Lecture 4.1 - Distributed Deep Learning with High Performance Computing

End-to-End Machine Learning with High Performance and Cloud Computing - Tutorial IGARSS 2022

17.07.2022

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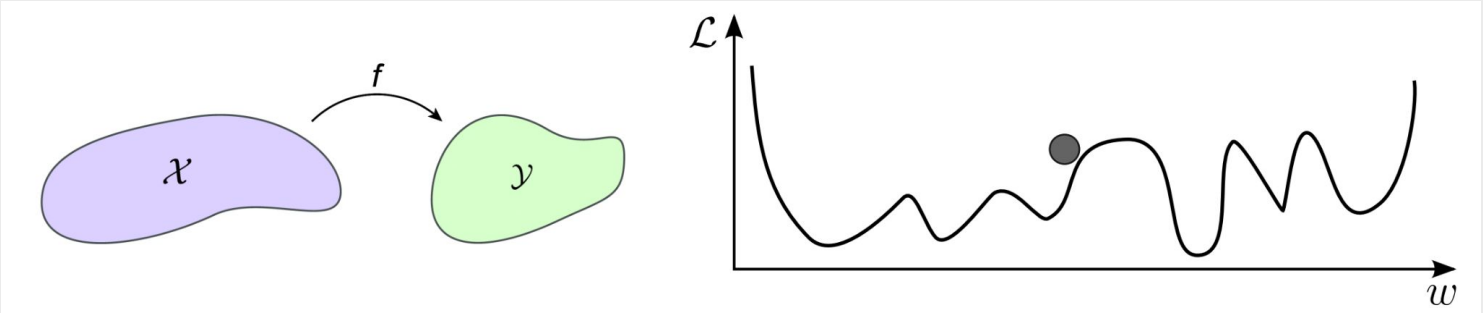
Outline

- Recap of basic concepts of Deep Learning
- Introduction to HPC
- MPI and other communication backends
- Introduction to Distributed Deep Learning
- Frameworks
- Final Remarks

Recap of basic DL concepts

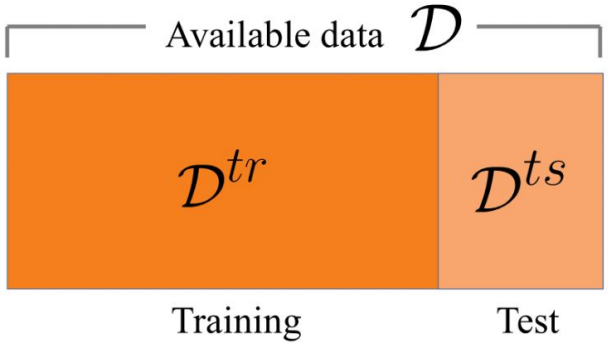
Optimization

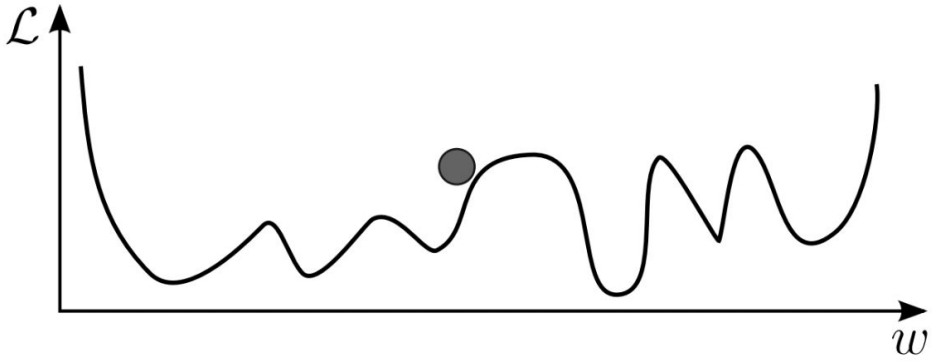
- Optimizing loss (objective) of a (complex) model f on data D
- a (complex) model: function (or distribution) family $f(X;\theta)$ $(p(X;\theta))$
- parameters θ are to adapt ("fit") given the data $X \in D$
- optimization: defining a loss $L(f(X;\theta), D)$
- loss L: measure of quality ("fit") of the model f in terms of a task solution on D
- Objective: minimize $L(f(X;\theta), D)$



Generalization

- Estimate $L(f(X;\theta), D^{unseen})$: aiming for good generalization capability
- General approach: split D into disjoint D_{tr} and D_{ts}, $D_{tr} \cap D_{ts} = \varnothing$
- train on D_{tr}
- generalization error on D_{ts} after training

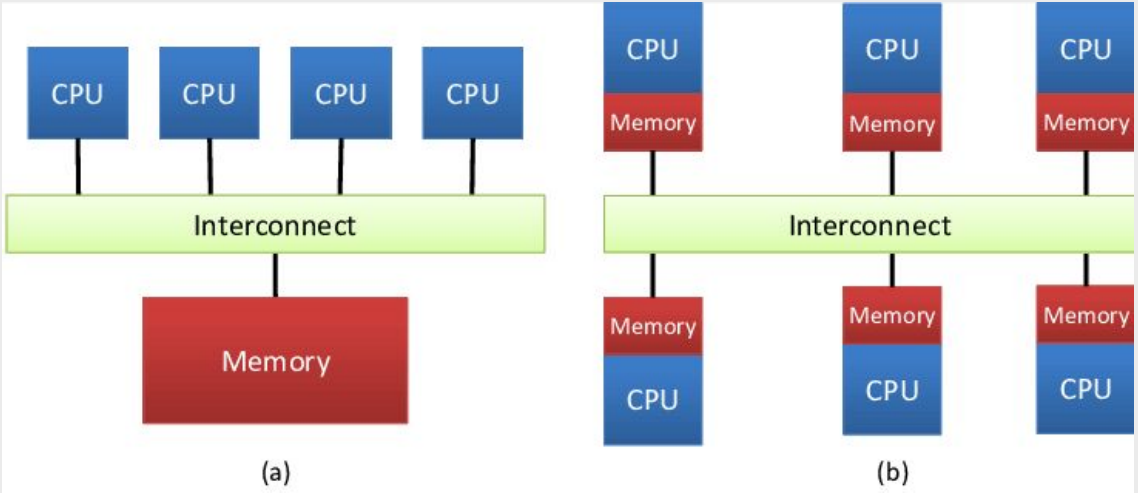




HPC

Hardware Levels of Parallelism

- (a) Single-machine (shared memory) (b) Multi-machine (distributed memory)



https://www.researchgate.net/publication/302245489_Adaptation_Strategies_in_Multiprocessors_System_on_Chip

