JUQUEEN

Best Practices

17. Mai 2013 | Florian Janetzko

Outline

Production Environment

- Module Environment
- Job Execution

Basic Porting

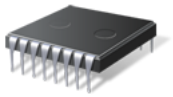
- Compilers and Wrappers
- Compiler/Linker Flags

Tuning Applications

- Advanced Compiler/Linker Flags
- QPX

JUQUEEN – System Architecture

IBM Blue Gene/Q JUQUEEN



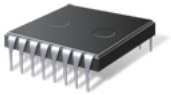
- IBM PowerPC A2 1.6 GHz, 16 cores/node, 4-way SMT, 64-bit
- 4-wide (dbl) SIMD (FMA)

- 16 GB RAM per node
- Torus network
- 28 racks, 458,752 cores

- 5.9 Petaflop/s peak

- Connected to a Global Parallel File System (GPFS) with 10 PByte online disk and 37 PByte offline tape capacity

JUQUEEN – Challenges



Chip
- 4-way SMT with1 integer + 1FPU instruction per cycle → filling pipes
- 4-wide SIMD → efficient vectorization

Memory
- 1 GB/core and *0.5 GB/core for pure MPI codes* → memory consumption
- HW support for transactional memory → efficient usage

Network
- Torus network → Mapping of tasks, communicators (communication pattern)

I/O
- Processing large amounts of data → Efficient I/O strategy and management

Parallelism
- MPP system → Scalability

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Module Environment

Module concept

- Provides overview over available software packages
- Eases use of software packages
  - Access to software packages, libraries
  - Supply of different versions of applications
  - Supply of application-specific information
- Enables dynamic modification of users' environment
  - Environment variables (**`PATH`**, **`LD_LIBRARY_PATH`**, **`MANPATH`**, …) are set appropriately
  - Detection of conflicts between applications

Module Environment

```
$ module <options> <module>
```

Option	Description
`<no option>`	Lists available options of the module command
`avail`	Lists all available modules
`list`	Lists modules currently loaded
`load`	Loads a module
`unload`	Unloads a module
`help`	Lists information about a module
`show`	Information about settings done by the module
`purge`	Unloads all modules

Module Environment

Six module categories

- COMPILER
  - *Different compilers and versions of compilers*
- IO
  - *I/O libraries and tools*
- MATH
  - *Mathematical libraries and software packages*
- MISC
  - *Software not fitting into another category*
- SCIENTIFIC
  - *Software packages from different scientific fields*
- TOOLS
  - *Performance analysis, debugger, etc.*

Software for

Compute Nodes:

`/bgsys/local`

Front-end Nodes:

`/usr/local`

Module Environment

```
$ module avail
------------ /bgsys/local/modulefiles/TOOLS ------------
------------ /bgsys/local/modulefiles/SCIENTIFIC ------------
cp2k/2.2.12394          cpmd/3.15.1_c(default) namd/2.8
cpmd/3.15.1             lammps/30Aug12         namd/2.9(default)
cpmd/3.15.1_a           lammps/5May12(default)
cpmd/3.15.1_b           libint/1.1.4
```

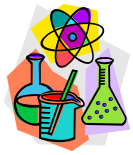
```
------------ /usr/local/modulefiles/COMPILER ------------
cmake/2.8.8(default)
------------ /usr/local/modulefiles/MATH ------------
------------ /usr/local/modulefiles/SCIENTIFIC ------------
------------ /usr/local/modulefiles/IO ------------
------------ /usr/local/modulefiles/TOOLS ------------
UNITE/1.1
------------ /usr/local/modulefiles/MISC ------------
```

Module Environment – Applications & Libraries

Mathematical applications and libraries

arpack (2.1)	gsl (1.15)	mumps (4.10.0)	scalapack (2.0.1)
fftw (2.1.5,3.3.2)	hypre (2.8.0)	parmetis (3.2.0,4.0.2)	sprng (1.0, 2.0)
gmp (5.0.5)	lapack (3.3.0)	petsc (3.3)	sundials (2.5.0)

