

# CP2K Open Source Molecular Dynamics

This document is intended to be a recipe for building and running the Intel branch of CP2K which uses the Intel Development Tools and the Intel runtime environment. Differences compared to CP2K/trunk may be incorporated into the mainline version of CP2K at any time (and subsequently released). For example, starting with CP2K 3.0 an LIBXSMM integration is available which is (optionally) substituting CP2K's "libxsmm" library.

## Getting the Source Code

The source code is hosted at GitHub and is supposed to represent the master version of CP2K in a timely fashion. CP2K's main repository is actually hosted at SourceForge but automatically mirrored at GitHub.

```
git clone https://github.com/hfp/libxsmm.git
git clone --branch intel https://github.com/cp2k/cp2k.git cp2k.git
ln -s cp2k.git/cp2k cp2k
```

## Build Instructions

In order to build CP2K/intel from source, make sure to rely on one of the recommended compiler versions:

- Intel Compiler 15.0.3.187 (Build 20150407)
- Intel Compiler 16.0.0.109 (Build 20150815)
- Intel Compiler 16.0.1.150 (Build 20151021)

For Intel MPI, usually any version is fine.

```
source /opt/intel/composer_xe_2015.3.187/bin/compilervars.sh intel64
source /opt/intel/mpi/5.1.0.069/intel64/bin/mpivars.sh
```

For product suites, the compiler and the MPI library can be sourced in one step.

```
source /opt/intel/compilers_and_libraries_2016.0.109/linux/bin/compilervars.sh intel64
```

To build the CP2K application, building LIBXSMM separately is not required (it will be build in an out-of-tree fashion as long as the LIBXSMMROOT path is supplied). Since CP2K 3.0, the mainline version (non-Intel branch) is also supporting the LIBXSMM however the library needs to be built separately.

```
cd cp2k/makefiles
make ARCH=Linux-x86-64-intel VERSION=psmp LIBXSMMROOT=/path/to/libxsmm -j
```

To further adjust CP2K at build time of the application, additional key-value pairs can be passed at make's command line (similar to ARCH=Linux-x86-64-intel and VERSION=psmp).

- **LIBXSMM\_PREFETCH**: set LIBXSMM\_PREFETCH=1 to unconditionally enable software prefetches.
- **LIBXSMM\_MNK**, **LIBXSMM\_M**, **LIBXSMM\_N**, **LIBXSMM\_K**: see LIBXSMM documentation.
- **JIT**: set JIT=0 to disable JIT code generation (enabled by default), and to statically specialize LIBXSMM.
- **MPI**: set MPI=3 to experiment with more recent MPI features e.g., with remote memory access.
- **SYM**: set SYM=1 to include debug symbols into the executable e.g., helpful with performance profiling.
- **DBG**: set DBG=1 to include debug symbols, and to generate non-optimized code.

Please note that the arch-files for the versions "popt", "sopt", and "ssmp" are provided for convenience and are actually based on the "x"-configuration (Linux-x86-64-intel.x) by using even more of the above key-value pairs (OMP, ACC, etc.).

## Running the Application

Running the application may go beyond a single node, however for the purpose of an example the command line shown below is limited to a single node. Running an MPI/OpenMP-hybrid application, a number of processes (MPI ranks) which is half the number of cores might be a good starting point (below command could be for an HT-enabled dual-socket system with 16 cores per processor and 64 hardware threads).

```
mpirun -np 16 \
  -genv "I_MPI_PIN_DOMAIN=auto" \
  -genv "KMP_AFFINITY=compact,granularity=fine,1" \
  cp2k/exe/Linux-x86-64-intel/cp2k.psmtp workload.inp
```

For an actual workload, one may try cp2k/tests/QS/benchmark/H2O-32.inp, or any workload under cp2k/tests/QS/benchmark\_sing For latter set of workloads however LIBINT and LIBXC may be required. The CP2K/intel branch aims to enable a

performance advantage by default. However, there are some options allowing to re-enable default behavior (compared to CP2K/trunk).

