Simplifying Usability of Simulation Frameworks using a UI for ASTRA-sim

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Abstract

this is not the abstract, write one instead

Contents

Acronyms

AI	Artificial Intelligence
API	Application Programming Interface
ASTRA-Sim	Accelerator Scaling for TRAining Simulator
CLI	Command-line Interface
CSV	comma-seperated values
DML	Distributed Machine Learning
ENIAC	Electronic Numerical Integrator and Computer
ET	Execution Trace
FIFO	First-In, First-Out
GEMM	General Matrix Multiplication
GPU	Graphics Processing Unit
GUI	Graphical User Interface
HBM	High Bandwidth Memory
HCI	Human-Computer Interaction
HPE	Hewlett Packard Enterprise
HTSim	High Throughput Simulator
HW	Hardware
JSON	JavaScript Object Notation
LIFO	Last-In, Last-Out
LLM	Large Language Model
LSQ	Logical Scheduling Queues
ML	Machine Learning
NIC	Network Interface Card
NPU	Neural Processing Unit
NS-3	Network Simulator 3
SGD	Stochastic Gradient Descent
SOU	States of Understanding
SSOU	Simulated States of Understanding
SSP	Stale Synchronous Parallel
SW	Software
TCP	Transmission Control Protocol
TXT	Text
UI	User Interface
UX	User Experience

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1 Introduction

1.1 Motivation

Machine Learning is used in many aspects of daily life, business and research. To fit demands of high scalability, distribution of the training is used. Distributed Machine Learning (DML) is dependable of configurations such as parallelization strategy, topologies and communication. Important is to find configurations to minimize used training time and optimize computation and communication distribution. Finding such configurations is difficult, as it depends on an expensive hardware base and a huge variety of available system choices. Optimizing choices uses many resources, such as money, time and power. To reduce these costs, simulation can be used. One simulator for research of DML is Accelerator Scaling for TRAining Simulator (ASTRA-Sim). When companies want to train their own Machine Learning (ML) model, they face similar challenges. Here Hewlett Packard Enterprise (HPE) could provide solutions such as the necessary hardware infrastructure, making those companies their customers. Additionally, they should provide associated system choices to use the system efficiently. To gain the companies as their customers, they should provide realistic insights in how long the training would take. To find and help evaluate such information, a simulator like ASTRA-Sim can be used. As it is a research tool and not designed for a sales use case like this, its usage is challenging. It's multiple versions and parameters, that need prior training and expertise, make usage for a non-expert user group like HPE customers difficult.

1.2 Problem Statement

1.3 Objectives

1.4 Structure

2 Literature and State of the Art

In this chapter, the current state of the art and literature get presented. First, the development of machine learning to distributed machine learning gets sketched. Then, ASTRA-Sim gets presented and compared to alternative DML (simulation) approaches. Lastly, User Interface (UI) and User Experience (UX) best practices, with a focus on evaluation criteria and UI for scientific tools get presented.

2.1 History of Distributed Machine Learning

DML is a concept based on ML distributed on multiple machines. To deeply understand it, one needs to know basics of ML first.

Development of Machine Learning

The concept of machines learning similar to human learning was first proposed in 1950 by Turing [1]. He proposed the first known of theoretical description of the concept that later became known as Artificial Intelligence (AI). In his paper, he introduces basics such as the idea that machines could simulate human intelligence, if they are given the right data and algorithms. He states that learning, similar to children education is central and supports it with evolutionary algorithms. He claims that machines, which can be seen as discrete-state machines, can simulate anything, which enables them to universal computational capabilities useable for ML.

Following this basic idea, the first working ML program was introduced in 1959 by Samuel [2]. Samuel presents a program that is able to play the game checkers better than its programmer, with only 8 – 10 hours of playing and information such as rules of the game. This program is based on self-improvement, it adjusts its strategy based on previous outcomes. Therefor it is the first documented “self learning” algorithm. The learn process has two approaches; one is memorizing each board positions evaluation and the other one to adjust this evaluation function based on experiences. In this version, it uses the delta between expected and actual result to update expected parameters.

At this time early ML begun and these concepts were expanded, as in 1963 Abramson presents further pattern recognition and machine learning approaches [3]. Here, statistical

approaches were introduced and data was first viewed as vectors in a multidimensional space. He framed pattern recognition as a classification problem in vector spaces with two subproblems, being the partitioning techniques and choice of measurements. Also, the first idea of a distinction between supervised and unsupervised training was explained. But there were still gaps in research that only had to be discovered in the following years, like the selection of relevant features.

In the following years, many concepts of ML were revised and newly discovered. Such as backpropagation in the 80s [4], that introduced using gradient calculation for loss correction, or the big data field especially in the 2000s [5].

As ML grew and gained importance, problems regarding growing demands arose. One is the growing availability of datasets. With more data available, training once possible in a few ours might take days or even years to finish, if not optimized. The data is also more complex, forming vectors of increasing dimensions, compared to past data. Also, models are increasing in complexity, so do deep networks have trillions of parameters compared to shallow neural networks in 1990 [6]. These problems demand a solution. Parts of these problems could be solved by scaling with improved hardware as an option, as chips could be made more efficient by scaling with smaller transistors [7]. This approach, based on Moore's law [8], is not upholdable anymore, in the 2010s it was declared "dead" [9]. Naturally, the developed solution was distributing the training. DML is a subset of ML that splits the training process onto multiple Neural Processing Units (NPUs) [10]. In 2024, distributed training became the standard for large scale systems and remained the state of the art [11].

