

Mathematical Libraries and Application Software on JURECA and JUQUEEN

JSC Training Course

Outline

- General Informations
- Sequential Libraries
- Parallel Libraries and Application Systems:
 - Threaded Libraries
 - MPI parallel Libraries
 - Application Software
- Software for Materials Science
- Software for Computational Engineering
- Further Information

General Informations JUQUEEN

- All libraries as modules in `/bgsys/local/name`
- `module avail` lists names of available libraries
- `module avail name` lists available versions on *name*
- `module help name` tells how to use library
- `module load name` sets environment variables for `-L$(NAME_LIB)` and `-I$(NAME_INCLUDE)` to include in makefile
- Link sequence important, `.o` always before the libraries, sometimes double linking necessary
- Linking Fortran subroutines with the C linker needs
`mpixlc_r name.c -L/opt/ibmcmp/xlf/bg/14.1/bglib64
-lxl -lxlopt -lxlf90_r -lxlfmath -lm -lrt`

General Informations JURECA (I)

- `module spider name` shows whether a library is available in the current stage and in which versions
- `module spider name/version` shows which environment you have to load before you can load that version
- to check availability of other versions first say
`module use /usr/local/software/jureca/OtherStages`
after that
`module spider name`
shows all available versions of the software
(currently not working as expected)

General Informations JURECA (II)

- First you have to load a compiler,
module load Intel loads the current default intel compilers
version 2018.0.128,
- Then you load an MPI version
module load ParaStationMPI loads the single threaded
version of ParaStation MPI version 5.2.0-1
- module load imkl loads MKL 2018.0.128
- module load intel-para still works and loads the current
default intel compiler with ParaStationMPI and MKL

General Informations JURECA (III)

- after loading compiler and MPI module `avail` shows the software available with that environment
- `module avail name` and `module help name` also only work after loading a compiler and, if necessary MPI and imkl
- Many libraries available for more than one environment
- Write e-mail to sc@fz-juelich.de if you want special versions or new software
- `$EBROOTNAME` is the root directory where the library is installed, for most libraries `$NAME_ROOT` is also set
- Linking Fortran subroutines with the C linker requires `-lifcore -lifport` in the link command

Sequential Libraries and Packages (I)

Vendor specific Libraries

JURECA

- MKL Intel® Math Kernel Library
versions as mentioned in general informations,
2018.0.128 on JURECA

JUQUEEN

- ESSL (Engineering and Scientific Subroutine Library)
version 5.1.1-3 in /bgsys/local/lib

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: JUQUEEN and JURECA

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>

Contents of ESSL Version 5.1.1-3

Bibliotheken von den Herstellern

- BLAS level 1-3 and additional vector, matrix-vector, and matrix-matrix operations
- Sparse vector and matrix operations
- LAPACK computational routines for linear equation systems and eigensystems
- Banded linear system solvers
- Linear Least Squares
- Fast Fourier Transforms

Contents of ESSL Version 5.1.1-3 (II)

- Numerical Quadrature
- Random Number Generation
- Interpolation

For further information see

IBM Engineering and Scientific Subroutine Library for Linux on
POWER V5.1:

Guide and Reference

[http:](http://www.fz-juelich.de/ias/jsc/EN/Expertise/Support/Software/SystemDependentLibraries/ESSL_ESSL SMP.html)

[//www.fz-juelich.de/ias/jsc/EN/Expertise/Support/
Software/SystemDependentLibraries/ESSL_ESSL SMP.html](http://www.fz-juelich.de/ias/jsc/EN/Expertise/Support/Software/SystemDependentLibraries/ESSL_ESSL SMP.html)

Link to IBM documents Guide and Reference

Usage of MKL on JURECA (I)

- 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 on JURECA(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]
```

Usage of ESSL

- FORTRAN, C , and C++ callable,
- Arrays FORTRAN like, i.e. column-first
- Header file `essl.h` for C and C++
- Installed in `/bgsys/local/lib` (not as module)

Usage of ESSL (II)

Compilation and linking of program name.f calling ESSL routines

```
mpixlf90_r name.f -L/bgsys/local/lib -lesslbg
```

Compilation and linking of program name.c calling ESSL routines

