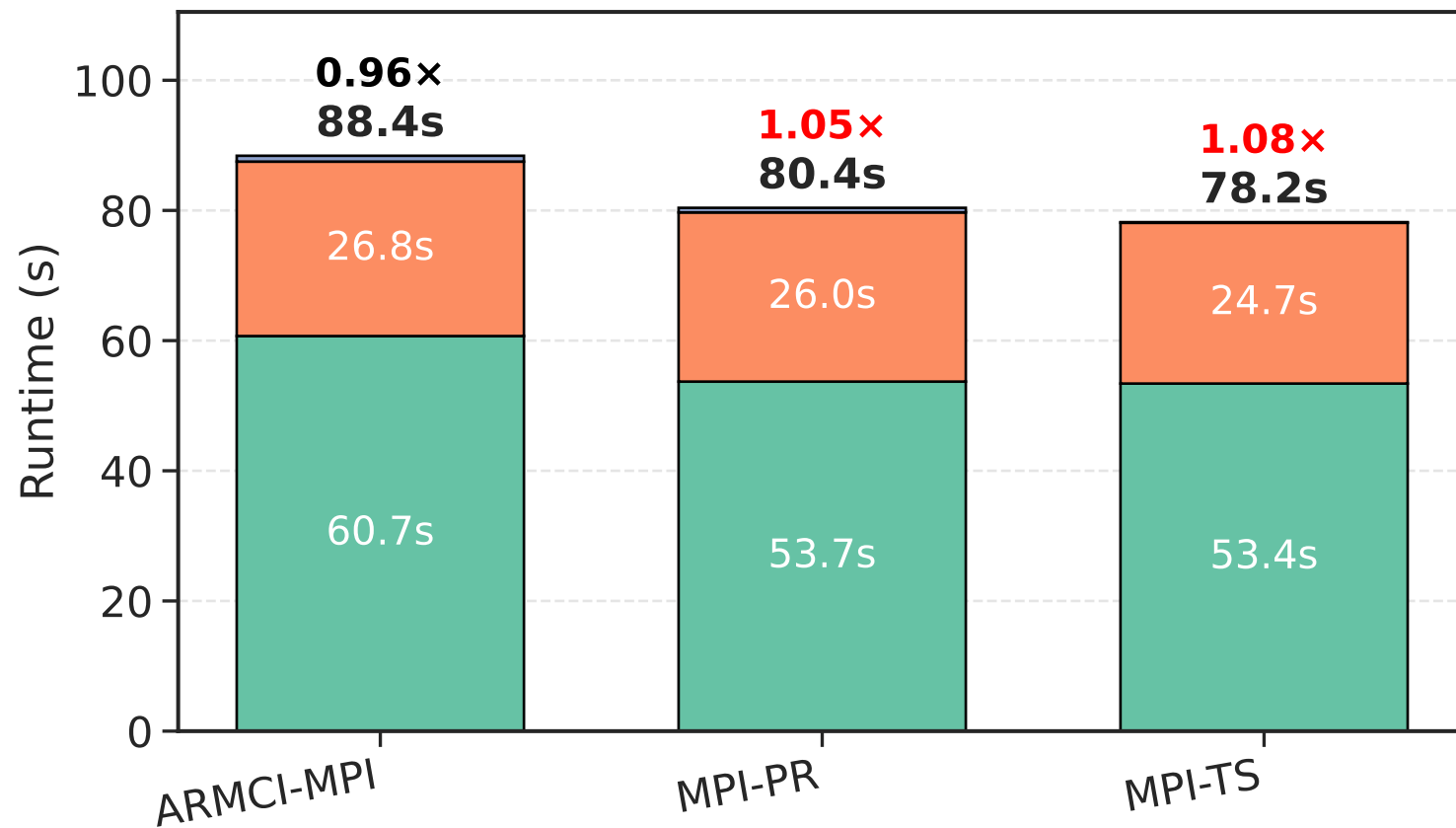


NWChem @ 4 Nodes (160 Cores)

