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Advancing Scientific Discovery: A High Performance Computing Architectures for AI and Machine Learning

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Abstract

In this time, when HPC and AI are converging, we are witnessing the era of combining HPC with AI, i.e. data, which will bring to bear new scientific discovery and innovation at unimagined speed. Computing approaches used in the past have been unable to keep up with growing datasets and increasingly sophisticated problems in research. With the combination of HPC systems and the power of analytic AI and machine learning, previously almost unsolvable problems are being tackled in areas such as climate, drug discovery, materials science, and many other. This paper presents how these cutting edge HPC architectures and technologies can support these breakthroughs, describes the challenges of delivering AI on HPC systems and what can be done about it and provides a strategy for organizations seeking to maximize the value of these powerful tools.

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The Need for HPC Catalyzed by AI

As the data science problems grow more complex and the data grows exponentially, scientific users are reaching the limits of what traditional HPC systems can provide. Like genomics, climate science and particle physics, FIELDS have datasets that commonly exceed peta and exa byte scales. But on the other hand, researchers strive more and more on ever more complex multi scale, multi physics simulations, moving further away from any existing supercomputer. They are promising in analyzing and speeding up simulations with the help of AI and machine learning techniques with massive datasets. These purposes can be served by AI agents that intelligently explore the huge parameter space to optimize simulations, or deep learning models that can find insIdentable patterns in nois, experimental data. AI can help scientists make more sense of what they do have, but also speed up their solutions to problems which would otherwise be intractable.[1-3]

Nevertheless, it is hard to successfully intertwine HPC and AI architectures and their related software systems. As a matter of fact, computational characteristics and required resource of AI workloads are completely different from those of HPC applications. As we want to deploy AI at scale in an HPC environment, we need to determine the hard and soft stacks that address both paradigms. The high performance computing (HPC) systems are required owing to rapid development of artificial intelligence (AI) and machine learning (ML). For AI applications, HPC, i.e., the use of advanced computing architectures that can carry out the processing of the complex computation at scale, is imperative. Deep learning based AI algorithms require large amount of computational power, data processing and storage and traditional computing systems frequently lack the capability to provide this. These needs are well suited for being met with HPC systems, with their large parallel processing capabilities, which will speedup and efficiency train AI models (Figure 1).[4]-[5]

Modern AI and ML algorithms that are used, especially in areas like Natural language processing, Computer vision, autonomous systems, has very complex demands for processing power. Processing large datasets while performing calculations that

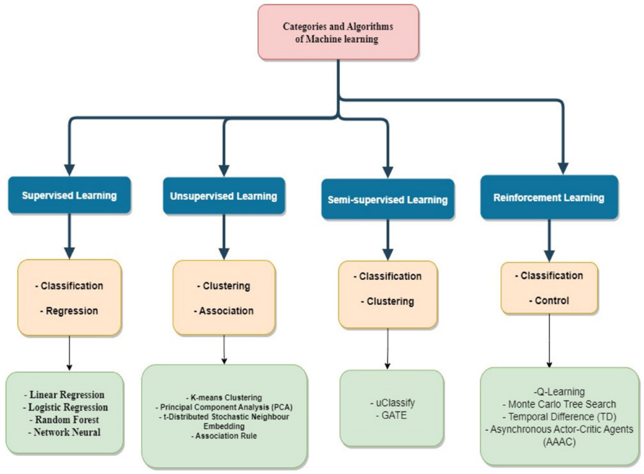

Fig. 1: HPC and AI architectures

require high level of processing power is an area of use for these algorithms. Taking the training of deep neural networks, for example, it is comprised of updating millions of parameters over a thousand of iterations and would take an unacceptable amount of time on standard computers. However, HPC systems can distribute these tasks amongst many processors, thereby greatly speeding up the training time.[6-7]

Another big reason why HPC in AI is used is in response to the amount of data an average AI model needs. Processing these big datasets use vast storage and computational capacity which is extensively needed by AI and ML applications. The ability of HPC platforms to handle and process large volumes of data in parallel makes them a very good fit to use to manage and analyze this information. Additional benefits of HPC in the area of real-time processing also enable AI models to come up with faster insights, which could prove to be extremely useful in industries like healthcare, finance and autonomous vehicles. The final conclusion is that the combination of AI and HPC is becoming a more important necessity to advance scientific discovery and innovation. Not only does the complexity of AI models require the need for HPC, also required is rapid speed of data processing and storage as well as real time analysis. With the evolution of the AI, the HPC will continue to be a fundamental component to achieve the full power of AI and machine learning.[8]

Artificial Intelligence and its Impact on HPC based on Key Architectural Considerations

Several key architectural considerations need to addressed to integrate AI capabilities into HPC systems.

