Beyond Desktop Computation: Challenges in Scaling a GPU Infrastructure

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Abstract—Enterprises and labs performing computationally expensive data science applications sooner or later face the problem of scale but unconnected infrastructure. For this up-scaling process, an IT service provider can be hired or in-house personnel can attempt to implement a software stack. The first option can be quite expensive if it is just about connecting several machines. For the latter option often experience is missing with the data science staff in order to navigate through the software jungle. In this technical report, we illustrate the decision process towards an on-premises infrastructure, our implemented system architecture, and the transformation of the software stack towards a scaleable Graphics Processing Unit (GPU) cluster system.

Index Terms—Shared Computing, GPU, Infrastructure, On-Premises, Cloud

I. INTRODUCTION

In the course of computing history, sufficient computing power often exhibited a basis for the application of novel ideas. But it often also has been the basis for research ideas that were not superior because of the idea, but simply because of sufficient computing power available. Here, in some kind of sense, the increasing computational power drove the development of research ideas [1]. The steadily increasing amount of computational power was long driven by Moore’s Law, whereas the producing industry is not driven by this observation anymore [2]. Also the field of Artificial Intelligence (AI) gained popularity due to the amount of increased computational power, and evolved in new fields, like Deep Learning (DL) [3], [4].

Due to the promising results by applications of AI methods, a lot of research is currently performed in the field of AI based methods. Working with AI especially DL the question of the computational resources arises sooner or later. We observed, that in a lot of companies, Data Scientists are often the only ones with expertise in Computer Science. Besides their main function, they have to take care about computing infrastructure - even if it is not their field of expertise. This causes, that a huge amount of time is spent on research for applicable tools, systems, and environments to develop on.

Similar to other companies, start-ups, and universities, a simple GPU on-premises infrastructure is maintained within our institute, consisting of only a single server. This computing infrastructure was initially implemented as simple as possible, due to the lack of expertise and time. By using fair-share, one server with eight GPUs was set up. This machine specification can be found in Section IV line C.1. On this machine, for eligible people access was granted for research and training. When submitting a computation job, one user had to choose a not used GPU and start the job by only using this one dedicated resource. For multi-GPU jobs, several resources were allocated and blocked. With this setup it was likely to happen, that one user did not restrict a jobs resources according to the policy and blocked all computational resources. Additionally, inferences with other jobs are possible, leading to failures in all involved jobs. With a growing number of users on such a shared hardware, the demand for manageable permissions and restrictions increased.

Up-scaling and extending such an on-premises infrastructure, while preserving easy usage can be quite complex, without the help of experts in the field of IT infrastructure and High-Performance Computing. Also, the decision, on whether to move to the cloud shall be well defined, since this must be argued towards various stakeholders.

In the progress of planning the extension of our existing computational resources, several questions came up while being aligned with the set requirements:

Q1 Is a transition into the cloud financially beneficial or should the existing on-premises infrastructure be extended?

Q2 Are there preexisting solutions available?

Q3 What hardware components are needed and how to design the architecture?
Q4 What software components need to be part within the used software stack?

In this work, we are outlining the architecture of our established GPU computing infrastructure, as it scaled from a single server to a multi-instance computing cluster. This is based on the decision towards an on-premises infrastructure and the alignment with defined requirements. This report shall not give the impression of being a best practice, however, it is intended to show the considerations that are necessary when transforming infrastructure to a multi-instance cluster setup.

This report is structured as follows: In Section II we give a short overview of our considerations to decide on a Cloud or on-premises computing infrastructure within our institution. Section III outlines the requirements on the infrastructure, that lead to the architecture of the infrastructure Section IV and the setup of the cluster Section V. In Section VII we discuss about advantages and disadvantages of our implementation with an outlook and further considerations.

II. CLOUD VS. ON-PREMISES COMPUTING

Deciding on weather to run ones projects in the cloud or as an on-premise infrastructure involves many different aspects which are examined in the following. As one question this report shall answer is whether a transition for the computational tasks into the cloud is beneficiary, the emphasis in this section is put on factors which could lead or force ones intention to one or the other solution.

Like described in [5], there are models for grasping the scope of IT activities which shall not be our main focus here. Nevertheless, finding an appropriate solution for the own institution or company is key to a cost-effective solution. When further referring to [5] not just IT based Operations and Infrastructure (O&I) need to be considered but also ones that influence those. Thus, each of these may change when adopting from one model to another. Due to these manifold influencing factors in those areas and activities, a decision is highly based on the processes an institution applies.

