On Strong Scaling Open Source Tools for Mining Atom Probe Tomography Data

Markus Kühbach[1*], Priyanshu Bajaj[1], Andrew Breen[1], Eric A. Jägle[1] and Baptiste Gault[1]

[1.] Department for Microstructure and Alloy Physics, Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany.
* Corresponding author: m.kuehbach@mpie.de

There is an increasing demand in the atom probe tomography (APT) community for accurate and efficient open source tools for assessing the quality and content of increasingly large experimental datasets, combined with a mindset change towards open source reproducible methods [1]. APT is a microscopy and microanalysis technique which produces datasets in the form of point clouds representing a material's volume at the nanoscale with positional and chemical information for each ion. This information allows to characterize microstructures and portray snapshots of their evolutionary mechanisms. Currently, two software tool options exists: one is IVAS [2], the Integrated Visualization and Analysis Software, a functionally rich graphical front end solution; the other, complementary option, are scripts that are less functionally diverse, but cutting-edge proof-of-concept tools, developed by experimentalists [3,4] and primarily, like IVAS, using sequential algorithms and implementations. IVAS is proprietary, not cross-compatibly executable, and closed source which poses an effective barrier to rigorous functional verification and extension. In contrast, the source code to these individual, ad-hoc tools is usually open, they employ fully transparent algorithms and thus patch and complement functionalities that are missing in IVAS.

With increasing data volume, analysis sophistication level, and increasing level of detail queried from an atom probe dataset, it would be useful to employ scientific computing, i.e. parallelized analysis and visualization techniques. On the one hand to use software parallelization to speed-up existing analyses and make a timely execution of numerically more demanding tasks possible. Examples include the extraction of structural features (crystal defects, phase and grain boundaries) and querying of crystallographic pieces of information. On the other hand, scientific computing techniques can be employed to assist researchers with automatically running analyses and assist in report writing to save time when distilling the scientifically relevant content. Despite such evident benefits, the development of such tools is still at an early stage, focusing typically on isolated tasks [5] due to the time and computer science background knowledge required to make such software scale on modern computers. To this end, this work contributes PARAPROBE, an open source software [6,7], which employs a collection of tailored parallelized algorithms and data structures to achieve strong scaling efficiency for various spatial analysis tasks of relevance for APT practitioners.

Specifically, we report how batch processing of lists of ion-type-specific spatial statistics tasks, such as the computation of radial distribution functions, k-nearest neighbors, 3d spatial distribution maps, or clustering tasks can be accelerated and quantified rigorously using dataset boundary extraction methods to distance all ions of the dataset and probe farther spherical inspection areas. We report a method to compute full volume tessellations which form the basis for constructing three-dimensional micro-structural features inside the dataset. Finally, we report a parallelized method for characterizing fully automatically local crystallographic orientation within the dataset volume using discrete Fast Fourier Transform methods combined with indexing the intensity pattern in inclination space as such obtained via image template matching. Figures 1 and 2 offer a perspective on the contents of the talk [7].

References:

[1] AV Ceguerra et al., Current Opinion in Solid State & Materials Science **17** (2013), p. 224.

[2] R Ulfig et al., Microscopy and Microanalysis **15 (S2)** (2009), p. 294.

[3] P Felfer et al., Ultramicroscopy **132** (2013), p. 100.

[4] Atom Probe Workbench v1.0 released, http://www.massive.org.au/cvl/cvl-workbenches/atom-probe-workbench (accessed February 21th, 2019).

[5] H Lu et al., Proceedings of the 32nd IEEE International Parallel and Distributed Processing Symposium (IPDPS) (2018), p. 54.

[6] PARAPROBE, http://www.github.com/mkuehbach/PARAPROBE (accessed Febr. 21th, 2019).

