JÜLICH
FORSCHUNGSZENTRUM

Mathematical Libraries on JUQUEEN

JSC Training Course

May 10, 2012

Outline

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

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

- ESSL (Engineering and Scientific Subroutine Library) version 5.1 in /opt/ibmmath/essl/5.1/lib64

Public domain Software, planned

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

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

- 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 V5.1:

Guide and Reference

http://www.fz-juelich.de/ias/jsc/EN/Expertise/Support/Software/SystemDependentLibraries/ESSL.html

Guide and Reference

Usage of ESSL

Compilation and linking of program name.f calling ESSL routines

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

Compilation and linking of program name.c calling ESSL routines
not yet tested

Lapack (I)

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

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
```

Other sequential libraries

- ARPACK, ARnoldi PACKage, Version 2.1
- To be installed soon
- GSL, GNU Scientific Library
- To be installed soon
- GMP GNU Multiple Precision Library
- To be installed soon

Parallel Libraries and Systems

Threaded Parallelism

- ESSLsmp 5.1 (JUQUEEN)

Usage:

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

Parallel Libraries

MPI Parallelism, all planned

- 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)

- Status of ScaLAPACK 2.0.1

BLACS now part of ScaLAPACK, but LAPACK and BLAS have to be linked seperately

LAPACK 3.3.0 already installed,
BLAS from essl, srotm and drotm are missing, will be put into liblapack.a
ScaLAPACK compiled and „installed“, but tests give error with MPI
Executables from DD1 run without error
newly linked executables with all .o-files from DD1 run into error

MPI Parallelism (III)

- 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

Further Information

- http://www.fz-juelich.de/ias/jsc/EN/Expertise/JUQUEEN/JUQUEEN_node.html
- http://www.fz-juelich.de/ias/jsc/EN/Expertise/Support/Software/Software_node.html

JSC People

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