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Accelerating two-dimensional tensor network contractions using QR-decompositions

Infinite projected entangled-pair states (iPEPS) provide a powerful tool for studying strongly correlated systems directly in the thermodynamic limit. A core component of the algorithm is the approximate contraction of the iPEPS, where the computational bottleneck typically lies in the singular value or eigenvalue decompositions involved in the renormalization step. This is particularly true on GPUs, where tensor contractions are substantially faster than these decompositions. We propose a new contraction scheme for C4v-symmetric tensor networks that combines the corner transfer matrix renormalization group (CTMRG) with QR decompositions, are substantially faster –especially on GPUs. This approach achieves up to two orders of magnitude speedup over standard CTMRG, enabling state-of-the-art results for the Heisenberg and J1–J2 models in about one hour on an H100 GPU.

Authors: CORBOZ, Philippe (University of Amsterdam); YANG, Qi (University of Amsterdam); ZHANG, Yining (University of Amsterdam)

Presenter: ZHANG, Yining (University of Amsterdam)

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