Running MD on HPC architectures II. Bluegene/Q

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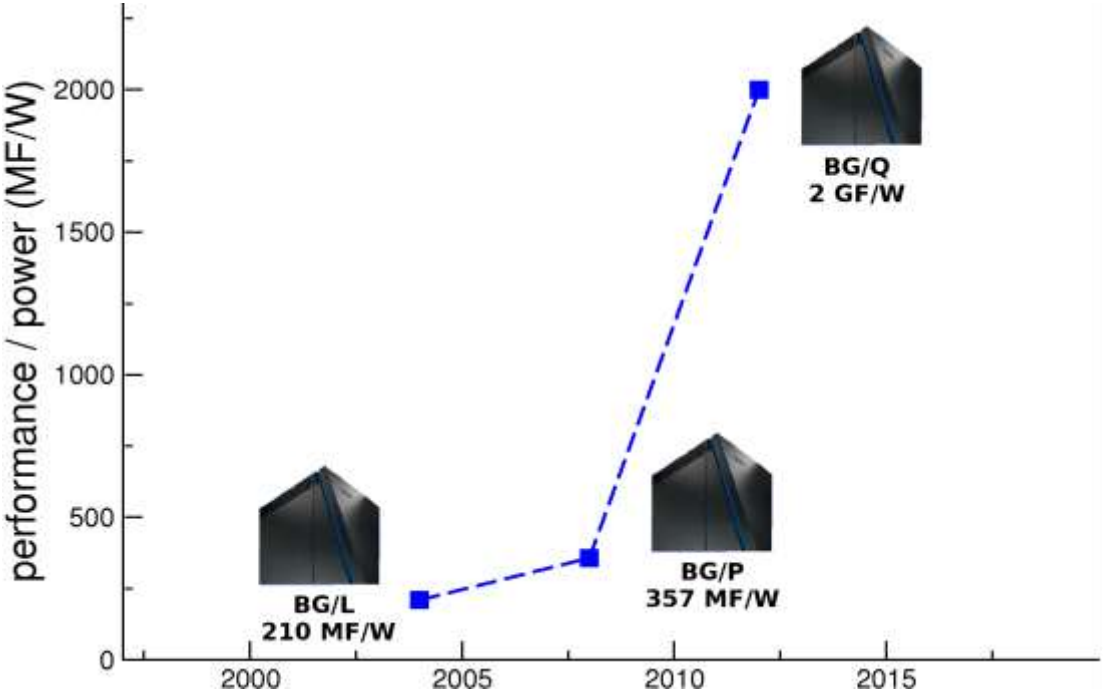
Outline

- Overview of Blue Gene/Q architecture
- Production environment
- How to launch a MD code on Fermi
- Example: Satellite Tobacco Mosaic virus with NAMD

- BG is a massively parallel supercomputer
- It holds different types of nodes (and networks)
- It is designed to have high energy-efficiency (performance/power)



BLUE GENE EVOLUTION

	Total		Biggest Config	Per rack		
	Performance [PF]	Efficiency [MF/W]	Max # of racks	Performance [TF]	Efficiency	# of cores
BG/L	0.596	210	104	5.7	2.02	2048
BG/P	1	357	72	13.9	4.96	4096
BG/Q	20	2000	96	209	20.83	16384

Towards higher and higher:

- Performance
- Efficiency
- Density of cores per rack

Content of a BGQ Rack

- 2 **midplanes** form a rack
- Each midplane has 16 **Node Cards**
- Each Node Card has 32 **Compute Nodes**
  - 2x32x16=1024 compute nodes per rack
- Flexible I/O nodes – node cards ratio
  (at least 512 cores per I/O node)
  - In our configuration: 2 rack con 1024 core per I/O node
    8 rack con 2048 core per I/O node

PARTNERSHIP FOR ADVANCED COMPUTING IN EUROPE

FERMI @ CINECA
PRACE Tier-0 System

Architecture: 10 BG/Q Racks
Model: IBM-BG/Q
Processor Type: IBM PowerA2, 1.6 GHz
Computing Cores: 163840
Computing Nodes: 10240
RAM: 1 GByte / core
Internal Network: 5D Torus
Disk Space: 2 PByte of scratch space
Peak Performance: 2 PFlop/s
Power Consumption: 1 MWatt

Note that..

The number of I/O nodes per rack constraints:

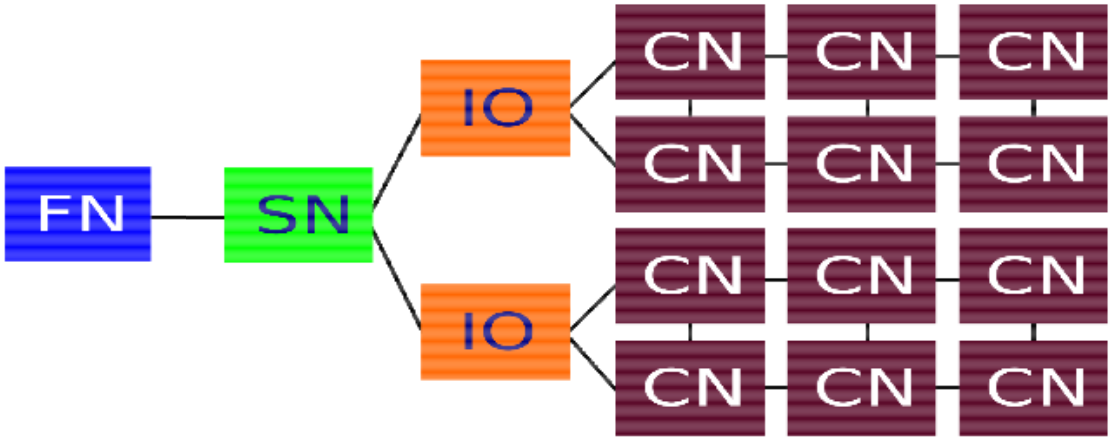
- I/O bandwidth to/from compute racks
  (each I/O node has 2 links (4GB/s in 4GB/s out))

