

Visual Interrogation of Gyrokinetic Particle Simulations

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Abstract. Gyrokinetic particle simulations are critical to the study of anomalous energy transport associated with plasma microturbulence in magnetic confinement fusion experiments. The simulations are conducted on massively parallel computers and produce large quantities of particles, variables, and time steps, thus presenting a formidable challenge to data analysis tasks. We present two new visualization techniques for scientists to improve their understanding of the time-varying, multivariate particle data. One technique allows scientists to examine correlations in multivariate particle data with tightly coupled views of the data in both physical space and variable space, and to visually identify and track features of interest. The second technique, built into SCIRun, allows scientists to perform range-based queries over a series of time slices and visualize the resulting particles using glyphs. The ability to navigate the multiple dimensions of the particle data, as well as query individual or a collection of particles, enables scientists to not only validate their simulations but also discover new phenomena in their data.

1. Introduction

As simulations evolve and grow into the peta-scale size it becomes increasingly important to have tools that allow scientists to explore their data in multiple ways. This is especially true when working with data that does not have any spatial coherence, which is often found when using particle in cell (PIC) codes or other codes that also utilize particles as part of their simulation. Fusion research is one important area that uses the PIC method to study the loss of energy due to microturbulence. Multi-dimensional visualizations, such as the ones we describe in this paper, expand the way scientists can explore and understand their data.

The approach described in Section 2 is a multivariate exploration interface that provides scientists a way of exploring and visualizing both physical and variable spaces from a global view to a refined selection of particles and field data over time [6].

Within the SCIRun Problem Solving Environment, the technique described in Section 3 allows the application scientist to create query driven visualizations of particle data.

2. Multivariate Exploration Interface

The system described here was designed with two goals for particle visualization: to allow scientists to visually confirm expected phenomena and to provide an exploration tool that

assists in scientific discovery. The challenge is how to relate multiple variables, both simulated values and post calculations with those values, within the visualization framework while still maintaining the advantage of interactivity. Our system addresses this issue by displaying the data using multiple views, which are grouped into either variable or physical visualization. Multiple-view interfaces have been widely used in the visualization community, and our work is closely related to the work of Akiba and Ma [1] and Rubel et al. [11], who also use parallel coordinates for data exploration. Introducing a variable space visualization not only expands the amount of displayed information, it also provides a tightly coupled user interface for intuitively selecting subsets of the particle data. In addition, the physical visualization provides interactive 3D exploration with transparency, lighting, and view control.

2.1. Physical Visualization

Since the particle data is time-varying, there are two ways the system can render the data. If only a single time step is being viewed, the particles are rendered as spherical glyphs. If a time interval is being viewed, the particles are rendered using illuminated pathlines. In both cases, a single scalar variable is mapped to color and opacity for that primitive using a 1D transfer function. The variable associated with the transfer function can be interactively chosen from a list of variables which have been read from the data or from an equation defined by the user.

For the single time step glyph representation of the particles, we utilize current GPU-based particle visualization methods that have been described by Gribble et al. [3]. As with the standard point primitive, no extra data storage beyond the single 3D position and scalar value is needed for rendering. Also, by using view-oriented billboards shaded via GPU hardware, the particles are given a 3D appearance with correct lighting and perspective size without intensive rendering requirements. The size of the glyphs can be interactively increased or decreased depending on user preference or to reduce overlapping problems. The result of this rendering technique is improved image quality and better depth cues, which allows for easier identification of single particles and physical location. Figure 1 shows a small subset of particles rendered with the spherical glyph.

One way the user can visualize particle changes over time is by animating the spherical glyphs. However, it is difficult to study the entire path of motion, especially if the time interval is very large. Our exploration system provides another solution by allowing particle trajectories to be rendered as illuminated pathlines [9]. Not only does the pathline visualization show where a particle was located during the specified time interval, it can also show the value of the particle across the time steps by coloring the pathline with the same 1D color map that is used for glyph coloring. Coloring the pathlines in this way also allows the user to selectively reduce clutter by changing the opacity values with the transfer function. In addition, the user can specify how many time steps forward or backward the pathline should traverse from the given time frame.