Scientific applications



CPMD (3.15.1)	Gromacs (4.5.5)	OpenFOAM*
CP2K (2.2.12394)	Lammps (5May12,30Aug12)	QuantumEspresso*
GPAW*	Namd (2.8, 2.9)	VASP**

* In preparation

** Software not installed but makefiles are available

Module Environment – Applications & Libraries

I/O libraries

darshan
HDF5
netCDF
SIONlib

Tools

Cmake (2.8.8)
DDT*
Extrae (2.2.1)
hpctoolkit (5.2.1)
PAPI (4.4.0)
Scalasca (1.4.2)
Tau (2.21.2, 2.21.3)
Totalview (8.11.0)

* In preparation

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Running Simulations – 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)
  - *Classes chosen by LoadLeveler according to core count of job*

For Information about LoadLeveler on JUQUEEN see

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

LoadLeveler - Commands

Command	Description
`llsubmit <jobfile>`	Sends job to the queuing system

`llq`
`llq -l <job ID>`
`llq -s <job ID>`
 	
`llq -u <user>`
	Lists all queued and running jobs
	detailed information about the specified job
	detailed information about a specific queued job, e.g. expected start time
	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

LoadLeveler – Command Examples

Submitting a batch job: **`llsubmit`**

```
$ llsubmit batch-job.js
llsubmit: Processed command file through Submit Filter:
"/bgdata/admin/loadl/extensions/filter".
llsubmit: The job "juqueen2c1.zam.kfa-juelich.de.35395" has been submitted.
```

Query status of submitted jobs: **`llq`**

```
$ llq -u userid
Id                       Owner      Submitted   ST PRI Class        Running On
------------------------ ---------- ----------- -- --- ------------ -----------
juqueen2c1.35395.0       userid     11/15 10:11 I  50  n001

1 job step(s) in query, 1 waiting, 0 pending, 0 running, 0 held, 0 preempted
```

Cancel a submitted job: **`llcancel`**

```
$ llcancel juqueen2c1.35395.0
llcancel: Cancel command has been sent to the central manager.
```

LoadLeveler – Job Command File

ASCII file containing two major parts

1. LoadLeveler job keywords block at the beginning of a file
   - LoadLeveler keywords have the form
     `#@<keyword>`
   - # and @ can be separated by any number of blanks

2. One or more application script blocks
   - Regular shell script
   - Can contain any shell command

LoadLeveler – Standard Keywords

Keyword	Description
`#@job_name=<name>`	Name of the job

`#@notification=`
`end`
`error`
`never`
`start`
`always`
	Send notification
	if the job is finished
	if the job returned an error code ≠ 0
	never
	upon the start of the job
	combination of `start, end, error`

`#@notify_use=<mailaddr>`	Mail address to send messages to
`#@wall_clock_limit=hh:mm:ss`	Requested wall time for the job

`#@input=<input file name>`
`#@output=<file name for stdout>`
`#@error=<file name for stderr>`
	Specifies corresponding file names

`#@environment=[<variable>,` COPY_ALL]	Environment variable to be exported to job
`#@queue`	Queue job

LoadLeveler – Blue Gene/Q Keywords

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

LoadLeveler – 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
m048*	16385 – **24576**	24:00:00	06:00:00
m056*	24577 – **57344**	24:00:00	06:00:00

INCREASING PRIORITY

*On demand only

You will be charged for the full partition (e.g. if you request 513 nodes you will be charged for 1024 nodes!) → Always use full partitions!

LoadLeveler – Job Scheduling

Backfill scheduler

- The biggest job has the highest priority (*Top Dog*)
- LoadLeveler fills gaps with smaller, short-running jobs while freeing the system for the Top Dog

Tip: Specify the wall time for your jobs as exact as possible, because jobs requesting a shorter wall time have a better chance to be executed.

