

JUQUEEN

Best Practices

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Outline

- Production environment
 - Module environment
 - Job execution
- General porting of applications
 - Compilers and wrappers
 - Compiler/linker flags
- Porting and tuning – selected topics
 - Static and shared libraries
 - Mapping
 - MPMD
 - MPI extensions
 - QPX

Module environment

Modules – Features

Overview of available products

- Provides fast overview over all available products
- Provides fast overview over all available versions of a selected product

Use of software and libraries

- Enables access to software packages and libraries
- Supports different versions of one product side by side
- Provides application-specific information

Dynamic modification of user environment

- Necessary environment variables are set appropriately, no need to set variables manually
- Detection of conflicts between applications

Module environment

Command `module [options] [module]`

Selected options

`<no option>`

Lists all available options of the module command

`avail`

Lists all available modules and versions

`list`

Lists modules currently loaded

`load/unload`

Loads/unloads a module

`help`

Lists information about a module

`show`

Displays information about environment settings applied by the module

`purge`

Unloads all currently loaded modules

Module environment

Module categories on JUQUEEN

COMPILER

IO

MATH

MISC

SCIENTIFIC

TOOLS

Software for compute nodes

/bgsys/local

Software for front-end nodes

/usr/local

Example

```

----- /bgsys/local/modulefiles/TOOLS -----
----- /bgsys/local/modulefiles/SCIENTIFIC -----
OpenFOAM/2.1.1-gcc(default)    cpmd/3.15.3
QuantumEspresso/5.0.1(default) lammps/30Aug12
[...]
----- /usr/local/modulefiles/COMPILER -----
cmake/2.8.11(default)  python3/3.4.1(default)
----- /usr/local/modulefiles/MATH -----
[...]
```

Module environment – available software

Selected mathematical software

Elemental (0.81)
 FFTW (2.1.5/3.3.3)
 GSL (1.15)
 hypre (2.9.0)
 LAPACK (3.4.2)
 MUMPS (4.10.0)
 P3DFFT (2.5.2)
 ParMETIS (4.0.2)
 PETSc (3.5.1)
 ScaLAPACK (2.0.2)
 SPRNG (2.0)
 sundials (2.5.0)

Science

cp2k (2.4.0)
 cpmd (3.15.3)
 lammmps (30AUG12)
 NAMD (2.9)
 OpenFOAM (2.1.1)
 QE (5.0.1)

I/O libraries and tools

cdo (1.6.1)
 darshan (2.2.8)
 HDF5 (1.8.9)
 Nco (4.3.4)
 netCDF (4.3)
 p-netCDF (1.3.1)
 SIONlib (1.5.2)

Tools

extrae (2.4.1)
 MUST (1.2.1)
 Scalasca (2.1)
 Scorep (1.3)
 Tau (2.23.1)
 Totalview (8.14.0)
 Vampir (8.4)

Compiler (tools)

cmake (2.8.11)
 clang (3.4)
 gcc (4.9.1)
 Not via modules
 bgxlc (12.01)
 bgxlf (14.01)

Job execution – Batch system

Execution of applications managed by LoadLeveler

- Users submit jobs using a job command file
- LoadLeveler allocates computing resources to run jobs
- The scheduling of jobs depends on
 - Availability of resources
 - Job priority (jobs with larger core counts are privileged)
- Jobs run in queues (job classes)
 - Chosen by LoadLeveler according to core count

More information about LoadLeveler on JUQUEEN

<http://www.fz-juelich.de/ias/jsc/EN/Expertise/Supercomputers/JUQUEEN/UserInfo/LoadLeveler.html>

Job execution – Job command file

ASCII file containing two major parts

Job command file	Keyword block
	• LoadLeveler keywords have the form #@<keyword> • # and @ can be separated by any number of blanks
	Shell script block
	• Regular shell script • Can contain any shell command

Job execution – LoadLeveler keywords

Keyword	Description
<code>#@job_name=<name></code>	Name of the job
<code>#@notification=</code> <code>end</code> <code>error</code> <code>never</code> <code>start</code> <code>always</code>	Send notification if the job is finished if the job returned an error code $\neq 0$ never upon the start of the job combination of start , end , error
<code>#@notify_user=<mailaddr></code>	Mail address to send messages to
<code>#@wall_clock_limit=hh:mm:ss</code>	Requested wall time for the job
<code>#@input=<input file name></code> <code>#@output=<file name for stdout></code> <code>#@error=<file name for stderr></code>	Specifies corresponding file names
<code>#@environment=[<variable>,COPY_ALL]</code>	Environment variable to be exported to job
<code>#@queue</code>	End of keyword section

Job execution – LoadLeveler keywords

Keyword	Description
<code>#@job_type=[serial, bluegene]</code>	Specifies the type of job step to process. Must be set to bluegene for parallel applications.
<code>#@bg_size=<number of nodes></code>	Size of the Blue Gene job, keywords bg_size and bg_shape are mutually exclusive.
<code>#@bg_shape=<A>xx<C>x<D></code>	Specifies the requested shape of a job (in midplanes).
<code>#@bg_rotate=[True, False]</code>	whether the scheduler should consider all possible rotations of the given shape
<code>#@bg_connectivity=[TORUS, MESH, EITHER] Xa Xb Xc Xd</code>	Type of wiring requested for the block (can be specified for each dimension separately)

Job execution – Shell script section

- Can contain any shell scripts commands
- Launching parallel applications:

