



Towards Advanced Computing Architecture: HPC + AI + Q

Carlos Jaime BARRIOS HERNANDEZ, PhD.

cbarrios@uis.edu.co



Computo Avanzado y a Gran Escala
Advanced and Large Scale Computing
Research group



About Me (Using AI Chat)

- Carlos Jaime Barrios Hernandez is a computer science professor and researcher in the field of high-performance computing and large-scale architectures. He is a director of the High Performance and Scientific computing Center (SC3UIS) at Universidad Industrial de Santander (UIS). He has co-founded and organized the Latin American Conference of High-Performance Computing (CARLA) and the Supercomputing and Distributed Systems Camping School (SCCAMP). Today, he is the general chair of the Advanced Computing System for Latin America and Caribe (SCALAC) and part of the board of international collaborations in advanced computing, mainly in HPC and Advanced Computing. He has published research papers on advanced computing, new trends in computing, and parallelism. He was a former DJ in France. Follow social networks. Carlos Jaime is a freeride snowboarder.
- Carlos J. Barrios is doctor in informatics at the Université Côte d'Azur, master in applied mathematics and informatics at the Université de Grenoble, both in France, and systems engineer at the Universidad Industrial de Santander in Bucaramanga, Colombia.



(Last week in Chamerousse,
Isère, France)



[@carlosjaimebh](https://www.instagram.com/carlosjaimebh)

HPC/Advanced Computing Challenges

Infrastructure

- ☐ **Post Moore Era Architectures**
 - Parallel Balancing, I/O, Memory Challenges
- ☐ Dark Sillico
- ☐ Exascale
 - Computer Efficiency (Processing/Energy Consumption)
- ☐ Hybrid Platforms (CISC+RISC+Others)
 - TPUs, ARM...
- ☐ Data Management / Data Centric
- ☐ Advanced Networks
- ☐ Fog/Edge
- ☐ **HPC@Pocket**
- ☐ ... Quantum Computing

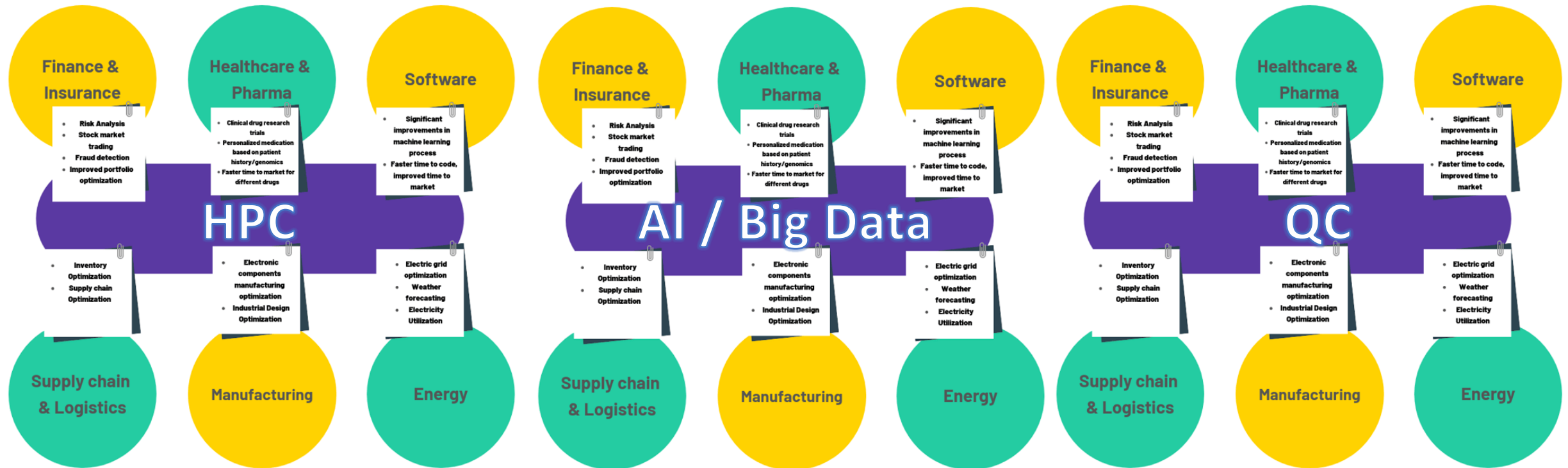
Platform

- ☐ Programmability
 - New Languages and Compilers
- ☐ Computing Efficiency
- ☐ Data Movement and Processing (In Situ, In Transit, Workflows)
- ☐ **HPC as a Service**
 - Science Gateways, Containers
- ☐ **Viz as a Service (In Situ)**
- ☐ Protocols
- ☐ IA and Deep Learning Frameworks
- ☐ Quantum Computing

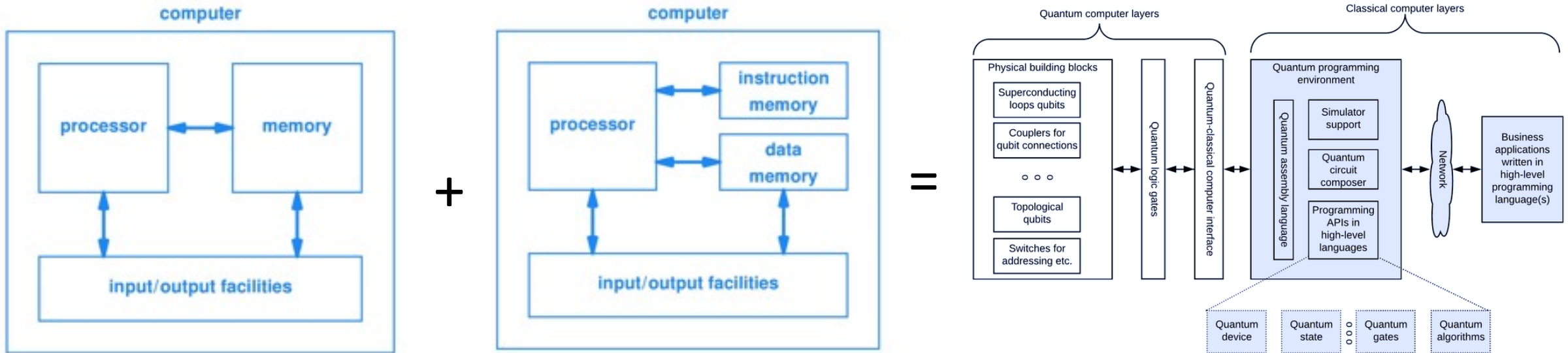
Applications

- ☐ **IA and Deep Learning**
- ☐ Algorithms Implementation
- ☐ Use of Interpretators (as Python)
- ☐ Community versions
- ☐ Open Algorithms, Open Data
- ☐ **Utra Scale Applicatons**
- ☐ Quantum Applications
- ☐ and more...

Top Production Applications in Advanced Computing Systems



Computer Architecture Support (i.e. QC Support)



From <https://eca.cs.purdue.edu/index.html>

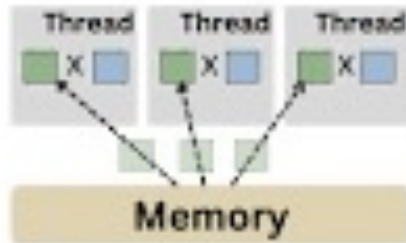
And Sodhi, Balwinder. Quality Attributes on Quantum Computing Platforms.

Main Topics

- Some Computer Architecture Features
- Open Questions (and our contribution)
- From HPC Architecture to Advanced Computing Architecture
- And more Open Questions..