- The minimum partition allocatable on a BG/Q system ("small block" jobs)

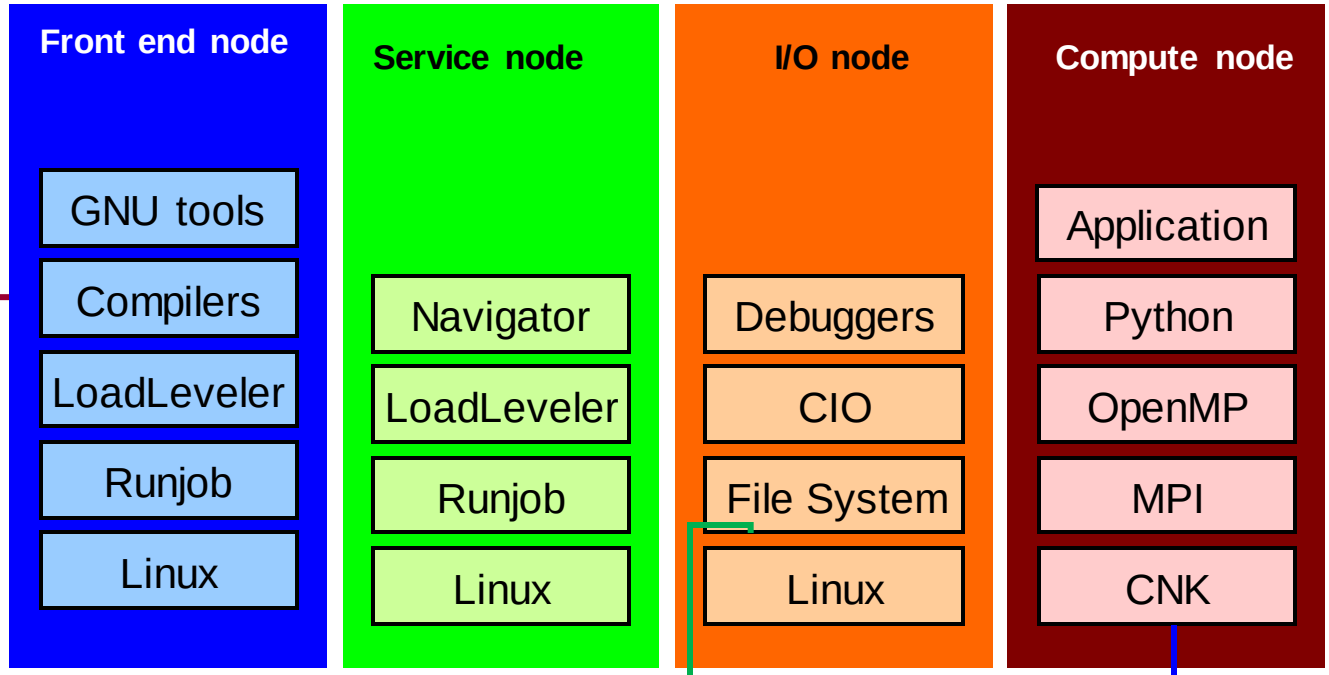
For FERMI:
  bg_size=64 (jobs running on R11 and R31) → 1024 cores
  bg_size=128 (jobs running on the other racks) → 2048 cores

BG/Q I/O architecture

- **Front-end nodes (FN)**, dedicated for user's to login, compile programs, submit jobs, query job status, debug applications
- **Service nodes (SN)**, perform system management services, create and monitoring processes, initialize and monitor hardware, configure partitions, control jobs, store statistics
- **I/O nodes (IO)**, provide a number of OS services, such as files, sockets, process management, debugging
- **Compute nodes (CN)**, run user application, limited OS services



Software stack: Overview



Cross compilation: executables are built to run on compute nodes

Not on compute nodes!

