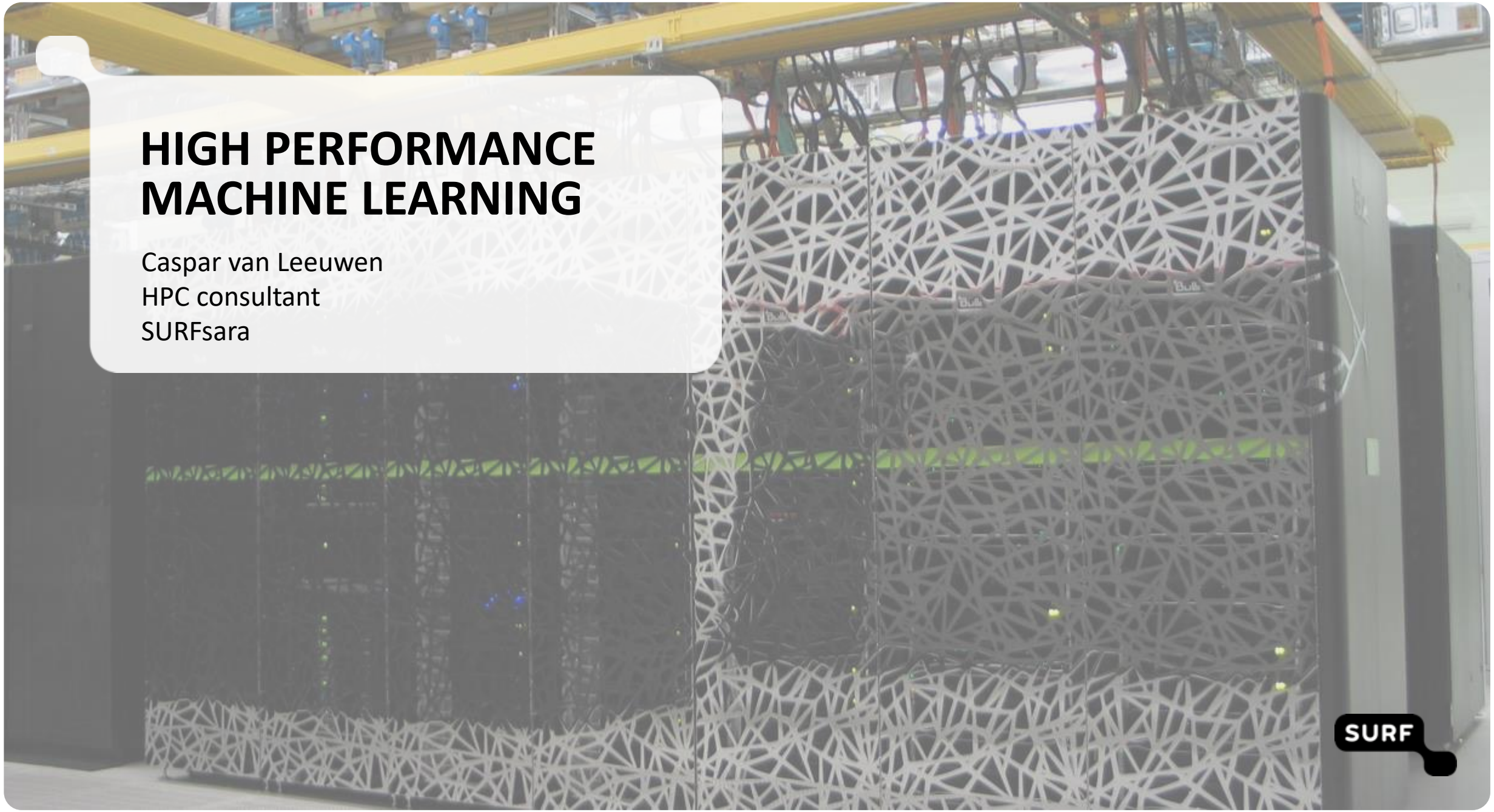


# HIGH PERFORMANCE MACHINE LEARNING

Caspar van Leeuwen
HPC consultant
SURFsara

# Program, 2nd day

- 9:00 – 9:30 Introduction to Parallel Computing (Caspar van Leeuwen)
- 9:30 – 10:30 Parallel Computing for Deep Learning: ideas, framworks, and hardware bottlenecks (Caspar van Leeuwen)
- 10:30 – 11:00 Coffee break
- 11:00 – 11:30 Structure of Deep Learning Frameworks: computational graph, autodiff, and optimizers (Ruben Hekster)
- 11:30 – 12:30 Hands-on: Profiling TensorFlow with TensorBoard (Ruben Hekster)
- 12:30 – 14:00 Lunch Break
- 14:00 – 15:00 Hands-on: Data Parallelism with Horovod (CIFAR10) (Maxwell Cai)
- 15:00 – 15:30 Coffee break
- 15:30 – 16:15 Introduction to hybrid parallelism (Caspar van Leeuwen)
- 16:15 – 17:00 Open Discussion

# Hardware

Goals:

- Understand what hardware bottlenecks could be limiting
- Understand pro’s and con’s of various hardware
- Know how to choose appropriate hardware for you DL task
- Know what to do to mitigate bottlenecks

# Hardware bottlenecks

- Compute (floating point operations per second, FLOPS)
- Memory bandwidth
- Memory size
- I/O
- Communication

# Hardware bottlenecks

- Compute (floating point operations per second, FLOPS)
- Memory bandwidth
- Memory size
- I/O