Compute Architecture

However, the workloads of deep learning training are quite computational intensive, with low precision demand. This makes them ideal for such acceleration hardware like GPUs or TPUs. But even today many HPC applications are still sensitive to diversity of computational needs and hence rely on general purpose CPUs (Table 1).[9]

The HPC architecture based on such an AI also requires to balance for both these requirements.

Table 1

Challenge	Description	Impact
Scalability and Resource Management	Managing large-scale resources and ensuring the system scales with growing data and processing demands.	Scalability issues can result in inefficient use of resources and slowdowns in processing time.
Data Throughput and Bandwidth Limitations	Ensuring the system can handle large datasets efficiently without bottlenecks in data transfer.	Data bottlenecks lead to system inefficiency and increased computation time.
Power Consumption and Cooling Issues	High-performance computing systems consume significant power and require advanced cooling solutions.	Excessive power consumption and poor cooling can lead to hardware failure and high operational costs.
Algorithm Optimization for HPC	Optimizing AI/ML algorithms to leverage the full potential of HPC architectures is a complex task.	Inadequately optimized algorithms can lead to suboptimal performance, limiting the effectiveness of HPC systems.
Interconnect Latency and Communication Overheads	Reducing communication delays and improving data transfer between processing units in multi-core or distributed systems.	Communication delays can significantly hinder overall performance, especially in parallel computing systems.

Conversely to leading solutions that use heterogeneous computing techniques, combining general purpose CPUs with AI accelerators, the performance of the attack available on the different computing platforms has not fully been investigated. In the example of Perlmutter supercomputer from the Lawrence Berkeley National Laboratory, AMD EPYC CPUs connected to NVIDIA A100 GPUs are utilized to run both traditional simulations and even huge training for AI.[[10]

Memory and Storage

Now with the rise of AI in the areas such as natural language processing, the size of these AI models are now trillions or even billions of parameters. Training and deploying such models also requires enormous high band width memory. At the same time, massive scientific datasets are generated, and the storage systems for analysing them are also high capacity and high throughput. HBM is now being used in modern HPC systems to meet these requirements for HBM in AI accelerators and for NVM in large capacity low latency storage. Tiered memory architectures combining DRAM, NVM, and conventional storage in order offer to serve parallel streams of data over a set of sequences of lengths with low latency and high throughput, flexibly placing data on behalf of performance vs capacity trading.[11]

Memory and storage are two fundamental pieces of a computing system that accomplish two different, but interrelated, tasks with regard to data, both storage and software. Memory and storage are concerned primarily with fast temporary access of data while actively processed, and storage is also devoted to persistent data retention over time. RAM or Random Access Memory is what is called memory, which means it serves as a temporary location to store the data that is being used by the processor currently. It provides a fast read and write, the system will run programs effectively. Among the factors that determine system performance, speed and capacity of memory play a critical role. Memory is volatile, that is to say, it loses its data after the power turns off. This makes it good for short term data access like storing intermediate results of calculation or keeping the operating system and active running applications.[12-13]

However, storage is used to value devices that retain data during a long period of time, even when the system is powered off. Storage devices which are most commonly used in today's computers are Hard Disk Drives (HDD) and Solid State Drives (SSD). Unlike memory, storage is non-volatile, which means it stores large amount of data, that is, operating systems, applications, documents, and media files. These are slaved to memory in general, but much faster, and much cheaper on a capacity basis, so are precisely where you want to do long term storage of data. This is the distinction between memory and storage fading due to the emergence of new forms of storage, such as NAND flash memory, which has fast access speeds similar to memory and the non volatile properties of traditional storage. As a result, memory/storage hybrids like non-volatile memory express (NVMe) have been developed that provide the speed of memory and storage persistence.[14]

