

# Mathematical Libraries and Application Software on JUROPA, JUGENE, and JUQUEEN

## JSC Training Course

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# Outline

- General Informations
- Sequential Libraries
- Parallel Libraries and Application Systems:
  - Threaded Libraries
  - MPI parallel Libraries
  - Application Software
- Further Information

# General Informations JUROPA (I)

- Five compiler versions
- Default: Intel 11.1.072 with MKL 10.2.5.035
- Module: Intel 11.0.074 with MKL 10.1.0
- Module: Intel 11.1.059 with MKL 10.2.2.025
- Module: Intel 12.0.3 or 12.0.4, MKL included
- Module: Intel 12.1.1, MKL included
- module unload intel, module unload mkl  
before loading a new intel (and MKL) Module

## General Informations JUROPA (I)

- Most libraries compiled with 11.1.059 and MKL 10.2.2.025, new versions with 12.0 or 12.1
- Module unload and module load must be called in batch scripts before execution, too
- Starting with intel/12.0.3 MKL is included with module load intel/12.\*
- For most libraries versions compiled with intel/12.0.\* and/or 12.1.\* available

## General Informations JUROPA (II)

- `module avail` shows what is available
- `module help name` shows how to use the library
- `module load name` prepends `LD_LIBRARY_PATH` and `INCLUDE` and sets `NAME_ROOT` to the correct directory
- Link sequence important, `.o` always before the libraries, sometimes double linking necessary

## General Informations JUGENE (I)

- 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$(*_LIB)` and `-I$(*_INCLUDE)` to include in makefile
- Link sequence important, `.o` always before the libraries, sometimes double linking necessary

## General Informations JUGENE (II)

- Up to now all libraries compiled with `-qarch=450`, to avoid misaligned variables calling programs must be compiled in the same way, compiler default is `-qarch=450d`
- Additional version with `-qarch=450d` for most libraries
- Additional version compiled with `-g` for most libraries
- See module avail for additional versions

## General Informations JUQUEEN (I)

- 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$(*_LIB)` and `-I$(*_INCLUDE)` to include in makefile
- Link sequence important, `.o` always before the libraries, sometimes double linking necessary



## General Informations JUQUEEN (II)

- First all libraries will be compiled with `-O3 -qstrict -g -qsimd=noauto`
- Additional version compiled without `-g` will be added
- Perhaps later on versions with `simd`, too
- See module avail for available versions
- Only the most recent versions will be installed

# Sequential Libraries and Packages (I)

## Vendor specific libraries

### **JUROPA only:**

- MKL Intel® Math Kernel Library

### **JUGENE and JUQUEEN:**

- ESSL (Engineering and Scientific Subroutine Library)

# Sequential Libraries and Packages (II)

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

# Contents of Intel® MKL 10.\*

- 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 10.\*

- GMP routines
- Poisson Library
- Interface for fftw

For more information see

*[.../JUROPA/Documentation/Documentation\\_node.html](#)*

# Contents of ESSL Version 4.4(JUGNE) and 5.1(JUQUEEN)

- 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

- Numerical Quadrature
- Random Number Generation
- Interpolation

All routines are thread-safe,  
i.e. can be used within OpenMP threads

For further information see

*IBM Engineering and Scientific Subroutine Library for Linux on POWER  
Version 4 Release 3 or Version 5.1:*

## **Guide and Reference**

[\*.../Support/Software/SystemDependentLibraries/ESSL.html\*](#)

Guide and Reference (Link to IBM documents)

## Usage of MKL (I)

- FORTRAN, C , and C++ callable
- Arrays FORTRAN like, i.e. column-first
- Three versions, old 10.1.0 and two variants of 10.2
- starting with intel/12.0.3 included in intel module

Compilation and linking of program name.f calling sequential MKL routines, default version

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



## Usage of MKL (II)

Compilation and linking of program name.f calling sequential MKL routines starting with intel/12.0.3

```
module unload mkl
module switch intel intel/12.0.3
ifort name.f -o name
-lmkl_intel_lp64 -lmkl_intel_thread
-lmkl_core -liomp5 -lpthread
```

Linking of MKL always dynamic, so modules must be switched before execution, too

## Usage of MKL (III)

To use CBLAS include mkl.h into source code

Compilation and linking of program name.c calling sequential MKL routines

```
[module unload mkl  
module switch intel intel/12.0.3]  
icc name.c -o name -lmkl_intel_lp64  
-lmkl_intel_thread -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` on JUGENE (not as module)
- Installed in `/opt/ibmmath/essl/5.1/lib64` on JUQUEEN

## Usage of ESSL II

Compilation and linking of program name.f calling ESSL routines

### JUGENE:

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

### JUQUEEN:

```
mpixlf90_r name.f  
-L/opt/ibmmath/essl/5.1/lib64 -lesslbg
```

## Usage of ESSL III

Compilation and linking of program name.c calling ESSL routines

### JUGENE:

