

LECTURE 1: MACHINE LEARNING FOR EARTH OBSERVATION POWERED BY SUPERCOMPUTING

GRSS ESI/HDCRS End-to-End Machine Learning with Supercomputing and in the Cloud - Tutorial IGARSS 2023 – 16 July, 2023

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JÜLICH
Forschungszentrum

SUPERCOMPUTING
CENTRE

UNIVERSITY
OF ICELAND



IMPACT
Interagency Implementation
and Advanced Concepts Team

C
EURO

ADMIRE
malleable data solutions for HPC

RAISE
Center of Excellence

EUPEX



HOW TO EXTRACT KNOWLEDGE IN A TIMELY MANNER?

From data acquired by diverse
observational systems



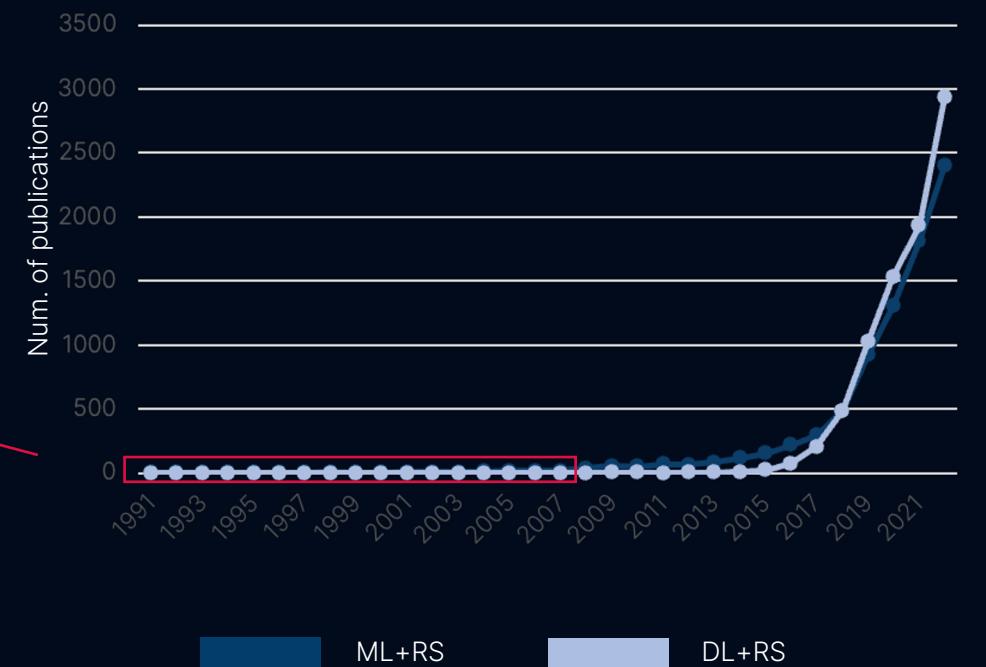
HOW TO USE ARTIFICIAL INTELLIGENCE FOR EARTH OBSERVATION?

MACHINE LEARNING AND DEEP LEARNING IN REMOTE SENSING

- Classical ML such as Support Vector Machine (SVM) and Random Forest (RF) since the '90s



- DL unleashed advances in the last decade
- Figures may differ depending on the source, but the overall trend remains consistent



HOW TO EXPLOIT EMERGING COMPUTING PARADIGMS?



Supercomputing



Specialized Hardware Computing



Quantum Computing



Edge Computing



Cloud computing

...



Blockchain

HIGH PERFORMANCE COMPUTING

SUPERCOMPUTERS

A high-performance computer for complex calculations that general-purpose computers cannot handle



- High number of processors, vast amounts of memory, and high-speed interconnects
- Optimal for scientific research, weather forecasting, engineering, and more
- Focus on maximum performance and maintainability reliability

DIFFERENCE BETWEEN LAPTOP AND SUPERCOMPUTER

Laptop	Supercomputer
Few cores	Lots of cores
Limited memory	Lots of memory
Slower than supercomputer	Faster than laptop
Personalized Operating System (OS)	Mostly linux based
Owned by you	Owed by public sector and located somewhere
Used by owner	Many users



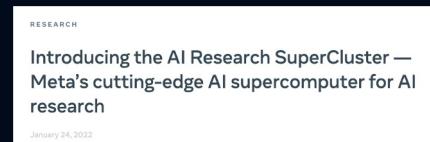
CURRENT POPULARITY OF SUPERCOMPUTERS



TPU v4: An Optically Reconfigurable Supercomputer for Machine Learning with Hardware Support for Embeddings

Industrial Product*

Norman P. Jouppi, George Kurian, Sheng Li, Peter Ma, Rahul Nagarajan, Lifeng Nai, Nishant Patil, Suvinay Subramanian, Andy Swing, Brian Towles, Cliff Young, Xiang Zhou, Zongwei Zhou, and David Patterson
Google, Mountain View, CA



- Big tech companies are announcing their AI supercomputers
- Supercomputing now goes far beyond traditional scientific computing, which was driven by large governments
- The field is currently propelled by major industries building highly specialized supercomputers

N. P. Jouppi, G. Kurian, et al., "TPU v4: An Optically Reconfigurable Supercomputer for Machine Learning with Hardware Support for Embeddings", 2023, <https://doi.org/10.48550/arXiv.2304.01433>

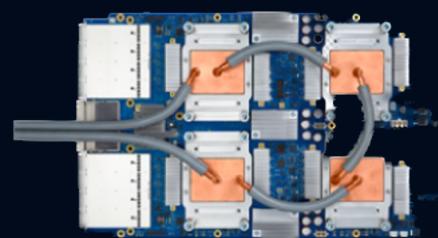
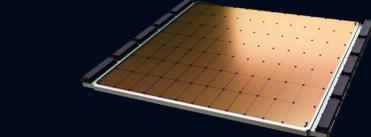
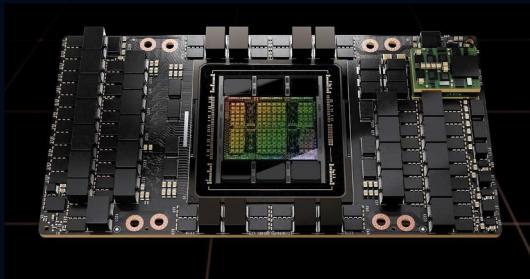
<https://www.forbes.com/sites/jamesmorris/2022/10/06/teslas-biggest-news-at-ai-day-was-the-dojo-supercomputer-not-the-optimus-robot/?sh=22ba4ab780bd>

<https://ai.facebook.com/blog/ai-rsc/>

<https://www.thesun.co.uk/tech/5072741/google-nasnet-ai-child-reinforcement-learning/>

Torsten Hoefer, "Efficient AI: From supercomputers to smartphones", Scalable Parallel Computing Lab @ ETH Zurich, <https://youtu.be/xxwT45ljG4o>

TRAINING OF DEEP LEARNING MODELS REQUIRES ACCELERATORS



- GPUs (currently NVIDIA dominant), TPUs (Google)
- GPUs: generic deep learning hardware (parallelizing matrix/tensor operations via vectorization)
- Specialized hardware, eg. in-memory computing chips, Graphcore IPU: Colossus MK2, Cerebras Wafer Scale Engine 2 (850k cores)

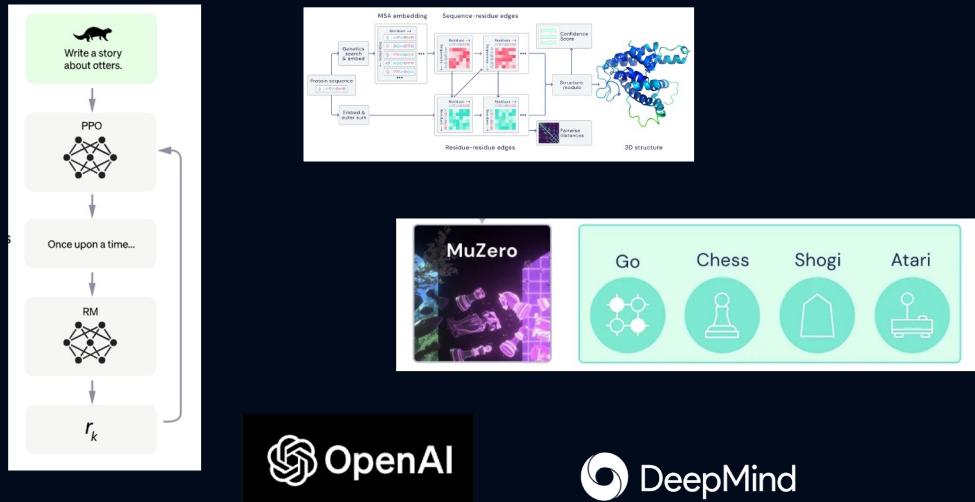
<https://www.nvidia.com/en-us/data-center/technologies/hopper-architecture/>

<https://cloud.google.com/tpu>

<https://www.graphcore.ai/products/ipu>

<https://www.cerebras.net/product-chip/>

MOST BREAKTHROUGHS REQUIRE HEAVY COMPUTE POWER, USING MANY ACCELERATORS SIMULTANEOUSLY



- GPT-3: natural language generation, language understanding
- CLIP, DALL-E 2, Stable Diffusion: image understanding and image generation
- AlphaFold 2: protein structure prediction
- AlphaZero, MuZero: learning control in highly dimensional state-action spaces

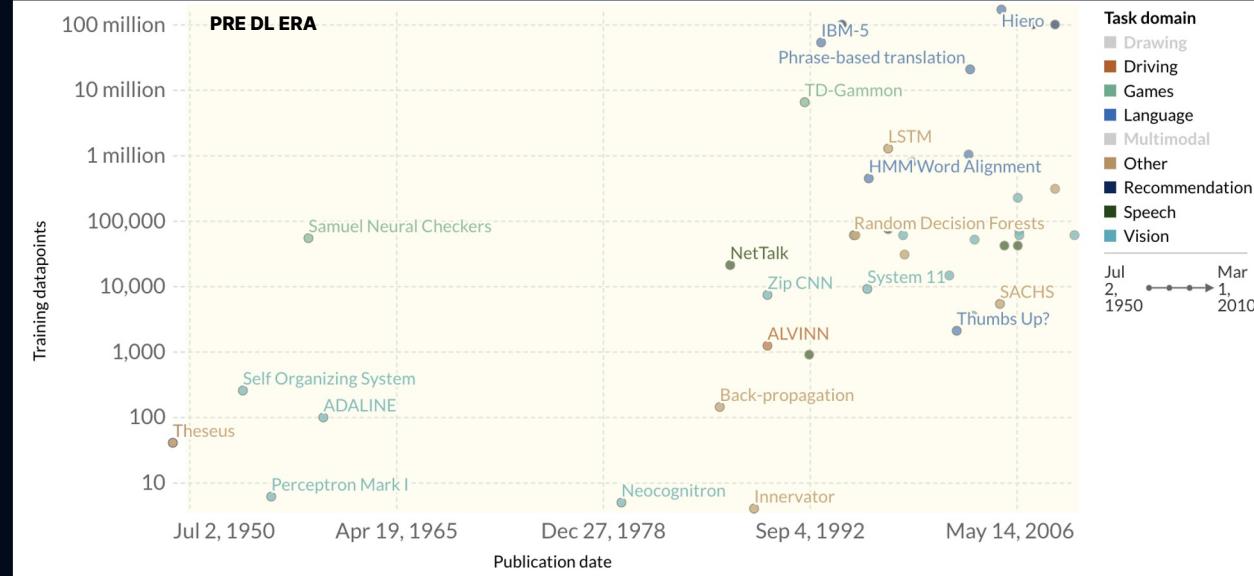
<https://openai.com/blog/chatgpt>

AlphaFold: a solution to a 50-year-old grand challenge in biology, <https://www.deepmind.com/blog/alphafold-a-solution-to-a-50-year-old-grand-challenge-in-biology>

MuZero: Mastering Go, chess, shogi and Atari without rules, <https://www.deepmind.com/blog/muzero-mastering-go-chess-shogi-and-atari-without-rules>

Jenia Jitsev, Towards Scalable Deep Learning, Scalable Learning & Multi-Purpose AI Lab, Helmholtz AI, LAION @ JSC

PRE DEEP LEARNING ERA (1950-2010)

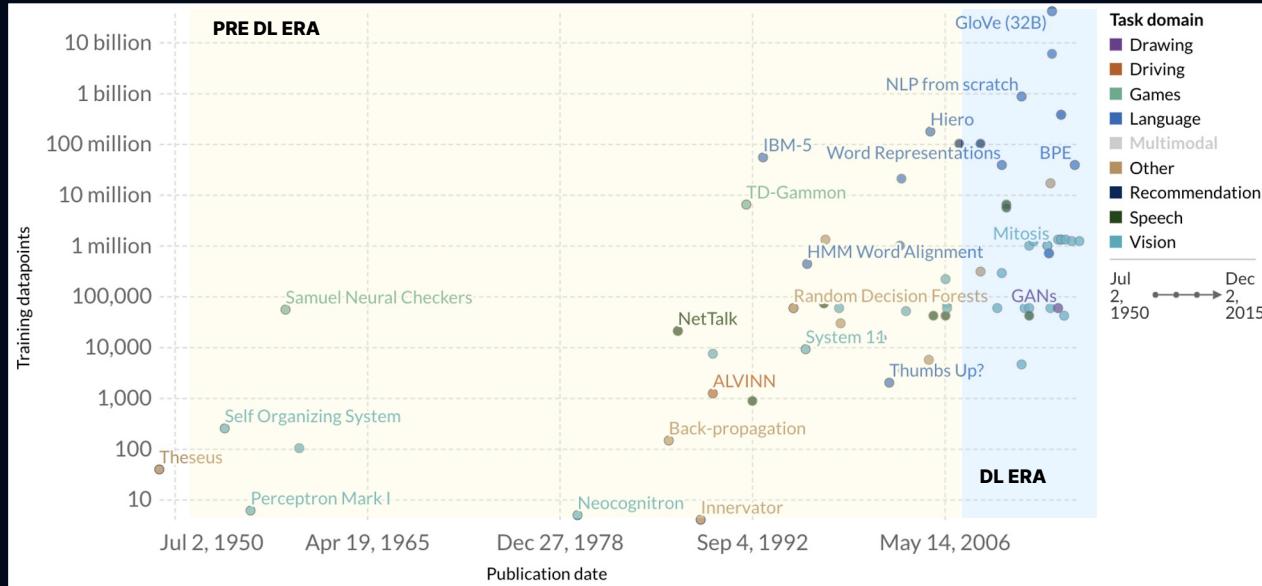


C. Giattino, et al., Artificial Intelligence, <https://ourworldindata.org/artificial-intelligence>

J. Sevilla, L. Heim, A. Ho, T. Besiroglu, M. Hobbahn and P. Villalobos, "Compute Trends Across Three Eras of Machine Learning," 2022 International Joint Conference on Neural Networks (IJCNN), pp. 1-8, 2022, <https://doi.org/10.1109/IJCNN55064.2022.9891914>

- Training compute doubled every 17 to 29 months
- This increase is roughly in line with Moore's Law

DEEP LEARNING ERA AROUND 2010



C. Giattino, et al., Artificial Intelligence, <https://ourworldindata.org/artificial-intelligence>

J. Sevilla, L. Heim, A. Ho, T. Besiroglu, M. Hobbahn and P. Villalobos, "Compute Trends Across Three Eras of Machine Learning," 2022 International Joint Conference on Neural Networks (IJCNN), pp. 1-8, 2022, <https://doi.org/10.1109/IJCNN55064.2022.9891914>

- The trend accelerated along with the popularity of deep learning
- From around 2010, compute doubles every 4 to 9 months

LARGE-SCALE ERA AROUND 2015



C. Giattino, et al., Artificial Intelligence, <https://ourworldindata.org/artificial-intelligence>

J. Sevilla, L. Heim, A. Ho, T. Besiroglu, M. Hobbahn and P. Villalobos, "Compute Trends Across Three Eras of Machine Learning," 2022 International Joint Conference on Neural Networks (IJCNN), pp. 1-8, 2022, <https://doi.org/10.1109/IJCNN55064.2022.9891914>

D. Silver et al., "Mastering the game of Go without human knowledge," Nature, vol. 550, pp. 354–359, 2017, <https://doi.org/10.1038/nature24270>

- In late 2015, a new trend of large-scale models emerged
- Computational capacity significantly higher than that of other models published in the same year (e.g., release of AlphaGo)
- This growth trend is slower than the overall DL trend, with a doubling time of roughly every 8 to 17 months

JUWELS

Exascale Pathfinder

- Ranking in November 2020
 - TOP500 (7 World, 1 Europe)
 - Green500 (1 in TOP100)
 - TOP10 AI (4)



Julich Supercomputing Centre, "JUWELS Cluster and Booster: Exascale Pathfinder with Modular Supercomputing Architecture at Julich Supercomputing Centre," Journal of large-scale research facilities, vol. 7, no. A138, 2021.