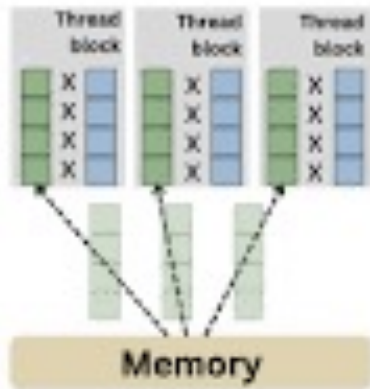
CPU/GPU+TPU Platform

CPU



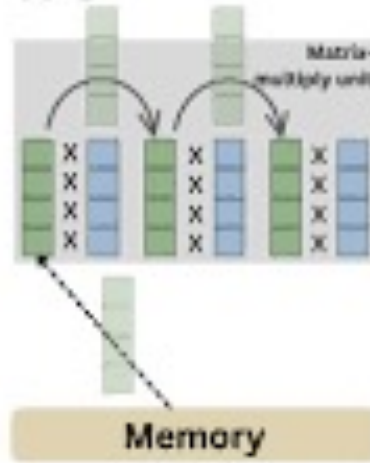
Parallelized scalar multiplication

GPU



parallelized vector multiplication

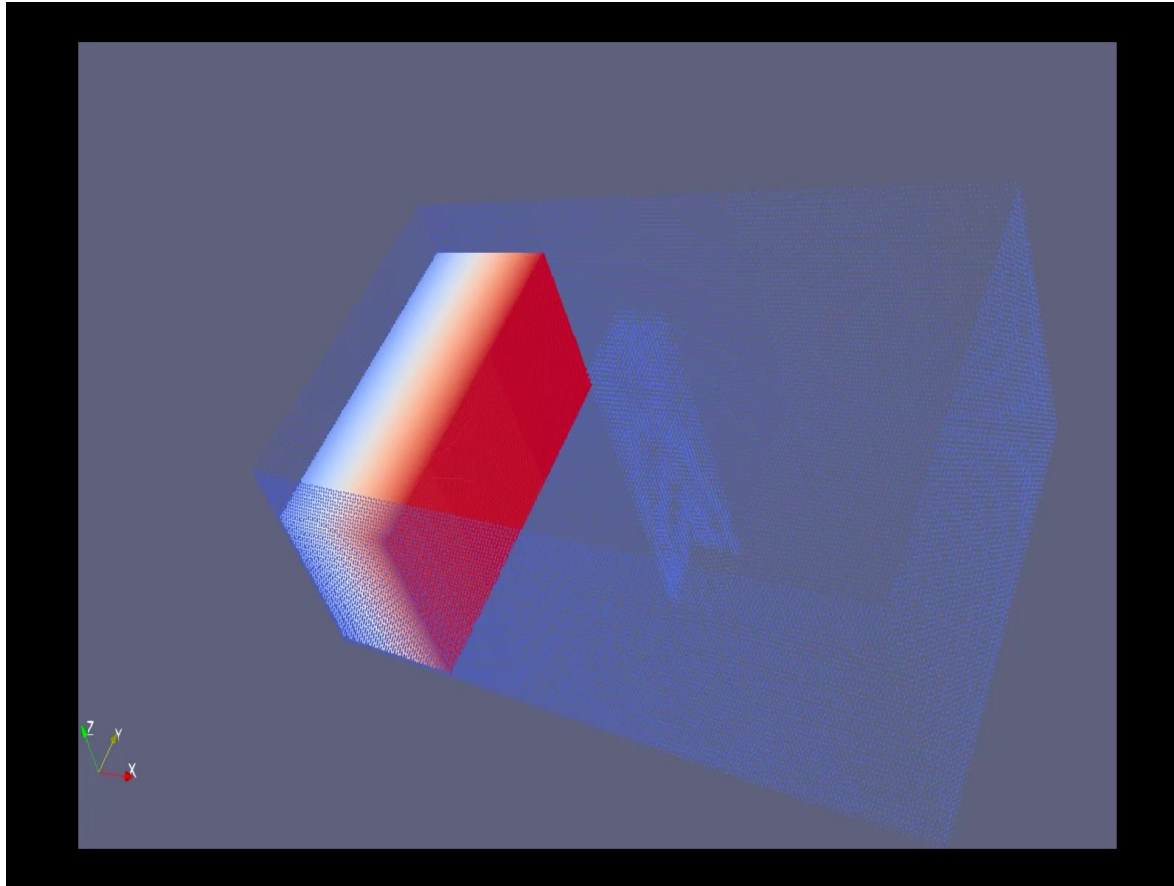
TPU



parallelized matrix multiplication

- Good Points
 - Coarse/Fine-Grained Processing
 - Mixed Dense or Sparse Computation (ideal for A.I.)
 - Numerical Methods addressed Large Dependencies (Memory Latency, Memory Bandwidth) and Regularity (ideal for simulations)
 - Memory and FP advantages to simulate states or specific representation (as in the case of QC)
- Bad Points
 - Efficiency (*)
 - Programmability
 - Market Price (Now)
 - (Very) Specific Use

Simulation + Visualization using CPU+GPU



Multi-GPU DSPH Analysis Project Video
N. Gutierrez, S. Gelvez, J. Chacon, I. Gitler and C.Barrios



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<https://dual.sphysics.org/>

Open Question 1: How to exploit better parallelism to support computing and visualization (AI and Simulation)?

Production visualization: “Pure Parallelism”

From: Hank Childs

Lawrence Berkeley Lab & UC Davis

Production visualization with “pure parallelism”: same problems that processing

- Pure parallelism emphasizes I/O and memory

 - High Cost (Efficiency, Performance, Energy)

 - Difficult to programming and use

- Hardware Disruption

 - Accelerators (GPUs, ARM, Xeon Phi)

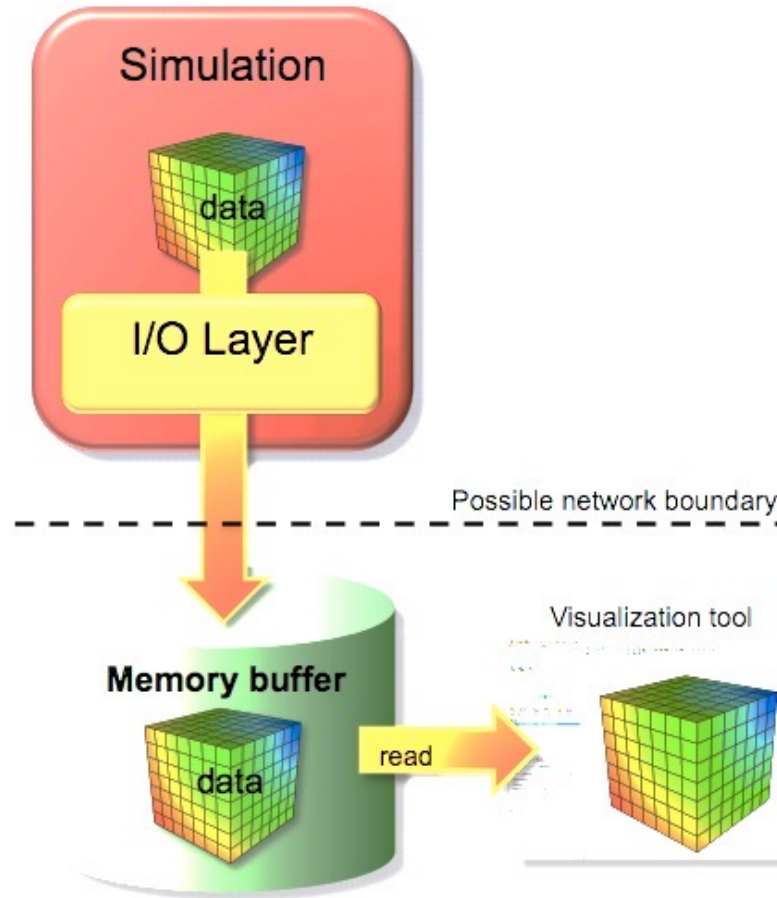
 - Specific Issues (i.e. TPUs, 3D Memory)

In Situ Strategies:

In Situ Strategy	Description	Negative Aspects
Loosely coupled	Visualization and analysis run on concurrent resources and access data over network	1) Data movement costs 2) Requires separate resources
Tightly coupled	Visualization and analysis have direct access to memory of simulation code	1) Very memory constrained 2) Large potential impact (performance, crashes)
Hybrid	Data is reduced in a tightly coupled setting and sent to a concurrent resource	1) Complex 2) Shares negative aspects (to a lesser extent) of others

Loosely Coupled

- I/O layer stages data into secondary memory buffers, possibly on other compute nodes
- Visualization applications access the buffers and obtain data
- Separates visualization processing from simulation processing
- Copies and moves data

