Chapter 1

Introduction
Why High Performance Computing?

Quote:

It is hard to understand an ocean because it is too big. It is hard to understand a molecule because it is too small. It is hard to understand nuclear physics because it is too fast. It is hard to understand the greenhouse effect because it is too slow. Supercomputers break these barriers to understanding. They, in effect, shrink oceans, zoom in on molecules, slow down physics, and fastforward climates. Clearly a scientist who can see natural phenomena at the right size and the right speed learns more than one who is faced with a blur.

Al Gore, 1990
Why High Performance Computing?

- Grand Challenges (Basic Research)
  - Decoding of human genome
  - Kosmogenesis
  - Global Climate Changes
  - Biological Macro molecules
- Product development
  - Fluid mechanics
  - Crash tests
  - Material minimization
  - Drug design
  - Chip design
- IT Infrastructure
  - Search engines
  - Data Mining
- Virtual Reality
  - Rendering
  - Vision
Examples for HPC-Applications: Finite Element Method: Crash-Analysis

Asymmetric frontal impact of a car to a rigid obstacle
Examples for HPC-Applications: Aerodynamics

Slotted Airfoil (8034 elements)

Inertial Method
Examples for HPC-Applications: Molecular dynamics

Simulation of a noble gas (Argon) with a partitioning for 8 processors: 2048 molecules in a cube of 16 nm edge length simulated in time steps of $2 \times 10^{-14}$ sec.

Barry Linnert, linnert@inf.fu-berlin.de, Cluster Computing SoSe 2020
Examples for HPC-Applications: Nuclear Energy

- 1946 Baker Test
- 23,000 Tons TNT
- Lots of nukes produced during the cold war
- Status today: Largely unknown

Examples for HPC-Applications: Visualization

Rendering (Interior architecture)

Rendering (Movie: Titanic)

Photo realistic presentation using sophisticated illumination modules
Examples for HPC-Applications: Analysis of complex materials

- \( \text{C}_{60}\)-trimer
- \( \text{Si}_{1600}\)
- MoS\(_2\)
- 4H-SiC

Source: Th. Frauenheim, Paderborn
"The performance of a computer increases (roughly) quadratically with the prize"

Consequence:
It is better to buy a computer which is twice as fast than to buy two slower computers.
(The law was valid in the sixties and seventies over a wide range of universal computers.)
Eighties

Availability of powerful Microprocessors

- High Integration density (VLSI)
- Single-Chip-Processors
- Automated production process
- Automated development process
- High volume production

Consequence:
Grosch's Law no longer valid:
1000 cheap microprocessors render (theoretically) more performance in (MFLOPS) than expensive Supercomputer (e.g. Cray)

Idea:
To achieve high performance at low cost use many microprocessors together

⇒ Parallel Processing
Eighties

- Wide spread use of workstations and PCs
  Terminals being replaced by PCs
  Workstations achieve (computational) performance of mainframes at a fraction of the price.

- Availability of local area networks (LAN) (Ethernet)
  Possibility to connect a larger number of autonomous computers using a low cost medium. Access to data of other computers. Usage of programs and other resources of remote computers.

- Network of Workstations as Parallel Computer
  Possibility to exploit unused computational capacity of other computers for computational-intensive calculations (idle time computing).
Nineties

- Parallel computers are built of a large number of microprocessors (Massively Parallel Processors, MPP), e.g. Transputer systems, Connection Machine CM-5, Intel Paragon, Cray T3E
- Alternative Architectures are built (Connection Machine CM-2, MasPar).
- Trend to use cost efficient standard components ("commercial-off-the-shelf, COTS") leads to coupling of standard PCs to a "Cluster" (Beowulf, 1995)
- Exploitation of unused compute power for HPC ("idle time computing")
- Program libraries like Parallel Virtual Machine (PVM) and the Message Passing Interface (MPI) allow for development of portable parallel programs
- Linux as operating system for HPC becomes prevailing
# Top 10 of TOP500 List (06/2001)

