Multivariate Volume Data: Achieving Deeper Insight through Multivariate Volume Rendering and Machine-Guided Exploration

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Meeting-report

Multivariate Volume Data: Achieving Deeper Insight through Multivariate Volume Rendering and Machine-Guided Exploration

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Detailed analysis of nanoscale imaging data plays an important role in guidance for future experiments and successful scientific discoveries. However, increasing complexity and production of nanoscale imaging data have made this analysis more difficult, and, in some situations, infeasible. Multivariate volumetric data, which contains more than one channel per voxel, has become increasingly prevalent in important industries such as battery technology. Due to its multidimensional nature, however, multivariate data is complex and usually requires substantial human effort to analyze. Oftentimes, each channel is visualized separately and individually. However, this does not reveal the complex yet frequently important interactions between the channels.

RadVolViz is a specialized application for direct volume rendering featuring a dedicated transfer function editor designed explicitly for handling multivariate volume data [1]. Based on a series of interviews conducted with several domain experts in nanoscale imaging, microscopy, and spectroscopy, *RadVolViz* was designed to visualize all channels simultaneously, automatically generate a meaningful first impression of the data through a semi-automated data-driven color mapping scheme, and provide support for interactive selection and filtering for exploring desired aspects of the data.

A multivariate information display (*B* in Fig. 1) was designed to provide an overview of the data and serve as a multivariate transfer function editor (MTE). Nodes corresponding to each channel/dimension are plotted on the outside, and a subsampled distribution of the voxels are plotted on the inside. Several modes of interaction with the MTE, including lens filtering (Fig. 2) and manual coloring, provide exploration for different aspects of the data. Automatic rearrangement of channel nodes by correlation is also possible, resulting in greater visual contrast between less correlated channels.

The analysis of several sample datasets exemplifies some of the deep insights which may be achieved through multivariate volume rendering. For example, in a chemically sensitive electron tomography study (Fig. 1 and 3) of a four-channel lithium-ion battery dataset, the distribution of elements was visualized to determine whether cathode materials were synthesized properly. Adjusting the opacity to reveal the interior, as shown in Fig. 3, revealed deficiencies in the sample's synthesis process. Another study on trace doping of lithium cobalt oxide in a lithium-ion battery, with a goal of increasing surface stability, is shown in Fig. 2. Several insights, including that the surface distribution of *Ti* provided an explanation for the long-term stability of the material, were obtained through the analysis. These examples, along with additional examples in the paper [1], including some from other scientific disciplines, demonstrate the (sometimes significantly) faster time-to-discovery that multivariate volume visualization enables.

Research is actively being performed to further enhance multivariate volume analysis through several approaches, including through making many of the visualization techniques within *RadVolViz* accessible in the widely used open source visualization applications ParaView [2] and Tomviz [3], accelerating multivariate data exploration through the use of AI-driven analysis, and simplifying the visualization of multimodal volumetric datasets through new data reduction techniques. All software produced for this research will be open source and freely available [4].

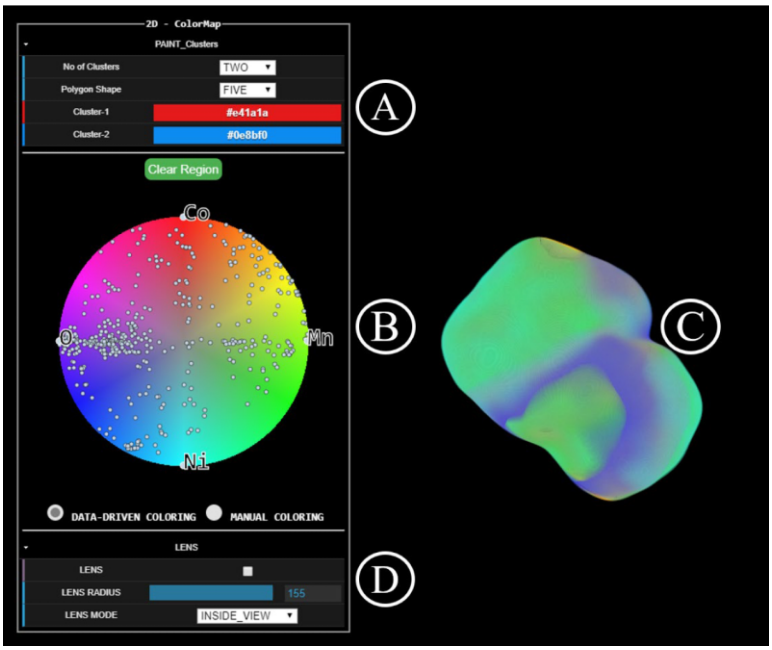

Fig. 1. Multivariate volume visualization using the *RadVolViz* application [1]; (C) rendered Chemically Sensitive Electron Tomography dataset; (B) interactive multivariate information display which doubles as the volume transfer function editor; (A) and (D) are manipulation controls.