```
mpixlc_r name.c -I/opt/ibmmath/essl/5.1/include  
-L/bgsys/local/lib -lesslbg  
-L/opt/ibmcmp/xlf/bg/14.1/bglib64 -lxl -lxlopt  
-lxlf90_r -lxlfmath -lm -lrt
```


LAPACK (I)

- Part of MKL on JURECA in libmkl_core.a
- Part of OpenBLAS/0.2.20 on JURECA if GCC is loaded
- Public domain version 3.6.0 and 3.7.0 on JUQUEEN
- Must be used together with ESSL (or ESSLsmp)
- Some routines already in ESSL
- Attention, some calling sequences are different!
- Experimental LAPACK header file available for C-usage of lapack on JUQUEEN
- Experimental C-LAPACK, liblapacke.a (3.6.0 and 3.7.0) on JUQUEEN

LAPACK (II)

Compilation and linking of FORTRAN program name.f calling LAPACK routines

JURECA: (see usage of MKL),

JUQUEEN:

```
module load lapack/3.7.0[_g][_simd]
mpixlf90_r name.f -Wl,-allow-multiple-definition
-L/bgsys/local/lib [-lessl[smp]bg] -L$(LAPACK_LIB)
-llapack -lessl[smp]bg
```

ESSL must be linked after LAPACK to resolve references, linking `essl[smp]` also before `lapack` takes `lapack` routines from `essl`

Arpack

- ARPACK, ARnoldi PACKAge, Version 2.1 and arpack-ng/3.5.0 on JUQUEEN
- ARPACK-NG/3.5.0 on JURECA
- Iterative solver for sparse eigenvalue problems
- Reverse communication interface
- FORTRAN 77
- Calls LAPACK and BLAS routines

GSL – GNU Scientific Library

- Version 2.1 on JUQUEEN (xlc), 2.4 JURECA (gcc and icc)
- Provides a wide range of mathematical routines
- Not recommended for performance reasons
- Often used by configure scripts
- `module load gsl/2.1_strict[opt] [g] JUQUEEN`
- `module load intel-para GSL/2.4`
for icc version on JURECA
- `module load GCC ParaStationMPI[/5.2.0-1] GSL/2.4`
for gcc version on JURECA

GMP- GNU Multiple Precision Library

Version 6.1.0 compiled with GCC on JUQUEEN,
version 6.1.2 on JURECA

NAG Libraries

- NAG Fortran Mark 22 on JUQUEEN: as module more than 1600 user-callable routines
- Mark 26 on JURECA only available with Intel compiler
- Please tell us if you really need it

Parallel Libraries

Threaded Parallelism I

- MKL (JURECA)
is multi-threaded or at least thread-safe
if OMP_NUM_THREADS not set, 48 threads used on
JURECA
Usage:

```
ifort name.f -o name -lmkl_intel_lp64  
-lmkl_intel_thread -lmkl_core -liomp5 -lpthread
```

Parallel Libraries

Threaded Parallelism II

- ESSLsmp 5.1.1-3 (JUQUEEN)

Usage: Fortran:

```
mpixlf90_r name.f -L/bgsys/local/lib -lesslsmpbg
```

C:

```
mpixlc_r name.c -L/bgsys/local/lib -lesslsmpbg  
-L/opt/ibmcmp/xlsmp/3.1/bglib64 -lxlsmp  
-I/opt/ibmmath/essl/5.1/include  
-L/opt/ibmcmp/xlf/bg/14.1/bglib64 -lxlf90_r -lxl  
-lxlfmath -lxlopt -lm -lrt -ldl
```

- FFTW 3.3 (Fastest Fourier Transform of the West)
Sequential, threaded, and OpenMP version on JUQUEEN
3.3.6 on JURECA Intel compiler and GCC

<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)
- 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)

Parallel Systems, MPI Parallelism

- PETSc, toolkit for partial differential equations

ScaLAPACK

JURECA: part of MKL with Intel compiler,
ScaLAPACK/2.0.2-OpenBLAS-0.2.20 with GCC

JUQUEEN: ScaLAPACK Release 2.0.2, contains already
BLACS

- FORTRAN, also C-Interface, scalapack.h incomplete
- LAPACK has to be linked, too, \$LAPACK_DIR set when loading scalapack
- <http://www.netlib.org/scalapack/index.html>

Contents of ScaLAPACK

- 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

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
```

