Colour Number Coding Scheme for Time-Varying Visualisation in Glassy Ion Trajectories

J. M. Sharif*†, M. S. A. Latiff† and M. A. Ngadi†
*Department of Computer Science, Swansea University, SA2 8PP, United Kingdom
†Department of Computer System & Communication, University Technology of Malaysia, 81310, Johor, Malaysia
Email: johan@fsksm.utm.my, shafie@fsksm.utm.my, asri@fsksm.utm.my
Telephone: (+607) 5532384, Fax: (+607) 5565044

***Abstract*— In physics, ion trajectories has totally relied on statistical analysis from experimental and computer simulation results[23][15][33][20][10]. 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 concept, 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. 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, colour scale, visualisation, time-varying data, spatio-temporal visualisation, molecular dynamics, scientific data, hybrid scheme, visual representation

I. Introduction

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 [3], fault tolerant or fault diagnosis/monitoring [26], analysis model [21], developing framework [24] and communication system [5]. Some of the effort combined with another field of research such as complexity theory [31], system theory [27] and test pattern generators [32]. Some researchers borrowed a technique from coding theory concept to solve some research problem such as in testing problems [2], cryptography [30], optical flow [14], adaptive radar [12], algorithm [38] and neural network [37].

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 [16] but differently with Ishikawa, he used to improving the communication performance in hypercube multiprocessor with bus connection through coding theory concept [13]. 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 [6]. For Rains, they improved the codes by determine the bound through finding the minimum distance of the codes using the length [25].

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 works for solving the problem in some research area with the help of coding theory concept such as in data security [30], optical flow [14], communication channel [12] and neural network [37]. 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 attention has been given in literature on timeline encoding especially in codes.

Location codes is a labelling technique that represented tetrahedral elements within a mesh. Lee et al. [17] used this technique for labelling triangular faces. There are also a few authors used this idea for their works such as Evans et al. [4] who use an array where the label of a node determines the node location in the array. Thus, Zhou et al. [39] 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 [8] for extracting isosurfaces at different levels of details. Location code also has been used in spatio-temporal database research for labeling purpose as well [34]. Since then, there is another labeling scheme has been introduce like LPT code [1]. It was extension from the location code itself. The origin idea for labeling codes has comes from Gargantini [7]. 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 [18] 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

[22]. 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. [19]. There is few more codes had been introduce in image representation such as sarkar's code [28] [29], logicodes [36], restricted logicodes [36] and symbolic codes [11]. 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.

The paper is organized as follows. Firsts, we discuss existing and relevant codes which is available in time-varying visualisation. In Section 3, we divided the explanation into two concrete situations. We highlight the issue of timeline events which is before collaboration takes place and after collaboration which is called collaborative events. In the first 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. We elaborate the issues of collaborative events in the following subsection. Finally, in section 4 we concluded our study.

II. Visualising Ion Trajectories

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 colour scale and code 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. Temporal Encoding

When using visualisation to summarise 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 determine the time of an event but also for the identification corresponding parties involved in collaborative, but collaborative events is not included at moment.

We divided our temporal encoding scheme into two major part. The purpose of global colour scale is to allow the viewer to determine a time frame at global scale and the purpose of local colour scale is to enhance the accuracy our scheme in order to differentiating a different vector segments.

In the next section, we would like to shows our implementation of local colour scale in depicting a series of timeline in ion trajectory.

1) 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;

$$((m + 1)k^m) \geq n \quad (1)$$

Figure 1 shows a quaternary colour coding scheme for ion tracks with 1000 vectors.

