BUILDING CP2K

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Machine Access

- Where can you run CP2K?
  - Own Laptop
    - Serial / OpenMP build
  - Institute workstation / cluster
  - ARCHER accounts
    - Cray XC30 @ EPCC
    - CP2K 3.0 psmp pre-installed
      - massively parallel calculations

  - Use "`qsub -q short`" for testing (<20m, < 8 nodes)

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Prerequisites - Environment

- POSIX-compliant OS
  - Linux, UNIX (e.g. AIX) …
  - Cygwin, Mac OS X also possible
- Build tools
  - GNU Make, Python 2.x (or later)
- Compilers
  - GNU gcc / gfortran 4.6 (or later)
  - Intel ifort 15.x (or later, 14.x possible with care)
  - IBM XLF 14.1

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Prerequisites - Libraries

- BLAS & LAPACK (required)
  - Vendor-tuned libraries preferred (MKL, ACML, ESSL)
  - Free auto-tuned libraries (GotoBLAS, ATLAS)
  - Reference BLAS + LAPACK from Netlib (last resort, very slow!)

- MPI & ScaLAPACK (required for MPI parallel build)
  - Usually provided by your cluster / HPC
  - Require MPI 2.x (3.x optional)
  - OpenMPI. MPICH, Intel MPI, Cray MPT all tested
  - ScaLAPACK provided by vendor maths libraries…
    - … or download from Netlib
  - `-D__parallel -D__SCALAPACK`

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Prerequisites - Libraries

- FFTW3 (Recommended)
  - CP2K has an inbuilt FFT implementation
  - FFTW3 will give much better performance
    - + freely available
    - + easy to compile / install
  - Enable using `-D__FFTW3`

Optional Libraries

- LibXC
  - CP2K has various common XC functionals e.g. PBE, LDA, BLYP…
  - Many more available via libxc
  - Version 2.2.2 or later
  - `-D__LIBXC` and `-I$(LIBXC_DIR)/include`
- Libint
  - Required for all hybrid functional calculations
  - Version 1.1.4 only
  - `-D__LIBINT`

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Optional Libraries

- ELPA
  - Optimised diagonalisation routines
  - Build process optimises for specific architecture
  - < June 2014 version : `-D__ELPA`
  - >= June 2014 and < Nov 2015 version : `-D__ELPA2`
  - >= Nov 2015 version : `-D__ELPA3`

- All other libraries / options / flags
  - See http://www.cp2k.org/howto:compile
  - and `cp2k/INSTALL`

- Auto-tuned performance libraries (libsmm, libgrid)
  - More on Tues…

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Arch files and compilation

- Compiler and architecture-specific options are given in an ‘arch file’
  - Examples in `cp2k/arch`
  - e.g. `Linux_x86-64-gfortran.popt`
  - Copy/customise for your environment

- To build CP2K
  - in the `cp2k/makefiles` directory:

corresponding to arch file

```
make -j 4 ARCH=Linux-x86-64-gfortran VERSION=popt
```

parallel build

Errors? Ask me!

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Arch files and compilation

- CP2K binary should be built in
  - `cp2k/exe/<ARCH>/cp2k.<VERSION>`
- Very quick test:

  `cp2k.sopt --version`

  - MPI binaries (`popt`) should be run with `mpirun`
  - Maybe within a batch script?
- Quick test
  - in the `cp2k/tests/QS` directory:

```
../../exe/ARCH/cp2k.sopt C.inp
```

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Testing CP2K

- CP2K comes with a suite of >2600 test input files

- Good for checking you have correctly compiled CP2K
  - Tests that all enabled features of CP2K run
  - Most tests compare against a reference result

- To execute regression tests:
  - Instructions in `cp2k/tools/regtesting`
  - Also online: http://cp2k.org/dev:regtesting

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Testing CP2K

- `do_regtest` script
  - SVN update, builds CP2K (`--nosvn -nobuild` to skip)
  - Runs all tests (in parallel, if possible)
  - Takes ~10 mins – a few hours
  - Summary of results and details of any failing tests

```
-------------------------------- Summary -------------------------------
Number of COMPILE warns 0
Number of FAILED  tests 2
Number of WRONG   tests 51
Number of CORRECT tests 2589
Number of NEW     tests 0
Total number of   tests 2642
```

Test failed to complete

Test completed, but does not match reference

Test completed for first time (and no reference result available)

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Testing CP2K

- Automatic testing on 30+ different platforms
  - Test failures automatically reported to developers
- Results available online at http://dashboard.cp2k.org
- Check here when using an SVN trunk version

Building CP2K

Questions?