



**nVIDIA**





# NVIDIA THE AI COMPANY

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Romuald Josien

# GPUS FOR HPC AND DEEP LEARNING

Huge demand on compute power (FLOPS)

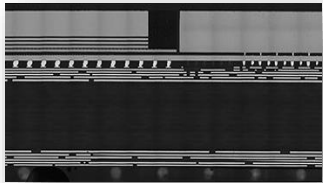
NVIDIA Tesla V100



5120 energy efficient cores + TensorCores  
7.8 TF Double Precision (fp64), 15.6 TF Single Precision (fp32) ,  
125 Tensor TFLOP/s mixed-precision

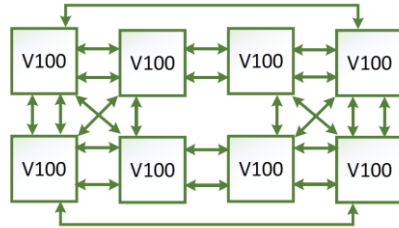
Huge demand on communication and memory bandwidth

CoWoS with HBM2



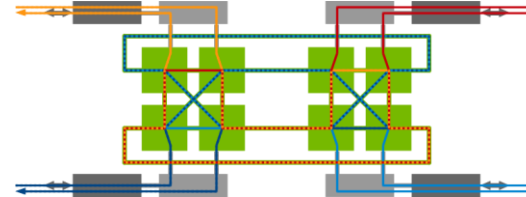
900 GB/s Memory Bandwidth  
Unifying Compute & Memory  
in Single Package

NVLink



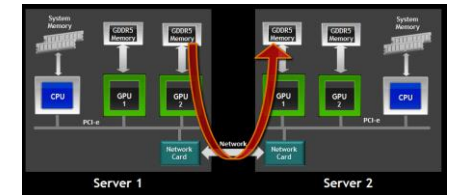
6 links per GPU a 50 GB/s bi-directional for maximum scalability between GPU's

NCCL



High-performance multi-GPU  
and multi-node collective  
communication primitives  
optimized for NVIDIA GPUs

GPU Direct /  
GPU Direct RDMA

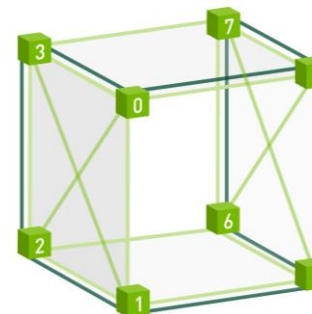
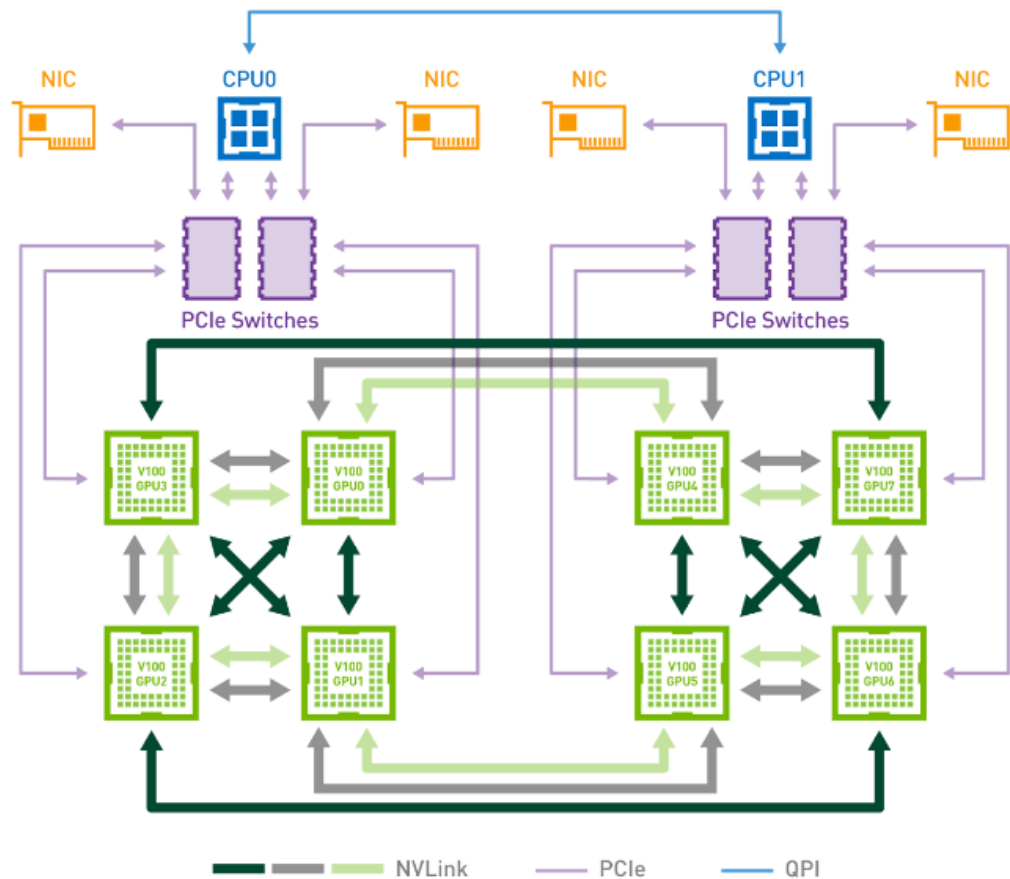


Direct communication  
between GPUs by  
eliminating the CPU from  
the critical path

The background features a complex network of glowing green lines and nodes. The nodes are small, bright green circles of varying sizes, some appearing as larger, fainter bokeh-like shapes. The lines are thin, green, and crisscross the dark space, creating a sense of interconnectedness and data flow. The overall aesthetic is futuristic and technical.

**DL MULTI GPU**

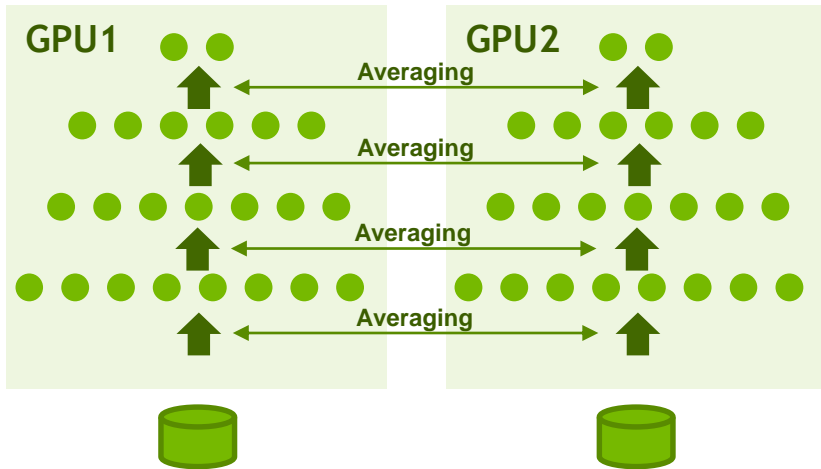
# DL DATA PARALLELISM - NVLINK



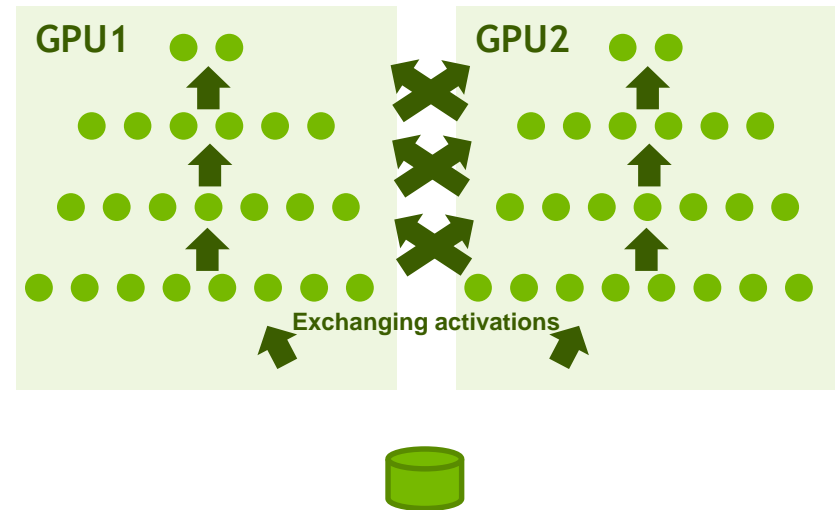
# DATA VS MODEL PARALLELISM

## Comparison

### ▶ Data Parallelism



### ▶ Model Parallelism



# DATA VS MODEL PARALLELISM

## Comparison

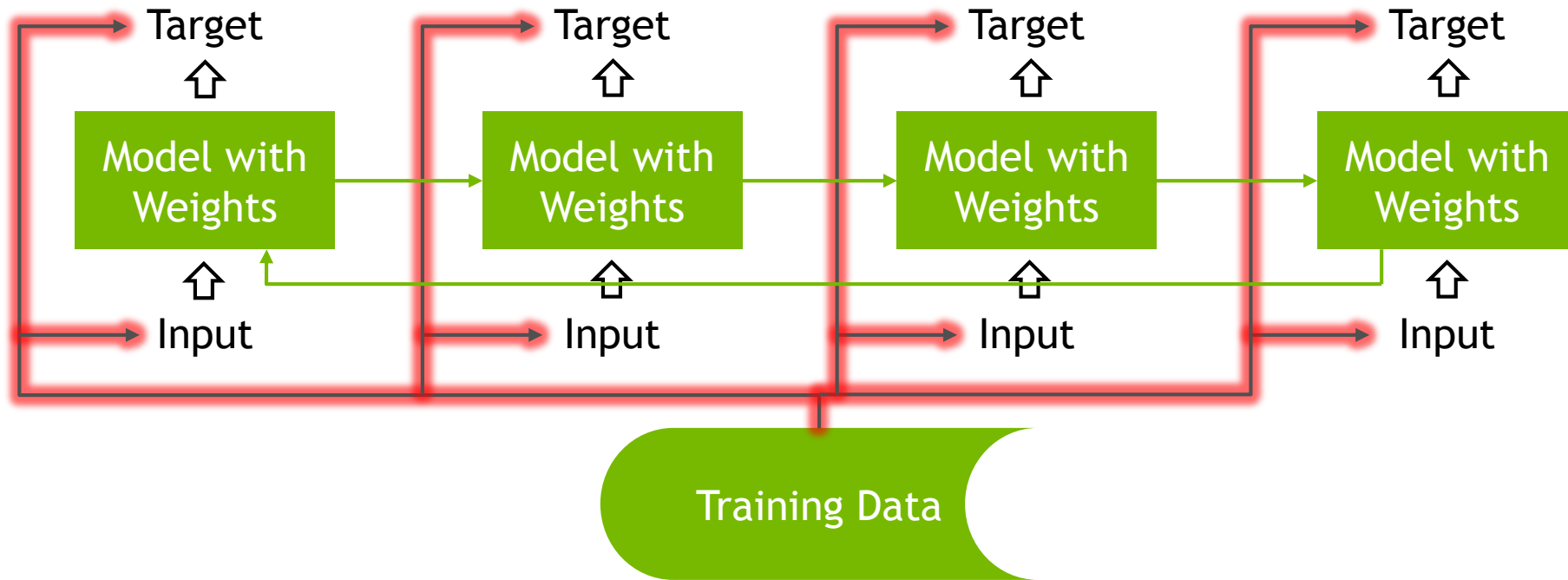
### ▶ Data Parallelism

- ▶ Allows to speed up training
- ▶ All workers train on different data
- ▶ All workers have the same copy of the model
- ▶ Neural network gradients (weight changes) are exchanged

### ▶ Model Parallelism

- ▶ Allows for a bigger model
- ▶ All workers train on the same data
- ▶ Parts of the model are distributed across GPUs
- ▶ Neural network activations are exchanged