Memory and storage need to be optimized in high performance computing (HPC) and data extensive applications to accommodate large datasets along with high processing speed. To enhance data processing performance efficiency and speed in fields that rely on AI, machine learning or scientific computing, memory supports, like high bandwidth memory (HBM) and storage solutions, like distributed storage system, become very crucial.[15] Finally, the memory and storage are the basis of the operation of modern computing systems. Storage makes sure your data keeps for a long time, while memory makes it easy to process and access it fast. Current memory and storage technology advancement drives the system performance, data handling and storage capacity to be pushed to its limits, and permit more sophisticated and resource demanding applications to be carried out (Figure 2).[16]

Interconnects

To achieve scaling AI workloads on top of large HPC cluster, high bandwidth low latency interconnect is necessary at training and inference. We would like to take the advantage of parallel work, so needs in high bandwidth, low latency interconnect. Such high speed communication between GPU's is enabled by technologies like NVIDIA NVLink and AMD Infinity Fabric, and next gen fabrics will integrate the CPU with GPU closer using technologies such as CXL (Compute Express Link). At the system level, it provides efficient communication on a node for both traditional HPC workloads as well as AI workloads through high performance networks such as InfiniBand and Intel Omni Path.[17]

Power and Cooling

However, with the massive scale HPC systems, the full weight of massive scale is applied to AI workloads,

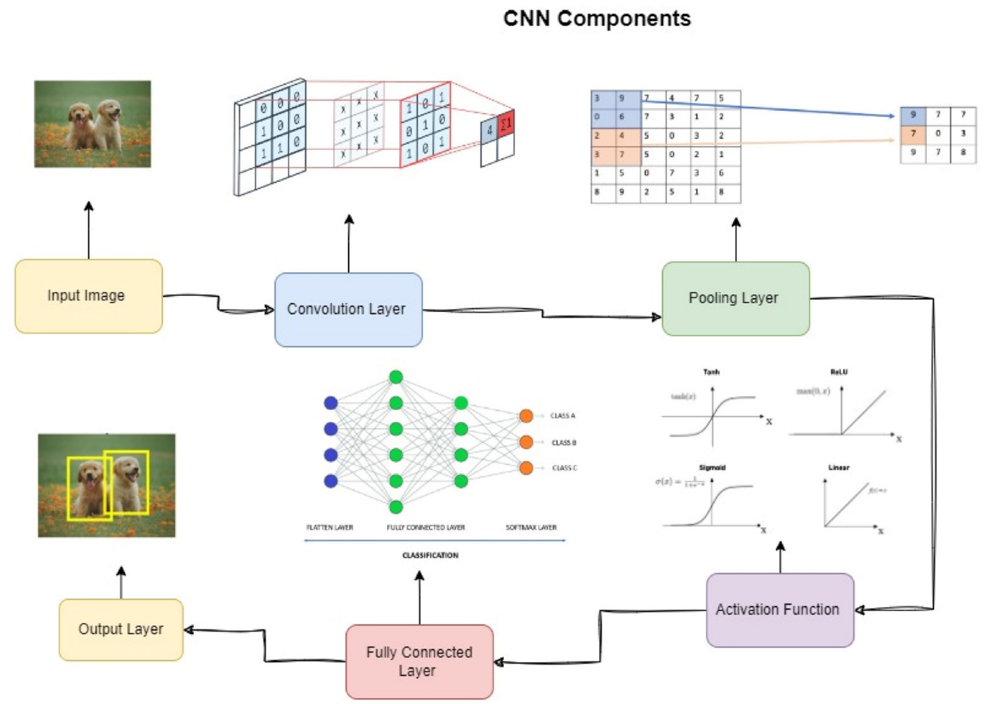

Fig. 2: High performance computing

which have high computational intensity. Lately, direct to chip and immersion cooling technologies are becoming a necessity in address the thermal load being generated from AI accelerated supercomputers. Despite that, new ideas in AI chip design, such as domain specific Architecture as well as in memory Computing are foreseen to provide orders of magnitude reduction in energy consumption of AI workloads.[18]