2.2. Variable Visualization

While the physical rendering allows the user to explore a single variable by modifying a color transfer function, another visualization is necessary for providing information about multiple variables simultaneously. To provide the multivariate visualization and interface, we turn to the popular information visualization technique of parallel coordinates, which was introduced by Inselberg [5]. Parallel coordinates have been successively used to show relationships between variables, and with effective rendering techniques, scientists can quickly discern patterns, outliers, or common groups. The conventional construction begins with one parallel axis for each of the variables being shown. Then for each primitive, in this case particles, a single, semi-transparent line strip is used to intersect every axis to coincide with the primitive's values for those variables [13]. However, this approach alone suffers from over saturation and low scalability in cases like ours where the number of data items can be very large.

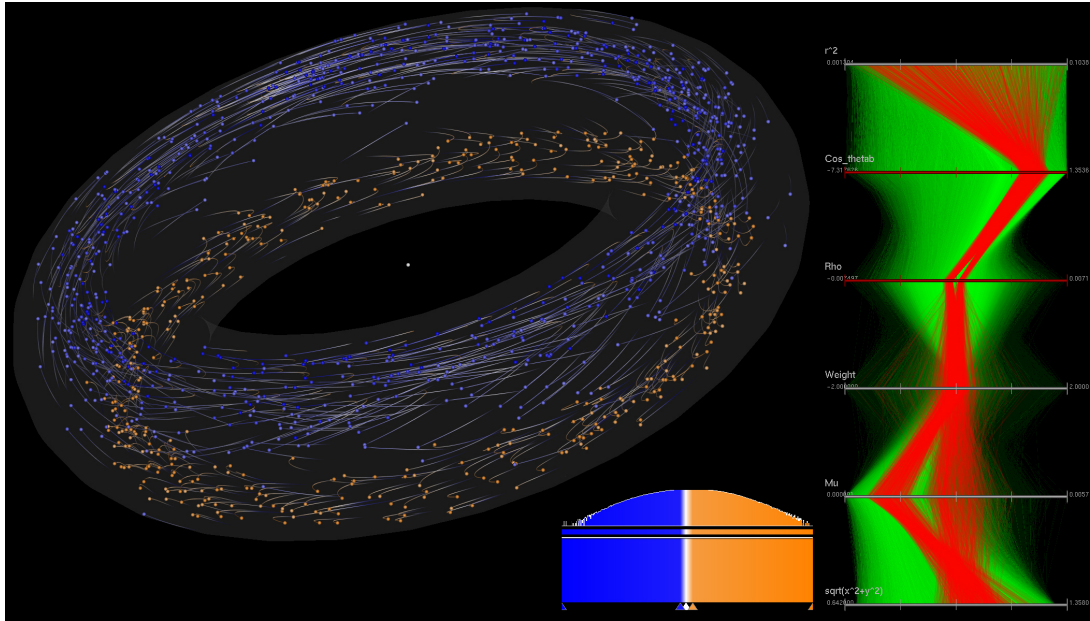


Figure 1. The multivariate exploration interface consists of a parallel coordinates view and a physical view of the data, along with a transfer function editor. In this example, particles were chosen using the particle selection lock to modify a selection of trapped particles based on specific time-varying conditions, and their values correspond to red polylines on the parallel coordinates. The change in sign of parallel velocity as the particles change direction can be seen from the pathline coloring, going from negative (blue) to positive (orange) or vice versa.

For our application we use a 2D bin approach that was utilized by Novotny and Hauser [10]. This technique addresses many of the large-scale data issues by rendering the global view from a 2D histogram of the data lines where the bins are colored and ordered by intensity.

