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

JSC Training Course

May 22, 2012
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-save, 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

```bash
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/ibmmmath/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:**

```bash
mpixlc_r name.c -L/usr/local/lib
-leslbg -lm
-L/opt/ibmcmp/xlf/bg/11.1/lib -lxlf
-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
-lessslbg
-L/opt/ibmcmp/xlf/bg/14.1/lib64 -lxlf
-1xlopt -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
-llapack
```

ESSL must be linked after LAPACK to resolve references
Lapack (III)

**JUQUEEN:**

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

ESSSL 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.

```fortran
module load arpack
ifort name.f -larpack -lmlk_lapack
  -lmlk_intel_lp64 -lmlk_intel_thread
  -lmlk_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

```bash
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 fl90
- Fortran 77 Mark 22:
  More than 1600 user-callable routines
- NAG C Mark 8:
  more than 1000 user-callable routines
- fl90 Release 4,
  43 new generic user-callable routines
Parallel Libraries and Systems
Threaded Parallelism

- MKL (JUROPA)
  is multi-threaded or at least thread-save 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 \texttt{name.f} calling routines from ScaLAPACK, default version:

\begin{verbatim}
mpif77 name.f -lmlkl_scalapack_lp64 -lmlkl_blacs_intelmpi_lp64 -lmlkl_lapack -lmlkl_intel_lplp64 -lmlkl_intel_thread -lmlkl_core -liomp5 -lpthread
\end{verbatim}
Availability and Usage on JUROPA

ScaLAPACK and BLACS in MKL

Linking a program \textit{name.f} calling routines from ScaLAPACK, new version:

\begin{verbatim}
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
   -lpthread
\end{verbatim}
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
mpiixlf77[+_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
devolved 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
SPRNG

The Scalable Parallel Random Number Generators Library for ASCI 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

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✔ Package available

✔️ Installation in progress/planned
Visualization Software for Materials Science

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✔️ 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
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