Introduction to the Practical Aspects of Programming for IBM Blue Gene/P

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IBM Science and Technology Center

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- IBM Rational software
- Smarter Commerce for Retail
- Smarter Cities

Outline

1. Blue Gene architecture in the HPC world
2. Blue Gene/P architecture
3. Conclusion
4. References

Outline

1. Blue Gene architecture in the HPC world
   - Brief history of Blue Gene architecture
   - Blue Gene in TOP500
   - Blue Gene in Graph500
   - Scientific applications
   - Gordon Bell awards
   - Blue Gene installation sites
2. Blue Gene/P architecture
3. Conclusion
4. References

Brief history of Blue Gene architecture

- **1999** — US$100M research initiative, novel massively parallel architecture, protein folding
- **2003,** Nov — Blue Gene/L first prototype — TOP500, #73
- **2004,** Nov — 16 Blue Gene/L racks at LLNL — TOP500, #1
- **2007** — Second generation — Blue Gene/P
- **2009** — National Medal of Technology and Innovation
- **2012** — Third generation — Blue Gene/Q
- Features:
  - Low frequency, low power consumption
  - Fast interconnect balanced with CPU
  - Light-weight OS

Blue Gene in TOP500

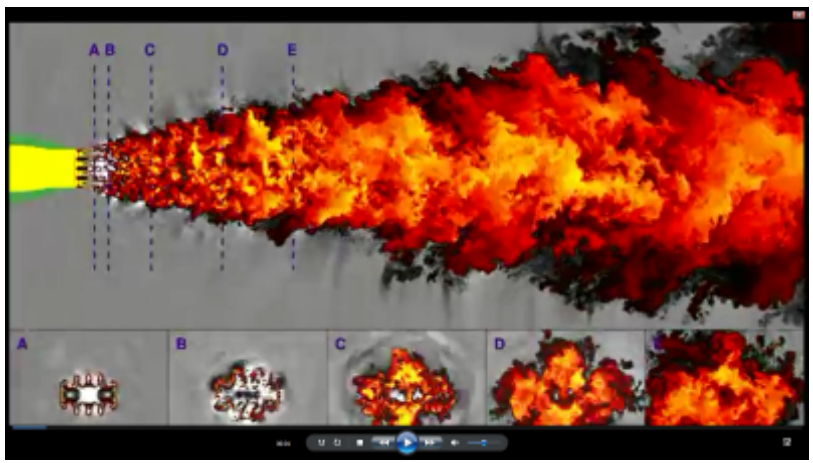
Date	#	System	Model	Nodes	Cores
Jun'14 / Nov'14	3	Sequoia	Q	96k	1.5M
Jun'13 / Nov'13	3	Sequoia	Q	96k	1.5M
Nov'12	2	Sequoia	Q	96k	1.5M
Jun'12	1	Sequoia	Q	96k	1.5M
Nov'11	13	Jugene	P	72k	288k
Jun'11	12	Jugene	P	72k	288k
Nov'10	9	Jugene	P	72k	288k
Jun'10	5	Jugene	P	72k	288k
Nov'09	4	Jugene	P	72k	288k
Jun'09	3	Jugene	P	72k	288k
Nov'08	4	DOE/NNSA/LLNL	L	104k	208k
Jun'08	2	DOE/NNSA/LLNL	L	104k	208k
Nov'07	1	DOE/NNSA/LLNL	L	104k	208k
Jun'07	1	DOE/NNSA/LLNL	L	64k	128k
Jun'06 / Nov'06	1	DOE/NNSA/LLNL	L	64k	128k
Nov'05	1	DOE/NNSA/LLNL	L	64k	128k
Jun'05	1	DOE/NNSA/LLNL	L	32k	64k
Nov'04	1	DD2 beta-system	L	16k	32k
Jun'04	4	DD1 prototype	L	4k	8k

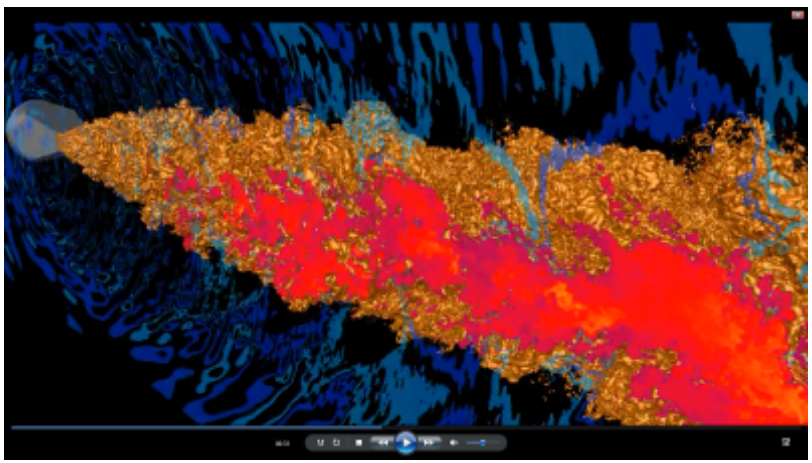
Blue Gene in Graph500

Date	#	System	Model	Nodes	Cores	Scale	GTEPS
Nov'14	1	Sequoia	Q	96k	1.5M	41	23751
Jun'14	2	Sequoia	Q	64k	1M	40	16599
Nov'13	1	Sequoia	Q	64k	1M	40	15363
Jun'13	1	Sequoia	Q	64k	1M	40	15363
Nov'12	1	Sequoia	Q	64k	1M	40	15363
Jun'12	1	Sequoia/Mira	Q	32k	512k	38	3541
Nov'11	1	BG/Q prototype	Q	4k	64k	32	253
Jun'11	1	Interpid/Jugene	P	32k	128k	38	18
Nov'10	1	Interpid	P	8k	32k	36	7

Jet Engine Noise CFD Simulation

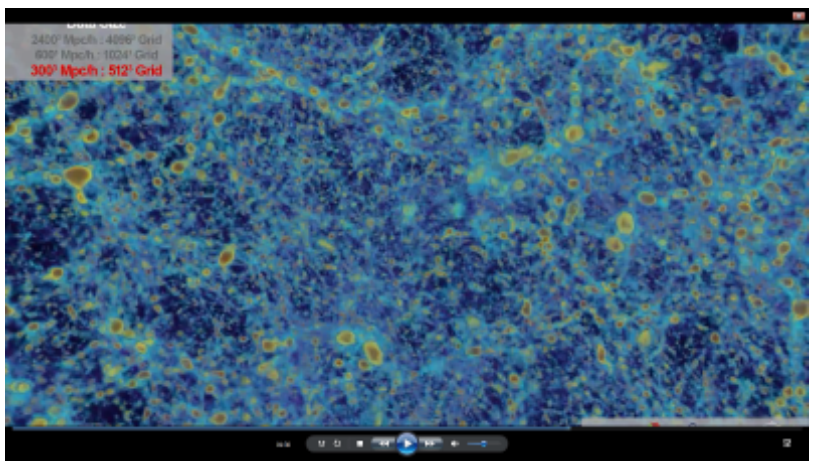
- Supersonic jet noise simulation, effects of chevrons on jet noise
- 128k Blue Gene/P cores — ≈ 100 hours
- 1M Blue Gene/Q cores — ≈ 12 hours
- IBM Blue Gene Q Sequoia, Lawrence Livermore National Laboratory
- `https://youtu.be/cjoz5tncRUs`
- `https://youtu.be/uxT-VmY3OWc`
- Video: Joseph W. Nichols, Stanford Center for Turbulence Research

