HPC-based fusion of quantum simulation, experiment analysis and data-driven science

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Several new features were added in 2DMAT [1-6], an open-source data-analysis software for advanced experimental measurement techniques. 2DMAT was developed by the PASUMS project at FY2020, 2021[1]. A major achievement was the efficient massively parallel computation of the population annealing Monte Carlo (PAMC) method [7]. An almost ideal parallel efficiency was found not only on the ISSP supercomputer (ohtaka) but also on the Fugaku supercomputer with upto 8×10^5 nodes, a half of the Fugaku supercomputer. We used 2DMAT for the data analysis of total-reflection high-energy positron diffraction (TRHEPD) at Slow Positron Facility, KEK [8]. The experimental setup of TRHEPD is similar to that of reflection high-energy electron diffraction (RHEED) but TRHEPD reveals the surface sensitivity and was used for the determination of surface structure. 2DMAT was applied to the analysis of the three-dimensional coordinates (x, y, z) for Ge(001)-c4x2 surface structure by the Bayesian inference using PAMC. [8] The PAMC analysis, as a global search, determined the correct surface structure without any initial guess. In addition, a new algorithm was proposed for a faster computation of the forward problem of TRHEPD analysis. [9]

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