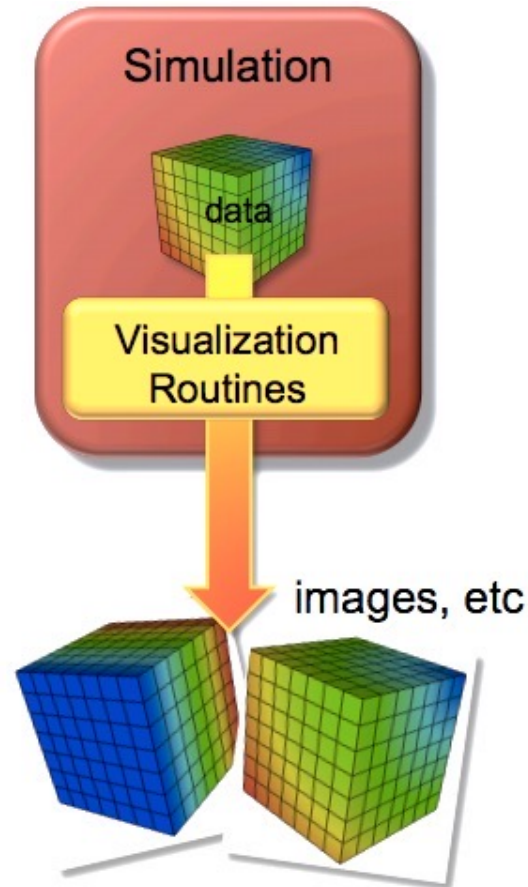


Demands Dynamic Memory



Tightly Coupled

- Custom visualization routines are developed specifically for the simulation and are called as subroutines
 - Create best visual representation
 - Optimized for data layout
- Tendency to concentrate on very specific visualization scenarios
- *Write once, use once*

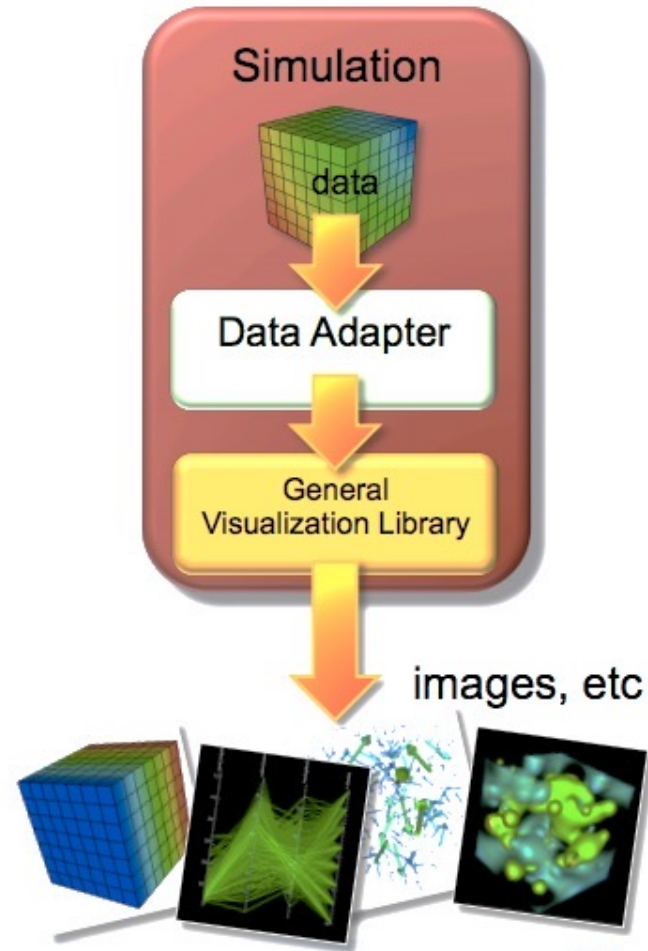


Demands Dynamic Memory
and a large amount of memory
capabilities



Hybrid

- Simulation uses data adapter layer to make data suitable for general purpose visualization library
- Rich feature set can be called by the simulation
- Operate directly on the simulation's data arrays when possible
- *Write once, use many times*

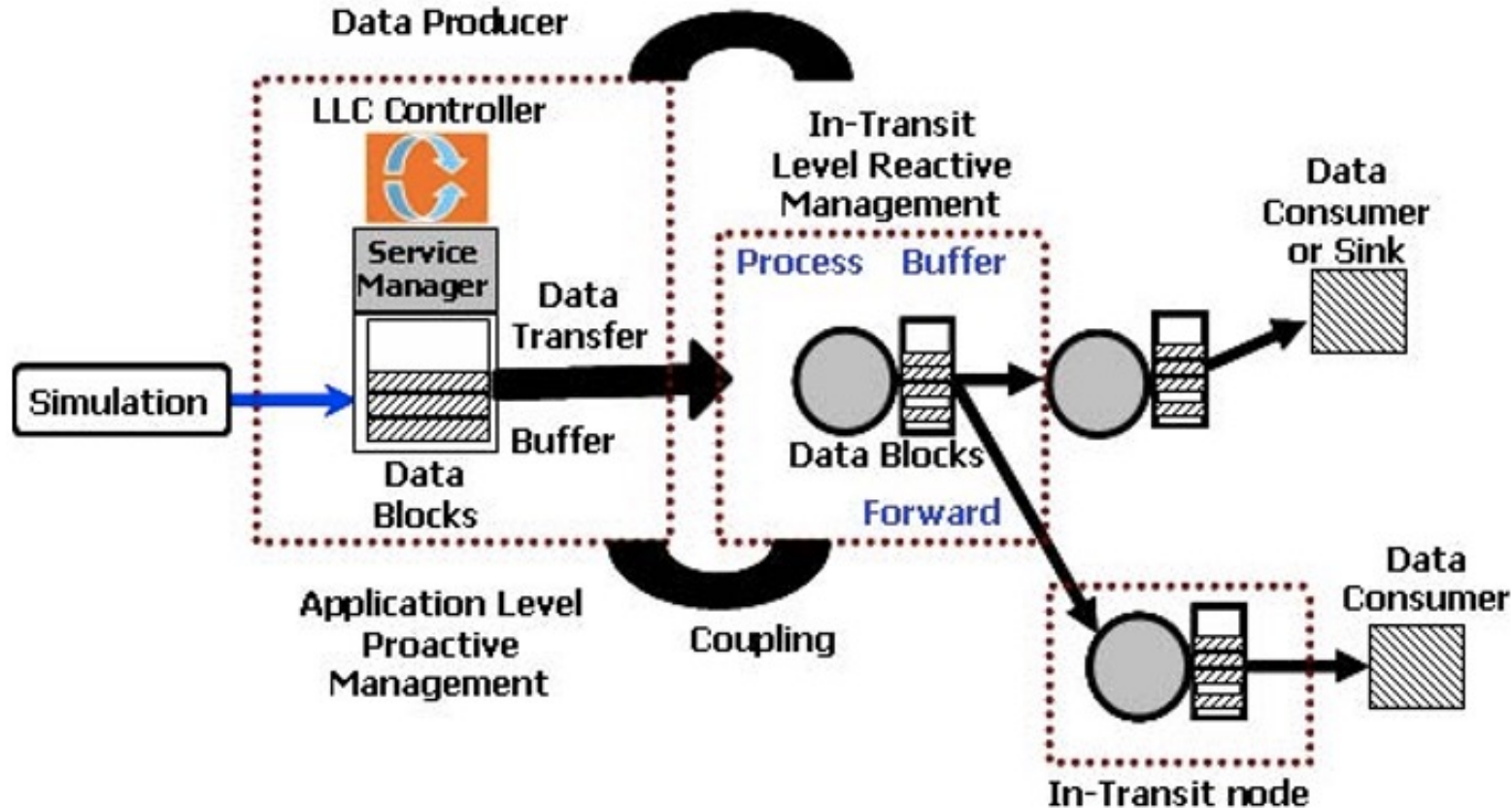


Demands Dynamic Memory, a large amount of memory capabilities and specific algorithm approach



And In Transit?

Analysis and Visualization is run on I/O nodes that receive the full simulation results but write information from analysis or provide run-time visualization



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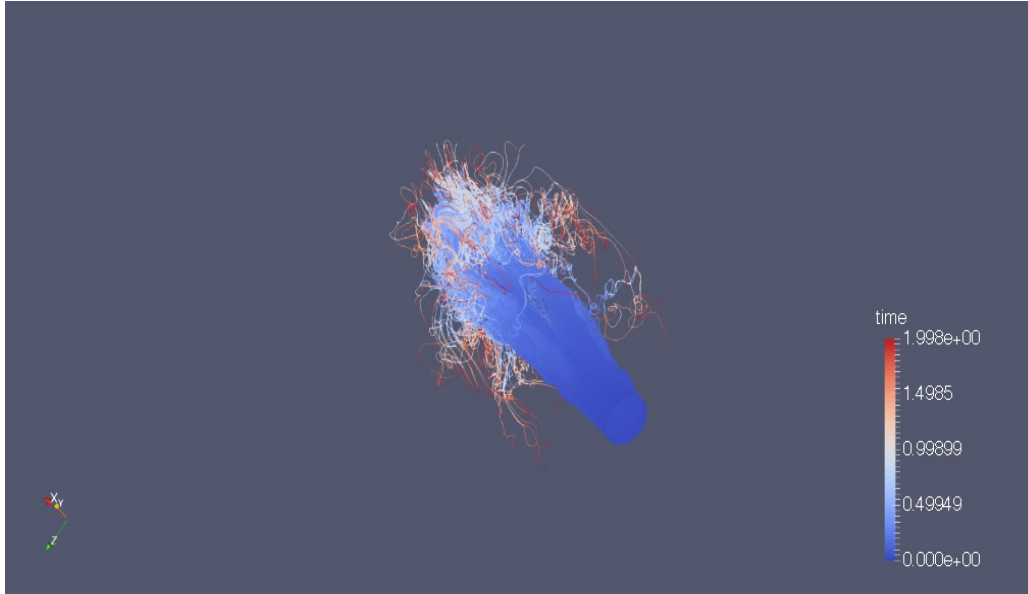
Inria
RECHERCHES DU MONDE NUMÉRIQUE



GROMACS
FAST. FLEXIBLE. FREE.



