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Acquisition, Reconstruction and Curation of Multimodal 3D TriBeam Data

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A broad objective in materials science is to understand and control the structure of materials for materials discovery and development as well as optimization and prediction of material properties. The recent development of TriBeam tomography [1, 2] enables acquisition of mm^3-scale multimodal datasets containing EDSD, EDS, BSE and/or SE image data. Datasets of multiple classes of materials, including metallic alloys, ceramics, composites and geological materials have been acquired, with individual dataset volumes of multiple terabytes. To rigorously extract 3D information from these datasets, entirely new sets of reconstruction algorithms and workflows as well as 3D structure and property analysis tools are under development, as described below. Furthermore, early efforts to advance the infrastructure for the curation, distribution, and sharing of workflows and data through the Bisque platform [3] are reported.

A critical first step for reconstruction of 3D datasets using multimodal information is the correction of distortions that develop due to optics, electronics and detectors. A new approach to distortion correction has been developed [4]. Segmented BSE or SE images along with corresponding EBSD images are subjected to an image-based speckling strategy in both imaging modalities. The speckled data is meshed and a covariance matrix adaption evolution strategy (CMA-ES) distorts the mesh until speckles superimpose, enabling automated development of polynomial functions that describe the mesh distortion. This fully automated strategy requires no manual annotation and has been demonstrated using datasets of nickel alloys that contain microstructural features at the 1 μm scale.

Beyond distortion correction, subsequent reconstruction workflows have been developed within the Dream.3D platform [5]. For large datasets, the development of robust Dream.3D workflows is challenged by linear nature by which critical reconstruction parameters, such as misorientation tolerance, can be adjusted to properly identify features such as grains, Fig. 1. We have integrated the Dream.3D toolkit with BisQue to greatly facilitate selection of critical reconstruction parameters when working with these large 3D datasets in the HDF5 format. To accomplish this, pipelines are parameterized and run in parallel, Fig. 1, across multiple compute nodes to generate many 3D reconstruction instantiations from the initial raw dataset.

BisQue is a cloud-based system that uses a web browser interface to interact with 2D images as well as the complexity of 3D datasets [3]. The database architecture of BisQue is such that every processing execution, dataset (input and output) and workflow processing pipeline receives a unique web address URL. These URLs are useful for at least two reasons: tracking data provenance and data sharing. Data provenance with BisQue is automatically captured and can be easily accessed through visualized workflows. The workflow shows where input data is located, the parameters of a module execution are captured in the metadata and the output data is located. Therefore, passing data between research groups becomes straightforward due to the data operation transparency. Furthermore, data sharing is facilitated due to the data all being stored and accessed remotely, mitigating versioning problems common to large data operations. Other tools include web-based 3D data visualizers, data array viewers and table viewers, which make possible data analysis exclusively in the cloud. An example of an application of this system is on a 3D dataset of a melt pool generated via an electron beam additively manufactured process. A large parameter space has been explored in an automated fashion via 200 reconstructed dataset variants generated in parallel. The parameter studies of these additive manufactured 3D datasets are crucial for understanding what material defects emerge from the printing process and the structure that results from different printing parameters [6].

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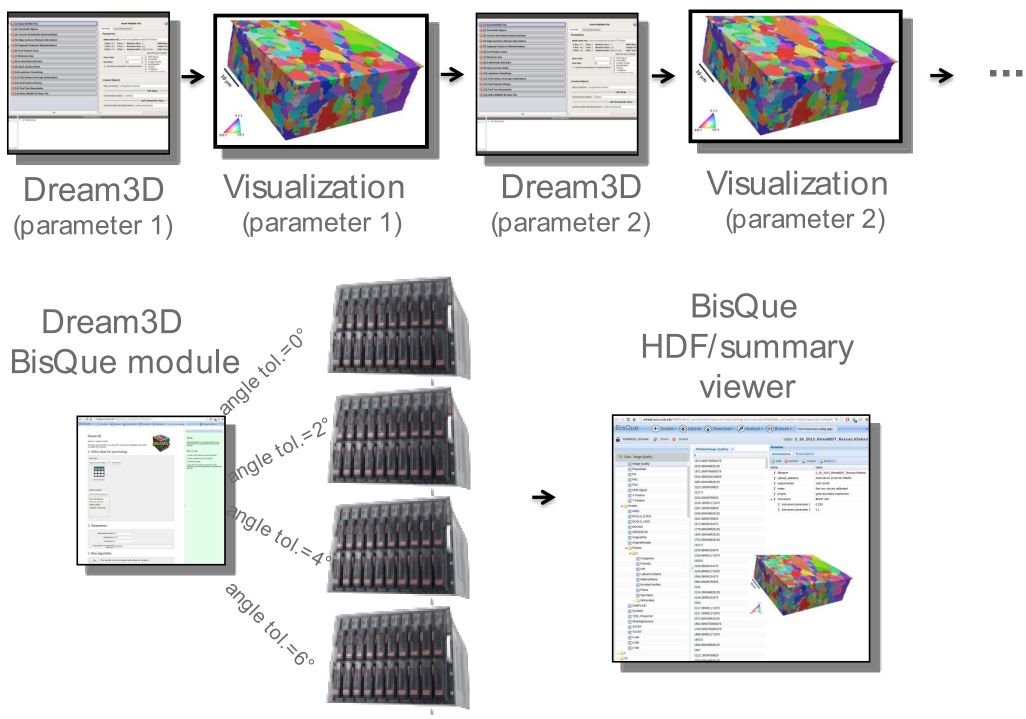

Figure 1. The Bisque infrastructure for parameterized reconstruction workflows within Dream.3D, which eliminates the slow, linear investigation of parameter space (top) with parallel reconstruction workflows (bottom).

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