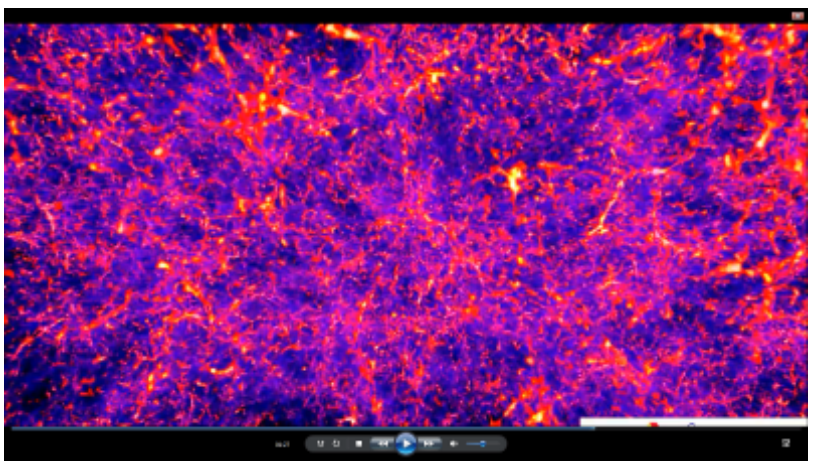




Secrets of the Dark Universe

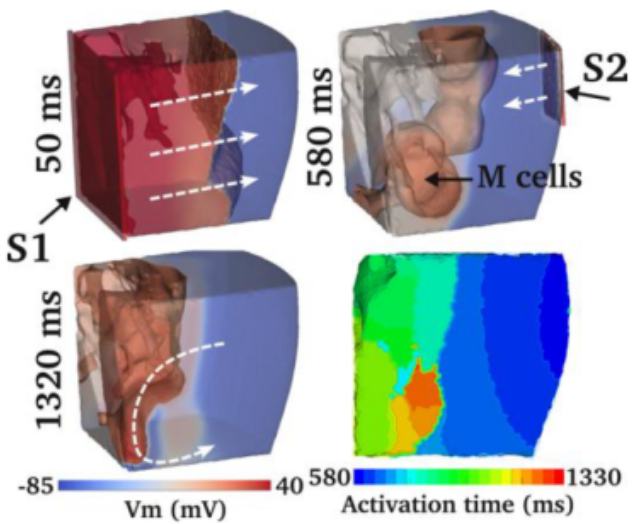
- The evolution of the Universe simulation, understanding the physics of the dark matter and energy
- 1 BG/Q rack — 68B particles
- 32 BG/Q racks — 1.1T particles
- `http://www.youtube.com/watch?v=tdv8yrJk4VE`
- `http://www.youtube.com/watch?v=-S-T_iTiAxQ`
- Video: ANL, LANL, LBNL

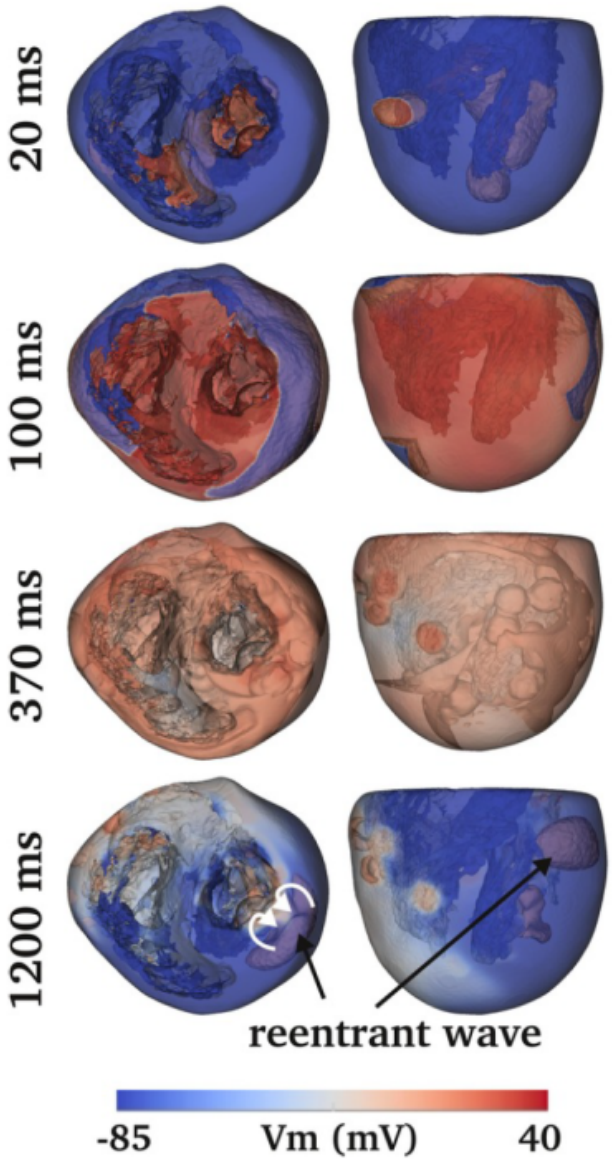




Real-Time Modeling of Human Heart Ventricles

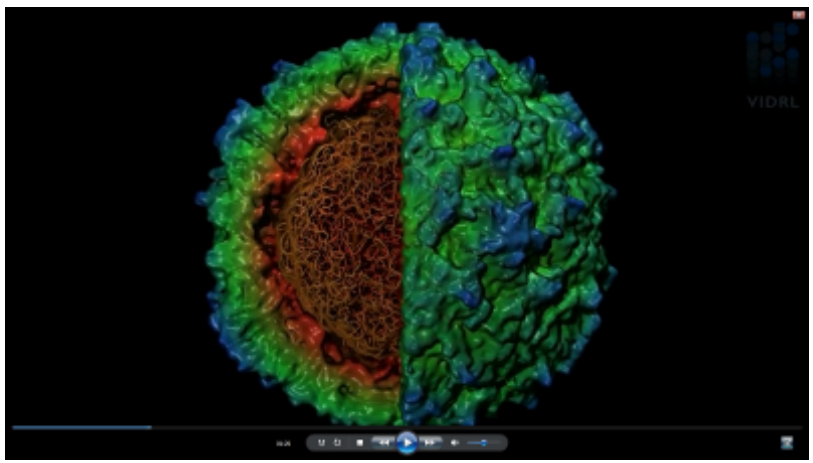
- Simulation of drug-induced arrhythmias
- Resolution — 0.1 mm
- 768k Blue Gene/Q cores
- 43% peak
- http://dl.acm.org/citation.cfm?id=2388999
- LLNL, IBM Research, IBM Research Collaboratory for Life Sciences