DML Characteristics

With DML a solution for scaling was introduced, and new challenges have to be solved. Distributing the machine learning process is not straightforward—it depends on many factors, such as the way of splitting, network latencies and communication strategies.

The basic DML process combines individual computation of different workers with a communication between them. That way they can train one model together by separating tasks. This separation can follow two approaches visualized in figure 2.1 by the official PyTorch website (https://docs.pytorch.org/torchrec/high-level-arch.html) [**<empty citation>**]. One, called data parallelism, is splitting the data that the model is supposed to train on. That way, all workers iteratively train a part of the data onto the same model and communicate the models parameters and gradients between computation iterations. While data parallelism has the advantage of being easily implementable and reduce computation times nearly linearly (TODO check if true lol), its communication can create new overheads if workloads are distributed unevenly and a synchronous communication is used. Detailed on that and

further advantages and disadvantages get discussed in section 2.1. The other parallelization, called model parallelism, a type being for example pipeline parallelism, is focussing on splitting the models parts onto the workers. Here, the layers of the model are divided and trained separately with according communication. This has the advantage of enabling training to include large models, but requires more complicated communication than data parallelism. Common are also hybrid approaches in which both data and models get split. This combines advantages such as a high scalability and the possibility for an efficient training performance, but new introduced challenges are finding the optimal distribution between data and model parallel strategies as well as for load balancing communication and computation efficiently [12].

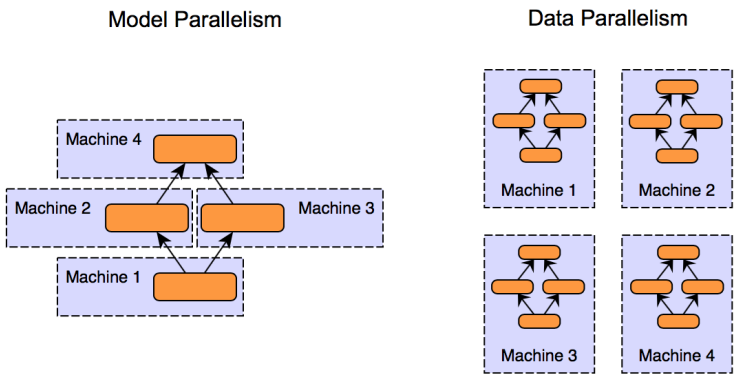

Figure 2.1: Parallelism Strategies

Hardware Details

The workers used in the DML process, generally called NPUs, are usually Graphics Processing Units (GPUs). They can appear in high amounts, from 8 GPUs for research purposes to 1000s for Large Language Models (LLMs) like GPT-5 [**<empty citation>**].

A set of NPUs structured together is called cluster, and each cluster is able to take different amounts of them. How they are connected in each cluster is described by a physical network topology. Every cluster in one machine, or called node, respectively, communicates via intra-node-communication. NPUs communicating between different nodes is possible over Network Interface Cards (NICs), which are connected in an inter-node-network. While intra-node communication has low latencies and high bandwidths, inter-node-communication has rater high latencies and low bandwidths. This would make a distributed training with few machines attractive, but realistic distribution onto many machines is much more scalable [**<empty citation>**]. That is due to the limited amount of GPUs in one server [**<empty citation>**]. Therefore, large distributed systems use and depend on both, intra and inter-node-communication. The topologies of distributed systems can be

based on different architectures. Verbreaken presents that there are four types of topologies that can exist for distributed systems [13]. Generally they can be divided into centralized, decentralized and fully distributed topologies, based on the degree of the distribution. A structural overview can be found in 2.2.

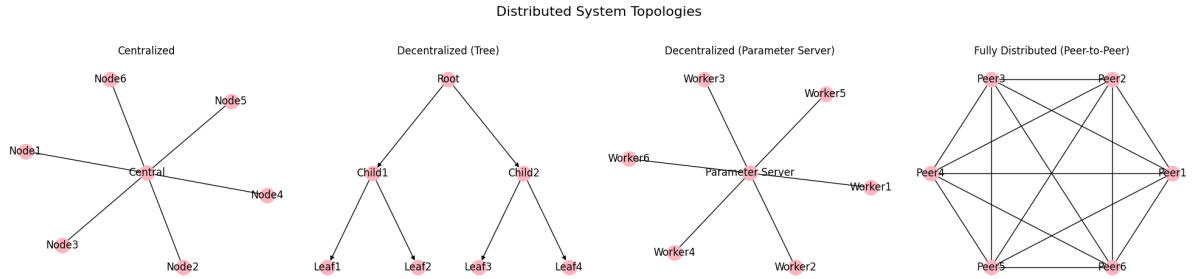

Figure 2.2: Network Topologies

The centralized topology is characterized by a strict hierarchical structure in which all nodes are connected with one central server that orchestrates them and performs the necessary steps for the combination of the machine learning. It serves a simple coordination but is limited in scalability due to having a single point of failure.

The tree topology is a decentralized topology in which the nodes are structured hierarchical. The communication takes place between the nodes in specific directions. Information is communicated upwards and distributed downwards. This is scalable as every node only communicates with children or parents.

