

SuperMUC @ Leibniz Supercomputer Centre



- [Movie on YouTube](#)

Peak Performance

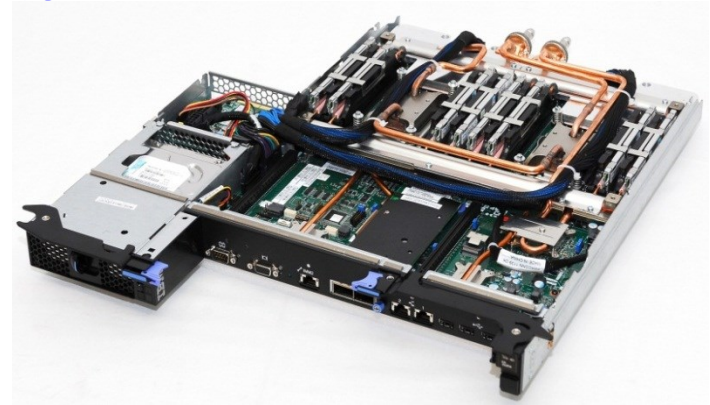
- Peak performance: 3 Peta Flops 3×10^{15} Flops

- | | | |
|-------|-----------|-------------|
| Mega | 10^6 | million |
| Giga | 10^9 | billion |
| Tera | 10^{12} | trillion |
| Peta | 10^{15} | quadrillion |
| Exa | 10^{18} | quintillion |
| Zetta | 10^{21} | sextillion |

- Flops: Floating Point Operations per Seconds

Distributed Memory Architecture

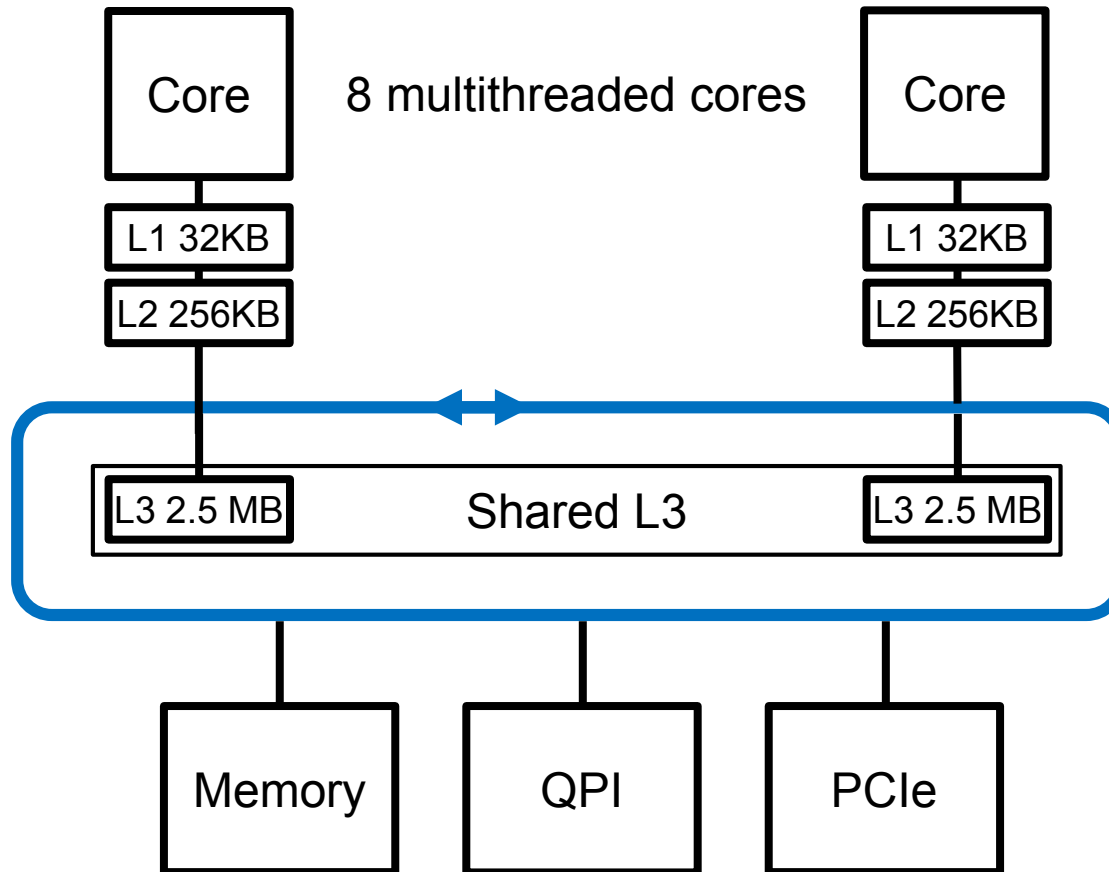
- 18 partitions called islands with 512 nodes
- Node is a shared memory system with 2 processors
 - Sandy Bridge-EP
Intel Xeon E5-2680 8C
 - 2.7 GHz (Turbo 3.5 GHz)
 - 32 GByte memory
 - Infiniband network interface
- Processor has 8 cores
 - 2-way hyperthreading
 - 21.6 GFlops @ 2.7 GHz per core
 - 172.8 GFlops per processor