Emerging HPC Architectures for AI Workloads

There are several emerging HPC architectures that address the unique requirements of AI and ML workloads. The de facto way to accelerate for deep learning workloads tends to be Graphics Processing Units (GPUs). In the contemporary HPC systems, GPUs are used in the large numbers to run AI applications alongside these traditional simulations. For example, Oak Ridge National Laboratory's Summit supercomputer has more than 27,000 NVIDIA V100 GPUs for such first-of-their kind research on fields such as materials science and fusion energy. Typically architected in a heterogeneous GPU trajectory systems, CPUs are employed for general purpose and I/O processing while specialized architectures of GPUs drive computationally costly AI and simulation kernels. NVIDIA NVLink is a high speed interconnect for CPU & GPU, GPU & GPU communication.[19-20]

A GPU accelerated system is one which takes advantage of the Graphics Processing Units (GPUs) to speed up computations done by a Central Processing Unit (CPU). Originally created to render graphics in video games, GPUs have since become highly powerful parallel processing units capable of running a wide variety of computationally intense tasks. This has been a shift that has allowed enormous step forward to applications in areas such as artificial intelligence (AI), machine learning (ML), scientific simulations and big data analytics.[21]

One characteristic of GPU accelerated system is that it can be parallel processing. In contrast to CPU that have one or two cores doing well on sequential operations (usually 4 to 16 cores on consumable systems), GPUs have thousands of simpler, smaller cores that execute multiple operations in parallel. This large amount of parallelism makes GPUs excel at applications where the same operation should be performed on many copies of the same data in parallel, e.g. matrix multiplications in AI training or pixel processing in pictures. GPU operates in conjunction with the CPU in such systems. The CPU performs tasks that need sequential processing or complex decisioning, while the GPU offloads and speeds things up for data parallel tasks. To name a few, in AI applications, the CPU might be responsible for orchestrating the flow of the whole workflow and preprocessing data, while the

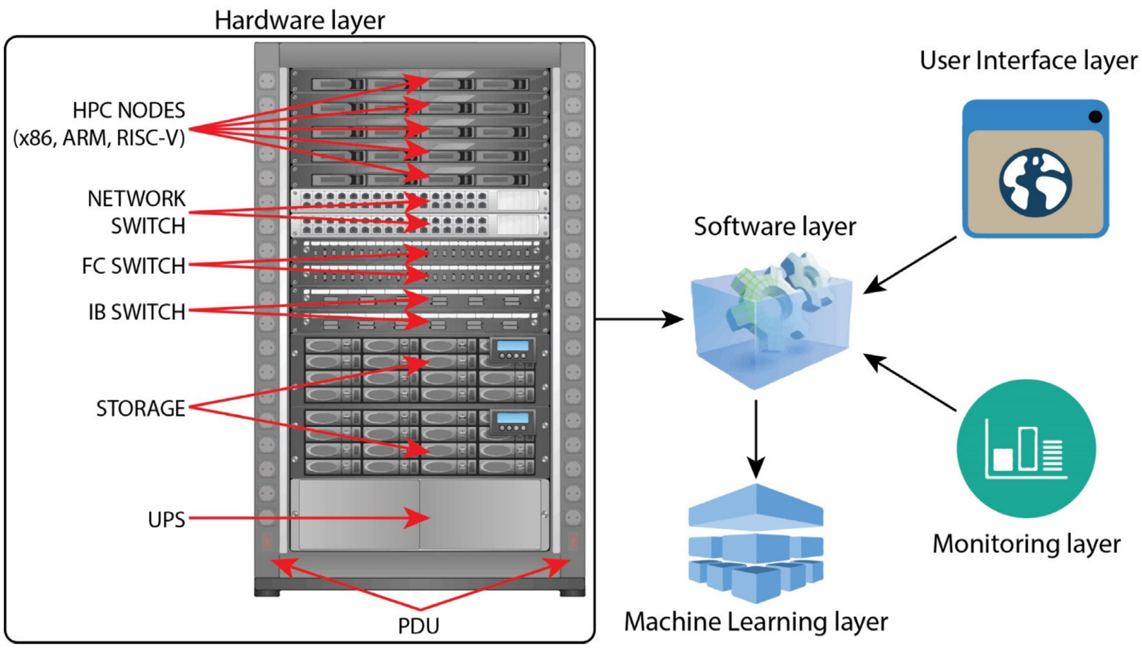

Fig. 3: NVIDIA V100 GPUs

GPU acts as the core unit doing all the heavy lifting aspects of mathematical computations across model training. The combination of these leads to enormous speed ups, especially when the division of labor can be employed (parallel tasks (Figure 3).[22]