The parameter server topology is a second decentralized topology that combines centralized parameter servers to store and retrieve gradients with decentralized ML nodes. These servers have a shared memory, so the parameters can be synchronized between multiple parts. The disadvantage of this is that all communication happens at the parameter servers, creating bottlenecks if many workers are combined with few servers.

A fully distributed topology works like a peer-to-peer network, meaning each node holds its own copy of the models parameters and is able to communicate with all other nodes. Communication is possible in every direction and at any time. This is very scalable, as new workers can be added without a high centralized overload, but it has the disadvantage that the communication can create a high overhead if every worker broadcasts its information.

Topologies can be asymmetric or symmetric, depending on if the connections are bidirectional or unidirectional. For fully distributed systems both could be possible, while all other topologies depend on bidirectional connections [14].

Communication Strategies

While physical topologies are showing different ways of organizing and centralizing the connections of machines, logical topologies can be used to specify how the actual communication is practiced. For this two main communication strategies a distinction between two new types of parallelization has to be made. They can either be synchronous, meaning all machines communicate at the same time collaboratively, or asynchronous, where each worker communicates as soon as it is finished with its own computation. Both are not applicable to every physical topology. Asynchronous communication is best suited for decentralized topologies with parameter servers. In that case workers push and pull parameters anytime necessary without the need for waiting for other workers to finish. Possible are also more varying approaches such as a trade-off version, called local Stochastic Gradient Descent (SGD), that allows workers to communicate asynchronous for a set amount of time until needing to synchronize [13] or Stale Synchronous Parallel (SSP), which additionally allows for cached parameters to be used for synchronization for the set amount of time [15].

Depending on the parallelization strategies and split of the training process varying types of communication have to be performed. While data parallelism relies on frequent exchange of calculated gradients, for example tensor parallelism, a type of model parallelism, needs to communicate between steps as early as in the forward pass [16].

Those types of communications can be achieved by using for example communication collectives. That are a set of synchronized communication patterns, which can be used for sharing and combining information across multiple machines in distributed systems, for instance *All-Reduce*, *All-to-All* or *Reduce-Scatter*. These collectives are most common for data parallelism, as they help to synchronize and combine gradients, and share parameters. They are blocking, meaning, nodes have to wait for each other's computation to finish, and they have to be orchestrated by a centralized controller. Generally, collectives can be separated into redistributive operations, that share data and consolidative operations, that aggregate data. The most common collective used for data parallelism is *All-Reduce*. In the following the approach of collectives is explained, based on *All-Reduce* as an example. For guidance, figure 2.3 shows a visualization of the collective. The source for this explanation is the 25th course lecture of UC Berkeley's course *CS 168* in spring 2025 [17].