Usage on JUQUEEN

Compilation and linking of a program name.f calling ScaLAPACK routines:

```
module load scalapack/2.0.2[_g] [-simd]
mpixlf90_r name.f -L$SCALAPACK_LIB -lscalapack
-L$LAPACK_LIB -llapack
-L/bgsys/local/lib -lessl[smp]bg
```

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
- JUQUEEN pure MPI and hybrid version 2015.11.001 and 2016.05.003
- JURECA pure MPI and hybrid version 2017.05.002

Elemental

- C++ framework, two-dimensional data distribution element by element
- <http://libelemental.org/about/>
- 0.87.7 on JURECA, hybrid version
- 0.85 on JUQUEEN only available with CLANG compiler, pure MPI version

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
- Version 5.0.0 and 5.1.1 on JUQUEEN, version 5.1.1 on JURECA
- <http://graal.ens-lyon.fr/MUMPS/>

ParMETIS

Parallel Graph Partitioning and Fill-reducing Matrix Ordering
developed in Karypis Lab at the University of Minnesota
Version 3.2.0 and 4.0.3 on JUQUEEN, 4.0.3 on JURECA

[http:](http://glaros.dtc.umn.edu/gkhome/metis/parmetis/overview)

[//glaros.dtc.umn.edu/gkhome/metis/parmetis/overview](http://glaros.dtc.umn.edu/gkhome/metis/parmetis/overview)

Hypre

High performance preconditioners

Version 2.12.1 on JURECA, also version with bigint,
2.9.0b, 2.10.1, and 2.11.1 also version with bigint, on JUQUEEN,
bigint cannot be used together with essl

<http://www.llnl.gov/CASC/hypre/software.html>

FFTW

- Version 2.1.5, this old version contains an old MPI-parallel version of FFTW on JUQUEEN
(`module avail fftw2`)
- Version 3.3.2 and 3.3.3 on JUQUEEN,
3.3.6 on JURECA, (Intel and GCC modules)
all with MPI parallel version
On JUQUEEN ask
`module avail fftw3`

PARPACK

- ARPACK Version 2.1 and arpack-ng/3.5.0 JUQUEEN
- ARPACK-NG/3.5.0 on JURECA
- PARPACK MPI-Version
- 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 Generators Library for
ASCI Monte Carlo Computations

Version 2.0 [JUQUEEN] and 5.0[JURECA]:

various random number generators in one library

Version 1.0 separate library for each random number generator,
on JUQUEEN and JURECA

<http://sprng.cs.fsu.edu/>

Sundials (CVODE)

Package for the solution of ordinary differential equations,
Version 2.6.2 on JUQUEEN and 3.0.0 JURECA

[https:](https://computation.llnl.gov/casc/sundials/main.html)

[//computation.llnl.gov/casc/sundials/main.html](https://computation.llnl.gov/casc/sundials/main.html)

PETSc

- Portable, Extensible Toolkit for Scientific Computation
- Numerical solution of partial differential equations
- version 3.7.3 on JUQUEEN and 3.8.0 on JURECA
- with several other packages included on both systems
- complex version and version with 8-Byte integer
- <http://www.mcs.anl.gov/petsc/>
- JUQUEEN:

```
module avail petsc
```

```
module help petsc/[whatever version you want]
```
- JURECA:

```
module spider petsc
```

Software for Materials Science

| Package | JUQUEEN | JURECA |
|-----------------|---------|--------|
| Abinit | | yes |
| ADF | | yes |
| Amber | | yes |
| CP2K | yes | yes |
| CPMD | yes | yes |
| Gromacs | yes | yes |
| LAMMPS | yes | yes |
| Molpro | | yes |
| NAMD | yes | yes |
| NWChem | | yes |
| QuantumEspresso | yes | yes |
| TURBOMOLE | | yes |

Software for Computational Engineering

- CFD Package **OpenFOAM** is installed on
JUQUEEN Versions 2.1.1
JURECA Version 4.1 and some older versions
and OpenFOAM-Extend 3.1 and 3.2, only in
older stages up to now
- 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/juqueen>

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

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