Designed for simulation and large-scale machine learning

Funded through SiVeGCS (BMBF, MWK-NRW)

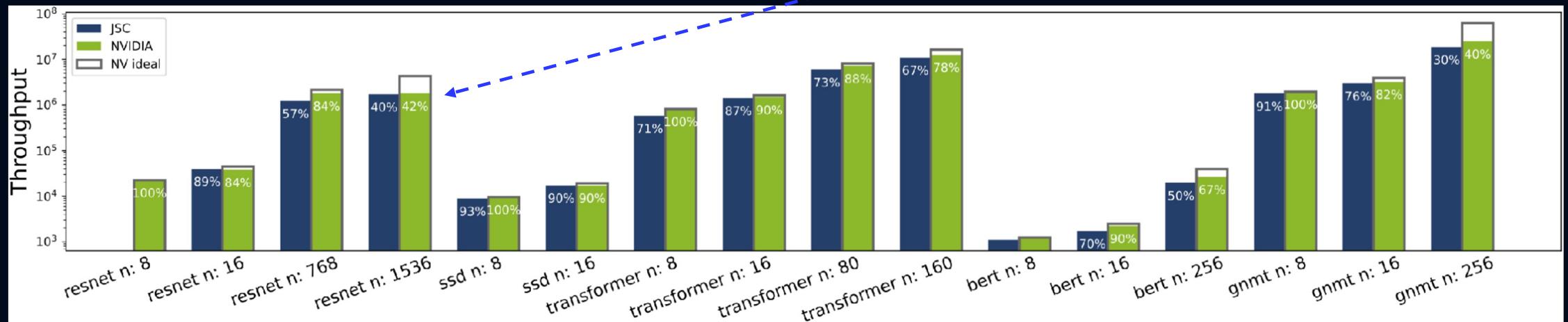
JUWELS BOOSTER – A “DUAL USE” SYSTEM

Benchmark result

- Benchmark: NVIDIA’s submission to MLPerf training v0.7
- Metrics: Throughput in Samples/sec
- 5 Benchmarks on up to 1536 GPUs
- Reference: NVIDIA’s results on specific AI system Selene

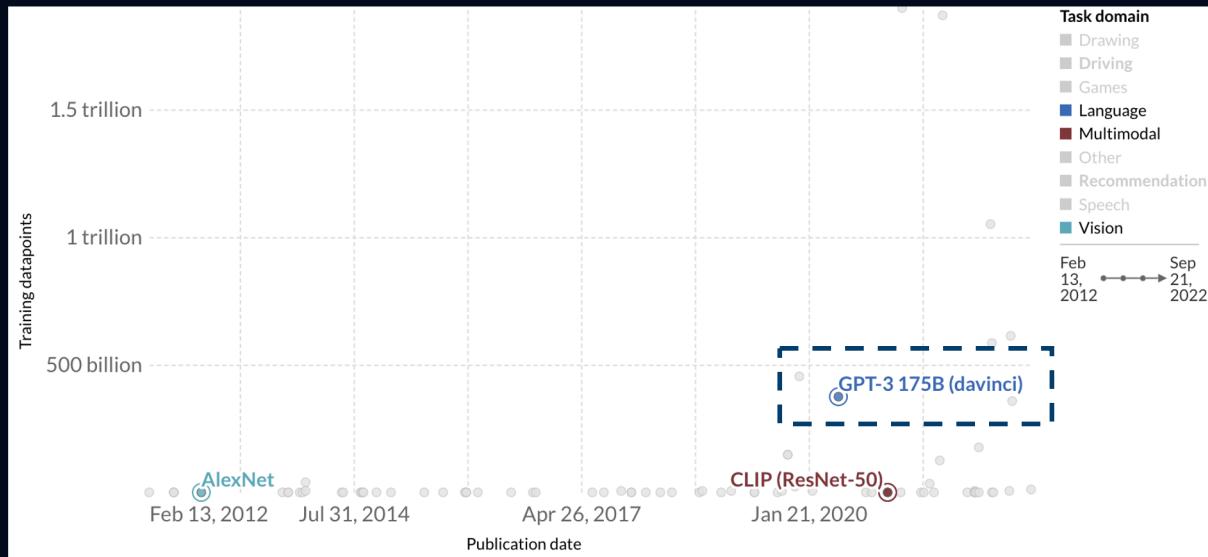
Example

- Task: Train Resnet50 on ImageNet
- GPUs: 1536
- Throughput: 1.7 Million Images / Sec
- Training complete after 43 seconds!
- Parallelization efficiency: 40%



S. Kesselheim, A. Herten, K. Krajsek, J. Ebert, J. Jitsev, M. Cherti, M. Langguth, B. Gong, S. Stadtler, A. Mozaffari, G. Cavallaro, R. Sedona, A. Schug, A. Strube, R. Kamath, M. G. Schultz, M. Riedel, and T. Lippert, “JUWELS Booster – A Supercomputer for Large-Scale AI Research,” in High Performance Computing (H. Jagode, H. Anzt, H. Ltaief, and P. Luszczek, eds.), (Cham), pp. 453–468, Springer International Publishing, 2021.

GPT-3 MODEL (175 BILLION WEIGHT PARAMETERS)



- AlexNet, winner ILSRVC 2012 – 60M
- ResNet-50, winner ILSRVC 2015 – 25M
- CLIP ViT L/14, multi-modal learning, 2021 - 600M

TIME REQUIRED FOR A FULL TRAINING OF GPT-3 MODEL



- ≈ 355 years with one Nvidia Volta 100 GPU
- ≈ 90 years with one Nvidia Ampere 100 GPU
- ≈ 16 days if scaled well with 2,000 A100 GPUs on JUWELS Booster

Jülich Wizard for European Leadership Science (JUWELS), <https://www.fz-juelich.de/en/ias/jsc/systems/supercomputers/juwels>

Jenia Jitsev, Towards Scalable Deep Learning, Scalable Learning & Multi-Purpose AI Lab, Helmholtz AI, LAION @ JSC

TIME REQUIRED FOR A FULL TRAINING OF GPT-4 MODEL



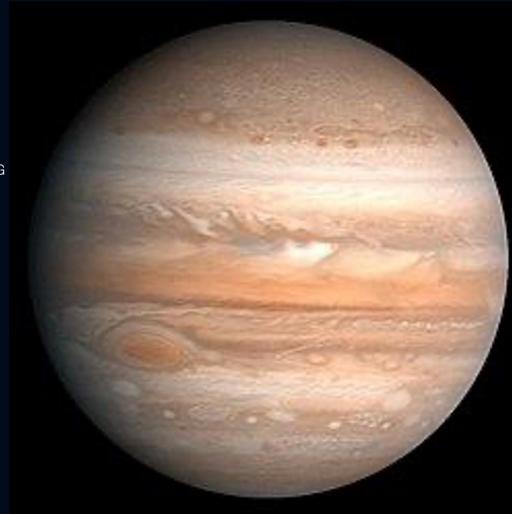
- ≈ 5500 years with one Nvidia Ampere 100 GPU
- ≈ 1200 years with one Nvidia Hopper 100 GPU
- ≈ 900 days if scaled well with 2,000 A100 GPUs on JUWELS Booster

JU PIONEER FOR INNOVATIVE AND TRANSFORMATIVE EXASCALE RESEARCH (JUPITER)



Mars
(JUWELS)

Jupiter



Mars: d= 6,800 Km
Jupiter: d= 143,00 Km

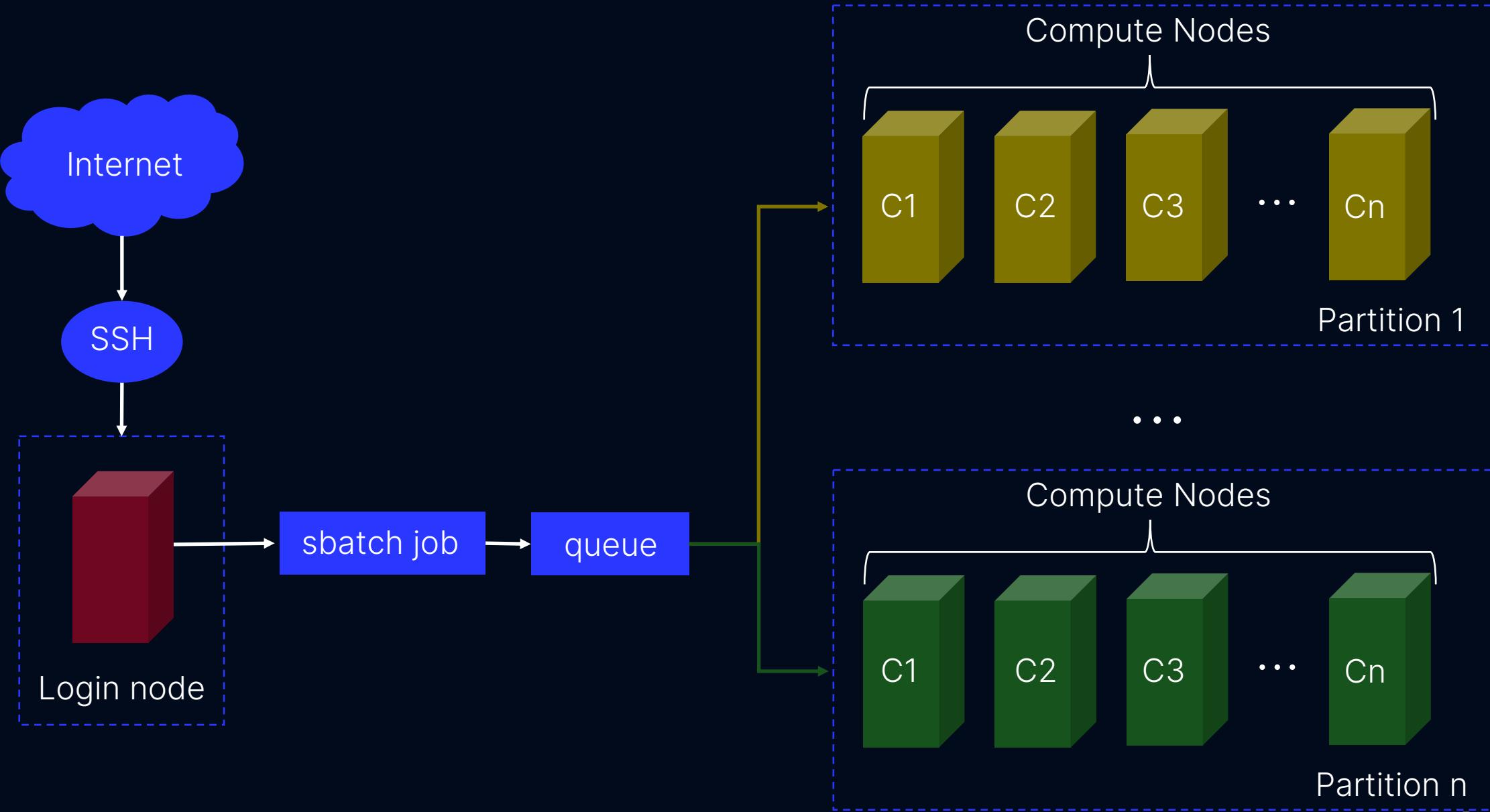
JUWELS: 85 PF/s peak
JUPITER: 1,300 PF/s peak

Thomas Lippert, "Jupiter Ascending, Driving the Forefront of Europe's HPC Effort", EuroHPC Summit 2023, <https://www.eurohpcsummit.eu/>

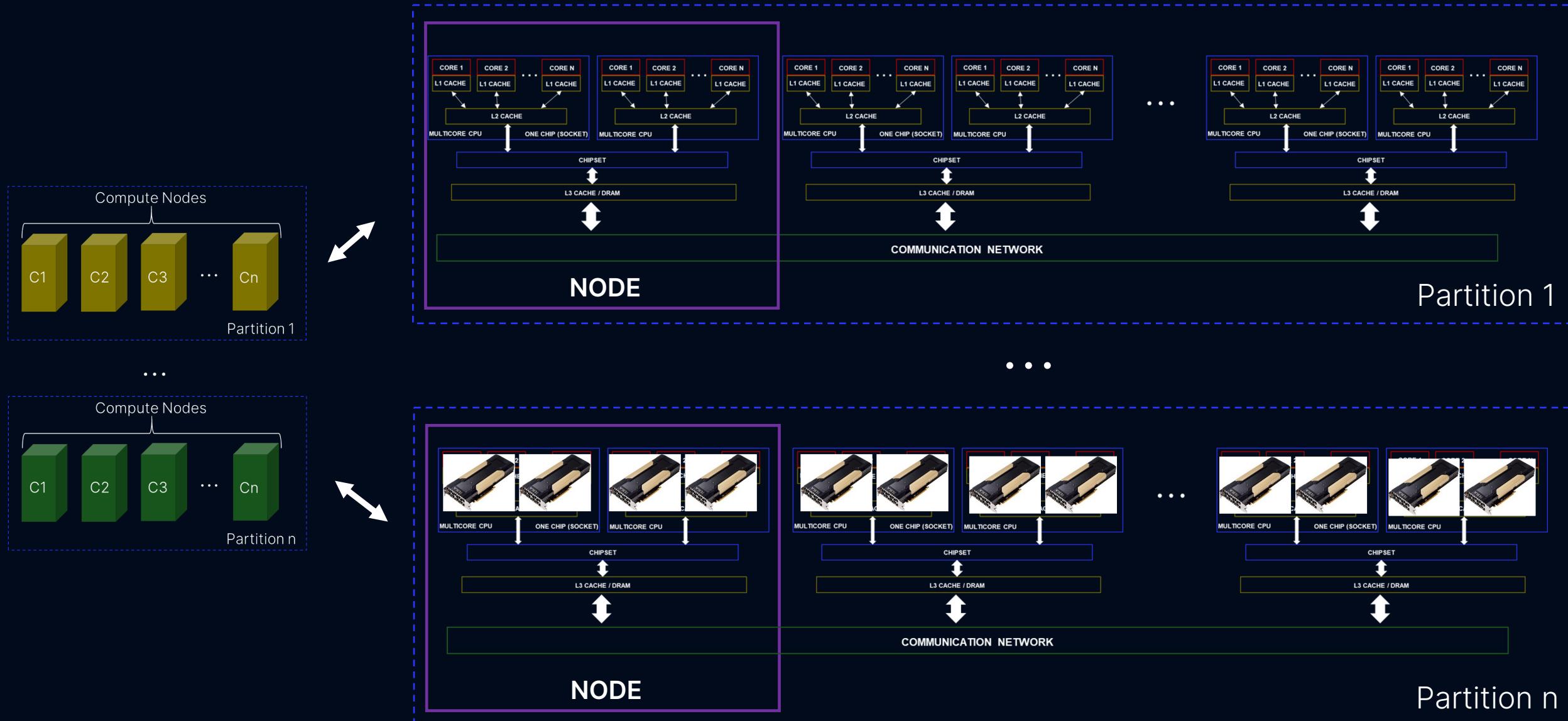
JUPITER | The Arrival of Exascale in Europe, <https://www.fz-juelich.de/en/ias/jsc/jupiter>

