Mathematical Libraries and Application Software on JURECA and Booster

JSC Training Course

June 2018 | I. Gutheil, D. Alvarez | JSC
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
Figure: Current toolchain tree in JURECA
Modules environment

Figure: Current toolchain tree in Booster
Hierarchical modules

- GCCcore/.5.5.0 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
- Then you can load any other packages
  - ml QuantumESPRESSO/6.2
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 and the Booster 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
  `ml use /usr/local/software/jureca[booster]/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
Vendor specific Libraries

- MKL Intel® Math Kernel Library versions as mentioned in general informations, 2018.2.199 on JURECA and Booster
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

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

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

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

Arpack

- ARPACK-NG/3.5.0
- 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-para GSL/2.4 for icc version on JURECA
- module load GCC/7.3.0 ParaStationMPI[/5.2.1-1] GSL/2.4 for gcc version on JURECA
- 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
MKL (JURECA) is multi-threaded if OMP_NUM_THREADS not set, 48 threads used on JURECA 68 threads on Booster

Usage:
```bash
ifort name.f -o name -lmkl_intel_lp64 -lmkl_intel_thread -lmkl_core -liomp5 -lpthread
```
Parallel Libraries
Threaded Parallelism II

- FFTW 3.3 (Fastest Fourier Transform of the West) 3.3.7 on JURECA Intel compiler and GCC 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 on JURECA

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 uses ScaLAPACK, must be linked together with scalapack

- FORTRAN 95, same data-distribution as ScaLAPACK
- JURECA pure MPI and hybrid version 2017.11.001
- Booster 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 Partitioning 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

Hypre

FFTW

3.3.7 on JURECA, (Intel and GCC modules) all with MPI parallel version

PARPACK

- PARPACK MPI-Version, part of ARPACK-NG/3.5.0
- 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_pack.html
SPRNG

The Scalable Parallel Random Number Generators Library for ASCI Monte Carlo Computations
version 5.0:
various random number generators in one library
Version 1.0 separate library for each random number generator
http://sprng.cs.fsu.edu/

Sundials (CVODE)

Package for the solution of ordinary differential equations, Version 3.1.0
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 3.9.0
- 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

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<th>JURECA</th>
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<td>NWChem</td>
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<td>QuantumEspresso</td>
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</tr>
<tr>
<td>TURBOMOLE</td>
<td>yes</td>
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</tbody>
</table>
Software for Computational Engineering

- JURECA only
- 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
  - 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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