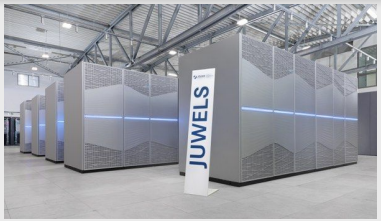
HPC

HPC at the frontline of computing power

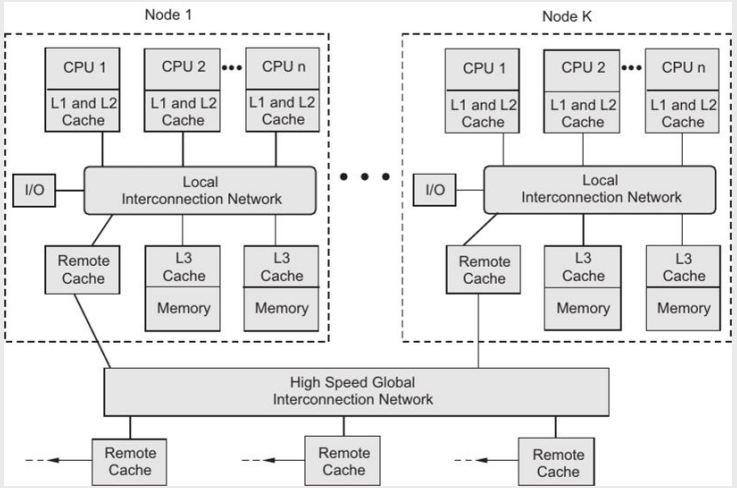
It includes work on ‘four basic building blocks’:

- Theory (numerical laws, physical models, speed-up performance, etc.)
- Technology (multi-core, supercomputers, networks, storages, etc.)
- Architecture (shared-memory, distributed-memory, interconnects, etc.)
- Software (libraries, schedulers, monitoring, applications, etc.)

Architecture: Shared-memory building blocks interconnected with a fast network (e.g., InfiniBand)



https://www.fz-juelich.de/de/ias/jsc

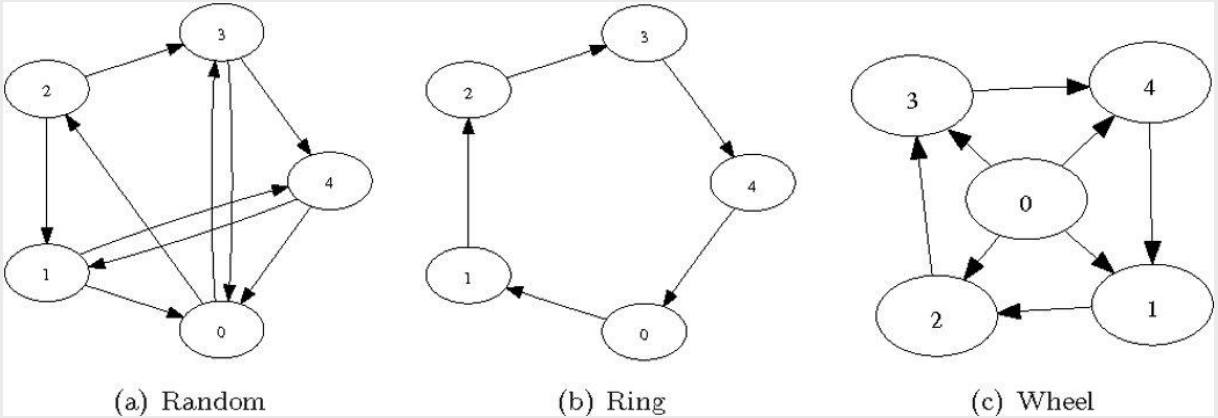


https://ebrary.net/206293/computer_science/distributed_shared_memory_multiprocessors_numa_model

Communication Backend

MPI

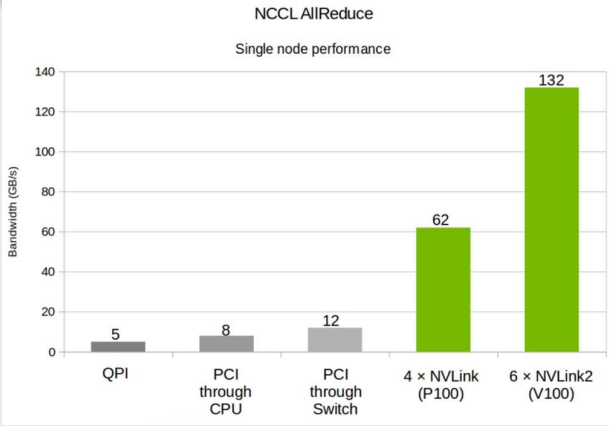
- MPI is a **standard** for **exchanging messages** between multiple computers running a parallel program across **distributed memory**
- Point-to-point and collective communication are supported
- **Different topologies** can be implemented
- Parallel I/O operations
- Blocking and non blocking statements

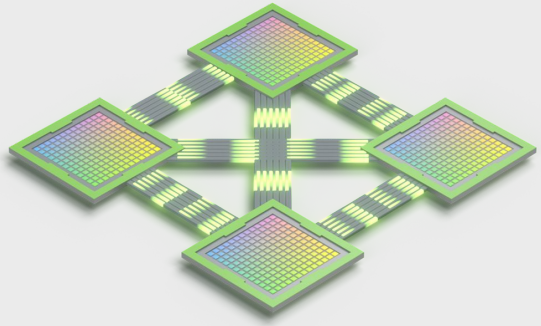


Hoefler, T., Rabenseifner, R., Ritzdorf, H., de Supinski, B. R., Thakur, R., & Träff, J. L. (2010). The scalable process topology interface of MPI 2.2. Concurrency and Computation: Practice and Experience, 23(4), 293–310. https://doi.org/10.1002/cpe.1643

NCCL

- NVIDIA Collective Communications Library (NCCL) [19]
- Provides **optimized implementation of inter-GPU communication** operations, such as allreduce and variants
- Optimized for **high bandwidth and low latency** over PCI and NVLink/NVSwitch high speed interconnect for intra-node communication (up to 16 GPUs)
- Sockets and InfiniBand for inter-node communication
- For a comparison between communication backends look at: [https://mlbench.github.io/2020/09/08/communication-backend-comparison/]





https://developer.nvidia.com/blog/scaling-deep-learning-training-nccl/

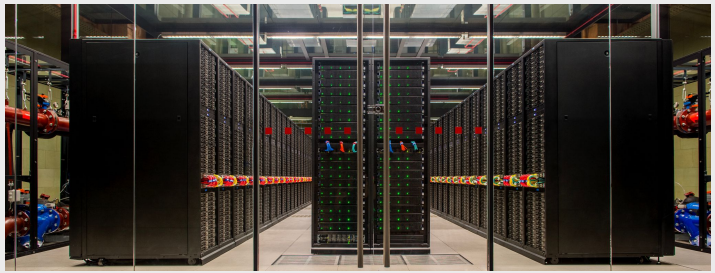
RCCL

- AMD's port of NCCL: ROCm Communication Collectives Library (RCCL) uses the same C API as NCCL
- NCCL APIs do not need to be converted

https://github.com/RadeonOpenCompute/ROCm

https://lumi-supercomputer.eu/easybuild-lumis-primary-software-installation-tool-introduced/