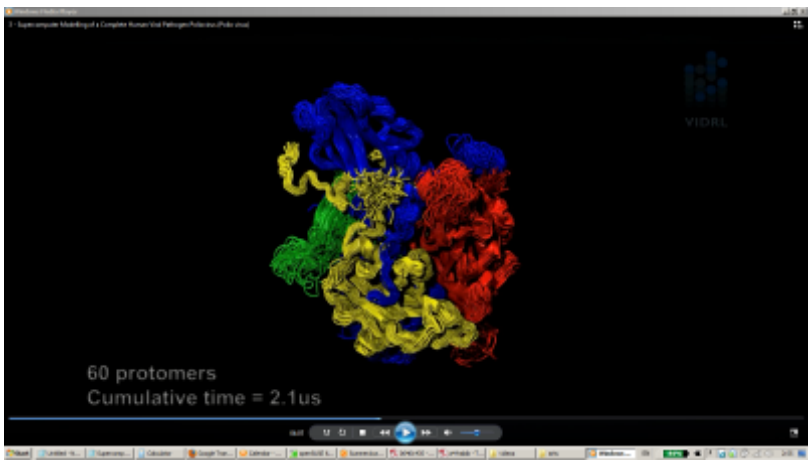




Modelling of a Complete Human Viral Pathogen Poliovirus

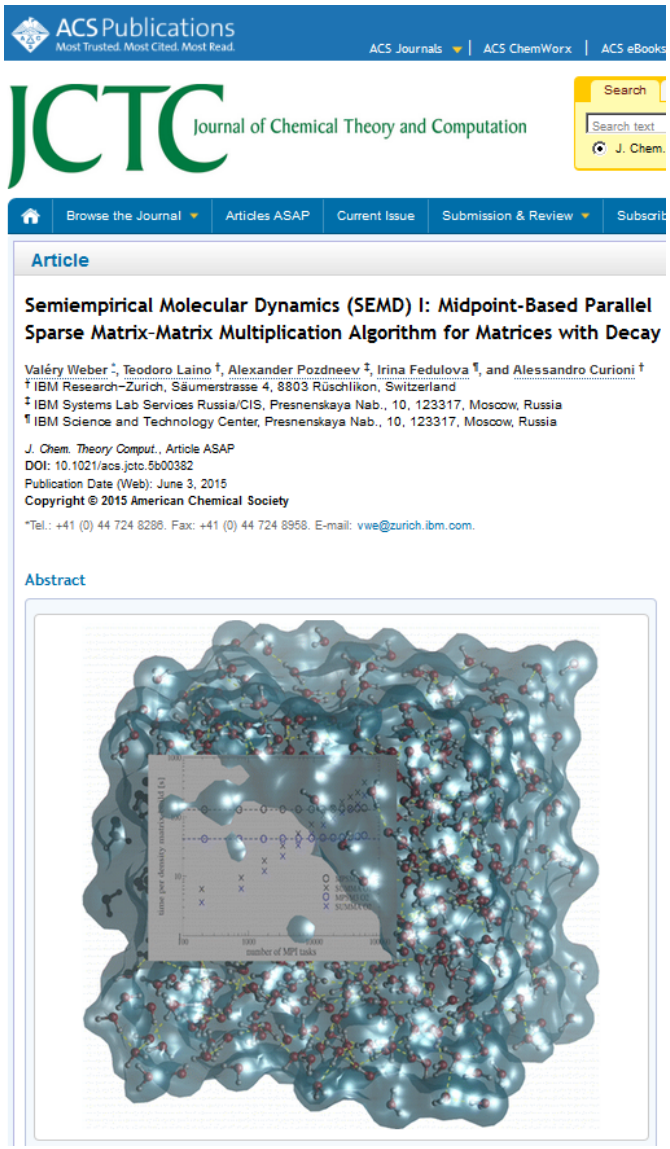
- Reconstruction and simulation of poliovirus
- Antiviral drugs, virus infection, modelling related viruses
- 3.3M–3.7M atoms
- Blue Gene/Q, Victorian Life Sciences Computing Initiative
- `http://www.youtube.com/watch?v=Nih0Qa673FY`





Parallel Sparse Matrix–Matrix Multiplication

- Semiempirical Molecular Dynamics (SEMD) I: Midpoint-Based Parallel Sparse Matrix–Matrix Multiplication Algorithm for Matrices with Decay
- Inspired by the midpoint method
- Approaching a perfect linear scaling
- Up to 185 193 processes on BG/Q
- doi: 10.1021/acs.jctc.5b00382

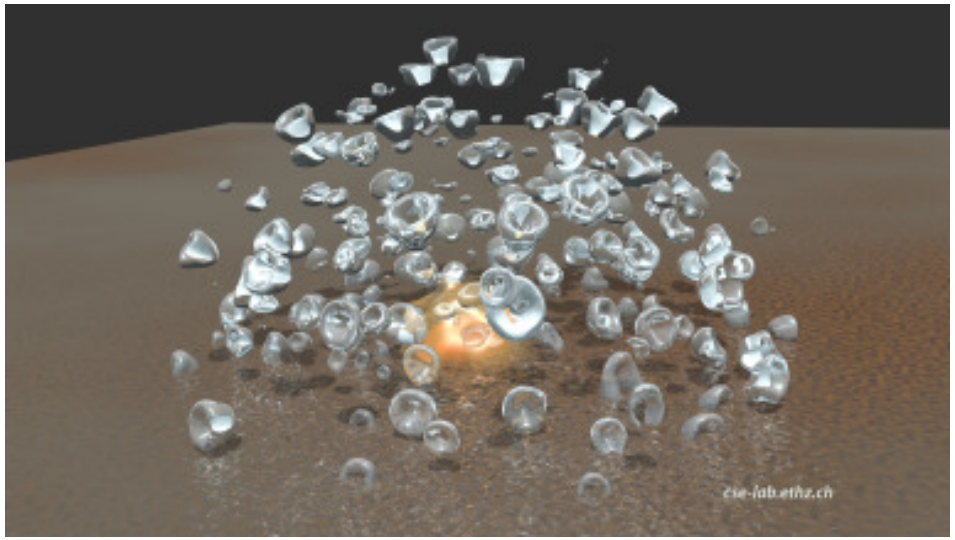


Gordon Bell prize — 7 awards

- **2005** — 100+ TFlop Solidification Simulations on Blue Gene/L
- **2006** — The Blue Gene/L supercomputer and quantum ChromoDynamics
- **2006** — Large-scale Electronic Structure Calculations of High-Z Metals on the Blue Gene/L Platform
- **2007** — Extending stability beyond CPU millennium: a micron-scale atomistic simulation of Kelvin-Helmholtz instability
- **2008** — Linearly scaling 3D fragment method for large-scale electronic structure calculations
- **2009** — The cat is out of the bag: cortical simulations with 10^9 neurons, 10^{13} synapses
- **2013** — 11 PFLOP/s simulations of cloud cavitation collapse

11 PFLOP/s simulations of cloud cavitation collapse

- ACM Gordon Bell Prize 2013
- IBM Blue Gene/Q Sequoia
  - 96 racks, 20.1 PFLOPS peak
  - 1.5M cores (6.0M threads)
  - 73% peak (14.4 PFLOPS)
  - 13T grid points
  - 15k cavitation bubbles
- Destructive capabilities of collapsing bubbles
  - high pressure fuel injectors and propellers
  - shattering kidney stones
  - cancer treatment
- doi: 10.1145/2503210.2504565
- https://youtu.be/zfG9solC6_Y



- IBM Research Zurich
- ETH Zurich
- Technical University of Munich
- Lawrence Livermore National Laboratory (LLNL)