- No shell interpreter
- No fork/exec support

BGQ Networks

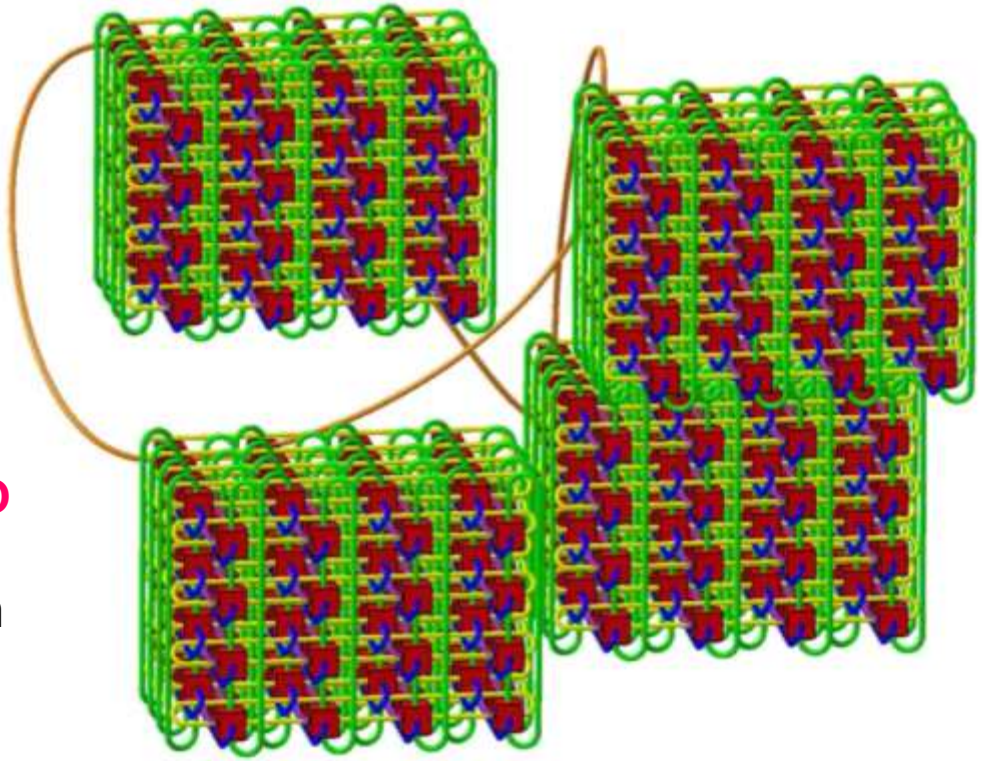
5D Torus Network

5D topology for point-to-point communication

- 2 GB/s bidirectional bandwidth on all (10+1) links, 5D nearest neighbour exchange at 1.75 GB/s per link
- Collective and barrier networks embedded in 5-D torus network.

External, independent and dynamic I/O system

- I/O nodes in separate drawers/rack with private interconnections
- I/O network to/from Compute rack: 2 links (4 GB/s in 4 GB/s out)