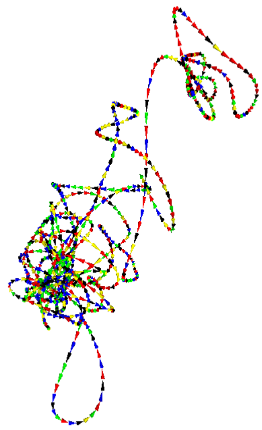


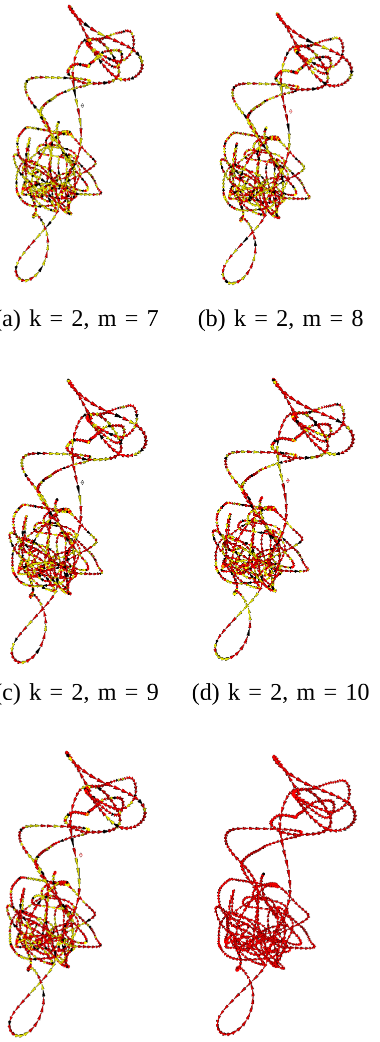
Fig. 1. Quaternary Colour Coding Scheme on trajectory of sodium #169

2) Results: In this section, as an example, we present a visual study of ion trajectory. In our case, quaternary colour coding scheme is considerable suit to represent the time series in ion trajectories. Here, we shows the results in relation to determine the best value for the parameter m and k based on equation 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 determine the temporal position of each vector.

3) Remarks: In this section, we consider the selection of m and k will dealing with our local colour scale. According to Equation 1, we will shows all possibility of parameter m and k have been applied on ion #169 trajectory. Our targeting goal from this method is to improve the correlation of each vector segment with the timeline more accurately and hence totally enhanced the differentiation of different vector segments. We introduced a *Colour Number Coding Scheme* in our visualisation.

Again based on 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 m reaches 1000 which is the

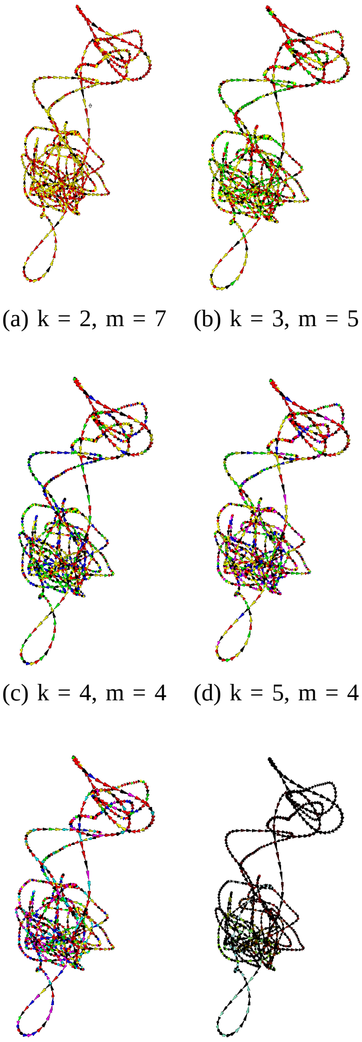


(a) k = 2, m = 7 (b) k = 2, m = 8

(c) k = 2, m = 9 (d) k = 2, m = 10

(c) k = 2, m = 11 (d) k = 2, m = 1000

Fig. 2. Experimental images for satisfying m parameter



(a) k = 2, m = 7 (b) k = 3, m = 5

(c) k = 4, m = 4 (d) k = 5, m = 4

(c) k = 6, m = 4 (d) k = 256, m = 2

Fig. 3. Experimental images for satisfying k parameter

maximum number of vector segment. This comparison task will illustrated in Figure 2. This figure show to us that when we increase the value of m until $m = 1000$, its loss the accuracy of local scale timeline because its does not give any meaning to the viewers.