Some of Blue Gene installation sites

- USA:
  - DOE/NNSA/LLNL (2)
  - DOE/SC/ANL (3)
  - University of Rochester
  - Rensselaer Polytechnic Institute
  - IBM Rochester / T.J. Watson (4)
- Germany:
  - Forschungszentrum Juelich (FZJ)
- Italy:
  - CINECA
- Switzerland:
  - Ecole Polytechnique Federale de Lausanne
  - Swiss National Supercomputing Centre (CSCS)
- Poland:
  - Interdisciplinary Centre for Mathematical and Computational Modelling, University of Warsaw
- France:
  - CNRS/IDRIS-GENCI
  - EDF R&D
- UK:
  - University of Edinburgh
  - Science and Technology Facilities Council — Daresbury Laboratory
- Japan:
  - High Energy Accelerator Research Organization/KEK (2)
- Australia:
  - Victorian Life Sciences Computation Initiative
- Canada:
  - Southern Ontario Smart Computing Innovation Consortium/University of Toronto

Outline

1. Blue Gene architecture in the HPC world
2. Blue Gene/P architecture
   - Air-cooling
   - Hardware overview
   - BG/P at Lomonosov MSU
   - Computing node
   - Execution process modes
   - Memory subsystem
   - Networks
   - Compilers
   - Software
   - Software stack
   - I/O nodes psets
   - Double Hammer FPU
3. Conclusion
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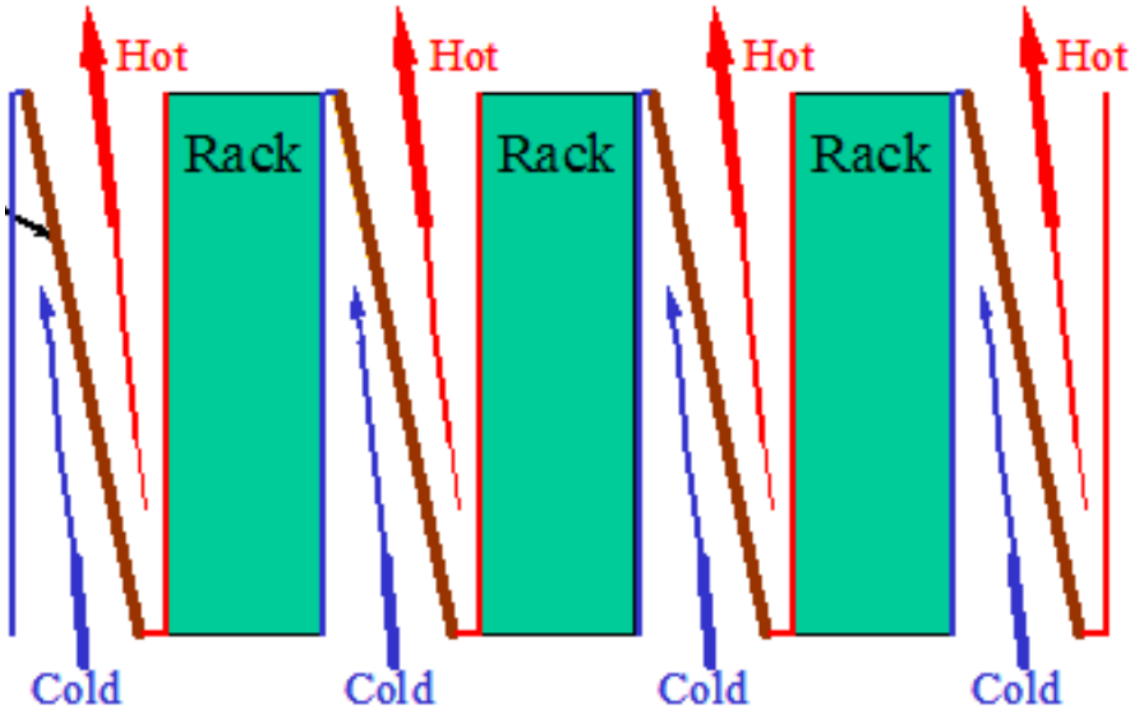
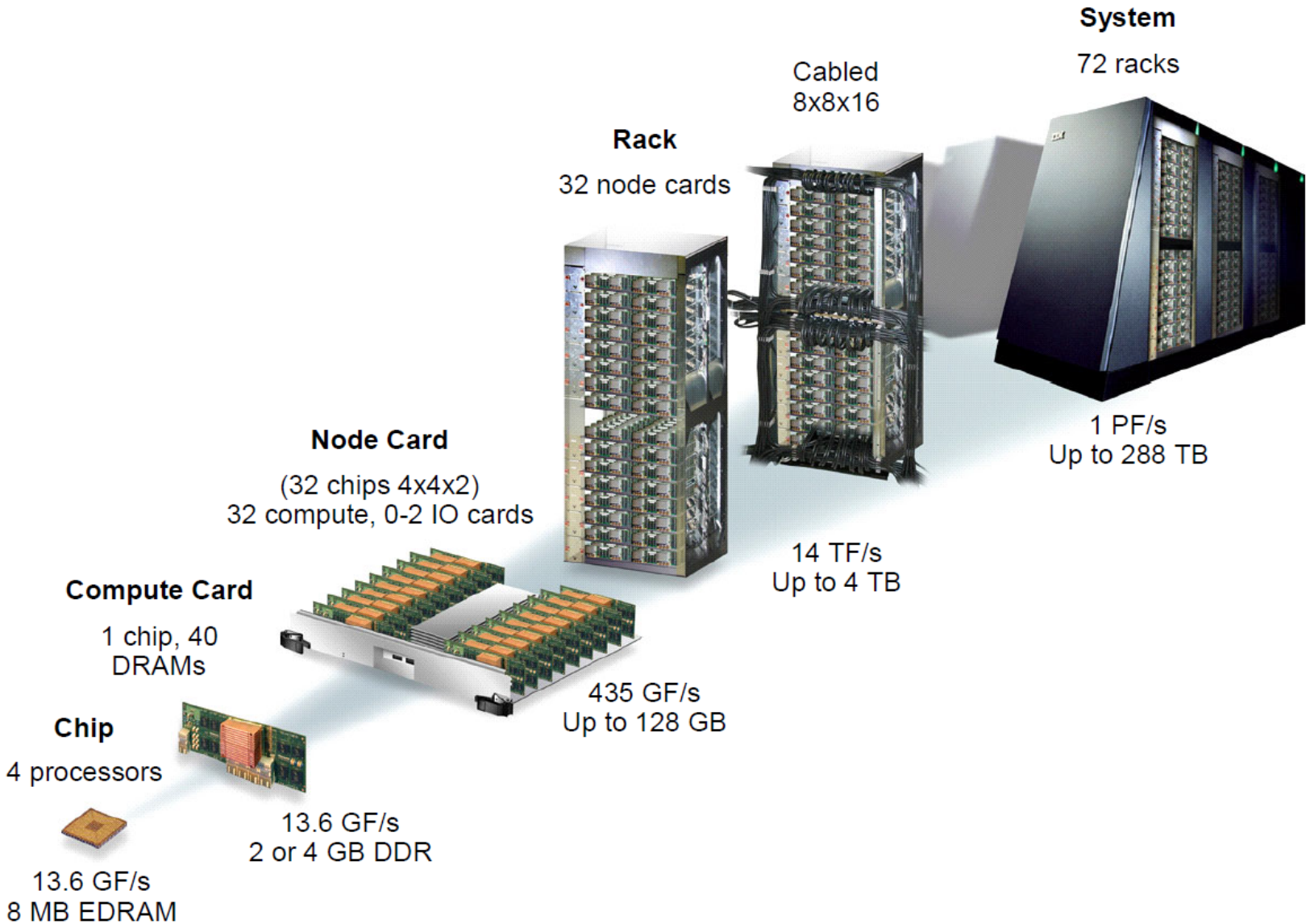
Blue Gene/P air-cooling