The variable visualization also provides a means for selecting particles by a simple brushing operation. For each axis of the parallel coordinates plot, the user may select and deselect ranges of values via mouse drags. The focus of both the physical and variable visualizations becomes the current selection of particles based on the brushed ranges. An example of both the global and focused portions of parallel coordinates can be seen in Figure 1. Also, scientists can expand their understanding of any single variable by opening a XY time-variable plot to see how the selected particles change over time with respect to the given variable.

To provide additional control over the combinations of variables, each axis of the plot can be toggled between the *union* or *intersection* operator. In union mode (inclusive OR), the particles selected by that axis are simply added to the collective selection. In intersection mode (logical AND), the final collective selection can only include particles that are selected on every intersecting axis. The resulting particles exhibit a specific parameter subset, where each particle meets all intersected ranges.

When the user decides to animate the particles or modify the selection through time, the parallel coordinates can be set to one of two modes. The first mode is *particle selection lock*, which causes subsequent changes in time to keep the same particles selected. Particle selection lock is useful for seeing how particles chosen at one time step change and move over time, such as the example given in Figure 1 that shows the pathlines of selected trapped particles. The other mode is *range selection lock*, which causes changes in time to regenerate the particle selection based on the same defined parameter ranges. This mode allows the user to see the impact of

a specific variable constraint over time by showing the amount and location of particles within the collection at each new frame.

3. Query-Driven Visualization

Query driven visualizations are particularly useful in the verification and validation process of developing a simulation code as it allows the application scientist to interrogate their simulation results very precisely. Two examples of other query-driven visualization systems that are most closely related to ours is that of Swift-3D [7] and TimeFinder [4]. Swift-3D utilizes C-style query expressions that are translated into C-code, compiled into shared libraries, and then dynamically linked into the application. The advantage of this type of approach is its speed and flexibility. SCIRun also makes use of dynamic compilation not only for query based operations but many other operations. TimeFinder allows for interactive exploration of time varying data sets, presenting the query results in a manner that allows for subsequent data-mining.

When performing a query on a single time the results can immediately be visualized. This is because all of the data has been fully interrogated. When the data is a series of times slices, it is possible to visualize the query results on a slice-by-slice basis. However, this may not give the desired results. For instance, when interrogating particle in cell data, a particle may pass the query in one or more time slices. If the particle is visualized only when it passes the query, it will appear and disappear during the course of the visualization. As such, we have implemented a two-pass operation, performing the query over all of the particles in all of the time steps in the first pass and visualizing the results during the second pass. During the second pass a particle is displayed if it has passed the query for at least one or more time steps. For example, even though a particle may pass only the last time step, it will be displayed through all time steps. This provides visual continuity throughout the entire visualization.

It is also possible for the user to further refine the query in between passes. For instance, a histogram that shows the range of the number of time steps particles have passed a particular query is presented to the user. From this they can refine the query simply by stating that the particles must not only pass the query but pass the query for at least N time steps. The ability to produce histograms or other meta data and incorporate it into queries, which themselves may be composed of multivariate data, is an important part of the visualization and analysis process, as it allows the application scientist to more actively interrogate their data.

3.1. Multivariate Glyphs

For our initial application of magnetic fusion PIC data, it was desirable to visualize three data values associated with each particle, the velocity parallel to magnetic field, the radius of the charged ring about which the particle gyrates (gyro-radius), and the statistical weight based on their departure from equilibrium, Figure (2). Visualizing multivariate data that represents both scalar and vector values presents several unique challenges, [12].

For instance, taking the naive approach and representing each data value as a separate glyph leads to unacceptable results as shown in Figure (3) where the weight sphere occluded the velocity vector in one case. This is just one example of occlusion that can be shown. To visualize multivariate data, a single glyph with enough degrees-of-freedom to represent each data value must be used or, if multiple glyphs are used, they must be unified to prevent occlusion. We have taken the latter approach and utilized two glyphs, a cone and a torus, each of which has two degrees of freedom. We have unified them through the radius, which is common to both (implicit in this is the orientation which is also common to both). As such, there is a total of three degrees-of-freedom that can have data values mapped to them. For the cone, the velocity magnitude naturally maps the length and the gyro-radii maps to the radius. While for the torus, the gyro-radii maps to the major radius and the weight to the minor radius, Figure (4). Because the gyro-radii is used in both glyphs, it is not possible for either glyph to occlude the other.

