Introduction to IBM Blue Gene

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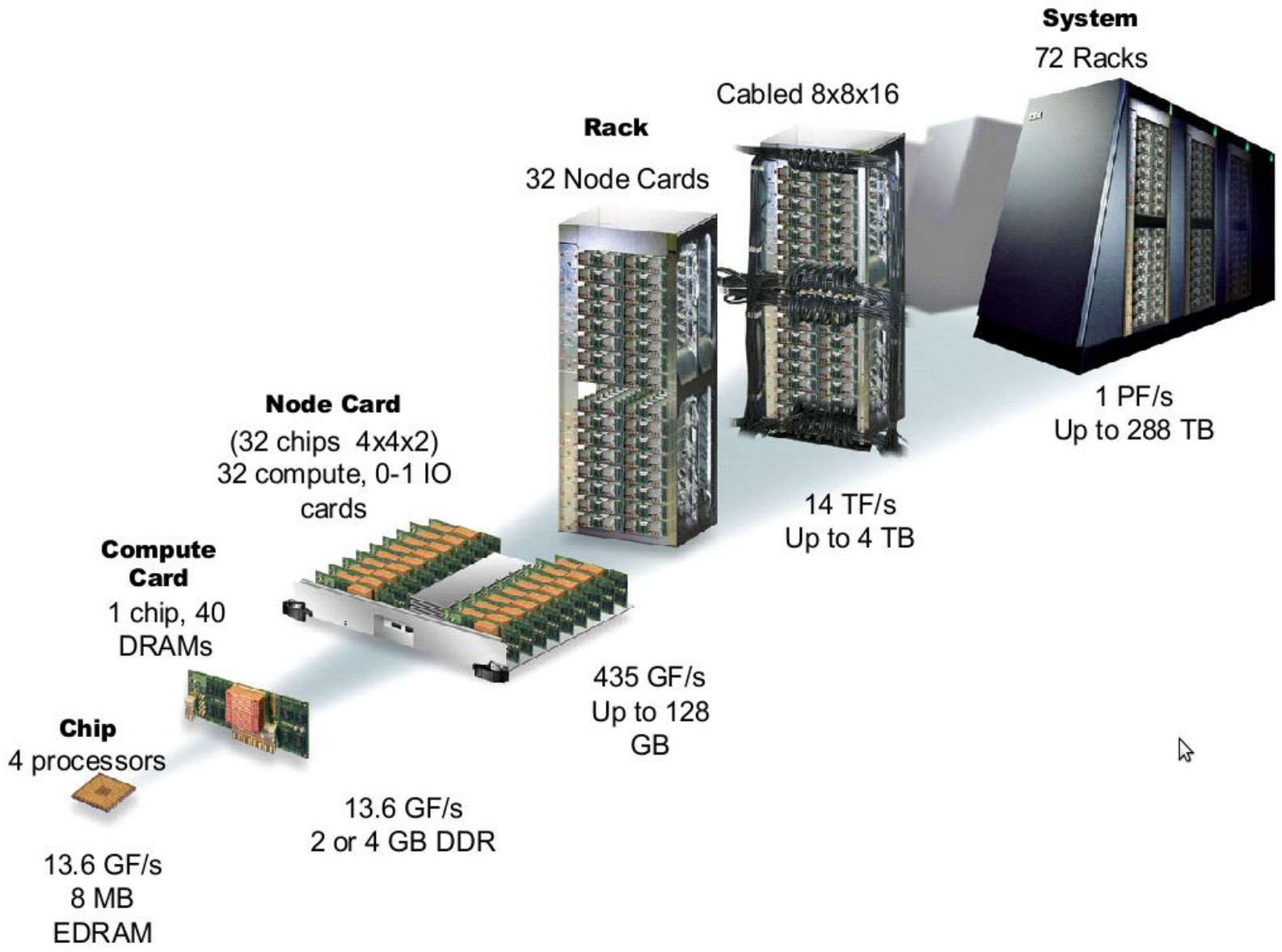
Specification

- Bulgarian Supercomputing Centre (BGSC) works with and provides access to a supercomputer IBM Blue Gene/P, consisting of 2048 computing nodes (8192 PowerPC cores @ 850 MHz, 4TB RAM)
- Connection between the computing nodes and the rest of the infrastructure: *16 channels x 10 Gb/s*
- Disk storage capacity: *12 TB*
- Front-end OS: *SLES10, externally accessible through SSH*
- Performance rating: *27.85 Tflops*
- Energy efficiency: *371.67 Mflops/W*