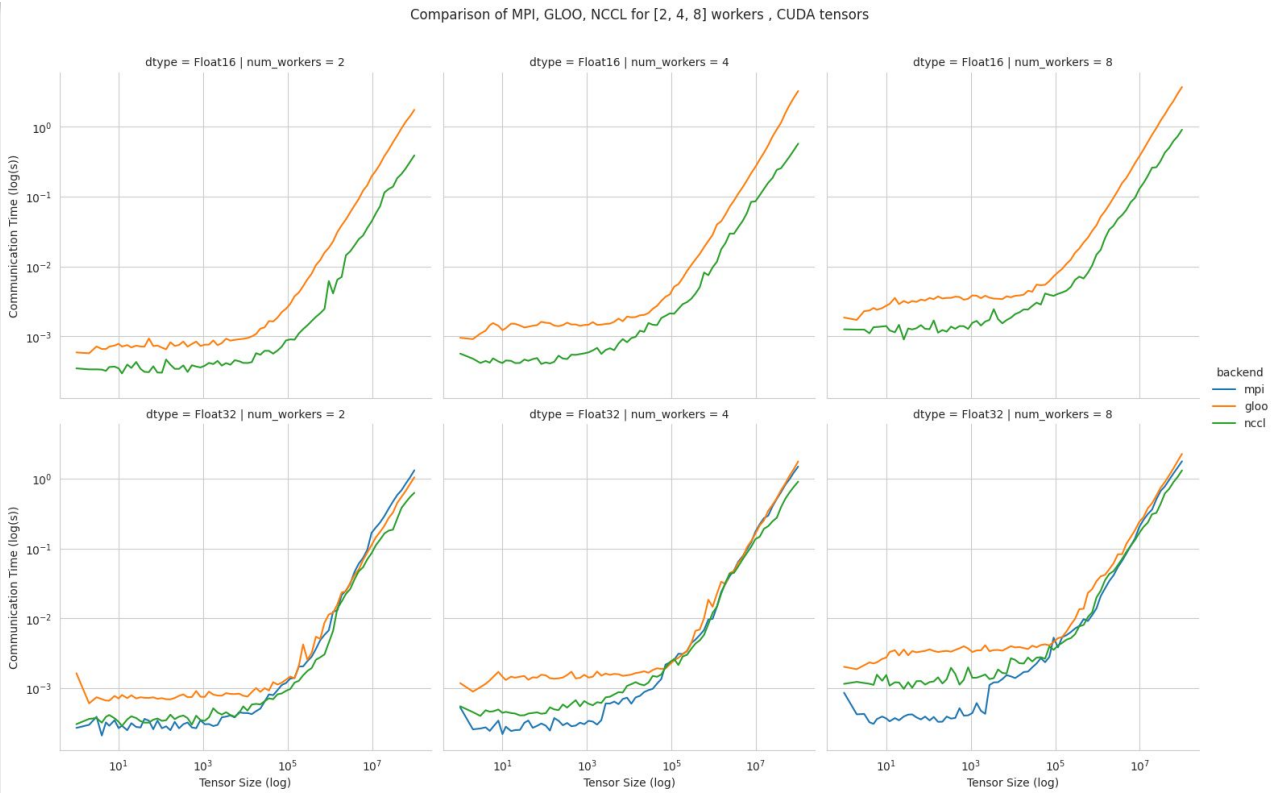
https://hwrig.com/amd-instinct-gpu-and-epyc-are-making-lumi-in-2021/



https://www.bsc.es/innovation-and-services/technical-information-cte-amd

Benchmark

- For a comparison between communication backends look at: [https://mlbench.github.io/2020/09/08/communication-backend-comparison/]
- MPI vs Gloo vs NCCL



Motivation

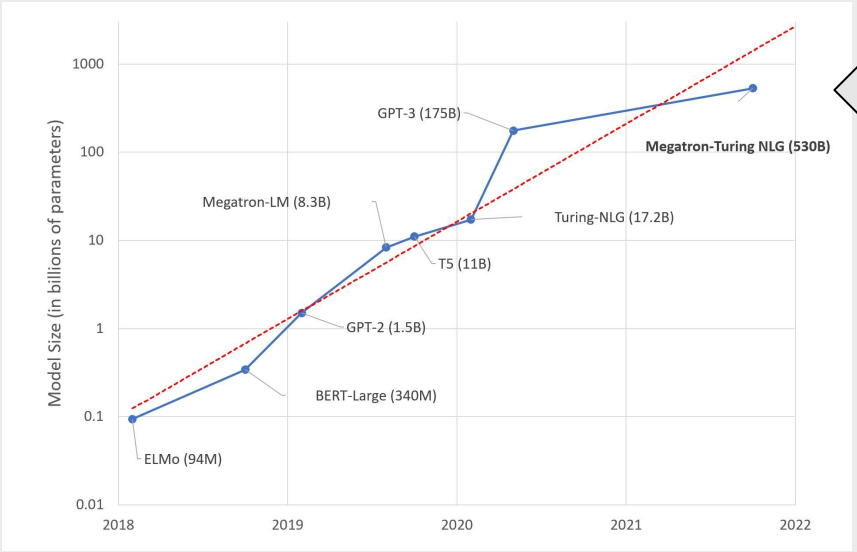
Motivation

In recent years almost exponential increase of number of parameters of the models

2020

https://www.microsoft.com/en-us/research/blog/a-deep-generative-model-trifecta-three-advances-that-work-towards-harnessing-large-scale-power/