Command `runjob [options]: <executable> [arguments]`

Selected options

`--envs <ENV_Var=Value>`

Sets the environment variable **ENV_Var=Value**

`--exp-env <ENV_Var>`

Sets the environment variable **ENV_Var**

`--np <number>`

Total number of (MPI) tasks

`--ranks-per-node <number>`

Number of (MPI) tasks per compute node

Job execution – Example Job command file

```
#@job_name           = MPI_code
#@comment            = "32 ranks per node"
#@output              = test_$(jobid).out
#@error               = test_$(jobid).err
#@environment         = COPY_ALL
#@job_type            = bluegene
#@notification        = never
#@bg_size             = 512
#@bg_connectivity     = torus
#@wall_clock_limit    = 14:00:00
#@queue

runjob --np 16384 --ranks-per-node 32 : app.x
```



Pure MPI applications need to use 32 tasks per node in order to use the architecture efficiently, i.e., to fill all pipe lines and registers and to avoid idle times!



Job execution – MPI/OpenMP hybrid jobs

```
#@job_name          = hybrid_code
#@comment           = "16x4 configuration"
#@output            = test_$(jobid).out
#@error             = test_$(jobid).err
#@environment       = COPY_ALL
#@job_type          = bluegene
#@notification      = never
#@bg_size           = 512
#@bg_connectivity   = torus
#@wall_clock_limit  = 14:00:00
#@queue

runjob --np 8192 --ranks-per-node 16\
      --env OMP_NUM_THREADS=4 : app.x -i input
```

! Several process/thread configurations are possible:

- $\text{ntasks} \times \text{nthreads} = 64$
- $\text{ntasks} = 2^n, 0 \leq n \leq 6$

Test which configuration gives the best performance for your application and setup!

Job execution – Job classes

Class name	#Nodes	Max. run time	Default run time
n001	1 – 32	00:30:00	00:30:00
n002	33 – 64	00:30:00	00:30:00
n004	65 – 128	12:00:00	06:00:00
n008	129 – 256	12:00:00	06:00:00
m001	257 – 512	24:00:00	06:00:00
m002	513 – 1024	24:00:00	06:00:00
m004	1025 – 2048	24:00:00	06:00:00
m008	2049 – 4096	24:00:00	06:00:00
m016	4097 – 8192	24:00:00	06:00:00
m032*	8193 – 16384	24:00:00	06:00:00
m056*	24577 – 57344	24:00:00	06:00:00

* On demand only

↑
INCREASING PRIORITY
↓



You will be charged for **full partitions** (e.g. when requesting 513 nodes you will be charged for **1024** nodes!) → Always use full partitions!



Job execution – Loadleveler commands

Command	Description
llsubmit <jobfile>	Sends job to the queuing system
llq	Lists all queued and running jobs
llq -l <job ID>	detailed information about the specified job
llq -s <job ID>	detailed information about a specific queued job, e.g. expected start time
llq -u <user>	lists all jobs of the specified user
llcancel <job ID>	Kills the specified job
llstatus	Displays the status of LoadLeveler
llclass	Lists existing classes and their properties
llqx	Shows detailed information about all jobs