- The Forschungszentrum Jülich in Germany will house Europe's first exascale computer, named JUPITER
- This machine is set to surpass the threshold of one quintillion (a "1" followed by 18 zeros) calculations per second
- JUWELS 20 = JUPITER (when using the diameters of planets as a measurement scale)

ANATOMY OF A SUPERCOMPUTER



PARTITIONS AND NODES



KEY INFORMATION ABOUT A SUPERCOMPUTER

TYPE OF PARTITIONS

NUMBER OF NODES

PERFORMANCE

ACCELERATORS

RAM

NETWORK:
BANDWIDTH, LATENCY

CPU, NUMBER OF CORES

...

JÜLICH RESEARCH ON EXASCALE CLUSTER ARCHITECTURES - DATA CENTRIC (JURECA-DC)



- 98,304 CPU cores, 768 GPUs
- 3.54 (CPU) + 14.98 (GPU) Petaflops per second peak performance
- Mellanox InfiniBand HDR (HDR100/HDR) DragonFly+ network
 - Ca. 15 Tb/s connection to Booster via gateway nodes
- 350 GB/s network connection to JUST for storage access

<https://www.fz-juelich.de/en/ias/jsc/systems/supercomputers/jureca>

JURECA-DC – CONFIGURATION



576 COMPUTE NODES

2× AMD EPYC 7742, 2× 64 cores, 2.25 GHz

Partition 1

192 ACCELERATED COMPUTE NODES

2× AMD EPYC 7742, 2× 64 cores, 2.25 GHz

4× NVIDIA A100 GPU, 4× 40 GB HBM2e

Partition 2

19 LOGIN NODES

2× AMD EPYC 7742, 2× 64 cores, 2.25 GHz

Partition 3

ACCESS SUPERCOMPUTERS AT JSC

Secure Shell (SSH)



Cryptographic protocol for operating services securely over an unsecured network

Jupyter-JSC



Supercomputing in your Browser

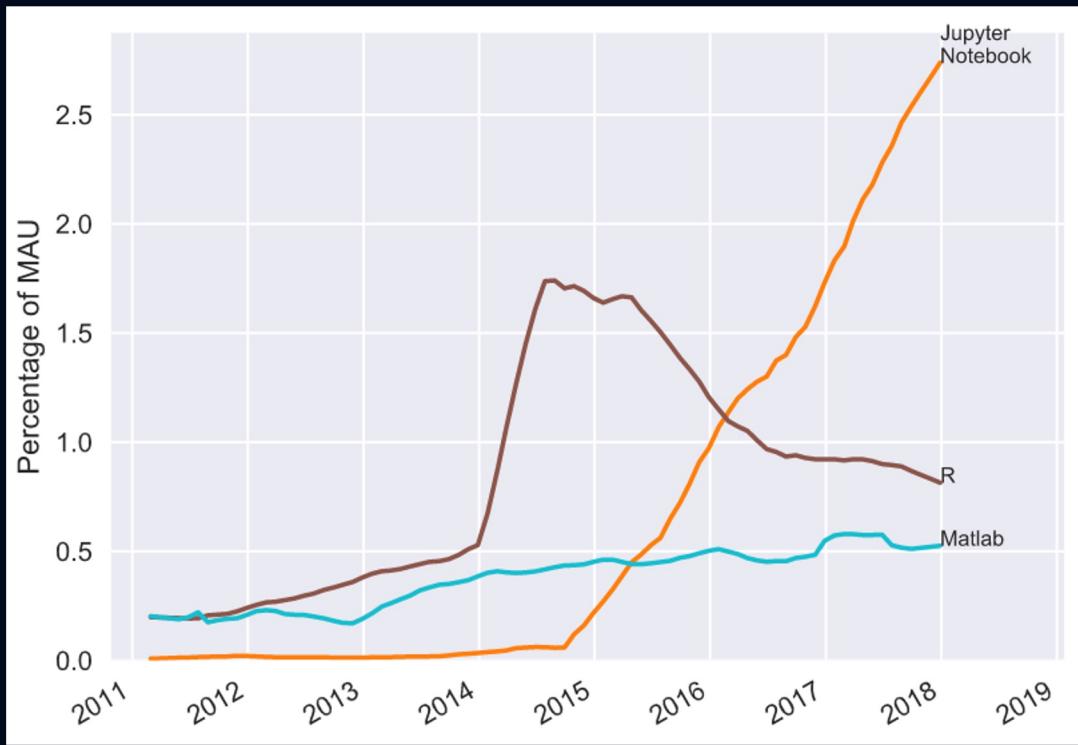
UNICORE



Uniform Interface to Computing Resources

RISE OF JUPYTER'S POPULARITY

Monthly aggregated number of user interactions with GitHub repos (= Monthly Active Users (MAU))

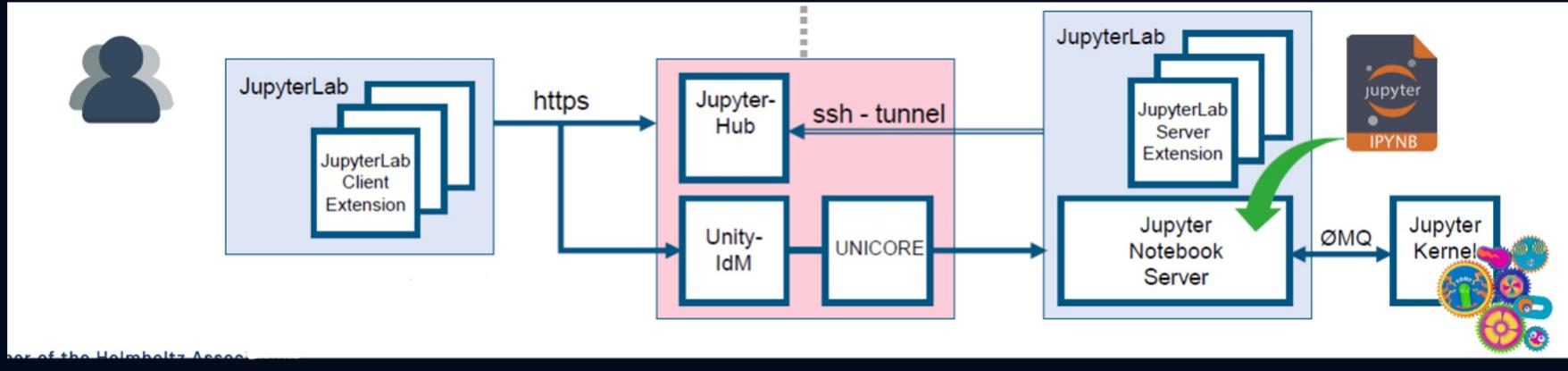


Jupyter Notebooks have seen significant and steady growth over the last years

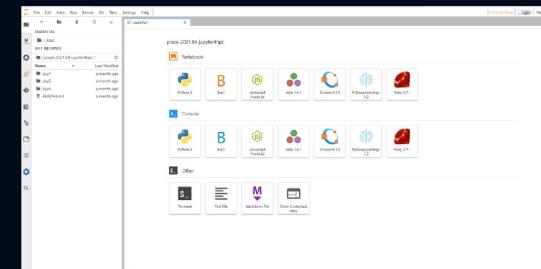
Python is pushing this trend

<https://www.benfrederickson.com/ranking-programming-languages-by-github-users/>

JUPYTER-JSC WEB SERVICE



Browser

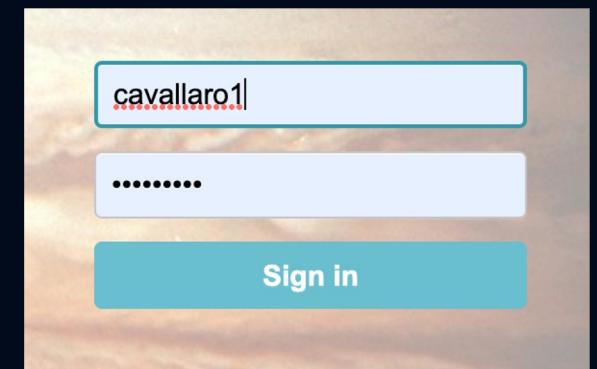


HPC system

ACCESS JUPYTER-JSC

- Go to <https://jupyter-jsc.fz-juelich.de/>, login

The screenshot shows the Jupyter-JSC homepage. At the top left is the Jülich Forschungszentrum logo. The top navigation bar includes links for Start, Links, JSC Status, and Documentation. The main content area features a large image of server racks. Overlaid on this image is a white box containing the text "Supercomputing in Your Browser". Below this, a paragraph explains the service: "We are pleased to bring "Supercomputing in your browser". Jupyter-JSC is designed to provide the rich high performance computing (HPC) ecosystem to the world's most popular software: web browsers. JupyterLab is a web-based interactive development environment for Jupyter notebooks, code, and data. JupyterLab is flexible to support a wide range of workflows in data science, scientific computing, and machine learning. [Read more.](#)" A navigation bar at the bottom of this section has four items: Jupyter-JSC (selected), JUWELS, JURECA, and JUSUF. To the right of the main image is a sidebar with the JSC logo and the heading "Jupyter-JSC Supercomputing in Your Browser". It describes the service and provides instructions for logging in or registering. At the bottom is a "Login" button highlighted with a yellow border, a user icon, and a "Register" button.



JURECA DC – HPC SYSTEM

Hardware Configuration of the JURECA DC Module (Phase 2: as of May 2021)

- **480 standard compute nodes**
 - 2x AMD EPYC 7742, 2x 64 cores, 2.25 GHz
 - 512 (16x 32) GB DDR4, 3200 MHz
 - InfiniBand HDR100 (NVIDIA Mellanox Connect-X6)
 - diskless
- **96 large-memory compute nodes**
 - 2x AMD EPYC 7742, 2x 64 cores, 2.25 GHz
 - 1024 (16x 64) GB DDR4, 3200 MHz
 - InfiniBand HDR100 (NVIDIA Mellanox Connect-X6)
 - diskless
- **192 accelerated compute nodes**
 - 2x AMD EPYC 7742, 2x 64 cores, 2.25 GHz
 - 512 (16x 32) GB DDR4, 3200 MHz
 - 4x NVIDIA A100 GPU, 4x 40 GB HBM2e
 - 2x InfiniBand HDR (NVIDIA Mellanox Connect-X6)
 - diskless
- **12 login nodes**
 - 2x AMD EPYC 7742, 2x 64 cores, 2.25 GHz
 - 1024 (16x 64) GB DDR4, 3200 MHz
 - 2x NVIDIA Quadro RTX8000
 - InfiniBand HDR100 (NVIDIA Mellanox Connect-X6)
 - 100 Gigabit Ethernet external connection

CREATE A NEW JUPYTERLAB

- Partition: login node

JupyterLabs

You can configure your existing JupyterLabs by expanding the corresponding table row.

	Name	System	Partition	Project	Status	Actions
+	NEW JUPYTERLAB					
Lab Config	Name	IGARSS tutorial 2023 - Login Node				
Resources	Version	JupyterLab - 3.4				
Kernels and Extensions	System	JURECA				
	Account	cavallaro1				
	Project	training2308				
	Partition	LoginNode				

► Start

CREATE A NEW JUPYTERLAB

S

ing JupyterLabs by expanding the corresponding table row.