2022

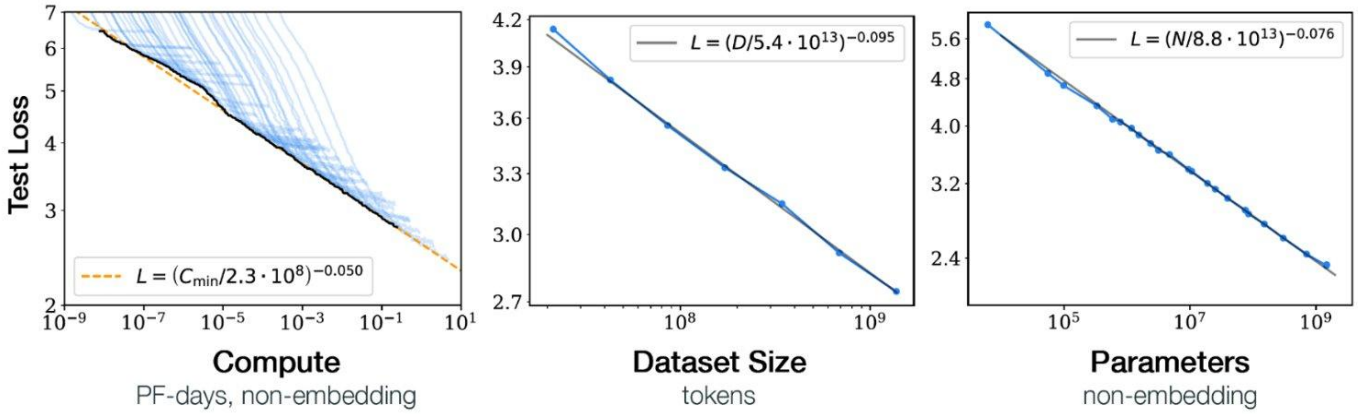


https://huggingface.co/blog/large-language-models

Motivation

- Bigger models require bigger datasets
- Consequence -> More resources are needed (both memory and computation power)

	Data Set	Type	Task	Size
small	MNIST	Image	Classification	55,000
small	Fashion MNIST	Image	Classification	55,000
small	CIFAR-10	Image	Classification	45,000
large	ImageNet	Image	Classification	1,281,167
large	Open Images	Image	Classification (multi-label)	4,526,492
large	LM1B	Text	Language modeling	30,301,028
large	Common Crawl	Text	Language modeling	~25.8 billion

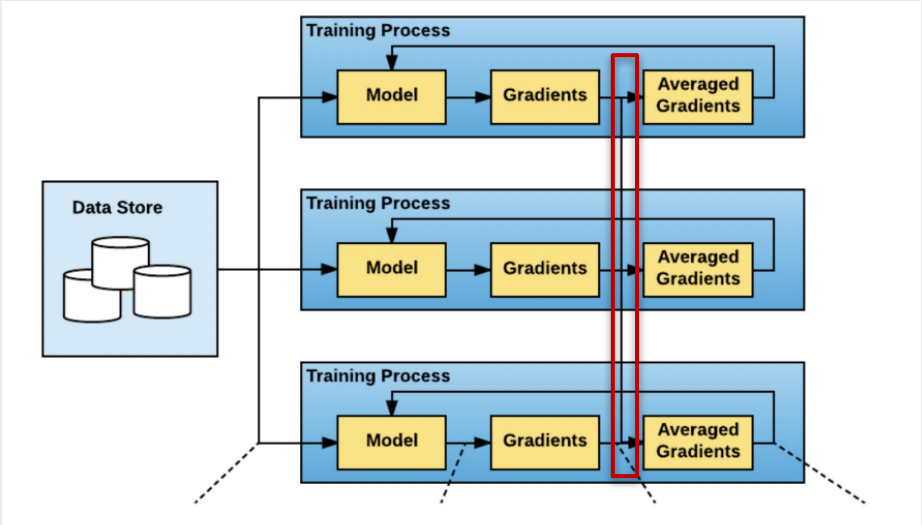


Kaplan et al., “Scaling Laws for Neural Language Models”, 2020, https://arxiv.org/abs/2001.08361

Distributed Deep Learning

Data Parallelism

- Concept: split the data
- The gradients for different batches of data are calculated separately on each node
- But averaged across nodes to apply consistent updates to the model copy in each node

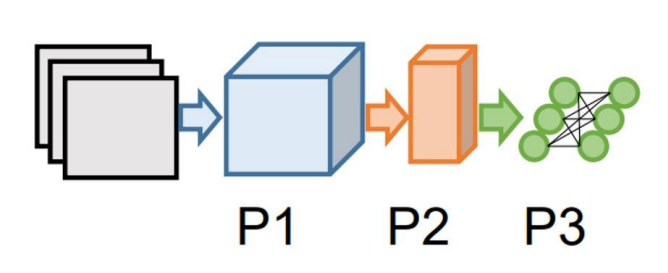


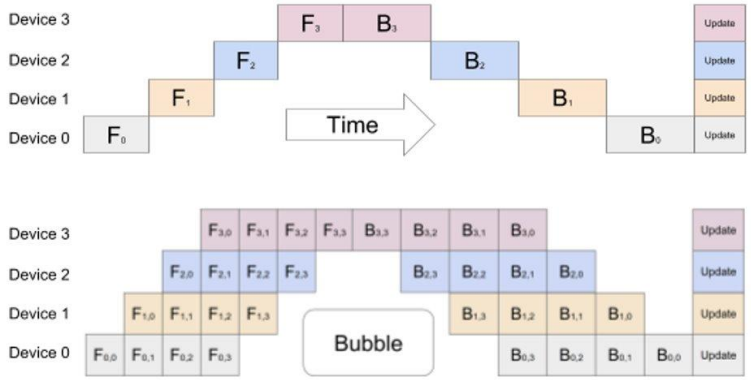
A. Sergeev and M. D. Balso, "Horovod: Fast and Easy Distributed Deep Learning in TensorFlow", arXiv:1802.05799, 2018

Model Parallelism

Concept: split the model
Pipelining:

- partitioning the DNN according to depth, assigning layers to specific processors
- overlapping computations, i.e., between one layer and the next (as data becomes ready)





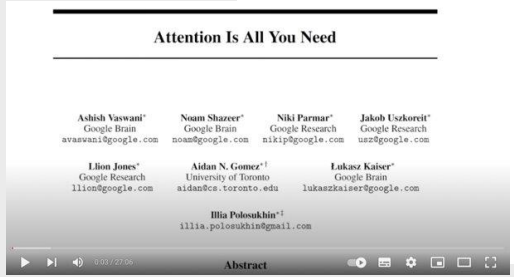
Top: The naive model parallelism strategy leads to severe underutilization due to the sequential nature of the network. Only one accelerator is active at a time. Bottom: GPipe divides the input mini-batch into smaller micro-batches, enabling different accelerators to work on separate micro-batches at the same time.