- Communication

E.g. training a compute intensive network on a single node

# Hardware bottlenecks

- Compute (floating point operations per second, FLOPS)
- Memory bandwidth
- Memory size
- I/O
- Communication

- Data needs to get to the processor in time in order to do compute!
- Many codes are limited by memory bandwidth

# Hardware bottlenecks

- Compute (floating point operations per second, FLOPS)
- Memory bandwidth
- Memory size
- I/O
- Communication

- Very deep or wide networks, or networks with very large input/output layers (e.g. high resolution images) may be limited by memory size.
- Not a performance bottleneck, but a no-go!

# Hardware bottlenecks

- Compute (floating point operations per second, FLOPS)
- Memory bandwidth
- Memory size
- I/O
- Communication

- HPC systems typically have shared file systems, usually with good bandwidth, but (relatively) low IOPS
- (Very) common bottleneck in distributed learning! Many nodes reading from the same filesystem.
- Other users (& sysadmins) will dislike you if you do I/O in a naive way!

# Hardware bottlenecks

- Compute (floating point operations per second, FLOPS)
- Memory bandwidth
- Memory size
- I/O
- Communication

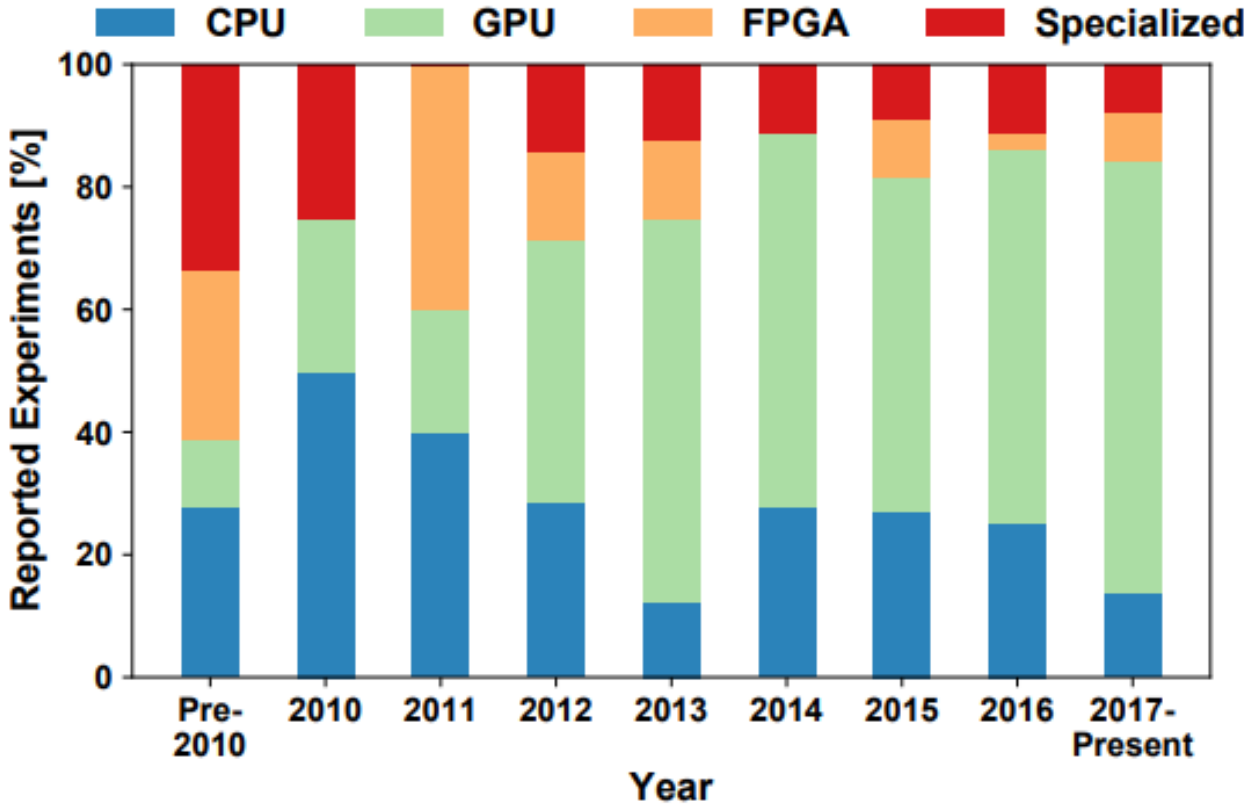
Communication can be limiting in several ways:

