Development of A Novel Method For 3D Scientific Datasets in Ion Dynamics

J.M. Sharif [1,2], M.S.A. Latiff [2] and M.A. Ngadi [2]

[1] Swansea University, School of Physical Science, Department of Computer Science, UK

[2] University Technology of Malaysia, Faculty of Computer Science & Information System, Department of Computer System & Communication, Malaysia

Abstract

In physics, structure of glass and ion dynamics are essentially based on statistical analysis of data acquired through experimental measurement and computer simulation [1, 2]. Invariably, the details of the structure-transport relationships in the data have been mistreated in favor of ensemble average [3, 4]. In this study, we demonstrate a visual approach of such relationship using surface-based visualisation schemes. In particular, we demonstrate a scientific datasets of simulated 3D time-varying model and examine the temporal correlation among ion dynamics. We propose a scheme that uses a three dimensional visual representation with colour scale for depicting the timeline events in ion dynamics and this scheme could be divided into two major part such as global and local time scale. With a collection of visual examples from this study, we demonstrate that this scheme may offer an effective tool for visually mining 3D timeline events of the ion dynamics. This work will potentially form a basis of a novel analysis tool for measuring the effectiveness of visual representation to assist physicist in identifying

possible temporal association among complex and chaotic atom movements in ion dynamics.

1.0 Spatio-Temporal Datasets

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, $F : E^d \, x \, T \rightarrow R^n$, where E^d denotes d-dimensional Euclidean space, $T = R^* \cap \{\infty\}$ the domain of time and 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.

2.0 Timeline Colour Scale

In colour science, colour scale is a series of ordered numbers which represents observable gradations of an attribute or combination of attributes of colour perception. Mostly in colour scale, visualisation is commonly used to represent a numerical information.

Normally, a sequence of N distinct numerical values v0, v1,…,vN can be respectively represented by the colours c0, c1,…,cN, which can comprise as steps of an attribute.

In data visualisation, commonly they used to convey a wide variety of information. Generally, every scientific visualisation need a colour to enhance the ability to analysis, evaluate, assess and examine the large datasets. In time-varying visualisation, colour also become popular lately to achieve their objective. Rheingans[5] introduced such a colour scale which can be useful for univariate, bivariate or multivariate data. Colour scales also has been used extensively in many applications, including automotive, medical, topography and fluid mechanics. In perceptual point of view, Healey and Enns[6] presents perceptual colour scale algorithm based on variety of colour model such as Munsell, CIELUV and RGB or CIEXYZ.

Some researcher use a colour scale for visual representation purpose. Chuah and Eick[7] used a rainbow colour to encode the attributes of object in circle shape for managing a large software project. While, Gall et. al.[8] were modified rainbow scale to 21 colour scale that uses in 2D and 3D graphs. However, Vos and Spoelder[9] were decided rainbow colour scale would lead to misinterpretation or distinguished in visualising corneal shape. We would like to introduce our scheme that uses rainbow colour scale as a core idea but we manipulate in different way for visualising of timeline events in ion dynamics. Our method consists two time scale which is global and local colour time scale as shown in Figure 1.

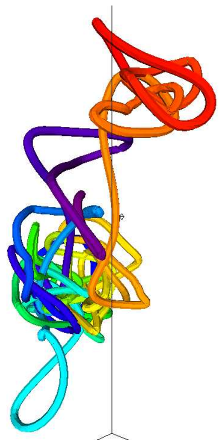


Figure 1a

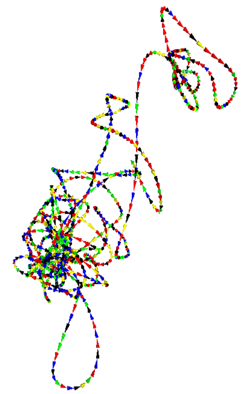
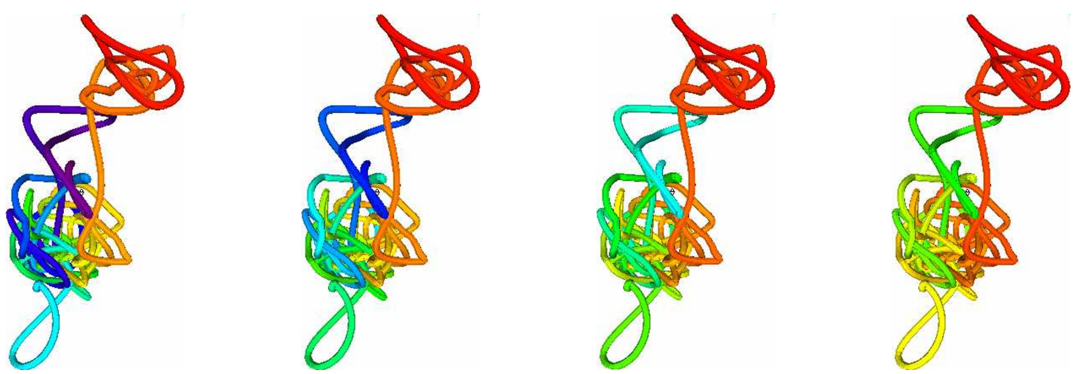