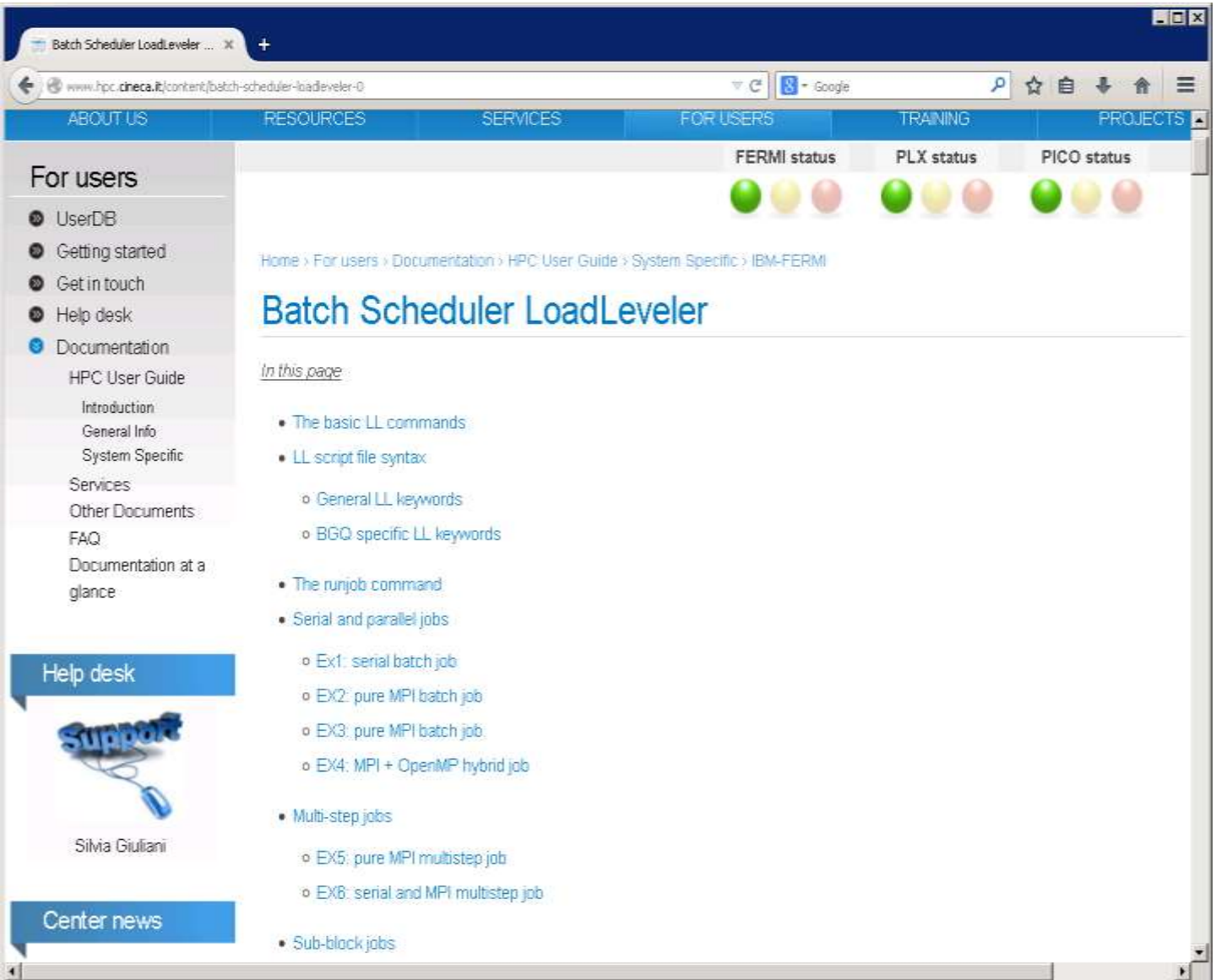


Fermi Production environment

queue name	ComputeNodes	max wall time	defined on	notes	priority
debug	64	00:30:00	2 rack with 16 I/O nodes	Maxqueued(*)=1	high
longdebug	64	24:00:00	2 rack with 16 I/O nodes	Maxqueued(*)=2	low
smallpar	128	24:00:00	8 rack with 16 I/O nodes	Maxqueued(*)=4	high
parallel	256 - 512	24:00:00	2 rack with 8 I/O nodes	Maxqueued(*)=2	high
bigpar	1024 - 2048 (1-2 racks)	24:00:00	6 rack with 8 I/O nodes	Maxqueued(*)=2	very high
keyproject	1024 - 6*1024 (1-6 racks)	24:00:00	8 rack with 8 I/O nodes	Ask to superc@cineca.it Due to the geometry of the system, the max number of usable racks is 6	very high
serial	1 core	06:00:00	front-end node	to be requested with @#class=serial	high

FERMI User's Guide:

http://www.hpc.cineca.it/content/ibm-fermi-user-guide
http://www.hpc.cineca.it/content/batch-scheduler-loadleveler-0



How to submit your job script: LL commands

llsubmit

Example:
$> llsubmit job.cmd

llq
Example:
llq -u $USER
$> llq -u amarani0

```
Id                       Owner        Submitted     ST  PRI Class      Running On
------------------------ ---------- ----------- -- --- ------------ -----
fen04.7334.0             amarani0     9/21 15:11    I     50  parallel

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

How to submit your job script: LL commands

$> llq -l <job_id>
• will print a more verbose output will be generated for job_id
• In particular you'll be notified about the bgsize you requested and the real bgsize allocated:

……
……
BG Size Requested: 1024
BG Size Allocated: 1024
BG Shape Requested:
BG Shape Allocated: 1x1x1x2
BG Connectivity Requested: Mesh
BG Connectivity Allocated: Torus Torus Torus Torus
……
……

$> llcancel
Example:
>llcancel <job_id>

Job script: general structure

```
#!/bin/bash
# @ job_name  = bgsize.$(jobid)
# @ output  = z.$(jobid).out
# @ error   = z.$(jobid).err
# @ shell = /bin/bash
# @ job_type  = bluegene
# @ wall_clock_limit  = 02:00:00
# @ notification = never
# @ bg_size  = 256
# @ class = keyproject
# @ account_no  = cinstaff
# @ restart = no
# @ queue


cd /gpfs/scratch/userinternal/cin0753a/mydir

runjob –ranks-per-node  64 ./program.exe
```

LL keywords

Application block

runjob

Applications always need to be executed with **runjob** command to run on the compute nodes

- Syntax:
  - runjob [options]
  - runjob [options] binary [arg1 arg2 ... argn]
- Parameters can be set
  - by command-line options (higher priority!)
  - environment variables
- runjob –h for a complete list

runjob options – I (job)

Command line option	Environment variable	Description
--exe executable	RUNJOB_EXE= executable	Specifies the full path to the executable (this argument can be also specified as the first argument afer ":") runjob --exe /home/user/a.out runjob : /home/user/a.out
--args "prg_args"	RUNJOB_ARGS="prg_args"	Passes "prg_args" to the launched application on the compute node runjob : a.out hello world runjob --args hello world --exe a.out
--envs "ENVVAR=values"	RUNJOB_ENVS= "ENVVAR=value"	Sets the environment variable ENVVAR=value in the job environment on the compute nodes
-exp_env ENVVAR	RUNJOB_EXP_ENV =ENVVAR	Exports the environment variable ENVVAR in the current environment to the job on the compute nodes

runjob options – II (resources)

Command line option	Environment variable	Description
--ranks-per-node		Specifies the number of processes per compute node. Valid values are:1,2,4,8,16,32,64
--np n	RUNJOB_NP=n	Number of processes in the job(<= block_size*ranks-per_node)
--mapping	RUNJOB_MAPPING= mapfile	Permutation of ABCDET or a path to a mapping file containing coordinates for each rank

runjob options – III

Command line option	Environment variable	Description
--start_tool		Path to tool to start with the job
--tool_args		Arguments for the tool

Fermi Production environment