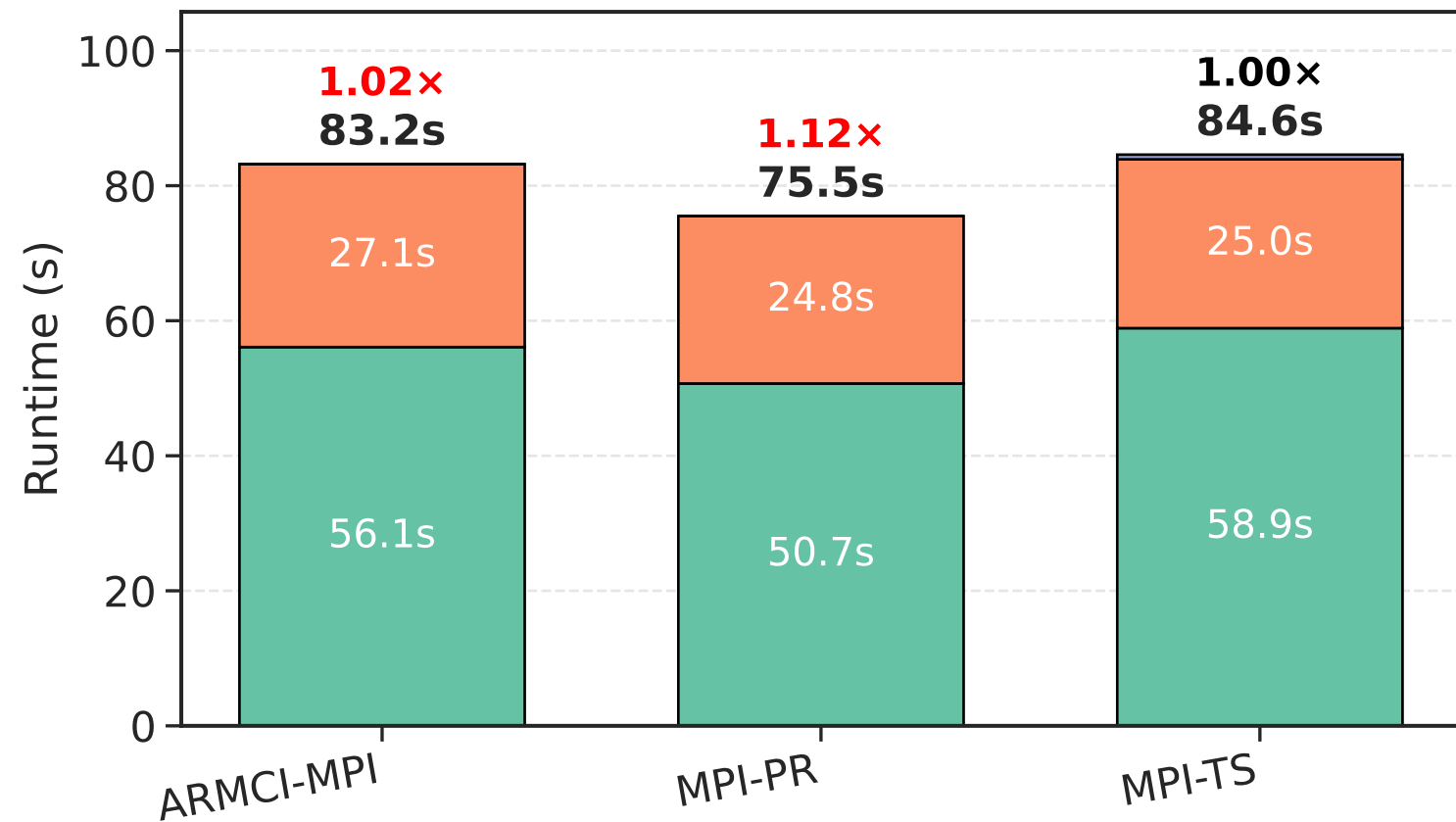
MPI Communication Strategies per Software Stack (SCF / DFT / Other)

