

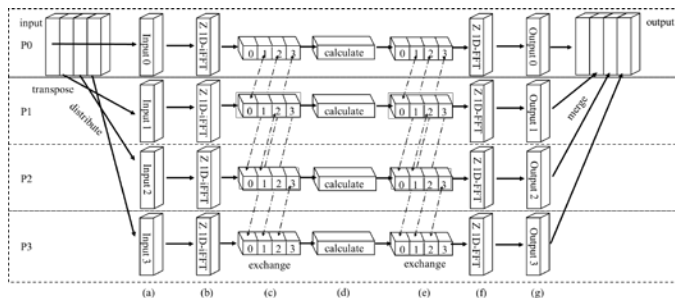
Accelerating the Cryo-EM Structure Determination in RELION on GPU Cluster

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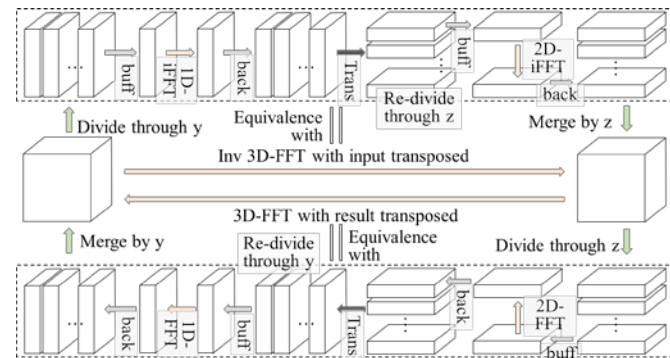
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Problems & Ideas

- Problems of the waste of resources significantly deteriorates the computation efficiency of RELION
 - We perform a comprehensive analysis of the performance of RELION and identify several performance bottlenecks for optimization.
- Ideas: Propose several optimization strategies to improve the performance of RELION
 - Computation redundancy optimization
 - Parallelization of M-Step
 - The computation acceleration of symmetries
 - Memory affinity optimization

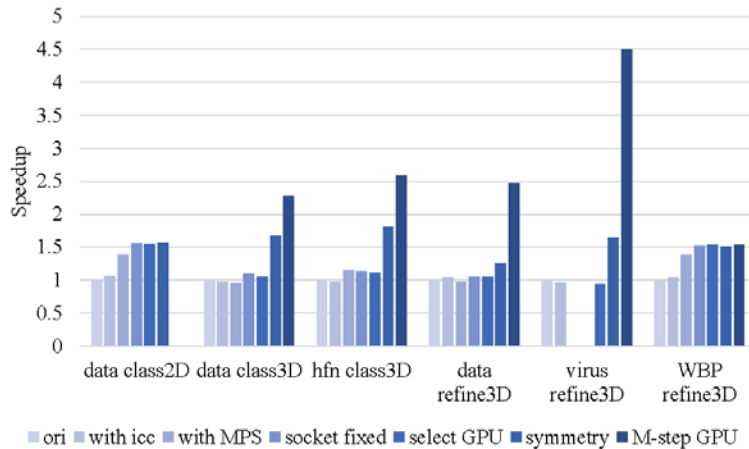


The Pipe & Menon algorithm optimized with intra-group parallelization



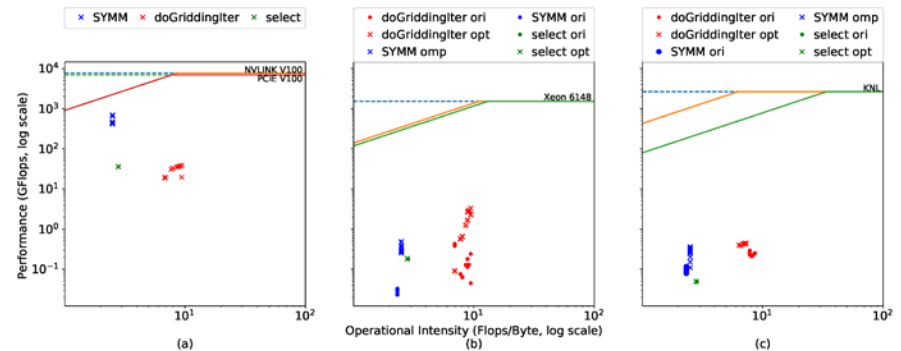
The FFT schedule partitioning and data buffering method on GPU.

Main Contributions



The performance improvement of RELION with the proposed optimizations.

- The experiment results show that our proposed optimizations achieve 4.5x performance speedup. In addition, our proposed optimizations are able to scale to the GPU cluster for acceleration.
- We provide the roofline model analysis to demonstrate our proposed optimizations achieve high computation efficiency.



The roofline model of RELION running on (a) Nvidia V100 GPU, (b) Intel Xeon Gold 6148, and (c) Intel Xeon Phi 7210 (KNL).