, i - w + 1, ..., i + w - 1$$

We have:

$$\psi_3 = \left(1 - \frac{std\left(d_j \,|\, j = i - w, ..., i + w - 1 \right)}{mean\left(d_j \,|\, j = i - w, ..., i + w - 1 \right)} \right)^{D_3}$$

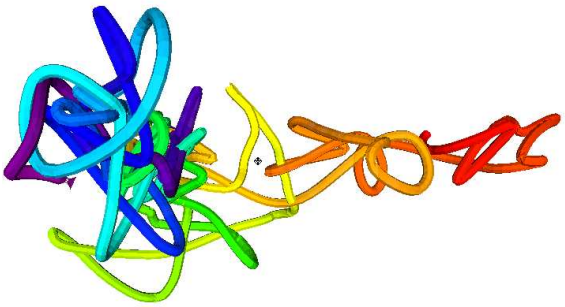
where D_3 is similar to D_1 for ψ_1, *std()* and *mean()* are the standard deviation and mean functions of the samples d_{i-w}, d_{i-w+1} ,….., d_{i-w-1}. When the window goes beyond the two end points of a trajectory, we simply include less sample in the calculation.

Once we have computed $\psi \in [0,1]$, we can highlight or de-highlight the corresponding vector segments. Three different methods of highlighting the probability of collaboration are shown in Figure 5. We chose a small sample because it is easy for clarification purpose.

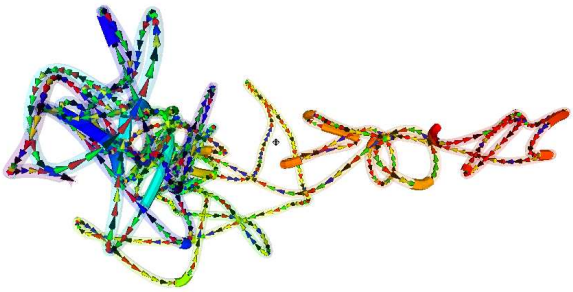
In Figure 5(a), we applied an opacity to a vector glyph only and the tube would remain unchanged. Here, the viewer should be able to come closer to the object and choose randomly based on global colour scale at which time frame they want to visualise it.

While in Figure 5(b), we applied an opacity of tube around the glyphs with a high ψ value which, in effect defines the opacity of the tube. This method looks better than a previous method because a viewers will know instantly as compared to previous method. However, this method is only beneficial for small set of datasets.

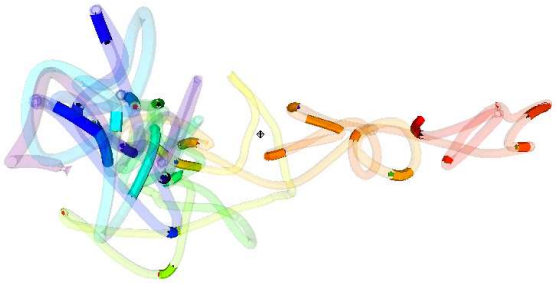
In Figure 5(c), we used the value of ψ to modify an opacity of the corresponding tube and vector segment.If there is a high probability of collaboration, the tube and vector glyphs are fully opaque and if there is a low probability, they are almost totally transparent. The last method seems to convey information with more certainty to human observer.



(a) method 1



(b) method 2



(c) method 3

Figure 5 : The possibility of collaboration between Na #211 and Na #106, when ψ was computed with ψ_1 (only #106 is shown)

Figure 5, shows the probability computed, using ψ_1 between each of the ion trajectories Na #106 and