```
mpixlc_r name.c -L/usr/local/lib  
-lesslbg -lm  
-L/opt/ibmcmp/xlf/bg/11.1/lib -lxl  
-lxlopt -lxlf90_r -lxlfmath  
-L/opt/ibmcmp/xlsmp/bg/1.7/lib -lxlomp_ser  
-lpthread
```

## Usage of ESSL IV

Compilation and linking of program name.c calling ESSL routines

**JUQUEEN:**

```
mpixlc_r name.c  
-I/opt/ibmmath/essl/5.1/include  
-L/opt/ibmmath/essl/5.1/lib64  
-lesslbg  
-L/opt/ibmcmp/xlf/bg/14.1/lib64 -lxlf  
-lxlopt -lxlf90_r -lxlfmath -lm
```

# Lapack (I)

- Part of MKL on Juropa, until intel/11.1.\* separate file, starting with intel/12.0.3 in libmkl\_core.a
- Public domain version 3.1 and 3.3 on JUGENE
- Public domain version 3.3 on JUQUEEN
- Must be used together with ESSL (or ESSLsmp)
- Some routines already in ESSL
- Attention, some calling sequences are different!

## Lapack (II)

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

**JUROPA:** (see usage of MKL) ,  
-lmkl\_lapack only up to intel/11.1.072

**JUGENE:**  
module load lapack[/3.3.0]  
mpixlf77\_r -qarch=450 -qtune=450 name.f  
-L/bgsys/local/lib [-lessl[smp]bg]  
-L\$(LAPACK\_LIB) -llapack  
-lessl[smp]bg

ESSL must be linked after LAPACK to  
resolve references



## Lapack (III)

### JUQUEEN:

```
module load lapack/3.3.0_g  
mpixlf77_r name.f  
-L/opt/ibmmath/essl/5.1/lib64  
[-lessl[smp]bg]  
-L$(LAPACK_LIB) -llapack  
-lessl[smp]bg
```

ESSL must be linked after LAPACK to  
resolve references

# Arpack

- ARnoldi PACKage, Version 2.1
- Iterative solver for sparse eigenvalue problems
- Reverse communication interface
- FORTRAN 77
- Calls LAPACK and BLAS routines

## Arpack (II)

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

**JUROPA:** versions with default and old compiler only.

```
module load arpack
ifort name.f -larpack -lmkl_lapack
-lmkl_intel_lp64 -lmkl_intel_thread
-lmkl_core -liomp5 -lpthread
```

## Arpack (III)

### JUGENE:

```
module load arpack
```

```
mpixlf77_r -qarch=450 -qtune=450 name.f  
-L$(ARPACK_LIB) -larpack -L$(LAPACK_LIB)  
-llapack -L/bgsys/local/lib -lessl[smp]bg
```

## GSL – GNU Scientific Library

- Version 1.13 and 1.14(default) on JUROPA and JUGENE, 1.15 with intel/12.0.4 on JUROPA, 1.15 on JUQUEEN
- Provides a wide range of mathematical routines
- Not recommended for performance reasons
- Often used by configure scripts
- `module load gsl[/1.13] JUGENE`
- `module load gsl/1.15_g JUQUEEN`
- `module load gsl [ /1.13] [ /1.15] JUROPA`

# NAG Libraries

- JUROPA only, NAG Fortran 77, NAG C, and NAG f190
- Fortran 77 Mark 22:  
More than 1600 user-callable routines
- NAG C Mark 8:  
more than 1000 user-callable routines
- f190 Release 4,  
43 new generic user-callable routines

# Parallel Libraries and Systems

## Threaded Parallelism

- MKL (JUROPA)  
is multi-threaded or at least thread-safe  
usage as with sequential routines  
if OMP\_NUM\_THREADS not set, 8 threads used
- FFTW 3.2.2 and 3.3 (Fastest Fourier Transform of the West) <http://www.fftw.org>
- ESSLsmp 4.4 (JUGENE) 5.1 (JUQUEEN)

Usage:

```
mpixlf90_r name.f -L/bgsys/local/lib  
[-L/opt/ibmmath/essl/5.1/lib64]  
-lesslsmpbg
```

# Parallel Libraries

## MPI Parallelism

- ScaLAPACK (Scalable Linear Algebra PACKage)
- FFTW (Fastest Fourier Transform of the West)
- MUMPS (Multifrontal Massively Parallel sparse direct Solver)
- ParMETIS (Parallel Graph Partitioning)
- hypre (high performance preconditioners)
- PARPACK (Parallel ARPACK)



## MPI Parallelism (II)

- 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
- PDE2D, Finite Element Package (JUROPA only)

# ScaLAPACK

## ScaLAPACK

**JUROPA** part of MKL

**JUGENE** Release 1.8 public domain library  
together with

BLACS v1.1 public domain version

and Release 2.0.1, now BLACS already part of  
ScaLAPACK

*<http://www.netlib.org/scalapack/index.html>*

FORTRAN, also C-Interface

LAPACK has to be linked, too

# 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

# Availability and Usage on JUROPA

## ScaLAPACK and BLACS in MKL

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