Big jobs

- Jobs requesting ≥8 racks are collected and run in dedicated time slots (e.g. after a maintenance) at least once a week

Running Simulations – runjob Command

Launch command for parallel applications

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

Option	Description
`--args <prg_arg>`	Passes "**`prg_arg`**" to the launched application on the compute node.
`--exe <executable>`	Specifies the full path to the executable
`--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

LoadLeveler – Example Job Command File I

```
#@job_name          = MPI_code
#@comment           = "32 ranks per node"
#@output            = test_$(jobid)_$(stepid).out
#@error             = test_$(jobid)_$(stepid).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 --exe app.x
```

Pure MPI applications need to use 32 tasks per node in order use the architecture efficiently!

Running Simulations – MPI/OpenMP Codes

- On Blue Gene/P
  - Three modes were available
    1. VN mode (4 MPI tasks, no thread per task)
    2. DUAL mode (2 MPI tasks with 2 OpenMP threads each)
    3. SMP mode (1 MPI task with 4 OpenMP threads)
- On Blue Gene/Q
  - One node has 16 cores with 4-way SMT each
  - Several configurations possible
    - $\texttt{ntasks} \times \texttt{nthreads} = 64$
    - $\texttt{ntasks} = 2^{n},\ 0 \leq n \leq 6$

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

LoadLeveler – Example Job Command File II

```
#@job_name          = hybrid_code
#@comment           = "16x4 configuration"
#@output            = test_$(jobid)_$(stepid).out
#@error             = test_$(jobid)_$(stepid).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
```