- Latency (many, small message send between nodes)
- Bandwidth (few, large messages send between nodes)
- Load imbalance (some workers in distributed job are slower / have more work; others have to wait when synchronization is needed)
- CPU ⇔ GPU

# Hardware overview

A look at the hardware, from a DL perspective:

- Nvidia Pascal / Volta GPUs
- AMD Vega / Vega20
- Intel Xeon Scalable
- AMD Zen
- Specialized hardware
- I/O
- Interconnects




Source: Demystifying Parallel and Distributed Deep Learning: An In-Depth Concurrency Analysis, Ben-Nun & Hoefler 2018

# Hardware overview

| | INT8 [TOPS] | FP16 [TFLOPS] | FP32 [TFLOPS] | FP64 [TFLOPS] | Memory [GB] | Memory Bandwidth [GB/s] | PCIe [GB/s] | Proprietary Interconnect [GB/s] |
|---|---|---|---|---|---|---|---|---|
| AMD MI25 | - | 24.6 | 12.29 | 0.77 | 16 | 484 | 15.75 | - |
| AMD MI50 | 53.6 | 26.8 | 13.4 | 6.7 | 16 | 1024 | 31.51 | 200 (2 × 100) |
| AMD MI60 | 58.9 | 29.5 | 14.7 | 7.4 | 32 | 1024 | 31.51 | 200 (2 × 100) |
| NVIDIA P100 | - | 21.2 | 10.6 | 5.3 | 16 | 732 | 15.75 | 160 (4 × 40) |
| NVIDIA V100 | 62.8 | 31.4 / 125 | 15.7 | 7.8 | 16/32 | 900 | 15.75 | 300 (6 × 50) |
| Intel Xeon Scalable 8180 (per socket) | - | - | 3.0 / 4.2 | 1.5 / 2.1 | 768 (max) | 119 (max) | 15.75 | - |
| AMD EPYC 7601 (per socket) | - | - | 1.1 / 1.4 | 0.56 / 0.69 | 2000 (max) | 159 (max) | 15.75 | - |

Source: Prace best practice guide – deep learning
http://www.prace-ri.eu/IMG/pdf/Best-Practice-Guide-Deep-Learning.pdf

# Hardware overview

GPUs support reduced precision, has higher performance

| | INT8 [TOPS] | FP16 [TFLOPS] | FP32 [TFLOPS] | FP64 [TFLOPS] | Memory [GB] | Memory Bandwidth [GB/s] | PCIe [GB/s] | Proprietary Interconnect [GB/s] |
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Source: Prace best practice guide – deep learning
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# Hardware overview

GPUs have a lot of FLOPS compared to CPUs

| | INT8 [TOPS] | FP16 [TFLOPS] | FP32 [TFLOPS] | FP64 [TFLOPS] | Memory [GB] | Memory Bandwidth [GB/s] | PCIe [GB/s] | Proprietary Interconnect [GB/s] |
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Source: Prace best practice guide – deep learning
http://www.prace-ri.eu/IMG/pdf/Best-Practice-Guide-Deep-Learning.pdf