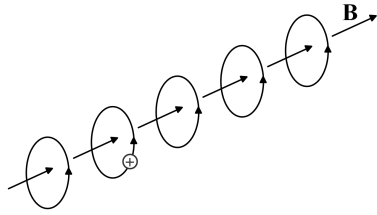


Figure 2. *The physical representation of a particle that is traveling along a magnetic field B while gyrating around a charged ring, [2].*

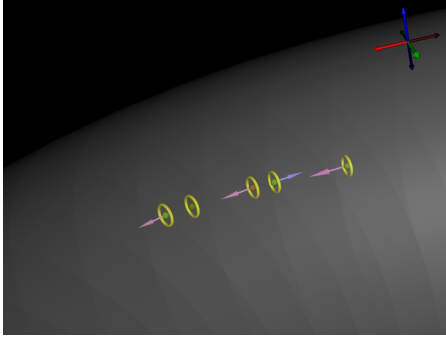


Figure 3. *A visualization of five particles using three distinct glyphs. Note the velocity arrow for one particle is occluded by the weight glyph.*

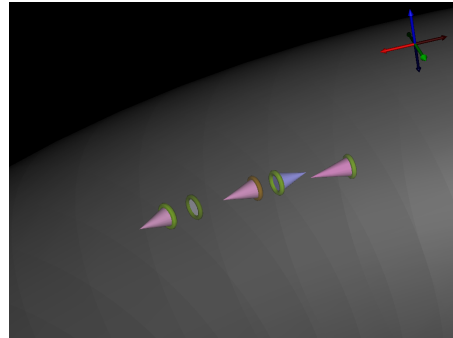


Figure 4. *A visualization of five particles using two unified glyphs, a cone and a torus.*

3.2. Colormapping

Although not necessary, utilizing color reinforces the physical mapping. For multivariate glyphs, colormaps were needed that would emphasize the changes in the paired signed values of the parallel velocity magnitude and the weight. At the same time, the colormaps had to contrast each other no matter where in the color spectrum a pair of values layed. We accomplished this using a tetrad grouping of colors from the color wheel [8]. A tetrad are four colors equally spaced apart on the color wheel, giving a high contrast between each color, Figure (5). This resulted in a blue and a red-violet tint colormap, with a narrow band of white in the center for the velocity magnitude and a yellow-green and a orange bivariate shade colormap with a narrow band of black in the center for the weight. These colormaps are used in Figures (4) and (6).

4. Conclusion

In this paper we have described two new applications that have advanced the way plasma scientists visually explore particle simulation data. The ability to find individual particles within a multi-dimensional space means that troublesome particles can be singled out for detailed study. For example, the systems allow for easy selection and rendering of trapped particles, which have significantly more impact on plasma transport than do passing particles. In addition, the multivariate exploration interface provides a visualization for displaying a global context of all the variables, and conditions such as the influence of other variables or location in toroidal space can be examined for individual particles. The understanding provided by our system may lead to discovering solutions to problems facing turbulent plasma flow.

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Figure 5. A tetrad on a color wheel, four colors equally spaced apart from each other, giving a high contrast between each.