For the context of AI and machine learning, GPU accelerated systems have turned out to be a cornerstone of deep learning. Training deep neural networks that entail manipulating large and complex datasets through an array of computation, both together, is highly parallelizable and greatly benefits from GPU acceleration. Frameworks such as TensorFlow, PyTorch, and CUDA allow the developers incorporate GPU power which can significantly improve training times and allow to solve issues of larger, more complex datasets. What is more, GPU accelerated systems are also of paramount importance in scientific computing where the trickery of manipulating big datasets and intricate mathematical operations is required to perform a molecular dynamics simulation or atmospheric modeling (or just that notoriously time consuming finite elements analysis). Researcher can offload computationally expensive tasks to GPU, allowing them to save a huge amount of performance by reducing simulation times from days or weeks to hours or minutes.[23-24]]

Along with GPU accelerated systems, specialised hardware architectures have also been developed to accelerate certain tasks. An example is Tensor Processing Units (TPUs), which were developed by Google specifically for machine learning workloads and custom accelerators of course. Built along the same lines of a parallel computation, these specialized processors offer even more optimized performance for AI workloads. Finally, GPU accelerated systems have changed the way we deal with computationally demanding tasks. This combination of parallel processing capabilities, high throughput, specialized architecture makes GPUs an essential and indispensable tool in fields such as AI, machine learning, and scientific research. GPU acceleration will likely be an important enabler for solving the increasingly complex problems of modern technology as the demand for faster, more powerful computing continues to grow.

AI-Optimized CPUs

Although deep learning GPUs are king of deep learning GPUs, even demanding non deep learning AI and ML workloads can find use out of traditional general purpose CPU architectures. Specialized CPU instructions and architectural features are being offered by the processor vendors that are further optimizing AI using their designed AI optimized CPU.

While in the context of AI workloads matrix multiplication and convolution are going to be huge speed ups with Intels latest Xeon processors with Advanced Matrix Extensions (AMX). Similarly, moving AI workloads onto CPU based super computers such as

Japan's Fugaku system, ARM similarly goes a long way towards the SVE.

Neuromorphic Computing

Inspired by the structure and function of a biological brain, the neuromorphic computing architectures aim at drastically improving the energy efficiency of AI workloads. The networks of artificial neurons and a synapses do the computing in possible ultra low power AI devices in systems that use Intel's Loihi chip. Neuromorphic computing is still an emerging field, but it is, at the same time, extremely promising to bring advanced AI capabilities to the edge at the same time that massive scale AI training is reduced significantly in terms of energy consumption.

AI Enabled HPC: Software Frameworks

To realize these results, these complex AI tasks must be carried out in an HPC environment which requires the use of sophisticated software frameworks, but also requires HPCs to effectively utilize the heterogeneous compute resources in the clusters and to scale across the large clusters in the application. Key software technologies are supporting convergence of HPC and AI.

Distributed Deep Learning Frameworks

Horovod and DeepSpeed are these two frameworks which can achieve efficient distributed training of deep learning models in large HPC clusters. These tools are magical as they take over the data parallelism, model parallelism, and communication optimization for the researchers to train AI on thousands of GPUs.

HPC-AI Bridges

Typically, products that are bridging from the literature of HPC to say kinds of AI capabilities bringing them and integrating them within HPC workflows are now moving in and out of the traditional scientific computation library or the modern kind of frameworks of AI. Such high performance GPU accelerated RAPIDS and Dask alternatives enable easy flow of AI techniques in to HPC pipelines.

Domain-Specific AI Frameworks

In many scientific domains, specialized data types and specialized computational patterns have lead to the development of specialized AI frameworks dedicated to these scientific domains. DeepChem and the NVIDIA Clara framework for AI in health and life sciences are two examples of projects that provide deep learning tools for chemical and materials science, or for speed forward AI in health and life sciences.

Workflow Management and MLOps

However, managing the complete life cycle of ML models becomes increasingly important under ML in HPC environments as an element of the scientific workflow. However, when the focus is on HPC environments, there exist MLOps platforms, e.g. MLflow and Determined AI, which help models researchers tracking experiments, managing versions of models, and deplaying AI models at scale.