# Hardware overview

CPUs have a lot of memory compared to GPUs

| | INT8 [TOPS] | FP16 [TFLOPS] | FP32 [TFLOPS] | FP64 [TFLOPS] | Memory [GB] | Memory Bandwidth [GB/s] | PCIe [GB/s] | Proprietary Interconnect [GB/s] |
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| Intel Xeon Scalable 8180 (per socket) | - | - | 3.0 / 4.2 | 1.5 / 2.1 | 768 (max) | 119 (max) | 15.75 | - |
| AMD EPYC 7601 (per socket) | - | - | 1.1 / 1.4 | 0.56 / 0.69 | 2000 (max) | 159 (max) | 15.75 | - |

Source: Prace best practice guide – deep learning
http://www.prace-ri.eu/IMG/pdf/Best-Practice-Guide-Deep-Learning.pdf

# Hardware overview

Memory bandwidth relative to FLOPS is approximately the same

| | INT8 [TOPS] | FP16 [TFLOPS] | FP32 [TFLOPS] | FP64 [TFLOPS] | Memory [GB] | Memory Bandwidth [GB/s] | PCIe [GB/s] | Proprietary Interconnect [GB/s] |
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Source: Prace best practice guide – deep learning
http://www.prace-ri.eu/IMG/pdf/Best-Practice-Guide-Deep-Learning.pdf

# Nvidia Pascal / Volta GPUs

Generally *you* are responsible for specifying a reduced precision: DL frameworks don't do this automatically since it may impact your networks accuracy, convergence, etc

Features

- INT8 & FP16 support
- (Volta) Tensor cores: fused multiply-add units that support mixed precission (multiply in FP16, add in FP32). High performance: 120 TOPS.

$$D = \begin{pmatrix} A_{0,0} & A_{0,1} & A_{0,2} & A_{0,3} \\ A_{1,0} & A_{1,1} & A_{1,2} & A_{1,3} \\ A_{2,0} & A_{2,1} & A_{2,2} & A_{2,3} \\ A_{3,0} & A_{3,1} & A_{3,2} & A_{3,3} \end{pmatrix} \begin{pmatrix} B_{0,0} & B_{0,1} & B_{0,2} & B_{0,3} \\ B_{1,0} & B_{1,1} & B_{1,2} & B_{1,3} \\ B_{2,0} & B_{2,1} & B_{2,2} & B_{2,3} \\ B_{3,0} & B_{3,1} & B_{3,2} & B_{3,3} \end{pmatrix} + \begin{pmatrix} C_{0,0} & C_{0,1} & C_{0,2} & C_{0,3} \\ C_{1,0} & C_{1,1} & C_{1,2} & C_{1,3} \\ C_{2,0} & C_{2,1} & C_{2,2} & C_{2,3} \\ C_{3,0} & C_{3,1} & C_{3,2} & C_{3,3} \end{pmatrix}$$

FP16 or FP32 FP16 FP16 FP16 or FP32

- High bandwidth memory, 2nd generation (HBM2)
- NVLink: allows direct $GPU_1 \Leftrightarrow GPU_2$ communication in a multi-GPU node (much faster than having to go over PCIe)

# Nvidia Pascal / Volta GPUs

(Low-level) library support

- CUDA
- cuBLAS: basic linear algebra
- cuSPARSE: sparse matrix algebra
- cuDNN: primitives for deep neural networks
- NCCL: NVIDIA collective communications library (implements efficient allreduce and supports e.g. NVLink & RDMA)

Efficient low-level libraries are just as important as hardware itself! Otherwise, theoretical hardware specs might be great, but you'll never get that performance!

# AMD Vega / Vega20

Features

- INT8 & FP16 support
- High bandwidth memory, 2nd generation (HBM2)
- PCIe 4.0 support (large bandwidth CPU ⇔ GPU)
- Infinity fabric: proprietary interconnect for high bandwidth GPU ⇔ GPU communication in a multi-GPU node.

# AMD Vega / Vega20

(Low-level) library support

- Heterogeneous-computing Interface for Portability (HIP): a C++ dialect that was designed to ease conversion of CUDA applications to portable C++ code
- MIOpen: machine learning primitives (based on the OpenCL or HIP)
- rocBLAS: basic linear algebra
- ROCm: software ecosystem for GPU computing
- ROCm: has forks of TensorFlow, Caffe 2, PyTorch, MxNet and CNTK with MIOpen support.

