Mathematical Libraries and Application Software on JUQUEEN and JURECA

JSC Training Course

November 2015 | I. Gutheil
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
  mpi$xlc_r name.c -L/opt/ibmcmp/xlf/bg/14.1/bglib64 -lxlfmath -lm -lrt
General Informations JURECA (I)

- `module spider name` shows whether a library is available and how to load it
- `module load intel-para` loads the current default toolchain with intel compilers version 15.0.3, MKL 11.2, and parastation MPI version 2015.07
- Other toolchains available: gpsolf/2015.07, intel/2015.07, and intel-para/2015.07-mt with multi-threaded parastation MPI
- after loading the toolchain `module avail` shows the software available with that toolchain
General Informations JURECA (II)

- Many libraries available for more than one toolchain
- 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
- Linking Fortran subroutines with the C linker requires -lifcore -lifport in the link command
Tips and Tricks, not recommended! Only works for sequential libraries compiled with another compiler.
If you want to link software name only available through a different toolchain, e.g. gpsolf/2015.07 with the intel-para toolchain, do the following:
module load gpsolf/2015.07
module load name
echo $EBROOTNAME
export NAME_ROOT=$EBROOTNAME
module purge
module load intel-para
Allows you to link -I$NAME_ROOT/include
-L$NAME_ROOT/lib
If you want to link a dynamic library you have to add $NAME_ROOT/lib to $LD_LIBRARY_PATH
Sequential Libraries and Packages (I)

Vendor specific Libraries

JURECA

- MKL Intel® Math Kernel Library
  versions as mentioned in general informations,
  11.2 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
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://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:
  module load intel-para
  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
module load intel-para
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 -lxlf -lxlopt -lxlf90_r -lxlfmath -lm -lrt
LAPACK (I)

- Part of MKL on JURECA in libmkl_core.a
- Part of libopenblas.so on JURECA if gpsof/2015.07 is loaded
- Public domain version 3.3, 3.4.2, and 3.5.0 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 3.3 on JUQUEEN (may also be tried with 3.4.2)
- Experimental C-LAPACK, liblapacke.a in versions 3.4.2 and 3.5.0 on JUQUEEN
LAPACK (II)

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

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

**JUQUEEN:**

```
module load lapack/3.4.2[_g][_simd]
mpixlf90_r name.f -Wl,-allow-multiple-definition
-llapack -lessl[smp]bg
```

ESSSL 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
- arpack-ng/3.1.3 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,
  1.16 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-para GSL/1.16`
  for icc version on JURECA
- `module load gpsolf/2015.07 GSL/1.16`
  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-para
Parallel Libraries
Threaded Parallelism I

- MKL (JURECA)
  is multi-threaded or at least thread-save usage as with sequential routines
  if OMP_NUM_THREADS not set, 56 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 and JURECA,
  additional version in MKL and FFTW/3.3.4 coming with gpsof/2015.07 on JURECA
  `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-para and intel,
ScaLAPACK/2.0.2-OpenBLAS-0.2.14-LAPACK-3.5.0 with gpsof

**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](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 or intel-para toolchain:
```
mpif77 name.f -lmkl_scalapack_lp64
-lmkl_blacs_intelmpi_lp64 -lmkl_intel_lp64
-lmkl_intel_thread -lmkl_core -liomp5 -lpthread
```
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
- JUQUEEN MPI and hybrid version 2013.11 and 2014.06
- JURECA MPI and hybrid version 2014.06 and 2015.05.001 pure MPI version
Elemental

- C++ framework, two-dimensional data distribution element by element
- [http://libelemental.org/about/](http://libelemental.org/about/)
- 0.85 on JURECA, 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 5.0.0 on JURECA
- [http://graal.ens-lyon.fr/MUMPS/](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://glaros.dtc.umn.edu/gkhome/metis/parmetis/overview

Hypre

High performance preconditioners
Version 2.10.0b on JURECA,
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 MPI-parallel version of FFTW on JURECA and JUQUEEN
- Version 3.3.2 and 3.3.3 on JUQUEEN, 3.3.4 on JURECA
- [http://www.fftw.org](http://www.fftw.org)
PARPACK

- ARPACK Version 2.1 on JUQUEEN
- arpack-ng/3.1.3 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
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 seperate 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 2.5.0 on JUQUEEN, version 2.6.1 on JURECA
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 and 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

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<th>Package</th>
<th>JUQUEEN</th>
<th>JURECA</th>
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Software for Computational Engineering

- CFD Package **OpenFOAM** is installed on
  - **JUQUEEN** Versions 2.1.1
  - **JURECA** in process

- Commercial **FEM Software**
  - **ANSYS**, **LS-DYNA**, **COMSOL** are technically maintained (in future) on **JURECA**
  - **Licenses** must be provided by **User**!
Further informations and JSC-people

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

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