	System	Partition	Project
NEW JUPYTERLAB			
Name	IGARSS tutorial 2023 - Login Node		
Version	JupyterLab - 3.4		
System	JURECA		
Account	cavallaro1		
Project	training2308		
Partition	LoginNode		

576 COMPUTE NODES

2× AMD EPYC 7742, 2× 64 cores, 2.25 GHz

Partition 1

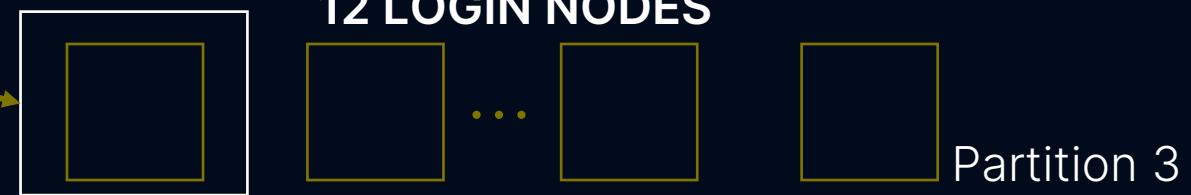
192 ACCELERATED COMPUTE NODES

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Partition 2

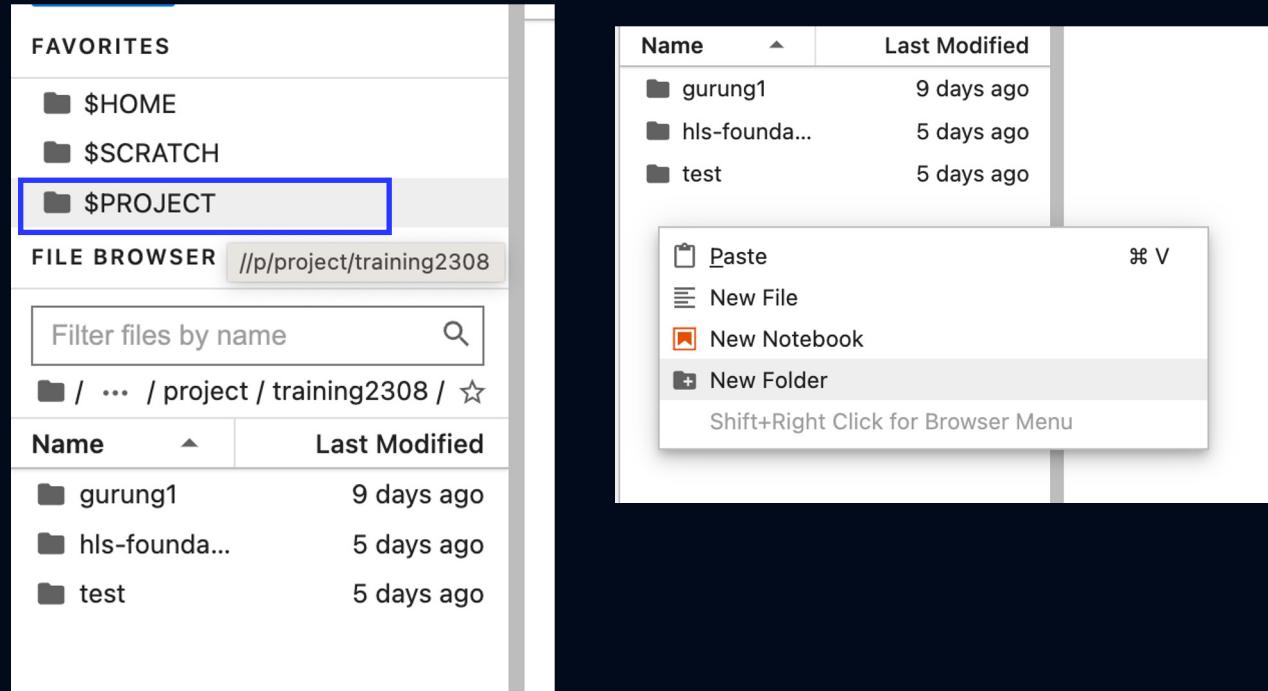
12 LOGIN NODES



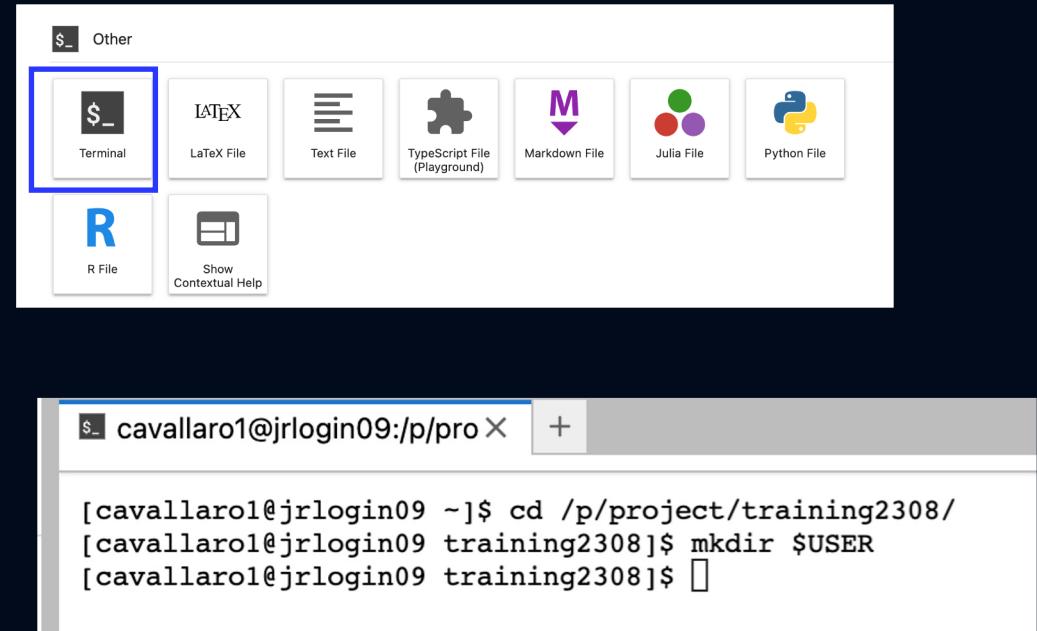
Partition 3

CREATE YOUR OWN FOLDER IN THE PROJECT

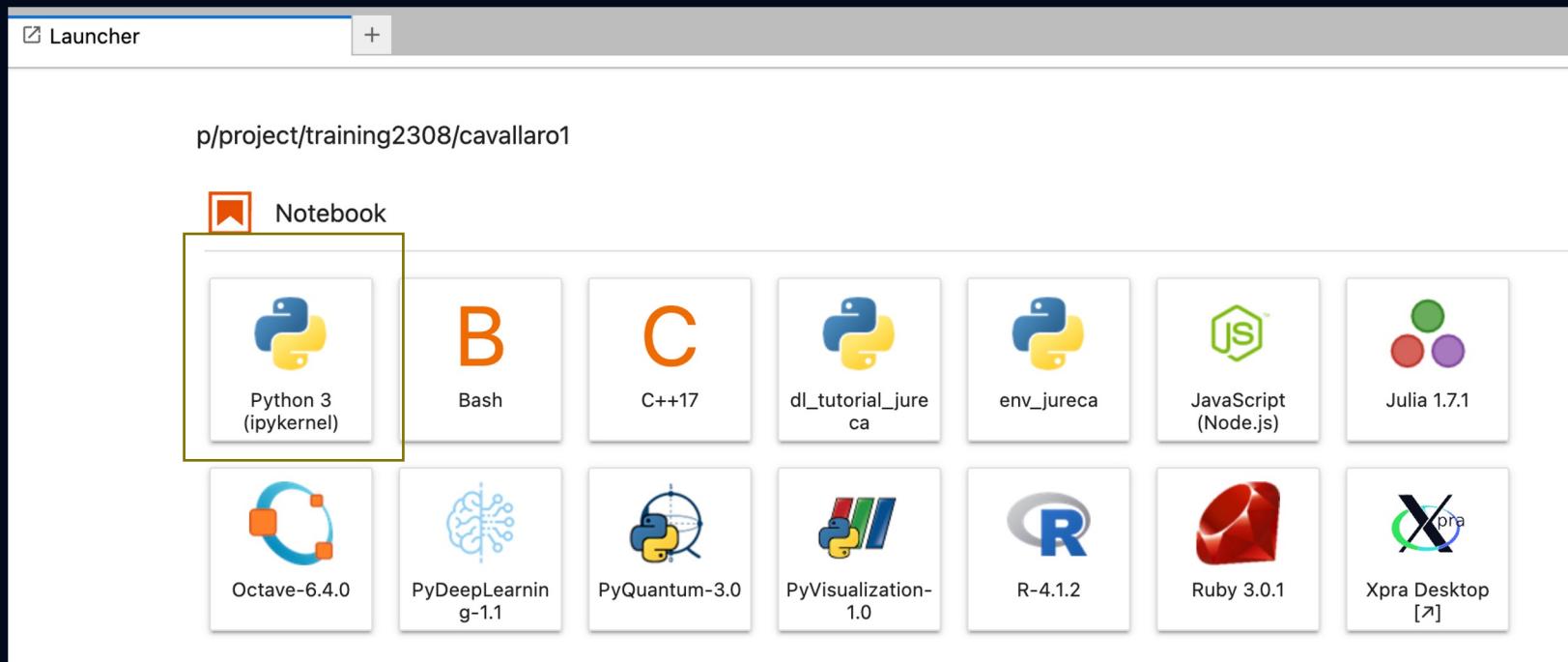
METHOD 1



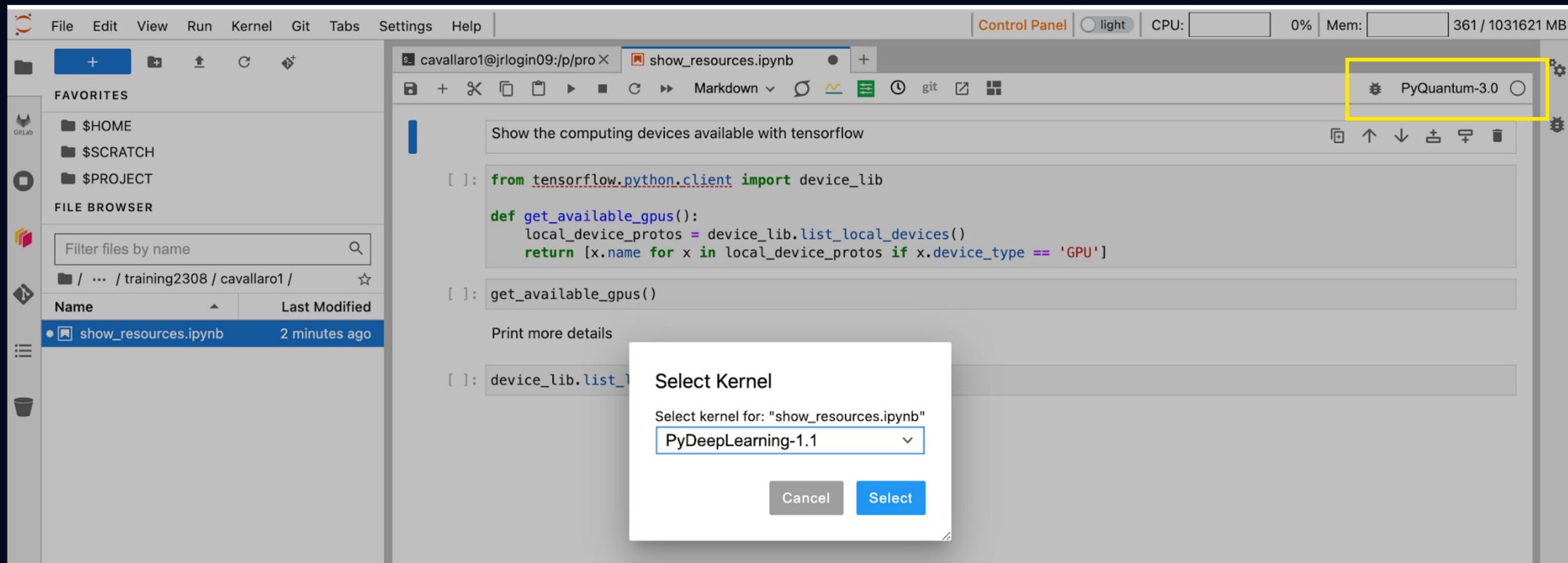
METHOD 2



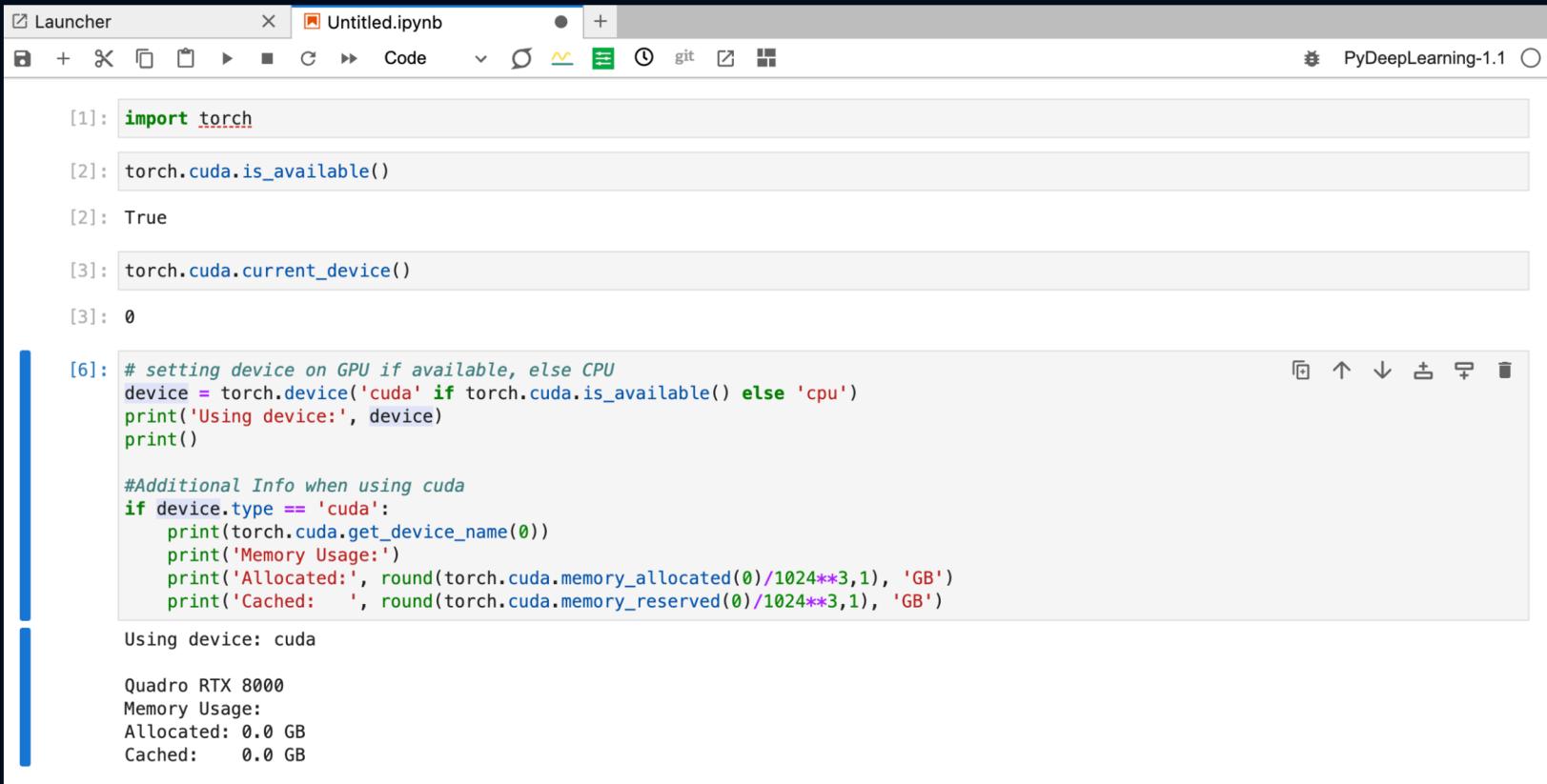
LAUNCH A NEW NOTEBOOK



SELECT THE KERNEL



CHECK COMPUTING RESOURCES



The screenshot shows a Jupyter Notebook interface with the title "Untitled.ipynb". The code cell [1] contains the command `import torch`. The output [2] shows the result of `torch.cuda.is_available()`, which is `True`. The output [3] shows the result of `torch.cuda.current_device()`, which is `0`. The code cell [6] contains a script to set the device to GPU if available, or CPU if not. It prints the device type and additional information about memory usage and allocation. The output shows that the device is a Quadro RTX 8000 with 0.0 GB of memory allocated and cached.

```
[1]: import torch
[2]: torch.cuda.is_available()
[2]: True
[3]: torch.cuda.current_device()
[3]: 0
[6]: # setting device on GPU if available, else CPU
device = torch.device('cuda' if torch.cuda.is_available() else 'cpu')
print('Using device:', device)
print()

#Additional Info when using cuda
if device.type == 'cuda':
    print(torch.cuda.get_device_name(0))
    print('Memory Usage: ')
    print('Allocated:', round(torch.cuda.memory_allocated(0)/1024**3,1), 'GB')
    print('Cached: ', round(torch.cuda.memory_reserved(0)/1024**3,1), 'GB')

Using device: cuda
Quadro RTX 8000
Memory Usage:
Allocated: 0.0 GB
Cached: 0.0 GB
```

Login nodes are used for job submission, code compilation, and file management, not for computation. They serve as a gateway to HPC resources and aren't designed to handle heavy computational loads

CREATE A NEW JUPYTERLAB

Lab Config

Name: IGARSS tutorial 2023 - Compute Node

Version: JupyterLab - 3.4

Resources !