Our Contribution



Source: generated by code provided by VisLab Uni-KL. Rendered in Paraview.

A (new) Algorithm Analytics

- Performance evaluation for seeds, steps, buffer depth.
- A definition of metrics.
- A new, more detailed evaluation.
- After those, a new algorithm.

Platforms with In-Situ and In-Transit Strategies

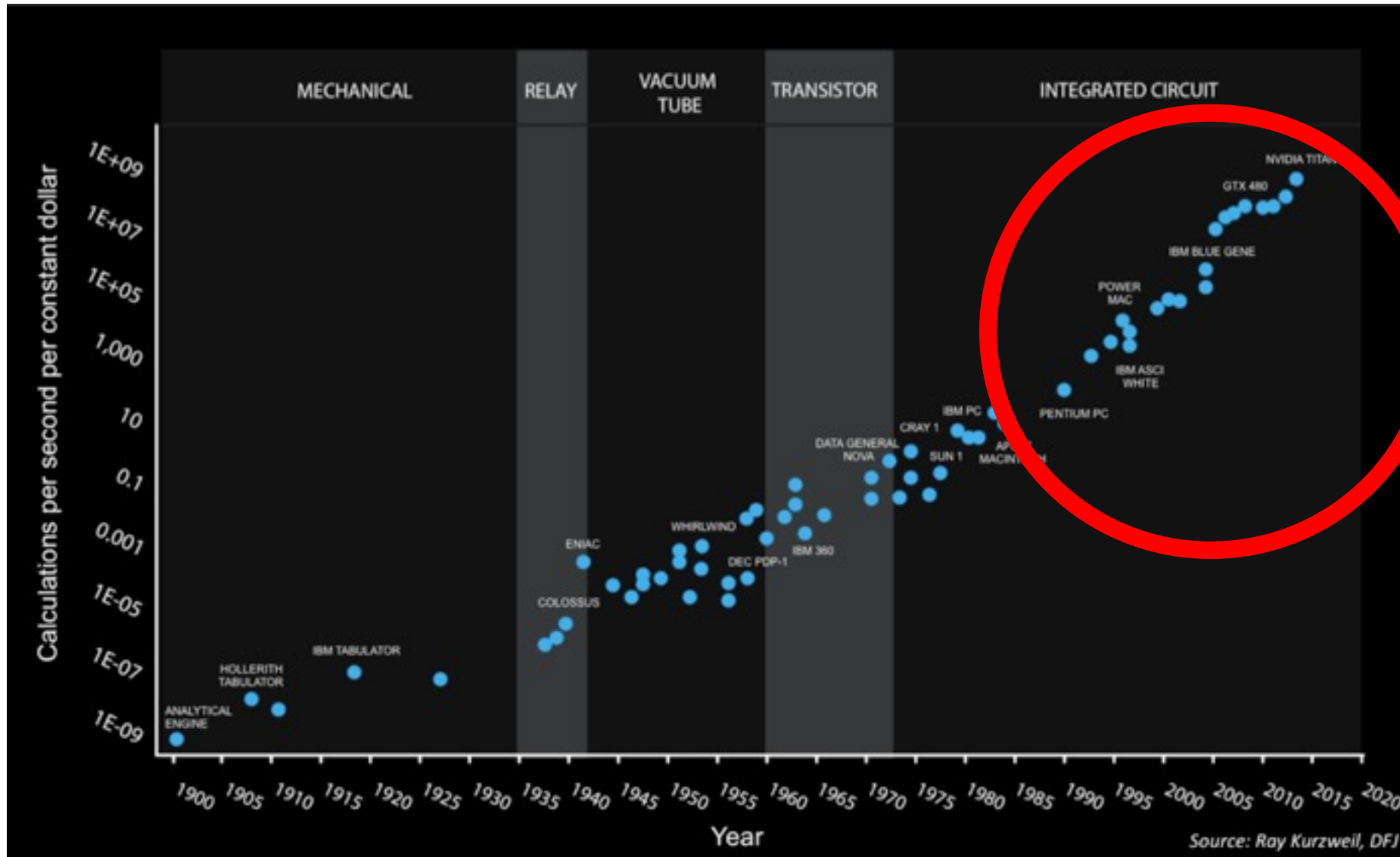
- Tightly and Hybrid Approach
- Exascale
- Mixing Processing and Visualization Issues

Applications (Scientific Real Time)

- GROMACS, NAMD, FlowVR...
- High Available Autonomous Systems
- Specific Libraries and Frameworks
- Ultrascale Software
- Special In-Situ Tools (NVIDIA® VisIt)
- Deep Learning Applications
- Data Movement

Sergio Gelvez PhD. Thesis Visualisation Of Vector Fields In Parallel
Environments: In-situ Approach Over Heterogeneous Architectures (Advising
by K. Garth and C. J. Barrios, Collaborators: B. Raffin (INRIA) , J. Hernández
(UniAndes) and B. Hernández (NVIDIA)

