Mathematical Libraries and Application Software on JURECA, Booster, and JUWELS

JSC Training Course

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JÜLICH Forschungszentrum | JÜLICH SUPERCOMPUTING CENTRE

Outline

- Navigating modules
- Compiling for the Booster
- Sequential Libraries
- Parallel Libraries and Application Systems:
  - Threaded Libraries
  - MPI parallel Libraries
  - Application Software
- Software for Materials Science
- Software for Computational Engineering
- Further Information

Modules environment

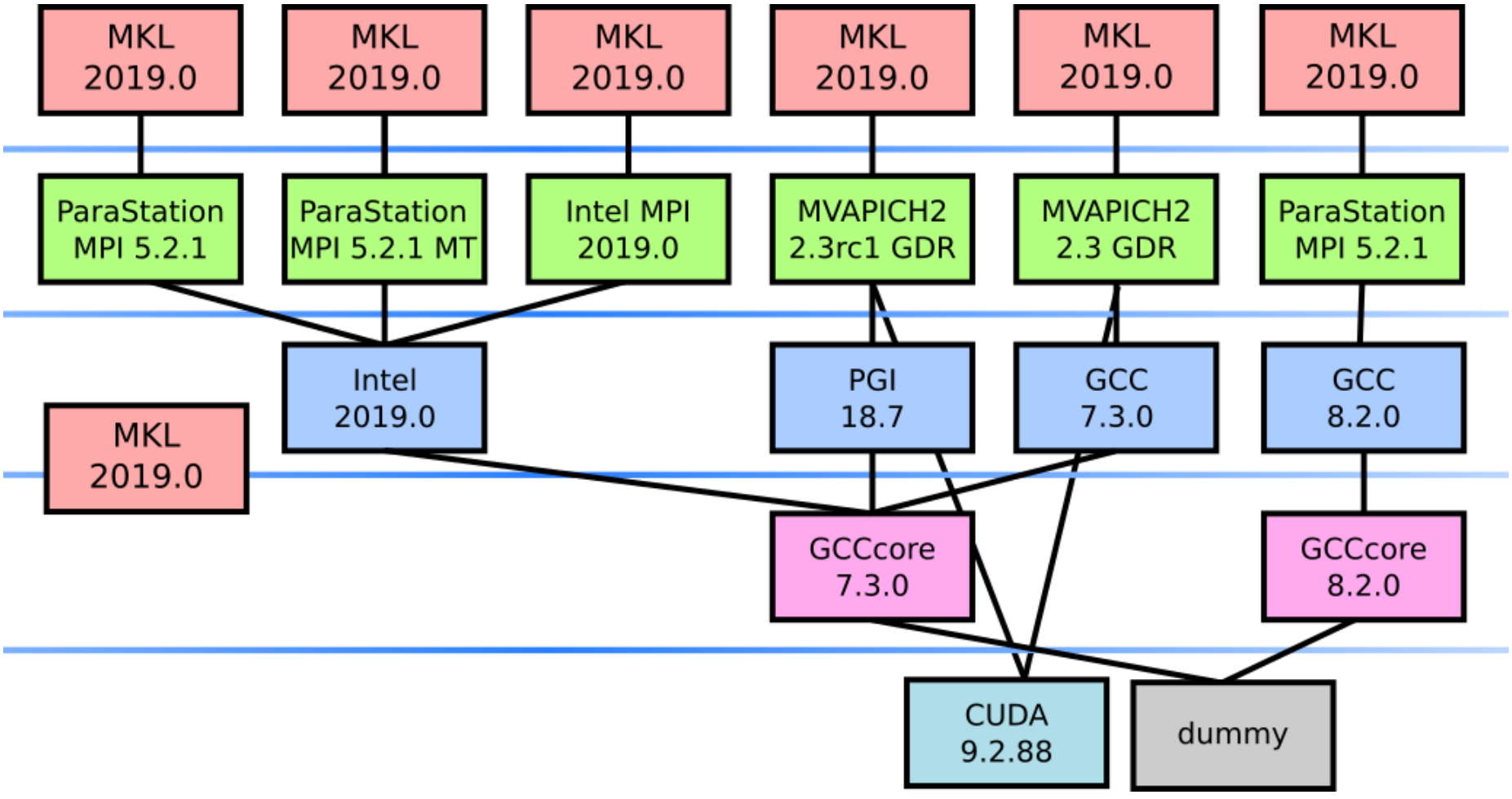

Figure: Current toolchain tree in JURECA and JUWELS

Modules environment

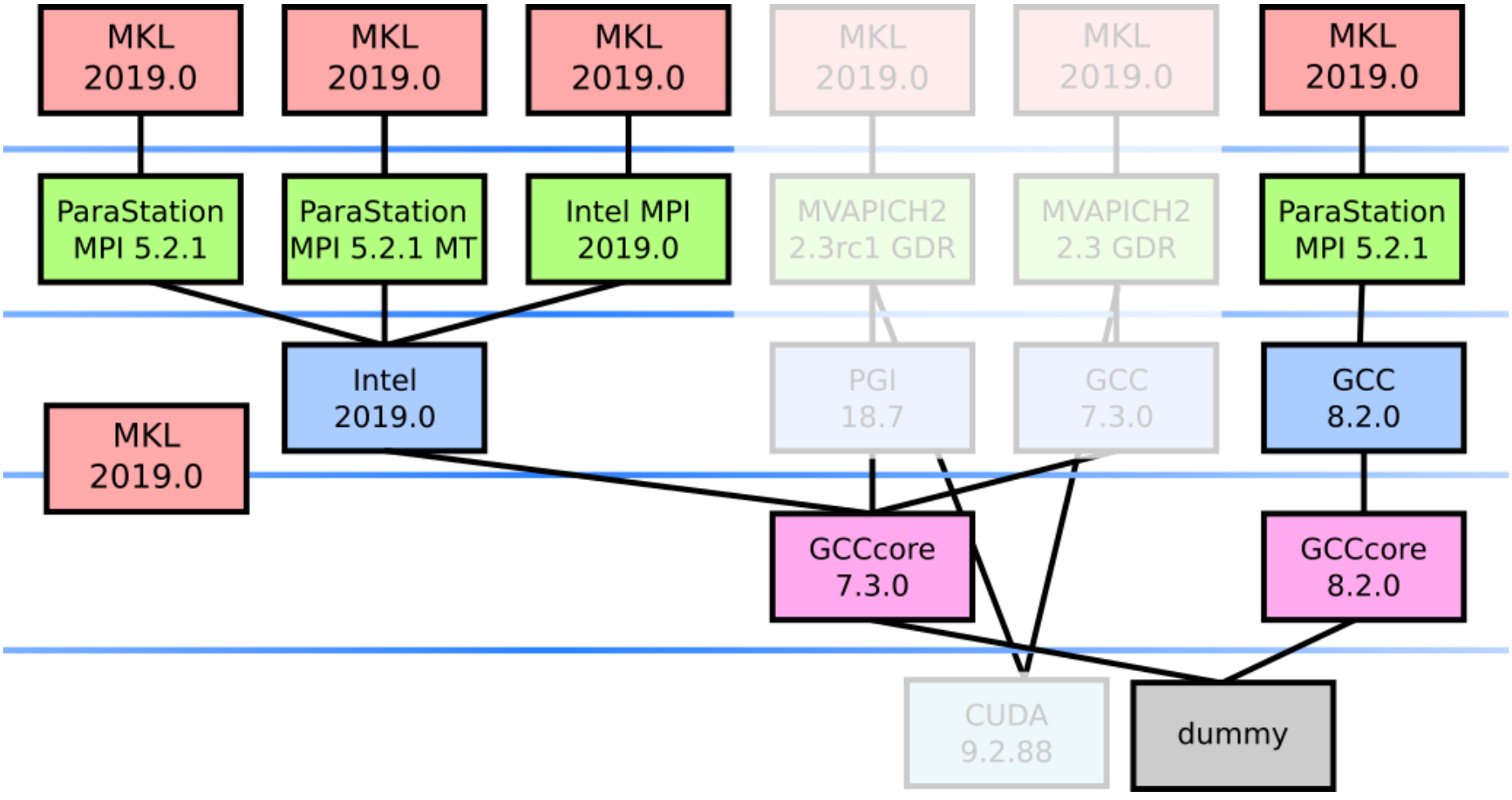

Figure: Current toolchain tree in Booster

Modules environment

Hierarchical modules

- `GCCcore/.7.3.0` is preloaded, which enables a lot of base software
- For HPC software you have to load a compiler, to expand the module tree

  `ml Intel`
- Then you load an MPI version

  `ml ParaStationMPI`

  Default version is `5.2.1-1` (ie: `MPI_THREAD_MULTIPLE` is not supported, you need `5.2.1-1-mt`)
- Then you can load any other packages

  `ml QuantumESPRESSO/6.3`

Modules environment

- After loading compiler and MPI `ml avail` shows the software available with that combination
- `ml avail` *name* and `ml help` *name* will show you details about the *name* package
- Many libraries are available for more than one combination/toolchain

- Write e-mail to `sc@fz-juelich.de` if you want special versions or new software
