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Optimized PETSc-HYPRE Library for GPU-Accelerated Simulation in OpenFOAM

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Abstract The GPU accelerated CFD simulation has been widely studied recently. Commercial software like ANSYS Fluent and Simcenter STAR-CCM+ has shown a powerful GPU-acceleration performance compared to traditional CPU-based parallelism; the open-source CFD platform OpenFOAM was originally designed to realize the parallel computing in multi-CPU cores, however, the GPU acceleration for matrix in OpenFOAM is constrained by its special matrix structure: Lower triangle – Diagonal – Upper triangle (LDU) structure; another open-source package PETSc, with GPU parallelism imbedded, has been implemented to replace the original linear algebra solver in OpenFOAM through API petsc4FOAM, the LDU matrix is transformed into the CSR structure inside of the API, which is commonly used in GPU parallelism, however, due to its complex matrix-converting process, most of the solving time is consumed during the matrix conversion. Another lagging factor is the default GAMG-CG solver in PETSc, especially the GAMG method, uses "smoothed aggregation" AMG, which has better theoretical properties for high order and elasticity problems and the algorithm's implementations and default parameters have been optimized for these types of problems, not for fluid equations. Thus, the combination platform shows a weak acceleration performance than expected in GPU mode. This project replaces the GAMG solver with HYPRE boomerAMG, modified the matrix conversion among OpenFOAM, PETSc and HYPRE to reduce additional waste. Optimized results show around 8.7x-speed up than the CPU (40 cores) simulation, around 9x-speedup than the original combination platform in GPU simulation.