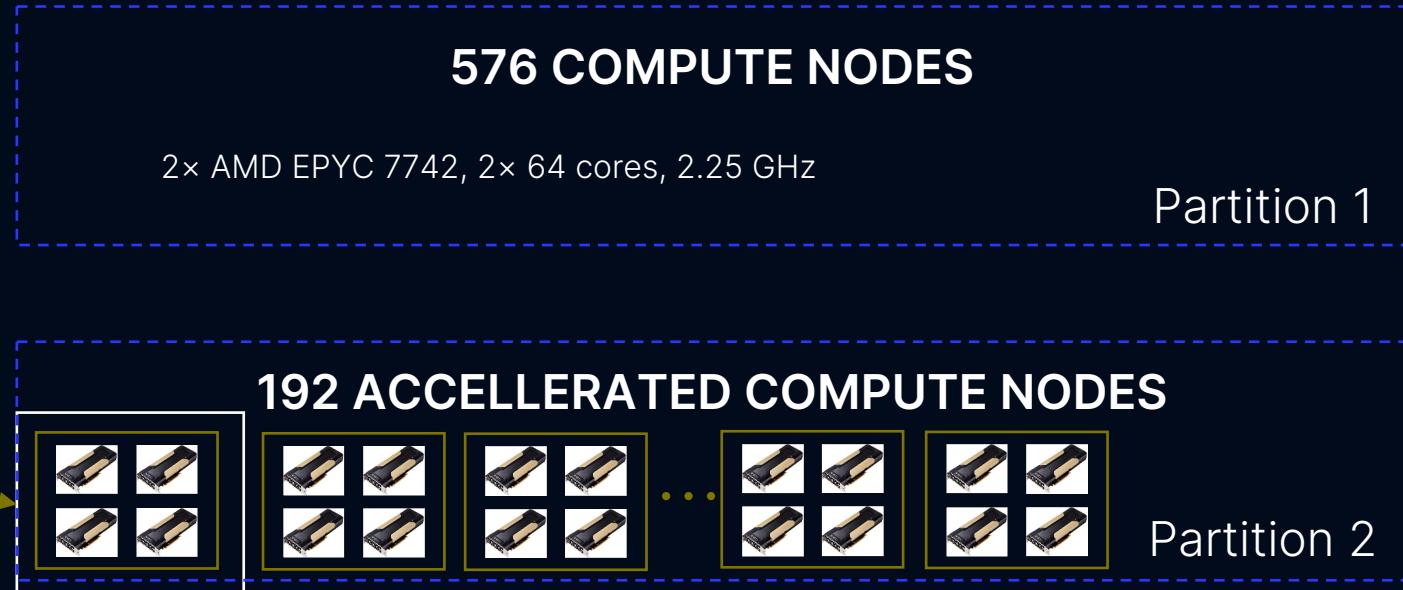
System: JURECA

Kernels and Extensions !

Account: cavallaro1

Project: training2308

Partition: dc-gpu



+

Nodes [1,24]: 1

GPUs [1,4]: 4

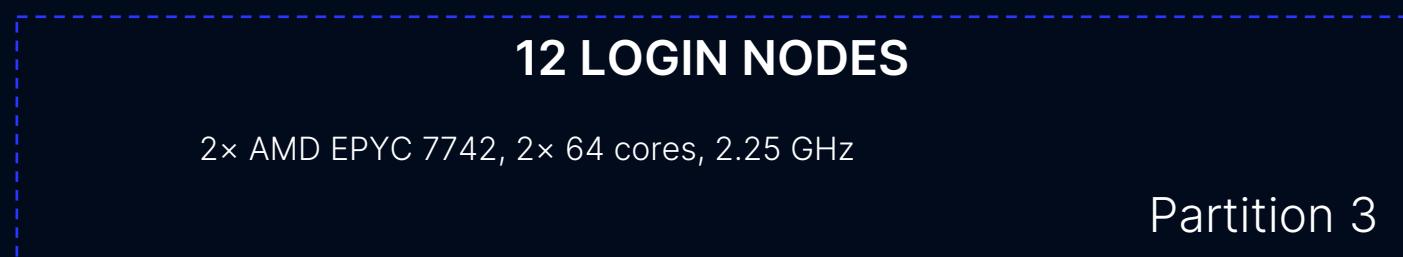
Resources

Runtime (minutes) [10,1440]: 30

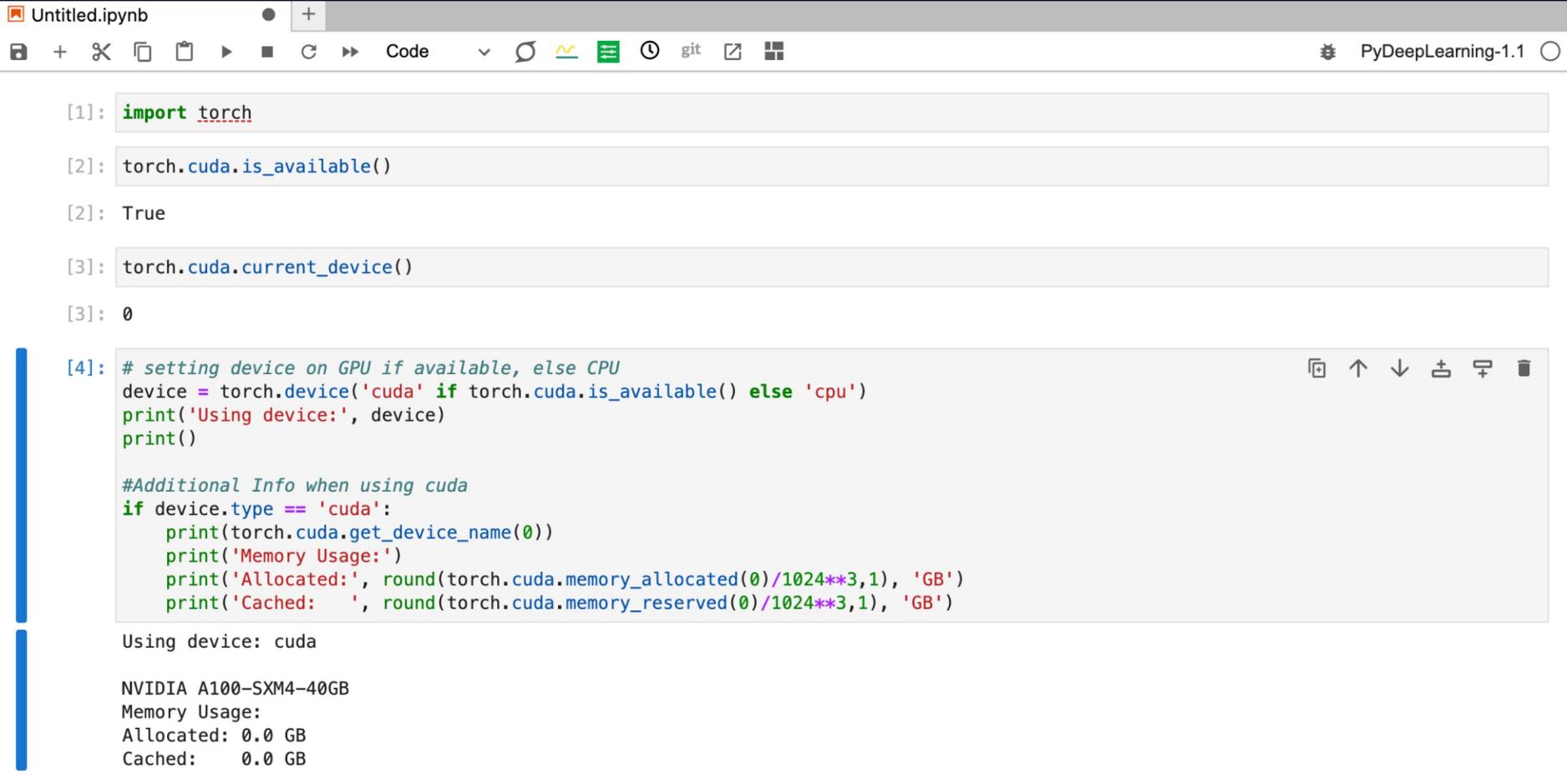
Lab Config

Kernels and Extensions

NEW JUPYTERLAB



CHECK COMPUTING RESOURCES



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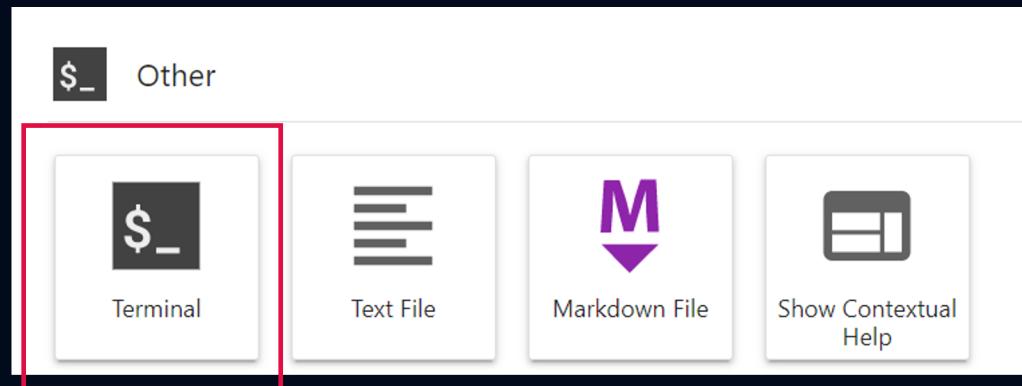
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[1]: import torch
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[3]: torch.cuda.current_device()
[3]: 0
[4]: # setting device on GPU if available, else CPU
device = torch.device('cuda' if torch.cuda.is_available() else 'cpu')
print('Using device:', device)
print()

#Additional Info when using cuda
if device.type == 'cuda':
    print(torch.cuda.get_device_name(0))
    print('Memory Usage:')
    print('Allocated:', round(torch.cuda.memory_allocated(0)/1024**3,1), 'GB')
    print('Cached:   ', round(torch.cuda.memory_reserved(0)/1024**3,1), 'GB')
```

The output of the code is displayed below the code cells:

```
Using device: cuda
NVIDIA A100-SXM4-40GB
Memory Usage:
Allocated: 0.0 GB
Cached: 0.0 GB
```

CHECK COMPUTING RESOURCES IN THE TERMINAL

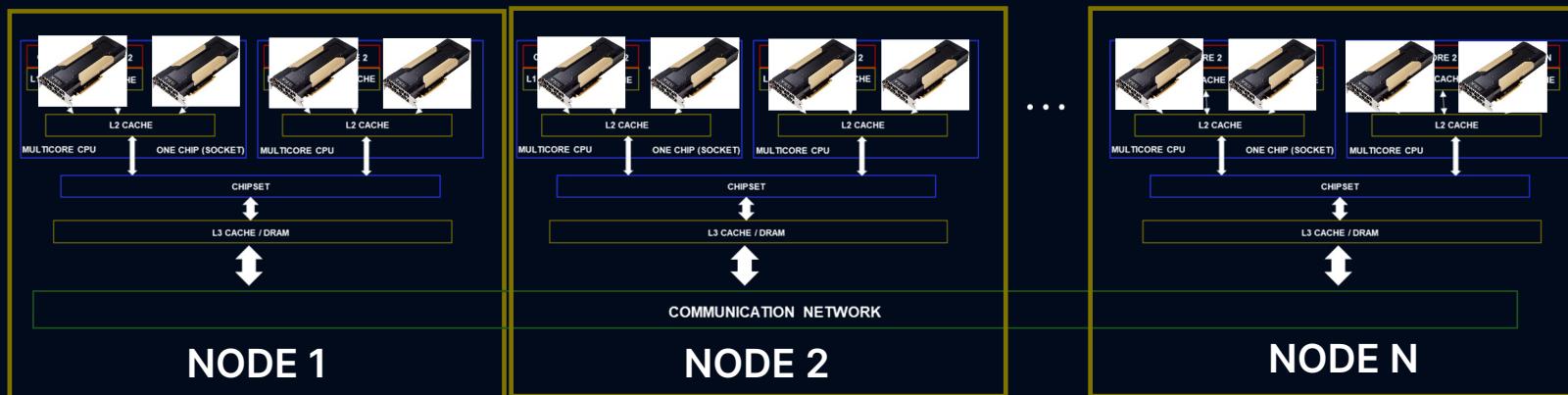


