Global and Local Color Time Scales to Encode Timeline Events in Ion Trajectories for Glassies

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Abstract: Glassy compounds lead directly to high ionic conductivity. Ionic conductivity generates ion trajectories. However, these trajectories have been represented by two-dimensional graph in order to visualize the timeline events in ion trajectories. This study addresses this problem by encoding the timeline events in ion trajectories with global and local color scales. Two time scales have been introduced namely Global Color Time Scale and Local Color Time Scale. The rainbow color has been chosen to represent global time scale meanwhile solid color has been used to generate local time scale. Based on evaluation, these techniques are successful in representing timeline events in ion trajectories for understanding the complicated heterogeneous movement of ion trajectories.

Keywords: glassy, ionic conductivity, color scale, coding theory, visualization.

1. Introduction

Formerly, the old-fashioned conventional batteries were made with liquid electrolytes, which have very high ionic conductivity. However, for safety and to improve on the stability of liquid electrolytes, the solid-state battery was developed. A solid-state battery is a battery that has solid electrodes and solid electrolytes. For the solid-state battery, ionic conductivity remained an issue for many years until glassies (glassy compounds) were found suitable for use as solid electrolytes, as well as higher in ionic conductivity [1, 2]. The reasons that glassies are preferred among other ionic conduction models because it is lighter, slower to drain, high power density and no leakage. Because of these advantages, glassies are now being used in many applications such as robotics, solar technologies, mobile phones and computer industries.

Materials are categorized in term of conductivity values such as conductors, semiconductors or dielectrics Electric current in conductors is either (insulators). electronic or ionic. Electronic conduction is found in metals, graphites, carbons, some oxides, inorganic compounds (tungsten, carbide) and some organic substances, whereas ionic conductivity is a form of electrical conductivity from ionic conduction. Glass is a material notable for ionic conductivity. It is a noncrystalline or amorphous solid material. A common fundamental constituent of glass is silica (silicon dioxide) with the chemical formula SiO₂. A mixture of glass and other compounds through chemical processes permits the movement of ions called ion dynamics that generates electrical conductivity, so that the movement of ions between anode and cathode generates electrical energy [3].

The movement of ions in glassies generates a path of ions where it is called ion trajectories. Ion trajectories represents one of the properties in ionic conductivity in glassies such as spatial structure, timeline and collaborative events. These properties have been represented by two-dimensional graph in order to understand the complicated heterogeneous movement of ions trajectories [4]. However, two-dimensional graph could not represent these properties in three- dimensional space even a data sets in three-dimensional coordinates.

Many techniques have been proposed in order to represent ion dynamics in glassies, ranging from chemical reactions to computer simulations. Funke and Banhatti [5] proposed a technique to represent ionic conductivity using chemical reactions. Meanwhile, Todorov et al. [6] used computer simulation to understand ionic conductivity and Habasaki and Hiwatari [3] represented ionic conductivity by two-dimensional graph.

Besides ionic conductivity, orientation of ion dynamics becomes an issue because it represents the movement of ions, including direction, magnitude and timeline of ion trajectories. Each position of an ion in three-dimensional coordinates has to be represented as a vector segment. Thus, each of the vector segments is used to represent ion trajectories including direction or orientation and velocity or magnitude. An iconic representation is proposed to represent the choreography of ion trajectories in order to represent each of the vector segments in ion trajectories. Though the main concern is to represent the time steps for each vector segment, unfortunately the shape of an icon only makes a trivial contribution in representing ion trajectories, such as position, magnitude and direction, while failing to address the representation of time series or timelines for each vector segment in ion trajectories.

This paper presents a technique to represent timeline events in ion trajectories. There are two types of techniques for global and local time scales. The global time scale for cylinder trajectories uses the Global Color Time Scale, while the local time scale for cone trajectories uses the Local Color Time Scale to distinguish each vector segment in the cone trajectories. To demonstrate the representation of timeline events, six clusters of ion trajectories have been chosen, three sodium ions and three oxygen ions. The following section elaborates in detail the representation techniques of timeline events in ion trajectories.