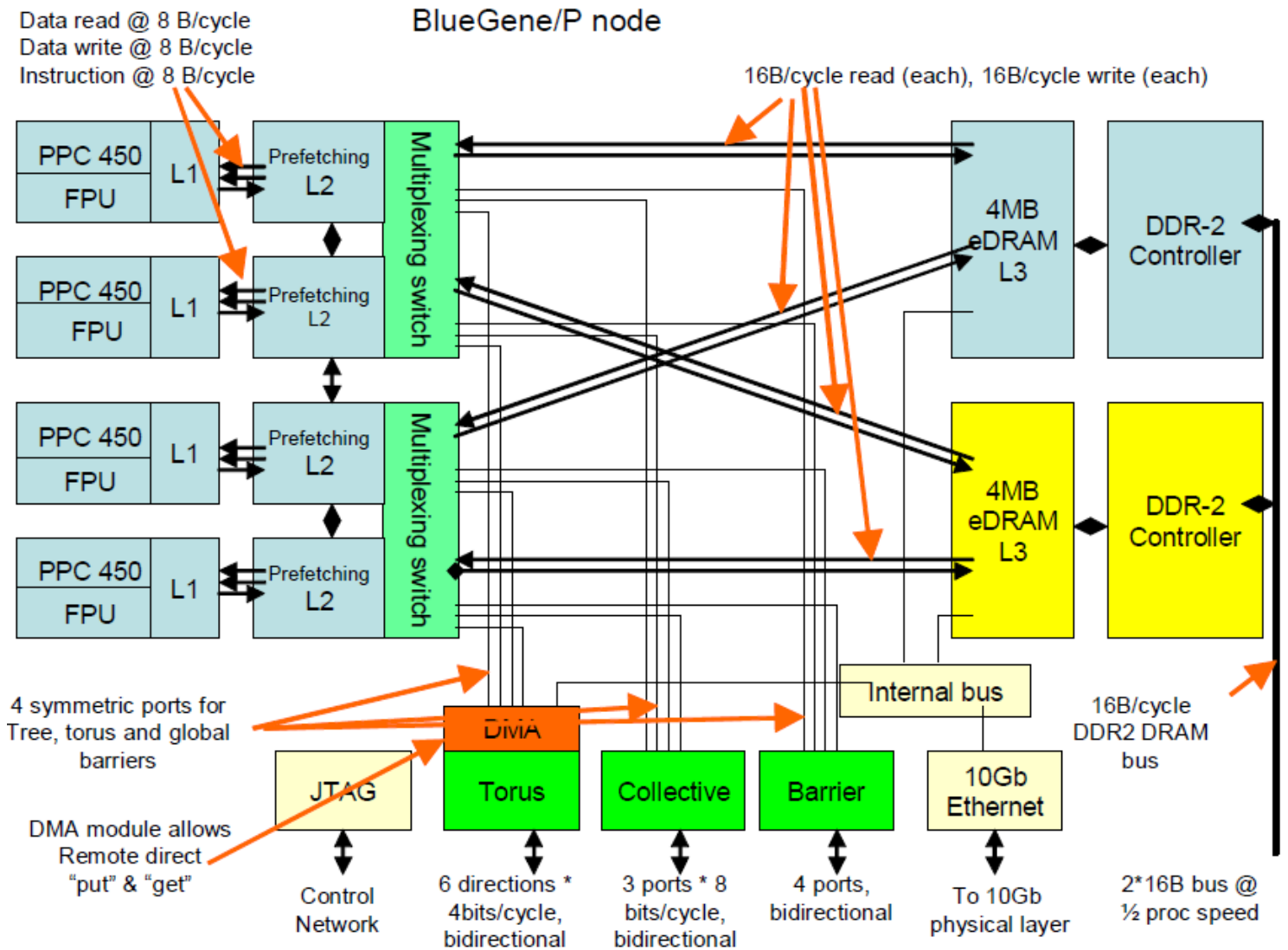
Blue Gene/P hardware overview



Blue Gene/P at Lomonosov MSU

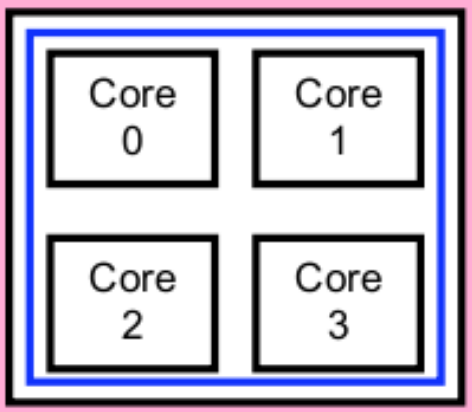
- Two racks
- 4 TB RAM
- 27.2 TFLOPS peak
- 23.2 TFLOPS on LINPACK (85% peak)