[7] The work was partially supported by BiGmax, the Max Planck Society's Research Network on Big-Data-Driven Materials-Science.
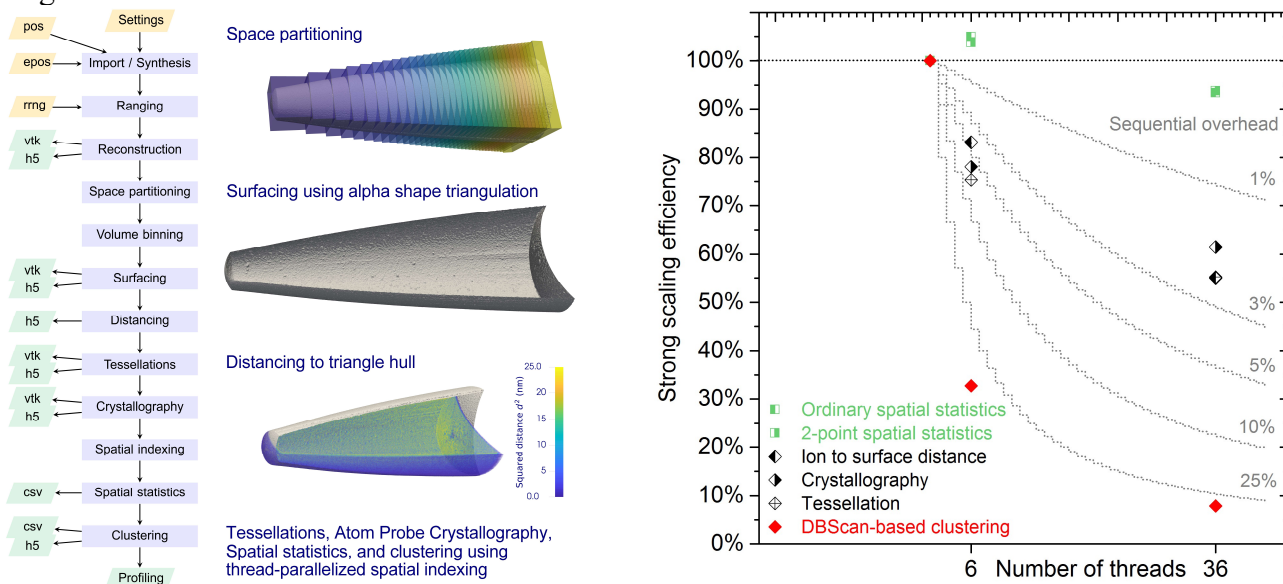
Figure 1. We present an open source scientific computing tool for assessing APT experiments.
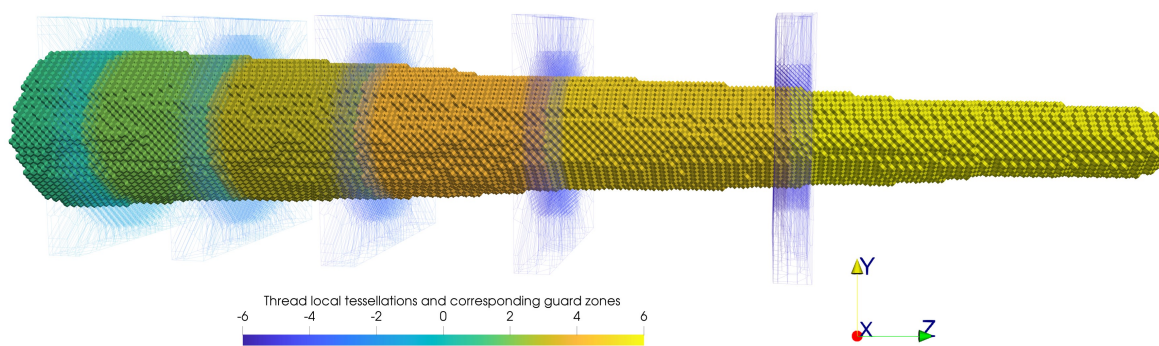
Figure 2. We use tailored implementation strategies and data structures to partition the ion point cloud spatially and balance the computational load. Guard zones about the computational sub-domains enable for a careful distributing and delegating of the work across the computing units. This is exemplified for a Voronoï tessellation of the entire dataset, where the guard zones, highlighted here with light-blue wire-frames, assure correct cell geometries across the sub-domain boundaries.