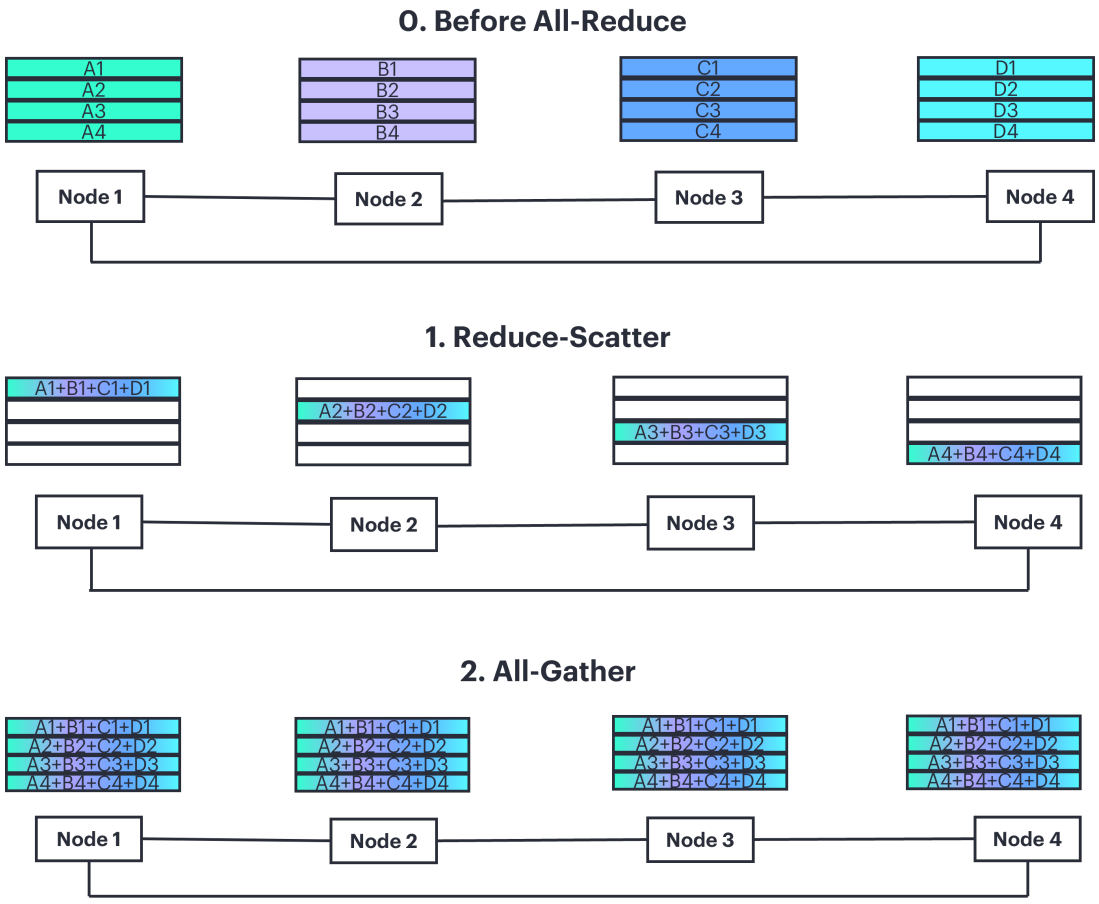

Figure 2.3: All-Reduce

This collective can be used for p nodes with each having a p-sized vector of values. This example uses $p = 4$, four nodes with each having four parameters that the model gets trained on. Every node needs to know the number of p and which index they have, meaning which parameter they are going to be responsible for. Also, this example uses a ring topology for easy visualization. The actual implementation can differ, in the following the theoretical background gets explained, more on that afterward.

In every iteration, the communication starts when all workers, here called nodes, are finished with their computation. Every Node has their four parameters stored. The first step of the *All-Reduce* is a *Reduce-Scatter*, which itself involves two steps, a *Scatter* and a *Reduce*. *Scatter* is the redistributive operation that shares every i-th parameter to the i-th node. With this, the first node receives all first parameters, the second all second ones and so on. *Reduce* is the consolidative operation, that combines the received set of parameters to one single aggregation. Together, they make every i-th node store one value in their i-th vector-place, combining the previous i-th values in every node's vector.

The second step is an *All-Gather*, which is an advanced version of *Gather*. That is an operation that is the reverse of *Scatter*, as it combines every i-th nodes i-th value in

one vector. *All-Gather* expands this by a *Broadcast*, which is the reverse of *Reduce* and distributes the resulting vector to all nodes. Afterward, the *All-Reduce* is finished, and every node has a p-sized vector of the combined and shared values.

The used operations can be implemented on top of various topologies, which influences how efficient the operation performs. In figure 2.4, common logical topologies are visualized. They can be for example a *Mesh*, *Tree*, or *Ring*.

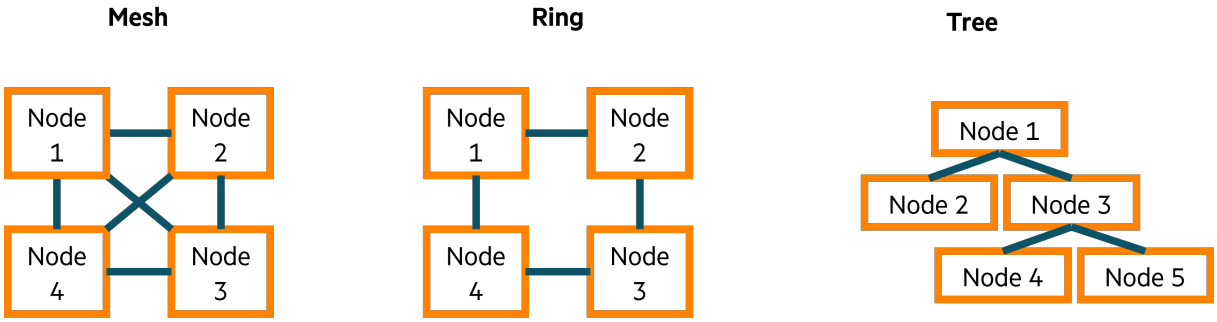

Figure 2.4: Logical Topologies

Depending on the underlying physical topology, different logical topologies can be useful for the different collectives, as different complexities of bandwidths are relevant. Also, overlay topologies can be used to create virtual links to support exchanging data between unconnected nodes. Furthermore, topologies can be defined on multiple dimensions. Examples are a two-dimensional ring or a three-dimensional torus.

DML Challenges

With many factors to consider, the DML process allows a high range of configurations. The first challenge is the communication overhead created when synchronizing shared parameters with workers that have different efficiency in their computations. Especially in centralized topologies with synchronized communication, workers waiting for others to finish should be avoided [18]. Additionally, when increasing computation allowance between communication times, a decrease of accuracy is likely to happen, as the model is trained less cohesively [19].

Yang et al. claim that nowadays configurations of large DML systems base on decentralized architectures with asynchronous communication [19]. Challenges like those get solved by research and evaluation tests of many configurations. Such adn apporach needs to consider model accuracy, energy consumption, throughput and latency, and cost[20]. To save resources and optimize configuration finding simulators can be used.

2.2 ASTRA-Sim and Related Simulation Tools

The most extensive publicly available DML simulator with a focus on Software (SW)/Hardware (HW)-Co-Design is ASTRA-Sim [21]. Its goal is to enable researchers to model and analyze configurations of DML. It has a focus on hierarchical systems and communication for both intra- and inter-node-communication. While there are many different versions of ASTRA-Sim the following explanation focusses on ASTRA-Sim 1.0 with an analytical backend. Explanations and comparison to other versions are provided in the subsection 2.2.