Benefits

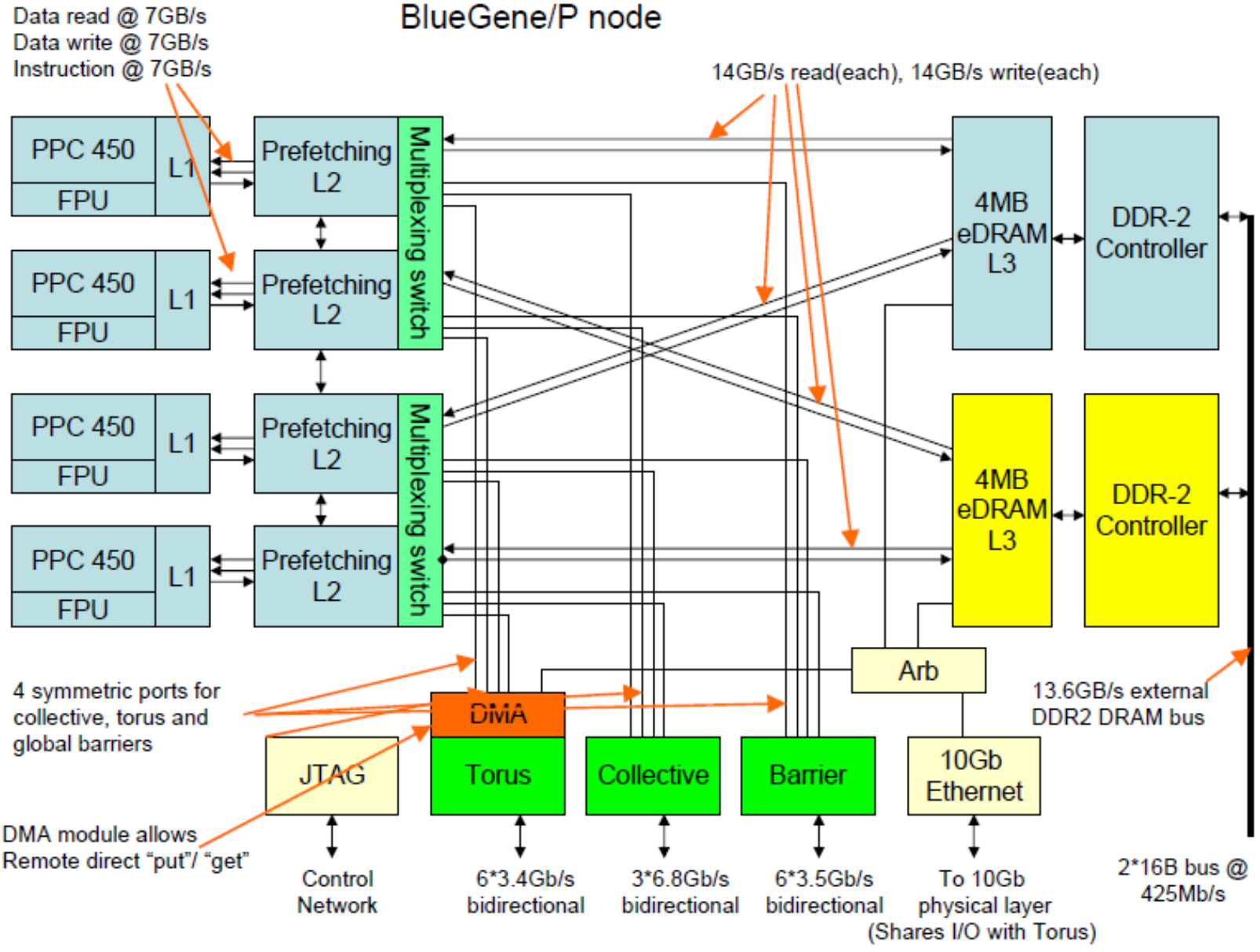
- Energy efficient
- Space saving
- Transparent, high availability, high speed network between the computing nodes
- Programming, based on standard API - MPI and OpenMP
- High scalability (thousands computing cores)
- High reliability