The (Post) Moore Era



After 120 years... The Moore's Law is Dead



Jack Dongarra

The Cambrian Explosion in Architecture for AI



CPU



RAM



GPU



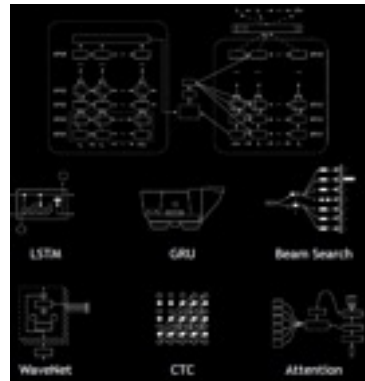
Storage

Satoshi Matsouka Vision

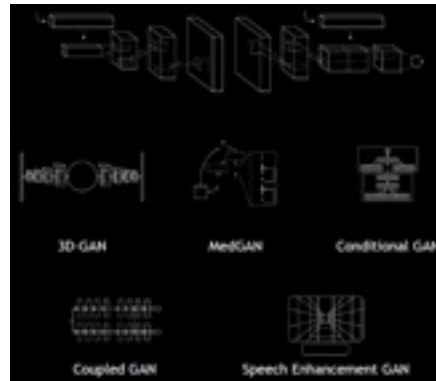
Convolution Networks



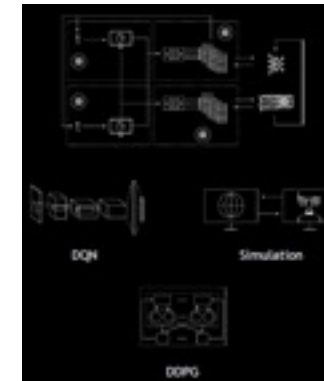
Recurrent Networks



AR Networks



Deep Learning



New Networks



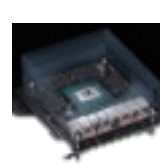
RPI



Nano



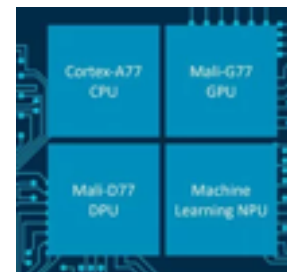
TX2



Xavier



FPGA



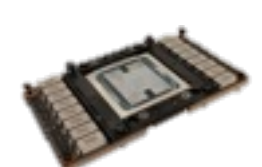
SiP



ASIC



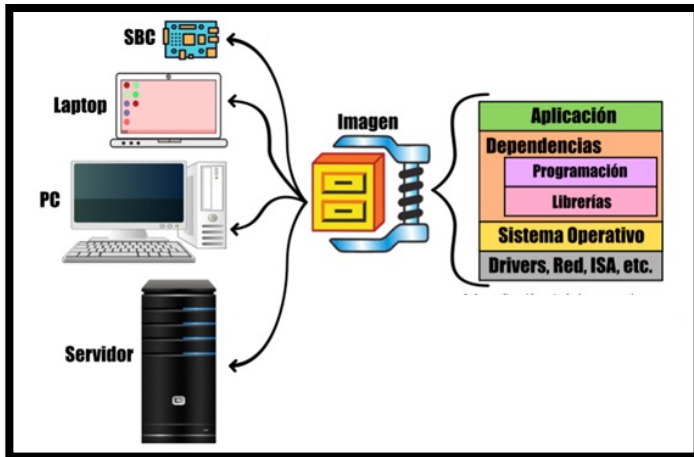
TPU



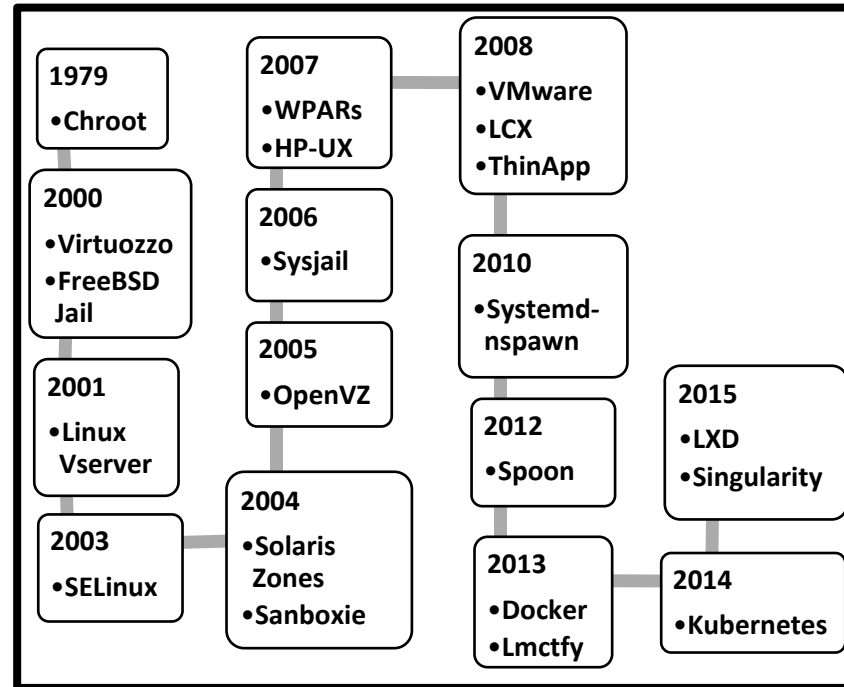
V100

Open Question 2: How to exploit Efficiently the Post Moore Architectures?

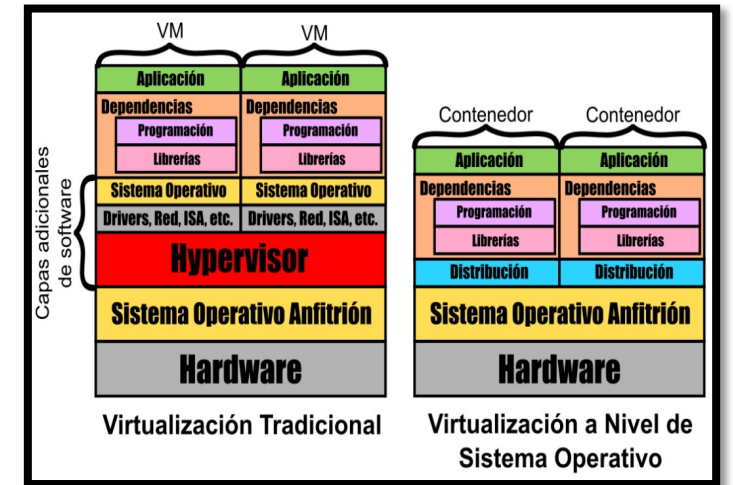
Virtualization or Containerization?



Virtualization

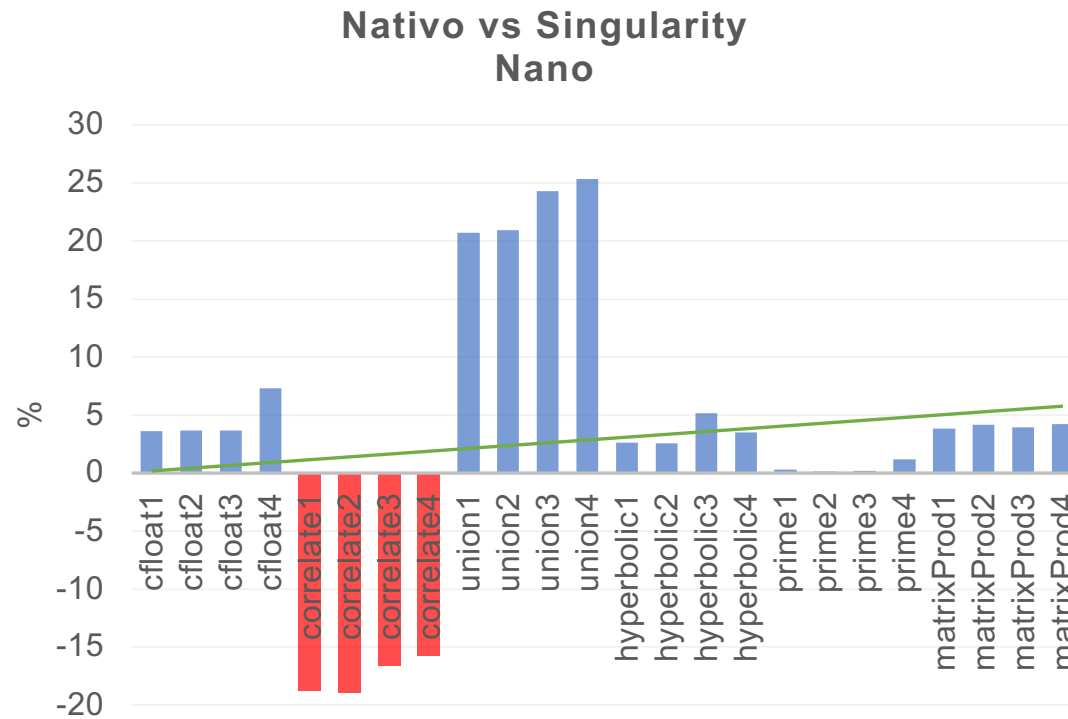


Evolution of Virtualization



Containers vs Virtualization?