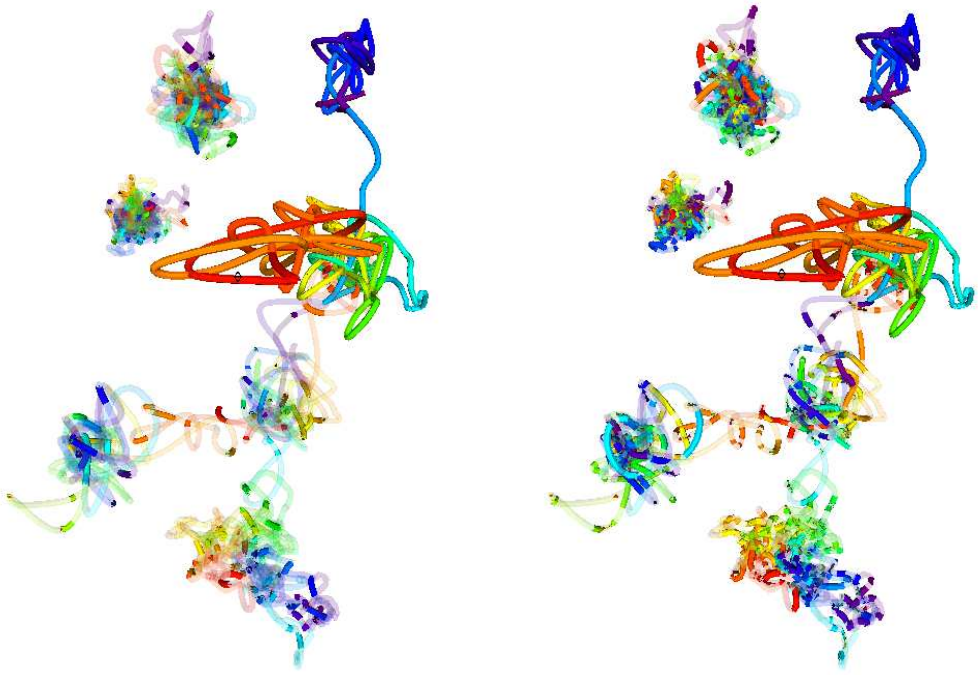
Na #211. From these visual examples, the scientists would be able to trigger the collaborative events effectively. Without highlighting and de-highlighting based on ψ, it would be difficult to observe these phenomena directly.

RESULTS AND DISCUSSION

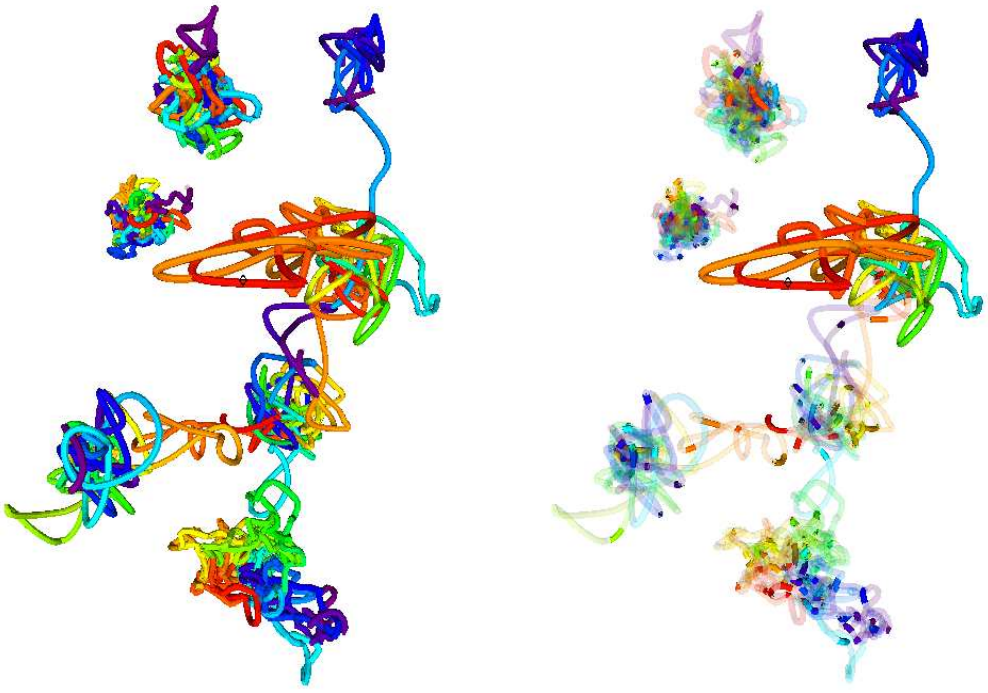
When collaborative events take place between ions in the simulation results, then the possible method that we could use is the second method as shown in Figure 5. But the technical details of this scheme will be presented in another paper work. Thus, in this paper, we are focusing on collaborative events with a visual study of the cluster of six ions.