2. Global Color Time Scale

The Global Color Time Scale is the representation technique for the global time scale of ion trajectories. The cylinder has been used to represent the Global Color Time Scale and a color scale has been set up for this. A color scale is a sequence of numbers for observing attribute gradations that also presents numerical information [7, 8]. Several analytical tests have been conducted to discover which color scale is possible to depict a timeline event on a global time scale. Given that an ion trajectory is a series of n+1 points, a_0 , a_1 , a_2 , ..., a_n . There are n consecutive vector segments, $\overline{a}_1, \overline{a}_2, \Box, \overline{a}_n$, where $\overline{a}_i = (a_i - a_{i-1})$. Next, a few possible schemes have been presented prior to decide a suitable scheme for a global time scale.

2.1 Single Color



Fig 1. Single color coding for trajectory of sodium #169

The single color is a representation technique where each vector segment is represented by the same color. Any color from RGB is selected, such as c_1 and assigned to each vector segment as shown below:

$$\begin{array}{cccc} a_1 & a_2 & \Box & a_n \\ c_1 & c_1 & \Box & c_1 \end{array}$$

Where n is the total number of vectors. Fig 1 shows a red color scheme for ion trajectories. However, this scheme does not represent an actual global time scale of timeline events. There is another technique where a small set of colors has been represented on cylinders repeatedly.

2.2 Discrete Color Cycle



Fig 2. Discrete color cycle for trajectory of sodium #169

With the small set of colors, a discrete color cycle scheme has been proposed. This scheme originated from Shoup (1979) for enhancement of the real-time animation capability. Given a series of color, $c_1, c_2, ..., c_k$

(k > 1), a color is assigned to each to vector segments as follows:

$$\overline{a}_1 \quad \overline{a}_2 \quad \cdots \quad \overline{a}_k \quad \overline{a}_{k+1} \quad \overline{a}_{k+2} \quad \cdots \quad \overline{a}_n$$
$$c_1 \quad c_2 \quad \cdots \quad c_k \quad c_1 \quad c_2 \quad \cdots \quad c_w$$

where w can be determined arithmetically. Fig 2 shows an example using three colors as a circular pattern or cyclic color. However, it is hard to represent the timeline of events along the trajectory of a cylinder because the color is repeated. The following section, there is another version of color technique for representing the global time scale of ion trajectory, where the small set of colors have been represented as three-dimensional points instead of vector segments as usual.

2.3 Continuous Color Spectrum

The continuous color spectrum has been introduced to represent the global time scale of ion trajectories. Given a series of colors in RGB, c_1 , c_2 , ..., c_k (k > 1 and normally k < n), then a color is assigned to each point as follows:

$$a_1 \ a_2 \ \cdots \ a_{k-1} \ a_k \ a_{k+1} \ a_{k+2} \ \cdots \ a_n$$

 $c_1 \ c_2 \ \cdots \ c_{k-1} \ c_k \ c_{k+1} \ c_{k+2} \ \cdots \ c_w$

where *w* is determined arithmetically. A continuous visual effect has been drawn by each vector segment \overline{a}_i with linear interpolation between two consecutive colors associated with a_{i-1} and a_i . However, in this case, smooth interpolation is unnecessary and does not serve well the purpose of showing the timeline [9, 10]. The next section, the same scheme is used but implemented on the vectors not for the point itself.

2.4 Key Colors



Fig 3. Four key colors namely red, orange, yellow and green

This is a scheme where each vector segment has been shown in order to represent the global time scale on the trajectory of cylinder. A small set of colors is used, c_1 , c_2 , ..., c_k (k > 1), colors are assigned to a specific vector in the vector series as follows :

$$\overline{a}_1 \quad \overline{a}_u \quad \cdots \quad \overline{a}_v \quad \cdots \quad \overline{a}_n$$

 $c_1 \quad c_2 \quad \cdots \quad c_i \quad \cdots \quad c_k$

where indices such as u and v are pre-determined. For each vector that has not been assigned a color, obtained by interpolate the two nearest neighbors with specified key colors in each direction. This scheme allows a time frame to be determined at a global scale with the help of key colors, as shown in Fig 3.