Our next experiment is to satisfied the value of parameter k. 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 Figure 3, those images rendered with small value of k are visually distinguishable than the images rendered with the high value of k.

It is clear that as the k or m are increase 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 1.

B. *Collaborative events*

The main objectives 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 collaborative events, although experiments suggested the existence of collaborative phenomena [9]. Therefore we have introduced a variable, ψ, representing the probability of collaborative. Given a set of m hypothesized criteria of collaborative, 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 two such criteria, namely (1) the ability for two or more ions to maintain similar orientation and (2) the ability for two or more ions to maintain similar velocity.

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 collaborative. With $\psi_1, v_{a,i}$ and $v_{b,i}$ are considered to be in collaborative, 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:

$$\psi_2 = \left(1 - \frac{abs(|v_{a,i}| - |v_{b,i}|)}{|v_{a,i}| + |v_{b,i}|} \right)^{D_2} \tag{4}$$

where D_2 is similar to D_1 for ψ_1. With $\psi_2, v_{a,i}$ and $v_{b,i}$ are considered to be in collaboration, if they are of a similar length. Once we have computed all those $\psi \in [0, 1]$, we can highlight or de-highlight the corresponding vector segments as shown in Figure 4.

1) Results: In this section, we shows the visual study of a cluster of six ions, including three sodium and three oxygen ions. Before visualisation, we make no assumption which ion may collaborate with each others in its motion. For each ions, we compute its probability of collaborative with each of the other ions in the cluster. We evaluate based on ψ_1 and ψ_2 as stated above.

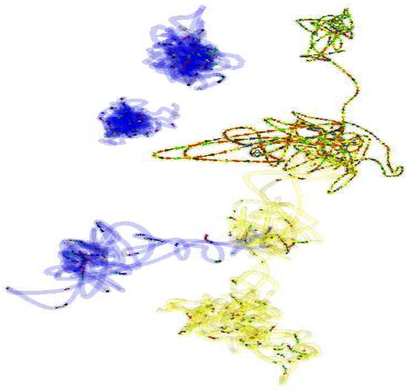
Below we present a small set of visualisation generated in the visual study. This image was computed using Na #211 as the reference ion, which displayed with a full set of its vector glyph. All other sodium ions are shown with a translucent tube in a warm colour, namely yellow or pink, while each oxygen trajectory is enclosed in a translucent tube in a cool colour. The glyphs are coloured using the quaternary colour number coding as in Figure 1.

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

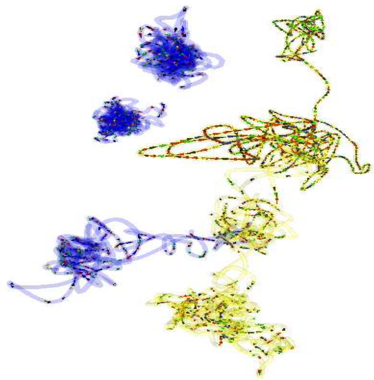
1) We have also confirmed that the collaboration in orientation is largely coincidental (Figure 4(a)).
2) While collaboration in velocity may also coincidental or at least influenced by the equispaced motion of different ions (Figure 4(b)).

III. Conclusion

We have developed an effective visual representation, which have combined benefits from several schemes, including the use of glyphs for conveying orientation and velocity and opacity for highlighting and de-highlighting appropriate events. Our main contribution have included the introduction of colour number coding scheme, which conveys temporal information in high degree of certainty and the effective deployment of visualisation in mining complex spatio-temporal data sets.



(a) When ψ_1.



(b) When ψ_2.

Fig. 4. The possible collaborative between Na #211 with other five ions, when probability was computed based on ψ_1 and ψ_2

From the above works, we can say that applying coding theory in ion trajectories can indicate some important activities in relation to the timeline event such as trigger collaborative events. This would help us to explore the insight of the chaotic movement of ion trajectories. In future, we would help to examine the spatio-temporal collaborative among ions and to identify possible collaborative behaviours and their spatial and temporal association among the complex and seemingly chaotic atom movements, we have made a few new discoveries, which will hopefully enhance our understanding of ion trajectories.