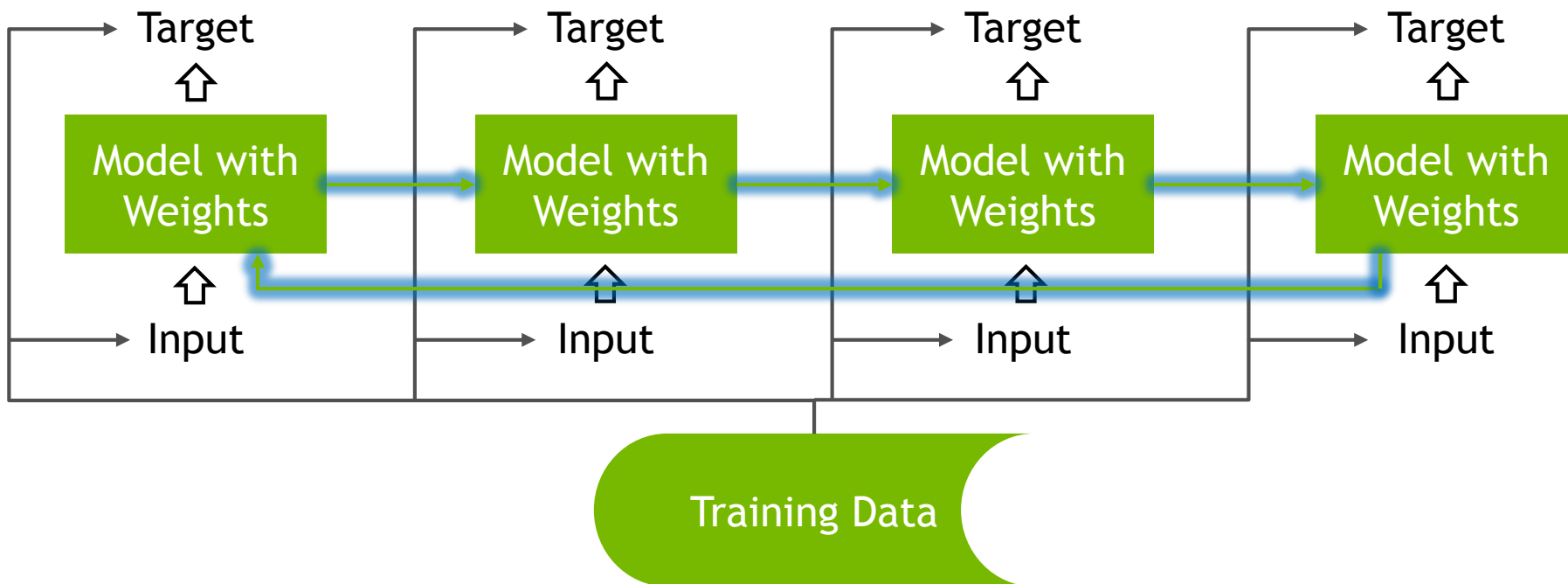
# MULTI GPU DATA PARALLEL DL TRAINING (SYNC SGD)



First load training data (different to each GPU)



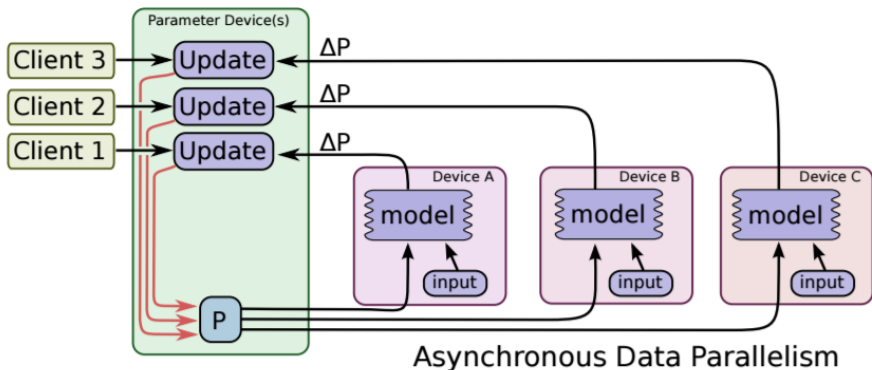
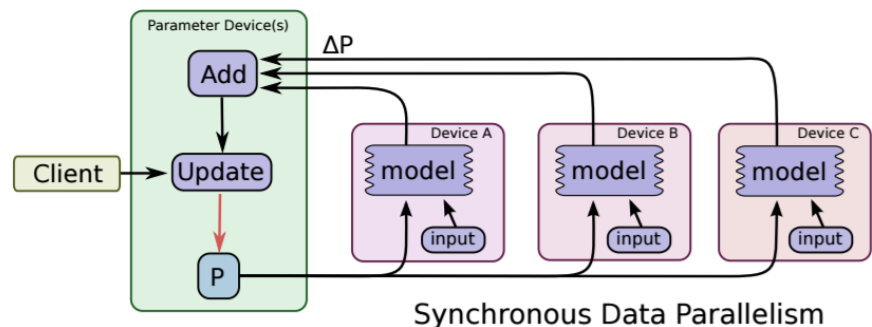
# MULTI GPU DATA PARALLEL DL TRAINING



Secondly, synchronize weights between the GPUs

# TF DEFAULT IMPLEMENTATION

## Parameter server



- ▶ Substantial limitations of the parameter server approach:
  - ▶ Server becomes a bottleneck
  - ▶ Generates substantially more communication than the all reduce based approach
- ▶ Makes sense when asynchronous SGD is being used (as all reduce assumes existence of a synchronisation point)

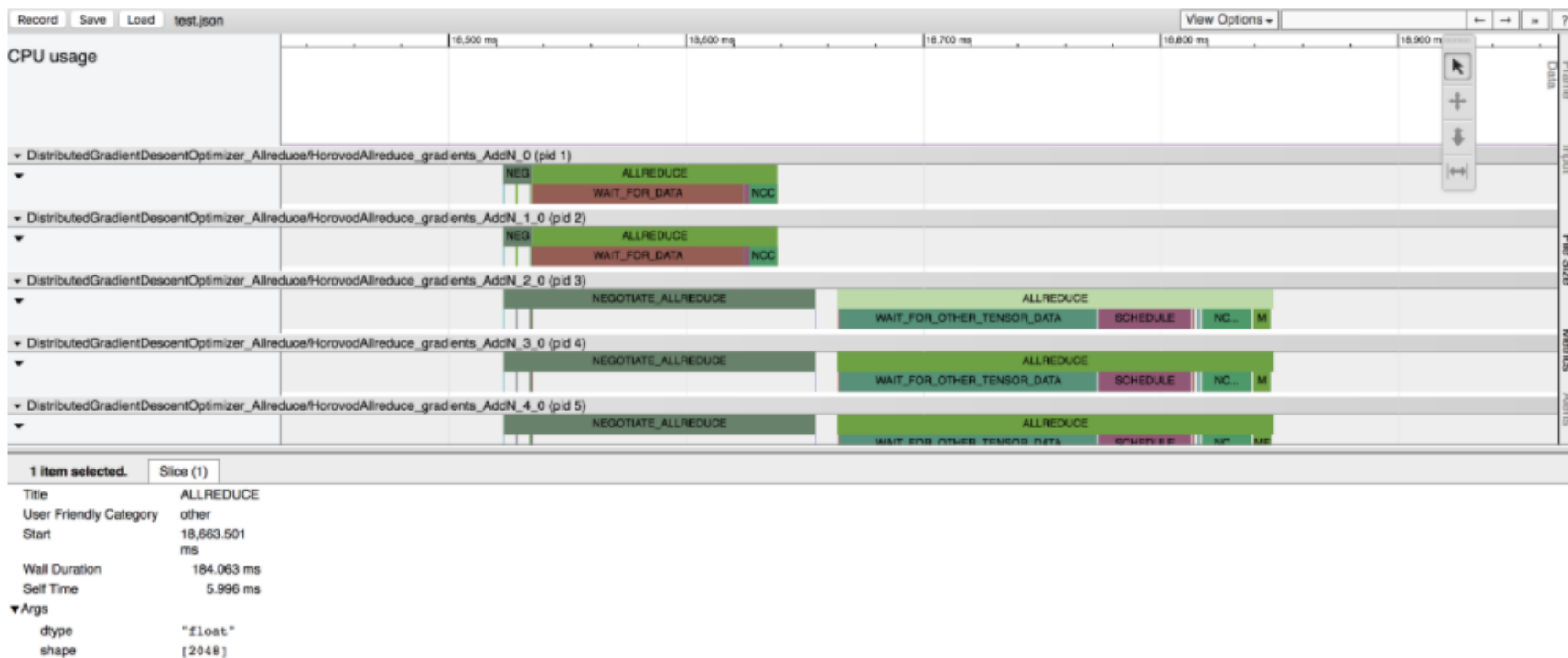
# HOROVOD

“Making distributed Deep Learning fast and easy to use”

- Leverages TensorFlow + MPI + NCCL 2 to simplify development of synchronous multigpu/multinode TensorFlow
- Instead of Parameter Server architecture leverages MPI and NCCL based all reduce
- Owing to NCCL it leverages features such as:
  - NVLINK
  - RDMA
  - GPUDirectRDMA
  - Automatically detects communication topology
  - Can fall back to PCIe and TCP/IP communication