<table>
<thead>
<tr>
<th>RANK</th>
<th>MANUFACTURER</th>
<th>COMPUTER</th>
<th>$R_{\text{MAX}}$ [TF/S]</th>
<th>INSTALLATION SITE</th>
<th>COUNTRY</th>
<th>YEAR</th>
<th>AREA OF INSTALLATION</th>
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## Top 10 of TOP500 List (06/2002)

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Earth Simulator (Rank 1, 2002-2004)

The Earth Simulator Center

Barry Linnert, linnert@inf.fu-berlin.de, Cluster Computing SoSe 2020
Earth Simulator

- 640 Nodes
- 8 vector processors (each 8 GFLOPS) and 16 GB per node
- 5120 CPUs
- 10 TB main memory
- 40 TFLOPS peak performance
- 65m x 50m physical dimension

Source: H. Simon, NERSC
<table>
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<tr>
<th>Rank</th>
<th>Site</th>
<th>Country/Year</th>
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| 1    | IBM/DOE                  | United States/2004   | \textit{BlueGene/L beta-System}  
\textit{BlueGene/L DD2 beta-System (0.7 GHz PowerPC 440)} / 32768  
IBM                          |                               | 70720                      | 91750          |
| 2    | NASA/Ames Research Center/NAS | United States/2004   | \textit{Columbia}  
SGI Altix 1.5 GHz, Voltaire Infiniband / 10160  
SGI                          |                               | 51870                      | 60960          |
| 3    | The Earth Simulator Center | Japan/2002           | \textit{Earth-Simulator} / 5120  
NEC                          |                               | 35860                      | 40960          |
| 4    | Barcelona Supercomputer Center | Spain/2004           | \textit{MareNostrum}  
eServer BladeCenter JS20 (PowerPC970 2.2 GHz), Myrinet / 3564  
IBM                          |                               | 20530                      | 31363          |
| 5    | Lawrence Livermore National Laboratory | United States/2004   | \textit{Thunder}  
\textit{Intel Itanium2 Tiger4 1.4GHz - Quadrics} / 4096  
California Digital Corporation |                               | 19940                      | 22938          |
| 6    | Los Alamos National Laboratory | United States/2002   | \textit{ASCI Q}  
\textit{ASCI Q - AlphaServer SC45, 1.25 GHz} / 8192  
HP                            |                               | 13880                      | 20480          |
| 7    | Virginia Tech            | United States/2004   | \textit{System X}  
\textit{1100 Dual 2.3 GHz Apple XServe/Mellanox Infiniband 4X/Cisco GigE} / 2200  
Self-made                    |                               | 12250                      | 20240          |
| 8    | IBM - Rochester          | United States/2004   | \textit{BlueGene/L DD1 Prototype (0.5GHz PowerPC 440 w/Custom)} / 8192  
IBM/ LLNL                    |                               | 11680                      | 16384          |
| 9    | Naval Oceanographic Office | United States/2004   | \textit{eServer pSeries 655 (1.7 GHz Power4+)} / 2944  
IBM                          |                               | 10310                      | 20019.2        |
| 10   | NCSA                     | United States/2003   | \textit{Tungsten}  
\textit{PowerEdge 1750, P4 Xeon 3.06 GHz, Myrinet} / 2500  
Dell                          |                               | 9819                       | 15300          |
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IBM Blue Gene
IBM Blue Gene
# TOP 10 / Nov. 2006

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## Top 500 Nov 2008

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## Top 500 Nov 2008

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<td>132800</td>
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<td>Ranger - SunBlade x6420, Opteron QC 2.3 Ghz, Infiniband / 2008 / Sun Microsystems</td>
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# Top 500 Nov 2011

