Mathematical Libraries and Application Software on JUQUEEN and JURECA

JSC Training Course

May 2016 | 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
  mpixc_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.
- 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` if you want special versions or new software
- `$EBROOT NAME` 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

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 -lesslblg

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 -lesslblg -L/opt/ibmcmp/xlf/bg/14.1/bglb64 -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
-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
- 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](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
- 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/](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 Partioning 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 2.11.0 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
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/

Package for the solution of ordinary differential equations,
Versions 2.6.1 on JUQUEEN and 2.6.2 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, 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

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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

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