Job execution – Monitoring of jobs

LoadLeveler

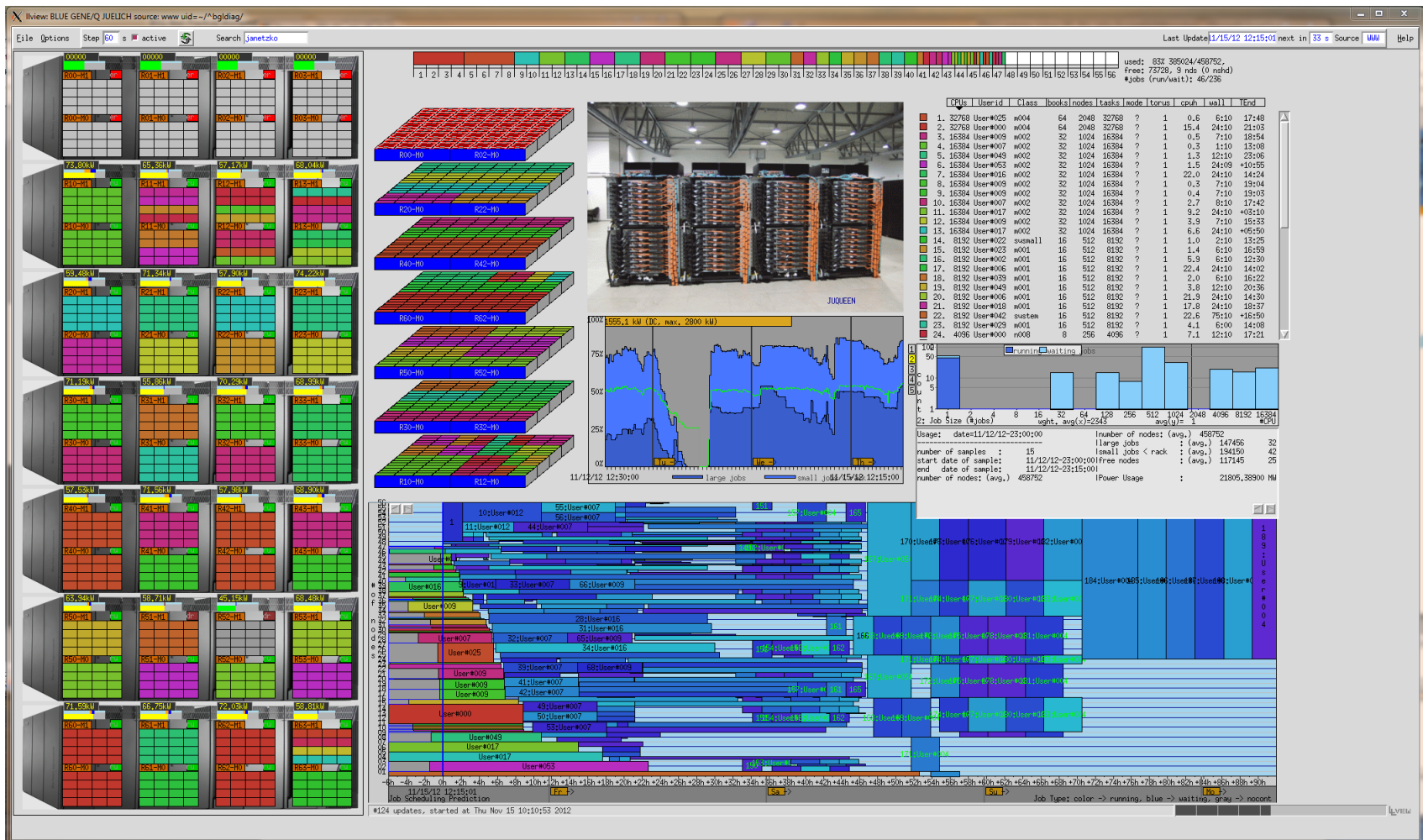
Command `llq [options]`

llview

- Client-server based application
- compact summary of different information (e.g. current usage of system, job prediction, expected and average waiting times, ...)
- Customizable
- Developed by W. Frings (JSC)

Command `llview`

Job execution – Ilview



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Compilers and wrappers

- Different compilers for front-end and compute nodes
- GNU and IBM XL family of compilers available
- For C/C++ also Clang compiler for compute nodes available
 - Full support of C++ 11 standard and special BGQ hardware features like QPX and vector intrinsics

Front – end nodes	Language		XL (thread-safe: add _r)	GNU	Clang
	C	xlc		gcc	---
	C++	xlc++, x1C		g++	---
	Fortran	x1f, x1f90, x1f95, x1f2003		gfortran	---

Compilers and wrappers

Compute nodes	Language		Compiler	MPI wrapper
	XL (thread-safe: add_r)	C	bgxlc, bgc89, bgc99	mpixlc
		C++	bgxlc++, bgxlC	mpixlcxx
		Fortran	bgxlf, bgxlf90, bgxlf95, bgxlf2003	mpixlf77, mpixlf90, mpixlf95, mpixlf2003
	GNU	C	powerpc64-bgq-linux-gcc	mpigcc
		C++	powerpc64-bgq-linux-g++	mpig++
		Fortran	powerpc64-bgq-linux-gfortran	mpigfortran
	Clang	C	bgclang	mpiclang
		C++	bgclang++	mpiclang++
		Fortran	---	---



If working with the XL suite of compilers, always use the thread-safe mpi wrappers when compiling for the compute nodes!





If you use OpenMP tasks, the gcc suite might lead to executables with a noticeable better performance than the XL suite of compilers!



MPI setups

Six different MPI setups available on JUQUEEN

Location of wrappers	/bgsys/drivers/ppcfloor/comm/<name>/bin	
<name>	Description	Usage
gcc	MPI library compiled with gcc, fine-grained locking, error checking and assertions enabled	Initial porting
gcc.legacy	MPI library compiled with gcc, coarse-grained locking, error checking and assertions enabled → slightly better latency for single-threaded codes	
x1	MPI library compiled with XL compilers, PAMI compiled with gcc, error checking and assertions enabled (default wrappers)	
x1.legacy	MPI library compiled with XL compilers, PAMI compiled with gcc, coarse-grained locking, error checking and assertions enabled	
x1.ndebug	MPI library compiled with XL compilers, PAMI compiled with gcc, fine-grained locking, error checking and assertions disabled	Correctly running production code
x1.legacy.ndebug	MPI library compiled with XL compilers, PAMI compiled with gcc, coarse-grained locking, error checking and assertions disabled	

XL: basic compiler and linker options

Increasing optimization Potential



Optimization Level	Description
-O2 -qarch=qp -qtune=qp	Basic optimization
-O3 -qstrict -qarch=qp -qtune=qp	More aggressive, not impact on acc.
-O3 -qhot -qarch=qp -qtune=qp	More aggressive, may influence acc. (high-order transformations of loops)
-O4 -qarch=qp -qtune=qp	Interprocedural optimization at compile time
-O5 -qarch=qp -qtune=qp	Interprocedural optimization at link time, whole program analysis

!

Some flags need to be used for compilation AND linking – Check the compiler manual. If you are not sure, include all flags used in the compile step in the linking step as well!

!