Some of the important key-factors are: Cost, Scalability / Upgradeability, Network Connectivity, Maintainability, Security, General Data Protection Regulation, Disaster Assistance, and Data Backup and Recovery. These factors are essential to consider when planning to deploy services to cloud providers. Nevertheless, cost is often the one considered first.

A. Costs

When comparing Cloud to On-Premise expenses, companies usually start looking at hardware bought for local usage and on-demand (virtual) hardware. But it is necessary to get a complete picture of the total costs which cannot be reduced to a plain procurement process.

As indicated in [5], O&I needs to be accounted for which translate to Capital Expenditures (CapEx) and Operation Expenditures (OpEx) when referring to economical terms. Additionally, it is noted, that especially for maintenance, it is necessary to spend a regular, potentially high amount for an on-premise solution compared to a similar cloud resource.

This is based on the companies needs: electricity costs, administrative staff, licenses and trainings.

Cloud resources, therefore, are incorporating those additional costs, offering services at a fixed price per resource and consumed time. However, it is still possible, to create solid cost efficient structures for machine learning when reducing OpEX and keeping CapEX at an acceptable level. Especially when dealing with Green AI. That may be the usage of renewable energy sources or facilitating outdated refurbished machines/hardware, in order to establish a GPU cluster.

For the decision on the extension of the institutes infrastructure experiments, regarding the usage of the existing infrastructure, where conducted. Over the period of four months (April - July 2021) the usage was monitored and logged. The usage over this period is used as a baseline for the calculation process. Overall 7366 hours of GPU usage were monitored, what translates to a 32% grade of operation.

In Table I an estimation of the costs over a period of 16 months is shown. The procurement costs are based on the existing on-premise infrastructure (C1). The costs of electricity are estimated based on the assumption, that 60% of the maximum power consumption is used in idle mode and the rest added based on the actual usage. The assumption on manpower is based on the fact, that the initial setup was done during the first two months and further maintenance was barely needed. With this on-premise solution, the initial costs were high, but the overall monthly costs were kept low.

For the calculation of the monthly costs, the mean monthly usage is considered (1843h/month). For both, MS Azure and Google Cloud, a setup was chosen with a commitment to min. three years.

Comparing all three variants (on-premises, Google Cloud and Microsoft Azure) with the observed rate of operation, on the "costs per month" the Azure configuration has a break-even at month 11 and the one from Google Cloud from month 3. Pessimistic baseline, since during the second half of the year (Aug - Dec) a much higher usage is observed.

1Rounded to full numbers. Break-even points indicated in bold.

2Prices (in EUR) as of 05.08.2021. Azure configuration: NC24s v3 instances with 24vCPU, 448 GiB Ram, 4x Tesla V100. Google Cloud: AI platform with BASIC GPU training tier. All platforms hosted in Europe.
16. Although, these systems are not completely equal in terms of hardware, the table provides a rough direction when an on-premises solution gets profitable.

Figure 1 illustrates the same data, where the black solid and dashed line represent the costs for the Google Cloud and on-premises solution, respectively, over time. The shadowed area around both lines indicate a calculated range of variance for a mean usage between 10% and 70%. Additionally, for both variants two further lines, indicating the theoretical trend for 20% and 40%, are indicated by the gray lines.

More specifically, Figure 1 renders the trade-off between cloud and on-premises computing in terms of costs. The on-premises solution faces the issue of high costs in the initial phase, but far less further costs. Using cloud services one pays exactly what is consumed. Depending on the actual usage, on-premises can pay-off sooner or later in case the system set-up may allow to save expenses during procurement or the running ongoing costs.

In literature also other comparisons on the costs of cloud vs. on-premises computing can be found, see [6].

B. GDPR

The protection of the intellectual properties and values of an institution or conforming to GDPR can be one of the reasons which force professionals to refrain from using cloud resources. Although, the large established cloud providers (e.g. Microsoft, IBM, Amazon, Google) provide possibilities to rent services which are hosted in particular regions, it is important to note that those are mainly American companies which may be forced to provide information, possibly sensitive data, even if stored in some other a non-us region.