While software stack is ‘young’ compared to NVidia, performance is competitive – provided the ROCm forks of the frameworks are used when computing on AMD hardware!

# Intel Xeon Scalable

Pro tip:
Low-end Xeon Scalable processors have only 1 AVX-512 FMA unit. AVX2 may perform better on these processors, because AVX-512 instructions are executed at lower clock speeds!

- Supports AVX-512 vector instructions
- Supports very large memory (more than 1 TB per node)
- Intel Math Kernel Library (MKL): optimized BLAS, LAPACK and FFTW routines
- Intel MKL-DNN: primitives for deep learning.

# AMD Zen

- Supports AVX-2 vector instructions
- Supports very large memory (more than 1 TB per node)
- BLIS: a BLAS implementation optimized for AMD EPYC processors
- libFLAME: portable library for dense matrix multiplications

Note: the Zen processor is not really marketed as a processor for DL task. DL frameworks don't generally support its low level libraries.

More info: PRACE AMD EPYC best practice guide, http://www.prace-ri.eu/IMG/pdf/Best-Practice-Guide-AMD.pdf

# Specialized hardware

Tensor processing units (TPU)

- Chip designed specifically for machine learning (tensor operations)
- Available only in Google Cloud
- Google Cloud TPU v3: 420 TFLOPS, 128 GB HBM. About 8 USD/TPU-hour
- Supported in TensorFlow

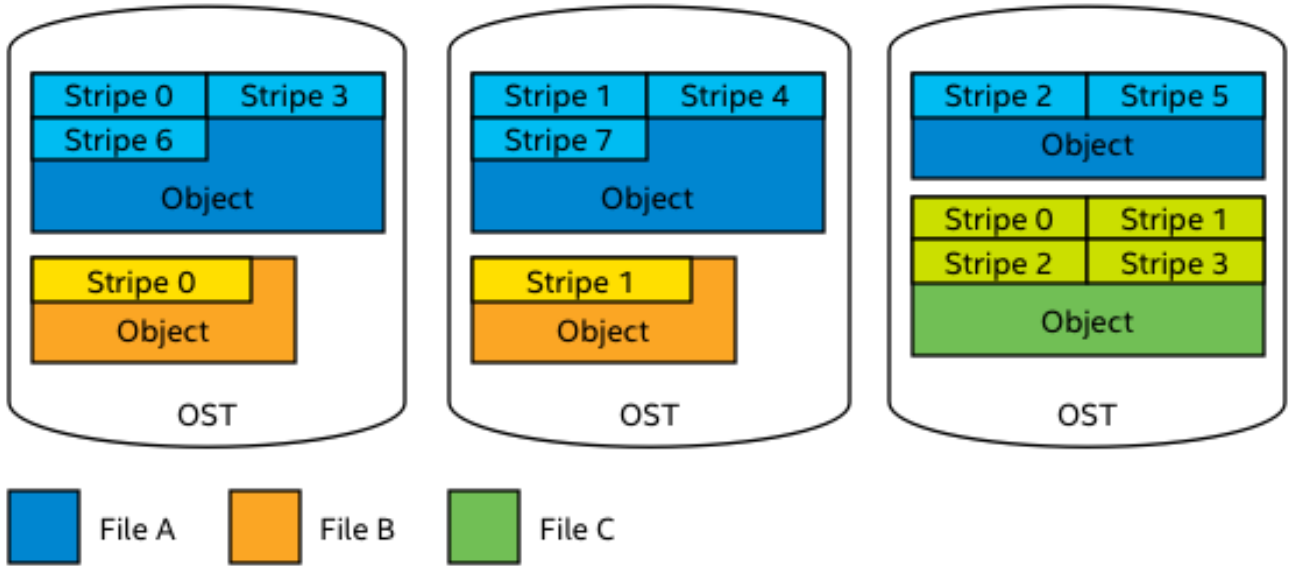
Field Programmable Gate Arrays (FPGA)

- Programmable chips
- Can do e.g. compute in any desired accuracy
- Very experimental, no framework support
- Maybe in the future…

# I/O

HPC systems typically use parallel shared file systems.

- Parallel file system: one file can be distributed over many physical disks, to increase I/O bandwidth.