ASTRA-Sim Approach and Implementation

Generally ASTRA-Sim consists of layers which enable users to configure and simulate specific input fields. The core of ASTRA-Sim features two parts. A workload layer that is used to specify the to be trained model, with expected layers of communication, and a system layer that can enable configure used collectives and scheduling policies. ASTRA-Sim is a network centered simulator, naturally an additional feature layer lets the user configure physical dependencies like topologies and bandwidths. Initially, ASTRA-Sim featured the existing Garnet network simulator [22].

The workload layer uses an external computation model, like Scale Sim [23] to calculate each layers used General Matrix Multiplications (GEMMs). Its inputs are based on the parallelization strategy *(Data, Model, Hybrid)*, size of communication and structure of layers.

The system layer implements collective operations dependent on logical topologies *(All-Reduce, All-Gather, ...)*. Other configurable dependencies are the scheduling policy *(Last-In, Last-Out (LIFO), First-In, First-Out (FIFO))* and specifics such as the amount of splits of the dataset or Logical Scheduling Queuess (LSQs), which are the active chunks processed per dimension. This layer is able to simulate different phases in the communication, like multistage collectives and real-time differences between multiple dimensions.

The network layer simulates the hardware dependencies. The analytical version is able to consider configurations for multiple dimensions too. For each dimension a topology *(Ring, Fully Connected, Switch)* with its amount of NPUs can be specified. The simulator includes latencies for links, routers and NICs and bandwidths for links. The number of links is also important. Lastly the network layer can also simulate High Bandwidth Memory (HBM), with its latency, bandwidth and memory scale.

Figure 2.5 shows the original architecture with the Garnet network simulator. The different network backends are interchangeable as they all implement the same AstraNetworkAPI.

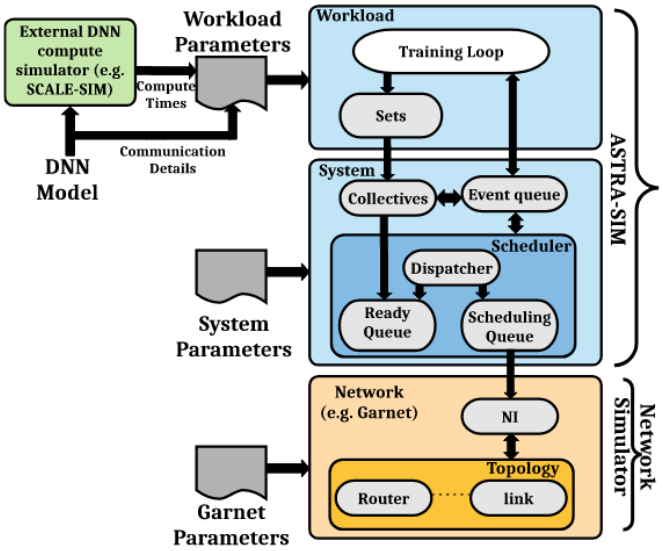

Figure 2.5: ASTRA-sim Architecture Overview, Official ASTRA-Sim 1.0 release [21]

Each simulation iteration start with the initialization, where the user can specify their configurations. In the implementation this is separated by layer to a JavaScript Object Notation (JSON) file for the network, a Text (TXT) file for the system and a TXT file for the workload. In the second step the workload gets produced. The loop produces sets of communication which again get separated into chunks for the processing. In the next step the chunks get sorted into LSQs and dispatched. This stream gets supervises and restarted if necessary. Next the final network simulation happens. In the analytical network the backend network gets simulated purely mathematically. Lastly, ASTRA-Sim exports its results into comma-seperated values (CSV) files. These show among other aspects the time of communication per layer, the distribution of computation vs communication and bottlenecks.

Versions and Modifications of ASTRA-Sim

Its initial release in 2020 includes a Garnet network. It was expanded later by an analytical network simulation. While Garnet is cycle accurate, so it simulates clock and packets in detail, the analytical network is based on mathematical approximate models. Therefore, the analytical model is slightly inaccurate, as it is for example not congestion aware, but it is more scalable than the garnet network.

In 2023 a second version of ASTRA-Sim was released [24]. It addresses the need for a higher scalable simulator, as deep learning models grew.

The loop is similar, with a few changes and extensions. First, the workload layer process. This workload layer was replaced with a chakra traced based workload layer. That is a

graph based workload documentation [25]. So, it replaces the previous static trainings loop with a dynamic one based on Execution Traces (ETs). An ET is a graph that reproduces a real ML training process. Each of its nodes represents either a GEMM, an access of memory or a collective communication. They can for example be extracted form frameworks such as PyTorch and converted to Chakra ETs. This workload layer supports more specific parallelization strategies than the 1.0 version *(Pipeline, Hybrid-Parallel, ...)*. This represents a more realistic model of parallelization, as the NPUs are capable of executing varying operations. After the ET is read and distributed on configures NPUs, each gets its own graph to simulate. Time spend on the computation, communication and usage of storage get collected. These use other layers information.

The system layer still manages the collective operations, depending on topoogies and scheduling strategies. A relevant difference to 1.0 is input got reduced to the only necessary parameters, ones reflected by chakra traces were crossed out. As a result it only features a topology, number of NPUs, internal bandwidth and internal latency. The idea is to completely abandon the inputs and retrieve them from chakra ET too.

