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PSCToolkit: Bringing Linear Algebra to the Exascale

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The growth of computational capabilities is ushering the era of exascale computing, presenting unprecedented opportunities and challenges for scientific applications. Sparse Linear algebra underpins a wide range of these applications: from simulating the transition to decarbonized energy in Europe to the construction of digital twins of the human body. The demands of exascale systems necessitate innovative approaches to algorithm design, scalability, and performance optimization.

PSCToolkit is a library designed to address these challenges by providing a scalable, portable, and efficient suite of linear algebra tools optimized for exascale architectures in the MPI+X framework. By leveraging hybrid parallelism and advanced GPU acceleration the PSCToolkit suite of libraries strives for optimal performance on heterogeneous systems. The toolkit integrates parallel sparse BLAS with Krylov methods and preconditioners.

In this poster, we present the architecture of PSCToolkit, highlight key design decisions [1]. We describe the most recent We describe the most recent additions from an algorithmic point of view [3] and demonstrate its performance through benchmarks on exascale-class systems [2,3].

1. D'Ambra, Pasqua, Fabio Durastante, and Salvatore Filippone. "Parallel Sparse Computation Toolkit." Software Impacts 15 (2023): 100463.

2. D'Ambra, Pasqua, Fabio Durastante, and Salvatore Filippone. "PSCToolkit: solving sparse linear systems with a large number of GPUs." arXiv preprint arXiv:2406.19754 (2024).

3. D'Ambra, Pasqua, Fabio Durastante, Salvatore Filippone, Stefano Massei, and Stephen Thomas. "Optimal Polynomial Smoothers for Parallel AMG." arXiv preprint arXiv:2407.09848 (2024).

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