FAST PARTICLE FUSION BASED ON JOINT REGISTRATION

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The particle-fusion approach by Heydarian et al. [1] based on an all-to-all registrations has proven to work well, but has a large computational cost and scales unfavorably with the number of particles N, namely as N^2. A fast particle fusion algorithm is needed to process large datasets, with N exceeding several 100s. Therefore, we propose a method that is capable of alleviating the computation cost of the all-to-all registration. Compared to it, the joint registration of multiple point clouds (JRMPC) [2] can reconstruct particles rapidly, as it scales linearly with N. In JRMPC input particles are iteratively transformed to fit in a continuously updated Gaussian mixtures model (GMM). However, the final outcome is not stable to different initializations. Different initial GMM centers will lead to different sets of particle rotations and translations. This is because JRMPC can easily get stuck in a locally optimum solution. It appears that such solutions usually contain several clusters of well registered particles, where the clusters have different poses. Instead of directly searching the globally optimal solution with huge efforts, the results of different initializations of JRMPC are classified by an unsupervised classification method [3]. The final step is to connect the set of different clusters from the different initializations into a single well-aligned structure containing the majority of the particles.

Our method has advantages in processing large quantities of data and the potential to deal with poor quality data. It can obtain clear structural detail with less computational time as shown in Figure 1.

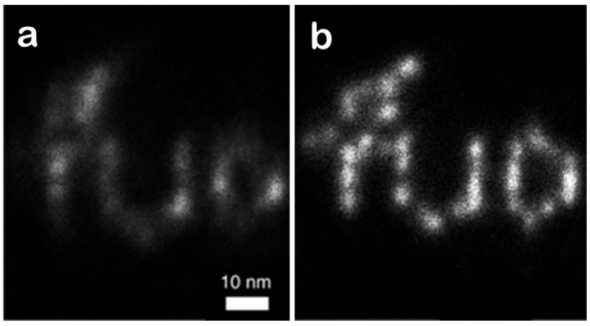

Figure 1: Comparison of particle-fusion performance by our method and all-to-all registration [1] on 549 experimental 'TUD logo' particles with 30% density of labeling. ***a)*** *Reconstruction of all to all method. The computational time is more than 2 hours.* ***b)*** *Reconstruction of our method. The computational time is about 12 minutes.*

[1] H. Heydarian, F. Schueder, M.T. Strauss et al., "Template-free 2D particle fusion in localization microscopy", Nature Methods 15, 781–784 (2018).
[2] G.D. Evangelidis, R. Horaud "Joint Alignment of Point Sets with Batch and Incremental Expectation-Maximization", IEEE PAMI (2018).
[3] T.A.P.M. Huijben, "Detecting structural heterogeneity in single-molecule localization microscopy data", TU Delft Master Thesis (2020).