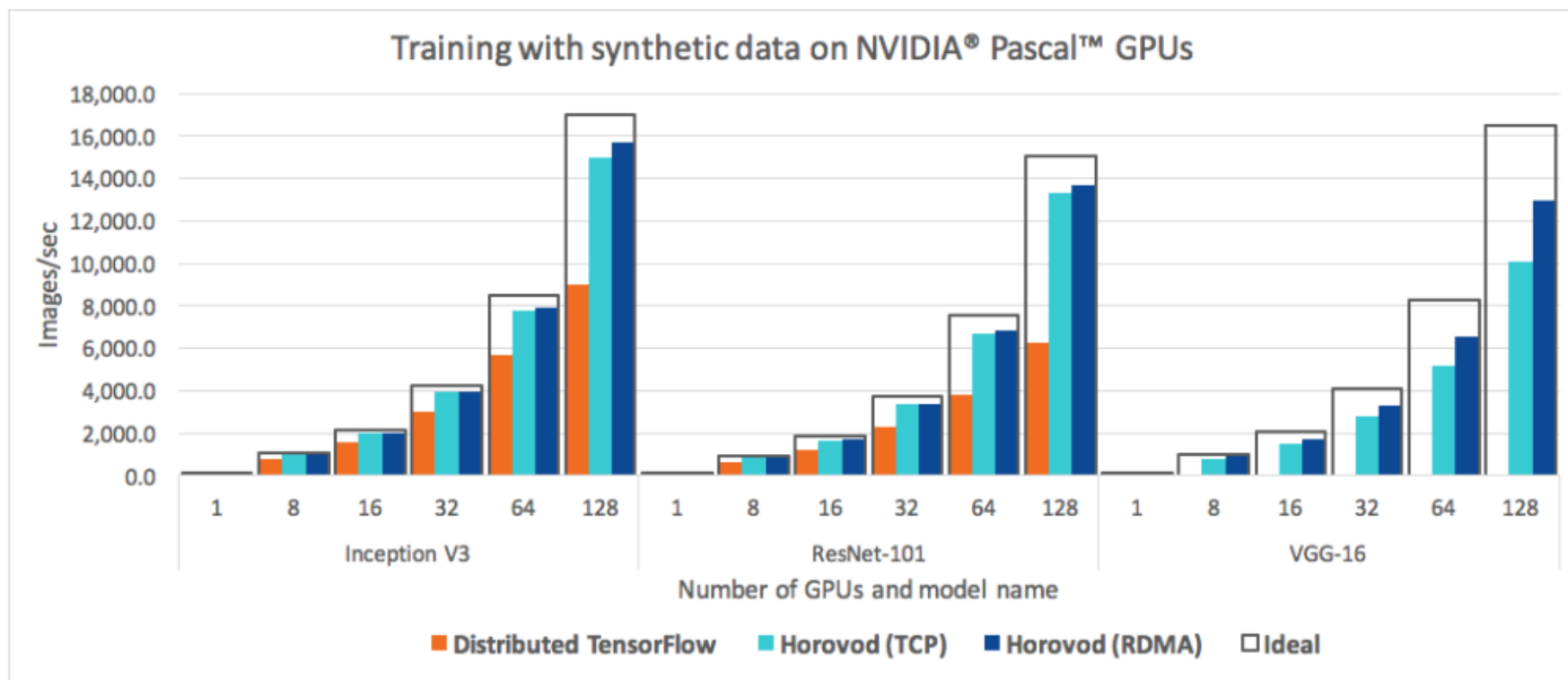
# HOROVOD TIMELINE

Powerful tool to help you understand the performance of your code

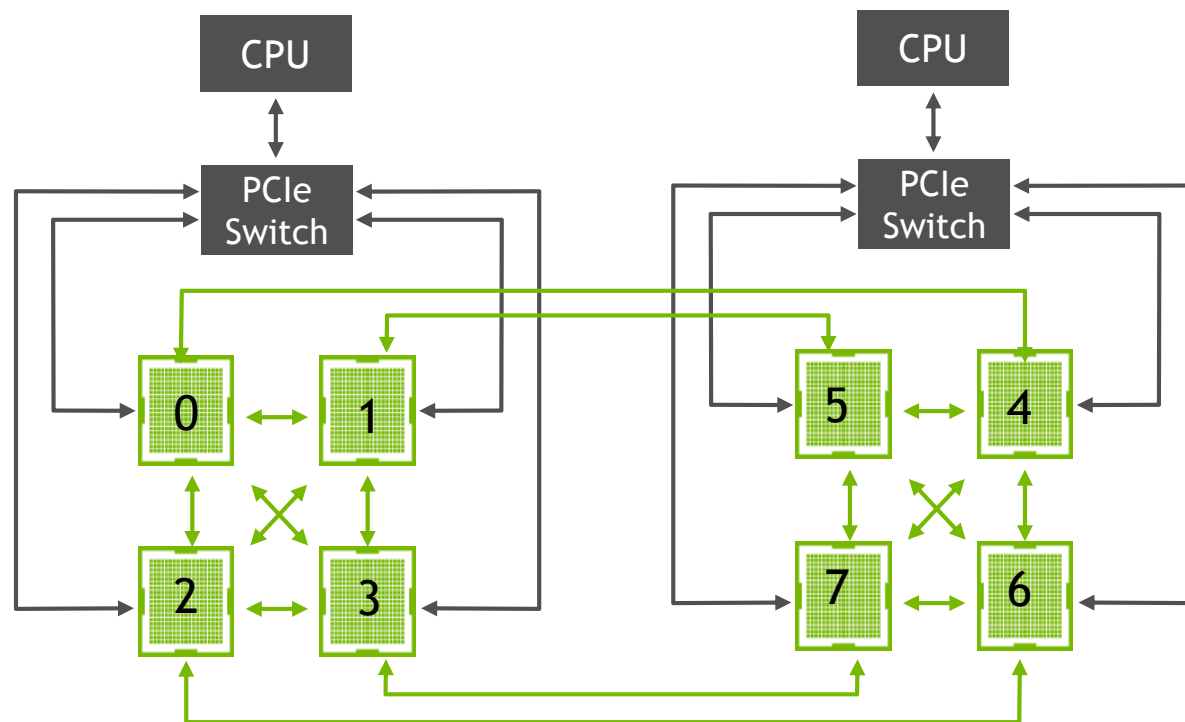


# HOROVOD

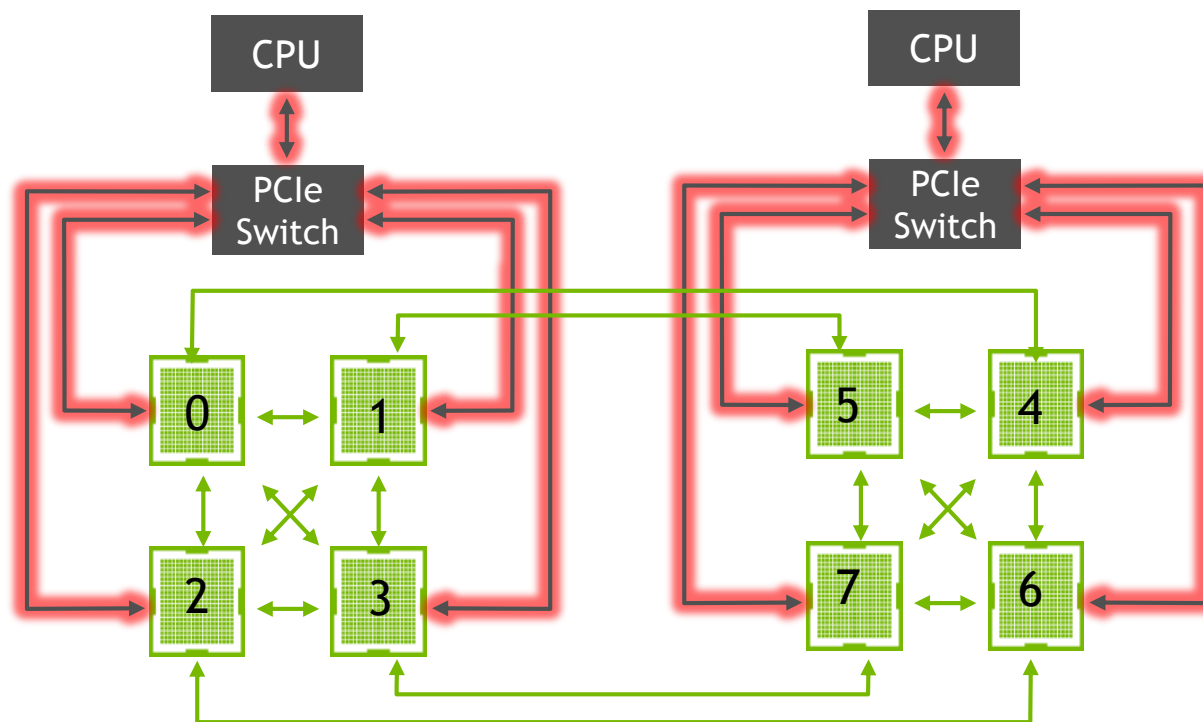
## Implications



# DL DATA PARALLELISM - NVLINK

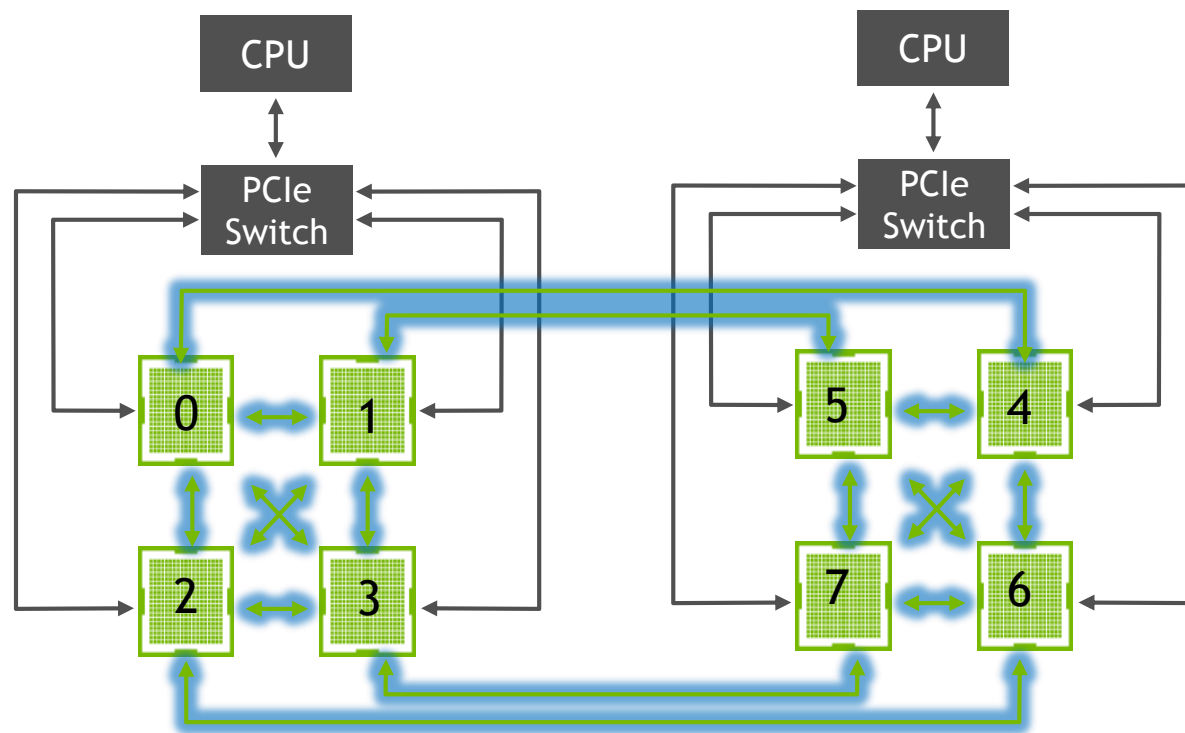


# DL DATA PARALLELISM - NVLINK



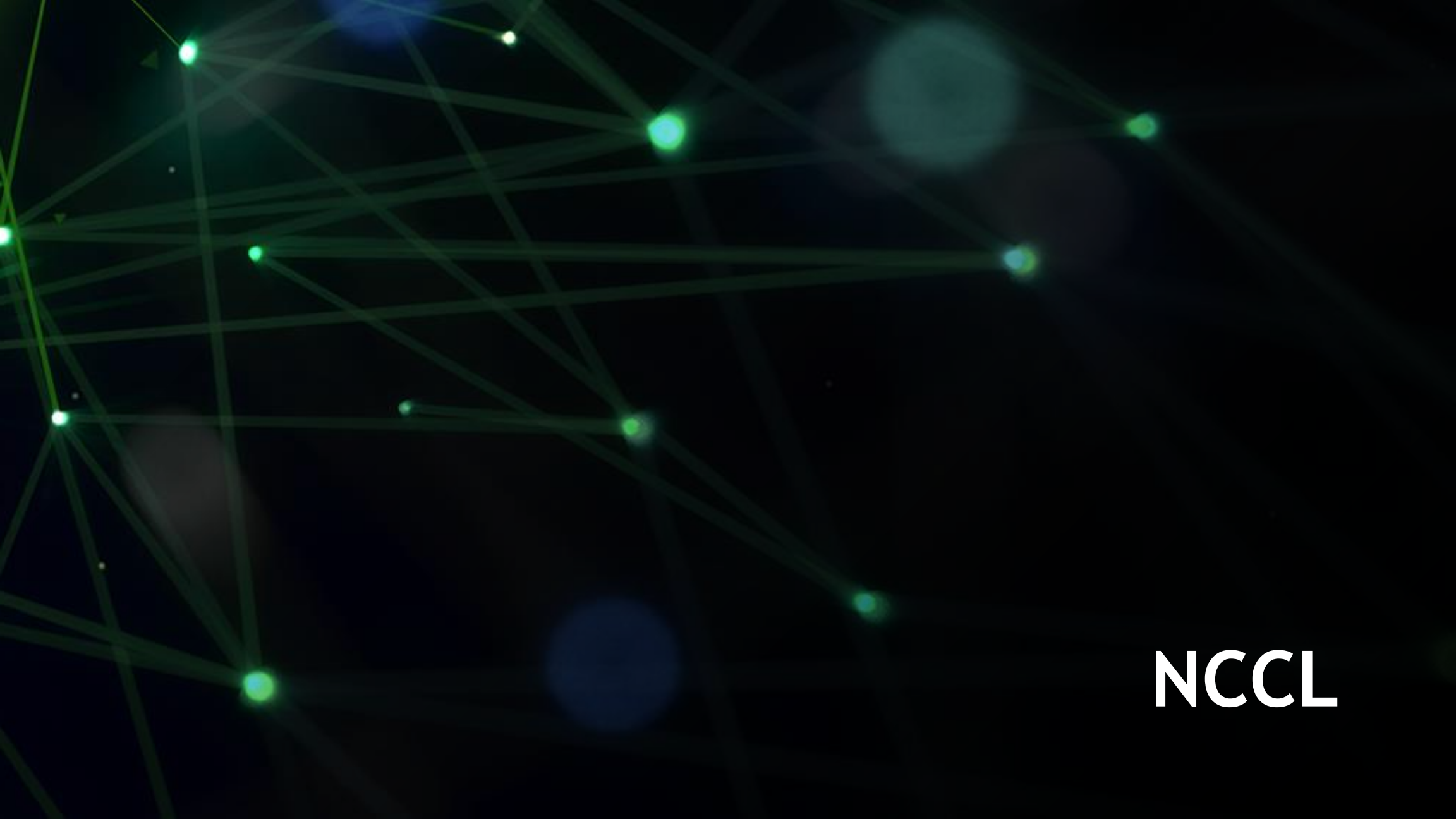
Data loading over PCIe

# DL DATA PARALLELISM - NVLINK



Gradient averaging over NVLink





**NCCL**

# NVIDIA Collective Communications Library (NCCL) 2

Multi-GPU and multi-node collective communication primitives

High-performance multi-GPU and multi-node collective communication primitives optimized for NVIDIA GPUs

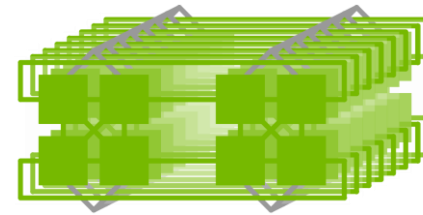
Fast routines for multi-GPU multi-node acceleration that maximizes inter-GPU bandwidth utilization

Easy to integrate and MPI compatible. Uses automatic topology detection to scale HPC and deep learning applications over PCIe and NVlink

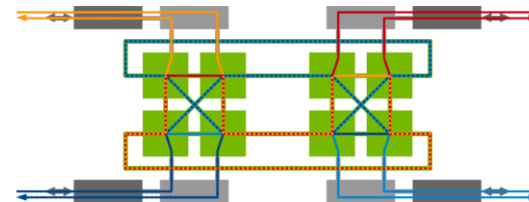
Accelerates leading deep learning frameworks such as Caffe2, Microsoft Cognitive Toolkit, MXNet, PyTorch and more