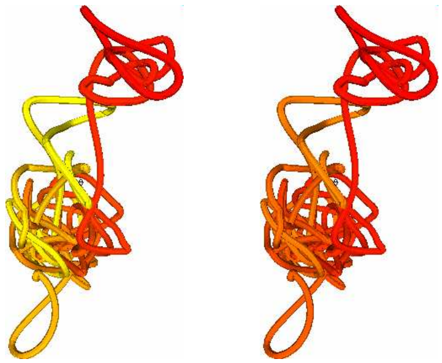
Figure 1b

Figure: (1a) *Global Colour Time Scale,* ***(1b)*** *Local Colour Time Scale*

3.0 Global Colour Time Scale : Key Colours



(a) (b) (c) (d)



(f) (g)

Figure: (2) shows the images of key colours scheme which is implemented on ion trajectories. In (2a), its shown seven key colours can represent ≈166 ions or time series event between two consecutive colours. In (2b), six key colours(200), (2c) five key colours(250), (2d) four key colours(333), (2e) three key colours(500) and (2f) two key colours(1000).

In this experiment we shown trajectory of sodium #169. These trajectory rendered with seven to two keys colour based on rainbow colour scale. Each of images represent how many time frame can be presented with the help of the key colours. In next part, we aim to show more accurately and hence to improve the differentiation of different vector segments that is why we introduce local colour time scale that we called colour number coding scheme

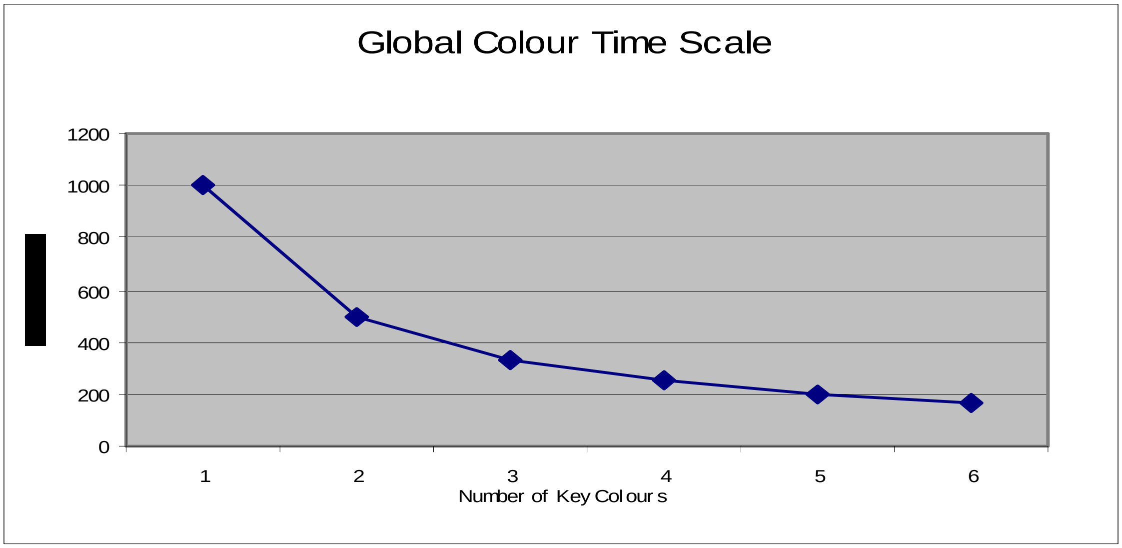


Figure: 3 Shows a number of ions that can be highlighted with Global Colour Time Scale. We understand more key colours will help to differentiate a vector segments in ion trajectory but unfortunately its hard to distinguish because interpolation between colour can make different vector segment indistinguishable.