```
s. cavallaro1@jrc0226:/p/projex +  
[cavallaro1@jrc0226 cavallaro1]$ nvidia-smi  
Fri Jul  7 10:50:54 2023  
+-----+  
| NVIDIA-SMI 525.105.17    Driver Version: 525.105.17    CUDA Version: 12.0 |  
+-----+  
| GPU  Name      Persistence-M | Bus-Id     Disp.A  Volatile Uncorr. ECC | | | | | | |
| Fan  Temp     Perf  Pwr:Usage/Cap | Memory-Usage | GPU-Util  Compute M. |  
|          |          |          |          |          |          |          | MIG M. |  
+-----+  
| 0  NVIDIA A100-SXM... On   00000000:03:00.0 Off | 0%          0 | Default Disabled |  
| N/A  45C     P0    61W / 400W | 3MiB / 40960MiB |  
+-----+  
| 1  NVIDIA A100-SXM... On   00000000:44:00.0 Off | 0%          0 | Default Disabled |  
| N/A  43C     P0    58W / 400W | 3MiB / 40960MiB |  
+-----+  
| 2  NVIDIA A100-SXM... On   00000000:84:00.0 Off | 0%          0 | Default Disabled |  
| N/A  44C     P0    59W / 400W | 3MiB / 40960MiB |  
+-----+  
| 3  NVIDIA A100-SXM... On   00000000:C4:00.0 Off | 0%          0 | Default Disabled |  
| N/A  44C     P0    58W / 400W | 3MiB / 40960MiB |  
+-----+  
+-----+  
| Processes:  
| GPU  GI  CI      PID  Type  Process name          GPU Memory Usage |  
|          ID  ID |  
+-----+  
| No running processes found |  
+-----+  
[cavallaro1@jrc0226 cavallaro1]$ █
```

LATER IN THIS TUTORIAL

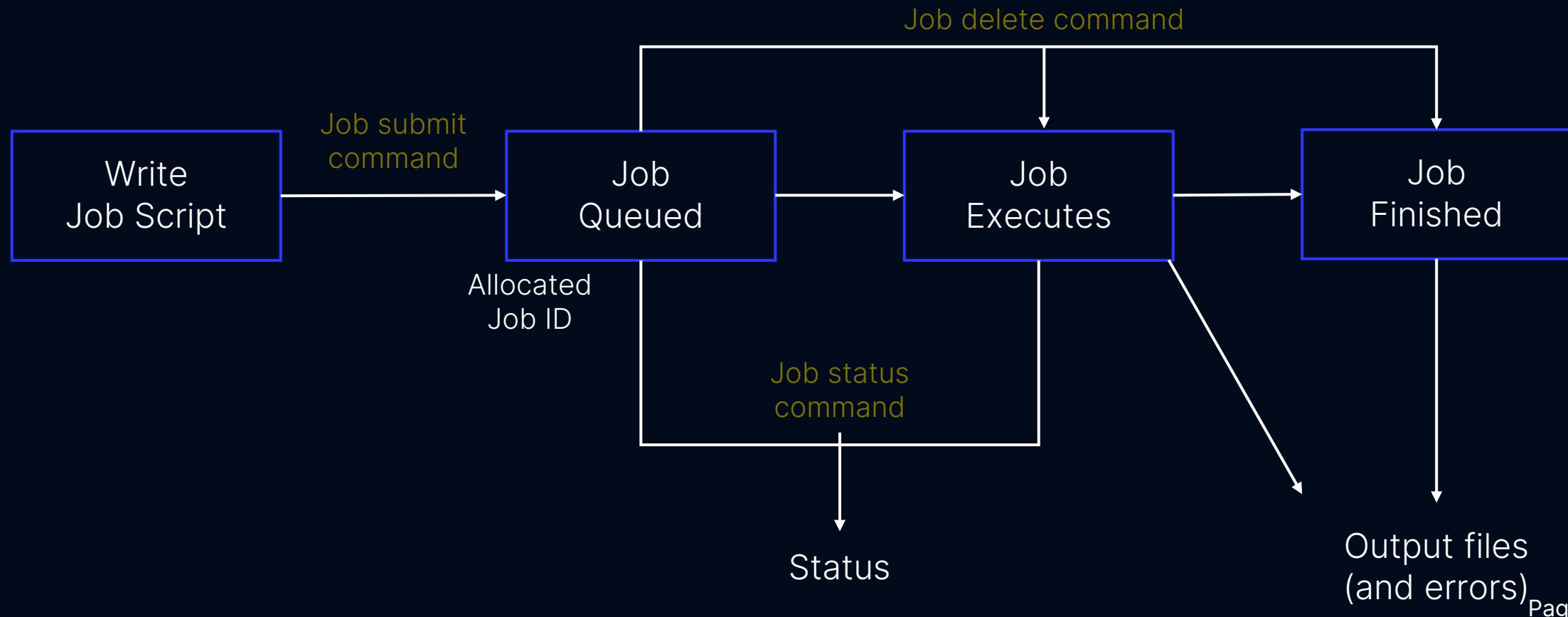
Hands-on - Distributed Deep Learning

- Workflow on the batch system
- Use job scripts to execute algorithms with more nodes (i.e., > 1 GPUs)

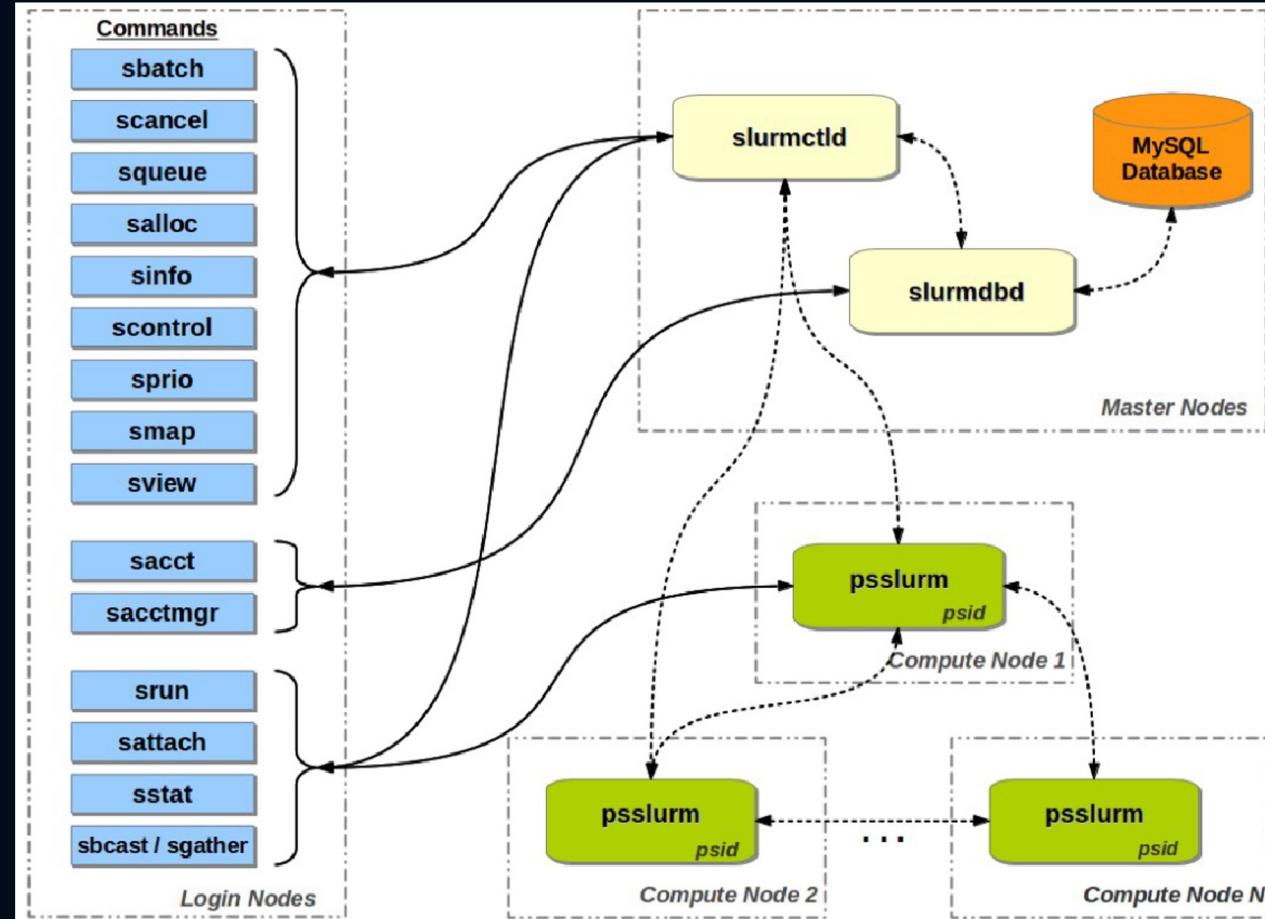


USING THE SUPERCOMPUTER MEANS SUBMITTING A JOB TO A BATCH SYSTEM

Job scheduling according to priorities. The jobs with the highest priorities will be scheduled next.



THE SLURM BATCH SYSTEM



NO NODE-SHARING



SUPERCOMPUTER USAGE MODEL AT JSC

Additional information

- Compute time allocation is based on compute projects. For every compute job, a compute project pays.
- Data projects allocate large amounts of storage, but no compute.
- To enable fair share, only relatively short job runs (24h) are allowed.
 - Please implement check pointing (or make your code fast enough).
- Solution for long-running tasks: Job arrays.

MODULE SYSTEM: SOFTWARE

All kind of software is already installed in modules.

Compiler/GCCcore/9.3.0		
AOCC/2.3.0	JupyterKernel-Ruby/2.7.1-2020.2.6	git/2.28.0
Autotools/20200321	JupyterProxy-Matlab/0.1.0-2020.2.6	gnuplot/5.2.8
Bazel/3.4.1	JupyterProxy-XpraHTML5/0.3.0-	h5py/2.10.0-serial-Python-
Bazel/3.6.0	2020.2.6	3.8.5
Boost_Python/1.74.0-nompi	LLVM/10.0.1	hwloc/2.2.0
Boost/1.74.0-nompi	METIS/5.1.0-IDX64	jemalloc/5.2.1
CFITSIO/3.490	MPFR/4.1.0	libvpx/1.9.0
CMake/3.18.0	Mercurial/5.5.2-Python-3.8.5	likwid/5.0.2
CVS/1.11.23	Meson/0.55.0-Python-3.8.5	likwid/5.1.0
Cirq/0.9.1-Python-3.8.5	NCCL/2.8.3-1-CUDA-11.0	magma/2.5.4
Clang/11.0.0	NSPR/4.25	meld/3.21.0-Python-3.8.5
Cling/0.7	NSS/3.51	memkind/1.10.1
Cling/0.9	Ninja/1.10.0	nano/5.5
CubeGUI/4.5	Nsight-Compute/2020.1.2	netCDF-C++4/4.3.1-serial
CubeGUI/4.6	Nsight-Compute/2020.2.0	netCDF-Fortran/4.5.3-serial
CubeLib/4.5	Nsight-Compute/2020.3.0	netCDF/4.7.4-serial
CubeLib/4.6	Nsight-Systems/2020.3.1	netcdf4-python/1.5.4-serial-
DWave/3.2.0-Python-3.8.5	Nsight-Systems/2020.4.1	Python-3.8.5
Doxygen/1.8.18	Nsight-Systems/2020.5.1	numba/0.51.1-Python-3.8.5
Eigen/3.3.7	Nsight-Systems/2021.1.1	parallel/20201122
Emacs/27.1	Octave/6.1.0-nompi	pyproj/2.6.1.post1-Python-
FriBidi/1.0.9	OpenAI-Gym/0.18.0-Python-3.8.5	3.8.5
GDB/10.1	OpenCV/4.5.0-Python-3.8.5	qccint/3.0.19
GEOS/3.8.1-Python-3.8.5	OpenEXR/2.5.2	re2c/1.3

MODULE SYSTEM: COMMANDS

`module avail`

`module purge # unload everything`

`module load`

`module spider`

module spider nano