Multi-GPU:  
NVLink  
PCIe



Multi-Node:  
InfiniBand verbs  
IP Sockets

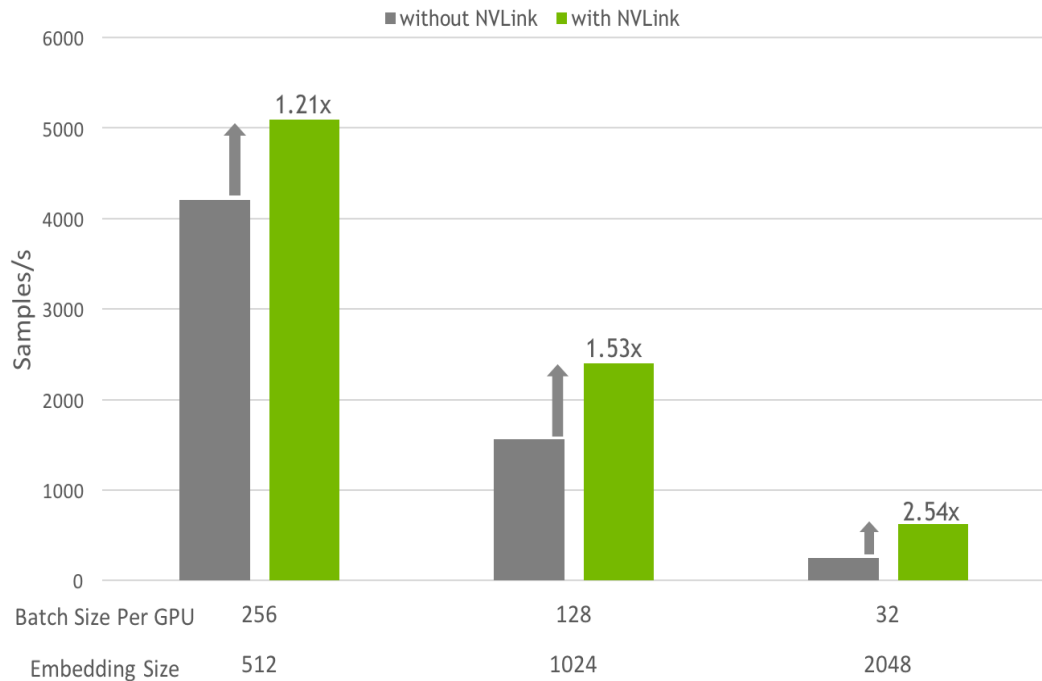


Automatic  
Topology  
Detection

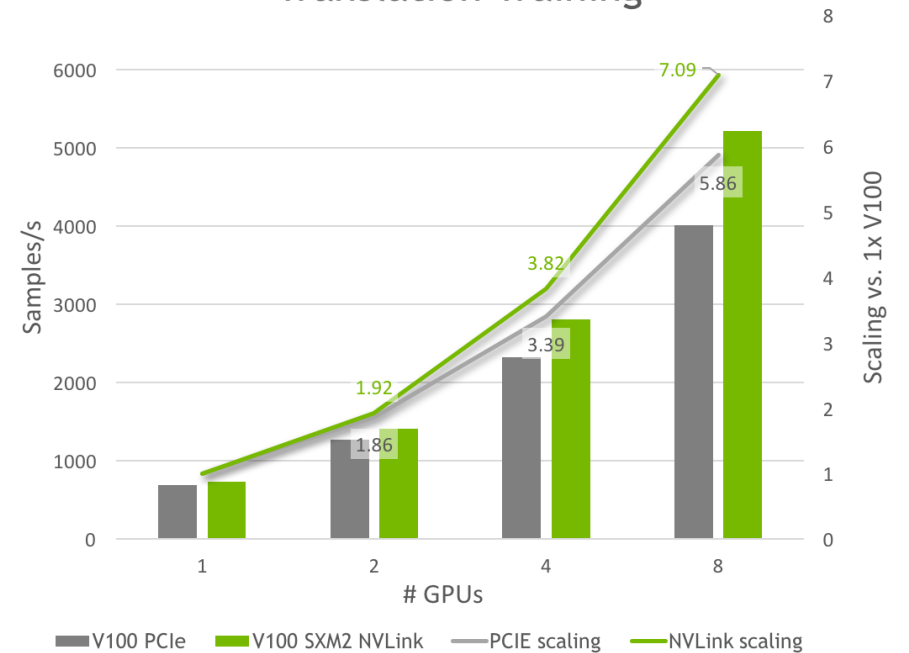
# IMPLICATIONS

Requirements highly dependent on the workload

### DGX-1 MXNet Neural Machine Translation Training



### DGX-1 MXNet Neural Machine Translation Training





**VOLTA AND TURING  
TENSOR CORE**

# TESLA V100

21B transistors  
815 mm<sup>2</sup>

80 SM  
5120 CUDA Cores  
640 Tensor Cores

16/32 GB HBM2  
900 GB/s HBM2  
300 GB/s NVLink



\*full GV100 chip contains 84 SMs

# VOLTA GV100 SM

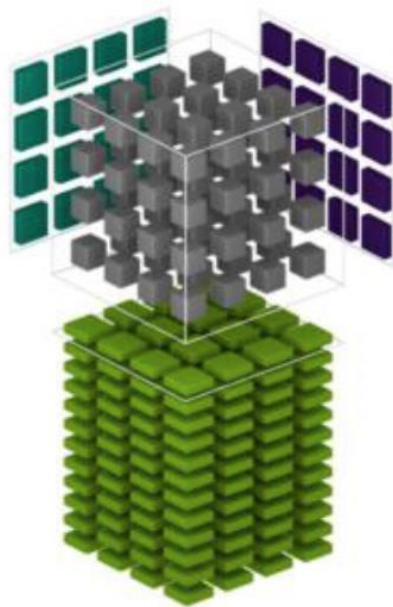
## Redesigned for Productivity

Completely new ISA  
 Twice the schedulers  
 Simplified Issue Logic  
 Large, fast L1 cache  
 Improved SIMT model  
 Tensor acceleration

	GP100	GV100
FP32 units	64	64
FP64 units	32	32
INT32 units	NA	64
Tensor Cores	NA	8
Register File	256 KB	256 KB
Unified L1/Shared memory	L1: 24KB Shared: 64KB	128 KB
Active Threads	2048	2048



# TURING TENSOR CORE



	FP16	Int8	Int4	Binary
<b>T4</b>	8x CUDA core 40-70 TFLOPs	16x CUDA core 80-140 TOPs	32x CUDA core 160-280 TOPs	128x CUDA core 640-1100 TOPs

SW at Launch

TensorRT, Libraries

CUTLASS Open Source Tensor Library, CUDA

# TENSOR CORE

## Mixed Precision Matrix Math - 4x4 matrices

New CUDA TensorOp instructions & data formats

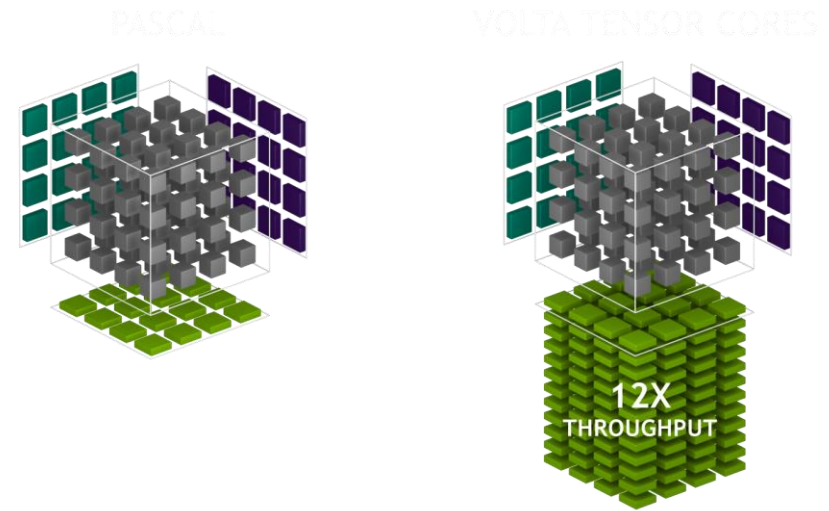
125 Tensor TFLOP/s mixed-precision

4x4x4 matrix processing array

$$D[\text{FP32}] = A[\text{FP16}] * B[\text{FP16}] + C[\text{FP32}]$$

Using Tensor cores via

- Volta optimized frameworks and libraries (cuDNN, CuBLAS, TensorRT, ..)
- CUDA C++ Warp Level Matrix Operations



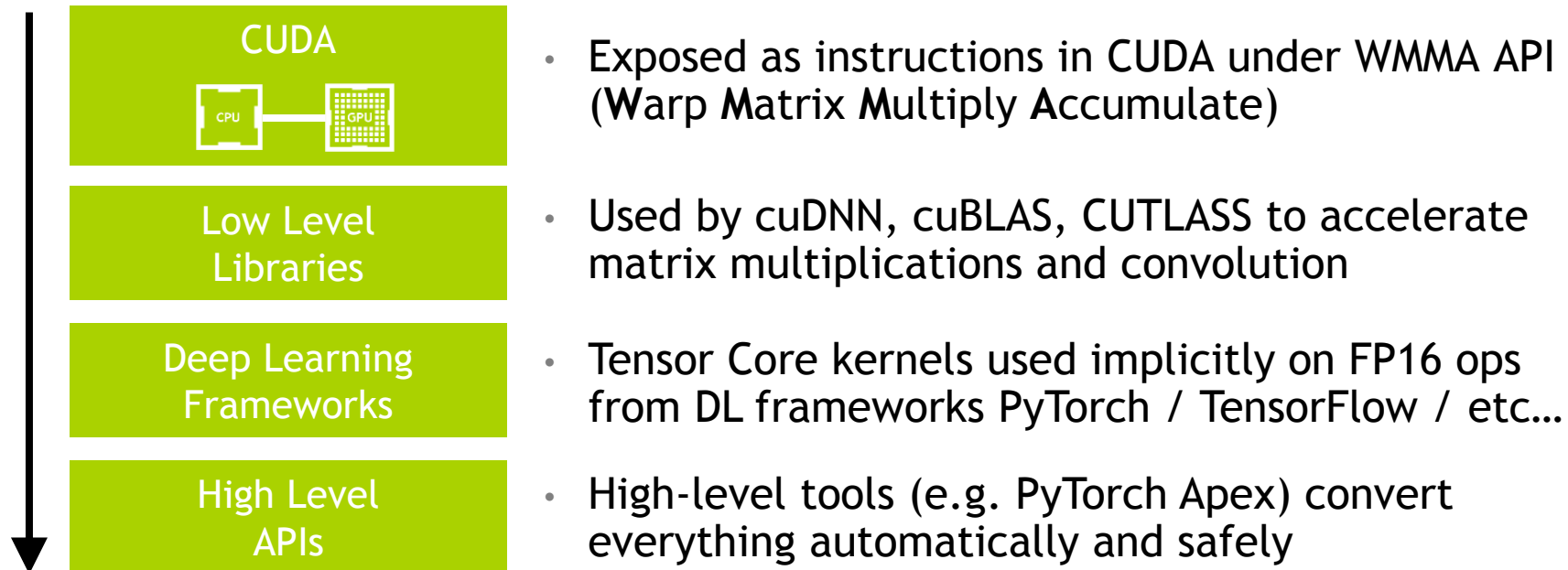
$$D = \begin{pmatrix} A_{0,0} & A_{0,1} & A_{0,2} & A_{0,3} \\ A_{1,0} & A_{1,1} & A_{1,2} & A_{1,3} \\ A_{2,0} & A_{2,1} & A_{2,2} & A_{2,3} \\ A_{3,0} & A_{3,1} & A_{3,2} & A_{3,3} \end{pmatrix} \begin{pmatrix} B_{0,0} & B_{0,1} & B_{0,2} & B_{0,3} \\ B_{1,0} & B_{1,1} & B_{1,2} & B_{1,3} \\ B_{2,0}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

FP16 or FP32                      FP16                      FP16                      FP16 or FP32

■ Activation Inputs   ■ Weights Inputs   ■ Output Results



# HOW TO USE TENSOR CORES



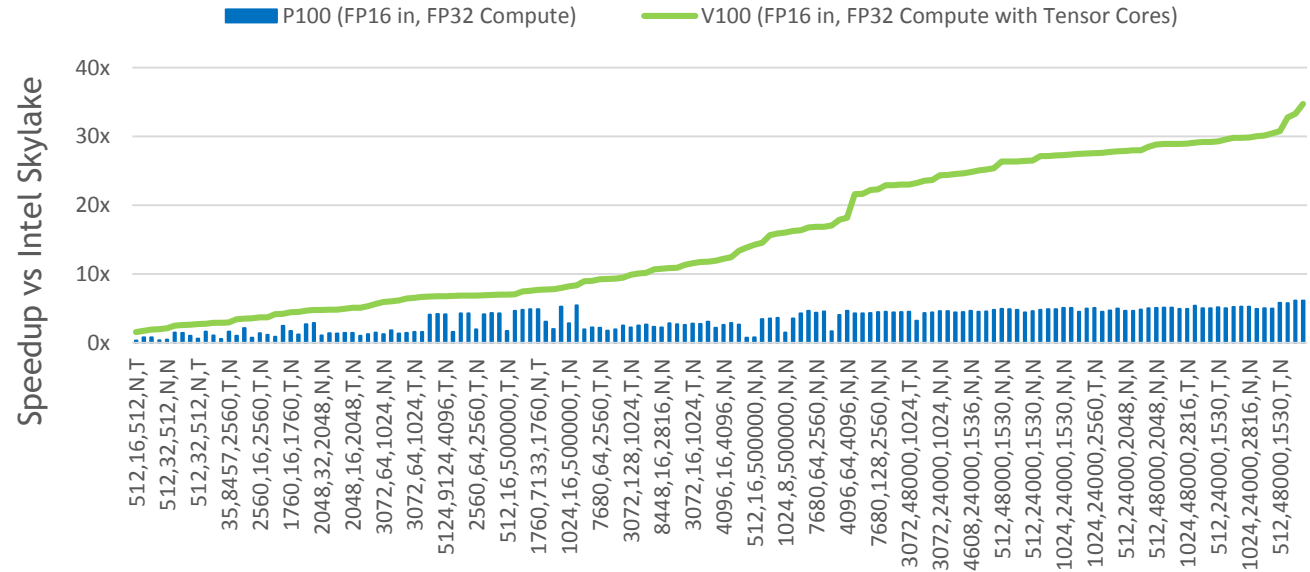
# cuBLAS 10.0

## Optimized GEMM Performance for Deep Learning

- ▶ Turing optimized GEMMs & GEMM extensions for Tensor Cores
- ▶ GEMM Performance Tuned for sizes used in various DL models
- ▶ API and Error Logging for debug and traceability

