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Versatile cross-platform compilation toolchain for Schrödinger-style quantum circuit simulation

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While existing quantum hardware resources have limited availability and reliability, there is a growing demand for exploring and verifying quantum algorithms. Efficient classical simulators for high-performance quantum simulation are critical to meeting this demand. However, due to the vastly varied characteristics of classical hardware, implementing hardware-specific optimizations for different hardware platforms is challenging. To address such needs, we propose CAST (Cross-platform Adaptive Schrödinger-style Simulation Toolchain), a novel compilation toolchain with cross-platform (CPU and Nvidia GPU) optimization and high-performance backend supports. CAST exploits a novel sparsity-aware gate fusion algorithm that automatically selects the best fusion strategy and backend configuration for targeted hardware platforms. CAST also aims to offer versatile and high-performance backend for different hardware platforms. To this end, CAST provides an LLVM IR-based vectorization optimization for various CPU architectures and instruction sets, as well as a PTX-based code generator for Nvidia GPU support. We benchmark CAST against IBM Qiskit, Google QSimCirq, Nvidia cuQuantum backend, and other high-performance simulators. On various 32-qubit CPU-based benchmarks, CAST is able to achieve up to 8.03x speedup than Qiskit. On various 30-qubit GPU-based benchmarks, CAST is able to achieve up to 39.3x speedup than Nvidia cuQuantum backend.

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