For network simulation the network layer was used, and the two existing implementations were revised and additional backends added. The analytical backend is still implemented as a scalable and fast approximate network simulator, but the Garnet backend was abandoned. Now instead the Network Simulator 3 (NS-3) [26] and the High Throughput Simulator (HTSim) [27] backend can be used for the network simulation. The NS-3 is a well established network simulator, that includes realistic network conditions with congestion and routing, which makes it suitable for simulation that needs to be very accurate and realistic. HTSim rather focusses on the integration of Ultra Ethernet, an alternative to the standard Transmission Control Protocol (TCP). It is more lightweight and an alternative to the NS-3 that includes view of network traffic as flows rather than individual packets, which is especially relevant for DML setups. Both are more accurate than the analytical model.

The 2.0 version also includes a new layer, called memory layer. It is connected via an own memory Application Programming Interface (API). This models the HBM previously managed by the system layer. It supports disaggregated memory architectures and realistic pipelines transfers with their according bandwidths, latencies and topologies. That way ASTRA-Sim is able to compare these different known memory architectures depending on underlying DML configurations.

In general, ASTRA-Sim 2.0 is more flexible that 1.0, by allowing many more configurations and realistic workloads. Its disadvantage is, that it is still being developed and changes are introduced. For a stable simulation 1.0 is the better choice, but in the future and for current research 2.0 will be more relevant.

Comparison to Further Simulation Tools

A specialty of ASTRA-Sim is that it supports hierarchical topologies, so it can model asymmetrical bandwidths. Also, it allows a differentiation between logical and physical topologies. This is especially relevant for research contexts. Additionally, it is easily extendable as layers can be exchanged and new factors such as new topologies or strategies can easily be added.

2.3 User Interface Design for Scientific Tools

Research tools in computer science are mostly based on Command-line Interfaces (CLIs). Including Graphical User Interfaces (GUIs) can increase use cases and amount of usage [28]. While UI refers to the visual and interactive design of a digital product, UX refers to the entire experience users go through when using digital tool. Both areas are highly interconnected and central for the users' satisfaction with a digital product [29]. The study of UI and UX is Human-Computer Interaction (HCI), which in return gives it a scientific base. In the following, design principles of UIs in general and in this projects specific context get explained and the current state of the art presented.

Human-Computer Interaction Foundations

HCI is an interdisciplinary area that deals with the design, evaluation and implementation of interactive computer systems [30]. Its goal is to improve these systems in their functionality and usability. Specific goals also include methods for designing and implementing user-friendly UIs as well as criteria for evaluating and comparing interfaces. HCI also focusses on the development of new interaction techniques and models to human machine interactions.

This discipline was relevant from the moment on the first electronic computer in 1946 was used, called the Electronic Numerical Integrator and Computer (ENIAC) [31], which was used for computation of military firing tables. Later, with the development of GUIs, the internet and a wide base of useable tools, HCI became an important field, also relevant for website design.

HCI claims that machines are worthless until they are properly useable. Two main aspects are the functionality and usability of machines. Functionality refers to the set of services a program provides. This value becomes only value if it is useable efficiency. Usability is the extent of which the system helps the users to activate their goals when using the

machine. It depends on the needs of the target user group. Generally, in HCI a system is only considered qualitative, if functionality and usability are balanced.

One important sub category of HCI is cognitive load. Kosch et al. [32] present its characteristics and measurements in the following way. Defining cognitive workload is a challenge, it describes the amount of complexity the human brain gets presented with when executing tasks. In the field of website GUI design this can be transferred as the complexity of brain processes a user goes through to navigate the website. Naturally, they should be minimized to ensure the least possible complexity when using the website. Because digital systems are getting increasingly more complex, measurements of cognitive workloads gets increasingly more difficult. They present metrics such as questionnaires, which are very subjective, physiological sensors which are very objective or presented behavior, like the users mouse activity. With those evaluations different layouts or navigation structures can be tested and compared.

Another important sub-field of HCI are feedback loops. Feedback is the direct response of a system to a users action and is central for users, especially when they interact with computers in the wrong way. In GUI design for example when entering values in a form or uploading files that are not meeting specific criteria, it needs to be made sure that users understand what went wrong and to give them feedback to reduce the possibility of this problem occurring again. No feedback, delayed feedback and wrong feedback can make the user feel frustrated and unable to take full advantage of functionalities. Pérez-Quiñones and Sibert present a foundational study on the feedback model based on the linguistic theory of States of Understanding (SOU) [33]. That is a model explaining which state humans think they are in during a conversation, based on expectations they have when communicating with each other. Instead of seeing communication as ping-pong iterations between two participants, here it is viewed as collaborative process based on Clark et Al. [34]. Basically, it includes four states a listener can be in after a speaker send a message. This original concept from the linguistic area was applied onto the HCI area. The resulting five Simulated States of Understanding (SSOU) represent states needed in communication between humans and computers to match the humans expectations. The stages are:

1. The system is ready to receive inputs,
2. The user entered an input and the system processes that,
3. The result gets reported by the system,
4. The system ignores the input,
5. The system stores the inputs for a later processing.

For every stage the computer needs to provide specific feedback, so the user feels informed, and unnecessary interactions can be reduced.