References

[1] F. Betul Atalay and David M. Mount. Pointerless implementation of hierarchical simplicial meshes and efficient neighbor finding in arbitrary dimensions. 2004.

[2] T. Berger and V. I. Levenshtein. Asymptotic efficiency of two-stage disjunctive testing. *IEEE Transactions on Information Theory*, 48(7):1741 – 1749, Jul 2002.

[3] D. J. Costello, J. Hagwnauer, H. Imai, and S. B. Wicker. Application of error-contol coding. *IEEE Transactions on Information Theory*, 44(6):2531–2560, Oct 2004.

[4] W. Evans, D. Kirkpatrick, and G. Townsend. Right-triangulated irregular networks. *Algorithmica*, 30(2):264–286, Mar 2001.

[5] A. Fujiwara and H. Nagaoka. Operational capacity and pseudoclassicality of quantum channel. *IEEE Transactions on Information Theory*, 44(3):1071 – 1086, May 1998.

[6] A. Garcia and H. Stichtenoth. algebraic function fields over finite fields with many rational places. *IEEE Transactions on Information Theory*, 41(6):1548 – 1563, Nov 1995.

[7] I. Gargantini. An effective way to represent quadtrees. *Communications of the ACM*, 25(12):905–910, Dec 1982.

[8] T. Gerstner and M. Rumpf. Multiresolutional parallel isosurface extraction based on tetrahedral bisection. *In Proceedings 1999 Symposium on Volume Visualization, ACM Press*, 1999.

[9] J. Habasaki and Y. Hiwatari. Fast and slow dynamics in single and mixed alkali silicate glasses. *Journal of Non-Crystalline 320*, 1-3:281–290, 2002.

[10] J. Habasaki, K.L. Ngai, and Y. Hiwatari. Time series analysis of ion dynamics in glassy ionic conductors obtained by a molecular dynamics simulation. *The Journal of Chemical Physics 122*, Feb 2005.

[11] D. J. Hebert. Symbolic local refinement of tetrahedral grids. *Journal of Symbolic Computation*, 17(5):457–472, May 1994.

[12] S. D. Howard and A. R. Calderbank. relationships between radar ambiguity and coding theory. In *IEEE International Conference on Acoustics, Speech, and Signal Processing, 2005. Proceedings. (ICASSP '05).*, pages 355 – 362. IEEE, 18-23 March 2005.

[13] T. Ishikawa. Hypercube multiprocessors with bus connections for improving communication performance. *IEEE Transactions on Computers*, 44(11):1338 – 1344, Nov 1995.

[14] M.A. Jabri, Ki-Young Park, Soo-Young Lee, and T.J. Sejnowski. properties of independent components of self-motion optical flow. In *30th IEEE International Symposium on Multiple-Valued Logic, 2000. (ISMVL 2000) Proceedings.*, pages 355 – 362. IEEE, 23-25 May 2000.

[15] P. Jund, W. Kob, and R. Jullien. Channel diffusion of sodium in a silicate glass. *Physics Review B*, 64, 2001.

[16] J. C. Kieffer. Sample converses in source coding theory. *IEEE Transactions on Information Theory*, 37(2):263 – 268, Mar 1991.

[17] M. Lee, L. De Floriani, and H. Samet. Constant-time neighbour finding in hierarchical tetrahedral meshes. *Proceedings of the Shape Modeling International 2001 (SMI'01)*, pages 286–295, 2001.

[18] S.-X. Li and M. H. Loew. Adjacency detection using quadcodes. *Communications of the ACM*, 30(7):627–631, Jul 1987.

[19] S.-H. Lin, P.-H. Wu, R.-P. Tzeng, and C.-Y. Huang. An efficient ,ethod for obtaining the level of the bincode. *CVGIP:Graphical Models and Image Processing*, pages 773–777, 2003.

[20] A. Meyer, J. Horbach, W. Kob, F. Kargl, and H. Schober. Channel formation and intermediate range order in sodium silicate melts and glasses. *Journal of Physics : Condensed Matter 1*, 2004.