[https://huggingface.co/docs/transformers/parallelism]

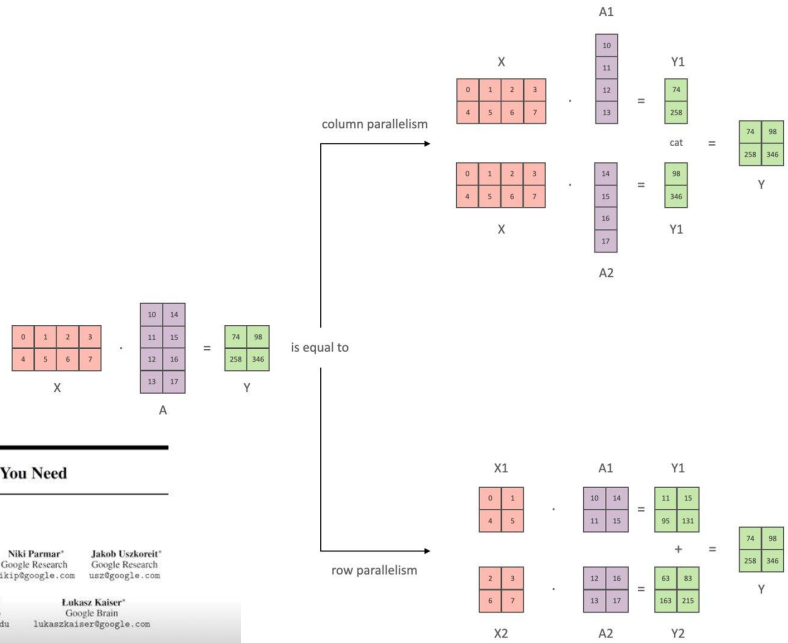
Model Parallelism

Tensor parallelism:

- matrix operations (f.e. matrix multiplication) can be split between multiple GPUs
- Scaling large transformers with multihead self-attention is based on this concept



[https://www.youtube.com/watch?v=iDulhoQ2pro&ab_channel=YannicKilcher]

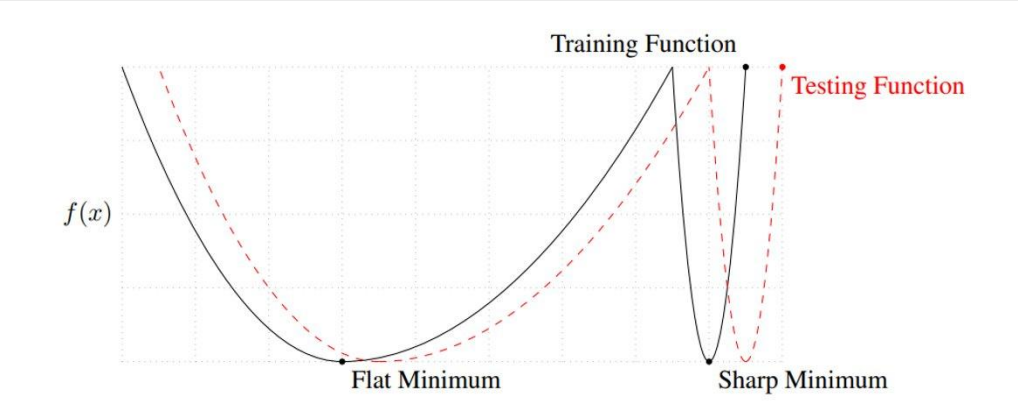


[https://huggingface.co/docs/transformers/parallelism]

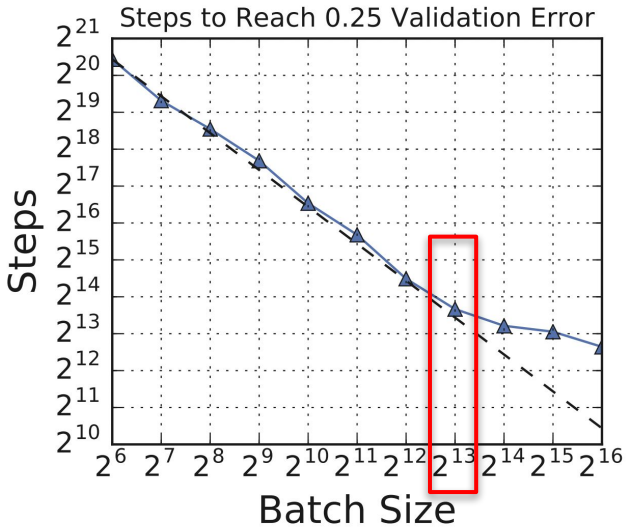
Challenges

- Poor generalization due to sharp minima

  [Hochreiter, Sepp and Schmidhuber, Jürgen. Flat minima. Neural Computation, 9(1):1–42, 1997]
- Time to accuracy does not decrease



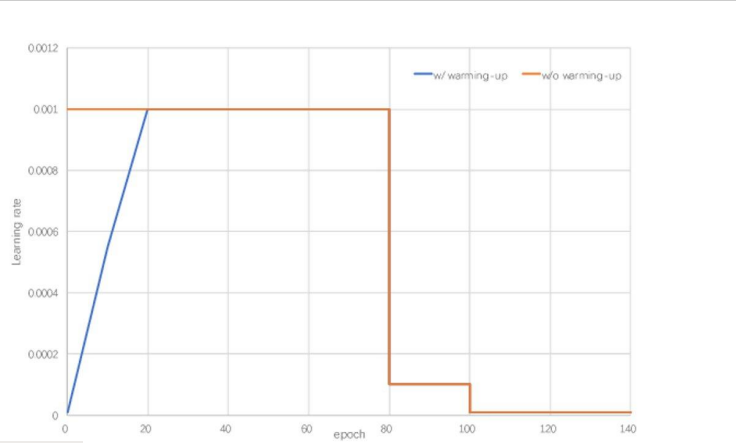
N. S. Keskar and D. Mudigere and J. Nocedal and M. Smelyanskiy and P.T.P. Tang, On Large-Batch Training for Deep Learning: Generalization Gap and Sharp Minima, 2016



Shallue et al., 2019, https://arxiv.org/pdf/1811.03600.pdf

Solution

- For batch size < 8000
  - Scale learning rate
  - Warm-up
- For batch size > 8000
  - Choice of the optimizer:
    - LARS
    - LAMB
    - post-local SGD



Warm-up

	Hardware	Software	Batch size	Optimizer	# Steps	Time/step	Time	Accuracy
Goyal *et al.* [3]	Tesla P100 × 256	Caffe2	8,192	SGD	14,076	0.255 s	1 hr	**76.3** %
You *et al.* [11]	KNL × 2048	Intel Caffe	32,768	SGD	3,519	0.341 s	20 min	75.4 %
Akiba *et al.* [10]	Tesla P100 × 1024	Chainer	32,768	RMSprop/SGD	3,519	0.255 s	15 min	74.9 %
You *et al.* [11]	KNL × 2048	Intel Caffe	32,768	SGD	2,503	0.335 s	14 min	74.9 %
Jia *et al.* [12]	Tesla P40 × 2048	TensorFlow	65,536	SGD	1,800	0.220 s	6.6 min	75.8 %
Ying *et al.* [16]	TPU v3 × 1024	TensorFlow	32,768	SGD	3,519	**0.037 s**	2.2 min	**76.3** %
Mikami *et al.* [13]	Tesla V100 × 3456	NNL	55,296	SGD	2,086	0.057 s	2.0 min	75.3 %
Yamazaki *et al.* [14]	Tesla V100 × 2048	MXNet	81,920	SGD	1,440	0.050 s	**1.2 min**	75.1 %

Osawa et al., 2020

Is that all?

