

# Mathematical Libraries and Application Software on JUQUEEN and JURECA

## 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

## General Informations JURECA (II)

- First you have to load a compiler,  
module load Intel loads the current default intel compilers  
version 2017.2.174,
- Then you load an MPI version  
module load ParaStationMPI loads the single threaded  
version of ParaStation MPI version 5.1.9-1
- module load imkl loads MKL 2017.2.174
- 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](mailto: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,  
2017.2.174 on JURECA

#### JUQUEEN

- ESSL (Engineering and Scientific Subroutine Library)  
version 5.1 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

- 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 (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/0.2.19-LAPACK-3.7.0 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/3.4.0 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), 2.3 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/2.3`  
for icc version on JURECA
- `module load GCC ParaStationMPI/5.1.9-1 GSL/2.3`  
for gcc version 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 (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-0.2.19-LAPACK-3.7.0 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](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 2016.05.004

## 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 2.11.2 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/3.4.0 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](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 2.7.0 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 3.7.6 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** Versions 2.0.1, 2.2.2, 2.3.1, 2.4.0. 3.0.0,  
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](http://www.fz-juelich.de/ias/jsc/EN/Expertise/Support/Software/_node.html)

### **Mailto**

Supercomputer support:

[sc@fz-juelich.de](mailto:sc@fz-juelich.de)

I. Gutheil: Parallel mathematical Libraries

[i.gutheil@fz-juelich.de](mailto:i.gutheil@fz-juelich.de)

B. Körfgen: Physics and Engineering software

[b.koerfgen@fz-juelich.de](mailto:b.koerfgen@fz-juelich.de)