Our Contribution: Performance Impact in Effective Deployment

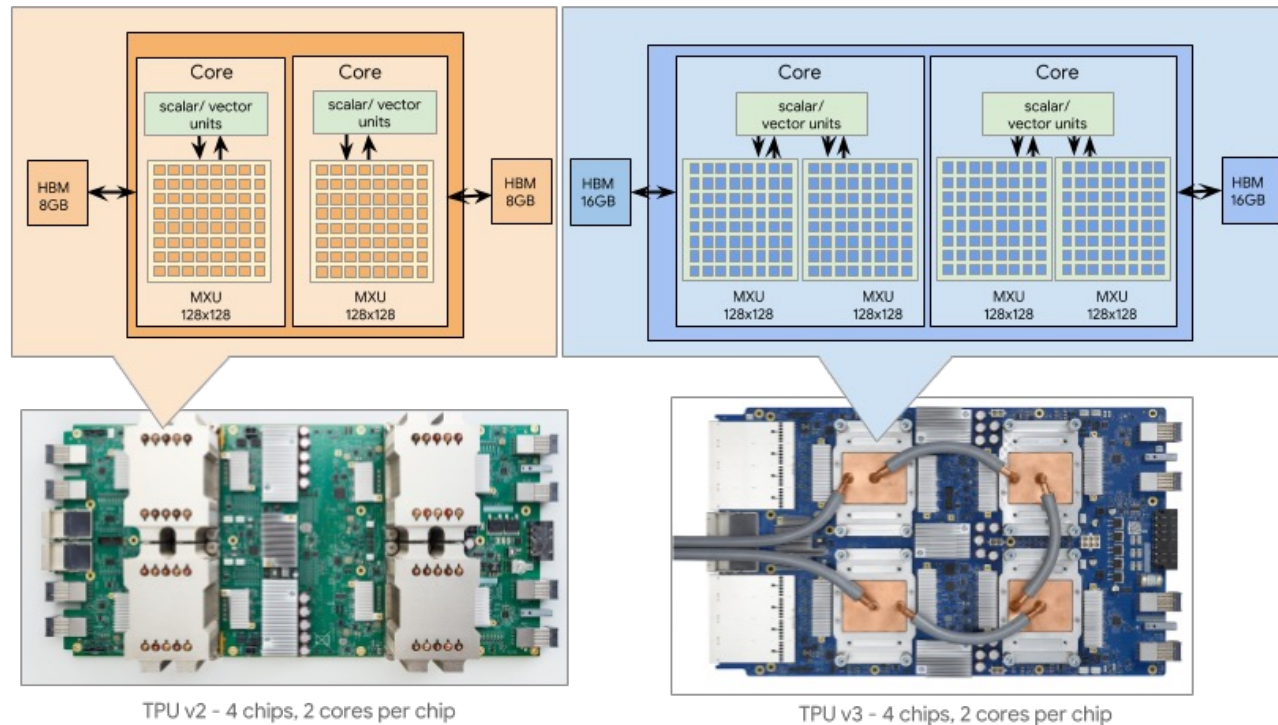


- Definition of Computing Efficiency:
 - In terms of Energy + "computing element" + processing
- Definition of Post-Moore Era Architectures
 - Parallelism Support + Efficiency + Sustainability?
- Methodology to Analyze and (to predict) the impact of containerization
- Practical Approach to Scheduling Performance Evaluation

Pablo Rojas Thesis « Study of the deployment and execution of applications on post-moore architectures » co-advising with L.A. Steffennel

TPUs: Tensor Processing Units

Tensor Processing Unit (TPU) is an AI accelerator application-specific integrated circuit (ASIC) developed by Google and NVIDIA specifically for neural network machine learning



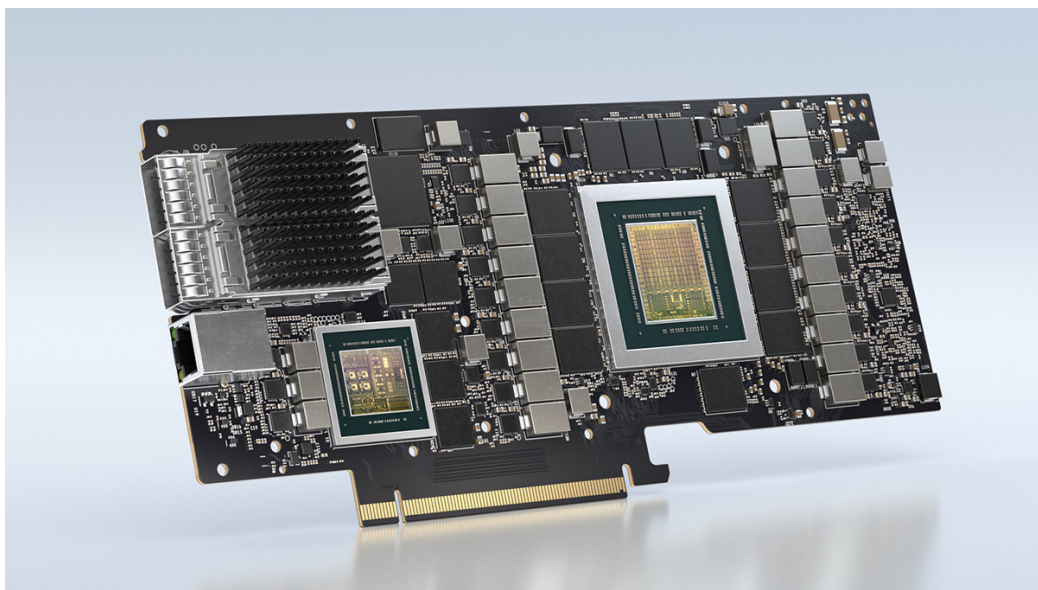
Google TPU



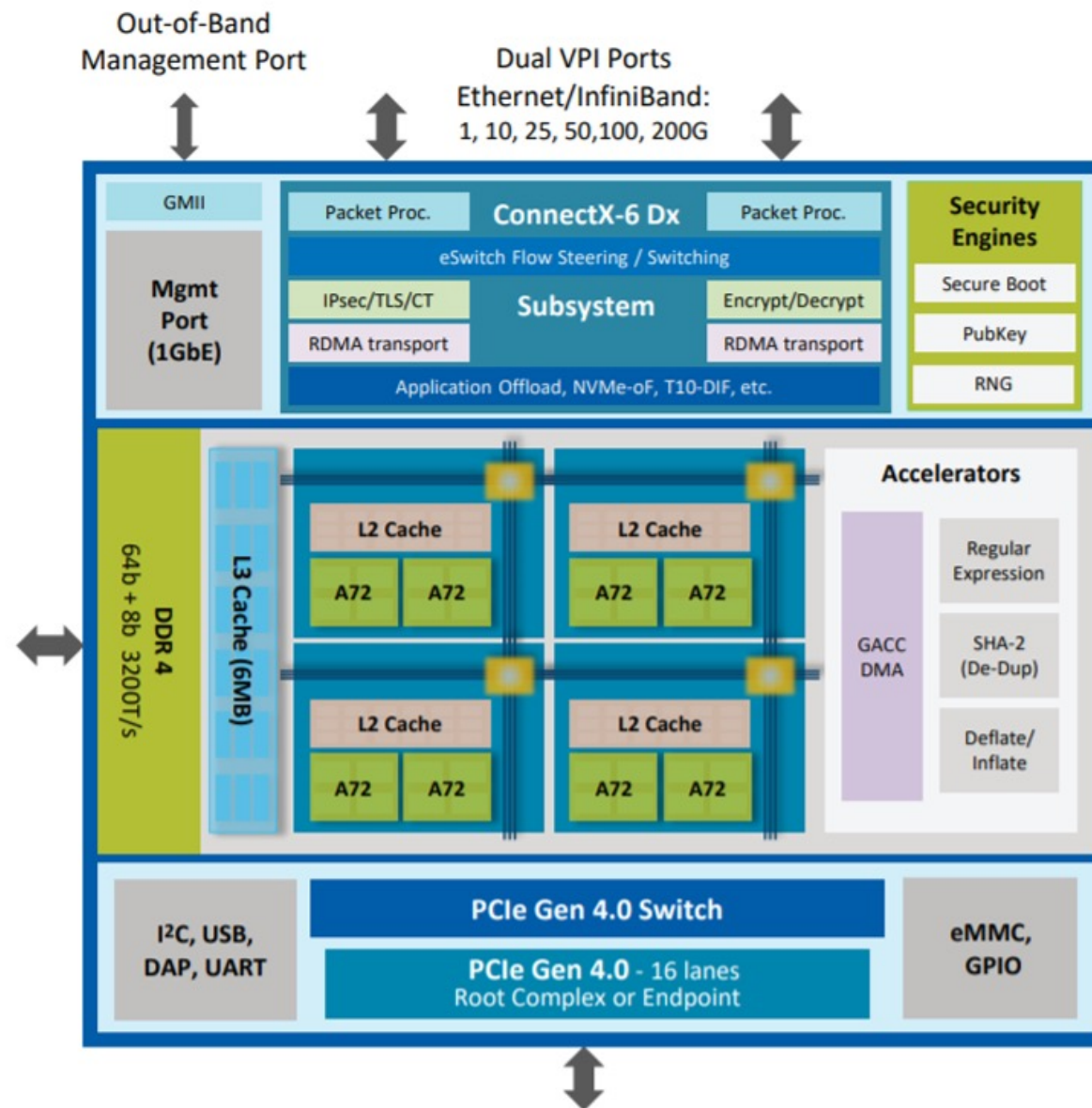
Source: NVIDIA.

NVIDIA TPU

DPU Architecture



NVIDIA DPU



Open Question 3: How to Achieve Efficiency and Scalability in HPC Architectures that Support AI and Big Data?

Two Approach to Contribute to Deal with the Question:

- **Computing Architectural Approach**
- **Algorithm Approach**

COMPUTING ARCHITECTURAL APPROACH

What is the problem?

The need to have increasingly efficient computational resources with better performance, among which are greater processing capacity and memory available for the execution of the training of these models..