XL: basic compiler and linker options

Compiler/linker flag	Description
<code>-qsmp=omp -qthreaded</code>	Switch on OpenMP support
<code>-qreport -qlist</code>	Generates for each source file <name> a file <name>.lst with pseudo code and a description of the kind of code optimizations which were performed
<code>-qessl -lessl[smp]bg</code>	Compiler attempts to replace some intrinsic FORTRAN 90 procedures by essl routines where it is safe to do so

More information about using ESSL

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

Example: compiler diagnostics

```
subroutine mult(c,a,ndim)
```

```
implicit none
```

```
integer :: ndim,i,j
```

```
double precision ::
```

```
a(ndim),c(ndim,ndim)
```

```
! Loop
```

```
do i=1,1000
```

```
do j=1,1000
```

```
c(i,j) = a(i)
```

```
enddo
```

```
enddo
```

```
end subroutine mult
```

```
>>>> LOOP TRANSFORMATION SECTION <<<<
```

```
1| SUBROUTINE mult (c, a, ndim)
```

```
[...]
```

```
Id=1 DO $$CIV2 = $$CIV2,124
```

```
10| IF (.FALSE.) GOTO lab_11
```

```
$$LoopIV1 = 0
```

```
Id=2 DO $$LoopIV1 = $$LoopIV1,999
```

```
[...]
```

```
-----
0 9 1 Loop interchanging applied
to loop nest.
```

```
0 9 1 Outer loop has been
unrolled 8 time(s).
```



XL: further compiler and linker options

Compiler/linker flag	Description
-qinline=auto:level=<number> -qinline+procedure1[:procedure2[:...]]	Function inlining 0 <= <number> <= 10
-qunroll[={auto yes}]	Unrolling of loops, default is -qunroll=auto
-qipa[=<suboptions_list>]	Intra/inter-procedural optimization, see manual
-qsimd[=auto noauto]	Switches on/off SIMD vectorization (check with -qreport -qlist !!)



Intra-procedural optimization (-O5 or -qipa=2) can cause very long compilation times, especially for C++ codes!



IBM XL compiler support for QPX

Usage of QPX

- Compiler flag `-qsimd=auto`
- Check that SIMD vectorization is actually done!
 - `-qreport`
 - `-qlist`

```
>>>> LOOP TRANSFORMATION SECTION <<<<
[...]
```

```
0 9 1      Loop with nest-level 1 and
           iteration count 1000 was
           SIMD vectorized
[...]
```

```
>>>> LOOP TRANSFORMATION SECTION <<<<
[...]
```

```
0 9 1      Loop was not SIMD vectorized
           because the loop is not the
           innermost loop.
0 10 1     Loop was not SIMD vectorized
           because it contains memory
           references with non-
           vectorizable alignment.
```

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User Information and Support

Information about JUQUEEN

- JSC websites at
http://www.fz-juelich.de/ias/jsc/EN/Expertise/Supercomputers/JUQUEEN/JUQUEEN_node.html
- IBM Blue Gene/Q Application Development Redbook
<http://www.redbooks.ibm.com/redpieces/pdfs/sg247948.pdf>

Dispatch and User Support

- Applications for accounts (for approved projects)

Forschungszentrum Jülich GmbH, JSC, Dispatch, 52425 Jülich
Tel: +49 2461 61 5642, Fax: +49 2461 61 2810
email: dispatch.jsc@fz-juelich.de

- User Support

Tel: +49 2461 61 2828
email: sc@fz-juelich.de

Creating static libraries

Preferred kind of library on BG/Q

```
bgxlc -c pi.c
bgxlc -c main.c
#
### Create the library
ar rcs libpi.a pi.o
#
### Create the executable program
bgxlc -o pi main.o -L. -lpi
```

Creating shared libraries

```
bgxlc -c pi.c
bgxlc -c main.c
### Create the dynamic library
bgxlc -qmkshrobj -Wl,-soname, libpi.so.0 \
      -o libpi.so.0.0 libpi.o
### Set up the soname
ln -s libpi.so.0.0 libpi.so.0
### Create a linker name
ln -s libpi.so.0 libpi.so
### Create the executable program
bgxlc -o pi main.o -L. -lpi -qnostaticlink \
      -qnostaticlink=libgcc
```



Shared libraries might become a bottleneck when using large core counts on Blue Gene systems! Try to avoid them!



Mapping

Mapping

The placement of MPI ranks on the cores of a partition, i.e., the physical layout of the MPI ranks, is called mapping.

Network topology of JUQUEEN

- 5 dimensional hypercube or torus
- Each node is connected to 10 nearest neighbors in directions $\pm A, \pm B, \pm C, \pm D, \pm E$
- A 6th dimension T is added to specify the hardware thread ID within one node ($0 < T \leq N-1$, where N is the number of MPI ranks per node)

Node location in the torus

$\langle A, B, C, D, E \rangle$

Process or thread location in the torus

$\langle A, B, C, D, E, T \rangle$

Mapping – Receiving partition information

Command `runjob : /bgsys/local/samples/personality/personality.elf`

Partition Information:
 block shape : `<2,2,2,2,2>` ← shape (A,B,C,D,E)
 torus links enabled : `<0,0,0,0,1>` ← TORUS enabled (A,B,C,D,E)

Setup: 32 nodes, -np 32 -p 1

IO Bridge Information:
 rank 0000017 of 0000032 location `<01,00,00,00,01>` core 00 hwthread 0 procid 00 ioBridge
`<01,00,00,00,01>` cn 'R63-M0-N06-J11' ion 'R63-ID-J03'
 rank 0000023 of 0000032 location `<01,00,01,01,01>` core 00 hwthread 0 procid 00 ioBridge
`<01,00,01,01,01>` cn 'R63-M0-N06-J06' ion 'R63-ID-J01'