```
$>module av

------------ /cineca/prod/modulefiles/base/applications --------
abinit/6.12.3        crystal09/1.01        qe/5.0bgq
amber/12             dl_poly/4.03           siesta/3.1
bigdft/1.6.0         gromacs/4.5.5         vasp/5.2.12
cp2k/2.3             lammps/20120816       vasp/5.3.2
namd/2.9             cpmd/v3.15.3
```

To load a specific module, i.e. set specific env vars
$> module load <module_name>

Show the variables set by a module
$> module show <module_name>

Retrieve informations of a module
$> module help <module_name>

Available MD packages on Fermi

Some of the currently installed MD codes on Fermi and available for use:

```
$> module av

------------ /cineca/prod/modulefiles/base/applications ------------

abinit/6.12.3              crystal09/2.0.1(default)   octopus/4.1(default)
amber/12(default)          dl_poly/4.03               openfoam/2.1.1
bigdft/1.6.0               dl_poly/4.05(default)      qe/5.0.3b(default)
cp2k/2.3                   gromacs/4.5.5(default)     qe/5.0bgq
cp2k/2.4(default)          gromacs/4.6.1              siesta/3.1
cpmd/3.15.3_rev2606        lammps/20120816            siesta/3.1-TS
cpmd/3.17.1(default)       namd/2.9(default)          vasp/5.2.12
namd/2.10                  enzo/2.2                   gromacs/4.5.5
crystal09/1.01             nwchem/6.3                 vasp/5.3.3(default)
```

NAMD template script for Fermi

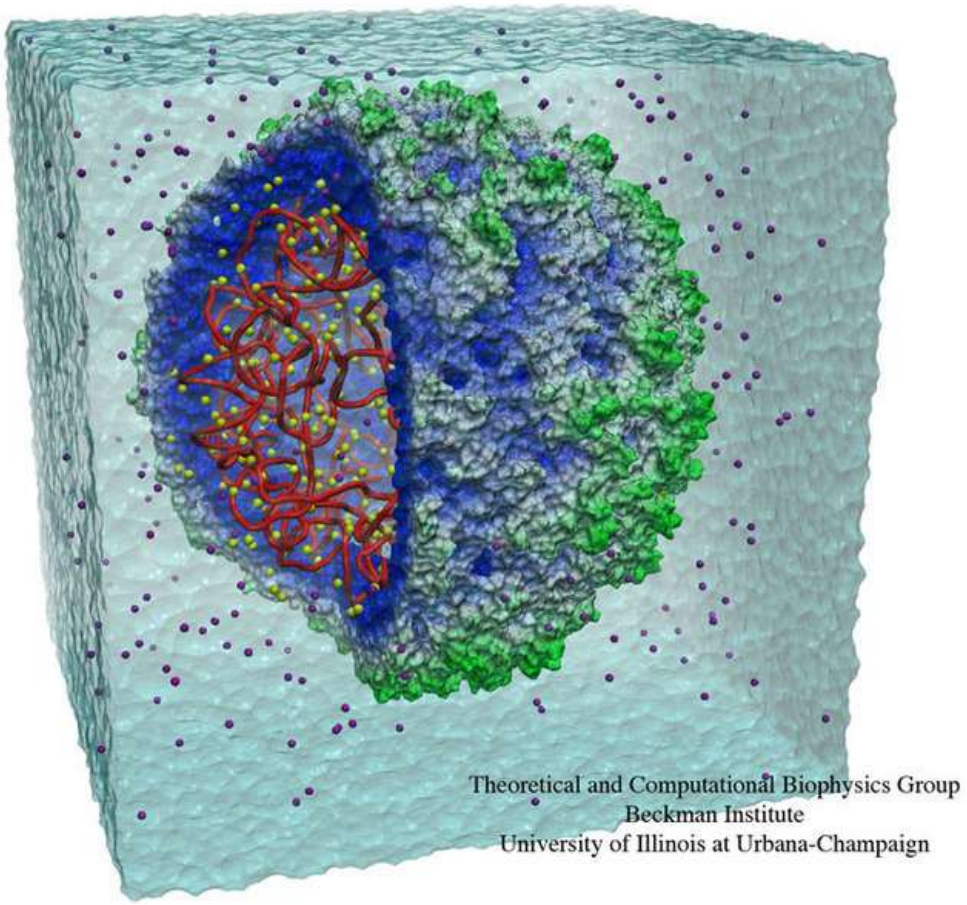
```
#!/bin/bash
# @ job_name  = namd.$(jobid)
# @ output  = $(job_name).out
# @ error = $(job_name).err
# @ shell = /bin/bash
# @ job_type  = bluegene
# @ wall_clock_limit  = 01:00:00
# @ bg_size  = 64
# @ account_no  = your_account_name
# @ queue