Blue Gene/P computing node

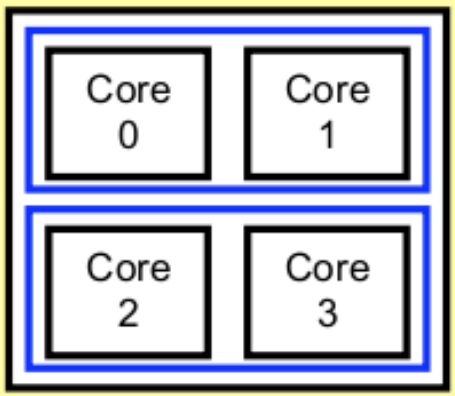


Execution process modes

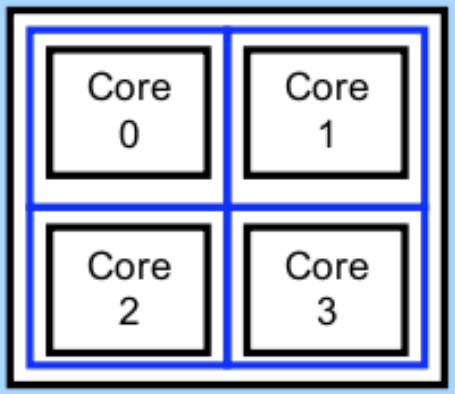
SMP Mode
1 Process
1-4 Threads/Process



Dual Mode
2 Processes
1-2 Threads/Process



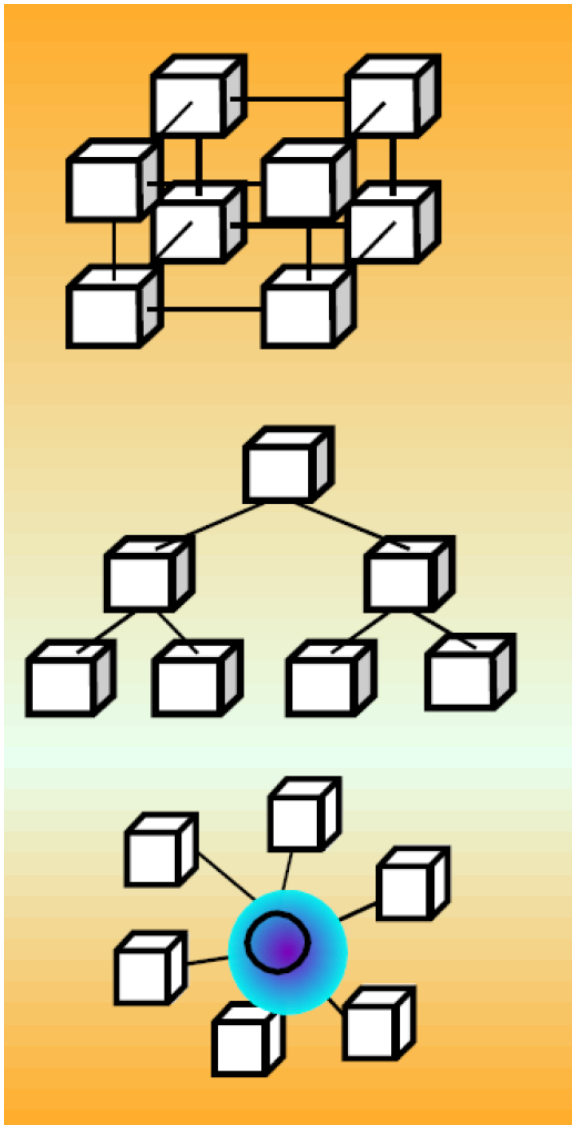
Quad Mode (VNM)
4 Processes
1 Thread/Process



Blue Gene/P memory subsystem

Cache	Total per node	Size	Replacement policy	Associativity
L1 instruction	4	32 KB	Round-Robin	▸ 64-way set-associative ▸ 16 sets ▸ 32-byte line size
L1 data	4	32 KB	Round-Robin	▸ 64-way set-associative ▸ 16 sets ▸ 32-byte line size
L2 prefetch	4	14 x 256 bytes	Round-Robin	▸ Fully associative (15-way) ▸ 128-byte line size
L3	2	2 x 4 MB	Least recently used	▸ 8-way associative ▸ 2 bank interleaved ▸ 128-byte line size
Double data RAM (DDR)	2	▸ Minimum 2 x 512 MB ▸ Maximum 4 GB	N/A	▸ 128-byte line size

Blue Gene/P networks



- 3D torus
  - 3.4 Gbit/s per each of 12 ports (5.1 GB/s per node)
  - Hardware latency: 0.5 ms (nearest neighbours), 5 ms (round-trip)
  - MPI latency: 3 ms, 10 ms
  - Main communication network
  - Many collectives take benefit of it
- Collectives (tree)
  - Global one-to-all communications (broadcast, reduction)
  - 6.8 Gbit/s per port
  - Round-trip latency: 1.3 ms (hardware), 5 ms (MPI)
  - Connects computing nodes and I/O nodes
  - Collectives on MPI_COMM_WORLD
- Global interrupds
  - Worst-case latency: 0.65 ms (hardware), 5 ms (MPI)
  - MPI_Barrier()

Blue Gene/P compilers

Compiler		C/C++		Fortran			
		C	C++	Fortran 77	Fortran 90	Fortran 95	Fortran 2003
GCC		mpicc	mpicxx	mpif77	—	—	—
IBM XL	non-threaded	mpixlc	mpixlcxx	mpixlf77	mpixlf90	mpixlf95	mpixlf2003
	thread-safe	mpixlc_r	mpixlcxx_r	mpixlf77_r	mpixlf90_r	mpixlf95_r	mpixlf2003_r

IBM XL compilers flags

- -qarch=450 -qtune=450
  - exploit only one of two FPUs
  - use when data is not 16-byte aligned
- -qarch=450d -qtune=450
  - alignment!
- -O3 (-qstrict)
  - minimal optimiazation level for Double Hammer FPU
- -O3 -qhot
- -O4 (-qnoipa)
- -O5
- -qreport -qlist -qsource
  - a lot of useful information in .lst file
- -qsmp=omp, -qsmp=auto

Blue Gene/P software

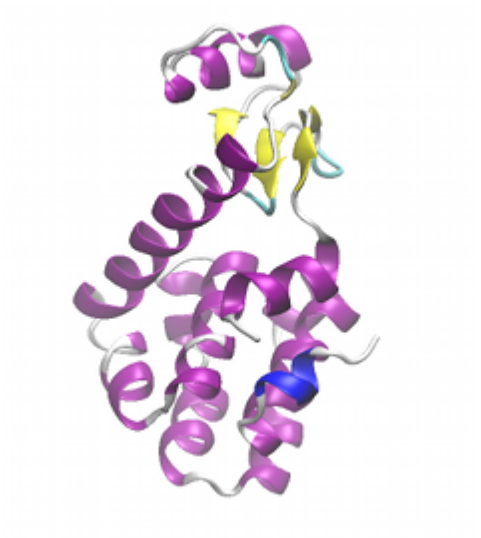
System software

- IBM XL and GCC compilers
- ESSL mathematical library (BLAS, LAPACK, etc.)
- MASS mathematical library
- LoadLeveler job scheduler