Coordinates of
 I/O bridge nodes
 A,B,C,D,E

Compute Node Information:

rank	location	core	hwthread	procid	Task	Coordinates	Node ID
0000023	<code><01,00,01,01,01></code>	00	0	00	Task 23 of 32	<code>(1,0,1,1,1,0)</code>	R63-M0-N06-J06
0000017	<code><01,00,00,00,01></code>	00	0	00	Task 17 of 32	<code>(1,0,0,0,1,0)</code>	R63-M0-N06-J11
0000022	<code><01,00,01,01,00></code>	00	0	00	Task 22 of 32	<code>(1,0,1,1,0,0)</code>	R63-M0-N06-J01
0000000	<code><00,00,00,00,00></code>	00	0	00	Task 0 of 32	<code>(0,0,0,0,0,0)</code>	R63-M0-N06-J17
0000016	<code><01,00,00,00,00></code>	00	0	00	Task 16 of 32	<code>(1,0,0,0,0,0)</code>	R63-M0-N06-J12
0000007	<code><00,00,01,01,01></code>	00	0	00	Task 7 of 32	<code>(0,0,1,1,1,0)</code>	R63-M0-N06-J27
0000021	<code><01,00,01,00,01></code>	00	0	00	Task 21 of 32	<code>(1,0,1,0,1,0)</code>	R63-M0-N06-J10
0000013	<code><00,01,01,00,01></code>	00	0	00	Task 13 of 32	<code>(0,1,1,0,1,0)</code>	R63-M0-N06-J20
0000025	<code><01,01,00,00,01></code>	00	0	00	Task 25 of 32	<code>(1,1,0,0,1,0)</code>	R63-M0-N06-J08
0000001	<code><00,00,00,00,01></code>	00	0	00	Task 1 of 32	<code>(0,0,0,0,1,0)</code>	R63-M0-N06-J22
0000027	<code><01,01,00,01,01></code>	00	0	00	Task 27 of 32	<code>(1,1,0,1,1,0)</code>	R63-M0-N06-J04
0000012	<code><00,01,01,00,00></code>	00	0	00	Task 12 of 32	<code>(0,1,1,0,0,0)</code>	R63-M0-N06-J19
0000019	<code><01,00,00,01,01></code>	00	0	00	Task 19 of 32	<code>(1,0,0,1,1,0)</code>	R63-M0-N06-J07
0000005	<code><00,00,01,00,01></code>	00	0	00	Task 5 of 32	<code>(0,0,1,0,1,0)</code>	R63-M0-N06-J23
0000029	<code><01,01,01,00,01></code>	00	0	00	Task 29 of 32	<code>(1,1,1,0,1,0)</code>	R63-M0-N06-J09
0000010	<code><00,01,00,01,00></code>	00	0	00	Task 10 of 32	<code>(0,1,0,1,0,0)</code>	R63-M0-N06-J30
0000031	<code><01,01,01,01,01></code>	00	0	00	Task 31 of 32	<code>(1,1,1,1,1,0)</code>	R63-M0-N06-J05

Coordinates
 A,B,C,D,E / A,B,C,D,E,T

Mapping

Changing the Mapping

Pre-defined mappings

Command `runjob --mapping <permutation of ABCDET>`

The rightmost coordinate is varied fastest. If no mapping is specified, the default is ABCDET, i.e., the processes are mapped first within one node before occupying the next node, etc.

User-defined mappings

Command `runjob --mapping <mapfile>`

`<mapfile>` is an ASCII file, where the n^{th} line specifies the 6 coordinates of the MPI rank n :

```
4 0 0 0 0 0 # task 0
0 0 0 2 0 0 # task 1
0 0 1 0 0 0 # task 2
[...]
```

Mapping

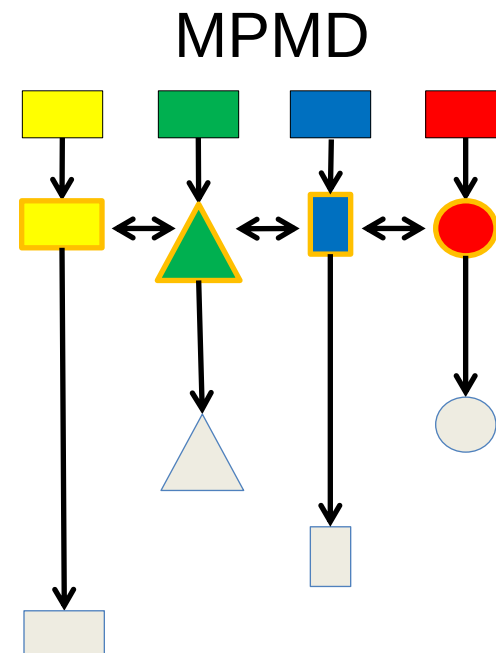
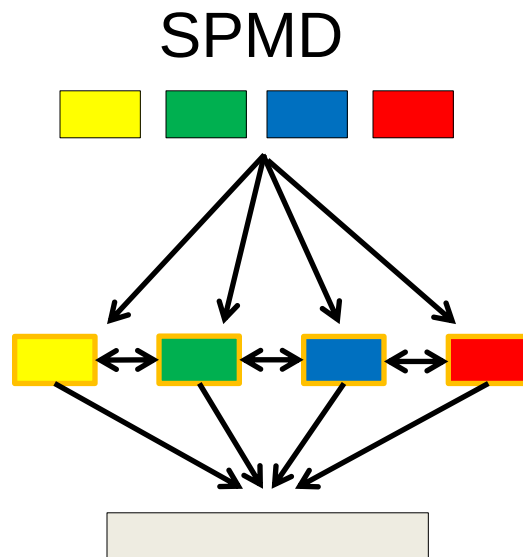
Hints for choosing an optimal mapping