- Still ongoing research
- Well-establish optimizers can match new ones with enough *hyperparameter tuning*

Batch size	Step budget	LAMB	Adam
32k	15,625	91.48	**91.58**
65k/32k	8,599	90.58	**91.04**
65k	7,818	–	**90.46**

https://openreview.net/pdf?id=Kloou2uk_Rz

Frameworks

Frameworks

Horovod

- *Data parallel*, each GPU has a copy of the model and a chunk of the data
- Efficient *decentralized framework*,

based on MPI and NCCL libraries, where actors exchange parameters without the need of a parameter server

- Works on top of Keras, TensorFlow, PyTorch and Apache MXNet

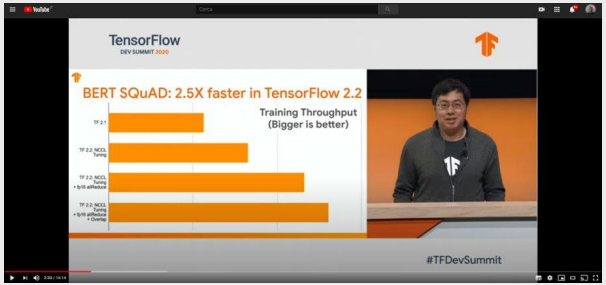
Tensorflow

- Parameter server for asynchronous training
- Mirrored strategy for synchronous training

Pytorch

- Distributed Data-Parallel Training (DDP)

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



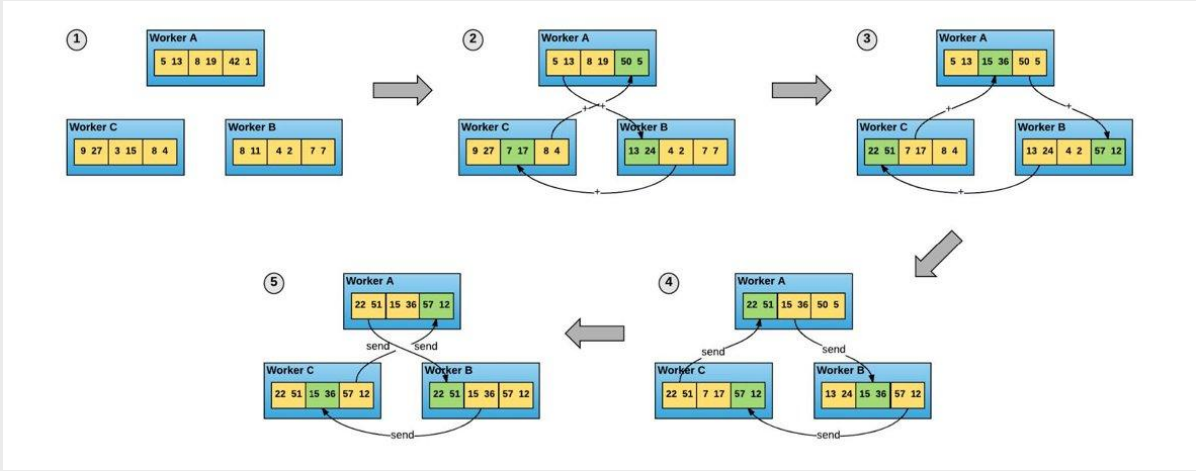
https://www.youtube.com/watch?v=6ovfZW8pepo&ab_channel=TensorFlow

Horovod

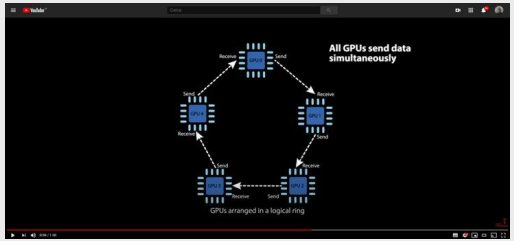
Ring allreduce

Two step process:

1. share-reduce step
2. share-only step



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



https://www.youtube.com/watch?v=4y0TDK3KoCA&t=585s&ab_channel=Uber Engineering

Distributed Training with TensorFlow

- tf.distribute.Strategy is a TensorFlow API that implements distributed training
- Easy to use and switching between strategies:
  - MirroredStrategy and MultiWorkerMirroredStrategy
  - TPUStrategy
  - ParameterServerStrategy
  - CentralStorageStrategy

- Use cluster resolver to read SLURM job configuration automatically

https://www.tensorflow.org/guide/distributed_training

Other Frameworks

TARANTELLA

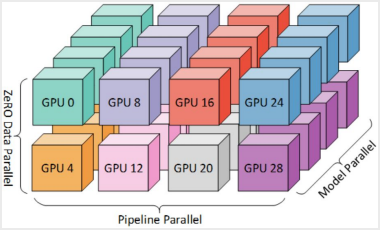
[https://github.com/cc-hpc-itwm/tarantella]

HEAT
Helmholtz Analytics Toolkit

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

Colossal-AI

[https://github.com/hpcaitech/ColossalAI]



raysgd

https://docs.ray.io/

Model size	Hidden size	Number of layers	Number of parameters (billion)	Model-parallel size	Number of GPUs	Batch size	Achieved teraFLOPs per GPU	Percentage of theoretical peak FLOPs	Achieved aggregate petaFLOPs
1.7B	2304	24	1.7	1	32	512	137	44%	4.4
3.6B	3072	30	3.6	2	64	512	138	44%	8.8
7.5B	4096	36	7.5	4	128	512	142	46%	18.2
18B	6144	40	18.4	8	256	1024	135	43%	34.6
39B	8192	48	39.1	16	512	1536	138	44%	70.8
76B	10240	60	76.1	32	1024	1792	140	45%	143.8
145B	12288	80	145.6	64	1536	2304	148	47%	227.1
310B	16384	96	310.1	128	1920	2160	155	50%	297.4
530B	20480	105	529.6	280	2520	2520	163	52%	410.2
1T	25600	128	1008.0	512	3072	3072	163	52%	502.0