SCF DFT Other

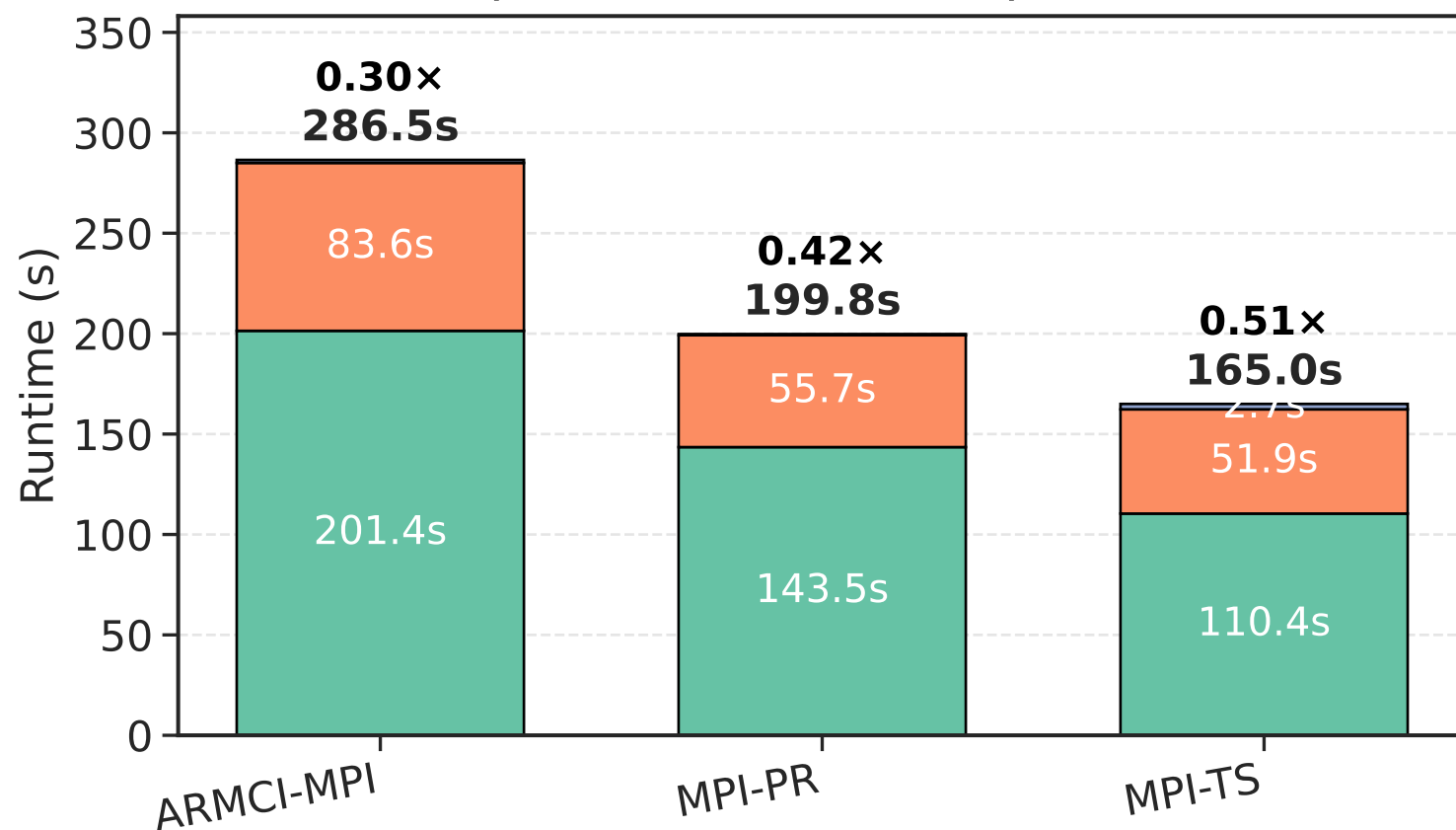
Intel MKL + Intel MPI



OpenBLAS + OpenMPI (GCC)



OpenBLAS + HPCX OpenMPI



OpenBLAS + OneAPI+OpenMPI