  - No guarantee the software will be installed
- $EBROOT*NAME* is the root directory where the library is installed

Modules environment

- `ml spider` *name* shows whether a library is available in the current stage and in which versions
- `ml spider` *name*/*version* shows which environment you have to load before you can load that version

- Many packages are hidden. To see them use
  `ml spider --show-hidden` *name*

Modules environment

- For R, Python and Perl we use bundles
  - You might be looking for a software package that is part of a bigger module
- Use `ml key software`
  `ml key numpy` will suggest `SciPy-Stack`
  - You might be looking for a software package that is part of a bigger module
- You can use then `ml spider` to find out how to load the module

Modules environment

Stages

- The whole software stack in JURECA, the Booster, and JUWELS is updated every 6 months
  - Right when there is an allocation for new projects
- Old stages are still accessible
- To check availability in other stages first type

  JURECA:

  ```
  ml use /usr/local/software/jureca/OtherStages
  ```

  Booster:

  ```
  ml use /usr/local/software/jurecabooster/OtherStages
  ```

  JUWELS:

  ```
  ml use /gpfs/software/juwels/otherstages
  ```

Compiling for the Booster (I)

- Cross-compilation on login nodes not recommended but technically possible
- `ml Architecture/KNL`
  - This should be the first module you load
  - Then you have the booster software stack available.