Sandy Bridge Processor

Latency:

- 4 cycles
- 12 cycles
- 31 cycles



Bandwidth:

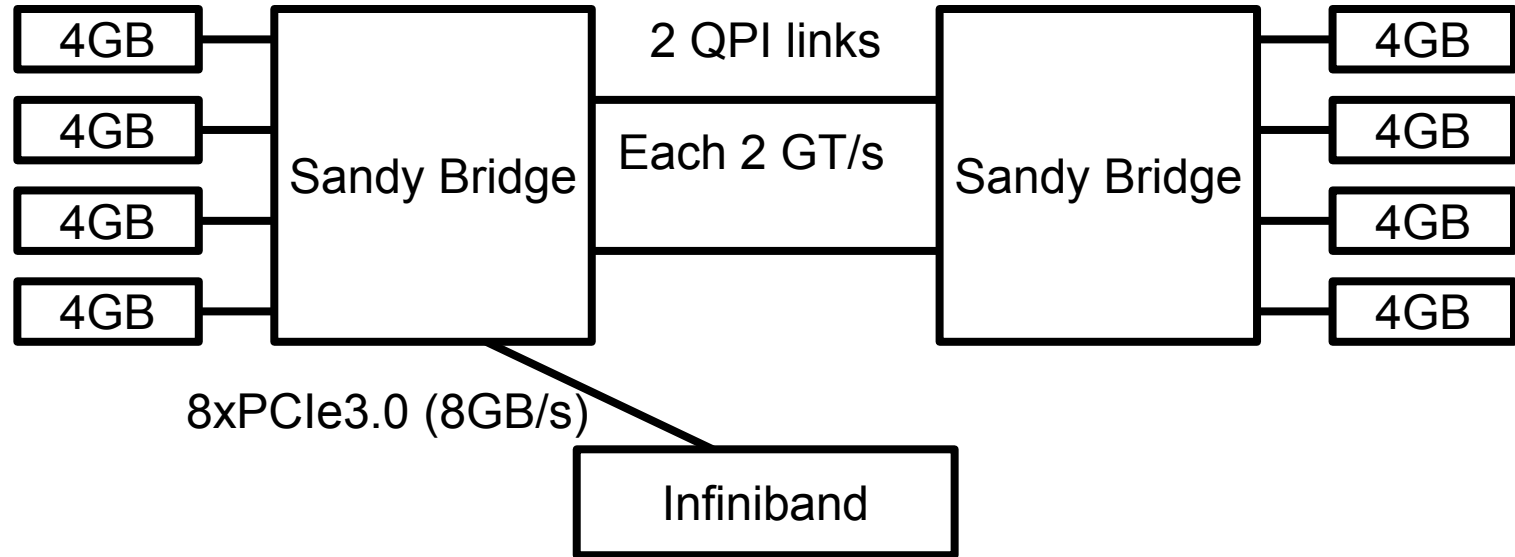
- $2 \times 16 / \text{cycle}$
- 32 / cycle
- 32 / cycle

Network frequency
equal to core frequency

- L3 cache

- Partitioned with cache coherence based on core valid bits
- Physical addresses distributed by a hash function