```
mpif77 name.f -lmkl_scalapack_lp64  
-lmkl_blacs_intelmpi_lp64 -lmkl_lapack  
-lmkl_intel_lp64 -lmkl_intel_thread  
-lmkl_core -liomp5 -lpthread
```

# Availability and Usage on JUROPA

## ScaLAPACK and BLACS in MKL

Linking a program *name.f* calling routines from ScaLAPACK, new version:

```
module unload mkl
module switch intel/12.0.4 or 12.1.1
mpif77 name.f -lmkl_scalapack_lp64
-lmkl_blacs_intelmpi_lp64 -lmkl_intel_lp64
-lmkl_intel_thread -lmkl_core -liomp5
-lpthreads
```

## Usage on JUGENE

```
Module load scalapack
```

```
mpixlf77[_r] name.f
```

```
-L$(SCALAPACK_LIB) -lscalapack
```

```
-L$(BLACS_LIB) -lblacsF77init
```

```
-lblacs -lblacsF77init
```

```
-L$(LAPACK_LIB) -llapack
```

```
-L/bgsys/local/lib -lessl[smp]bg
```

## Usage on JUGENE (II)

```
Module load scalapack/2.0.1
```

```
mpixlf77[_r] name.f
```

```
-L$(SCALAPACK_LIB) -lscalapack
```

```
-L$(LAPACK_LIB) -llapack
```

```
-L/bgsys/local/lib -lessl[smp]bg
```

## Usage on JUQUEEN

Not yet available due to BLACS problems

# 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 4.8.4, 4.9.2, and 4.10.0 on JUROPA, version 4.8.1, 4.9.2, and 4.10.0 on JUGENE  
<http://graal.ens-lyon.fr/MUMPS/index.html>



## ParMETIS

Parallel Graph Partitioning and Fill-reducing Matrix Ordering  
developed in Karypis Lab at the University of Minnesota

Version 3.1.1 and 3.2.0 on JUROPA and JUGENE

<http://glaros.dtc.umn.edu/gkhome/metis/parmetis/download>

## Hypre

High performance preconditioners

Version 2.0.0 and 2.6.0b on JUROPA and JUGENE

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

# FFTW

Version 2.1.5, this old version contains an MPI-parallel version of FFTW on JUROPA and JUGENE

Version 3.3 on JUROPA, compiled with intel/12.1.1

Version 3.3 on JUGENE

<http://www.fftw.org>

# PARPACK

- ARPACK Version 2.1 and
- 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 ASCII Monte Carlo Computations  
Version 2.0: 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 2.3.0 and 2.4.0 on JUROPA and JUGENE

*<https://computation.llnl.gov/casc/sundials/main.html>*

# PETSc

Version 3.0.0, 3.1.0-p8, and 3.2.0-p6 on JUROPA, 2.3.3,  
3.1-p1, and 3.2.0-p6 on JUGENE

Portable, Extensible Toolkit for Scientific Computation

Numerical solution of partial differential equation

<http://www.mcs.anl.gov/petsc/>

Usage at Research Centre Juelich:

module help petsc[/3.1-p2\_basic\_O3] on JUGENE

module help petsc/3.1.0-p8-basic on JUROPA

# PDE2D (JUROPA only)

- Solves quite general nonlinear, time-dependent, steady-state and eigenvalue systems of partial differential equations in 1D intervals, general 2D regions and 3D „boxes“
- Interactive user-interface, which makes it very easy to use
- Extensive graphical output capabilities
- Version 9.2

<http://www.pde2d.com/>

# Software for Materials Science

Simulation Package	Available on		
	JUGENE	JuRoPA	Workstations
ADF		✓	
Amber		✓	
CP2K		✓	
CPMD	✓	✓	
Dalton		✓	
Gromacs	✓	✓	
GPAW	✓	✓	
LAMMPS	✓	✓	
Molpro		✓	✓
NAMD	✓	✓	
NWChem		✓	
Tremolo	✓	✓	

✓ Package available

(✓) Installation in progress/planned

# Visualization Software for Materials Science

Visualization Package	Available on		
	JUGENE	JuRoPA	JUVIS
IDL		(✓)	✓
Molden	✓	✓	
RasMol		✓	
VMD	✓	✓	✓
Gnuplot	✓	✓	✓
grace	✓	✓	
gimp	✓	✓	
visit			✓
Pymol			✓

- ✓ Package available
- (✓) Package available but with limited functionality
- (✓) Installation in progress/planned



# Further Information

- <http://www.fz-juelich.de/ias/jsc/juropa>
- <http://www.fz-juelich.de/ias/jsc/jugene>
- <http://www.fz-juelich.de/ias/jsc/juqueen>
- [.../EN/Expertise/Support/Software/\\_node.html](.../EN/Expertise/Support/Software/_node.html)

# JSC People

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**M.Vaeßen: LAPACK**  
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**Software:**  
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