System

Ubuntu (18.04, 20.04, ...), Centos (7, 8) Architectures : x64 64, arm, ppc64le

Vendor Container

CUDA (x64_64, arm, ppc64le) OneAPI (x64_64)

BigDFT base SDK

lsim_sdk.py

Python (default, intel), Jupyter server

BigDFT SDK + Toolchain

Isim_toolchain.py

Compiler (GNU, LLVM, Intel, ARM Allinea studio, IBM), Linear algebra (MKL, OpenBLAS, default BLAS, ARM)

BigDFT SDK + Toolchain + MPI

Isim_mpi.py

CUDA-aware : OpenMPI, MVAPICH2-GDR Non CUDA-aware : OpenMPI, Intel MPI, MVAPICH2