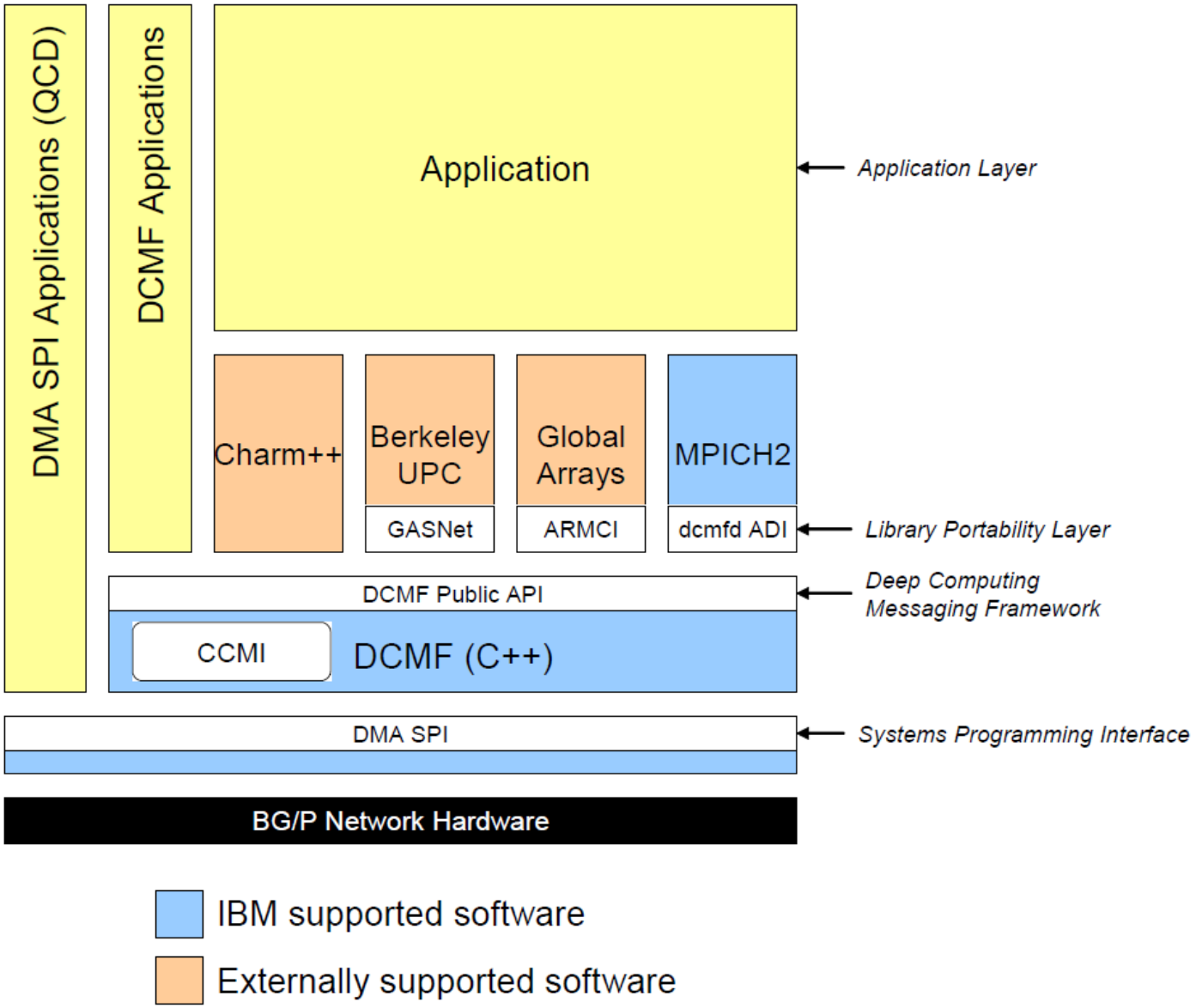
Application software and libraries

- FFTW
- GROMACS
- METIS
- ParMETIS
- szip
- zlib

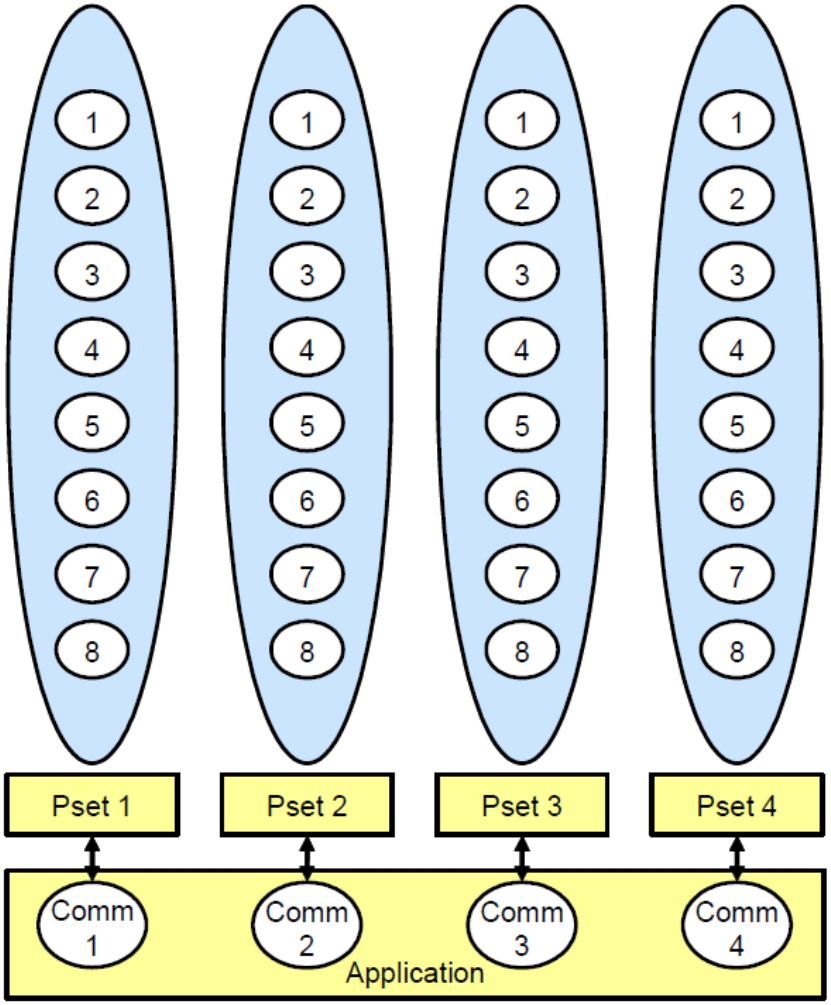
`http://hpc.cmc.msu.ru/bgp/soft`

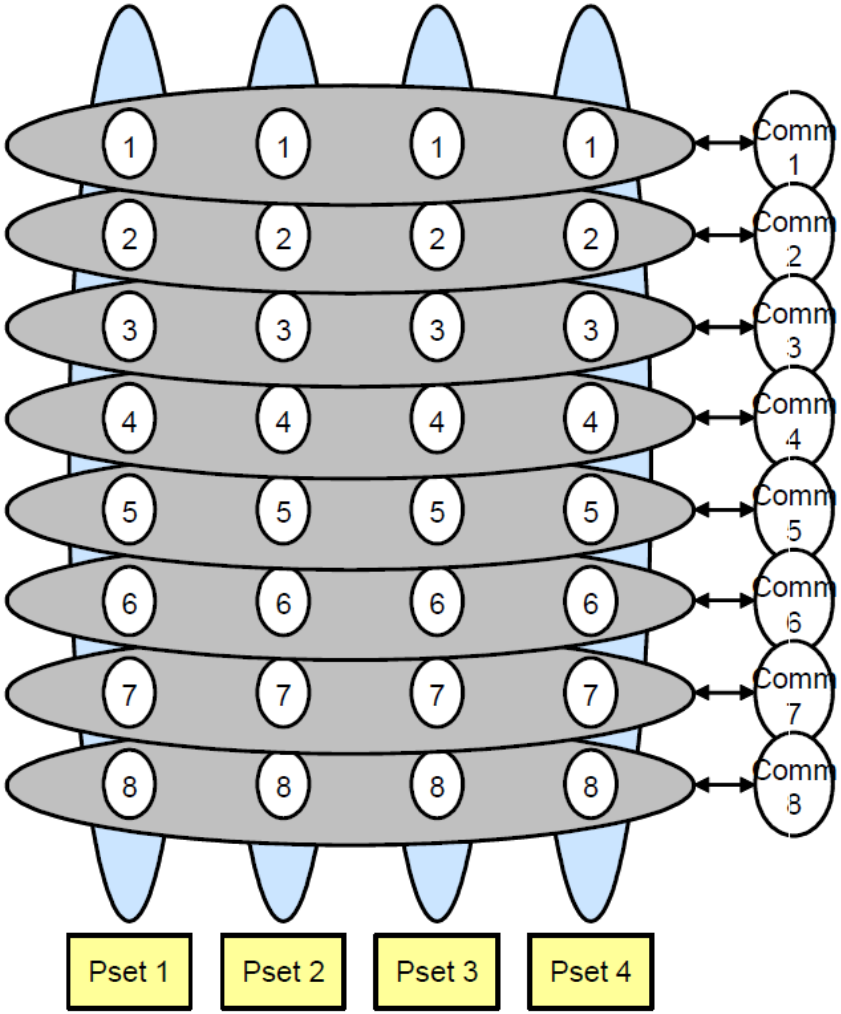


Blue Gene/P software stack



Grouping processes in respect to I/O nodes

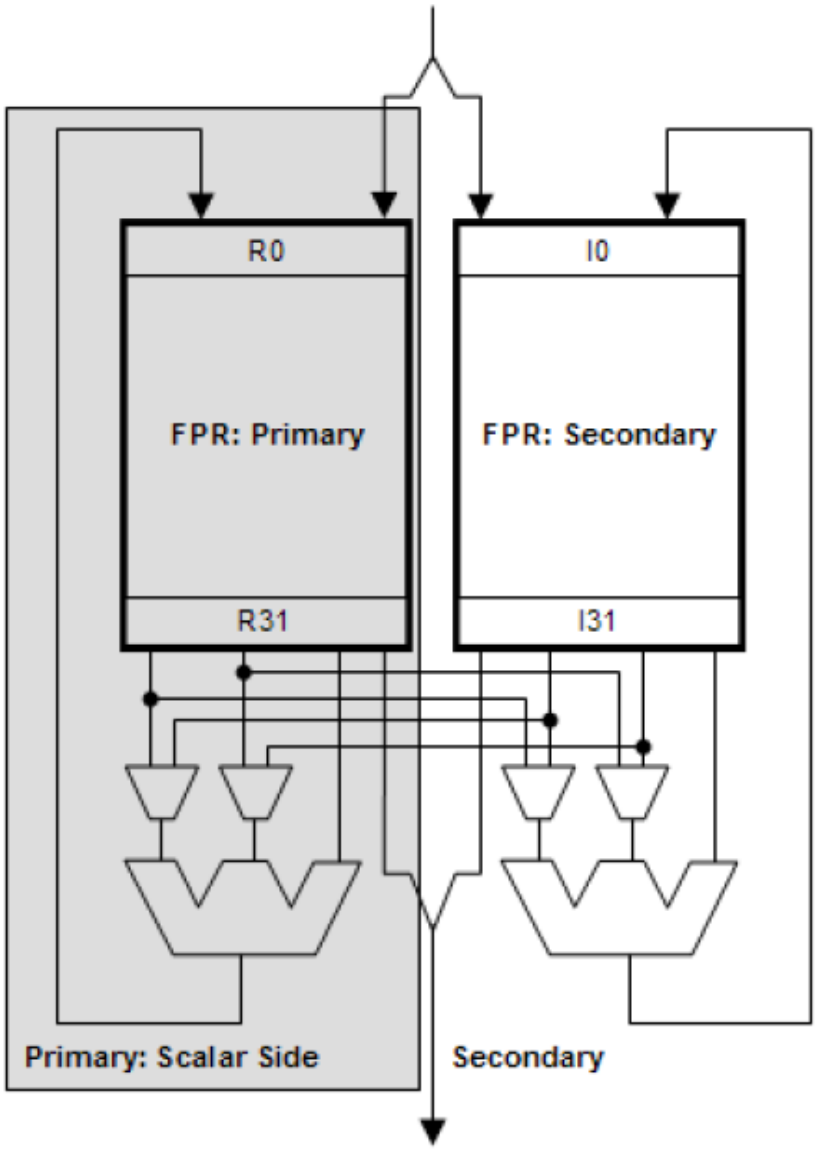


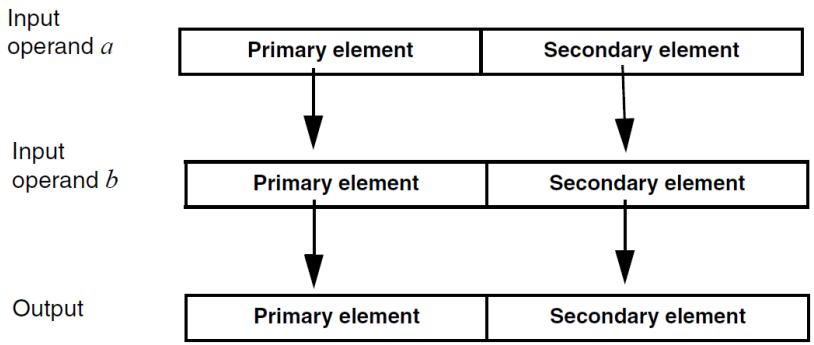



```
int MPIX_Pset_same_comm_create (MPI_Comm *pset_comm);
```

```
int MPIX_Pset_diff_comm_create (MPI_Comm *pset_comm);
```

Double Hammer FPU






```
#define MY_ALIGN __attribute__((aligned(16)))

int main() {
    double MY_ALIGN a[2] = { 2, 3 };
    double MY_ALIGN b[2] = { 4, 5 };
    double MY_ALIGN c[2] = { 6, 7 };
    double MY_ALIGN r[2]; // 2 * 4 + 6 = 14
                          // 3 * 5 + 7 = 22