# I/O

Two main types of parallel filesystems

- Lustre
  - Metadata (filename, size, location, etc) stored on separate server
  - Object Storage Target (OST) stores actual file
  - Striping over multiple OSTs can be managed by user
- GPFS
  - Metadata and actual file stored on the same server
  - Striping is managed automatically, by file system. User has no control.

# Mitigate hardware bottlenecks

- Compute (floating point operations per second, FLOPS)
- Memory bandwidth
- Memory size
- I/O
- Communication

- Use high-FLOP hardware (GPUs, TPUs)
- Use specialized vector instructions: AVX, AVX2, AVX-512 (CPUs)
- Use reduced precision training (GPUs)
- Use distributed learning

**Pro tip for Tensorflow CPU training**

'Pip install tensorflow' installs a TensorFlow binary with only AVX support. Poor performance on new CPU architectures!

- Build from source yourself (tricky, but allows perfect optimization for your system)
- Use prebuilt Intel optimized Tensorflow on Intel CPUs: pip install intel-tensorflow, or conda. (easy, but TF versions may lag behind) See https://software.intel.com/en-us/articles/intel-optimization-for-tensorflow-installation-guide

# Mitigate hardware bottlenecks

- Compute (floating point operations per second, FLOPS)
- Memory bandwidth
- Memory size
- I/O
- Communication

- Low level libraries (cuDNN, MKL-DNN) have optimized memory access patterns, meaning you get the most out of your memory bandwidth
- Make sure your DL framework is build against the appropriate low level libraries

# Mitigate hardware bottlenecks

- Compute (floating point operations per second, FLOPS)
- Memory bandwidth
- Memory size
- I/O
- Communication

- Choose different architecture. E.g. TPUs, or CPUs (distributed CPU training can provide as many FLOPS as serial training on GPUs, but much more memory!)
- Prune your model, if you can
- Model/pipeline parallelism

# Mitigate hardware bottlenecks

- Compute (floating point operations per second, FLOPS)
- Memory bandwidth
- Memory size
- I/O
- Communication

Depends on what's limiting:

- IOPS: pack small files into large files. Many frameworks provide dedicated file formats for this (TensorFlows: TFRecords, Caffe: LMDB), though other packed data formats such as HDF provide similar performance benefits. Particularly important if reading from Lustre filesystem: metadataservers don't scale!
- Bandwidth: exploit parallel filesystems. E.g. use Lustre striping. See PRACE Parallel I/O best practice guide http://www.prace-ri.eu/best-practice-guide-parallel-i-o/
- Stage on local disks, if nodes have it. This means read from shared filesystem only occurs once – further reads (each epoch) are done from local filesystem
- Stage in RAM (/dev/shm). Only an option for small datasets.

# Mitigate hardware bottlenecks

- Compute (floating point operations per second, FLOPS)
- Memory bandwidth
- Memory size
- I/O
- Communication

Depends on limiting factor:

- Latency: bundle small messages into larger ones (e.g. tensor fusion)
- Bandwidth: send as little data as possible (efficient reduction operation) using as much of the network between nodes as possible (parameter server = single bottleneck)
- Load imbalance: use homogeneous node types, all with same hardware.

More about tensor fusion:
https://github.com/horovod/horovod/blob/6f400014b8cb45aa013077aad0060032a4dda713/docs/tensor-fusion.rst