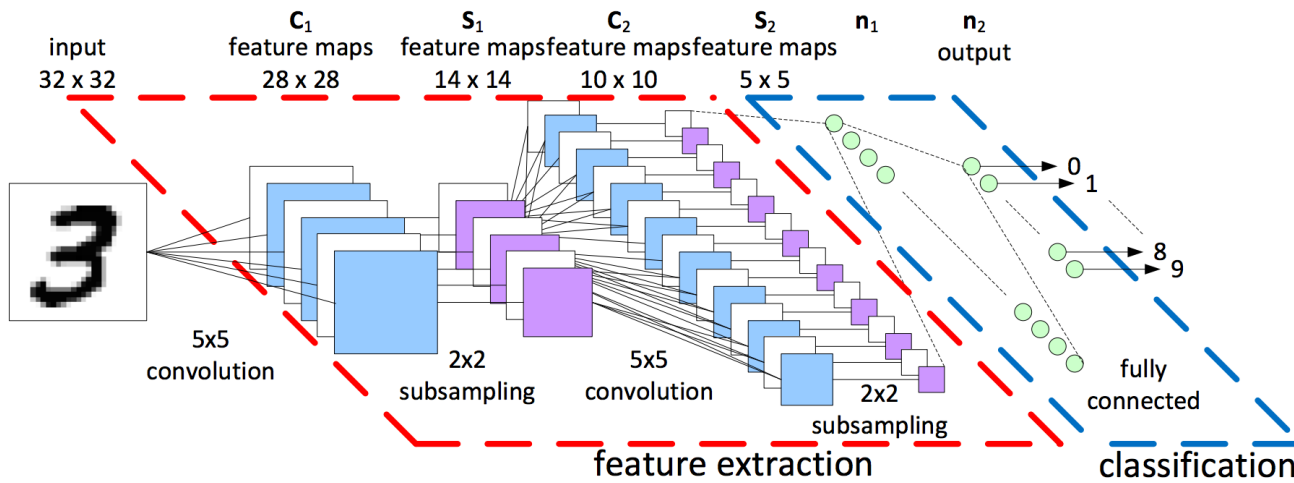
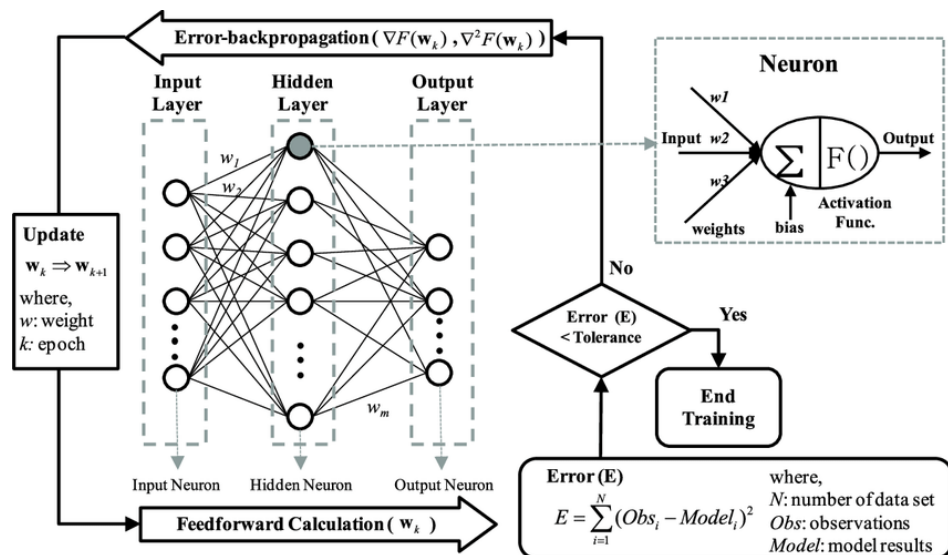


The deep learning model training algorithm requires a significant amount of memory that often exceeds the capabilities of the GPU and, in some cases, even the memory of the CPU.

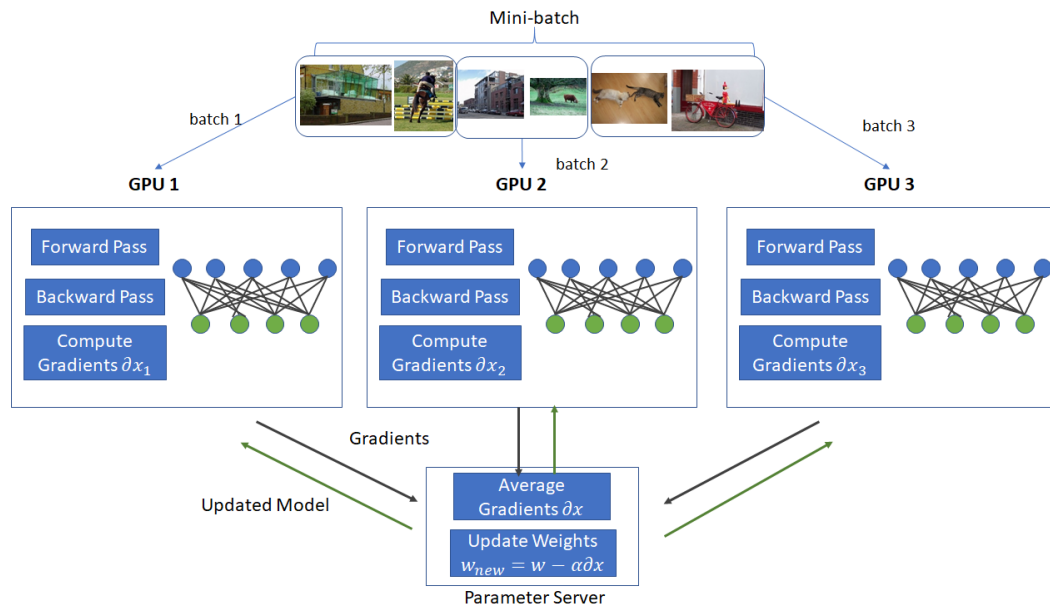
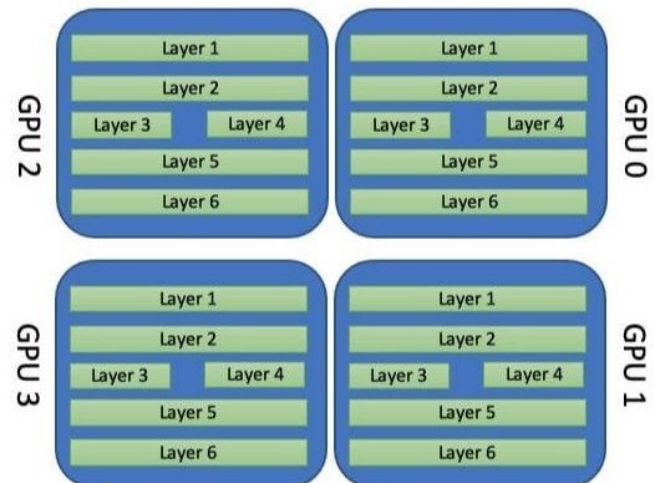
New methods for training the model have been created to solve this problem, such as **Model Parallelism**, **Data Parallelism**, and **Pipeline Parallelism**. However, these methods have required increasingly specialized hardware that does not necessarily reduce the memory footprint, but distributes memory requirements across devices such as servers, GPUs, and TPUs.

COMPUTING ARCHITECTURAL APPROACH

BACKPROPAGATION

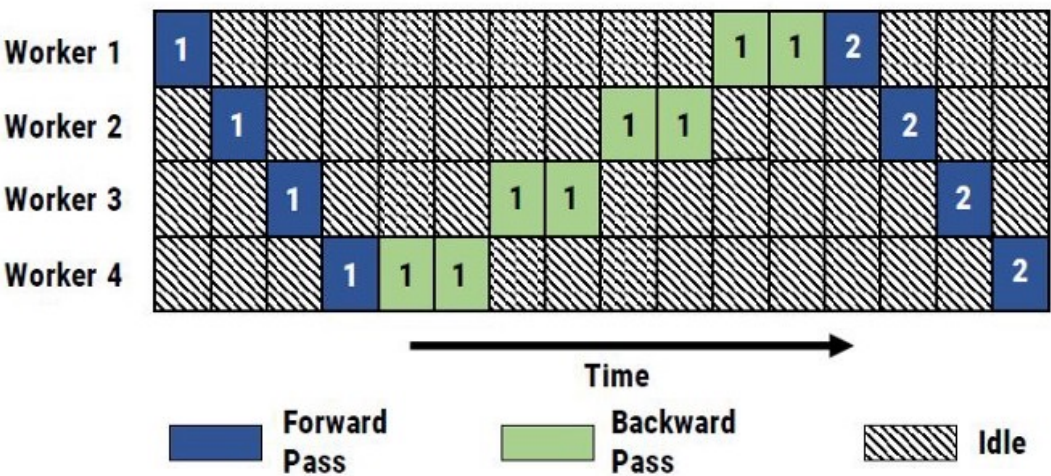
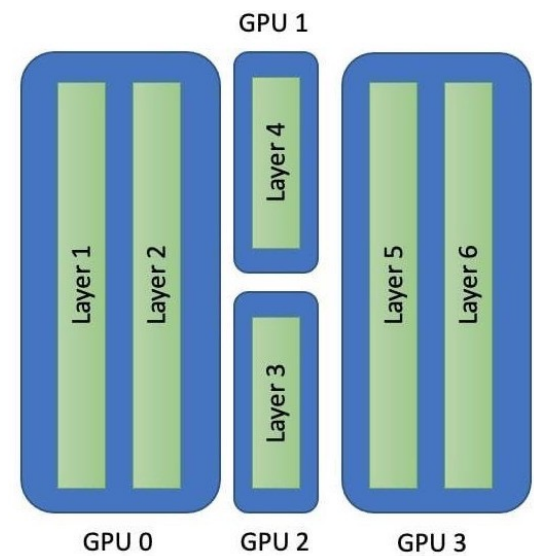