[21] O. Milenkovic. Analysis of bin model with applications in coding theory. In *International Symposium on Information Theory, 2004. ISIT 2004.*, page 224. IEEE, Jun 27 - Jul 2 2004.

[22] M. A Ouksel and A. Yaagoub. The interpolation-based bintree and encoding of binary images. *CVGIP:Graphical Models and Image Processing*, 54(1):75–81, 1992.

[23] J. Oviedo and J. F. Sanz. Molecular dynamics simulation of $(na_2o)_x(sio_2)_{1-x}$ glasses relation between distribution and diffusive behaviour of na atoms. *Physics Review B*, 58:9047, 1998.

[24] D.K. Pradhan. Logic transformation and coding theory-based frameworks for boolean satisfiability. In *Eighth IEEE International High-Level Design Validation and Test Workshop, 2003.*, pages 57 – 62. IEEE, 2003.

[25] E. M. Rains. shadow bounds for self-dual codes. *IEEE Transactions on Information Theory*, 44(1):134 – 139, Jan 1998.

[26] H. Ren, Z. Mi, J. Diao, and H. Zhao. A novel power system fdi scheme based on petri nets and coding theory. In *2004 International Conference on Power System Technology - POWERCON 2004*, pages 108 –113. IEEE, Nov 2004.

[27] J. Rosenthal. Some interesting problems in systems theory which are of fundamental importance in coding theory. In *Proceedings of the 36th IEEE Conference on Decision and Control*, pages 4574 – 4579 vol.5. IEEE, 10-12 Dec 1997.

[28] D. Sarkar. Boolean function-based approach for encoding of binary images. *Pattern Recognit. Lett.*, 17(8):839–848, 1996.

[29] D. Sarkar. Operation on binary images encoded as minimized boolean functions. *Pattern Recognit. Lett.*, 18:455–463, 1997.

[30] Silverberg, J. Staddon, and J. L. Walker. Applications of list decoding to tracing traitors. *IEEE Transactions on Information Theory*, 49(5), May 2003.

[31] D. A. Spielman. models of computation in coding theory. In *Thirteenth Annual IEEE Conference on Computational Complexity,*, page 120. IEEE, 15-18 June 1998.

[32] R. Srinivasan, S. K. Gupta, and M. A. Breuer. Novel test pattern generators for pseudoexhaustive testing. *IEEE Transactions on Computers*, 49(11):1228 – 1240, Nov 2000.

[33] E. Sunyer, P. Jund, W. Kob, and R. Jullien. Molecular dynamics study of the diffusion of sodium in amorphous silica. *Journal of Non-Crystalline*, 939:307–310, 2002.

[34] T. Tzouramanis, M. Vassilakopoulos, and Y. Manolopoulos. Multiversion linear quadtree for spatio-temporal data. *ADBIS: East European Symposium on Advances in Databases and Information Systems*, pages 279–292, 2001.

[35] A. Vardy. the intractability of computing the minimum distance of the code. *IEEE Transactions on Information Theory*, 43(6):1757 – 1766, Nov 1997.

[36] J.-G. Wu and K.-L. Chung. A new binary image representation : Logicodes. *Journal of Visual Communication and Image Representation*, 8(3):291–298, Sept 1997.

[37] L. Ying. Fractals, neural networks, cellular automata, formal language and coding theory. In *IEEE International Conference on Systems, Man and Cybernetics*, pages 1663 – 1669 vol.2. 1992, 18-21 Oct. 1992.

[38] J.-H. Youn and B. Bose. A topology-independent transmission scheduling in multihop packet radio networks. *Global Telecommunications Conference, 2001. GLOBECOM '01. IEEE*, 3:1918 – 1922, Nov 2001.

[39] Y. Zhou, B. Chen, and A. Kaufman. Multiresolution tetrahedral framework for visualizing regularvolume data. In *Proceedings of Conference on Computer Graphics(VISUALIZATION 97)*, pages 135–142. IEEE, Oct 1997.