

Inhomogeneities between Software Stacks of Developers, Testing Environments and Users

— A \LaTeX template —

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CP2K - A massively parallel electronic structure package

- Provides a wide range of electronic structure methods to tackle periodic systems containing from hundreds up to a few million atoms
- Written in Fortran 2008, performance critical code ported to CUDA or HIP
- Available on Github

Possible hardware

Piz Daint (CSCS, Lugano, Switzerland): position 3 of TOP500 (2017), today: position 28
Cray XC40/50, 21 PFLOPs (5704 compute nodes, each with NVIDIA P100)

LUMI (LUMI consortium, Kajaani, Finland): position 3 in TOP500, position 7 in GREEN500 (2023)
HPE Cray EX235a, 309 PFLOPs (2352 compute nodes, each with 4 AMD Instinct MI250X)

Compute clusters (testing, small workloads)
36-128 cores, with or without GPUs

Desktop machines/Notebooks (development, testing)
4-16 cores

CP2K Software Stack (I)

CP2K requires matching OpenMP-capable C, C++, Fortran compilers.

CP2K is designed to have a high performance independently of the platform, thus CP2K relies on vendor-provided implementations of common kernels.

Hardware/Compilers

Possible Accelerators:

- NVIDIA (CUDA)
- AMD (HIP/ROCM)
- FPGA
- OpenCL

Compiler Systems:

- GCC
- Intel
- Cray (partially)

General Libraries

BLAS+Lapack

MPI

BLACS+PBLAS+ScaLapack

FFTW

COSMA (replacing P?GEMM)

ELPA (replacing Eigenvalue
Solvers)

SPLA (replacing ?GEMM)

Domain-Specific Libraries

Libint

LibXC

LibXSMM

PEXSI

QUIP

Plumed

SPGLIB

SIRIUS

LibVori

Torch

Possible Solutions (I)

General recommendation:

The more complex your software package the more you should test the different combinations (CI, Dashboard)

Separation of concerns of build process with respective tools (installation of dependencies, configuration, building, ...).

Check recent versions of libraries and their provided functionality.

Problems	Solutions
Library/Code does not compile	drop it for the compiler
Compiler Bugs/ Missing Feature	Compiler support is still required: Workaround Otherwise: Drop the compiler support
Incompatibilities/Bugs in libraries	Workaround, drop the library
Bug after PR	Communication with Experts Workaround

THE END.

Thank you for your attention!