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<th>Total</th>
<th>Rmax</th>
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<tr>
<td>2</td>
<td>NUDT YH MPP, Xeon X5670 6C 2.93 GHz, NVIDIA 2050</td>
<td>National Supercomputing Center in Tianjin</td>
<td>China</td>
<td>186368</td>
<td>2566000</td>
<td>4701000</td>
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<td>3</td>
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<td>2331000</td>
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<td>HP ProLiant SL390s G7 Xeon 6C X5670, Nvidia GPU, Linux/Windows</td>
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<td>Japan</td>
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<td>1192000</td>
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<td>Cray XE6, Opteron 6136 8C 2.40GHz, Custom</td>
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<td>Bull bullx super-node S6010/S6030</td>
<td>Commissariat a l'Energie Atomique (CEA)</td>
<td>France</td>
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<td>BladeCenter QS22/LS21 Cluster, PowerXCell 8i 3.2 Ghz / Opteron DC 1.8 GHz, Voltaire Infiniband</td>
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<td>United States</td>
<td>122400</td>
<td>1042000</td>
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</tbody>
</table>
K-computer (AICS), Rank 1

- 800 racks with 88,128 SPARC64 CPUs / 705,024 cores
- 200,000 cables with total length over 1,000km
  - third floor (50m x 60m) free of structural pillars.
- New problem: floor load capacity of 1t/m² (avg.)
  - Each rack has up to 1.5t
  - High-tech construction required
- first floor with global file system has just three pillars
- Own power station (300m²)
The K-Computer

2013: Human Brain Simulation (Coop: Forschungszentrum Jülich)
Simulating 1 second of the activity of 1% of a Brain took 40 Minutes.
Simulation of a whole Brain possible with Exa-scale Computers?
Jugene (Forschungszentrum Jülich), Rank 13
<table>
<thead>
<tr>
<th>Rank</th>
<th>Name</th>
<th>Computer</th>
<th>Site</th>
<th>Country</th>
<th>Total Cores</th>
<th>Rmax</th>
<th>Rpeak</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Titan</td>
<td>Cray XK7, Opteron 6274 16C 2.200GHz, Cray Gemini interconnect, NVIDIA K20x</td>
<td>DOE/SC/Oak Ridge National Laboratory</td>
<td>United States</td>
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<tr>
<td>2</td>
<td>Sequoia</td>
<td>BlueGene/Q, Power BQC 16C 1.60GHz, Custom</td>
<td>DOE/NNSA/LLNL</td>
<td>United States</td>
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<td>16324751</td>
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<tr>
<td>3</td>
<td>K computer</td>
<td>K computer, SPARC64 VIIIfx 2.0GHz, Tofu interconnect</td>
<td>RIKEN Advanced Institute for Computational Science (AICS)</td>
<td>Japan</td>
<td>705024</td>
<td>10510000</td>
<td>11280384</td>
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<tr>
<td>4</td>
<td>Mira</td>
<td>BlueGene/Q, Power BQC 16C 1.60GHz, Custom</td>
<td>DOE/SC/Argonne National Laboratory</td>
<td>United States</td>
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<td>5</td>
<td>JUQUEEN</td>
<td>BlueGene/Q, Power BQC 16C 1.600GHz, Custom Interconnect</td>
<td>Forschungszentrum Juwelich (FZJ)</td>
<td>Germany</td>
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<td>6</td>
<td>SuperMUC</td>
<td>iDataPlex DX360M4, Xeon E5-2680 8C 2.70GHz, Infiniband FDR</td>
<td>Leibniz Rechenzentrum</td>
<td>Germany</td>
<td>147456</td>
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<tr>
<td>7</td>
<td>Stampede</td>
<td>PowerEdge C8220, Xeon E5-2680 8C 2.700GHz, Infiniband FDR, Intel Xeon Phi</td>
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# Top 500 Nov 2013

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<th>Rank</th>
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<th>Computer</th>
<th>Site</th>
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<th>Total Cores</th>
<th>Rmax</th>
<th>Rpeak</th>
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<tr>
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<td>United States</td>
<td>560640</td>
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<td>Sequoia</td>
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<td>Germany</td>
<td>147456</td>
<td>2897000</td>
<td>3185050</td>
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</tbody>
</table>
Tianhe-2 (MilkyWay-2), National Super Computer Center in Guangzhou, Rank 1