Monitoring of Jobs

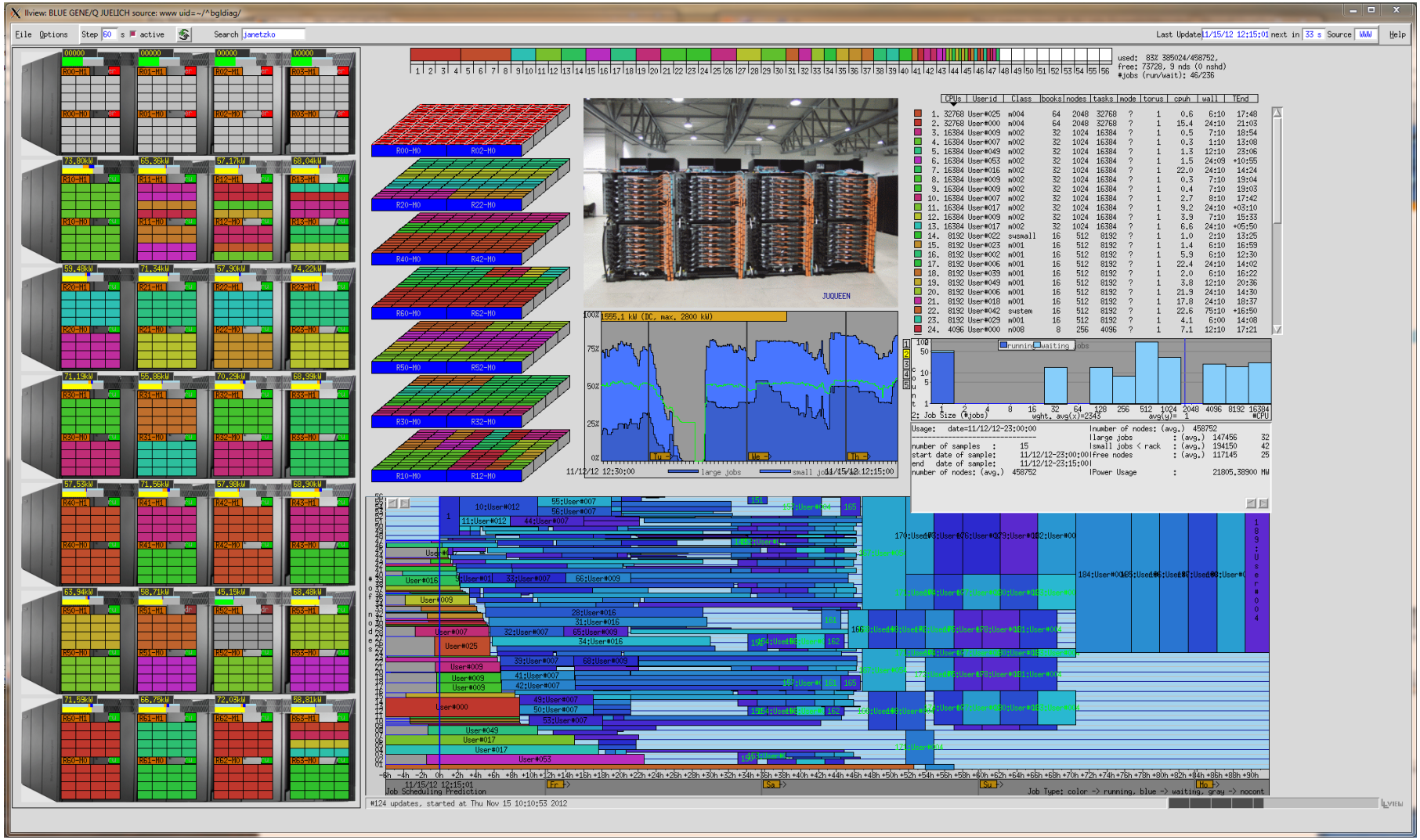
LoadLeveler

- 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)

Llview


llview: BLUE GENE/Q JUELICH source: www uid=~/^bgldiag/
File Options
Step 60 s active
Search janetzko
Last Update 11/15/12 12:15:01 next in 33 s Source WWW
Help
used: 83% 385024/458752,
free: 73728, 9 nds (0 nshd)
#jobs (run/wait): 46/236
JUQUEEN
1555.1 kW (DC, max. 2800 kW)
large jobs
small jobs
11/12/12 12:30:00
11/15/12 12:15:00
running
waiting
jobs
2: Job Size (#jobs)
wght. avg(x)=2343
avg(w)= 1
#CPU
Usage: date=11/12/12-23:00:00
number of samples : 15
start date of sample: 11/12/12-23:00:00
end date of sample: 11/12/12-23:15:00
number of nodes: (avg.) 458752
Number of nodes: (avg.) 458752
large jobs : (avg.) 147456 32
small jobs < rack : (avg.) 194150 42
free nodes : (avg.) 117145 25
Power Usage : 21805.38900 MW
Job Scheduling Prediction
#124 updates, started at Thu Nov 15 10:10:53 2012
Job Type: color -> running, blue -> waiting, gray -> nocont

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Compilers

- Different compilers for front-end and compute nodes
- GNU and IBM XL family of compilers available

Tip: It is recommended to use the XL suite of compilers for the CN since they produce in general better optimized code.

FRONT-END

Language	XL compiler	GNU compiler
C	`xlc, xlc_r`	`gcc`
C++	`xlc++, xlc++_r, xlC, xlC_r`	`g++`
Fortran	`xlf, xlf90, xlf95, xlf2003` `xlf_r, xlf90_r, xlf95_r, xlf2003_r`	`gfortran`

Compilers for CN

GNU (GCC)

Language	Compiler invocation	MPI wrapper
C	`powerpc64-bgq-linux-gcc`	`mpigcc`
C++	`powerpc64-bgq-linux-g++`	`mpig++`
Fortran	`powerpc64-bgq-linux-gfortran`	`mpigfortran`

XL COMPILERS

Language	Compiler invocation (thread-safe: *_r)	MPI wrapper (thread-safe: *_r)
C	`bgxlc, bgc89, bgc99`	`mpixlc`
C++	`bgxlc++, bgxlC`	`mpixlcxx`
Fortran	`bgxlf, bgxlf90, bgxlf95, bgxlf2003`	`mpixlf77, mpixlf90, mpixlf95, mpixlf2003`

Basic Compiler/Linker Options – XL Compilers I

Flags in order of 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 during compilation AND linking – Check the compiler manual. If you are not sure, include flags used for compiling also in the linking step!

Basic Compiler/Linker Options – XL Compilers II

Additional compiler flags

Compiler/Linker Flag	Description
`-qsmp=omp -qthreaded`	Switch on OpenMP support
`-qreport -qlist`	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
`-qessl –lessl[smp]bg`	Compiler attempts to replace some intrinsic FORTRAN 90 procedures by essl routines where it is safe to do so

How to link with ESSL routines, see

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

Creating static Libraries

Preferred kind of library on BG/Q

C/C++

```
  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

C/C++

```
  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!