```
[kesselheim1@jwlogin07 ~]$ module spider nano
```

```
nano: nano/5.5
```

Description:

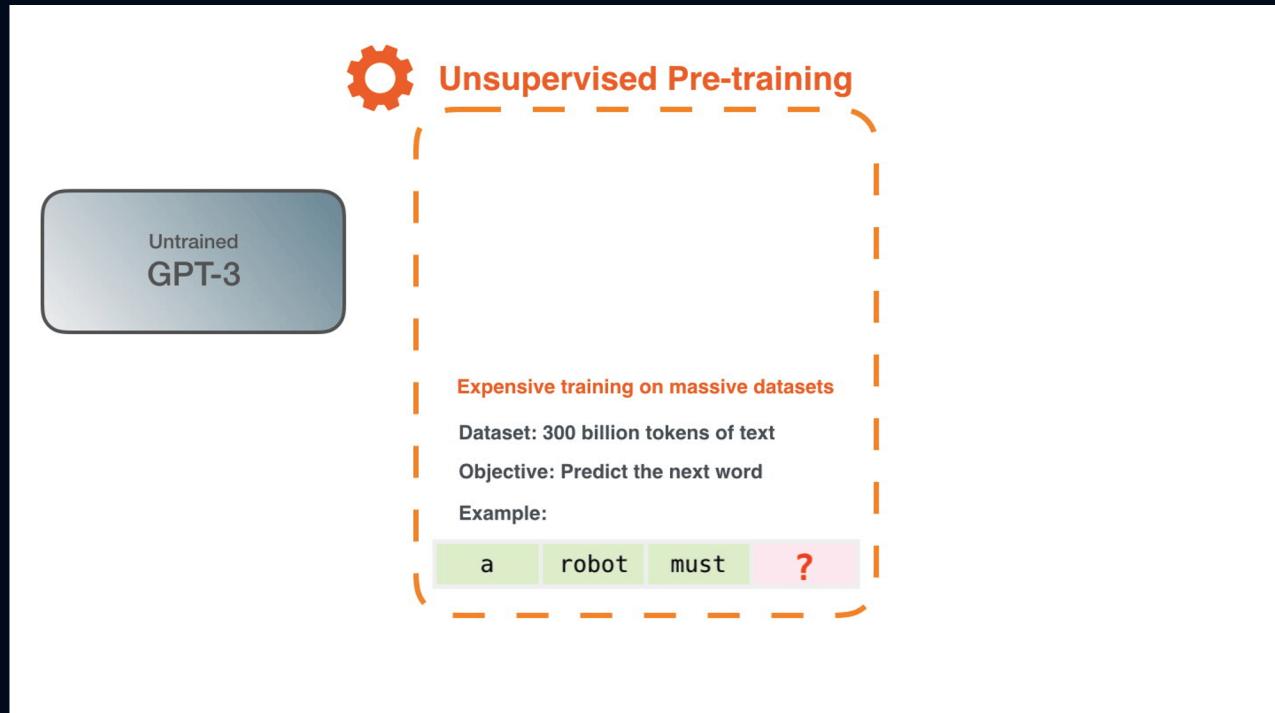
GNU nano is a small and friendly text editor. Besides basic text editing, nano offers features like undo/redo, syntax coloring, interactive search-and-replace, auto-indentation, line numbers, word completion, file locking, backup files, and internationalization support.

module load nano

`module avail`

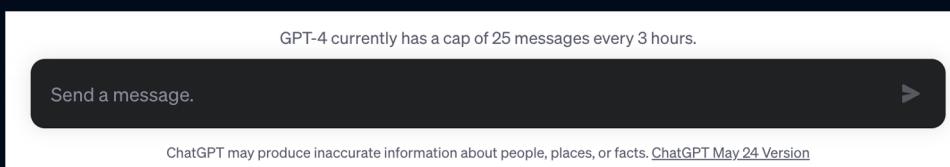
Core packages	(D)	(L)
Python/3.8.5		
R/4.0.2-nompi		
Ruby/2.7.1		
RusL/1.47.0		
SciPy-Stack/2020-Python-3.8.5		
Shapely/1.7.1-Python-3.8.5		
Singularity-Tools/2020-Python-3.8.5		
StdEnv/2020		
Subversion/1.14.0		
Tcl/8.6.10		
TensorFlow/2.3.1-Python-3.8.5		
TotalView/2020.1.13		
UCX/1.8.1		
UCX/1.9.0		
VTune/2019_update8		
Vampir/9.9.0		
VirtualGL/2.6.4		
Voron++/0.4.6		
X11/20200222		

FOUNDATION MODELS



- Large deep learning models trained on a vast quantity of data at scale (often by self-supervised learning or semi-supervised learning)
- They can be adapted to a wide range of downstream tasks
- Early examples of foundation models were pre-trained large language models, e.g., GPT foundation models

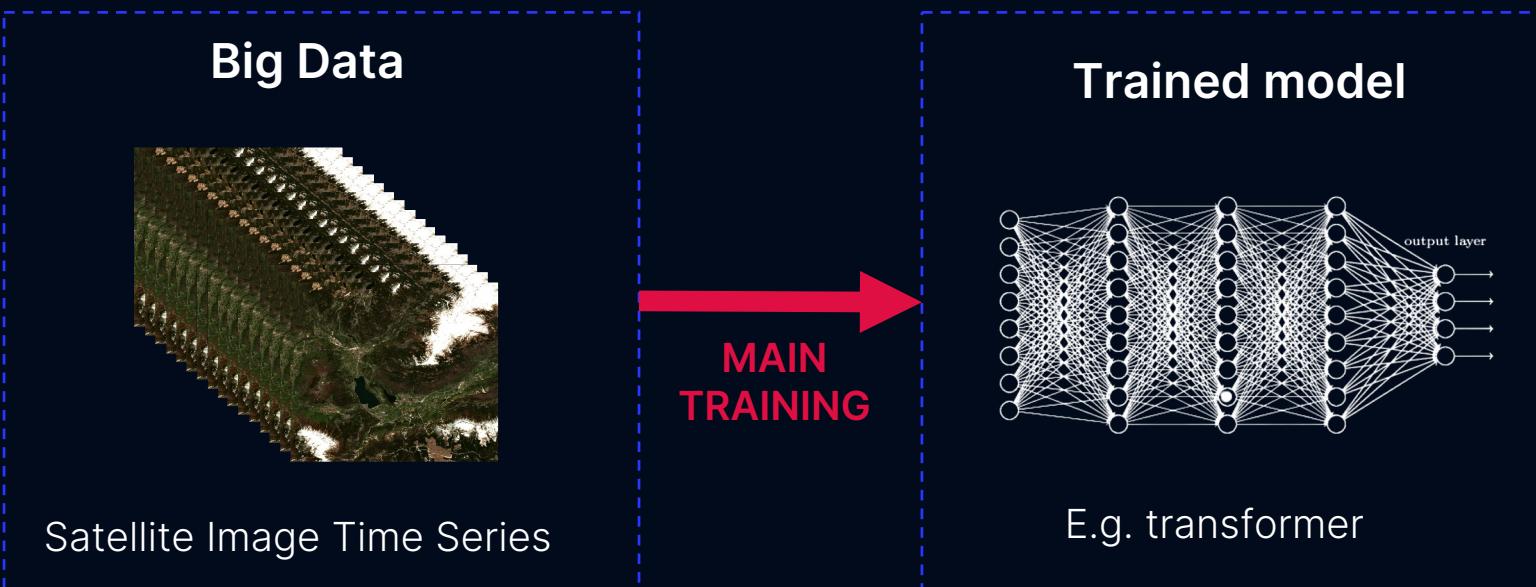
Jay Alammar, How GPT3 Works - Visualizations and Animations, <http://jalammar.github.io/how-gpt3-works-visualizations-animations/>



HOW TO CREATE A FOUNDATION MODEL?

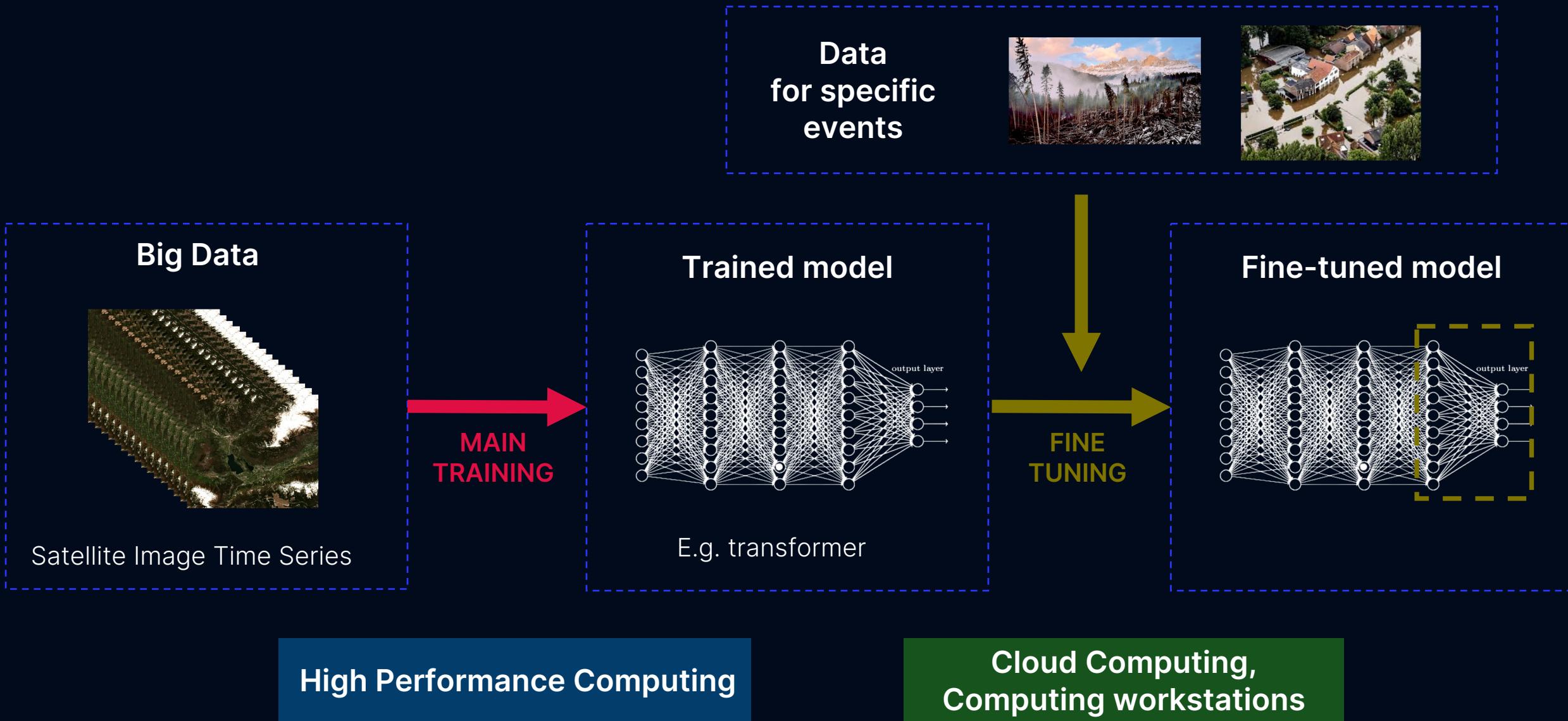
- 1) Gather data at scale
- 2) Train foundation model one time and evaluate
- 3) Fine-tune model for multiple downstream tasks
- 4) Inference (operational)

2. TRAIN FOUNDATION MODEL ONE TIME AND EVALUATE



High Performance Computing

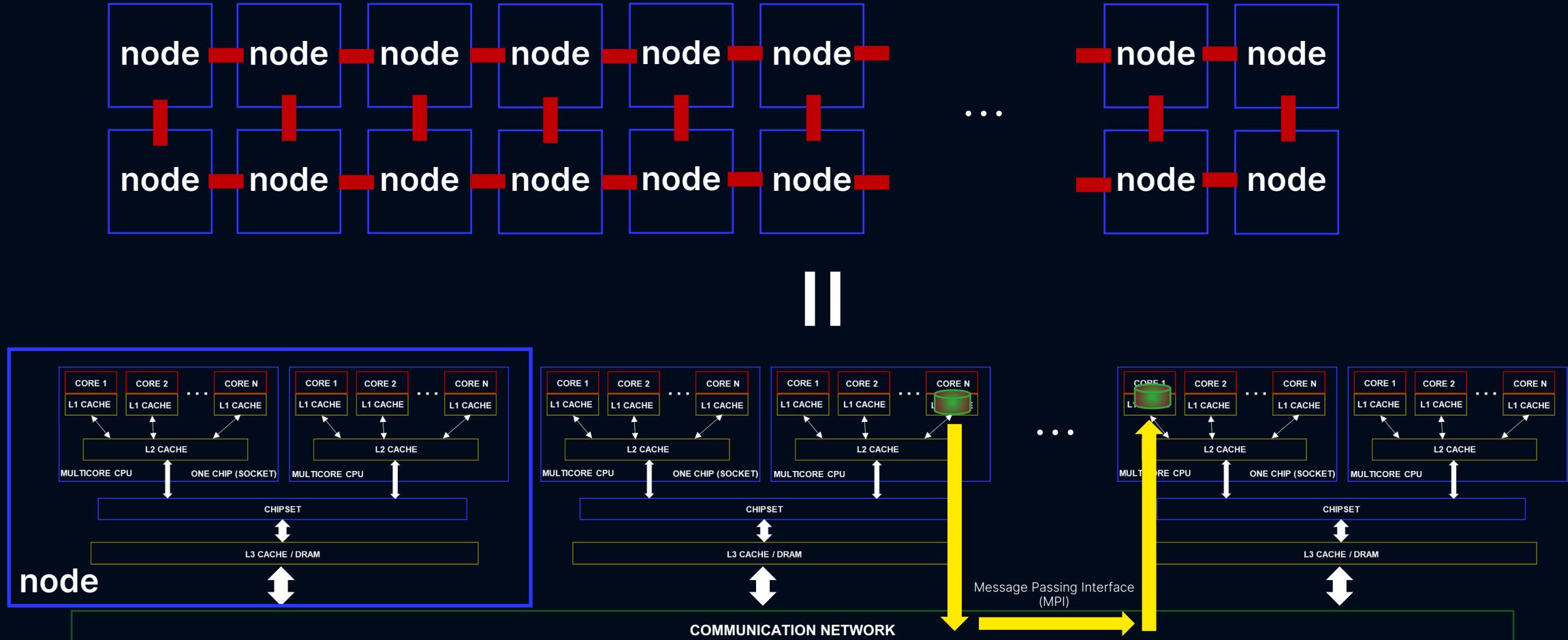
3. FINE-TUNE MODEL FOR MULTIPLE DOWNSTREAM USES



DISTRIBUTED DEEP LEARNING WITH HPC

WHAT IS A SUPERCOMPUTER?

Mixture of shared-memory and distributed-memory architectures



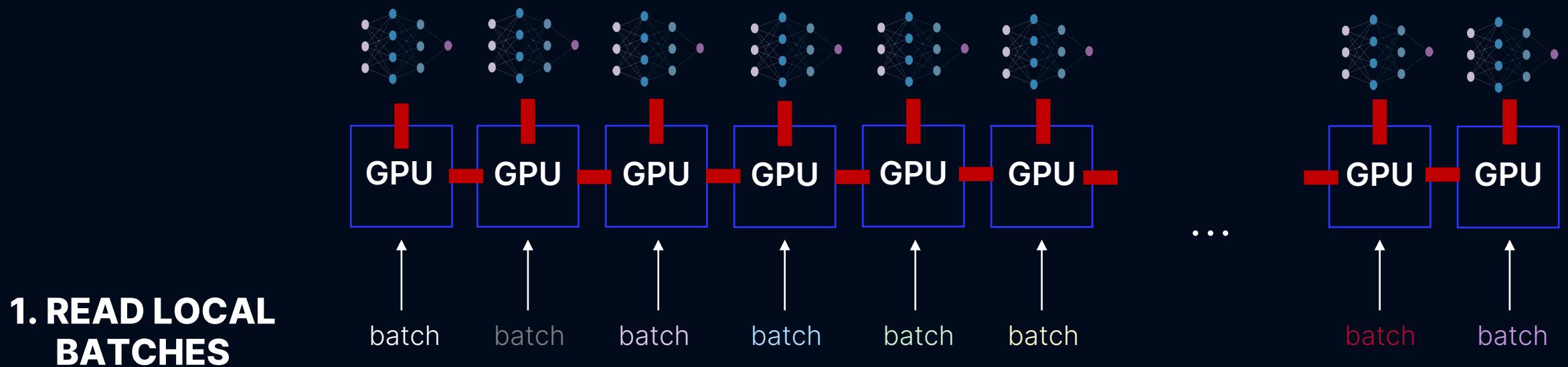
RECALL MINI-BATCH GRADIENT DESCENT

1. Initialize weights randomly $\sim \mathcal{N}(0, \sigma^2)$
2. Loop until convergence
3. Pick batch of B data points

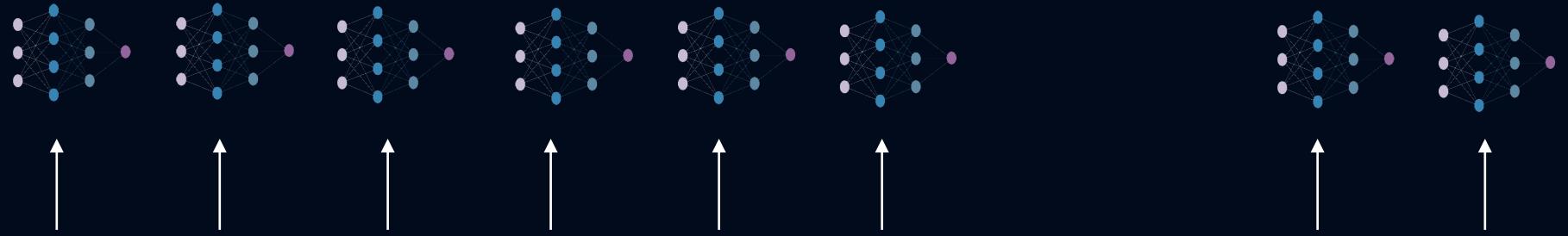
4. Compute gradient
$$\nabla h(W) = \frac{1}{B} \sum_{i=1}^B \nabla h_i(W)$$

Can use parallelization

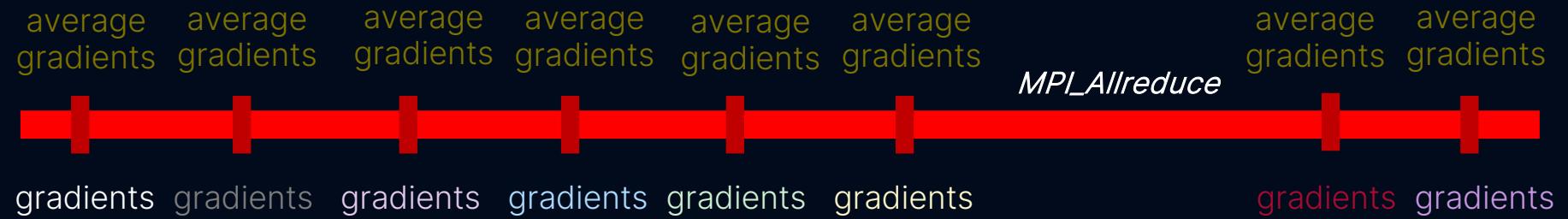
DISTRIBUTED TRAINING WITH DATA PARALLELISM: REPLICATE THE MODEL AND TRAIN ON LOCAL BATCHES



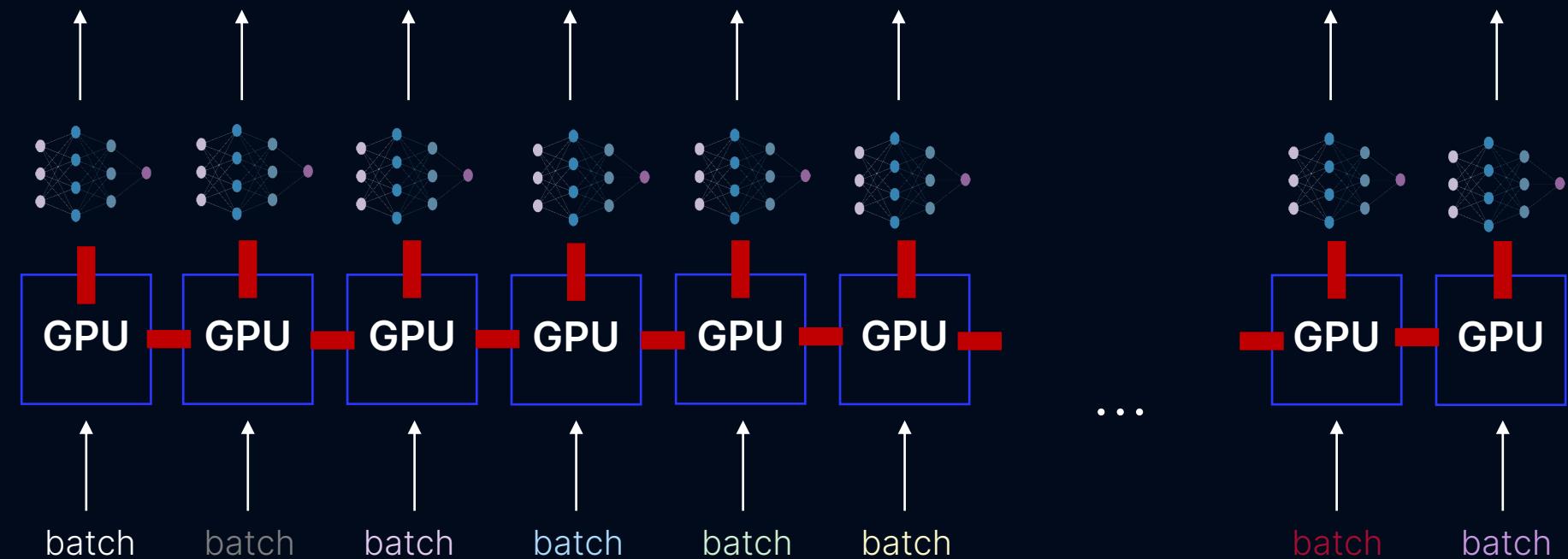
4. UPDATE MODEL



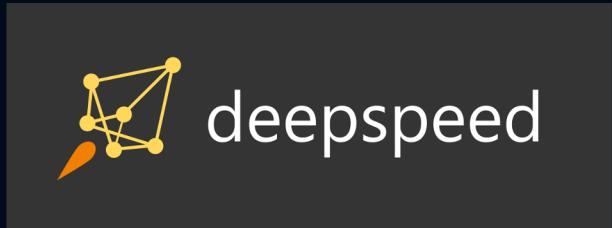
3. AVERAGE THE GRADIENTS



2. COMPUTE LOCAL GRADIENTS



DISTRIBUTED DEEP LEARNING FRAMEWORKS FOR HPC



<https://github.com/microsoft/DeepSpeed>



<https://github.com/horovod/horovod>

...

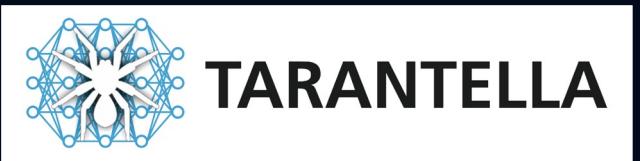


<https://github.com/helmholtz-analytics/heat>

...



<https://pytorch.org/tutorials/>



<https://github.com/cc-hpc-itwm/tarantella>

HOROVOD: DISTRIBUTED TRAINING FRAMEWORK WITH DATA PARALLELISM



Works on top of MPI and NCCL

On top of Tensorflow, Keras, PyTorch, MxNet

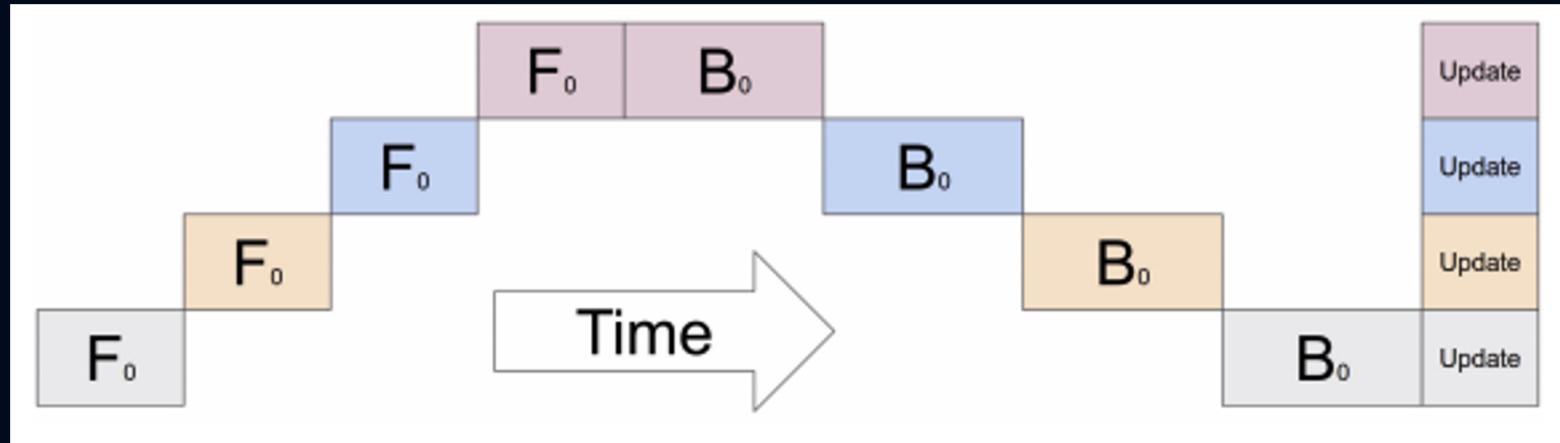
A. Sergeev and M. D. Baloo, "Horovod: Fast and Easy Distributed Deep Learning in TensorFlow", arXiv:1802.05799, 2018.

PYTORCH NATIVE DISTRIBUTED ALGORITHMS



PyTorch DDP similar to Horovod:

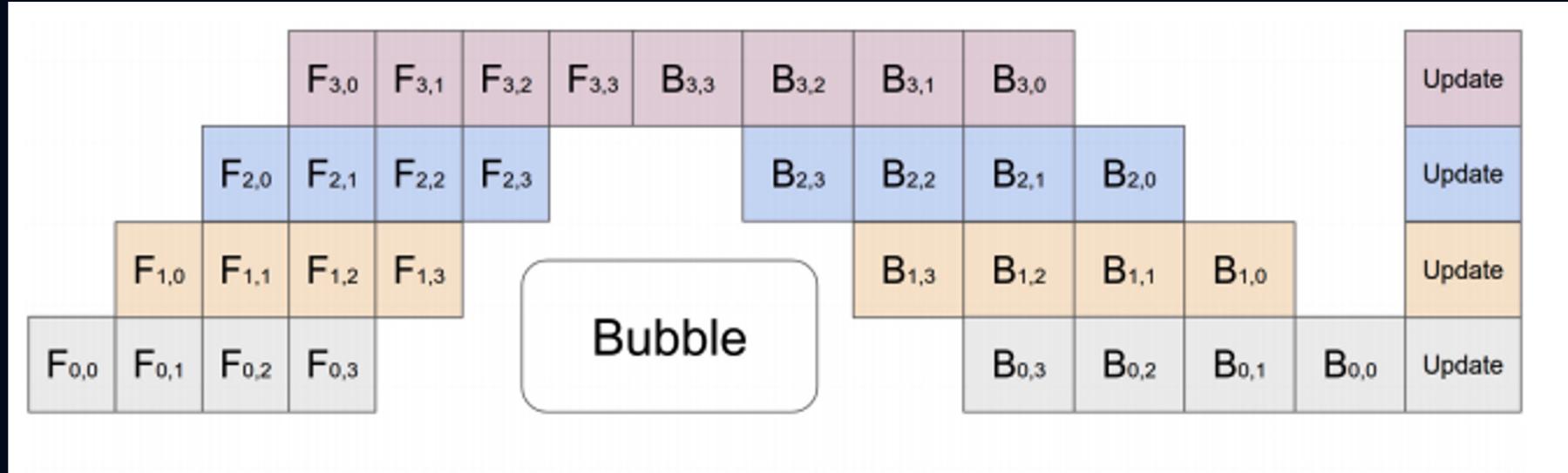
MODEL PARALLELISM



<https://pytorch.org/docs/stable/pipeline.html>

Model parallelism splits the model across multiple GPUs

PIPELINING



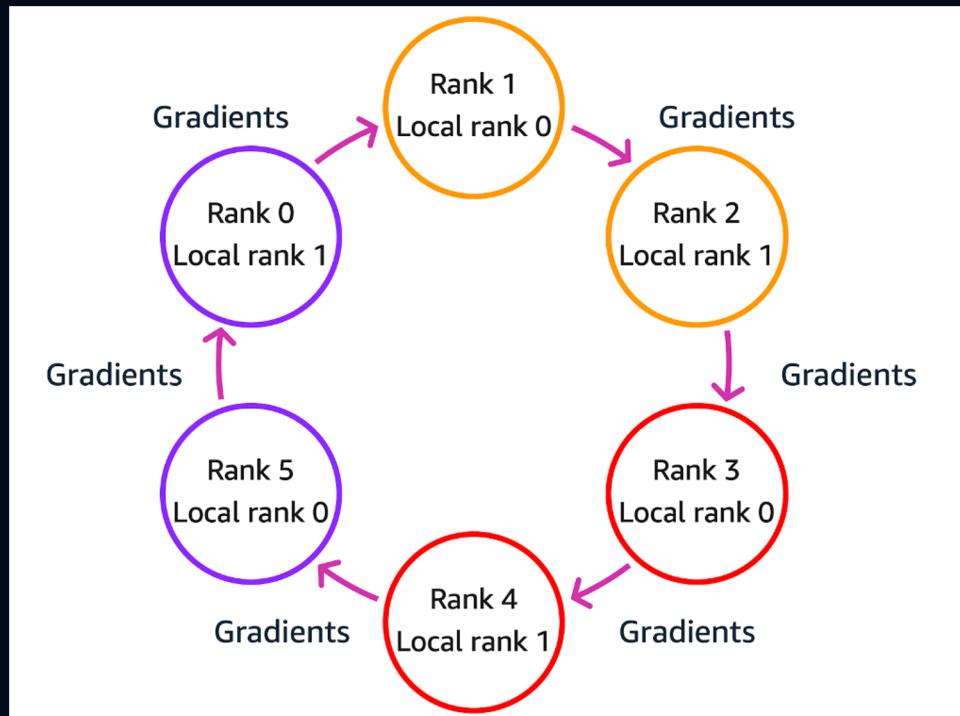
<https://pytorch.org/docs/stable/pipeline.html>