C. Other issues with Cloud Resources

In the following other important issues when dealing with cloud resources are listed:

- **Attacks:** cloud resources might be more vulnerable to attacks, not because they are more vulnerable in principle but with services, domains and exploits well-known by hackers they are rather under attack than custom services unknown to the (international) public.
- **Network connectivity dependency and downtimes:** Challenges arising due to technical outages of the world wide web may severely brake your manufacturing e.g. when thinking about production processes demanding real-time processing.
- **Limited control and flexibility:** Although, cloud providers getting richer in terms of tools and services, controlling remote hardware, servers or services may be still quite hard to deal with and may come with their own peculiarities which are difficult to manage.
- **Vendor lock-in:** provided services and interfaces are often highly proprietary and do not conform to cloud native structures or even basic IT standards.
- **Disaster Assistance and Data Backup and Recovery** may grow in complexity if e.g. a non-cloud based backup is required for cloud resources. However, for the GPU cluster backup only exists in form of a recovery image which restores the initial installation state. Further, as this cluster is used as a computing engine, which is doing batch processing, data on that cluster also resides on other systems and is not lost when data corruption occurs.

III. REQUIREMENTS TO OUR ON-PREMISES INFRASTRUCTURE

The intended infrastructure is used for different purposes (research, course work) and by different groups of people (faculty, scientific staff, and students). Each of the stake-holders has different requirements for the setup. Before the design of the architecture, the requirements were defined in order to select the components of the software stack and the topology of the cluster accordingly. For our setup, we identified requirements, which are discussed in the following.

(A) **Ease of usage** Development of all algorithms and jobs to be executed is done on local machines. To execute the jobs on the cluster, no modifications on code and no major changes on the call are necessary. Data and other necessary resources need to be available for the job, where ever it is scheduled to be executed. Additionally, no knowledge about the system itself is necessary for execution.

(B) **Scheduling of Jobs** A jobs execution is decoupled from the scheduling. This means, that a users, who submits a job, does not have to know about the architecture of the cluster or the setup of the computing nodes. When submitting a task, this is appended to a queue of jobs. When executing a job, the request for a certain type of resource is stated (e.g. type of CPU, memory, etc.). The system schedules the jobs according to first-in-first-out and the availability of the requested resources.
(C) **Workload Distribution** Resources shall be used equally over the system, where possible. If several computing nodes with likewise configuration exist, it must be assured that the load of work is distributed among those nodes. It must be avoided, that only few components take care of the whole computation, whereas the others are not used.

(D) **Permission Management** Different stakeholders use the cluster for different purposes. Hence it shall be possible to assign users to groups to restrict their usage to a defined policy. As a figurative example, members of the group *students* shall only be allowed to use *GPU* at a time for a maximum of *n* hours. This shall reduce the potential risk of misusing the infrastructure.

(E) **Maintainability and Scalability** It shall be possible to remove and exchange parts of the system, without too much time effort, and downtime. The same applies to the extension of the system: For future developments, the system must be designed in such a way, that additional computing power can easily be extended with no major modification to the system itself, which enhances complexity to the architecture and the configuration. Heterogeneous setups should be configurable.

(F) **Network Speed** When designing the topology of the connection between all the components within the system, it shall be taken care of to design this system in such a way, that the network speed is high and influences from other network traffic that reduce speed kept low. On the other hand, also the traffic between the components must not have any influence on the other resources on the network. Printing, access to the web or file servers must not be reduced in speed, just because of transferring data among two nodes.

(G) **Costs** The last requirement concerns the monthly costs of the infrastructure. Monthly costs are intended to be as low as possible, while initial costs must be below a certain predefined budget.

IV. INFRASTRUCTURE ARCHITECTURE

During the research, several solutions, offered by various companies were found, like [7]. All of these solutions posed the drawback to exceed the defined procurement budget.

The architecture of the up-scaled infrastructure is motivated by [9] and inspired by [7]. The designed architecture is illustrated in fig. 2. The whole cluster is completely abstracted from the public network by an interface router. This interface router creates a private network for the whole infrastructure, without putting load on the public network by data synchronization between the nodes. As a result, this hides the complexity of the infrastructure to the outside, while being still accessible from the public network. For the implemented cluster, a *MikroTik CRS-309-1G* is being used.

For the private, cluster network, instead of a conventional *Gigabit Ethernet*, a *SFP*+ connection is established. This protocol support data rates up to 10 Gbit/s. This enables faster synchronization between the nodes.