Fig 3 shows an image with four colors from rainbow color to represent the global time scale of timeline events. There are four key colors that have been chosen, red, orange, yellow and green. These four key colors are used to represent the global time scale of timeline events in ion trajectory from t = 0 until t = 1000. Between the key colors, it represents the interval timeline or time frame from t = 0 until t = 334 using Eq. 1. Eq. 1 is generated

from the linear interpolation function in order to generate colors among two key colors. Given n as the total number of vectors, then to find the time frame T between the key colors k that satisfies

$$T \approx \frac{n}{k-1}; k > 1 \tag{1}$$



Fig 4. Various time frames

If n = 1000 then k = 2 so that the time frame between two key colors are $T \approx 1000$ meanwhile value of T = 500 if k = 3, $T \approx 333.33$ if k = 4, $T \approx 250$ if k = 5, $T \approx 200$ if k = 6 and $T \approx 166.66$ when k reaches 7. All the above correlations between key colors and series of time are depicted in Fig 4. Fig 4 presented the time frame of Global Color Time Scale between two key colors for each of key colors. By increasing the number of key colors, it shows that the time frame between two colors can be reduced.

Fig 5 shows existing color scales with 256 colors, but it is hard to distinguish between key colors [11]. Almost all color scales, as depicted in Fig 5 generate ambiguities in between key colors in the Global Color Time Scale compared to the small set of key colors. As a result, it is easy to distinguish temporal events at high level or global time scale using small set of colors from any color model, as long as color interpolation exists between these colors [12]. The following section elaborates results from Local Color Time Scale in order to represent local time scale for each vector segment in the ion trajectory.



Fig 5. Existing Color Scales

3 Local Color Time Scale

Local Color Time Scale is a technique to represent local time scale for each vector segment in ion trajectory. At the local level, Global Color Time Scale can make different vector segments indistinguishable [11]. Therefore, the best representation technique is to use solid color. According to Ware and Bobrow [12], the possible number of colors that can be used only twelve, includes white and black. Since the number of colors is smaller than a one thousand timeline, manipulation of colors needs to be done in order to represent one thousand timeline events in ion trajectories.

A Color Number Coding Scheme for the trajectory of cones has been introduced in order to achieve the technique to represent local time scale. Given a small set of key colors, c_1 , c_2 , ..., c_k where k > 1 and distinctive interval-colors (e.g., white, black or grey depending on the background color), a group of consecutive vectors m that coded as a k-nary number can be used, separated by interval vector in the interval-color. Given n as the total number of vectors, the smallest integer m is obtained from Eq. 2.

$$(m+1)k^m \ge n \tag{2}$$

Given m = 5 for k = 3, m = 4 for k = 4 and m = 2 kreaches 19. The selection of m and k needs to address the balance between a smaller number of colors or a smaller number of color digits in each group of vectors. Fig 6 shows a quaternary color coding scheme for ion trajectory with 1000 vectors when m = 4 and k = 4.



Fig 6. Quaternary Color Number Coding Scheme

The quaternary color coding scheme is used for the Local Color Time Scale. Based on the result shown in Fig 6, the Local Color Time Scale helps the viewer to distinguish each vector segment in timeline events of ion trajectories. The following section, the optimum setting for parameters m and k are discussed.

3.1 Optimum Setting for *m*'s

Eq. 2, when k = 2, the minimum value for parameter m is 7. For n = 1000, the value of parameter m is increased until it reaches 1000 which is the maximum number of vector segments. Fig 7 illustrates some experimental images with varying m. Fig 7(d) demonstrates that when the value of m reaches 43 or more, the accuracy of Local Color Time Scale is lost, because it does not have any meaning. The following section determines the optimum setting for k value.



Fig 7. Experimental images for satisfying *m* parameter

3. Optimum Setting for *k*'s

This experiment was performed to satisfy the value of parameter k. Eq. 2 shows k represented the total of key colors. Based on the results obtained in Fig 8, in order to achieve appropriate representation of the Local Color Time Scale, the value of k and m should be balanced and not too large. This study, the maximum values of k was 10 because this is the maximum number of colors for differentiating between each other [12]. Meanwhile, the value of *m* can be varied, but images rendered with small values of *m* are visually distinguishable, compared with images rendered with the high values of m. In precise word, the small number of m is easy to represent the consecutive vector segment m, compared to the big number of m. Finally, the selection of m and k needs to address a balance between a smaller number of color k or smaller number of *m* in each group of vectors.