[https://github.com/NVIDIA/Megatron-LM]

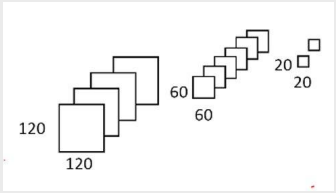
A Remote Sensing Use Case

BigEarthNet Classification

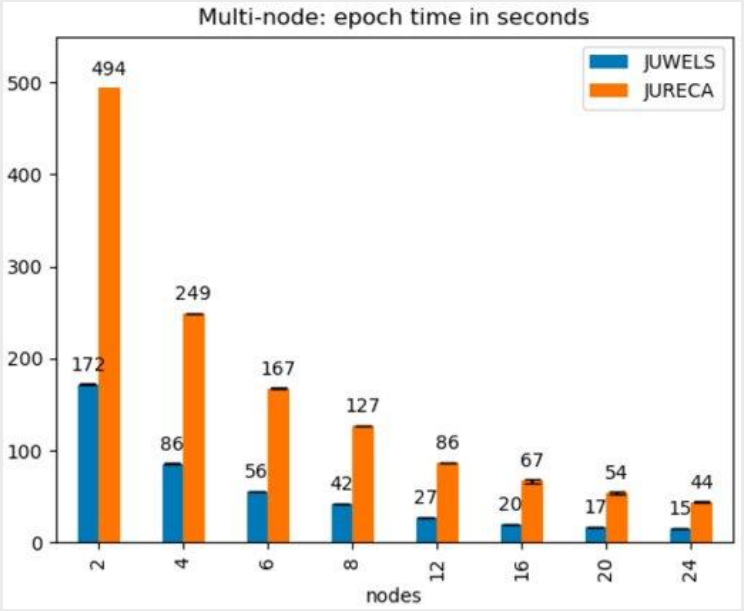
Dataset: BigEarthNet, Sentinel-2 Data Patches and Annotated with CORINE Land Covers

Model: ResNet50

0.74 F1-score up to 24 nodes - 96 GPUs with a global batch size of 8K samples



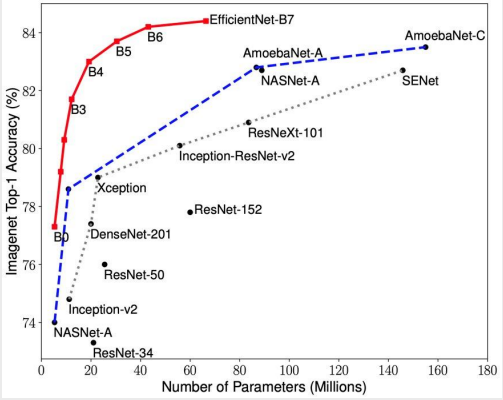
Patch and its dimension (px)



R. Sedona et al., Remote Sensing Big Data Classification with High Performance Distributed Deep Learning, 2019

Enhancements

- Adopted TensorFlow Dataset API to build a pipeline with integrated data augmentation, caching and prefetching of the data
- Deploying on 64 nodes / 256 GPUs of the Juwels Booster (Nvidia A100)
- New CNNs as EfficientNet, less parameters than ResNet, faster to train and higher accuracy
- Testing newer optimizers: LARS, LAMB, NovoGrad
- As the number of hyperparameters grows, there is the need to automatize the search for the optimal values (NAS)
- Hyper parameter tuning with **Ray Tune (embedded in Horovod)**: 'IGARSS2022 ACCELERATING HYPERPARAMETER TUNING OF A DEEP LEARNING MODEL FOR REMOTE SENSING IMAGE CLASSIFICATION', M. Aach, R. Sedona, A. Lintermann, G. Cavallaro, H. Neukirchen, M. Riedel, IGARSS2022 (accepted)



https://github.com/qubvel/efficientnet

Final Remarks

Final Remarks

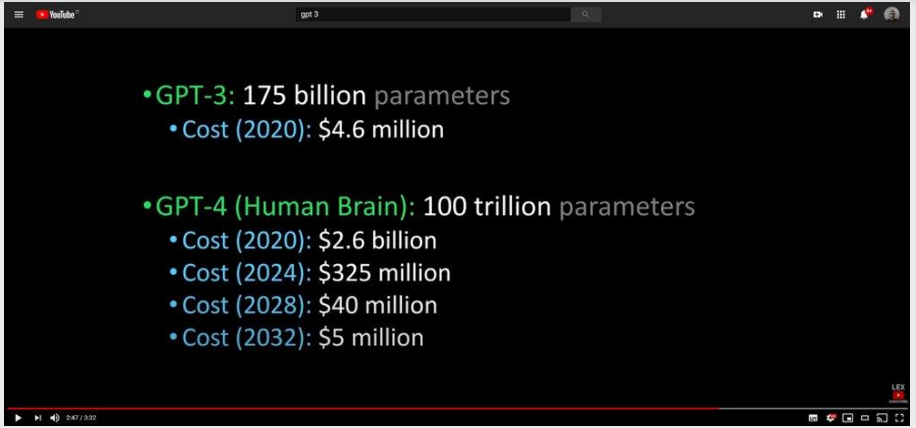
- The trend is to make distributed deep learning easier
- Not only frameworks, but integrated products
- Example: Dataflow-as-a-Service by SambaNova
- Intel's OpenAPI for heterogeneous computing
  [https://www.intel.com/content/www/us/en/developer/tools/oneapi/overview.html#gs.u1eb1g]
- AMD's GPUs using ROCm (similar to Nvidia's NCCL)

[f.e. https://www.bsc.es/innovation-and-services/technical-information-cte-amd]

[https://www.hpcwire.com/2020/12/09/ai-newcomer-sambanova-gas-product-lineup-and-offers-new-service/]

DL and Cloud Computing

- Trend towards cloud-based HPC
- What about costs?
- Let's have a look at **NCsv3-series** [25]
- **355 years** to train GPT-3 on a Tesla V100
- Training cost = 355Y×365D/Y×24H/D×0.9792$/H = **3.045.116$**



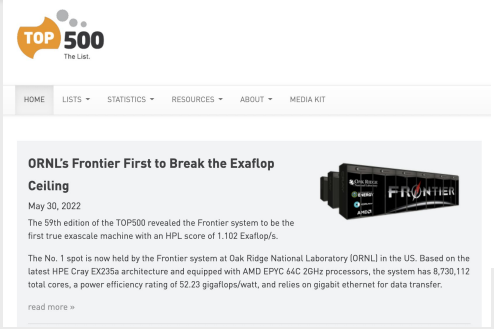
https://www.youtube.com/watch?v=kpiY_LemaTc&ab_channel=LexFridman