NUMA Node

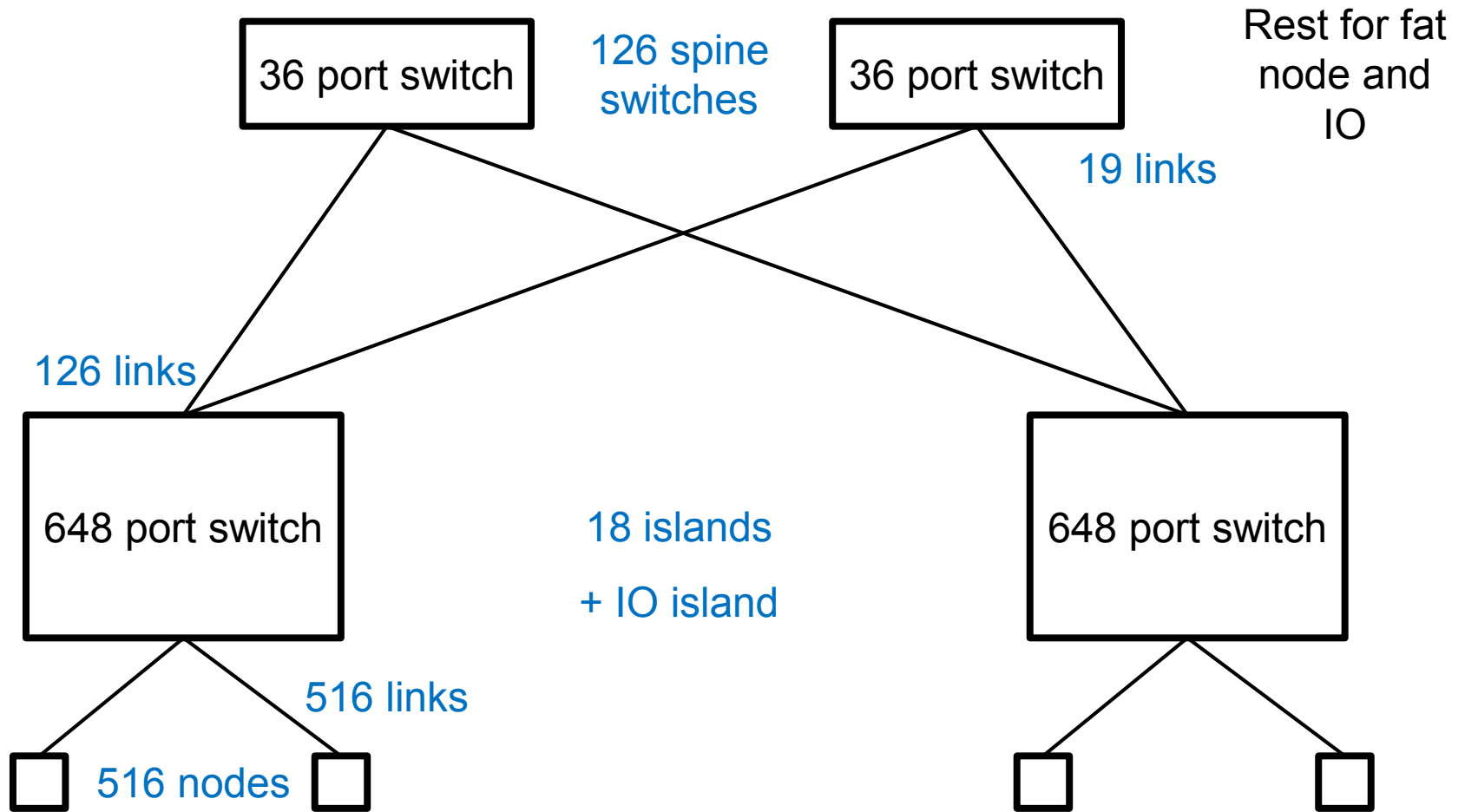


- 2 processors with 32 GB of memory
- Aggregate memory bandwidth per node 102.4 GB/s
- Latency
 - local ~50ns (~135 cycles @2.7 GHz)
 - remote ~90ns (~240 cycles)