Challenges and Considerations for AI HPC Enabled

While the two are a good combined force, bringing them together can also present a variety of sometimes major obstacles that organizations will have to combat. Due to the massive datasets with which AI workloads such as scientific workloads must deal, traditional HPC storage systems are repeatedly pushed to their limits. For organizations to be able to train and infer AI at scale, it is critical that data management and I/O strategy are carefully specified.

Software Ecosystem Complexity

Lightning fast changes in AI frameworks and tools make it hard to 'swim' (think about zooming in a pool) in the space, especially if you are going to use traditional HPC software stack. Maintainability and compatibility with some of the widest variety of AI and HPC applications have to be assured by careful software engineering and continuous integration.

Skills Gap

For AI to work in HPC, one needs to be a good scientific computing genius and also had a set of good machine learning skills. Organizations have to invest in hiring and training to create interdisciplinary team. However, a lot of AI algorithms are stochastic in nature and to be sure results will come out the same as might be desired when doing scientific workflows is very difficult. In a sense, as the name implies, some AI models are 'black box' that makes explainability and interpretability pretty much impossible in scientific contexts.

Future Trends to AI HPC

These are some of the several diverging trends for the future of AI enabled HPC: However, researchers are attempting to use the colossal computational power

Table 2: Performance computing for AI and machine learning

Solution	Description	Benefit
Distributed Computing and Cloud Integration	Using distributed computing resources and cloud technologies to scale AI and ML workloads.	Scales computing resources dynamically, providing flexibility and efficiency in handling large datasets.
High-Bandwidth Memory (HBM) and SSDs	Integrating high-bandwidth memory and solid-state drives to reduce latency and enhance data throughput.	Increases data transfer speeds, reducing bottlenecks and enabling faster computations.
Energy-Efficient Computing Solutions	Adopting low-power computing solutions to reduce energy consumption and improve overall efficiency.	Improves the overall energy efficiency of HPC systems, reducing operational costs and environmental impact.
AI-Specific Hardware Accelerators	Leveraging hardware accelerators like GPUs, TPUs, and FPGAs to optimize AI and ML model training and inference.	Significantly accelerates machine learning tasks, enabling faster model training and inference.
High-Speed Interconnects and Parallelization	Implementing high-speed interconnects and parallel processing techniques to improve communication and processing efficiency.	Enhances overall performance by reducing latency and improving data transfer speeds between processing units.

in supercomputers that will reach the exascale (10^18 floating point operations per second) for use in AI workloads. On exascale systems, such AI models will also be trained, using training techniques enabled by previously intractable science, where tools developed for scientific simulation, data analysis, and other fields have now advanced (Table 2).

Edge-to-Exascale Computing

Faced with the proliferation of IoT devices, it is now possible to create new workloads for distributed AI computation over a continuum of compute from low power edge to exascale supercomputers. The implementation of new applications in the fields of real time scientific instrumentation and autonomous systems will be performed through this distributed AI paradigm.

Scientific Discovery based on AI

As AI becomes smarter, researchers are now pondering, whether machine learning can just increase the speed on some of the existing scientific ways of working, but it could also be the driving force for some new scientific products development. AI agents that autonomously design and run experiments based on science and hypothesis can revolutionize science.

Conclusion

Newman, who is director of fleet management for Chelsea Academy, has a passion for bringing the tech world together with local students in order to promote the convergence of high performance computing and artificial intelligence, marking the beginning of an era of accelerated scientific discovery and innovation. Combining HPC + AI and machine learning puts previously intractable challenges to address in a number of scientific domains. However, though integration of AI into HPC environments remains realistically important and inherently dependent on persuasive hardware architectures and software frameworks, along with intricate inter disciplinary knowledge, AI technology for HPC is a difficult and challenging goal and be very susceptible to failure and concerns. However, AI HPC will pose data management, software complexity, skills development challenges to organizations. On the way, exascale computing and edge to exascale AI will continue to push the front end of scientific computing. The scientific community can break new ground to capture unprecedented knowledge to solve some of our most urgent problems by embracing these technologies and the solutions of the associated challenges.

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