System organization

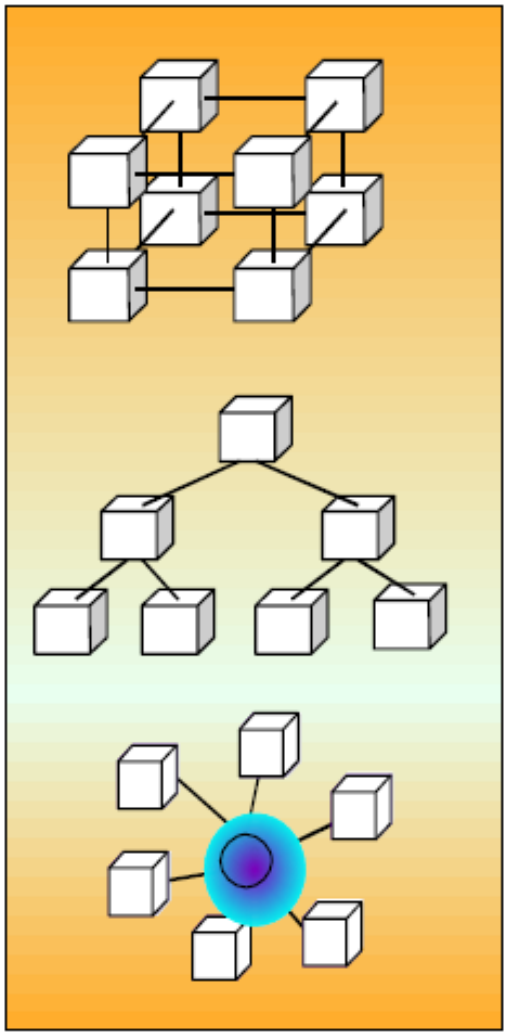


Technical data

Property		BG/P
Node Properties	Node Processors	4* 450 PowerPC
	Processor Frequency	0.85GHz (target)
	Coherency	SMP
	L1 Cache (private)	32KB/processor
	L2 Cache (private)	14 stream prefetching
	L3 Cache size (shared)	8MB
	Main Store/node	2GB
	Main Store Bandwidth	13.6 GB/s (2*16B wide)
	Peak Performance	13.6 GF/node
Torus Network	Bandwidth	6*2*425MB/s=5.1GB/s
	Hardware Latency (Nearest Neighbor)	160ns (32B packet) 500ns(256B packet)
	Hardware Latency (Worst Case)	5us(64 hops)
Collective Network	Bandwidth	2*0.85GB/s=1.7GB/s
	Hardware Latency (round trip worst case)	4us
System Properties	Peak Performance (72k nodes)	1PF
	Total Power	2.7 MW


BlueGene/P node
Data read @ 7GB/s
Data write @ 7GB/s
Instruction @ 7GB/s
14GB/s read(each), 14GB/s write(each)
PPC 450
FPU
L1
Prefetching L2
Multiplexing switch
4MB eDRAM L3
DDR-2 Controller
Arb
4 symmetric ports for collective, torus and global barriers
DMA
JTAG
Torus
Collective
Barrier
10Gb Ethernet
13.6GB/s external DDR2 DRAM bus
DMA module allows Remote direct "put"/ "get"
Control Network
6*3.4Gb/s bidirectional
3*6.8Gb/s bidirectional
6*3.5Gb/s bidirectional
To 10Gb physical layer
(Shares I/O with Torus)
2*16B bus @ 425Mb/s

Blue Gene/P Interconnection Networks



3 Dimensional Torus

- Interconnects all compute nodes
  - Communications backbone for computations
- Adaptive cut-through hardware routing
- 3.4 Gb/s on all 12 node links (5.1 GB/s per node)
- 0.5 µs latency between nearest neighbors, 5 µs to the farthest
  - MPI: 3 µs latency for one hop, 10 µs to the farthest
- 1.7/2.6 TB/s bisection bandwidth, 188TB/s total bandwidth (72k machine)

Collective Network

- Interconnects all compute and I/O nodes (1152)
- One-to-all broadcast functionality
- Reduction operations functionality
- 6.8 Gb/s of bandwidth per link
- Latency of one way tree traversal 2 µs, MPI 5 µs
- ~62TB/s total binary tree bandwidth (72k machine)

Low Latency Global Barrier and Interrupt

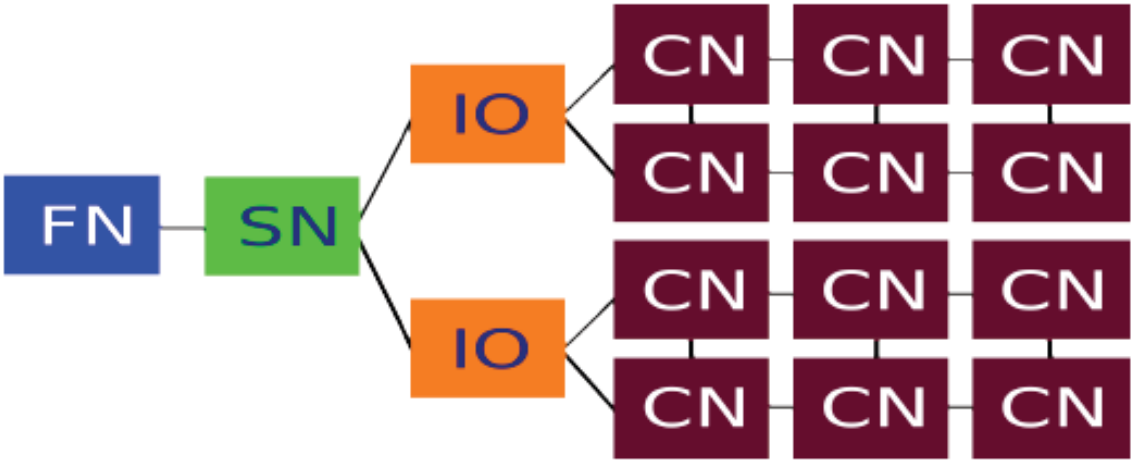
- Latency of one way to reach all 72K nodes 0.65 µs, MPI 1.6 µs

