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JÜLICH
FORSCHUNGSZENTRUM

Mathematical Libraries and Application Software on JUQUEEN and JUROPATEST

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

General Informations JUROPATEST (I)

- `module spider` *name* shows whether a library is available and how to load it
- `module load intel-para` loads the current toolchain with intel compilers version 15.2 and MKL 11.2
- after loading the toolchain `module avail` shows the software available with that toolchain
- $EBROOT*NAME* is the root directory where the library is installed
- Only latest version of each library available
- Write e-mail to `sc@fz-juelich.de` if you want special versions or new software
- Linking Fortran subroutines with the C linker requires `-lifcore -lifport` in the link command

General Informations JUROPATEST (II)

Tips and Tricks, not recommended!
If you want to link software *name* only available through gpsmpi with the intel-para toolchain, do the following:

```
module load gpsmpi
module load name
echo $EBROOTNAME
export NAME_ROOT=$EBROOTNAME
module unload gpsmpi
module load intel-para
```

Allows you to link -I$NAME_ROOT/include
-L$NAME_ROOT/lib

Sequential Libraries and Packages (I)

Vendor specific Libraries

JUROPATEST

- MKL Intel® Math Kernel Library
  versions as mentioned in general informations,
  11.2 on JUROPATEST

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, JUROPATEST planned

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/SystemDependentLibraries.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://www.fz-juelich.de/ias/jsc/EN/Expertise/Support/Software/SystemDependentLibraries/ESSL_ESSLSMP.html
Link to IBM documents Guide and Reference

Usage of MKL on JUROPATEST (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 JUROPATEST(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 -lessslbg
```

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 -lessslbg
-L/opt/ibmcmp/xlf/bg/14.1/bglib64 -lxl -lxlopt
-lxlf90_r -lxlfmath -lm -lrt
```

LAPACK (I)

- Part of MKL on JUROPATEST in libmkl_core.a
- Public domain version 3.3 and 3.4.2 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 version 3.4.2 on JUQUEEN

LAPACK (II)

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

JUROPATEST: (see usage of MKL),

JUQUEEN:

```
module load lapack/3.4.2[_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
- arpack-ng/3.1.3 on JUROPATEST
- 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 JUROPATEST
- 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 JUROPATEST

NAG Libraries

- NAG Fortran Mark 22 on JUQUEEN: as module
  more than 1600 user-callable routines
- planned on JUROPATEST

Parallel Libraries

Threaded Parallelism I

- MKL (JUROPATEST)
  is multi-threaded or at least thread-save
  usage as with sequential routines
  if OMP_NUM_THREADS not set, 56 threads used on JUROPATEST
  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 JUROPATEST,
  additional version in MKL on JUROPATEST
  http://www.fftw.org

Parallel Libraries

MPI Parallelism

- ScaLAPACK (Scalable Linear Algebra PACKage)
- ELPA (Eigenvalue SoLvers for Petaflop-Applications)
- 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

JUROPATEST: part of MKL
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 together with 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 JUROPATEST

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

```
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
- JUQUEEN MPI and hybrid version 2013.11 and 2014.06
- JUROPATEST MPI and hybrid version 2014.06

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 JUROPATEST
- http://graal.ens-lyon.fr/MUMPS/

ParMETIS

Parallel Graph Partinioning 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 JUROPATEST
http://glaros.dtc.umn.edu/gkhome/metis/parmetis/overview

Hypre

High performance preconditioners
Version 2.10.0b on JUROPATEST,
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 JUROPATEST and JUQUEEN
- Version 3.3.2 and 3.3.3 on JUQUEEN, 3.3.4 on JUROPATEST
- http://www.fftw.org

PARPACK

- ARPACK Version 2.1 on JUQUEEN
- arpack-ng/3.1.3 on JUROPATEST
- 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[JUROPATEST]:
various random number generators in one library
Version 1.0 seperate library for each random number generator, on JUQUEEN and JUROPATEST
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 JUROPATEST
https://computation.llnl.gov/casc/sundials/main.html

PETSc

- Portable, Extensible Toolkit for Scientific Computation
- Numerical solution of partial differential equations
- version 3.5.3 on JUQUEEN and JUROPATEST
- 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]
```

- JUROPATEST:

```
module spider petsc
```

Software for Materials Science

Package	JUQUEEN	JUROPATEST
ADF		planned
Amber		planned
CP2K	yes	yes
CPMD	yes	planned
Gromacs	yes	yes
GPAW	planned	yes
LAMMPS	yes	yes
Molpro		yes
NAMD	yes	planned
NWChem		yes
QuantumEspresso		yes
TURBOMOLE		planned

Software for Computational Engineering

- CFD Package **OpenFOAM** is installed on

JUROPA	Versions 1.7.x, 2.0.1, 2.2.2, 2.3.0
JUQUEEN	Versions 2.1.1
JUROPATEST	**in process**

- Commerical **FEM Software**
  - **ANSYS**, **LS-DYNA**, **COMSOL** are technically maintained on **JUROPA** and (in future) on **JUROPATEST / JURECA**
  - **Licenses** must be provided by **User !**

Further informations and JSC-people

http://www.fz-juelich.de/ias/jsc/juropa
http://www.fz-juelich.de/ias/jsc/juropatest
http://www.fz-juelich.de/ias/jsc/juqueen
http://www.fzjuelich.de/ias/jsc/EN/Expertise/Support/Software/Software_node.html

Mailto

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