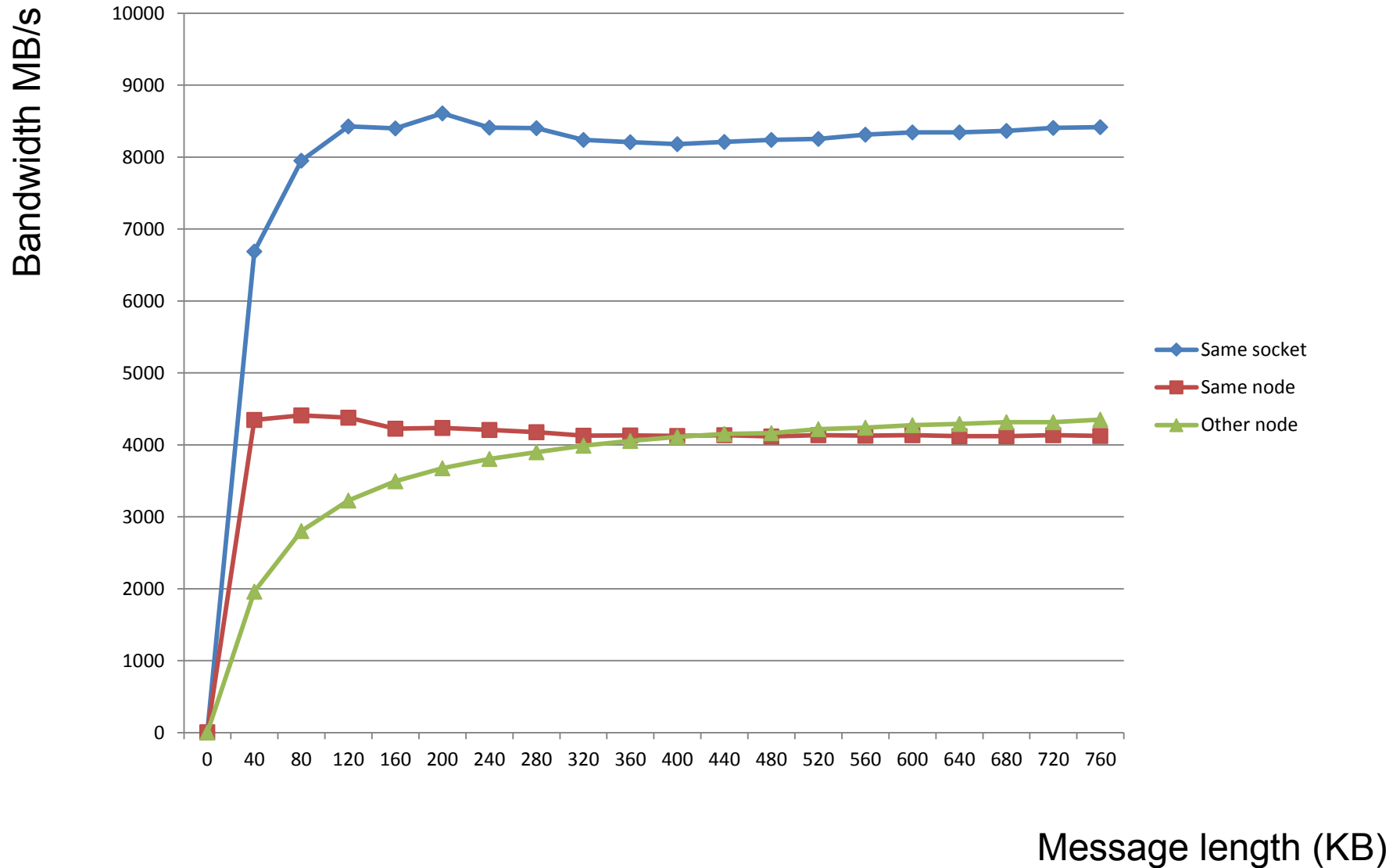
Interconnection Network

- Infiniband FDR-10
 - FDR means Fourteen Data Rate
 - FDR-10 has an effective data rate of 38.79 Gbit/s
 - Latency: 100 nsec per switch, 1usec MPI
 - Vendor: Mellanox
- Intra-Island Topology: non-blocking tree
 - 256 communication pairs can talk in parallel.
- Inter-Island Topology: Pruned Tree 4:1
 - 128 links per island to next level