Other networks

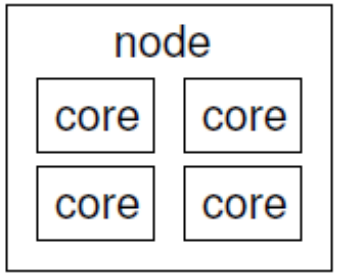
- 10Gb Functional Ethernet
  - I/O nodes only
- 1Gb Private Control Ethernet
  - Provides JTAG access to hardware. Accessible only from Service Node system

Blue Gene Hierarchical Organization

- Front-end nodes - dedicated for user's to login, compile programs, submit jobs, query job status, debug applications
- Compute nodes – run user applications, use simple compute node kernel (CNK) operating system, ship I/O-related system calls to I/O nodes
- I/O nodes – provide a number of Linux/Unix typical services, such as files, sockets, process launching, signals, debugging; run Linux
- Service nodes - perform partitioning, monitoring, synchronization and other system management services. Users do not run on service nodes directly.

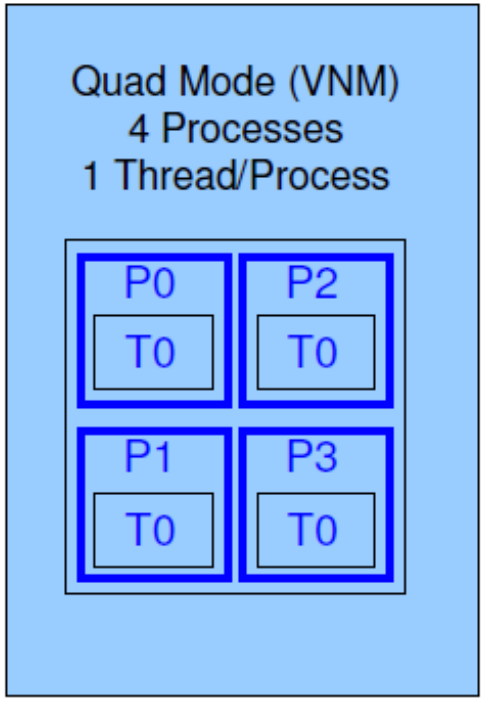


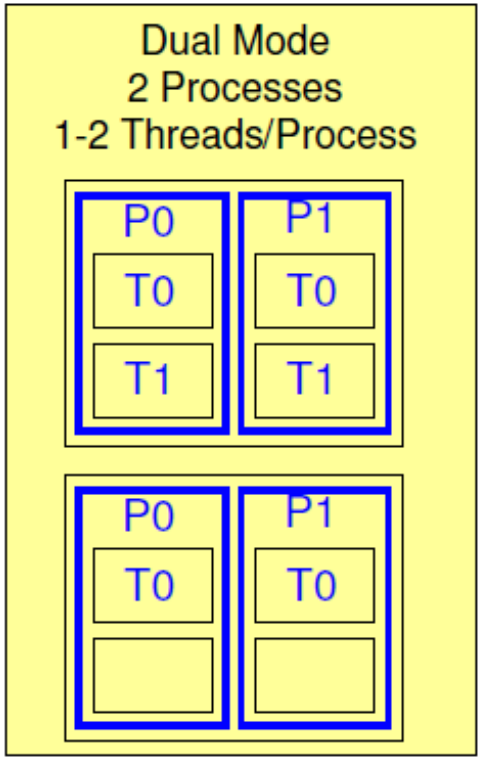
Execution Modes in BG/P per Node

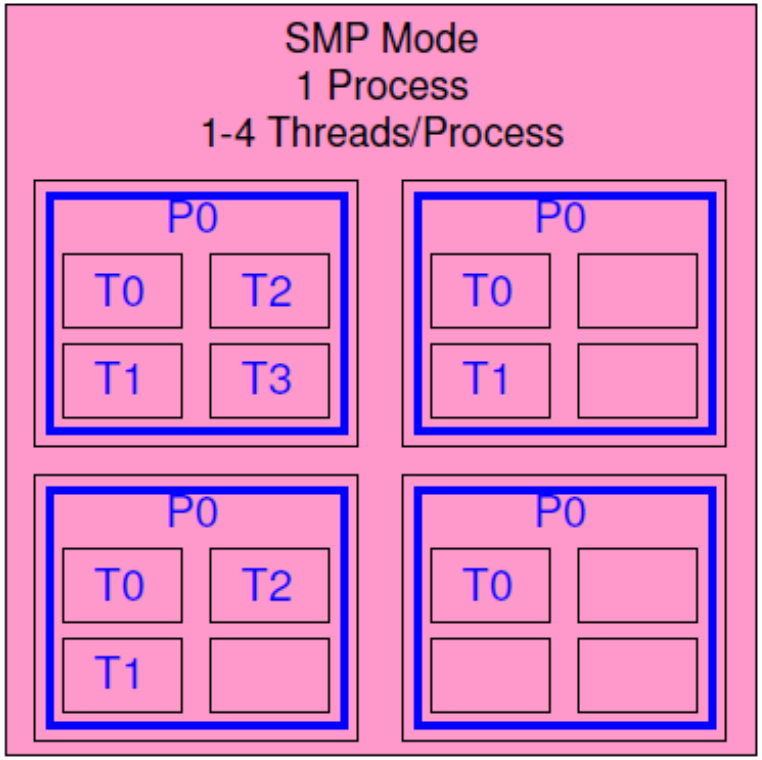


Software Abstractions Blue

- Next Generation HPC
  - **Many Core**
  - **Expensive Memory**
  - **Two-Tiered Programming Model**