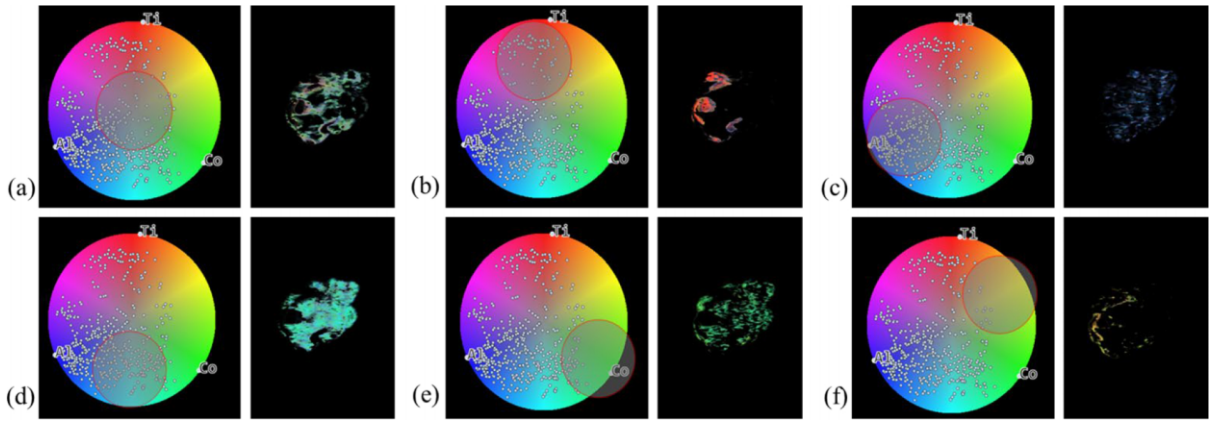

Fig. 2. Rendering results due to various lens placements using the LiCoO2 dataset described in the *RadVolViz* paper [1]: (a) relatively homogeneous samples, (b-f) samples with relatively high Titanium (b), Aluminum (c), mixtures of Aluminum and Cobalt (d), Cobalt (e), and mixtures of Titanium and Cobalt.

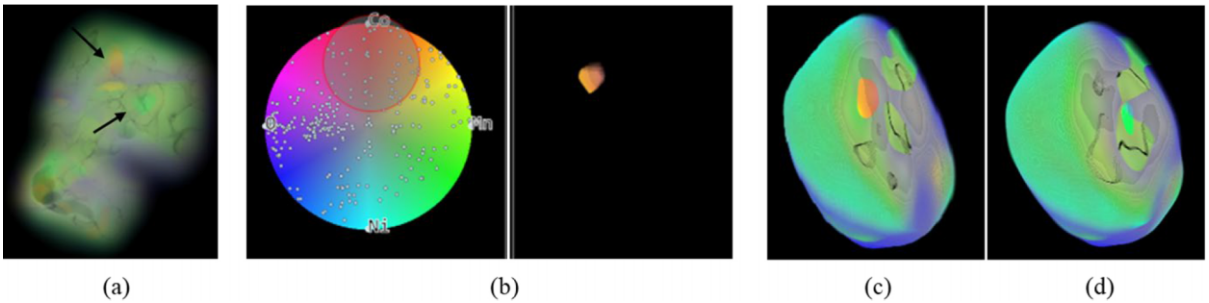

Fig. 3. Multivariate volume rendering of a lithium-ion battery sample described in the *RadVolViz* paper [1]. (a) Setting a low opacity threshold (0.05) reveals interesting interior structures (indicated by arrows). (b) Using the lens confirms that one of the embedded structures is metallic cobalt. (c-d) Subsequent clipping then fully exposes their presence, namely (c) metallic cobalt and (d) nickel-rich magnesium in the core of the sample. Both discoveries point to deficiencies in the sample's synthesis process. Images were taken from different viewpoints.

References

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