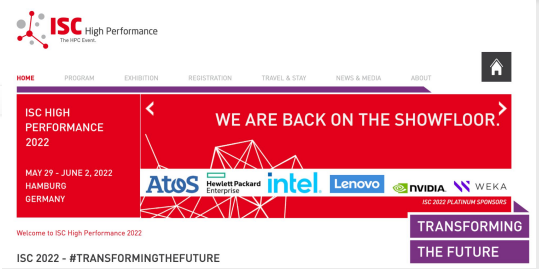
Add to estimate	Instance	Core	RAM	Temporary storage	GPU	Pay as you go	1 year reserved (% Savings)	3 year reserved (% Savings)	Spot (% Savings)
⊕	NC6s v3	6	112 GiB	736 GiB	1X V100	$3.06/hour	$1.9492/hour (~36%)	$0.9792/hour (~68%)	$0.306/hour (~90%)
⊕	NC12s v3	12	224 GiB	1.474 GiB	2X V100	$6.12/hour	$3.8984/hour (~36%)	$1.9585/hour (~68%)	$0.612/hour (~90%)
⊕	NC24rs v3	24	448 GiB	2.948 GiB	4X V100	$13.464/hour	$8.5766/hour (~36%)	$5.1002/hour (~62%)	$1.3464/hour (~90%)
⊕	NC24s v3	24	448 GiB	2.948 GiB	4X V100	$12.24/hour	$7.7970/hour (~36%)	$3.9169/hour (~68%)	$1.224/hour (~90%)

https://azure.microsoft.com/en-us/pricing/details/virtual-machines/linux/

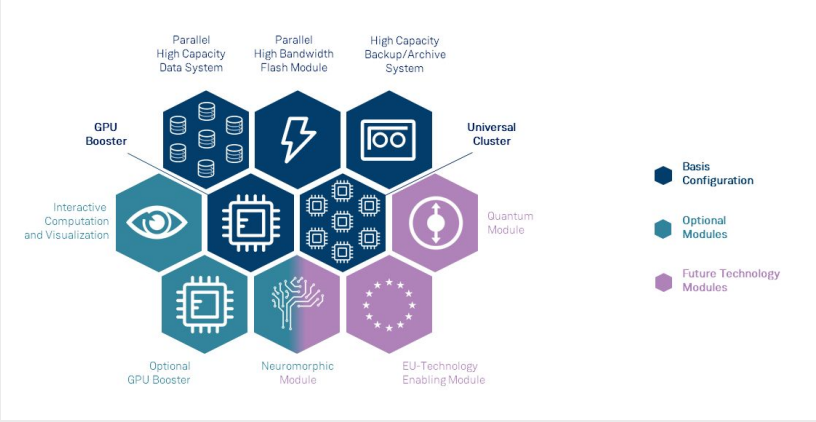
Towards Exascale

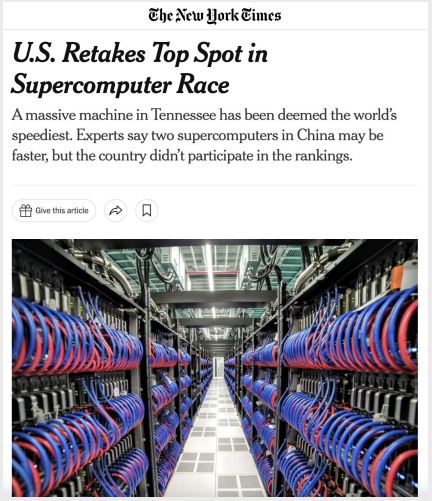
Frontier (First supercomputer to Break the Exaflop Ceiling at Oak Ridge National Laboratory (ORNL) in the US





Exascale Application Readiness
[https://www.olcf.ornl.gov/caar/frontier-caar/?fbclid=IwAR0JvTHz9rc_um_OGQbN28J8MDw5sv5yMF2OBWy2u5RKdMVyxODseWlnP7E]





https://www.fz-juelich.de/en/news/archive/press-release/2022/first-european-exascale-supercomputer-coming-to-julich

Final Remarks

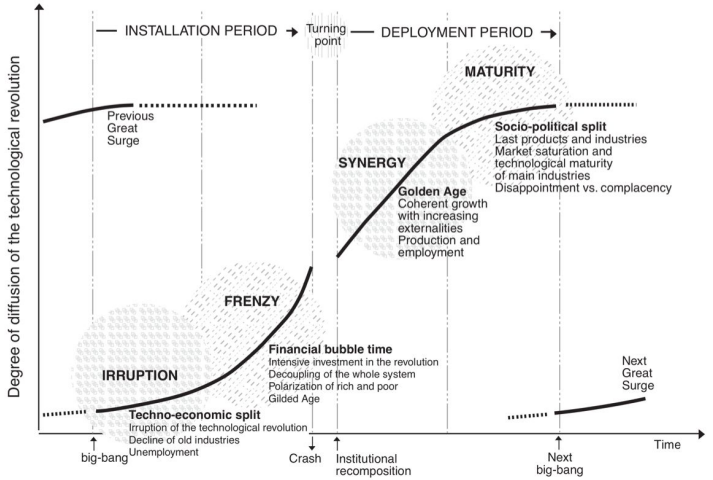
- Takeaways:
  - Frontier technology is fast paced
  - But successful solutions tend to become stable
  - Great opportunities for Distributed Deep Learning with the increased availability of computing resources

- Aknowledgement: Helmholtz AI Consultants

[https://www.helmholtz.ai/themenmenue/our-research/consultant-teams/helmholtz-ai-consultants-fzj/index.html]

[PRACE course "Introduction to Scalable Deep Learning" https://events.prace-ri.eu/event/1310/]

Figure 5.1 Recurring phases of each great surge in the core countries



Carlota Perez, 2002. "Technological Revolutions and Financial Capital," Books, Edward Elgar Publishing, number 2640.

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RAISE Center of Excellence

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Follow us:

Practical

- STEP 1: git clone
- STEP 2: codice train.py (TF mirrored strategy)
- STEP 3: (if enought time) participants will create SLURM job script, otherwise we provide it
- STEP 4: run the code
- STEP 5: check error and output file and that the model is saved
- -> load the model onto AWS

Have scripts ready to show in case Jupyter JSC is down

https://www.tensorflow.org/guide/distributed_training#other_strategies