

# 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 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/xf/bg/14.1/bglib64  
-lxl -lxlopt -lxlf90_r -lxlfmath -lm -lrt`

## General Informations JURECA (I)

- `module spider name` shows whether a library is available and how to load it
- First you have to load a compiler,  
`module load Intel` loads the current default Intel compilers version 2016.2 **without MKL**
- Then you load a MPI version  
`module load ParaStationMPI` loads the single threaded version of ParaStation MPI version 5.1.5
- `module load intel-para` still works and loads the current default Intel compiler with ParaStationMPI **including MKL** Version 11.3.2
- after loading compiler and MPI `module avail` shows the software available with that environment

## General Informations JURECA (II)

- 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
- 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,  
11.3.2 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 11.\*

- 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 11.\*

- GMP routines
- Poisson Library
- Interface for FFTW

For more information see <http://www.fz-juelich.de/ias/jsc/EN/Expertise/Support/Software/SystemDependentLibraries/MKL.html?nn=1742064>

## 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
```

or for threaded version:

```
ifort name.f -o name -lmkl_intel_lp64  
-lmkl_intel_thread -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 (for Intel and PGI compiler)
- Part of OpenBLAS on JURECA (for GCC)
- Public domain version (3.4.2) 3.5.0, and 3.6.0 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 in versions 3.4.2, 3.5.0, and 3.6.0 on JUQUEEN



## LAPACK (II)

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

**JURECA:** (see usage of MKL),

**JUQUEEN:**

```
module load lapack/3.6.0[_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
- module ARPACK-NG/3.3.0 on JURECA
- Iterative solver for sparse eigenvalue problems
- Reverse communication interface
- FORTRAN 77
- Calls LAPACK and BLAS routines

## GSL – GNU Scientific Library

- Version 1.15 on JUQUEEN,  
2.1 with gcc and icc on JURECA
- Provides a wide range of mathematical routines
- Not recommended for performance reasons
- Often used by configure scripts
- `module load gsl/1.15_03 JUQUEEN`
- `module load Intel GSL/2.1`  
for icc version on JURECA
- `module load GCC GSL/2.1`  
for gcc version on JURECA

## NAG Libraries

- NAG Fortran Mark 22 on JUQUEEN: as module more than 1600 user-callable routines
- Mark 24 on JURECA only available with Intel compiler

## Parallel Libraries

### Threaded Parallelism I

- MKL (JURECA)  
is multi-threaded or at least thread-safe  
usage as with sequential routines  
if OMP\_NUM\_THREADS not set, 48 threads used on  
JURECA  
always use  

```
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:

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

- FFTW 3.3 (Fastest Fourier Transform of the West)  
Sequential, threaded, and OpenMP version on JUQUEEN  
FFTW 3.3.4 on JURECA for Intel and GCC modules  
<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 (JURECA only)
- 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-0.2.15-LAPACK-3.6.0 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_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 2014.06 and 2015.11
- JURECA pure MPI and hybrid version 2015.11.001

## Elemental

- C++ framework, two-dimensional data distribution element by element
- <http://libelemental.org/about/>
- 0.85 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 and MPI
- Version 4.10.0 and 5.0.0 on JUQUEEN, version 5.0.1 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 4.0.2 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 2.11.0 on JURECA, also version with bigint,  
2.8.0b and 2.9.0b, 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 JURECA and JUQUEEN
- Version 3.3.2 and 3.3.3 on JUQUEEN, 3.3.4 on JURECA  
all with MPI parallel version
- <http://www.fftw.org>

## PARPACK

- ARPACK Version 2.1 on JUQUEEN
- module ARPACK-NG/3.3.0 on JURECA
- PARPACK MPI-Version
- Must be linked with LAPACK and BLAS
- Reverse communication interface, user has to supply parallel matrix-vector multiplication

[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,  
Versions 2.6.1 on JUQUEEN and 2.6.2 on 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 3.6.0 on JUQUEEN, 3.7.0 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
ADF		yes
Amber		yes
CP2K	yes	yes
CPMD	yes	yes
GPAW	planned	yes
Gromacs	yes	yes
LAMMPS	yes	yes
Molpro		yes
NAMD	yes	yes
NWChem		yes
QuantumEspresso		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
- 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:

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