Pipelining splits the input minibatch into multiple microbatches and pipelines the execution of these microbatches across multiple GPUs

HOROVOD USES RING-ALLREDUCE TO AVERAGE GRADIENTS AND UPDATE ALL COPIES OF THE MODELS

Arranges processes in a logical ring

Each process receives data from it's "left" neighbor and sends data to it's "right" neighbor



Makes communication cost independent of the number of processes

HDCRS

GEOSCIENCE AND REMOTE SENSING SOCIETY (GRSS)

One of the 39 societies of IEEE



Mission



Develop concepts and techniques of RS of the Earth, oceans, atmosphere, and space, as well as processing, interpretation, and dissemination of this information for the benefit of society

Facts



Founded in 1961

~4,200 members in 94 countries

69 chapters, 22 student chapters, and 11 ambassadors all over the world

GRSS TECHNICAL COMMITTEES

Earth Science Informatics



Geoscience Spaceborne Imaging Spectroscopy



Instrumentation and Future Technologies



Remote sensing Environment, Analysis and Climate Technologies



Frequency allocations in Remote Sensing



Image Analysis and Data Fusion



Modeling in Remote Sensing



GRSS Standards for Earth Observations



EARTH SCIENCE INFORMATICS (ESI) TECHNICAL COMMITTEE

Objectives

Advance application of informatics to
geoscience and remote sensing

<https://www.grss-ieee.org/technical-committees/earth-science-informatics/>

Chairs



Peter Baumann



Manil Maskey

TWO WORKING GROUPS

High-performance and Disruptive Computing in Remote Sensing (HDCRS)



Gabriele Cavallaro



Dora Blanco Heras



Jin Sun

Databases in Remote Sensing (DBRS)



Dai-Hai Ton
That



Kesheng (John)
Wu



Khalid
Belhajjame

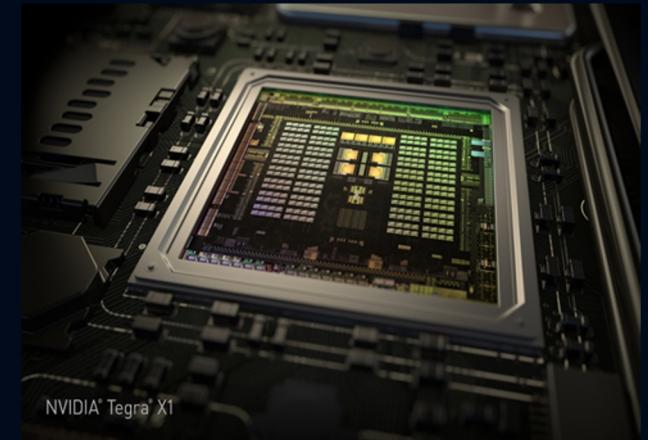
High Performance and Disruptive Computing in Remote Sensing Working Group

Main Objective:

Connect and support the community of interdisciplinary researchers in remote sensing who are specialized in emerging computing paradigms

The idea:

Innovative computing technologies applied to efficient computation of remote sensing problems



<https://www.grss-ieee.org/community/groups-initiatives/high-performance-and-disruptive-computing-in-remote-sensing-hdcrs/>

COME ABOARD

About Earth Science Informatics



MISSION

The Earth Science Informatics Technical Committee (ESI TC) provides a venue for informatics professionals to exchange ideas and share knowledge. It aims at advancing application of informatics to geosciences and remote sensing, assessing technology to support data stewardship and management, and promoting best practices and lessons learned.

The mission of the ESI TC is to bring together informatics experts and practitioners to share ideas and information to support open science and maximize the use of science data for research and applications.

JOIN ESI

<https://www.grss-ieee.org/technical-committees/earth-science-informatics/>

Activities

HDCRS SUMMER SCHOOL - 2023



Teaching material and videos will be soon available

<https://www.grss-ieee.org/community/groups-initiatives/high-perfomance-and-disruptive-computing-in-remote-sensing-hdcrs/hdcrs-summer-school-2023/>



ACTIVITIES AT IGARSS 2023

Tutorial on End-to-End Machine Learning with Supercomputing and in the Cloud



Hands-on experience in Supercomputer Systems and Cloud Computing Services for Remote Sensing Applications

Community Contributed Sessions



- (1) Scalable Parallel Computing for Remote Sensing
- (2) Quantum computing next generation HPC
- (3) Quantum Machine Learning algorithms for EO



<https://2023.ieeeigarss.org/>

Thank you for your attention