  - This doesn't work on the cluster compute nodes!

- Remember, cross-compiling is not recommended unless you know what you are doing

Compiling for the Booster (II)

Recommended way to compile for the Booster

- Start an interactive session, by
  `salloc --partition=develbooster`
- After the allocation is successful start a remote shell from within the salloc session and connect it to a pseudo terminal using
  `srun --cpu_bind=none --nodes=1 --pty /bin/bash -i`

- In batch scripts add
  `module load Architecture/KNL`
  before all other module commands

Sequential Libraries and Packages (I)

Remember that with intel compilers you need to link Fortran subroutines if using the C linker -lifcore -lifport

Vendor specific Libraries

- MKL Intel® Math Kernel Library
  versions as mentioned in general informations,
  2019.0.117 on JURECA, Booster, and JUWELS

For more information see
`http://www.fz-juelich.de/ias/jsc/EN/Expertise/Support/Software/SystemDependentLibraries/MKL.html?nn=1035570`

Sequential Libraries and Packages (II)

Public domain Libraries

- LAPACK (Linear Algebra PACKage)
- ARPACK (Arnoldi PACKage)
- GSL (Gnu Scientific Library)
- GMP (Gnu Multiple Precision Arithmetic Library)

Commercial library

NAG Fortran Library: JURECA only

Contents of Intel® MKL

- BLAS, Sparse BLAS, CBLAS
- LAPACK
- Iterative Sparse Solvers, Trust Region Solver
- Vector Math Library
- Vector Statistical Library
- Fourier Transform Functions
- Trigonometric Transform Functions

