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Microsoft MPI (MS-MPI) is a Microsoft implementation of the Message Passing Interface standard for developing and running parallel applications on the Windows platform.. MS-MPI offers several benefits:

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Quick and dirty cluster
installation¶. On a
cluster where users are
expected to be running
across multiple nodes
using MPI, make one

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installation similar to the above, and another using `-DGMX_MPI=on` and which is building only `mdrun`, because that is the only component of GROMACS that uses MPI. The latter will install a single simulation engine binary, i.e. `mdrun_mpi` when the default suffix is used.

**Installation guide —
GROMACS 2020.4**

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explains how to run MPI applications after MPICH is installed and working correctly. MPICH README is a basic README for MPICH beginners. It contains the simplest set of instructions to get started with MPICH.

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an MPI library installed that supports the MPI 1.3 standard, and; wrapper compilers that will compile code using that library. The GROMACS team recommends OpenMPI version 1.6 (or higher), MPICH version 1.4.1 (or higher), or your

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hardware vendor's MPI installation. The most recent version of either of these is likely to be the best.

Installation Instructions 5.0 - Gromacs

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