UI/UX Best Practices and Evaluation Metrics

One aspect that needs to be considered is the difference that target user groups bring with them. One technique to characterize user groups is by using personas [35]. Using personas is supposed to help developers understand expectations, goals and contexts of users, to optimize the end product for the user. That way the user is central for the design process and can specifically be targeted. How efficient personas are depends on the quality of data it is based on and the depth of them. There are many possible strategies of building personas based on existing datasets. If there is no dataset available, an approach including expert interviews, existing knowledge and assumptions have to be used [36]. Each personas specification should include information such as daily routines, goals, fears, attitudes, technology behaviour, demographics, and existing knowledge. Personas can be used to design specific usability tests or specifications of necessary functionality. Combined with HCI it can be used to evaluate the necessity of certain aspects such as the extent of necessary feedback.

One classification that could be made for users is weather they are experts or non-experts in the field of the website. This is especially important for scientific tools.

3 Design

3.1 Requirements

3.2 Requirements Analysis

3.3 Technology Selection

Figure 3.1: Methodology flowchart

3.4 UI/UX Design Process

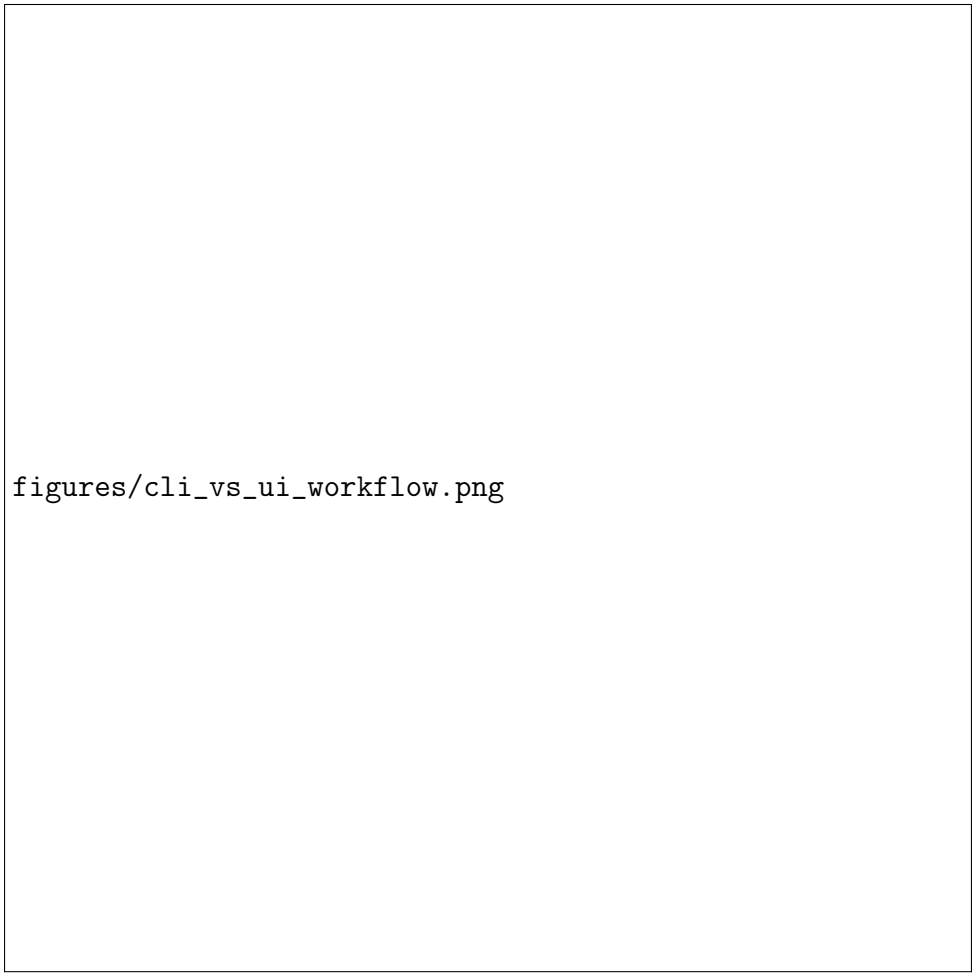

Figure 3.2: Concept diagram: CLI workflow vs UI workflow

4 Implementation

4.1 Optional: Overall Architecture

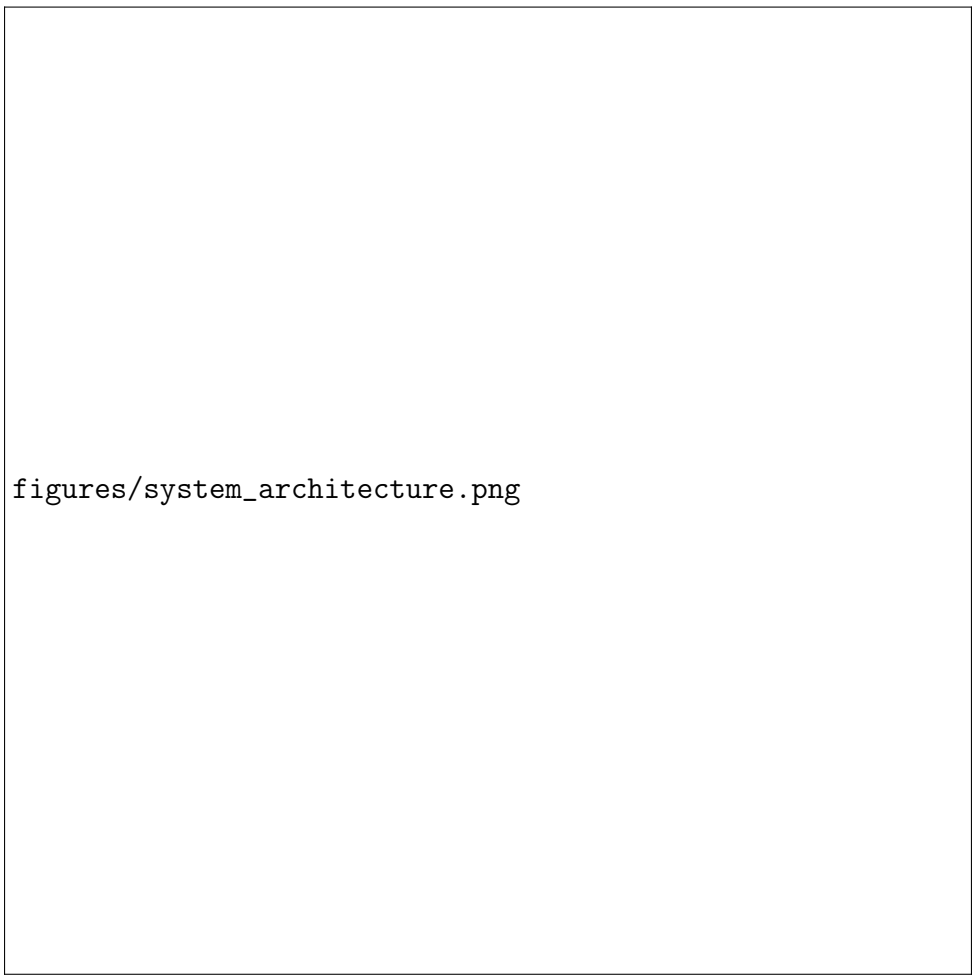

Figure 4.1: System architecture diagram

4.2 Frontend Design

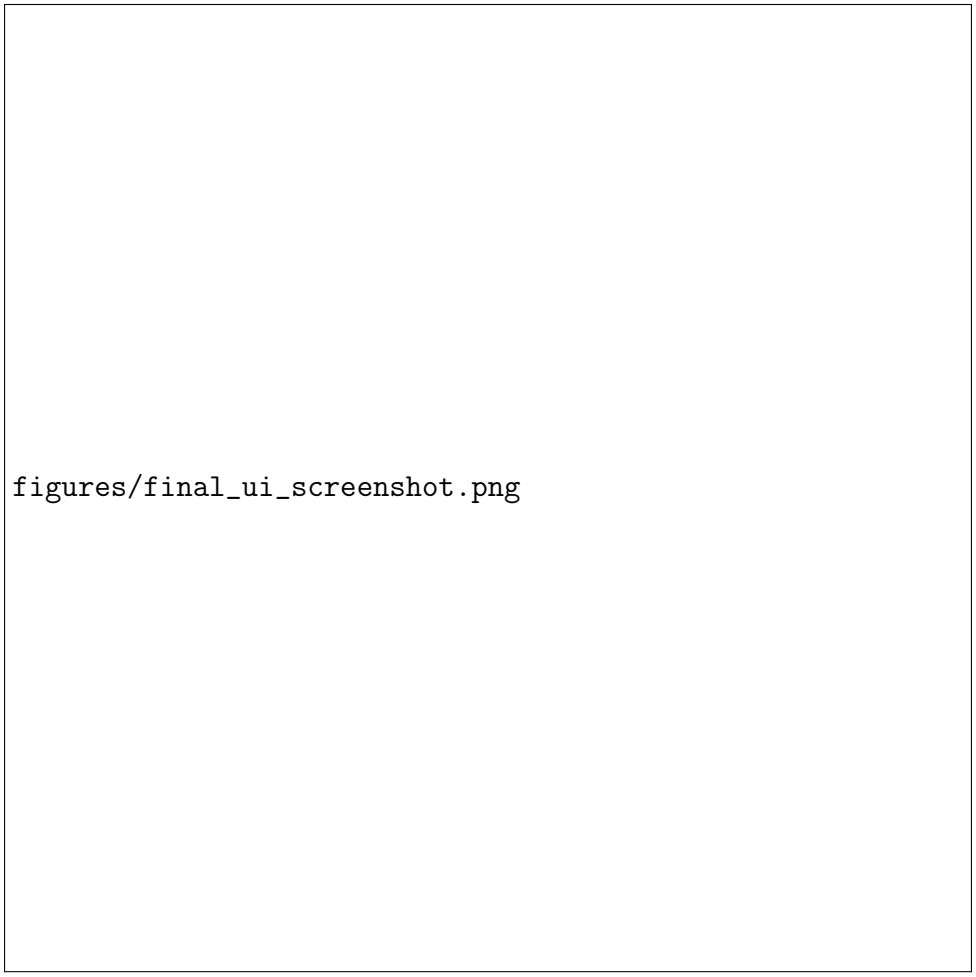

Figure 4.2: Final UI screenshot

4.3 Backend Integration

5 Evaluation

5.1 Feedback Integration

5.2 Challenges

5.3 Solutions

6 Conclusion and Future Work

6.1 Summary of Findings

6.2 Limitations

6.3 Next Steps

6.4 Future Work

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