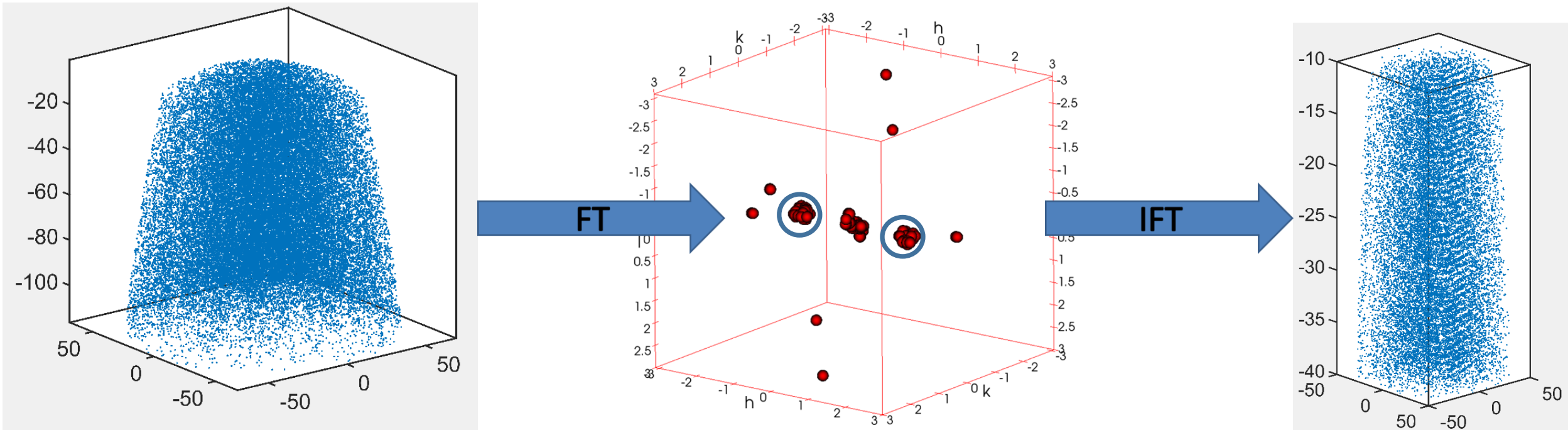


Development of efficient computational and visualization methods  
Hermann Lederer, Markus Rampp (Max Planck Computing and Data Facility).



A Python-based and GPU-accelerated analysis workflow was established for identifying crystalline sub-volumes of large APT samples (millions to billions of atoms). Accurate direct Fourier summation is used to transform between real space of atom coordinates and reciprocal space. The workflow employs the PyNX for computing the Fourier transformation (FT) from real to reciprocal space, and a fast inverse transformation (IFT) has been newly implemented for GPUs. Both transforms can now be computed within a few seconds on a modern GPU, paving the way from interactive, visual analysis by masking crystalline regions in reciprocal space using tools like ParaView, towards fully automated calibration of APT samples.