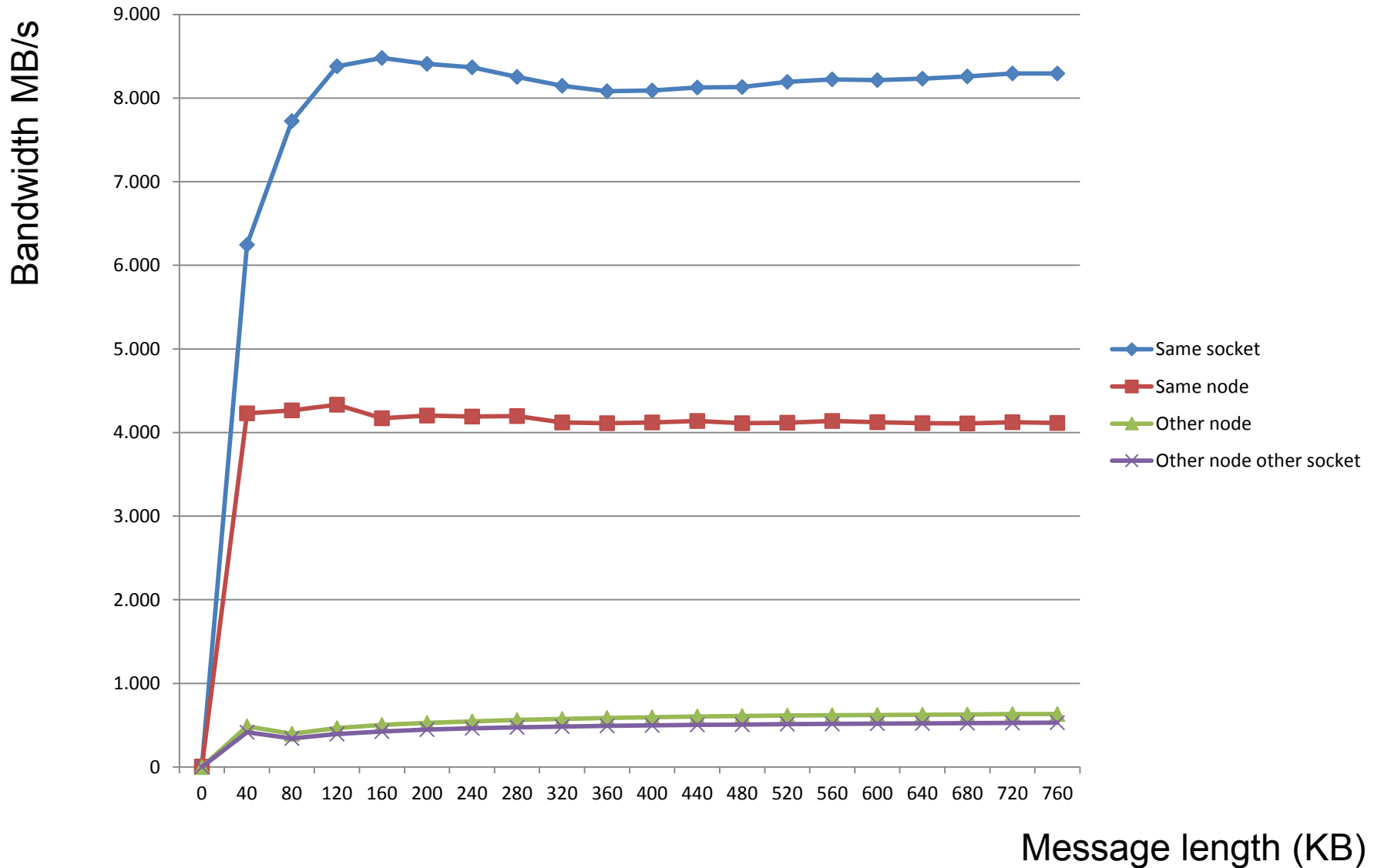
Peak Performance



MPI Performance – IBM MPI over Infiniband



MPI Performance – IBM MPI over Ethernet



9288 Compute Nodes

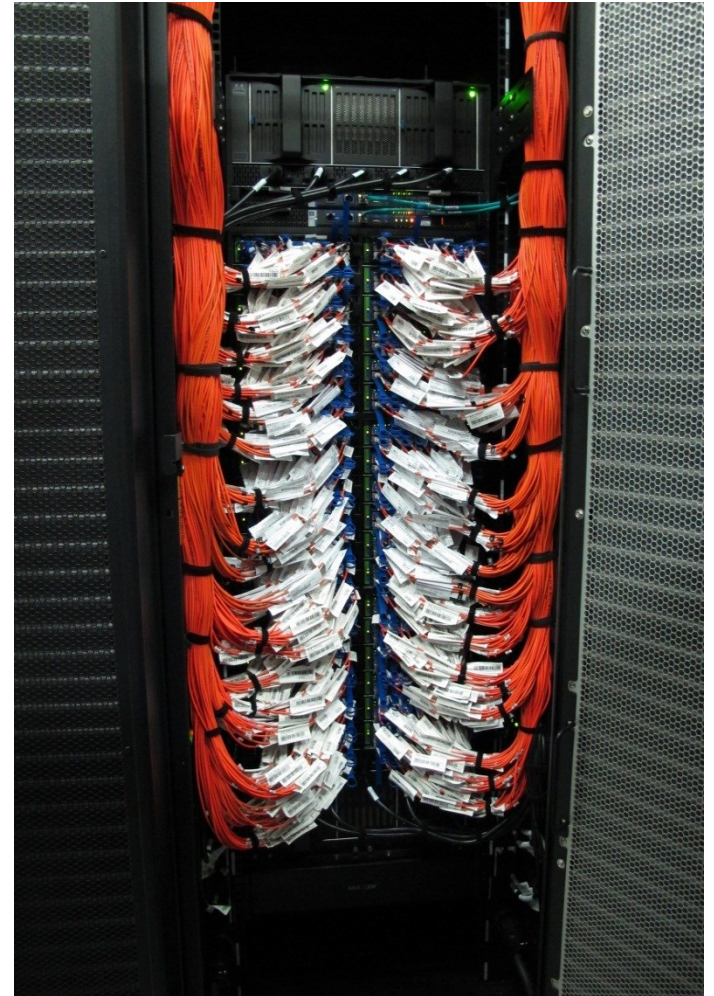
Cold Corridor
Infiniband (red)
and
Ethernet (green)
cabling



Infiniband Interconnect

19 Orcas 126 Spine Switches

11900 Infiniband Cables



Run jobs in batch

- Advantages

- Reproducible performance
- Run larger jobs
- No need to interactive poll for resources

- Test queue

- Max 1 island, 32 nodes, 2h, 1 job in queue

- General queue

- Max 1 island, 512 nodes, 48 h

- Large

- Max 4 islands, 2048 nodes, 48 h

- Special

- Max 18 islands ...

Job Script

```
#!/bin/bash
#@ wall_clock_limit = 00:4:00
#@ job_name = add
#@ job_type = parallel
#@ class = test
#@ network.MPI = sn_all,not_shared,us
#@ output = job$(jobid).out
#@ error = job$(jobid).out
#@ node = 2
#@ total_tasks=4
#@ node_usage = not_shared
#@ queue
. /etc/profile
cd ~/apptest/application
poe appl
```

- **llsubmit job.scp**
 - Submission to batch system
- **llq -u \$USER**
 - Check status of own jobs
- **llcancel <jobid>**
 - Kill job if no longer needed

Limited CPU Hours available

- Please

- Specify job execution as tight as possible.
- Do not request more nodes than required. We have to „pay“ for all allocated cores, not only the used ones.
- SHORT (<1sec) sequential runs can be done on the login node.
- Even SHORT OMP runs can be done on the login node.

Login to SuperMUC, Documentation

- First change the standard password
 - <https://idportal.lrz.de/r/entry.pl>
- Login via
 - lxhalle due to restriction on connecting machines
 - `ssh <userid>@supermuc.lrz.de`
 - No outgoing connections allowed
- Documentation
 - <http://www.lrz.de/services/compute/supermuc/>
 - <http://www.lrz.de/services/compute/supermuc/loadleveler/>
 - Intel compiler:
<http://software.intel.com/sites/products/documentation/hpc/compilerxe/en-us/2011Update/cpp/lin/index.htm>

Batch Script Parameters

- #@ energy_policy_tag = NONE
 - Switch of automatic adaptation of core frequency for performance measurements
- #@ node = 2
- #@ total_tasks= 4
- #@ task_geometry = {(0,2) (1,3)}
- #@ tasks_per_node = 2
 - Limitations on combination documented at LRZ web page
- Use Intel MPI
 - `module unload mpi.ibm`
 - `module load mpi.intel`