Contents of Intel® MKL

- GMP routines
- Poisson Library
- Interface for fftw

For more information see `http://www.fz-juelich.de/ias/jsc/EN/Expertise/Support/Software/SystemDependentLibraries/SystemDependentLibraries/MKL.html?nn=1035570`

Usage of MKL (I)

- Can be loaded with Intel compiler or GCC
- MPI has to be loaded before imkl
- FORTRAN, C, and C++ callable
- Arrays FORTRAN like, i.e. column-first (except cblas)
- Compilation and linking of program name.f calling sequential MKL routines:

```
ifort name.f -o name -lmkl_intel_lp64 -lmkl_sequential
-lmkl_core [-liomp5 -lpthread]
```

Usage of MKL (II)

To use CBLAS include mkl.h into source code

Compilation and linking of program name.c calling sequential MKL

```
icc name.c -o name -lmkl_intel_lp64 -lmkl_sequential
-lmkl_core [-liomp5 -lpthread -lifcore -lifport]
```

For flags to compile with other compilers (PGI, GCC) or multithreaded versions take a look at:

`https://software.intel.com/en-us/articles/intel-mkl-link-line-advisor`

LAPACK

- Part of MKL in libmkl_core.a
- Can be loaded with Intel or GCC on JURECA, Booster, and JUWELS
- In older Stages also part of OpenBLAS with GCC (JURECA only)

Arpack

- ARPACK-NG/3.6.3
- Iterative solver for sparse eigenvalue problems
- Reverse communication interface
- FORTRAN 77
- Calls LAPACK and BLAS routines, MKL necessary

GSL – GNU Scientific Library

- `module load Intel GSL/2.5`
  for icc version on JURECA and JUWELS
- `module load GCC/8.2.0 GSL/2.5`
  for gcc version on JURECA and JUWELS
- Provides a wide range of mathematical routines
- Not recommended for performance reasons
- Often used by configure scripts

GMP- GNU Multiple Precision Library

version 6.1.2 on JURECA

NAG Libraries

- NAG Fortran Mark 26 on JURECA only available with Intel compiler
- Please tell us if you really need it

Parallel Libraries

Threaded Parallelism I

- MKL
  is multi-threaded when linked with
  `-lmkl_[intel,gnu,pgi]_threaded`
  if OMP_NUM_THREADS is not set,
  48 threads used on JURECA
  68 threads on Booster
  96 threads on JEWELS (80 in accelerated nodes)
  Usage:
  ```
  ifort name.f -o name -lmkl_intel_lp64
  -lmkl_intel_thread -lmkl_core -liomp5 -lpthread
  ```
- FFTW 3.3 (Fastest Fourier Transform of the West)
  MPI, OpenMP and threads version
  http://www.fftw.org

Parallel Libraries

MPI Parallelism

- ScaLAPACK (Scalable Linear Algebra PACKage)
- ELPA (Eigenvalue SoLvers for Petaflop-Applications)
- Elemental, C++ framework for parallel dense linear algebra
- FFTW (Fastest Fourier Transform of the West)
- MUMPS (MUltifrontal Massively Parallel sparse direct Solver) not yet on Booster
- ParMETIS (Parallel Graph Partitioning)
- Hypre (high performance preconditioners)

MPI Parallelism (II)

- PARPACK (Parallel ARPACK), Eigensolver
- SPRNG (Scalable Parallel Random Number Generator)
- SUNDIALS (SUite of Nonlinear and DIfferential/ALgebraic equation Solvers)
- All three not yet on Booster

Parallel Systems, MPI Parallelism

- PETSc, toolkit for partial differential equations

ScaLAPACK

- part of MKL,
- Parallel BLAS 1-3, PBLAS Version 2
- Dense linear system solvers
- Banded linear system solvers
- Solvers for Linear Least Squares Problem
- Singular value decomposition
- Eigenvalues and eigenvectors of dense symmetric/hermitian matrices
- `http://www.netlib.org/scalapack/index.html`