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Diagnostic Compiler Flags (XL Compilers)

Diagnostic messages are given on the terminal and/or in a separate file

- **`-qreport`**: compilers generate a file **`name.lst`** for each source file
- **`-qlist`**: compiler listing including an object listing
- **`-qlistopt`**: options in effect during compilation included in listing

Listen to the compiler!

- **`-qflag=<listing-severety>:<terminal-severety>`**
- i: informal messages, w: warning messages, s: severe errors
- Use **`-qflag=i:i`** to get all information
- **`-qlistfmt=(xml|html)=<option>`**

Example: Compilers 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).
```

Single-Core Optimization – Compiler/Linker Flags

Insertion of prefetch instructions

```
-qprefetch=(no)aggressive
```

Function inlining

```
-qinline=auto:level=5
-qinline+procedure1[:procedure2[:…]]
```

Aggressive loop analysis and transformations

```
-qhot=level=[0-2]
```

Loop unrolling

```
-qunroll
```

Intra-/inter-procedural optimization (compiling + linking!)

```
-qipa
```

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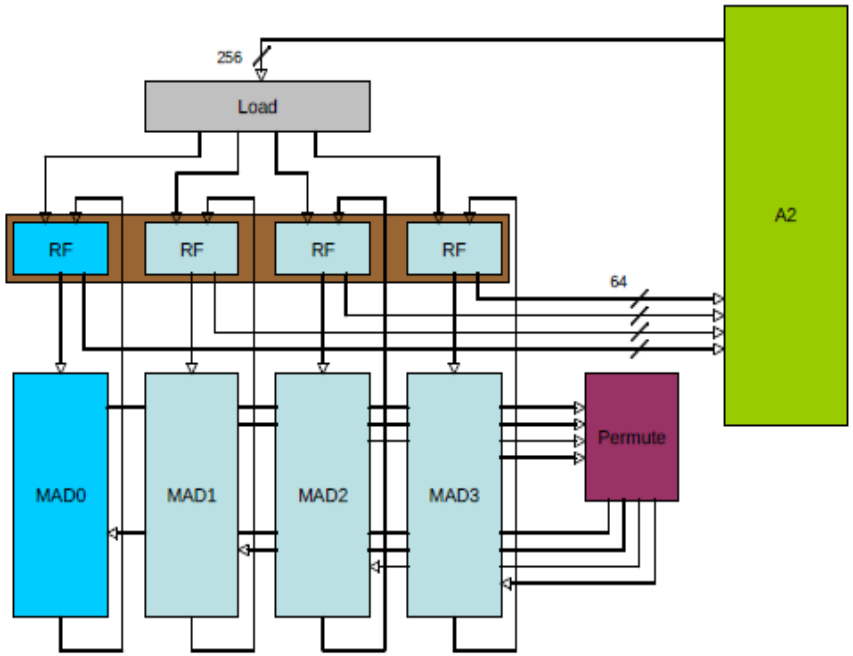
Quad Floating Point Extension Unit (QPX)

4 double precision pipelines, usable as:

- scalar FPU
- 4-wide FPU SIMD (Single Instruction Multiple Data)
- 2-wide complex arithmetic SIMD

8 concurrent floating point ops (FMA) + load + store



QPX Expected Performance Improvements

Type of Code	Expected performance improvements
Linear algebra dominated code	Up to 4x performance improvement over scalar code convenient to leverage “IBM ESSL for BG/Q”
Runtime-dependent alignment dominated code	1-4x performance improvement over scalar code (depending on runtime alignment values)
Memory-latency dominated code	Similar performance to BG/L and BG/P

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.
```

QPX Usage – Hints for the Compiler

Compiler needs hints

- Hint compiler to 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 QPX Intrinsics

New intrinsic variable type

- C/C++: vector4double
- FORTRAN: vector(real(8))

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 (e.g. where no loop)

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] = xdipl[j];
  yd[i] = ydipl[j];
  zd[i] = zdipl[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

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)

  Forschunszentrum 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