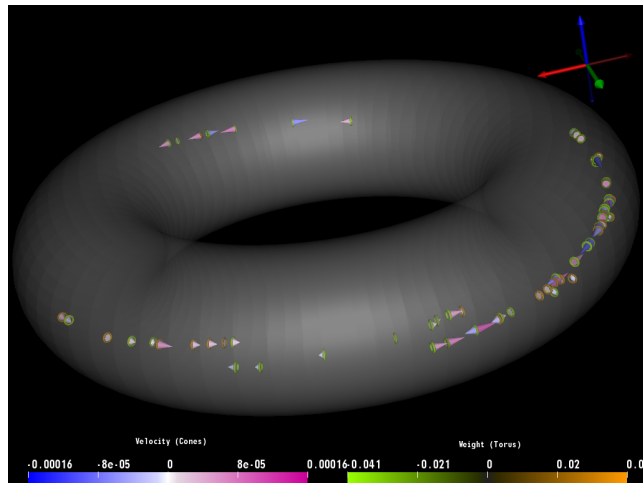


Figure 6. A visualization of particles from one time step using the unified glyphs.

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References

- [1] AKIBA, H., AND MA, K.-L. A tri-space visualization interface for analyzing time-varying multivariate volume data. In *Proceedings of Eurographics/IEEE VGTC Symposium on Visualization* (May 2007).
- [2] ETHIER, S., TANG, W., AND LIN, Z. Gyrokinetic particle-in-cell simulations of plasma microturbulence on advanced computing platforms. In *Proceedings of SciDAC 2005 Conference - Journal of Physics: Conference Series 16* (Philadelphia, 2005), Institute of Physics Publishing, pp. 1–16.
- [3] GRIBBLE, C. P., STEPHENS, A. J., GUILKEY, J. E., AND PARKER, S. G. Visualizing particle-based simulation datasets on the desktop. In *Workshop on Combining Visualization and Interaction to Facilitate Scientific Exploration and Discovery* (2006), pp. 111–118.
- [4] HOCHHEISER, H., AND SHNEIDERMAN, B. Visual specification of queries for finding patterns in time-series data. In *Discovery Science 2001, Lecture Notes in Artificial Intelligence #2226*, Springer-Verlag, pp. 441–446.
- [5] INSELBERG, A. The plane with parallel coordinates. *The Visual Computer V1*, 4 (December 1985), 69–91.
- [6] JONES, C., MA, K.-L., ETHIER, S., AND LEE, W.-L. An integrated visual exploration approach to particle data analysis. Tech. Rep. CSE-2007-20, University of California at Davis, March 2007.
- [7] KOUTSOFIOS, E., NORTH, S., TRUSCOTT, R., AND KEIM, D. Visualizing large-scale telecommunication networks and services (case study). In *Visualization '99: Proceedings of the conference on Visualization '04* (Washington, DC, USA, 1999), IEEE Computer Society, pp. 457–461.
- [8] MACDONALD, L. Using color effectively in computer graphics. *Computer Graphics and Applications 19* (1999), 20–35.
- [9] MALLO, O., PEIKERT, R., SIGG, C., AND SADLO, F. Illuminated lines revisited. In *IEEE Visualization 2005 Conference Proceedings* (2005), p. 3.
- [10] NOVOTNY, M., AND HAUSER, H. Outlier-preserving focus+context visualization in parallel coordinates. *IEEE Transactions on Visualization and Computer Graphics 12*, 5 (2006), 893–900.
- [11] RUBEL, O., WEBER, G., KERANEN, S., FOWLKES, C., HENDRIKS, C. L., SIMIRENKO, L., SHAH, N., EISEN, M., BIGGIN, M., HAGEN, H., SUDAR, D., MALIK, J., KNOWLES, D., AND HAMANN, B. Pointcloudxplore: Visual analysis of 3d gene expression data using physical views and parallel coordinates. *Eurographics/IEEE-VGTC Symposium on Visualization Proceedings* (2006), 203–210.
- [12] WALSUM, T. V., SILVER, F. P. D., AND POST, F. Feature extraction and iconic visualization. *IEEE Transactions on Visualization and Computer Graphics 2* (1996), 111–119.
- [13] WEGMAN, E. J., AND LUO, Q. High dimensional clustering using parallel coordinates and the grand tour. *Computing Science and Statistics 28* (1997), 361–368.