- Intel Xeon systems with Xeon Phi accelerators
  - 32000 Xeon E5-2692 (12 Core, 2.2 Ghz)
  - 48000 Xeon Phi 31S1P (57 Cores, 1.1 GHz)
  - Organization: 16000 Nodes, each
    - 2 Xeon E5-2692
    - 3 Xeon Phi 31S1P
- 1408 TB Memory
  - 1024 TB CPUs (64 GB per node)
  - 384 TB Xeon Phi (3x8 GB per node)
- Power 17.6 MW (24 MW with cooling)
Cray XK7

- 18,688 nodes with 299,008 cores, 710 TB (598 TB CPU and 112 TB GPU)
  - AMD Opteron 6274 16-core CPU
  - Nvidia Tesla K20X GPU
  - Memory: 32GB (CPU) + 6 GB (GPU)
- Cray Linux Environment
- Power 8.2 MW
JUQUEEN (Forschungszentrum Jülich), Rank 8 (2012: Rank 5)

- 28 racks (7 rows à 4 racks)
- 28,672 nodes (458,752 cores)
- Rack: 2 midplanes à 16 nodeboards (16,384 cores)
- Nodeboard: 32 compute nodes
- Node: 16 cores
  IBM PowerPC A2, 1.6 GHz

- Main memory: 448 TB (16 GB per node)

- Network: 5D Torus — 40 GBps; 2.5 μsec latency (worst case)

- Overall peak performance: 5.9 Petaflops
- Linpack: > 4.141 Petaflops
HERMIT (HLRS Stuttgart), Rank 39 (2012: Rank 27)

- Cray XE6
- 3,552 Nodes
- 113,664 Cores
- 126TB RAM

Barry Linnert, linnert@inf.fu-berlin.de, Cluster Computing SoSe 2020
## Top 500 Nov 2014

<table>
<thead>
<tr>
<th>R</th>
<th>Site</th>
<th>System</th>
<th>Cores</th>
<th>Rmax (TF/s)</th>
<th>Rpeak (TF/s)</th>
<th>Power (kW)</th>
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<td><strong>Tianhe-2 (MilkyWay-2)</strong></td>
<td>3,120,000</td>
<td>33,862.7</td>
<td>54,902.4</td>
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# Green 500 Top entries Nov. 2014

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<tr>
<th>Green500 Rank</th>
<th>MFLOPS/W</th>
<th>Site*</th>
<th>Computer*</th>
<th>Total Power (kW)</th>
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<tr>
<td>1</td>
<td>5,271.81</td>
<td>GSI Helmholtz Center</td>
<td>L-CSC - ASUS ESC4000 FDR/G2S, Intel Xeon E5-2690v2 10C 3GHz, Infiniband FDR, AMD FirePro S9150 Level 1 measurement data available</td>
<td>57.15</td>
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<td>2</td>
<td>4,945.63</td>
<td>High Energy Accelerator Research Organization /KEK</td>
<td>Suiren - ExaScaler 32U256SC Cluster, Intel Xeon E5-2660v2 10C 2.2GHz, Infiniband FDR, PEZY-SC</td>
<td>37.83</td>
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<td>GSIC Center, Tokyo Institute of Technology</td>
<td>TSUBAME-KFC - LX 1U-4GPU/104Re-1G Cluster, Intel Xeon E5-2620v2 8C 2.100GHz, Infiniband FDR, NVIDIA K20x</td>
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<td>4</td>
<td>3,962.73</td>
<td>Cray Inc.</td>
<td>Storm1 - Cray CS-Storm, Intel Xeon E5-2660v2 10C 2.2GHz, Infiniband FDR, Nvidia K40m Level 3 measurement data available</td>
<td>44.54</td>
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<td>5</td>
<td>3,631.70</td>
<td>Cambridge University</td>
<td>Wilkes - Dell T620 Cluster, Intel Xeon E5-2630v2 6C 2.600GHz, Infiniband FDR, NVIDIA K20</td>
<td>52.62</td>
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<td>6</td>
<td>3,543.32</td>
<td>Financial Institution</td>
<td>iDataPlex DX360M4, Intel Xeon E5-2680v2 10C 2.800GHz, Infiniband, NVIDIA K20x</td>
<td>54.60</td>
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<td>7</td>
<td>3,517.84</td>
<td>Center for Computational Sciences, University of Tsukuba</td>
<td>HA-PACS TCA - Cray CS300 Cluster, Intel Xeon E5-2680v2 10C 2.800GHz, Infiniband QDR, NVIDIA K20</td>
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<td>8</td>
<td>3,459.46</td>
<td>SURFsara</td>
<td>Cartesius Accelerator Island - Bullx B515 cluster, Intel Xeon E5-2450v2 8C 2.5GHz, InfiniBand 4x FDR, Nvidia K40m</td>
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<td>9</td>
<td>3,185.91</td>
<td>Swiss National Supercomputing Centre (CSCS)</td>
<td>Piz Daint - Cray XC30, Xeon E5-2670 8C 2.600GHz, Aries interconnect, NVIDIA K20x Level 3 measurement data available</td>
<td>1,753.66</td>
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<td>10</td>
<td>3,131.06</td>
<td>ROMEO HPC Center - Champagne-Ardenne</td>
<td>romeo - Bull R421-E3 Cluster, Intel Xeon E5-2650v2 8C 2.600GHz, Infiniband FDR, NVIDIA K20x</td>
<td>81.41</td>
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</tbody>
</table>
## Top 500 vs. Green 500