The following section is an analysis of timeline events in ion trajectories, in order to prove the correlation between Global Color Time Scale and Local Color Time Scale.



Fig 8. Experimental images for satisfying k parameter

4. Analysis of Timeline Events

The Global Color Time Scale has been proposed to represent global time scale in ion trajectories. With the help of key colors, it is used to determine global time scale of the ion trajectories. The Local Color Time Scale is proposed in order to increase the accuracy of global color scale and as a result, it can represent t = 0, 1, 2 and so on at the local level. The benefits from the Local Color Time Scale can be used later in another analysis such as collaboration or cooperation events in ion trajectories. This particular task shows the benefit of the proposed representation techniques to determine a timeline event of ion trajectories.

Six clusters of ions have been used which consist three oxygen ions and three sodium ions. The details image of ions can be found in Appendix B. It also shows the timeline event of ion trajectories in any chaotic pattern of movement. Each cluster of ions is used as experimental data sets. Each ion represents a series of timeline events. This analysis has been conducted in order to prove the correlation between Global Color Time Scale and Local Color Time Scale.

Some experimental activities to analyze the image of ion trajectories need to be done in order to visualize correct representation between global and local time scales. See Appendix C for further explanation about experimental activities and it has been presented in flowchart. It starts by choosing the appropriate region between 1 and 6, as shown in Fig 10. After that, it uses a navigation function to move into specific target or area and get the code by extracting the color coded cone before converting the color coded cone into the corresponding time.



Fig 9. Global Color Time Scale between 2 to 7 Key Colors

Fig 9 shows the time frame T for each of key colors. It started with two key colors up to seven key colors where the number of time frames T is decreased from 1000 to 167, when the number of key colors is increased.

Fig 10 shows the detail between interpolation of rainbow colors where k = 7. Each of the key colors represent the region of time series where each region has t = 167, so there are six regions that were identified.



Fig 10. Region in Global Color Time Scale



Fig 11. First Region of Global Time Scale for Ion Na\#211

At the beginning, the experiments were done with ion Na#211 (details in Appendix B). There are six regions for ion Na#211 (details in Appendix D) where the first region as shown in Fig 11, which is between red and orange may represent the initial position or beginning of the ion trajectory. Therefore, the global time scale is between t = 0 and t = 167. After that, by navigated towards the region, the local time scale has appeared. At last, with the help of the Local Color Time Scale, the local time scale can be identified.



Fig 12. Zoom-in effects of Ion Na#211 for the first, second and third region

Fig 12 shows the zoom-in effects for the first, second and third regions in ion Na#211. The leftmost images represent the every regions of the global time scale. Every region has been analyzed until the Local Color Time Scale appeared in the rightmost of the images.





Fig 13. First region of the right most images from Fig 12

Let starts with the 1st region and look into the rightmost of the images. After some steps are taken as mentioned in the previous paragraph, the final image of the 1st region is illustrated in Fig 13. It shows the Local Color Time Scale with a few combinations of colors such as green, green, red and red. Since quaternary color scheme has been chosen then the calculation to find t is as follows.

red = 0, vellow = 1, green = 2, blue = 3k is the number of colour to be used if m = 4, c_0, c_1, c_2, \Box , $c_{k,p}$, separator then $T_{t+0}, T_{t+1}, T_{t+i}, T_{t+i}$ based on the above image green, green, red, red, black (separator) so, the code is 2200 (two-two-zero-zero) equivalent to (green-green-red-red) To convert the code, $T = (4^{0} * 2) + (4^{1} * 2) + (4^{2} * 0) + (4^{3} * 0)$ T = 2 + 8T = 10 $t = (m+1)^* T \Longrightarrow From Eq. 2$ t = (4+1)*10t = 50 $T_{t+0}, T_{t+1}, T_{t+i}, T_{t+i(k-1)}$ T_{50} , T_{51} , T_{52} , T_{53}

This shows that the result of local time scale is located in the first region of the global time scale. The following paragraph, the 2nd region of global time scale has been chosen in order to prove the correlation between the global and local time scales.