- Can increase performance considerably
- Depends on the communication pattern of applications
- Ranks communicating with each other should be close
- Folding of dimensions according to decomposition

Job size: 1 midplane with 16 MPI ranks/node		
Example	Mapping ABCDET	Mapping TEDCBA
	Dimensions: $4 \times 4 \times 4 \times 4 \times 2 \times 16$ • Good for simulations with, e.g., following 2D decompositions: $256 \times 32 = (4^4) \times (2 \times 16)$ $64 \times 128 = (4^3) \times (4 \times 2 \times 16)$	Dimensions: $16 \times 2 \times 4 \times 4 \times 4 \times 4$ • Good for simulations with a 2D decomposition of $128 \times 64 = (16 \times 2 \times 4) \times 4^3$

MPMD – Multiple Program Multiple Data

Instead of using only one executables several different executables can be used at the same time sharing one JUQUEEN partition



MPMD job execution – Job command file

Example

MPMD setup

app1.x: 4 MPI processes

app2.x: 4 MPI processes

app3.x: 8 MPI processes

Job command file

```
#@job_name           = MPMD
#@comment            = "MPMD Example"
#@environment        = COPY_ALL
#@job_type           = bluegene
#@notification       = never
#@bg_size            = 32
#@bg_connectivity    = torus
#@wall_clock_limit   = 00:30:00
#@queue
```

```
runjob -n 16 -p 4 -mapping mpmd_mapfile : dummy.x
```

Mapfile for MPMD – Section I

Example

MPMD setup

app1.x: 4 MPI processes

app2.x: 4 MPI processes

app3.x: 8 MPI processes

mpmd_mapfile (ASCII file) – Section I

```
#mpmdbegin 0-3  
#mpmdcmd app1.x  
#mpmdend
```

app1.x with rank 0 to 3

```
#mpmdbegin 4-7  
#mpmdcmd app2.x  
#mpmdend
```

app2.x with rank 4 to 7

```
#mpmdbegin 8-15  
#mpmdcmd app3.x  
#mpmdend
```

app3.x with rank 8 to 15

Mapfile for MPMD – Section II

MPMD setup

app1.x: 4 MPI processes

app2.x: 4 MPI processes

app3.x: 8 MPI processes

mpmd_mapfile (ASCII file) – Section II positions in the 6D torus (ABCDET)

Example

```
0 0 0 0 0 0
0 0 0 0 0 1
0 0 0 0 0 2
0 0 0 0 0 3
```

app1 . x with rank 0 to 3,
first node, core 0 to 3

```
0 0 0 0 1 0
0 0 0 0 1 1
0 0 0 0 1 2
0 0 0 0 1 3
```

app2 . x with rank 4 to 7,
second node in E, core 0 to 3

```
0 0 0 1 0 0
0 0 0 1 0 1
0 0 0 1 0 2
0 0 0 1 0 3
0 0 1 0 0 0
0 0 1 0 0 1
0 0 1 0 0 2
0 0 1 0 0 3
```

app3 . x with rank 8 to 15,
first node in D and C,
cores 0 to 3 on each node

MPMD – important hints

- On one node only one executable can run.
- The number of ranks specified in the `runjob` command (`-p` or `--ranks-per-node`) must be the largest number of ranks per node needed.
- The memory available to an MPI task depends on the number of ranks per node specified in the `runjob` command (`-p 8` → 2 GB per rank, regardless how many ranks per node are actually started).
- The executable specified in the `runjob` command is a dummy argument

Obtaining information about the allocated partition and the distribution of processes

<http://www.fz-juelich.de/ias/jsc/EN/Expertise/Supercomputers/JUQUEEN/UserInfo/ShapeMapping.html#doc1413730bodyText4>

MPI extensions for Blue Gene/Q

IBM offers extensions to the MPI standard for Blue Gene/Q

- *Not* part of the official MPI standard!
- C (and Fortran77 interface for most functions)
- Functions start with `MPiX_` instead of `MPI_`

Overview over all available extensions

<http://www.fz-juelich.de/ias/jsc/EN/Expertise/Supercomputers/JUQUEEN/UserInfo/MPIextensions.html>