module  load namd/2.9

#launch with 256 processes (grouping 4 processes per node) using multi-thread (16 threads per process)
runjob  --rank-per-node  4 : $NAMD_HOME/namd2  +ppn16  input.namd  > output.log
```

64*4 = 256 MPI tasks

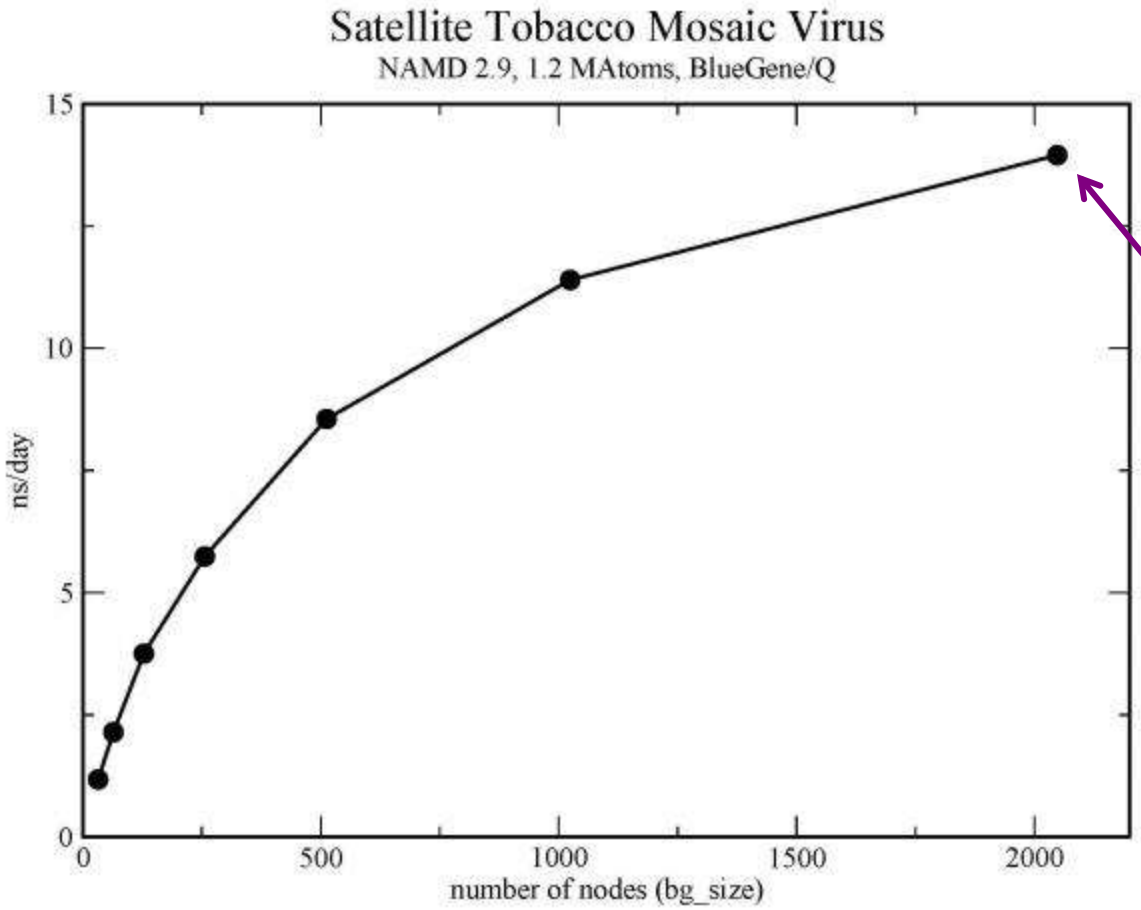
*16 = 4096 threads

Optimized by IBM namd version: adopts a mixed MPI/OpenMP thread approach for the parallel computation.