Usage of ScaLAPACK

Linking a program name.f calling routines from ScaLAPACK, default version, Intel compiler:

```
mpif77 name.f -lmkl_scalapack_lp64
-lmkl_blacs_intelmpi_lp64 -lmkl_intel_lp64
-lmkl_intel_thread[-lmkl_sequential]
-lmkl_core -liomp5 -lpthread
```

ELPA

Eigenvalue SoLvers for Petaflop-Applications

ELPA uses ScaLAPACK, must be linked together with scalapack

- FORTRAN 95, same data-distribution as ScaLAPACK
- `http://elpa.rzg.mpg.de/elpa-english?set_language=en`
- JURECA pure MPI and hybrid version 2018.05.001
- Version with GPU acceleration on JURECA and JUWELS
- Booster and JUWELS special version with AVX512 kernels for ELPA2

Elemental

- C++ framework, two-dimensional data distribution element by element
- `http://libelemental.org/about/`
- 0.87.7

MUMPS

MUltifrontal Massively Parallel sparse direct Solver

- Solution of linear systems with symmetric positive definite matrices, general symmetric matrices, general unsymmetric matrices
- Real or Complex
- Parallel factorization and solve phase, iterative refinement and backward error analysis
- F90 with MPI and OpenMP since 5.1.1
- current version 5.1.2
- `http://graal.ens-lyon.fr/MUMPS/`

ParMETIS

Parallel Graph Partinioning and Fill-reducing Matrix Ordering
developed in Karypis Lab at the University of Minnesota
4.0.3 on JURECA
http://glaros.dtc.umn.edu/gkhome/metis/parmetis/overview
Version with double precision real values available

Hypre

High performance preconditioners
Version 2.15.0 on JURECA and JUWELS, also version with bigint,
http://www.llnl.gov/CASC/hypre/software.html

FFTW

3.3.8 on JURECA and JUWELS, (Intel and GCC modules)

PARPACK

- PARPACK MPI-Version, part of ARPACK-NG/3.6.3
- Must be linked with LAPACK and BLAS
- Reverse communication interface, user has to supply parallel matrix-vector multiplication

`https://github.com/opencollab/arpack-ng`
`http://www.caam.rice.edu/~kristyn/parpack_home.html`

SPRNG

The Scalable Parallel Random Number
not yet on Booster
Generators Library for ASCI Monte Carlo Computations
version 5.0:
various random number generators in one library
Version 1.0 seperate library for each random number generator
http://sprng.cs.fsu.edu/

Sundials (CVODE)

Package for the solution of ordinary differential equations, Version 3.2.1
not yet on Booster
https://computation.llnl.gov/casc/sundials/main.html

PETSc

- Portable, Extensible Toolkit for Scientific Computation
- Numerical solution of partial differential equations
- version 3.10.2
- with several other packages included
- complex version and version with 8-Byte integer
- debug versions in Devel Stages only
- http://www.mcs.anl.gov/petsc/
- `ml spider petsc`

Software for Materials Science

Package	JURECA	JUWELS
Abinit	yes	yes
ADF	yes	no
Amber	yes	yes
CP2K	yes	yes
CPMD	yes	no
GPAW	yes	yes
Gromacs	yes	yes
LAMMPS	yes	yes
Molpro	yes	no
NAMD	yes	yes
NWChem	yes	no
QuantumEspresso	yes	yes
TURBOMOLE	yes	no

Software for Computational Engineering

- JURECA and JUWELS
- CFD Package **OpenFOAM**
  Version 4.1 in Stages/2017b and some older versions in older stages
  and OpenFOAM-Extend 3.1 and 3.2, only in older stages
- Commercial **FEM Software**
  - **ANSYS**, **LS-DYNA** , **COMSOL** are technically maintained on **JURECA** only
  - **Licenses** must be provided by the **User !**

Further information and JSC-people

http://www.fz-juelich.de/ias/jsc/jureca
http://www.fz-juelich.de/ias/jsc/EN/Expertise/Support/Software/_node.html

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