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TRANSPARENT EXECUTION OF NUMERICAL LIBRARIES ON DISTRIBUTED HPC PLATFORMS

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The usage of numerical software libraries is well established in scientific computing as they can provide advanced methods and efficient implementations for solving common problems of scientific applications. One major goal of using these libraries is to improve the application performance by fully exploiting the available computational hardware. For example, BLAS libraries, such as OpenBLAS or cuBLAS provide efficient implementations of linear algebra operations that exploit modern multicore processors or graphics processing units. In this contribution, we propose a method for redirecting the execution of an existing numerical software library to a distributed HPC platform. The redirection is transparent in the sense that the application does not have to distinguish whether the utilized library functions are executed locally or distributed. Thus, the method allows to exploit the computational power of HPC platforms even in non-parallel application codes. Our proposed solution provides replacements of the utilized library functions, that can be used without additional programming efforts for adapting the application code. Furthermore, by providing the replacement functions as a shared library, the redirection can also be applied to applications that are only available as a binary executable. We demonstrate the approach for several numerical software libraries, such as BLAS and LAPACK libraries for linear algebra operations, the FFTW library for fast Fourier transforms, and the ScaFaCoS library for fast Coulomb interactions in particle systems. This includes sequential libraries as well as parallel libraries based on multi-threading or MPI. The implementation utilizes the Simulation Component and Data Coupling library [1] for performing the program interactions and the data transfers between the locally executed application and the numerical software library executed on a distributed HPC platforms. Experimental results are presented to investigate the overhead of the required data transfers and the achieved performance improvements.

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