Within this private network, several nodes are connected. The interface node poses as the entry point to the cluster and the only accessible machine within the network for users. On this device, all tasks are scheduled and distributed according to the set policy and configuration. This node does not have any *GPU*, so no accidental blocking of resources may happen.

For the setup, the interface node is the standard gateway for the *SSH* access.

The actual computing tasks are scheduled to the computing nodes (*C_1* . . . *C_n*). These machines are equipped with sufficient computing power, *GPU*, and memory. For the implementation, the already available machine (old infrastructure) *C_1* is being used. Additionally, a further machine *C_2* is added to the system. The configuration of all machines (*C_1*, *C_2*, and *I*) are described in Section IV.

As indicated, this architecture also makes it easy to increase the number of further nodes. In fig. 2 a dedicated storage node is indicated. This storage is available by all components within the cluster and enables access to all data by all nodes. For the current implementation, this storage is not included in the setup. A dedicated storage will be added with one of the future extensions. Currently, only the storage from the nodes *C_1* and *C_2* is used by all nodes.

All devices and nodes in the implemented setup are chosen, so that they are easily built into a existing server rack within the in-house server room.

V. CLUSTER SETUP

For the setup of the cluster and the software stack, extensive research was needed. This was caused by the variety of software products available and their interoperability, enterprise products on the market, and expensive reference solutions. The following setup is inspired by the huge computing infrastructure of the University of Massachusetts [9]. The selection and installation of the software stack is based on the instructions in [10].

Each node in the initial setup of the cluster is based on a *Ubuntu 20.04 LTS Server* is used. The decision towards a *LTS*
version was done for a long lifetime support. Among others, consumer options used in practice are CentOS Linux 7 [9], and Ubuntu 20.04 LTS [10]. A comprehensive overview and comparison of the operating systems and components used in other clusters can be found on the TOP 500 list.

On each of the computing nodes, the appropriate CUDA driver is installed. The correct driver and CUDA version is dependent on the GPU and operating system.

Since the jobs to be executed are scheduled by a central entity on a machine within the cluster, storage synchronization is crucial. A user is only able to access the interface node. All data and environments also need to be synchronized to the cluster. The storage integrated in both computing nodes, $C_1$ and $C_2$, is provided as storage for the cluster. The storage is used as a ZFS (Zetta file system) and mounted from all other nodes within the cluster. Each machine mounts that storage to the same mount point in the file system. With other setups different approaches can be found, where either everything is mounted using only one directory [10] or the storage split among several directories for different purposes (e.g. home directories, research storage, scratch space, temporary Space) [11]. Within the implemented cluster, only the home directories and a data directory are shared within the cluster.

For password-less connections from the master to all worker nodes, the ssh keys are exchanged and munge is used as an authentication service. For the application of the used workload manager, MariaDB is used.

As a workload manager, the decision was made towards SLURM [12]. Another workload managers commonly used is HTCCondor [13]. The decision towards SLURM is not only based on the reference implementations, but also since SLURM is easy to use. Let’s consider a simple script, name execute_me.py. Using SLURM, applying a standard configuration, it is scheduled as simple as sbatch python execute_me.py. No further adaptations are needed to be taken care of.

Additionally, SLURM, which has a large community, is well documented, and even has enterprise support. Furthermore, over 60% of all supercomputers use SLURM in their setup [14]. SLURM can be used for any size of clusters and works well with over 1, 200, partially different, GPUs [9] and to smaller setups and clusters. Both, HTCCondor and SLURM, can be used interoperable. An overview on this and on both tools itself is given by [15] and [16].

SLURM is a highly configurable component. This workload manager can be configured in the most basic approach, where it works only as a simple workload manager that balances jobs on all nodes, up to a system were it is a part of a software stack, that not only restricts access to resources for certain users but also interconnects with other plugins like for accounting for the actual usage. For the implemented system, the initial configuration has two groups of users, where different types of GPUs are restricted to certain user groups. For instance, users of the group factuly may use all GPUs and members of students are restricted to GPUs on computing node $C_1$. Additionally, users from the first group can schedule as much jobs as needed, while the jobs are executed as soon as possible, and members of the latter can only have one job running at a time.