C

```
#include <mpix.h>
```

Fortran

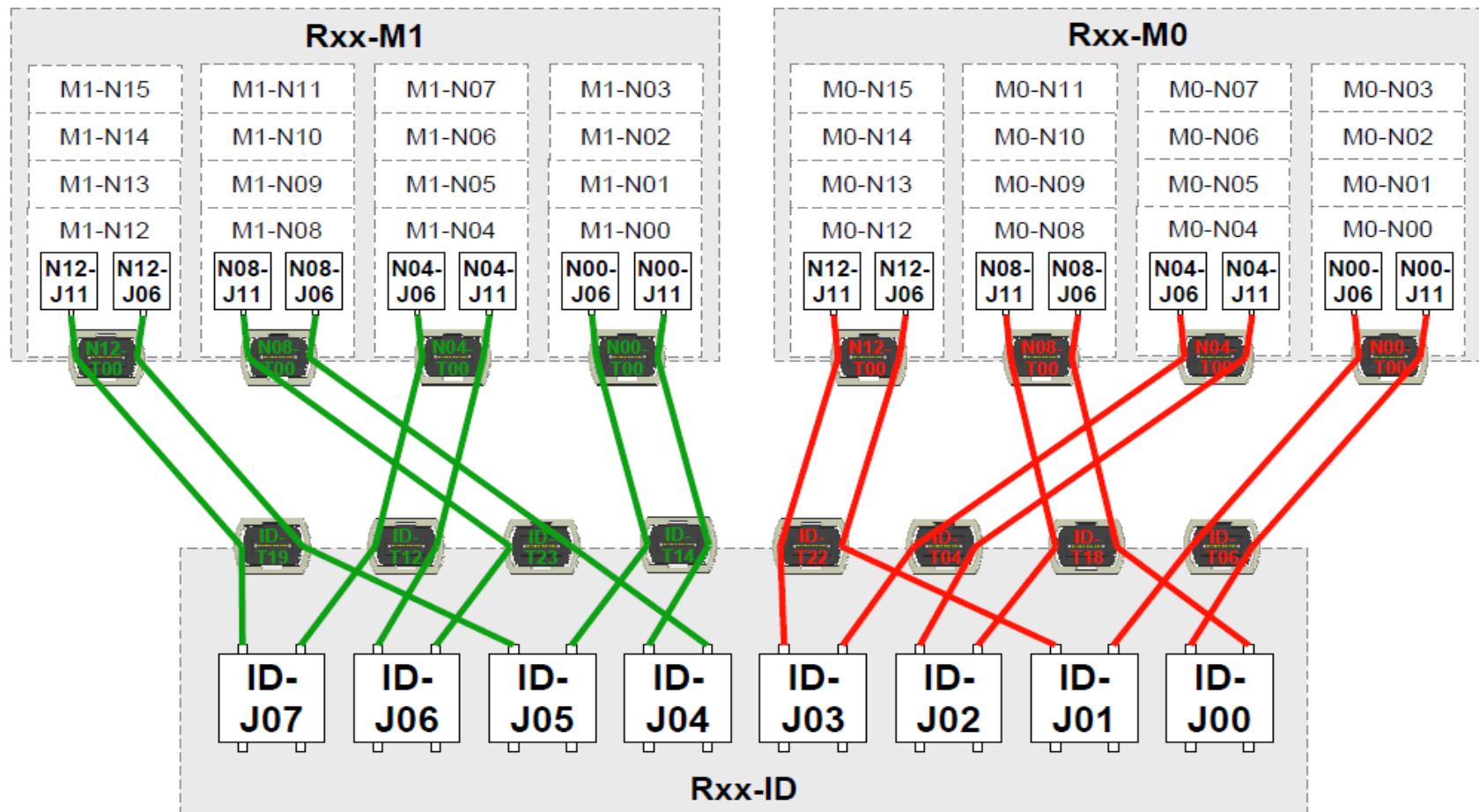
```
include 'mpif.h'
```

MPI extensions for Blue Gene/Q

```
MPIX_Hardware(MPIX_Hardware_t *hw)

typedef struct
{
    unsigned prank;           // Physical rank of node
    unsigned psize;           // Size of partition
    unsigned ppn;             // Processes per node
    unsigned coreID;          // Process ID
    unsigned clockMHz;        // Frequency in MHz
    unsigned memSize;         // Memory in MB
    unsigned torus_dimension; // Actual torus dimension
    unsigned Size[MPIX_TORUS_MAX_DIMS]; // Max. torus dimensions
    unsigned Coords[MPIX_TORUS_MAX_DIMS]; // Node's coordinated
    unsigned isTorus[MPIX_TORUS_MAX_DIMS]; // Wrap-around dims?
    unsigned rankInPset;      // Zero on Blue Gene/Q
    unsigned sizeOfPset;      // Zero on Blue Gene/Q
    unsigned idOfPset;        // Zero on Blue Gene/Q
} MPIX_Hardware_t;
```

Blue Gene/Q: I/O Node Cabling (8 ION/Rack)



MPI BGQ Extensions – I/O related functions

C

```
int MPIX_Pset_diff_comm_create(MPI_Comm *pset_comm_diff)
int MPIX_Pset_same_comm_create(MPI_Comm *pset_comm_same)
```

Fortran

```
MPIX_PSET_DIFF_COMM_CREATE(PSET_COMM_DIFF, IERROR)
MPIX_PSET_SAME_COMM_CREATE(PSET_COMM_SAME, IERROR)

INTEGER PSET_COMM_DIFF, PSET_COMM_SAME, IERROR
```

- Collective call on `MPI_COMM_WORLD`
- Returns a communicator which contains only MPI ranks which run on nodes belonging to different/same I/O Bridge Nodes
- The name of this function is chosen for backwards compatibility, since there are no psets on the Blue Gene/Q anymore

