

## **Characterizing the impact of compiler and MPI version differences in Containers using Spack**

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Containers are becoming an increasingly common solution to help meet the need for software flexibility on HPC systems. They allow for user-defined software stacks where users can install and manage their own software configurations on HPC resources. While working with containers on HPC machines, LANL scientists have noted that different compiler and MPI versions inside the container may affect the containerized application's results and/or performance. Previous studies have examined performance differences between container implementations and bare metal, but they have not explored how specific compiler and MPI implementation version combinations affect software and performance. We addressed this gap by analyzing the results of the CTS-2 benchmark scientific mini-apps, LAGHOS and HPCG, inside containers built with a matrix of different GCC and OpenMPI versions using the Spack package manager. The acceptance tests passed for every container combination but not without observable differences. Our results for HPCG indicated that the GCC and OpenMPI version combinations had little effect but there was a slight decrease in performance overall. Our results for LAGHOS indicated that the GCC version slightly affected performance while the OpenMPI version did not. Our results suggest specific compiler and MPI versions may lead to slightly improved performance. Future work includes: 1) experimenting with different compiler and MPI implementations, e.g., intel, intel-mpi, etc., 2) using other figure of merit acceptance tests for next-generation hardware in containers, e.g., SNAP, and Quicksilver, 3) experimenting with different compiler flags to help optimize the compiler, e.g., binutils, nvptx, etc.