The number of MPI process per node are selected with the --ranks-per-node option of LoadLeveler, while the number of OpenMP threads per MPI process with the +ppn flag of namd.

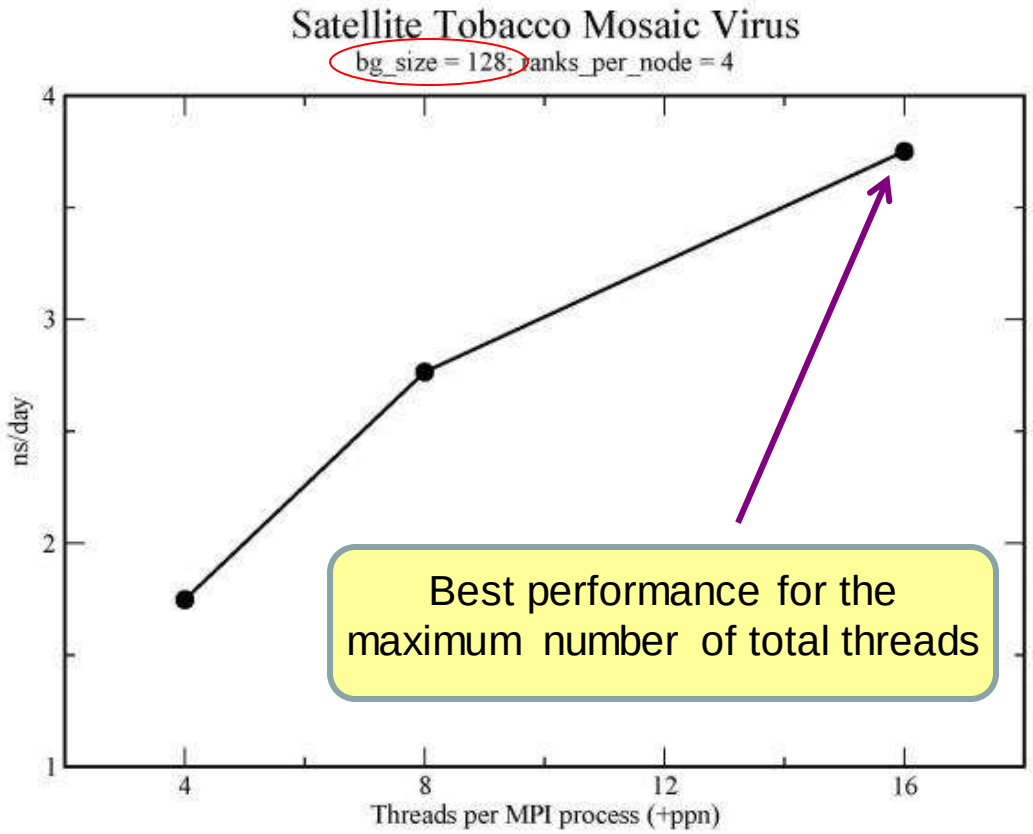
Satellite Tobacco Mosaic virus



STMV (virus) benchmark (1,066,628 atoms, periodic, PME)

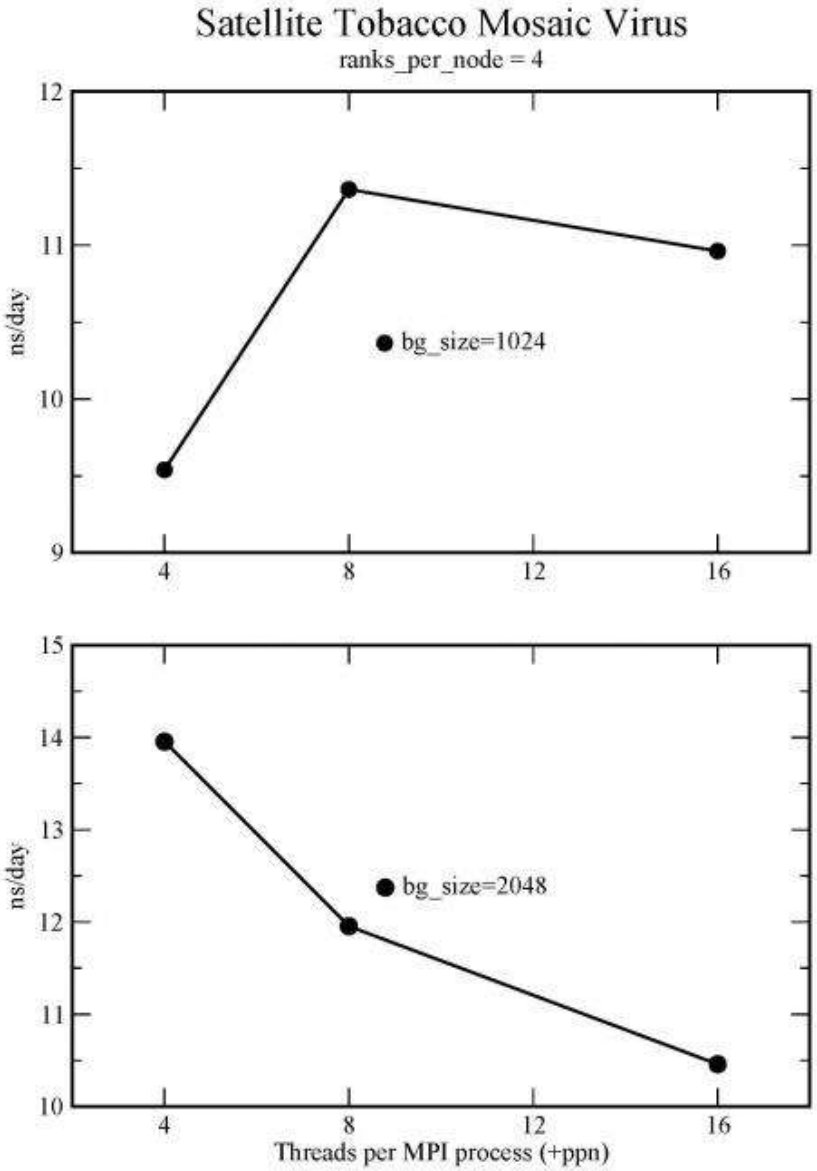


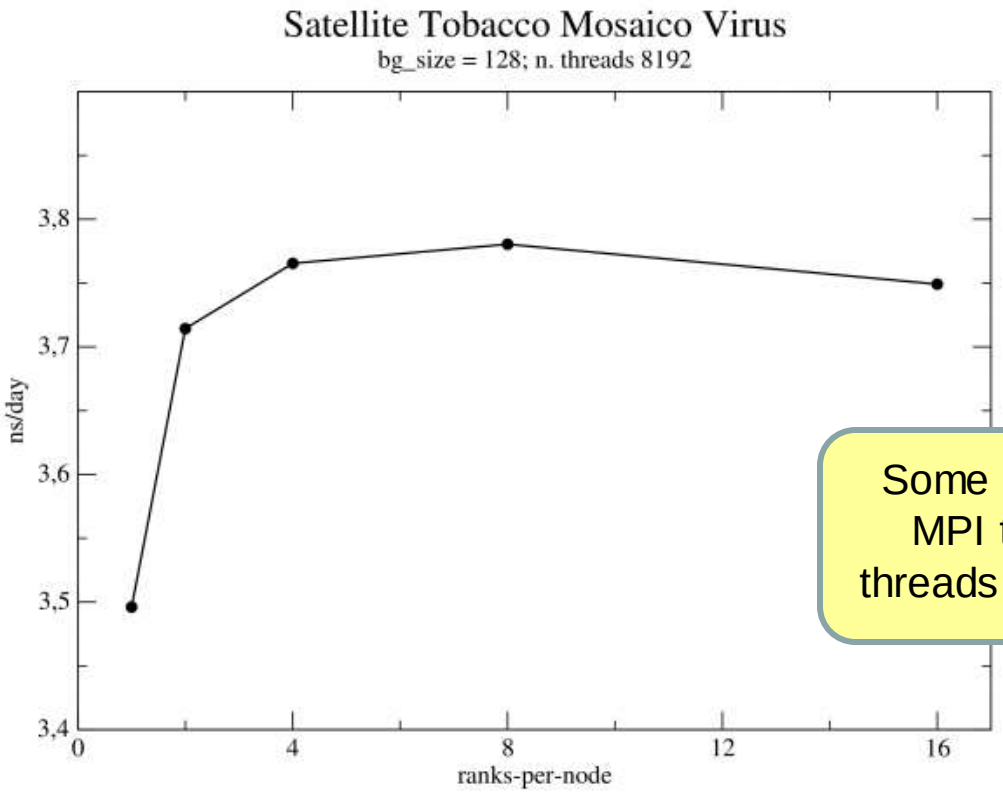
Increase of performance up to 32,768 cores! (bg_size=2048