File Systems

- Several places of interest for users (except the standard Linux dirs (/etc, /root, /usr, /dev and so on) are:
  - /shared1 – the fundamental user file system; its size is 4.4TB. It is visible from everywhere and this is where the jobs are run from.
  - /bgsys – BlueGene/P's system directory. This is where the system software, libraries, compilers, etc. is placed.

How to get access

- In order to get access to the machine you need:
  - Detailed description of your research project
  - The application must be shown to be scalable to at least 512 cores in order to benefit from the use of the supercomputer
  - Signed and written agreement with the usage policies. http://www.scc.acad.bg/index.php?option=com_content&view=article&id=102&Itemid=125&lang=bg
  - Send a request to bgteam@scc.acad.bg and we will send you the forms which you need to fill.
  - Your request will be duly reviewed by the management of the National Supercomputing Applications Consortium and accepted/rejected.

How to perform access

- Upon approval, an account will be created for you;
- The access is remote and performed via SSH (so it is secure);
- The name of the machine is: **bg-fen.scc.acad.bg**
- Example Linux command:
  - `ssh bg-fen.scc.acad.bg -l <username>`
- Be aware that SSH works on TCP port 22; If your organization has firewall, it has to be configured to let input and output trafic to this port for the specified machine;

Password change

- Upon your very first entering, the system will require you to change your password. Thus, please mind the messages that are written on the screen:

```
vpavlov@linux-hoe5:~> ssh bg-fen.scc.acad.bg -l vpavlov
Password:
Password change requested. Choose a new password.
Old Password:
New Password:
Reenter New Password:
Password changed.
Last login: Wed Oct 14 21:31:46 2009 from XXX.XXX.XXX.XXX


                                   ** BlueGene/P **

** This internal systems must only be used for conducting **
** IBM business or for purposes authorized by IBM management **
** Use is subject to audit at any time by IBM management. **
vpavlov@bgpfen:~>
```

How to copy your data

- Data to and from the machine can be copied by using a secure shell copy client, e.g. Scp:
  - `scp somefile username@bg-fen.scc.acad.bg:`
  - `scp -r somedir username@bg-fen.scc.acad.bg:`
- In the second example, the -r switch is used to specify recursive action – copy all files and sub-directories from the source path

Compiling your sofware

- Compiling applications (and libaries) to be used on the Computing Nodes is done via cross-compiling: the compiler works on the Front-end Node (FEN), but generates code targeted at the Computing Node (CN);
- The systam has 2 sets of C, C++ and FORTRAN compilers: GNU Toolchaing and IBM XL compilers;
- They are at:

```
/bgsys/drivers/ppcfloor/comm/default/bin/
```

- This directory can be added to the PATH env. Variable in order to be found by the shell. This can be done in your `~/.profile` file:

```
export PATH=/bgsys/drivers/ppcfloor/comm/default/bin/:$PATH
```

GNU Toolchain

- C compiler:

```
/bgsys/drivers/ppcfloor/comm/default/bin/mpicc
```

- C++ compiler:

```
/bgsys/drivers/ppcfloor/comm/default/bin/mpicxx
```

- FORTRAN-77 compiler:

```
/bgsys/drivers/ppcfloor/comm/default/bin/mpif77
```

- FORTRAN-90 compiler:

```
/bgsys/drivers/ppcfloor/comm/default/bin/mpif90
```

IBM XL compilers

- C/C++ compiler:

```
/bgsys/drivers/ppcfloor/comm/default/bin/mpixlc

/bgsys/drivers/ppcfloor/comm/default/bin/mpixlc_r
```

- FORTRAN-77 compiler:

```
/bgsys/drivers/ppcfloor/comm/default/bin/mpixlf77

/bgsys/drivers/ppcfloor/comm/default/bin/mpixlf77_r
```

- FORTRAN-90 compiler:

```
/bgsys/drivers/ppcfloor/comm/default/bin/mpixlf90

/bgsys/drivers/ppcfloor/comm/default/bin/mpixlf90_r
```

- The `_r` versions generate thread-safe code

How to perform compilation

- In order to perform a compilation, the Makefile or configure script (or whatever build system is used) must be instructed to use the cross-compiler instead of the standard gcc (or other).
- Usually, this is done by setting the env. Variables CC, FC, F77, CXX, etc. But in any case – the installation and configuration documentation of the package should be consulted.
- For example:

```
CC=mpixlc ./configure
```

IBM XL optimizations

- IBM XL compilers can produce code, specifically optimized for the PPC 450 double-hummer processor of the computing nodes. This is achieved by specifying the flags:

```
CFLAGS="-O3 -qarch=450d -qtune=450"
```