<table>
<thead>
<tr>
<th>Top 500</th>
<th>System</th>
<th>Rmax (TF/s)</th>
<th>Rpeak (TF/s)</th>
<th>Power (kW)</th>
<th>Green 500</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td><strong>Tianhe-2</strong> (MilkyWay-2)</td>
<td>33,862.7</td>
<td>54,902.4</td>
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<td>2</td>
<td><strong>Titan</strong></td>
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<td>27,112.5</td>
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<td><strong>Sequoia</strong></td>
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<td>20,132.7</td>
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<td>4</td>
<td><strong>K computer</strong></td>
<td>10,510.0</td>
<td>11,280.4</td>
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<td>5</td>
<td><strong>Mira</strong></td>
<td>8,586.6</td>
<td>10,066.3</td>
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<td>6</td>
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<td>7,788.9</td>
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<td><strong>Stampede</strong></td>
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<td>8,520.1</td>
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<td><strong>JUQUEEN</strong></td>
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<td>9</td>
<td><strong>Vulcan</strong></td>
<td>4,293.3</td>
<td>5,033.2</td>
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<td><strong>Cray CS-Storm</strong></td>
<td>3,577.0</td>
<td>6,131.8</td>
<td>1,499</td>
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</tr>
</tbody>
</table>
HLRN (Hannover + Berlin), Rank 120 + 121
Volunteer Computing

Great Internet Mersenne Prime Search (GIMPS)
Finding World Record Primes Since 1996

SETI@HOME

Folding@home
Grid’5000

Grid’5000 architecture

10 Gbps lambda activated for Grid’5000
Cloud Computing (XaaS)

- Usage of remote physical and logical resources

- Infrastructure as a service
- Platform as a service
- Software as a service
Supercomputer in the Cloud: Rank 64

- Amazon EC2 C3 Instance
- Intel Xeon E5-2680v2 10C 2.800GHz
- 10G Ethernet
- 26496 Cores (according to TOP500 list)
- Rmax: 484179 GFLOPS
- Rpeak: 593510,4 GFLOPS
Support for parallel programs

Parallel Application

Program libraries (e.g. communication, synchronization,..)

Middleware (e.g. administration, scheduling,..)

Distributed operating system

Connection network

node 1  node 2  node 3  node 4  node 5  node n
Tasks

**User’s point of view** (programming comfort, short response times)
- Efficient Interaction (Information exchange)
  - Message passing
  - Shared memory
- Synchronization
- Automatic distribution and allocation of code and data
- Load balancing
- Debugging support
- Security
- Machine independence

**Operator’s point of view** (High utilization, high throughput)
- Multiprogramming / Partitioning
  - Time sharing
  - Space sharing
- Load distribution / Load balancing
- Stability
- Security