Next, the second region of the global time scale has been chosen, as shown in Fig 14. Here are the steps taken to find t.

Fig 14. Second region of the right most images from Fig 12

red = 0, yellow = 1, green = 2, blue = 3k is the number of colour to be used if m = 4. c_0, c_p, c_2, \Box , c_{k-p} separator then $T_{t+0}, T_{t+1}, T_{t+i}, T_{t+0}$ based on the above image vellow, green, green, red, black (separator) so, the code is 1220 (one-two-two-zero) To convert the code. $T = (4^{0} * 1) + (4^{1} * 2) + (4^{2} * 2) + (4^{3} * 0)$ T = 1 + 8 + 32T = 41 $t = (m+1)^* T \Longrightarrow From Eq. 2$ t = (4+1)*41t = 205 $T_{t+0}, T_{t+1}, T_{t+i}, T_{t+0-1}$ $T_{205}, T_{206}, T_{207}, T_{208}$

It shows that the result of local time scale is located in the second region of global time scale. Next, the third region of global time scale has been chosen in order to prove the correlation between global and local time scale.



Fig 15. Third region of the right most images from Fig 12

Fig 15 shows the third region of global time scale. Here are the steps taken to find t. red = 0, vellow = 1, green = 2, blue = 3k is the number of colour to be used if m = 4. c_0, c_p, c_2, \Box , c_{kp} , separator then $T_{t+0}, T_{t+1}, T_{t+1}, T_{t+0}$ based on the above image green, green, red, yellow, black (separator) so, the code is 2201 (two-two-zero-one) To convert the code, $T = (4^{0} * 2) + (4^{1} * 2) + (4^{2} * 0) + (4^{3} * 1)$ T = 2 + 8 + 0 + 64T = 74 $t = (m+1)^* T \Longrightarrow from Eq. 2$ t = 370 $T_{t+0}, T_{t+1}, T_{t+i}, T_{t+i}$ T370, T371, T372, T373

This shows that the result of the local time scale is located in the second region of global time scale. Based on the result shown in the first, second and third regions of the global time scale, the Global Color Time Scale and Local Color Time Scale have been proven in order to represent the correct correlation between global and local time scales. The zoom-in images of six regions of global time scale for six clusters of ion trajectories can be found details in Appendix D to Appendix I.

5. Discussion

The beginning of this chapter, the highlight was on the technique for the representation of temporal information in ion trajectories. The proposed techniques, there are two schemes, the Global Color Time Scale and the Local Color Time Scale. The chapter started by represented the global time scale with Global Color Time Scale where each of ion trajectories was visualized globally or at a high level of visualization. Seven key colors were used in order to represent the global time scale of ion trajectories. A linear interpolation function was used in order to generate interval color between key color. The seven key colors come from rainbow colors, where each key color has interpolated colors existed between them. This technique, only selected colors for which an interpolation existed in the color model can be used to generate interpolation between key colors [12]. Finally, the rainbow color is the solution to represent the global time scales in ion trajectories, because the interpolation properties and the number of colors is neither too big nor too small.

The Local Color Time Scale was proposed to enhance the distinguishability of the global time scale so that each vector can be distinct. Moreover, with the small sets of colors, a Local Color Time Scale was initiated, the so-called Color Number Coding Scheme. The elaboration of the techniques can be found in Section 3. These techniques, parameters m and k were tested to verify a suitable value to represent the local time scales of ion trajectories. As a result, the small numbers of k and m are found sufficient to represent thousand of ions in one trajectory. An experiment was undertaken to verify the value of m and k.