- These are also valid for C++ and FORTRAN and so CXXFLAGS and FCFLAGS are usually set also

Example

- There is a sample program in /bgsys/local/samples/helloworld. It is equipped with a Makefile and a LoadLeveler JCF file.
- These can be used as skeleton examples for your own projects.
- In order to make the application you have to copy it to your own directory and then type 'make':

```
cp -r /bgsys/local/samples/helloworld ~/your-name

cd ~/your-name

make
```

- These commands create a file named `hello`, which can be executed on the BlueGene/P

Job execution

- Jobs are scheduled for execution by a system called LoadLeveler
- The prepared jobs are submitted for execution via the command `llsubmit`, which receives something called **Job Control File**, which describes the executing program and its environment
- This puts the job into a queue of waiting jobs. There are scheduling strategies via which the jobs are prioritized. When suitable resource is available, the next task in the queue will execute.
- You can see the contents of the queue with `llq`. If the status of the job is **R**, it is running, if **I** – it waits, and if **H**, there was a problem and you need to look at the error output and remove your job via `llcancel`.

Contents of a JCF

- /bgusr/local/samples/helloworld.jcf is an example Job Control File:

```
# @ job_name = hello
# @ comment = "This is a HelloWorld program"
# @ error = $(jobid).err
# @ output = $(jobid).out
# @ environment = COPY_ALL;
# @ wall_clock_limit = 01:00:00
# @ notification = never
# @ job_type = bluegene
# @ bg_size = 128
# @ class = n0128
# @ queue
/bgsys/drivers/ppcfloor/bin/mpirun -exe hello -verbose 1 -mode VN -np 512
```

This is how it is sent for execution:

```
cd /bgsys/local/samples/helloworld

llsubmit hello.jcf
```

JCF Parameters

- `# @ job_name = hello` The name for the job, could be anything
- `# @ comment = "This is a HelloWorld program"` Some comment
- `# @ error = $(jobid).err` Where to send the stderr. Writing to file descriptor 1 (in C) writes to this file. Note how $(jobid) is used to make this file unique. For example, if LoadLeveler gives the job an ID of 4242, then he name of the file will be 4242.err in the current working directory.
- `# @ output = $(jobid).out` Same here, but for the stdout (file descriptor 0 in C).
- `# @ environment = COPY_ALL;` This instructs LoadLeveler to copy the whole user environment when running the job. Thus, the job has the same environment as the user that executes llsubmit.

JCF Parameters (cont.)

- `# @ wall_clock_limit = 01:00:00` Time limit; after this time, the job is cancelled automatically. This cannot be more than a certain time limit imposed by the class of the job.
- `# @ notification = never` There is no infrastructure for notifications, so 'never' is a good value for this parameter.
- `# @ job_type = bluegene` This MUST be bluegene.
- `# @ bg_size = 128` This must be an integer, divisable by 128, but not larger than 2048. This gives the number of computing nodes that will be used in order to execute the job.This must correspond to the class of the job.

JCF parameters (cont.)

- `# @ class = n0128` This is the class of the job. The most important parameter. Different classes have different priorities.
- `# @ queue` This instructs LoadLeveler to put the job in the queue.
- `/bgsys/drivers/ppcfloor/bin/mpirun -exe hello -verbose 1 -mode VN -np 512` This is the actual command that sends the job to the BlueGene/P's computing nodes.
- Some parameters are:
- `-exe <executable_file>` – the executable file itself
- `-args "<arguments>"` – arguments to the executable file
- `-verbose 1` – write information about job startup/finalizing in the stderr file

JCF parameters (прод.)

- `-mode VN|SMP|DUAL` – This provides the mode of execution
- `-np N` – the number of processes on which the job will execute
- `- env BG_MAXALIGNEXP=-1` – **very important** (and not documented!) parameter, which instructs the CN kernel to ignore alignment traps. Most of the software is not intended to work on systems with alignment and if this parameter is lacking, many systems will crash.

Modes, processes and bg_size

- In order for the job to be correctly stated, the following must be true:

bg_size >= np / km

- **bg_size** is the value in the JCF file `# @ bg_size`
- **np** is the value of the -np argument to mpirun
- **km** is a coefficient of the mode: 1 за SMP, 2 за DUAL, 4 за VN
- bg_size must be divisable by 128 and correspond to the class of the job

bg_size examples

- `-mode VN -np 400` : bg_size = 128
- `-mode VN -np 600` : bg_size = 256
- `-mode DUAL -np 400` : bg_size = 256
- `-mode DUAL -np 600` : bg_size = 512
- `-mode SMP -np 400` : bg_size = 512
- `-mode SMP -np 600` : bg_size = 1024

Geometry

- A rack has two parts – midplanes (upper and lower).
- Each midplane has 512 CN
- **When bg_size >= 512** you can specify the geometry, which may improve performance with some packages (e.g. GROMACS)

Geometry (cont.)