By combining all the above methods, we provide an effective visual representation for visualising collaborative ion trajectories. As an example, we present a visual study of cluster of six ions, including three sodium ions and three oxygen ions. For each ion, we compute its probability of cooperation with other ions in the cluster. We evaluate ψ *based* ψ_1, ψ_2, ψ_3 *and* $(\psi_1 + \psi_2 + \psi_3/3)$.

Figure 6 gives a set of visualisation generated in the visual study using six ion trajectories. These images are all computed using Na #211 as the reference ion, which is displayed with a full set of its tube and vector glyphs. All other ions are shown with a translucent tube in global colour scale if there is a collaboration and the glyphs are coloured using local colour scale.



(a) When ψ_1 (b) When ψ_2



(c) When ψ_3 (d) When $(\psi_1 + \psi_2 + \psi_3)/3$

Figure 6 : The possible cooperation between Na \#211 with other five ions, when probability was computed based on ψ_1, ψ_2, ψ_3 *and* $(\psi_1 + \psi_2 + \psi_3/3)$

In this section, we want to highlight a collaboration event which is one of the main objectives of the study. Regarding to previous discussion, we decided to take advantage of that method (Figure 5c) because it looks more distinguishable for human observer. Here, we show those methods again but rendered on six clusters of ions. Actually, each of the method has its own advantages, depending on the nature of the task. If the global timeline is to be perceived, the method 1 (Figure 5a) is more effective because the viewer can look into the global colour scale if there is any cooperation events within such a segment or between key colours. To perceive the local colour scale codeword, method 2 (Figure 5b) is most suitable since it shows all the series of local timeline and the viewer will be able to convert the codeword. In such cases, the method 3 (Figure 5c) is more reliable when the viewer wants to fast spot if there is any collaboration in ions. All the results are illustrated in Figure 6.

From these visualisations, did we gain more understanding of the collaboration phenomena than what has already been understood in physics? In general, we are intrigued by the following findings:

i. We have confirmed that simulation of ion trajectories has shown a high degree of collaborative activities. We have pinpointed the main trigger event, that is, ion collaboration are maintaining a reasonably constant gap between each other as in Figure 6c almost all trajectories are highlighted.
ii. We have also confirmed that the collaboration in orientation is largely coincidental (Figure 6a), while collaboration in velocity may also coincidental or at least influenced by the equispaced motion of different ions (Figure 6b)
iii. We have helped extend the original hypothesis that only more mobile sodium ions are in collaboration and the visualisation (Figure 6c) has clearly shown that less mobile oxygen are also in collaboration with sodium
iv. We have also observed that even ions involved in highly cooperative activity may

temporarily disengage with each other or become less cooperative as shown in Figure 6c

By combining some above-mentioned methods together, we provide an effective visual representation for visualising spatio-temporal collaboration application. With the help of global colour scale, the scientists can determine the global time frame of the events, for example, t=0 can be easily found between two consecutive colours. For more details, local colour scale will help determine which corresponding ions are in collaboration. These will give such an idea to our future work to enhance the capability in helping the scientists to determine the corresponding parties involved in collaboration issues.

CONCLUSION

We have developed an effective application with visual study scheme which have combined several schemes including iconic representation for orientation, colour scale for time series events and opacity scheme for collaborative events. Our main contribution included the introduction of novel method to convey a temporal issues and collaborative events in complex spatio-temporal datatsets. We now aim to thumb up the ability of our tools for high numerical spatio-temporal datasets to enable excitation of any large spatio-temporal datasets in real time environment.

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