<https://developer.nvidia.com/cublas>

### Up to 90TF of Deepbench GEMM Performance



Deepbench training performance runs with Tesla P100, Tesla V100 and Intel Skylake 6140 Gold 2.3 GHz with hyperthreading off



# NVIDIA cuDNN 7

## Deep Learning Primitives

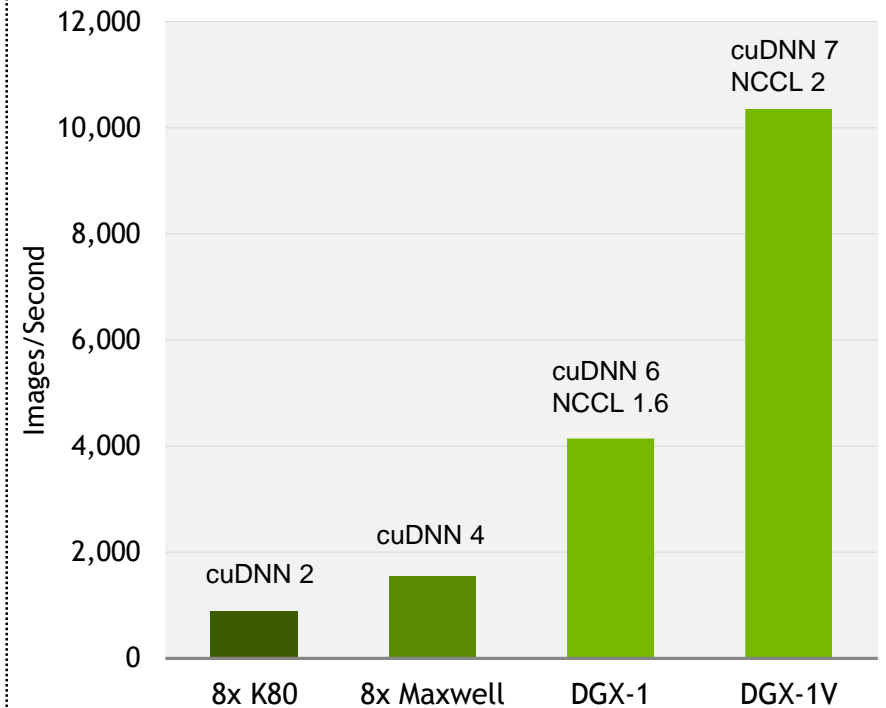
High performance building blocks for deep learning frameworks

Drop-in acceleration for widely used deep learning frameworks such as Caffe2, Microsoft Cognitive Toolkit, PyTorch, Tensorflow, Theano and others

Accelerates industry vetted deep learning algorithms, such as convolutions, LSTM RNNs, fully connected, and pooling layers

Fast deep learning training performance tuned for NVIDIA GPUs

## Deep Learning Training Performance



“ NVIDIA has improved the speed of cuDNN with each release while extending the interface to more operations and devices at the same time.”

— Evan Shelhamer, Lead Caffe Developer, UC Berkeley

# CUDNN EXAMPLE

```
// Set the compute data type (below as CUDNN_DATA_FLOAT):
checkCudnnErr( cudaSetConvolutionNdDescriptor(cudnnConvDesc,
                                                convDim,
                                                padA,
                                                convstrideA,
                                                dilationA,
                                                CUDNN_CONVOLUTION,
                                                CUDNN_DATA_FLOAT) );

// Set the math type to allow cuDNN to use Tensor Cores:
checkCudnnErr( cudaSetConvolutionMathType(cudnnConvDesc,
CUDNN_TENSOR_OP_MATH) );

// Choose a supported algorithm:
cudaConvolutionFwdAlgo_t algo =
CUDNN_CONVOLUTION_FWD_ALGO_IMPLICIT_PRECOMP_GEMM;
```

The background features a complex network of thin, light green lines connecting various nodes. The nodes are represented by small, glowing green circles of varying sizes and brightness. The overall aesthetic is technical and futuristic, set against a dark, almost black background.

# CUDA AND CUTLASS

# USING TENSOR CORES



NVIDIA cuDNN, cuBLAS, TensorRT

Volta Optimized  
Frameworks and Libraries

```
__device__ void tensor_op_16_16_16(  
    float *d, half *a, half *b, float *c)  
{  
    wmma::fragment<matrix_a, ...> Amat;  
    wmma::fragment<matrix_b, ...> Bmat;  
    wmma::fragment<matrix_c, ...> Cmat;  
  
    wmma::load_matrix_sync(Amat, a, 16);  
    wmma::load_matrix_sync(Bmat, b, 16);  
    wmma::fill_fragment(Cmat, 0.0f);  
  
    wmma::mma_sync(Cmat, Amat, Bmat, Cmat);  
  
    wmma::store_matrix_sync(d, Cmat, 16,  
        wmma::row_major);  
}
```

CUDA C++

Warp-Level Matrix Operations

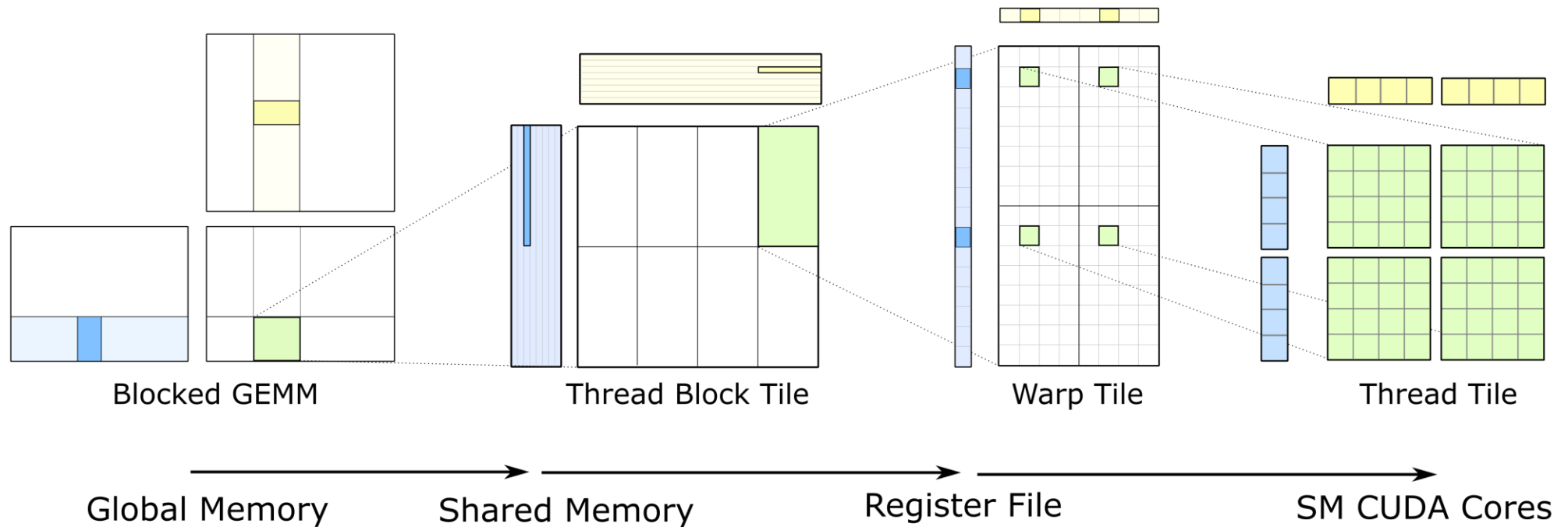
# DESIGN OBJECTIVES

Span the Design Space with Generic Programming

CUDA C++ templates for composable algorithms

Performance: Implement efficient dense linear algebra kernels

Structured, reusable components: flexibility and productivity



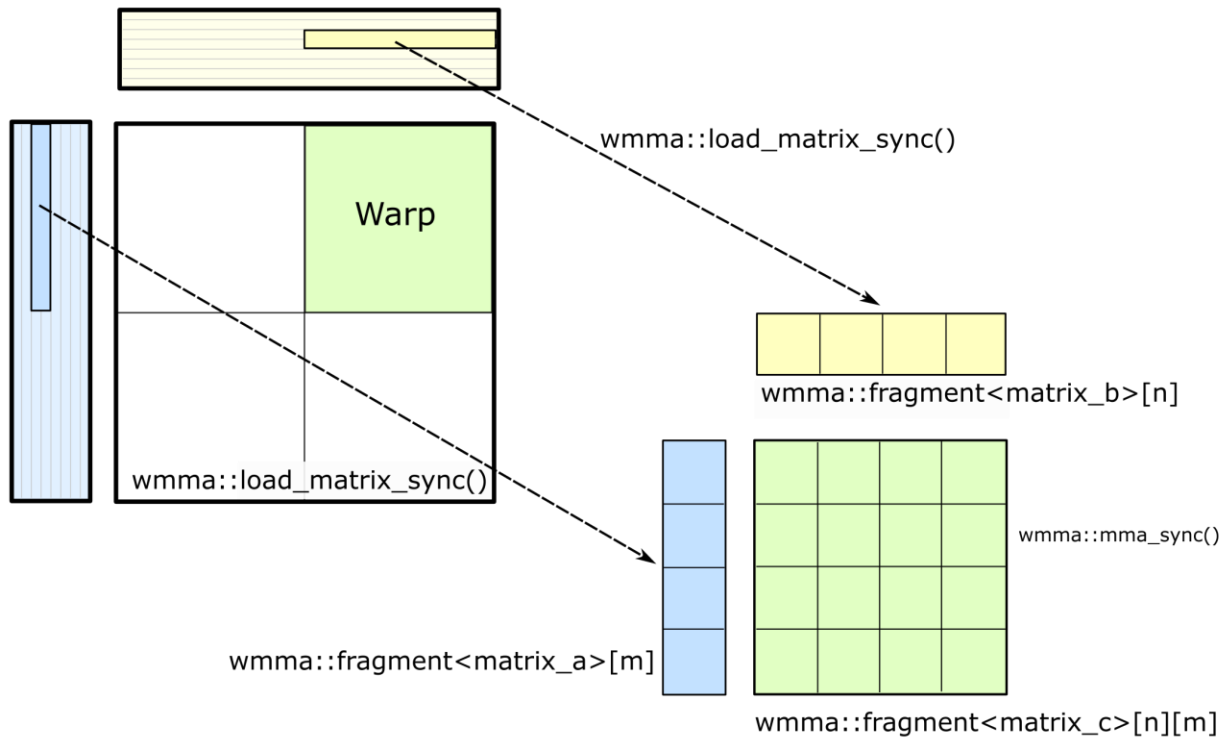


# EXAMPLE: VOLTA TENSOR CORES

## Targeting the CUDA WMMA API

### WMMA: Warp-synchronous Matrix Multiply-Accumulate

- API for issuing operations to Volta Tensor Cores



```
/// Perform warp-level multiply-accumulate using WMMA API
template <
  /// Data type of accumulator
  typename ScalarC,

  /// Shape of warp-level accumulator tile
  typename WarpTile,

  /// Shape of one WMMA operation - e.g. 16x16x16
  typename WmmaTile
>
struct WmmaMultiplyAdd {

  /// Compute number of WMMA operations
  typedef typename ShapeDiv<WarpTile, WmmaTile>::Shape
    Shape;

  /// Multiply: D = A*B + C
  inline __device__ void multiply_add(
    FragmentA const & A,
    FragmentB const & B,
    FragmentC const & C,
    FragmentD & D) {

    // Perform M-by-N-by-K matrix product using WMMA
    for (int n = 0; n < Shape::kH; ++n) {
      for (int m = 0; m < Shape::kW; ++m) {

        // WMMA API to invoke Tensor Cores
        nvcuda::wmma::mma_sync(
          D.elements[n][m],
          A.elements[k][m],
          B.elements[k][n],
          C.elements[n][m]
        );
      }
    }
  }
};
```