- # @ bg_connection = MESH | TORUS | PREFER_TORUS
  - MESH is the normal mode. The nodes are connected in cube (each with its 6 neighbours).
  - TORUS – toroidal connection in which the last in line is connected with the first in line. This halves the mean path and thus improves latency.
  - PREFER_TORUS – If possible – TORUS, if not – MESH

Geometry (cont.)

- # @ bg_shape = XxYxZ – X, Y and Z midplanes in each direction(see also bg_rotate)
- # @ bg_rotate = True | False – can rotate the geometry
- For our system this is only meaningful for bg_size = 1024, without permutations (bg_rotate = False). Then, bg_shape = 1x2x1 means that the two midplanes will be in 1 rack and bg_shape = 2x1x1 means they will be in different racks.

Job Classes

- The class of the job defines:
  - Priority – larger jobs take precedence
  - The maximum number of nodes that can be used
  - The maximum time that a job can run
- There is a limit how much jobs of each class can run simultaneously
- There are several classes:

Classes (cont.)

Class	Number of jobs	Max CNs	Time Limit
n0128	16	128	24h
n0128long	16	128	7d
n0256	6	256	24h
n0512	3	512	24h
n1024	1	1024	24h
n2048	1	2048	24h

Areas covered by the software and libraries installed on the IBM BlueGene/P at Bulgarian National Supercomputing Center (II)

- Computational fluid dynamics, large eddy simulations, nuclear reactor cooling simulations, gas combustions, coal combustions, pulverized coal furnaces (optimization, slagging, pollutants), semi-transparent radiation heat transfer, lagrangian modeling for multi-phase flows;
- Seismic wave propagation simulations, object impact and hazard risk calculations;
- Preconditioning Techniques for Large Linear Systems, Solving large sparse linear systems;
- Multi-scale linear solvers for very large linear systems etc.;

GROMACS

(GROningen Machine for Chemical Simulations)

- Primarily designed for biochemical molecules (proteins, lipids and nucleic acids) - a lot of complicated bonded interactions;
- Extremely fast at calculating the nonbonded interactions (that usually dominate simulations) – research on non-biological systems, e.g. polymers.
- Advantages:
  - Domain decomposition – particles;
  - PME 2D decomposition – long range electrostatics;
  - Leapfrog integration algorithm;
  - Variety of simulation box shapes;

http://www.gromacs.org

NAMD

(Not (just) Another Molecular Dynamics program)

- A parallel, object-oriented molecular dynamics code designed for high-performance simulation of large biomolecular systems.
- Developed using Charm++ - adaptive communication-computation overlap and dynamic load balancing.
- NAMD pioneered the use of hybrid spatial and force decomposition.
- Scales to thousands of processors. NAMD is tested up to 64,000 processors.
- Simulation preparation and analysis is integrated into the visualization package VMD.

LAMMPS

(Large scale Atomic / Molecular Massively Parallel Simulator)

- A classical molecular dynamics simulation code designed to run efficiently on parallel computers developed at Sandia National Laboratories.
- Integrates Newton's equations of motion for collections of atoms, molecules, or macroscopic particles that interact via short- or long- range forces with a variety of initial and/or boundary conditions.
- Uses spatial decomposition techniques to partition the simulation domain into small 3d sub domains.
- Most efficient (in a parallel sense) for systems whose particles fill a 3d rectangular box with roughly uniform density.

DL POLY 4

- DL_POLY is a general purpose classical molecular dynamics (MD) simulation software developed at Daresbury Laboratory by I.T. Todorov and W. Smith.
- DL_POLY_4 is based on the Domain Decomposition (DD) strategy and is best suited for large molecular simulations from 10^3 to 10^9 atoms on large processor counts.
- DL POLY 4 offers a selection of MD integration algorithms couched in both Velocity Verlet (VV) and Leapfrog Verlet (LFV) manner
- It is relatively easy to adapt DL POLY 4 to user specific force fields.

CP2K

(Car-Parrinello molecular dynamics 2000)

- A suite of modules:
  - variety of molecular simulation methods at different levels of accuracy, from ab-initio DFT to classical Hamiltonians, passing through semi-empirical NDDO approximation.
- Used for:
  - predicting energies, molecular structures, vibrational frequencies of molecular systems, reaction mechanisms;
- Ideally suited for performing molecular dynamics studies.
- Performs atomistic and molecular simulations of solid state, liquid, molecular, biological systems.