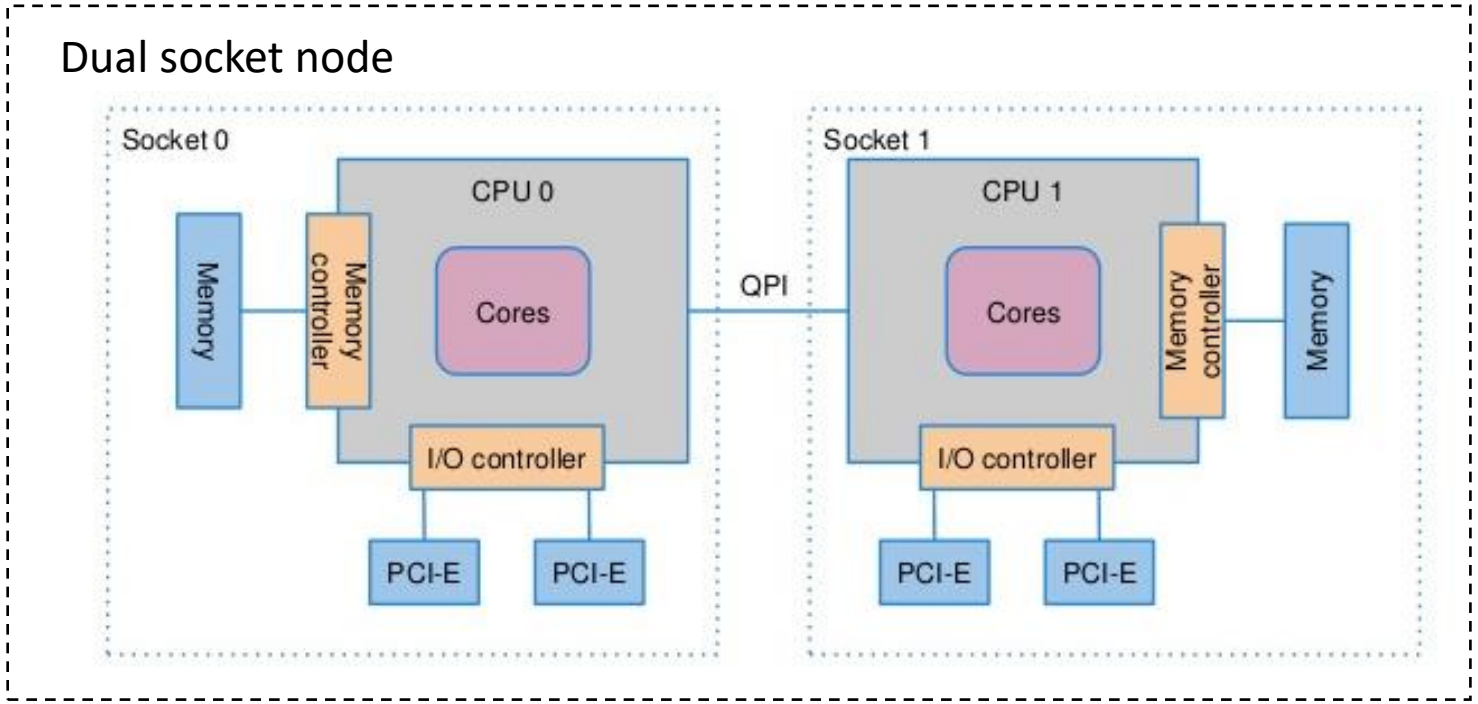


SURF

# Launching parallel workloads on CPU

NUMA domains

- Memory from CPU 0 and CPU 1 is ‘one memory’ from programmers point of view
- Cores from CPU 0 can access memory from CPU 1, but is slower!
- Dual socket: 2 tasks (data parallel) per node ≈ 20-50% faster than 1 task per node



# Launching parallel workloads on CPU

Problem:

- Performance hit if process moves from CPU 0 => CPU 1 (NUMA)
- Potential performance hit when multithreading across sockets (NUMA)
- Cache misses if thread is moved from one core to another (any multithreading application)

Solution:

- Launch 1 worker per socket
- Bind (MPI) processes to sockets
- Set number of threads to number of cores available per socket
- Bind threads to cores

# Launching parallel workloads

Binds threads to (hyperthreading)cores

Set nr of threads to nr of cores per socket

Example, 2-socket node, 12 cores per socket

- KMP_AFFINITY="granularity=fine,compact,1,0" OMP_NUM_THREADS=12 mpirun -np 2 --map-by ppr:1:socket --bind-to socket python train.py

Maps one process to each socket

Binds to socket

Launches two processes

- Tip: specify '--report-bindings' to get verbose output from *mpirun* on how processes are mapped / bound.
- Tip: specify 'KMP_AFFINITY="granularity=fine,verbose,compact,1,0" to get verbose output on how threads are bound

# Launching parallel workloads on GPU

Depends on the code!

Code designed for multi-GPU node (e.g. uses tf.device(‘/gpu:0’), tf.device(‘/gpu:1’) etc):

- Launch a single process per node

Code designed for single-GPU, but parallelized with e.g. Horovod:

- Typically: launch one (MPI) process per GPU

# Recap

Goals:

- Understand what hardware bottlenecks could be limiting
- Understand pro’s and con’s of various hardware
- Know how to choose appropriate hardware for you DL task
- Know what to do to mitigate bottlenecks