Section 4 shows the composite rendering of global and local time scales in order to prove the correct correlation between Global Color Time Scale and Local Color Time Scale. The previous techniques, Habasaki and Hiwatari [4] used a graph to represent the heterogeneous movements of ion trajectory from 2D data sets. However the proposed techniques were initiated to represent the movements of ion trajectory in 3D data sets. Six regions of global time scale were proposed where each of regions can represent 167t and one example of representation of Local Color Time Scale for the 1st region of ion trajectory was illustrated in Fig 13.

Appendix D to Appendix I were presented in details the zoom-in images of global time scale that have been performed on six clusters of ion trajectories. The next chapter demonstrates with a collection of visual examples that this scheme does not only identify the timeline events of such movements but can also confirm the presence of collaborative phenomena in ion dynamics.

6. Conclusion

This paper described about techniques to represent timeline events of ion trajectories. There are two color scales such as global and local color scales. Both color scales have been used to represent global and local time of ion trajectories. The result has shown these techniques have been succeeded based-on representation of the timeline events in global and local time scales. Each technique has been evaluated with previous techniques in order to represent timeline events in ion trajectories. The future work highlights the techniques for representing collaborative events in ion trajectories.

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Appendix A

Dataset

0	-2.000000	9.967	0.606	8.749
0	-2.000000	9.966	0.675	8.720
0	-2.000000	9.977	0.722	8.721
0	-2.000000	10.036	0.745	8.747
0	-2.000000	10.131	0.746	8.779
0	-2.000000	10.210	0.731	8.800
0	-2.000000	10.224	0.724	8.809
0	-2.000000	10.188	0.738	8.817
0	-2.000000	10.153	0.745	8.835
0	-2.000000	10.144	0.717	8.856
0	-2.000000	10.153	0.659	8.858
0	-2.000000	10.157	0.612	8.825
0	-2.000000	10.147	0.606	8.767
0	-2.000000	10.131	0.631	8.707
0	-2.000000	10.114	0.661	8.672
0	-2.000000	10.086	0.684	8.671
0	-2.000000	10.043	0.700	8.697
0	-2.000000	9.997	0.704	8.727

Appendix B

Six clusters of ion trajectories



(a) Na#211





(c) Na#106



(c) O#517



(d) O#928

Appendix C

Experimental Activities Flowchart



Appendix D

TIMELINE EVENT ANALYSIS FOR ION NA#211



Showing six regions of Global Time Scale for Ion Na#211



Zooming of Ion Na#211 for every region. From left to right, images indicated a zooming action taken for every single region until the viewer can see the color number coding for particular targeted portion.

Appendix E

TIMELINE EVENT ANALYSIS FOR ION NA#169



Showing six regions of Global Time Scale for Ion Na#169



169

Zooming of Ion Na#169 for every region. From left to right, images indicated a zooming action taken for every single region until the viewer can see the color number coding for particular targeted portion.

Appendix F



Showing six regions of Global Time Scale for Ion Na#106



106

Zooming of Ion Na#106 for every region. From left to right, images indicated a zooming action taken for every single region until the viewer can see the color number coding for particular targeted portion.

Appendix G



Showing six regions of Global Time Scale for Ion O#699



Zooming of Ion O#699 for every region. From left to right, images indicated a zooming action taken for every single region until the viewer can see the color number coding for particular targeted portion.

Appendix H



0t ≤ Time Frame ≤ 167t Red ≤ location ≤Orange



 $501t \le Time Frame \le 668t$ Green $\le location \le Cyan$



 $167t \le Time Frame \le 334t$ Orange $\le location \le Yellow$



688t ≤ Time Frame ≤ 835t Cyan ≤ location ≤ Blue



334t ≤ Time Frame ≤ 501t Yellow ≤ location ≤Green



 $\begin{array}{l} 835t \leq \text{Time Frame} \leq 1002t\\ \text{Blue} \leq \text{location} \leq \text{Indigo} \end{array}$



Showing six regions of Global Time Scale for Ion O#517



Zooming of Ion O#517 for every region. From left to right, images indicated a zooming action taken for every single region until the viewer can see the color number coding for particular targeted portion.

Appendix I



Showing six regions of Global Time Scale for Ion O#928



Zooming of Ion O#169 for every region. From left to right, images indicated a zooming action taken for every single region until the viewer can see the color number coding for particular targeted portion.