    double _Complex ra = __lfpd(a);
    double _Complex rb = __lfpd(b);
    double _Complex rc = __lfpd(c);

    double _Complex rr = __fpmadd(rc, rb, ra);

    __stfpd(r, rr);
}
```

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Conclusion

- Brief history of Blue Gene
  - BG/L, BG/P, BG/Q
  - National Medal of Technology and Innovation
  - TOP500, Graph500
  - Seven Gordon Bell awards
- Blue Gene/P architecture
  - Four cores per node
  - Two GB RAM per node
  - 1024 nodes per rack
  - Two BG/P rack at Lomonosov MSU
  - Compilers and software

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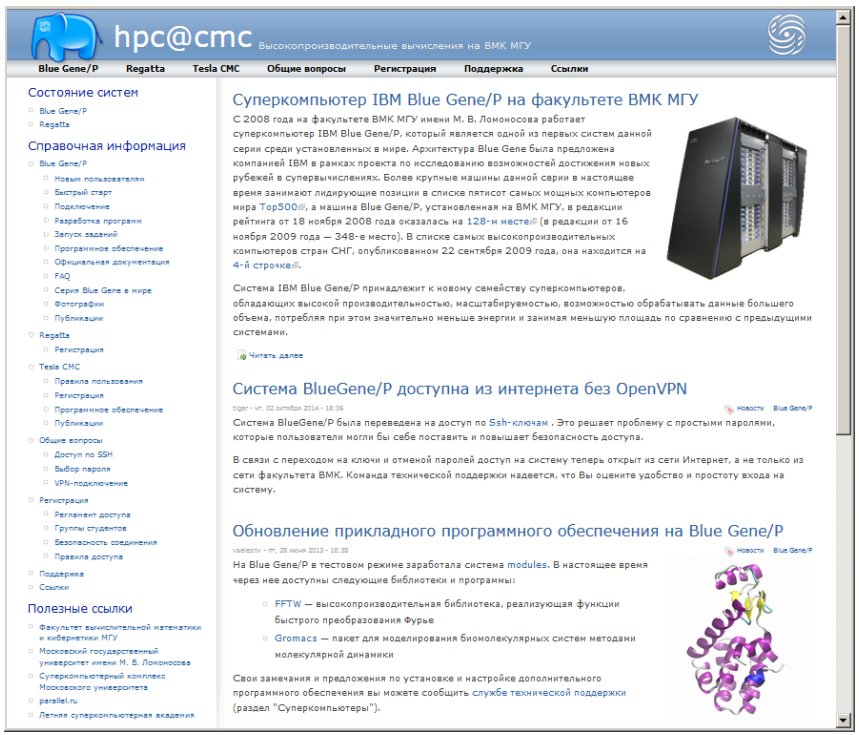

http://www.redbooks.ibm.com/abstracts/sg247287.html

http://hpc.cmc.msu.ru

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