Users and groups are managed using FreeIPA[7]. This software component offers an intuitive Web-UI for managing all accounts. For the initial setup, the clusters user accounts are intentionally independent of the organizational accounts for the rest of the official IT infrastructure. FreeIPA allows not only to add and delete users and groups, but it also allows to set validity periods, storage quotas, and much more.

VI. FUTURE ADAPTIONS

The purpose of this cluster is in computational power for research and academia. In both fields, it will be likely that the demand for computational power will increase in the following years. For this purpose, several adaptions to the cluster are planned already.

The first extensions on the number of computation nodes will be with a more ‘low-spec’ hardware. Using already available consumer hardware, the cluster will be extended, so that the number of computational devices increases. Using, e.g. several discarded, slower hardware can be offered in exchange for more jobs in parallel. Given the current situation on the international market, where only a small number and on overpriced GPUs are available, this is a very attractive option as long as the memory requirements of jobs are not too high. Additionally, from an economical perspective, this gives the hardware a second life instead of being recycled.

Depending on future usage, also more memory computational tasks may be executed on the machine. Therefore, SLURM also needs to be configured, so that no GPU, but a certain amount of memory can be allocated.

As noted in Section V, no dedicated storage is used within the implemented cluster. A further extension, where dedicated

https://www.top500.org/ https://www.freeipa.org/
storage is aimed. This storage is also planned to be fault-tolerant, by using formats of storage virtualization.

Maintaining a continuously growing infrastructure, it is not easy to keep an overview of the status on all machines and devices in the cluster simultaneously. To make administration easier, a cluster management system will be implemented. Observing the status of all connected nodes and devices, managing them, and taking actions on events will be the main task of the component implemented by this extension.

In Section II the comparison of the costs of using the cloud infrastructure is elaborated. Depending on the usage of the cluster, it is a further use case to overcome performance peaks by including cloud resources by an external vendor/provider. By starting a cloud instance while the cluster is in high demand, quick jobs can be outsourced to the cloud, which speeds up the execution of jobs.

Depended on future usage, it is also possible to improve the hardware to enable computational jobs, with a memory demand higher than the memory of a machine. RDMA\textsuperscript{8} is an extension technology with the ability to access memory from one host to another remote.

VII. DISCUSSION AND CONCLUSION

In this work, we focused on an overview of the transformation of a research machine with several GPUs to an extensible cluster of several computing nodes, each offering several GPUs.

The requirement on the ease of usage (requirement (req.) (A)) is preserved. Due to the usage of SLURM, no modifications need to be done on the code or the call itself, only the execution needs to be done using SLURM. Also, the scheduling of jobs (req. (B)) and the workload distribution (req. (C)) are handled by SLURM. The permission management (req. (D)) is also covered, commonly by SLURM and FreeIPA.

The requirement on maintainability and scalability (req. (E)), as well as on network speed (req. (F)) are both covered by the design of the clusters architecture. Further machines can be easily added with a minimum configuration effort. So even when starting with a small number of computing nodes, like in our case with two, it exhibits an effective and efficient platform to work with. The maximum speed within the network is above the standard network used within our institution and the traffic on the cluster does not influence the public network, due to its private scope.

The costs (req. (G)) are kept low and within budget. One might argue, that the components in this proposed setup are still not from a low-cost price range. However, all components described within this work can be replaced with existing and more budget-friendly components. Additionally, the monthly costs are controlled, without surprises by an unexpected increased demand.

In the introduction, we posed four questions that were asked before this project and answered within this work. Q1 was concerned, whether it is beneficial for the proposed use case to use cloud resources. In Section II, this topic is elaborated extensively. By showing a comparison of the costs, the decision was made against cloud solutions and to foster an on-premises infrastructure. Also, preexisting solutions (Q2) were not considered, since our research showed, that those solutions are above the given budgets limit. The design of the architecture (Q3) and the components of the software stack (Q4) are shown in Section IV and Section V respectively.

In growing enterprises, data science departments, and research facilities data scientists, often the only computer science or engineering experts, also have to take care of their infrastructure. A simple solution is established fast, but scaling is hard. A lack of expertise often results in sub-optimal or redundant solutions or endless research.

In this work, we showed from a data scientist perspective, how to scale an existing infrastructure with a limited budget, while, among other requirements, maintaining extensibility. We presented our architecture and the software stack of our cluster with job scheduling.

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\textsuperscript{8}Remote Direct Memory Access