# CUTLASS 1.3

## GEMM kernels targeting Volta Tensor Cores natively with `mma.sync`

Template abstractions for high-performance matrix-multiplication

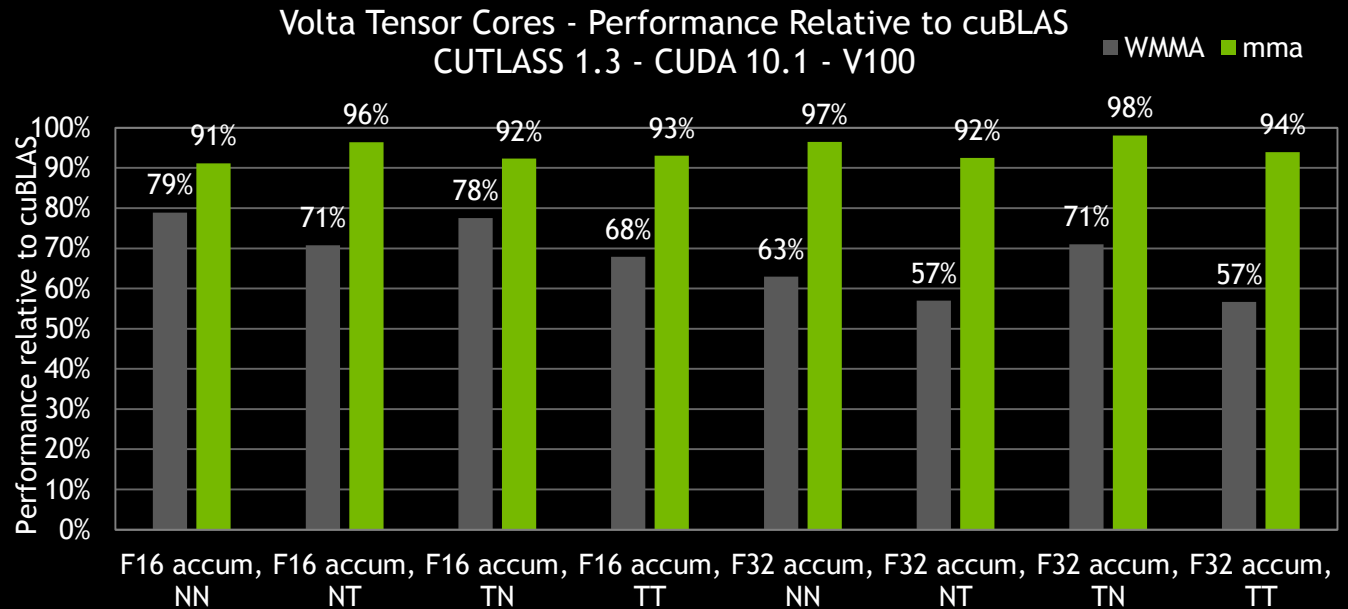
Header-only open source library

Thread-wide, warp-wide, block-wide, and device-wide primitives

Specialized data-movement and multiply-accumulate abstractions

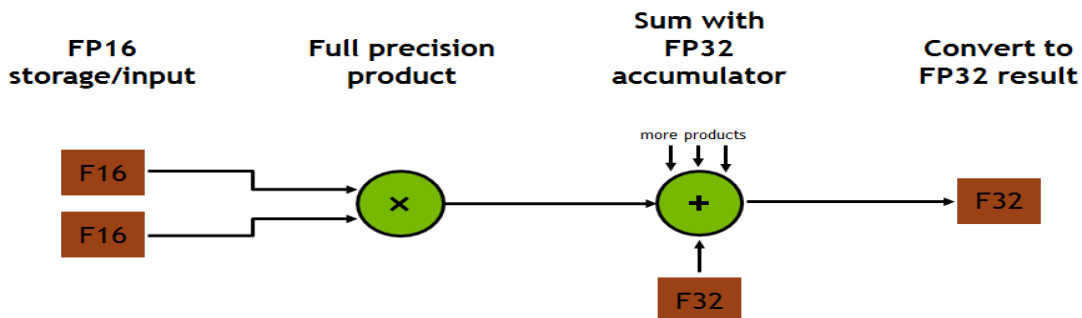
New in CUDA 10.1 & CUTLASS 1.3: `mma.sync`

- PTX assembly instruction enables maximum efficiency of Volta Tensor Cores operation



# TENSOR CORES FOR AI

- Simple trick for **2x to 5x faster deep learning training**
  - Accomplished in **few lines of code**
  - Models can use **same hyperparameters**
  - Models converge to **same accuracy**
- Half the memory traffic and storage **enabling larger batch sizes**
- AI community is trending towards **low precision as common practice**



# MIXED PRECISION TRAINING

- ▶ **Make an FP16 copy of the weights**
- ▶ Forward propagate using FP16 weights and activations
- ▶ **Multiply the resulting loss by the scale factor  $S$**
- ▶ Backward propagate using FP16 weights, activations, and their gradients
- ▶ **Multiply the weight gradients by  $1/S$**
- ▶ Optionally process the weight gradients (gradient clipping, weight decay, etc.)
- ▶ Update the master copy of weights in FP32

# 1. MODEL CONVERSION

- Make simple type updates to each layer:
  - Use FP16 values for the weights and inputs

```
# PyTorch
```

```
layer = torch.nn.Linear(in_dim, out_dim).half()
```

```
# TensorFlow
```

```
layer = tf.layers.dense(tf.cast(inputs, tf.float16), out_dim)
```

## 2. MASTER WEIGHTS

- FP16 alone is sufficient for some networks but not others; keep FP32 copy of weights

```
param = torch.cuda.FloatTensor([1.0])  
print(param + 0.0001)
```



1.0001

```
param = torch.cuda.HalfTensor([1.0])  
print(param + 0.0001)
```

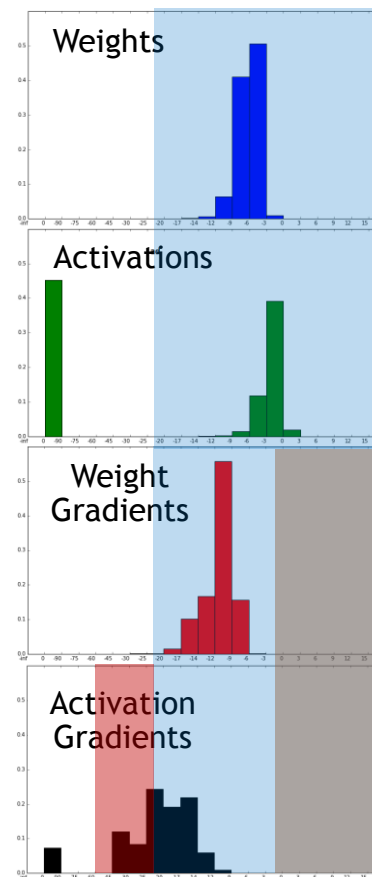


1

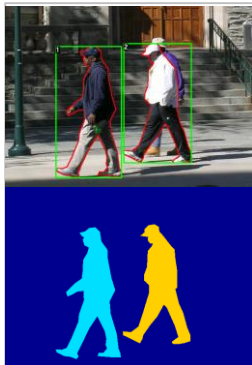
*When  $update/param < 2^{-11}$ , updates have no effect.*

# 3. LOSS SCALING

- Range representable in FP16: ~40 powers of 2
- Gradients are small:
  - Some lost to zero
  - While ~15 powers of 2 remain unused
- Loss scaling:
  - Multiply loss by a constant  $S$
  - All gradients scaled up by  $S$  (chain rule)
  - Unscale weight gradient (in FP32) before weight update



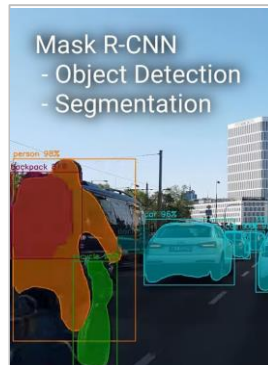
# AUTOMATIC MIXED PRECISION ADOPTION IN **PYTORCH** COMMUNITY



## TORCHVISION

Popular datasets, model architectures, common image transformations for computer vision

Facebook  
PyTorch



Mask R-CNN  
- Object Detection  
- Segmentation

## MASK R-CNN

Fast, modular reference implementation of Instance Segmentation and Object Detection

Facebook Research  
PyTorch



## PYTEXT

A natural language modeling framework

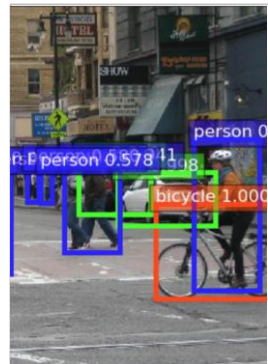
Facebook Research  
PyTorch



## PIX2PIXHD

Synthesizing and manipulating 2048x1024 images with conditional GANs

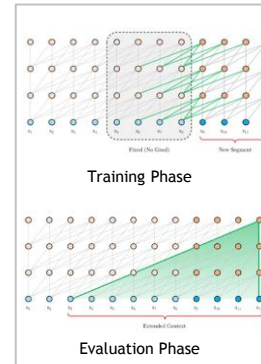
NVIDIA  
PyTorch



## GLUON-CV

Deep learning toolkit for computer vision

DMLC  
MXNet



## TRANSFORMER-XL

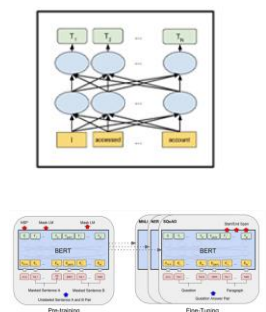
Attentive language models beyond a fixed-length context

CMU & Google  
PyTorch

[Link to NVIDIA Developer Page](#)  
[Link to Github NVIDIA DL Examples](#)

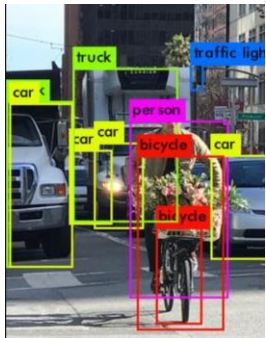


# AUTOMATIC MIXED PRECISION ADOPTION IN **TENSORFLOW** COMMUNITY



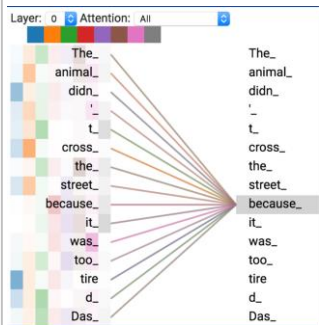
**BERT [TF2.0]**  
Unsupervised, deep-bidirectional encoders to deliver SOTA performance on many NLP tasks  
NVIDIA  
TensorFlow

The diagram shows a neural network with input tokens  $x_1, x_2, x_3$  and output tokens  $y_1, y_2, y_3$ . Below it, a flowchart illustrates the process: Pre-training (BERT) followed by Fine-Tuning (BERT) for various tasks like Text Classification, Question Answering, and Natural Language Inference.



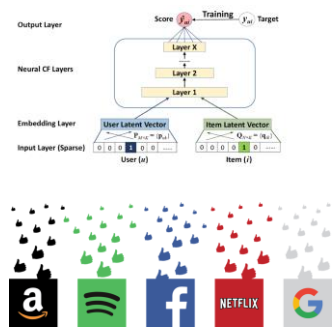
**Resnet-50 [TF2.0]**  
Image classification model based on residual blocks  
NVIDIA  
TensorFlow

The image shows a street scene with bounding boxes and labels for various objects: truck, traffic light, car, person, and bicycle.



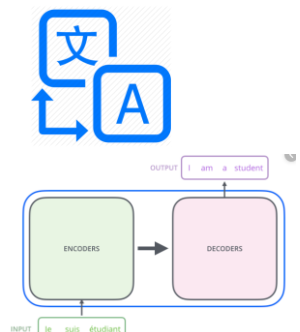
**Tensor2Tensor**  
Library of deep learning models & datasets maintained by Google Brain team  
NVIDIA  
TensorFlow

The visualization shows attention weights for the word 'because' in a sentence, highlighting its connections to other words in the context.




**NCF [TF2.0]**  
Neural Network based recommendation engine  
NVIDIA  
TensorFlow

The diagram shows a neural network architecture for recommendation. It includes an Input Layer (Users and Items), an Embedding Layer (User Latent Vector and Item Latent Vector), and Neural CF Layers (Layer 1, Layer 2, Layer X). The output is a Score  $f_{ui}$  compared against a Target. Logos for Amazon, Spotify, Facebook, Netflix, and Google are shown at the bottom.



**Transformer [TF2.0]**  
Image classification model based on residual blocks  
NVIDIA  
TensorFlow

The diagram illustrates the Transformer architecture with an encoder (INPUT: 'je suis étudiant') and a decoder (OUTPUT: 'I am a student').