MPI BGQ Extensions – I/O related functions

C `int MPIX_IO_node_id()`

Fortran

`MPIX_IO_NODE_ID(IO_NODE_ID)`
`INTEGER :: IO_NODE_ID`

- Returns the ID of the associated I/O node



NO IERROR parameter for Fortran



MPI BGQ Extensions – I/O related functions

C `int MPIX_IO_distance()`

Fortran `MPIX_IO_DISTANCE(IO_DISTANCE)`
`INTEGER :: IO_DISTANCE`

- Returns the distance to the associated I/O node in number of hops



NO IERROR parameter for Fortran



MPI BGQ Extensions – I/O related functions

C `int MPIX_IO_link_id()`

Fortran

```
MPIX_IO_LINK_ID(IO_LINK_ID)  
INTEGER      :: IO_LINK_ID
```

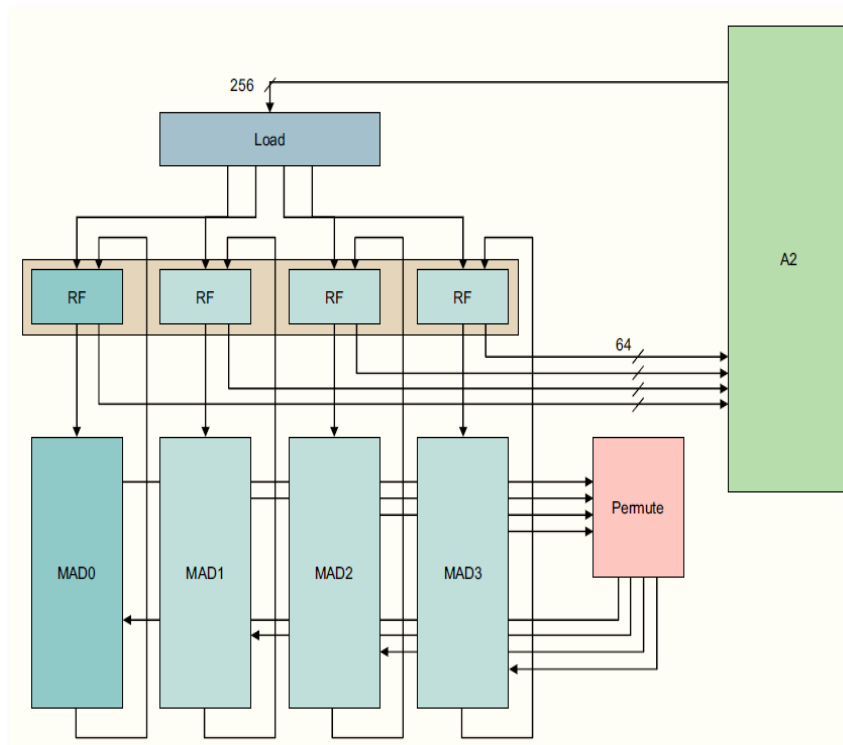
- Returns the ID of the link to the associated I/O node



NO IERROR parameter for Fortran



Quad-processing extension (QPX)



- Allows to perform 8 concurrent floating point operations (fused multiply-add, FMA) + load + store
- Four double precision pipelines, usable as
 - Scalar FPU
 - 4-wide double SIMD
 - 2-wide complex SIMD

IBM XL compiler support for QPX

Usage of QPX

- Compiler flag `-qsimd=auto`
- Check that SIMD vectorization is actually done!
 - `-qreport`
 - `-qlist`

```
>>>> LOOP TRANSFORMATION SECTION <<<<
[...]
```

```
0 9 1      Loop with nest-level 1 and
           iteration count 1000 was
           SIMD vectorized
[...]
```

```
>>>> LOOP TRANSFORMATION SECTION <<<<
[...]
```

```
0 9 1      Loop was not SIMD vectorized
           because the loop is not the
           innermost loop.
0 10 1     Loop was not SIMD vectorized
           because it contains memory
           references with non-
           vectorizable alignment.
```

IBM XL compiler support for QPX

Provide hints for the compiler

- Point to compiler likely iteration counts
- Instruct compiler to align fields
- Tell that FORTRAN assumed-shape arrays are contiguous
-qassert=contig

Fortran

```
real*8 :: x(:),y(:),a

!ibm* align(32, x, y)
!ibm* assert(itercnt(100))

do i=m, n
    z(i) = x(i) + a*y(i)
enddo
```

C/C++

```
double __align(32) *x, *y;
double a;
#pragma disjoint(*x, *y)
#pragma disjoint(*x, a)
#pragma ibm iterations(100)
for (int i=m; i<n; i++)
    z[i] = x[i] + a*y[i]
void foo(double* restrict a1,
         double* restrict a2){
    for (int i=0; i<n; i++)
        a1[i]=a2[i];}
```

IBM XL compiler QPX intrinsics

XL intrinsics	New intrinsic variable type	
	C/C++	<code>vector4double</code>
	Fortran	<code>vector(real(8))</code>
	Wide set of elemental functions available	
	LOAD, STORE, MULT, MULT-ADD, ROUND, CEILING, SQRT, ...	

Strengths:

- User may layout calculation by hand, if compiler not smart enough

Easy to use:

- Leave stack, register layout, load/store scheduling to compiler

QPX example using compiler intrinsics

```
...  
typedef vector4double qv;  
qv dx,dy,dz,dx2,dy2,dz2  
for (i=0;i<4;i++)  
{  
...  
    xd[i] = xdip1[j];  
    yd[i] = ydip1[j];  
    zd[i] = zdip1[j];  
}  
dx2 = vec_mul(dx,dx);  
dy2 = vec_mul(dy,dy);  
dz2 = vec_mul(dz,dz);  
d = vec_swsqrt(dx2+dy2+dz2);  
...
```

Source: IBM Corporation