```
runjob --np 512 --ranks-per-node 4 : $NAMD_HOME/namd2 stmv_ori.namd +ppn4 > stmv.out
runjob --np 512 --ranks-per-node 4 : $NAMD_HOME/namd2 stmv_ori.namd +ppn8 > stmv.out
runjob --np 512 --ranks-per-node 4 : $NAMD_HOME/namd2 stmv_ori.namd +ppn16 > stmv.out
```

That is not true anymore when increasing bg_size: Check the performance on your system!





Some combinations of MPI tasks/OpenMP threads are less efficient

```
runjob --np 2048 --ranks-per-node 16 : $NAMD_HOME/namd2 stmv_ori.namd +ppn4 > stmv.out
runjob --np 1024 --ranks-per-node  8 : $NAMD_HOME/namd2 stmv_ori.namd +ppn8 > stmv.out
runjob --np  512 --ranks-per-node  4 : $NAMD_HOME/namd2 stmv_ori.namd +ppn16 > stmv.out
runjob --np  256 --ranks-per-node  2 : $NAMD_HOME/namd2 stmv_ori.namd +ppn32 > stmv.out
runjob --np  128 --ranks-per-node  1 : $NAMD_HOME/namd2 stmv_ori.namd +ppn64 > stmv.out
```

Amber template script for Fermi

```
#!/bin/bash
# @ job_name  = amber.$(jobid)
# @ output  = z.$(jobid).out
# @ error = z.$(jobid).err
# @ shell = /bin/bash
# @ job_type  = bluegene
# @ wall_clock_limit  = 01:00:00
# @ notification = always
# @ bg_size  = 64
# @ account_no = my_account_no
# @ queue

module  load amber/12

# do any amber pre-processing on the front-end nodes (antechamber, tleaps, etc...

# get the path of the sander executable for the backend nodes
sander=$(which  sander.MPI)

# add any  sander options
exe="$sander  -i mdin  -o mdout  -p prmtop  -c inpcrd  -r restrt -ref refc -mtmd  mtmd  -x mdcrd"

#launch sander on all the allocated back-end nodes (note the : which must be present with  this syntax)
# if you have  memory problems reduce the --ranks-per-node option
runjob  --ranks-per-node  16 --env-all : $exe
```

GROMACS template script for Fermi

```
#!/bin/bash
# @ job_name  = gromacs.$(jobid)
# @ output  = $(jobid).out
# @ error = $(jobid).err
# @ shell = /bin/bash
# @ job_type  = bluegene
# @ wall_clock_limit  = 01:00:00
# @ notification = always
# @ bg_size  = 64
# @ account_no = <my_account_no>
# @ queue

module  load gromacs/4.6.5

# get the path of the mdrun  executable for the backend nodes
mdrun=$(which  mdrun_bgq)

# add any mdrun  options.
# Here we are using 4 OpenMP  threads for MPI task.
exe="$mdrun  -v -s topol.tpr  -ntomp  4"

#launch single precision mdrun  on all the back-end nodes
runjob  --ranks-per-node  16 --env-all : $exe
```

64*16 = 1024 MPI tasks
*4 = 4096 threads

mixed MPI/OpenMP thread version