**Sonnet**  
Library on top of TF designed to provide simple, composable abstractions for ML research.  
NVIDIA  
TensorFlow

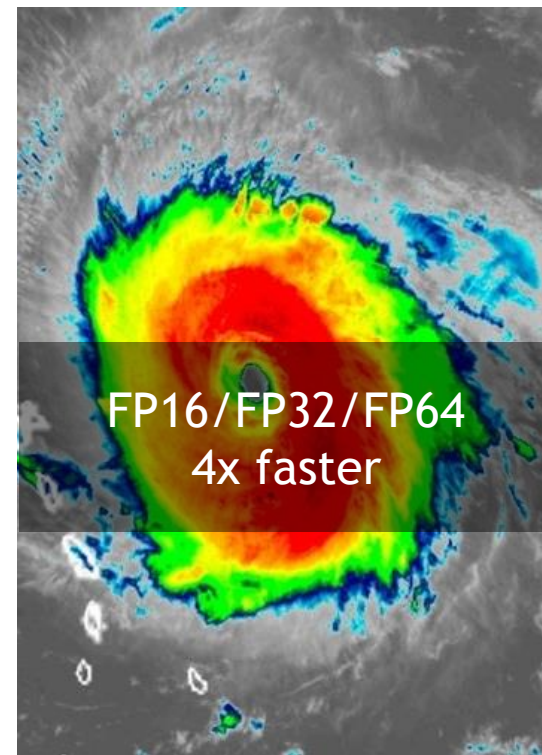
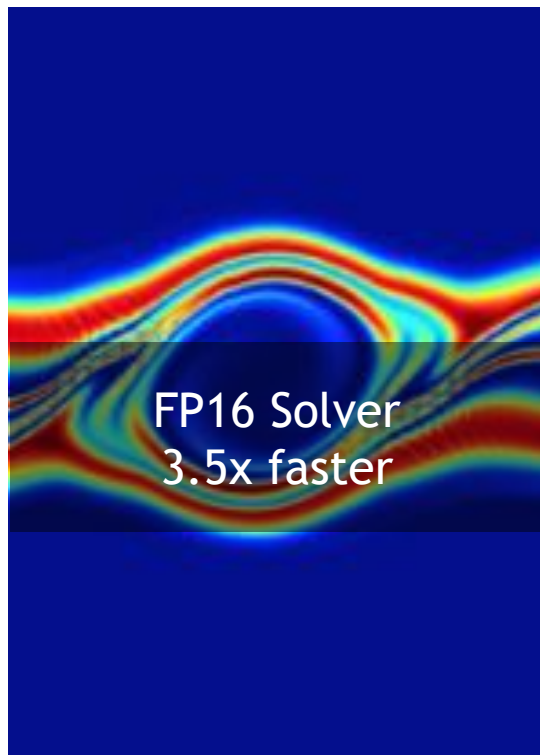
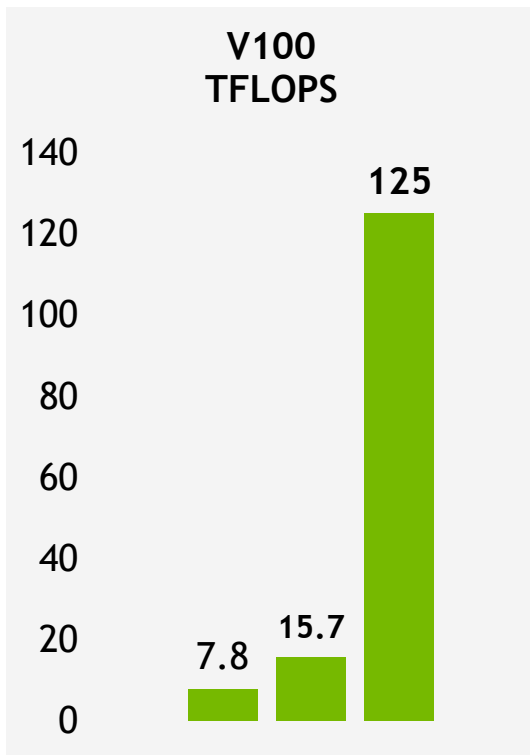
The Sonnet logo is a blue 3D cube-like shape.

# TENSOR CORES FOR HPC

- Mixed precision algorithms are **increasingly popular**
  - It is common to combine **double + single precision**, or **floating point + integer**
- Similar to AI:
  - Use low precision to **reduce memory traffic and storage**
  - Use Tensor Core instructions for **large speedups**

# TENSOR CORES FOR SCIENCE

## Mixed-Precision Computing



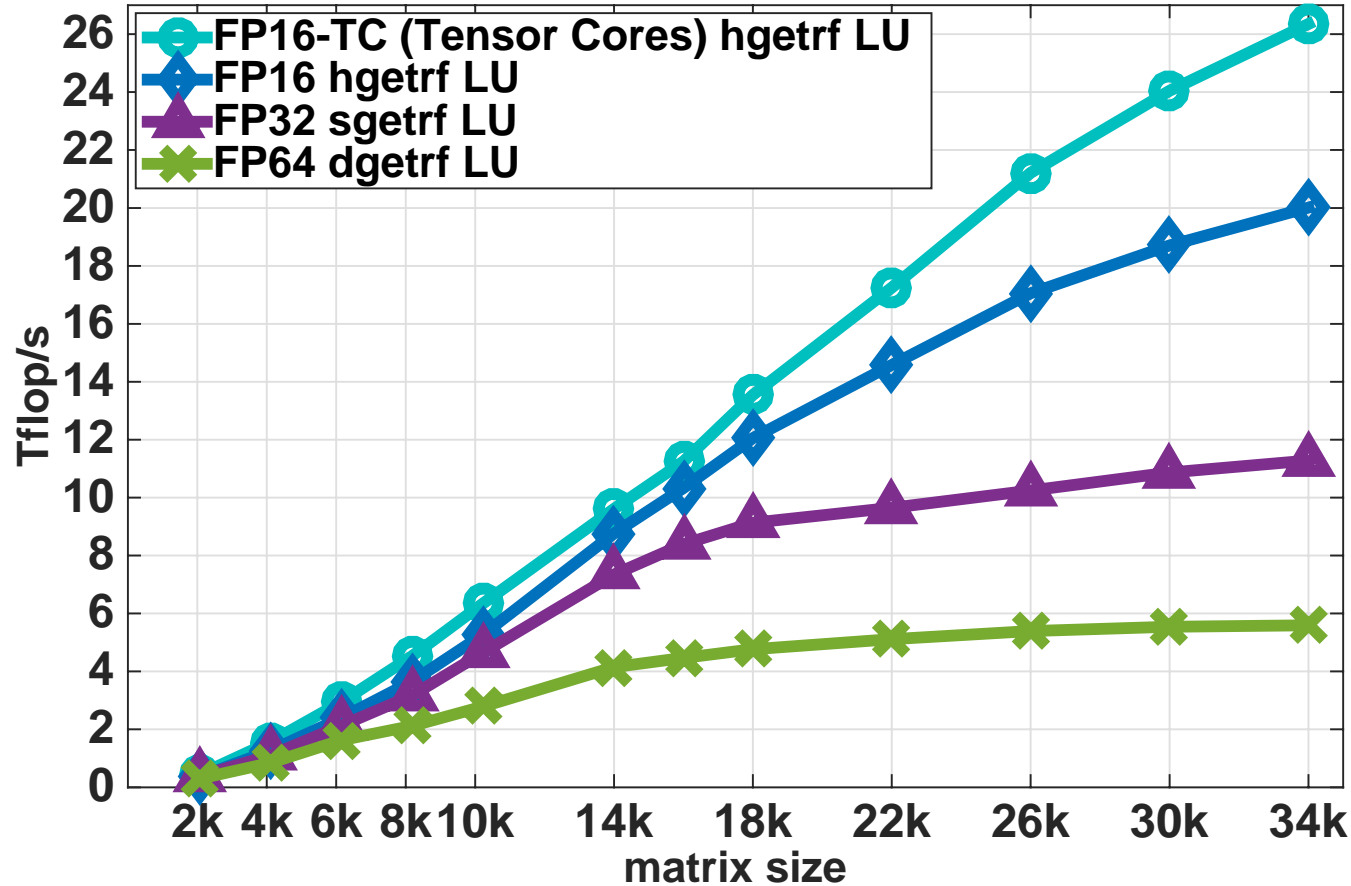
FP64+ MULTI-PRECISION

PLASMA FUSION  
APPLICATION

EARTHQUAKE SIMULATION

MIXED PRECISION WEATHER  
PREDICTION

# LINEAR ALGEBRA + TENSOR CORES



## Double Precision LU Decomposition

- Compute initial solution in FP16
- Iteratively refine to FP64

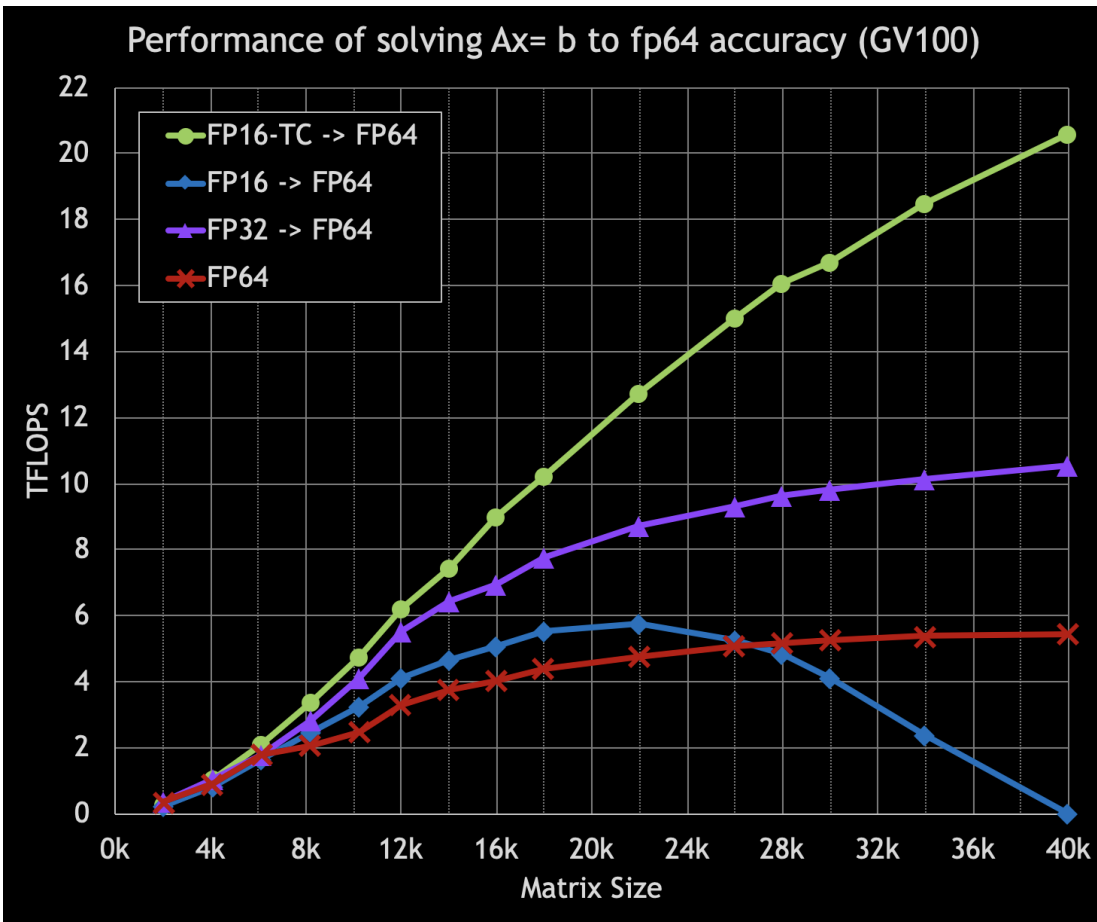
Achieved FP64 Tflops: **26**

Device FP64 Tflops: **7.8**

Data courtesy of: Azzam Haidar, Stan. Tomov & Jack Dongarra, Innovative Computing Laboratory, University of Tennessee  
"Investigating Half Precision Arithmetic to Accelerate Dense Linear System Solvers", A. Haidar, P. Wu, S. Tomov, J. Dongarra, SC'17  
GTC 2018 Poster P8237: *Harnessing GPU's Tensor Cores Fast FP16 Arithmetic to Speedup Mixed-Precision Iterative Refinement Solves*



