Benchmark of Linear Algebra Libraries Accelerated on Graphical Processors

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Computational chemistry increasingly relies on high-performance computing (HPC) to address complex scientific challenges. Graphics Processing Units (GPUs) have become a crucial tool for accelerating a wide range of simulations and calculations, offering new opportunities for efficiency and scalability. In this work, we provide a general overview of how numerical libraries for GPUs are influencing the development of computational chemistry. We discuss the benefits of using GPUs for typical computational tasks and highlight some of the challenges that arise when adapting traditional algorithms to GPU architectures. The use of GPU-accelerated computing enables researchers to study larger systems, perform longer simulations, and explore new areas of chemical research. As GPU hardware and software ecosystems continue to evolve, their impact on computational chemistry is expected to grow even further.