4.0 Local Colour Time Scale – Colour Number Coding Scheme

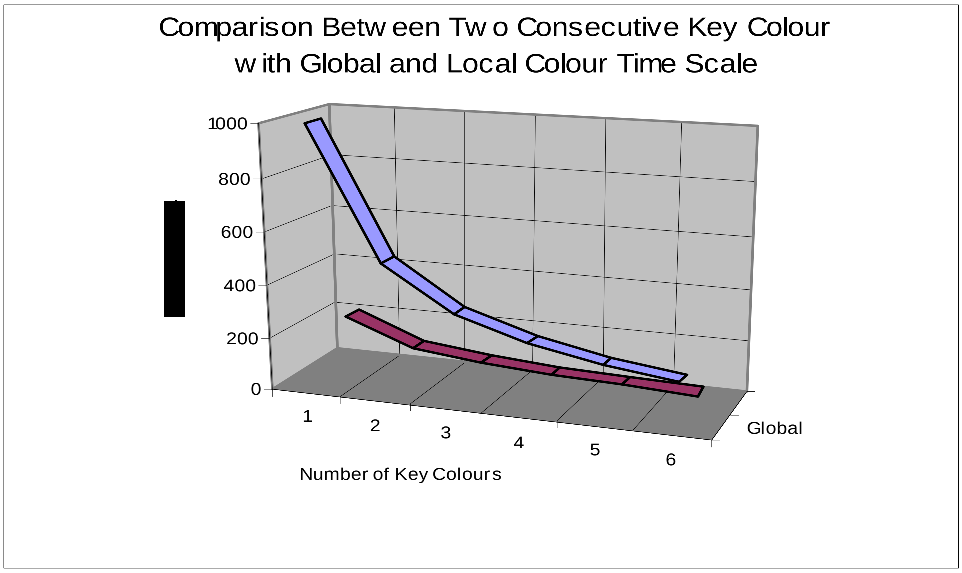


Figure: 4, comparison has been made between Global Colour Time Scale and Local Colour Time Scale. In Local Colour Time Scale, we combine hue and codeword to provide more accurately distinguishable display levels than interpolation. By doing this we hope a viewer especially physicists would be able to interpret the ion trajectory into the meaningful activities based on timeline events such as collaborative events.

Figure: 3 Shows a number of ions that can be highlighted with Global Colour Time Scale. We understand more key colours will help to differentiate a vector segments in ion trajectory but unfortunately its hard to distinguish because interpolation between colour can make different vector segment indistinguishable. In Figure 4, comparison has been made between Global and Local Colour Time Scale. In Local Colour Time Scale, we combine hue and codeword to provide more accurately distinguishable display levels than interpolation. By doing this we hope a viewer especially physicists would be able to interpret the ion trajectory into the meaningful activities based on timeline events such as collaborative events.

5.0 Remarks and Conclusion

The results show that our key colours scheme can be used to allow viewer to determine a time frame at global scale with the help of those key colours. In this study also we have shown that the colour number coding scheme can be used to visualise a time frame at low level of ion trajectory. 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 may enable us to form the basis of visually mining tools for time-varying visualisation.

6.0 Future Aims

We now aimed to enhanced our tools by the use of high numerical spatial-temporal datasets to enable excitation of any large spatio-temporal datasets. This will allow the visualisation of timeline events with collaborative events in real time environment.

References

1. Funke, K., *Jump Relaxation in Solid Electrolytes.* Progr. Solid State Chem, 1993. **22**: p. 111-195.
2. Smith, W., G.N. Greaves, and M.J. Gillan, *Computer Simulation of Sodium Disilicate Glass.* Journal Chemical Physics, 1995. **103**.
3. Greaves, G.N. and K.L. Ngai, *Reconciling ionic-transport properties with atomic structure in oxide glasses.* Phys. Rev. B 52, 1995.
4. Ngai, K.L., Y. Wang, and C.T. Moynihan, *The Mixed alkali effect revisited : importance of ion interactions.* Journal of Non-Crystalline, 2002. **307-310**: p. 999-1011.
5. Rheingans, P. *Task-based Color Scale Design*. in *Proceedings of Applied Image and Pattern Recognition '99*. 1999.

6. Healey, C.G., *Building a perceptual visualization architecture.* Behaviour and Information Technology 2000. **19**(1): p. 349-366.

7. Chuah, M.C. and S.G. Eick, *Managing Software with New Representations.* Proceedings IEEE Symposium on Information Visualization, 1997: p. 30-37,118.

8. Gall, H., M. Jazayeri, and C. Riva, *Visualizing Software Release Histories:The Use of Color And Third Dimension.* 15th IEEE International Conference on Software Maintenance (ICSM'99) 1999: p. 99.

9. Vos, F.M. and H.J.W. Spoelder, *Visualization In Corneal Topography*. Proceedings of IEEE Conference on Visualization, 1998: p. 427-430,559.