# TENSOR CORE-ACCELERATED ITERATIVE REFINEMENT SOLVERS



## Productization Plans

LU Solver

- ~August 2019
- Real & Complex FP32 & FP64

Cholesky Solver

- ~October-November 2019
- Real & Complex FP32 & FP64

QR Solver

- ~October-November 2019
- Real & Complex FP 32 & FP64

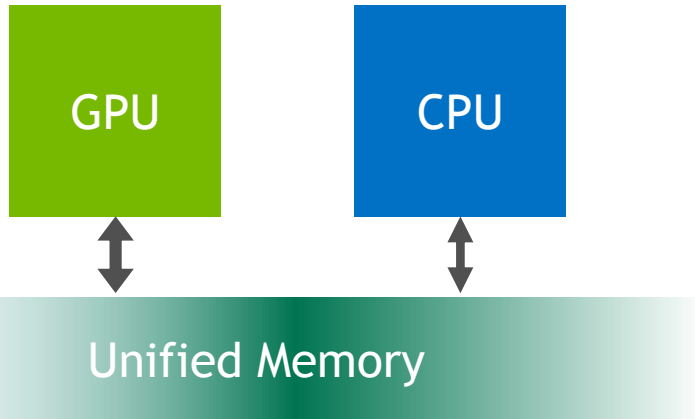


**UNIFIED VIRTUAL  
MEMORY**

# UNIFIED MEMORY

Large datasets, simple programming, High Performance

CUDA 8 and beyond



Allocate Beyond  
GPU Memory Size

Enable Large  
Data Models

Oversubscribe GPU memory  
Allocate up to system memory size

Tune  
Unified Memory  
Performance

Usage hints via cudaMemAdvise API  
Explicit prefetching API

Simpler  
Data Access

CPU/GPU Data coherence  
Unified memory atomic operations

# SIMPLIFIED MEMORY MANAGEMENT CODE

## CPU Code

```
void sortfile(FILE *fp, int N) {  
    char *data;  
    data = (char *)malloc(N);  
  
    fread(data, 1, N, fp);  
  
    qsort(data, N, 1, compare);  
  
    use_data(data);  
  
    free(data);  
}
```

## CUDA 6 Code with Unified Memory

```
void sortfile(FILE *fp, int N) {  
    char *data;  
    cudaMallocManaged(&data, N);  
  
    fread(data, 1, N, fp);  
  
    qsort<<<...>>(data, N, 1, compare);  
    cudaDeviceSynchronize();  
  
    use_data(data);  
  
    cudaFree(data);  
}
```



# UNIFIED MEMORY EXAMPLE

## On-Demand Paging

```
__global__  
void setValue(int *ptr, int index, int val)  
{  
    ptr[index] = val;  
}
```

```
void foo(int size) {  
    char *data;  
    cudaMallocManaged(&data, size);  
  
    memset(data, 0, size);  
  
    setValue<<<...>>>(data, size/2, 5);  
    cudaDeviceSynchronize();  
  
    useData(data);  
  
    cudaFree(data);  
}
```



Unified Memory allocation



Access all values on CPU



Access one value on GPU

# HOW UNIFIED MEMORY WORKS IN CUDA 6

## Servicing CPU page faults

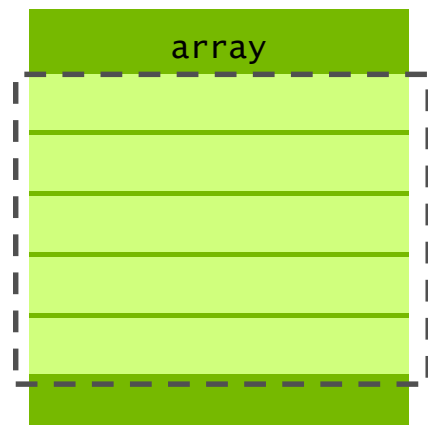
### GPU Code

```
__global__  
void setValue(char *ptr, int index, char val)  
{  
    ptr[index] = val;  
}
```

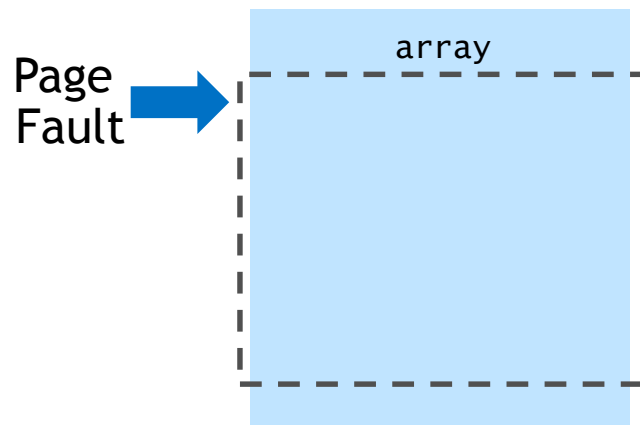
### CPU Code

```
cudaMallocManaged(&array, size);  
memset(array, size);  
setValue<<<...>>(array, size/2, 5);
```

### GPU Memory Mapping



### CPU Memory Mapping



Interconnect



# HOW UNIFIED MEMORY WORKS ON PASCAL

## Servicing CPU *and* GPU Page Faults

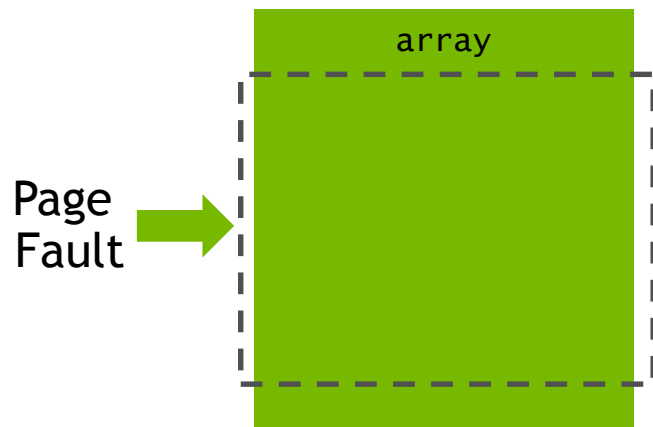
GPU Code

```
__global__  
void setValue(char *ptr, int index, char val)  
{  
    ptr[index] = val;  
}
```

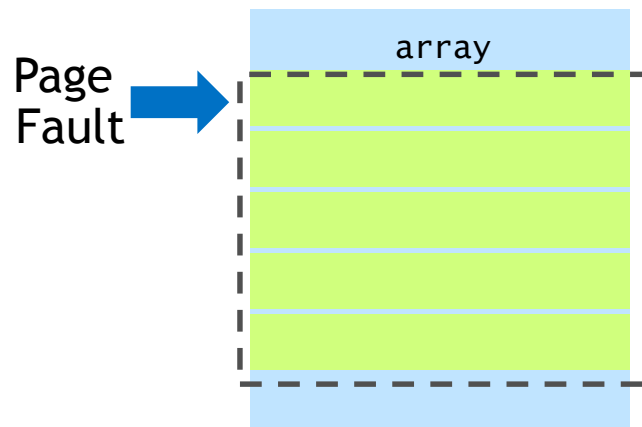
CPU Code

```
cudaMallocManaged(&array, size);  
memset(array, size);  
setValue<<<...>>(array, size/2, 5);
```

GPU Memory Mapping



CPU Memory Mapping

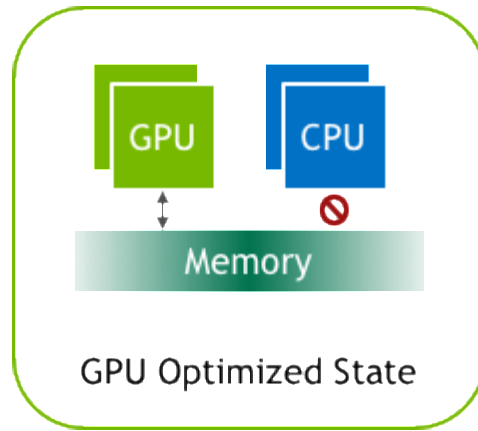


Interconnect

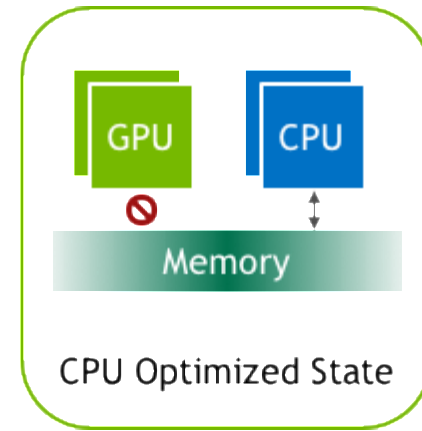


# VOLTA + UNIFIED MEMORY

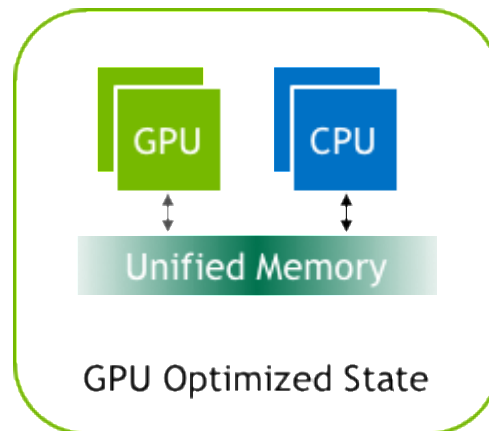
## VOLTA + PCIE CPU



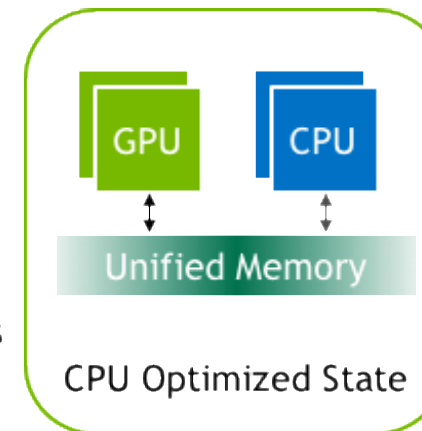
Page Migration Engine  
↔  
+ *Access counters*



## VOLTA + NVLINK CPU



Page Migration Engine  
↔  
+ *Access counters*  
+ *New NVLink Features*  
(*Coherence, Atomics, ATS*)





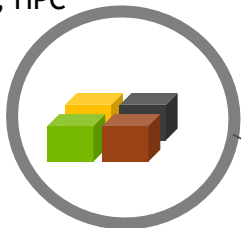
**NGC**

# NGC: GPU-OPTIMIZED SOFTWARE HUB

Simplifying DL, ML and HPC Workflows

50+ Containers

DL, ML, HPC

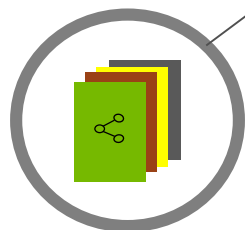


15+ Model Training Scripts

NLP, Image Classification, Object Detection & more



NGC



60 Pre-trained Models

NLP, Image Classification, Object Detection & more



Industry Workflows

Medical Imaging, Intelligent Video Analytics



DEEP LEARNING

TensorFlow | PyTorch | more



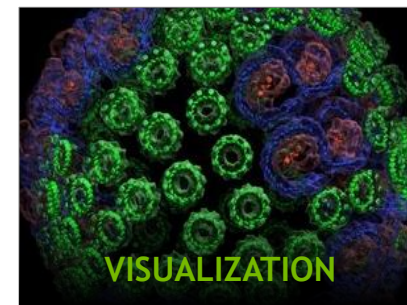
MACHINE LEARNING

RAPIDS | H2O | more



HPC

NAMD | GROMACS | more



VISUALIZATION

ParaView | IndeX | more

# NVIDIA GPU CLOUD REGISTRY

## Common Software stack across NVIDIA GPUs

### Deep Learning

All major frameworks with multi-GPU optimizations Uses NCCL for NVLINK data exchange Multi-threaded I/O to feed the GPUs

Caffe, Caffe2, CNTK, mxnet, PyTorch, Tensorflow, Theano, Torch

### HPC

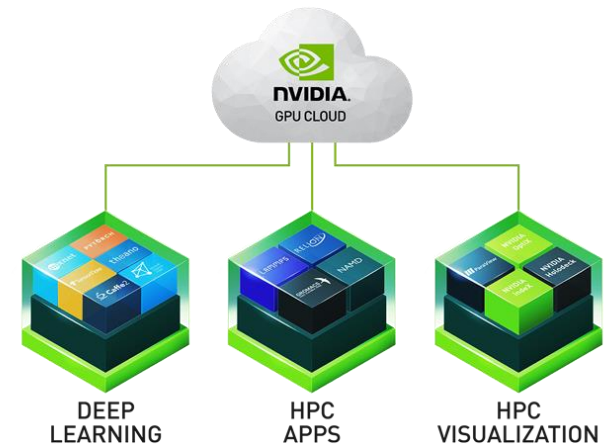
NAMD, Gromacs, LAMMPS, GAMESS, Relion, Chroma, MILC

### HPC Visualization

Paraview with Optix, Index and Holodeck with OpenGL visualization base on NVIDIA Docker 2.0, IndeX, VMD

### Single NGC Account

For use on GPUs everywhere - <https://ngc.nvidia.com>



**NVIDIA GPU Cloud** containerizes GPU-optimized frameworks, applications, runtimes, libraries, and operating system, available at no charge

Gunter Roeth ([gunterr@nvidia.com](mailto:gunterr@nvidia.com))



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