CPMD

(Car-Parrinello Molecular Dynamics)

- Ab Initio Electronic Structure and Molecular Dynamics Program.
- Includes ultrasoft pseudopotentials, free energy density functional, wavefunction optimization, geometry optimization,molecular dynamics:
  - constant energy, constant temperature and constant pressure, path integral MD, many electronic properties, time-dependent DFT,coarse-grained non-Markovian metadynamics, response functions and many electronic structure properties,hybrid quantum mechanical / molecular dynamics

NWChem 5.1
(Northwest Chemistry)

- Designed for parallel computer systems including parallel supercomputers and large distributed clusters.
- Scalable:
  - ability to treat large problems efficiently
  - utilization of available parallel computing resources.
- Molecular calculations including:
  - density functional, Hartree-Fock, Müller-Plesset, coupled-cluster, configuration interaction;
  - molecular dynamics, mixed quantum mechanics, geometry optimizations, vibrational frequencies, relativistic corrections;
  - ab-initio molecular dynamics;
  - extended DFT
- Periodic system modeling;

Quantum Espresso

Quantum Espresso can currently perform the following kinds of calculations:

- Ground-state energy and one-electron (Kohn-Sham) orbital's;
- Atomic forces, stresses, and structural optimization;
- Molecular dynamics on the ground-state Born-Oppenheimer surface, also with variable cell;
- Nudged Elastic Band (NEB) and Fourier String Method Dynamics (SMD) for energy barriers and reaction paths;
- Macroscopic polarization and finite electric fields via the modern theory of polarization (Berry Phases).

GAMESS

(General Atomic and Molecular Electronic Structure System)

- General purpose electronic structure code
- Primary focus is on ab initio quantum chemistry calculations
- Density functional theory calculations
- QM/MM calculations
- Energy-related properties
- Numerical Hessians from finite differences of analytic gradients
- Molecular dynamics Effective fragment potential (EFP) method

mpiBLAST and ScalaBLAST

- BLAST (Basic Local Alignment Search Tool) – the tool most frequently used for calculating sequence similarity.
  - Search large databases.
  - Comparison of nucleotide or protein sequences from the same or different organisms is a very powerful tool in molecular biology.
  - Finding similarities between sequences, scientists can infer the function of newly sequenced genes, predict new members of gene families, and explore evolutionary relationships.
- mpiBLAST is a parallel implementation of the Blast algorithm.
- ScalaBLAST: A Scalable Implementation of BLAST for High-Performance Data-Intensive Bioinformatics Analysis. A typical query list might contain thousands or millions of individual sequences, each of which is meant to be scored against a large database of publicly available sequence information, such as the non-redundant protein sequence database (nr).

SPECFEM3D
(seismic wave propagation)

- Unstructured hexahedral mesh generation is a critical part of the modeling process in the Spectral-Element Method (SEM).
- An advanced 3D unstructured hexahedral mesh generator that offers new opportunities for seismologist to design, assess, and improve the quality of a mesh in terms of both geometrical and numerical accuracy.
- The main goal is to provide useful tools for understanding seismic phenomena due to surface topography and subsurface structures such as low wave-speed sedimentary basins.

Code Saturne / Syrthes1.3.2

- **Code Saturne**:
  - Solve the Navier-Stokes equations in the cases of 2D, 2D axis symmetric or 3D flows.
  - The main module is designed for the simulation of flows which may be steady or unsteady, laminar or turbulent, incompressible or potentially dilatable, isothermal or not. Scalars and turbulent fluctuations of scalars can be taken into account.
  - Includes specific modules for the treatment of: lagrangian particle tracking, semi-transparent radioactive transfer, gas, pulverized coal and heavy fuel oil combustion, electricity effects (Joule effect and electric arcs) and compressible flows.
  - Engineering module (Matisse) - simulation of nuclear waste surface storage.

- **Syrthes –** conjugate heat transfer and transparent radiative heat transfer, Independent FE solver with tetrahedral mesh and arbitrary fluid-solid interface, Thermal shock, striping, fatigue Fuel combustion, ionic mobility under development.

Aster
(Structural mechanics code)

- A general code directed at the study of the mechanical behaviour of structures.
- For the expertise and the maintenance of power plants and electrical networks
- The main range of application is deformable solids: explains the great number of functionalities related to mechanical phenomena.
  - behaviour of industrial components – influence of physical phenomena (internal or external fluids, temperature, metallurgic phase changes, electro-magnetic stresses ...).
- Can « link » mechanical phenomena and thermal and acoustic phenomena together.
- Provides a link to external software, and includes a coupled thermo-hydro-mechanics kit.

Code Salome

- A generic platform for pre and post processing and code coupling for numerical simulation with the following aims:
  - Supports interoperability between CAD modeling and computation software;
  - Facilitate implementation of coupling between computing codes in a distributed environment;
  - Makes easier the integration of new components into heterogeneous systems for numerical computation;
  - Sets the priority to multi-physics coupling between computation software;
  - Pool production of developments (pre and post processors, calculation distribution and supervision) in the field of numerical simulation

Available libraries

- ✓ PETCs
- ✓ ParMETIS
- ✓ LAPACK
- ✓ Linpack
- ✓ ScalaPAck
- ✓ SuperLU
- ✓ MUMS
- ✓ HYPRE
- ✓ ParFE
- ✓ GotoBLAS
- ✓ FFTW
- ✓ GlobalArray
- ✓ PVFS2
- ✓ LUSTRE
- ✓ Trilinos

THE END
Thank you for your attention!