- **CP2K\_RECONFIGURE**: environment setting for reconfiguring CP2K (default depends on whether the ACCeleration layer is enabled or not). With the ACCeleration layer enabled, CP2K is reconfigured (as if CP2K\_RECONFIGURE=1 is set) e.g. an increased number of entries per matrix stack is populated, and otherwise CP2K is not reconfigured. Further, setting CP2K\_RECONFIGURE=0 is disabling the code specific to the Intel branch of CP2K, and relies on the (optional) LIBXSMM integration into CP2K 3.0 (and later).
- **MM\_DRIVER**: [http://manual.cp2k.org/trunk/CP2K\\_INPUT/GLOBAL/DBCSR.html#MM\\_DRIVER](http://manual.cp2k.org/trunk/CP2K_INPUT/GLOBAL/DBCSR.html#MM_DRIVER) gives a reference of the input keywords. For the CP2K/intel branch the MM\_DRIVER is set to XSMM by default (if LIBXSMMROOT was present).

## LIBINT and LIBXC Dependencies

To configure, build, and install LIBINT (Version 1.1.5 and 1.1.6 has been tested), one may proceed as shown below (please note there is no easy way to cross-build the library for an instruction set extension which is not supported by the compiler host). Finally, in order to make use of LIBINT, the key LIBINTROOT=\$(HOME)/libint needs to be supplied when building the CP2K application (make).

```
env \  
  AR=xiar CC=icc CXX=icpc \  
  ./configure --prefix=$(HOME)/libint \  
    --with-cc-optflags="-O1 -xHost" \  
    --with-cxx-optflags="-O1 -xHost" \  
    --with-libint-max-am=5 \  
    --with-libderiv-max-am1=4  
make  
make install  
make realclean
```

To configure, build, and install LIBXC (Version 2.2.2 has been tested), one may proceed as shown below. To actually make use of LIBINT, the key LIBXCROOT=\$(HOME)/libxc needs to be supplied when building the CP2K application (make).

```
env \  
  AR=xiar F77=ifort F90=ifort \  
  FC=ifort FCFLAGS="-O2 -xHost" \  
  CC=icc CFLAGS="-O2 -xHost" \  
  ./configure --prefix=$(HOME)/libxc  
make  
make install  
make clean
```

In case library needs to be cross-compiled, one may add --host=x86\_64-unknown-linux-gnu to the command line arguments of the configure script.

## Tuning

### Intel Xeon Phi Coprocessor

For those having an Intel Xeon Phi coprocessor in reach, an experimental code path using CP2K's ACCeleration layer (which was originally built for attached accelerators) is able to offload computation from the host system. However, the implementation leaves the host processor(s) unutilized (beside from offloading and transferring the work). Please note that although the host is only MPI-parallelized, the coprocessor uses OpenMP within each partition formed by a host-rank. For more details about affinizing the execution on the coprocessor, one may have a look at <https://github.com/hfp/mpirun>.

```
make ARCH=Linux-x86-64-intel VERSION=popt ACC=1 -j  
mpirun.sh -p8 -x exe/Linux-x86-64-intel/cp2k.popt workload.inp
```

For more details about offloading CP2K's DBCSR matrix multiplications to an Intel Xeon Phi Coprocessor, please have a look at <https://github.com/hfp/libxstream/raw/master/documentation/cp2k.pdf>. Further, cross-building CP2K for the Intel Xeon Phi coprocessor in order to run in a self-hosted fashion is currently out of scope for this document. However, running through CP2K's ACCeleration layer while executing on a host system is another possibility enabled by the universal implementation. However, the code path omitting the ACCeleration layer (see Running the Application) is showing better performance (although the code which is actually performing the work is the same).

```
make ARCH=Linux-x86-64-intel VERSION=psmp ACC=1 OFFLOAD=0 -j
```

## Eigenvalue Solvers for Petaflop-Applications (ELPA)

1. Download the latest ELPA from <http://elpa.rzg.mpg.de/elpa-tar-archive> (2015.05.001)
2. Make use of the `ELPAROOT` key-value pair (`ELPA=2` is used by default to rely on ELPA2).

## Memory Allocation Wrapper

Dynamic allocation of heap memory usually requires global book keeping eventually incurring overhead in shared-memory parallel regions of an application. For this case, specialized allocation strategies are available. To use the malloc-proxy of Intel Threading Building Blocks (Intel TBB), use the `TBBMALLOC=1` key-value pair at build time of CP2K. Usually, Intel TBB is just available due to sourcing the Intel development tools (see `TBBROOT` environment variable). To use `TCMALLOC` as an alternative, set `TCMALLOCROOT` at build time of CP2K by pointing to `TCMALLOC`'s installation path (configured with `./configure --enable-minimal --prefix=<TCMALLOCROOT>`).