DATA PARALLELISM

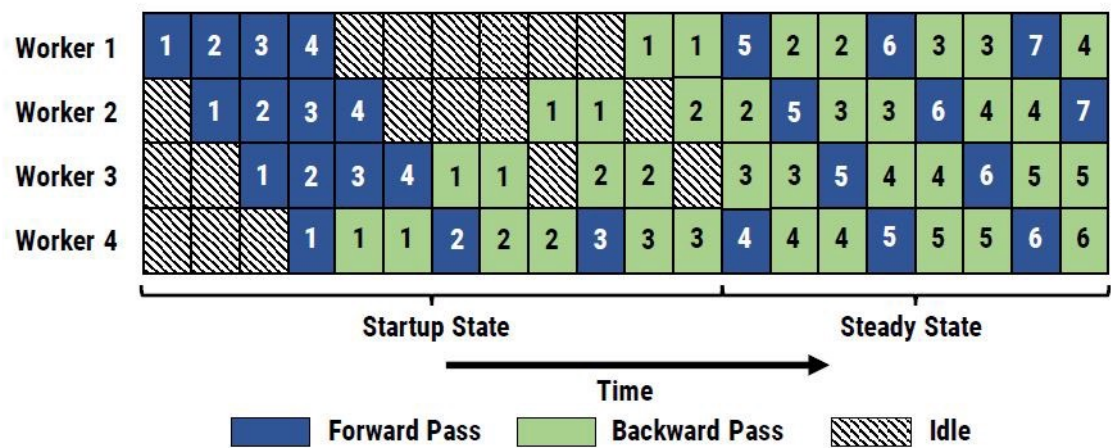
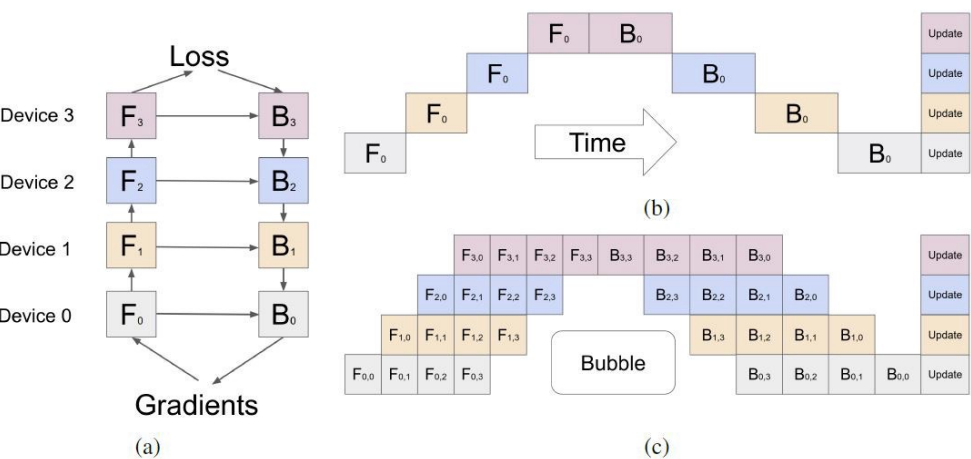


COMPUTING ARCHITECTURAL APPROACH

MODEL PARALLELISM

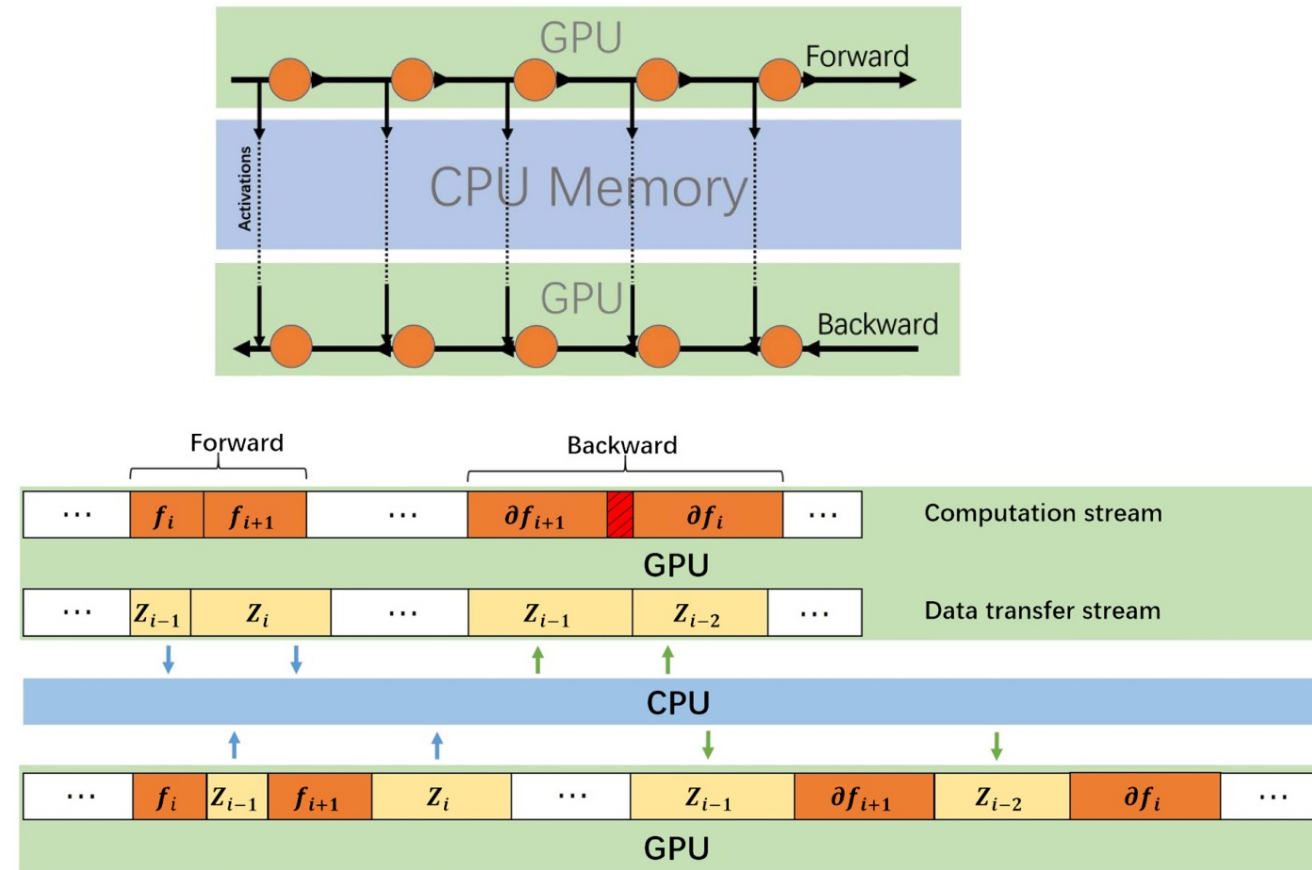


PIPELINE PARALLELISM



COMPUTING ARCHITECTURAL APPROACH

CPU OFFLOADING



Torres, L. A., Barrios, C. J., & Denneulin, Y. (2021). Computational Resource Consumption in Convolutional Neural Network Training – A Focus on Memory. *Supercomputing Frontiers and Innovations*, 8(1), 45–61. <https://doi.org/10.14529/jsfi210104>

Our Contribution: A New Parallelization Approach in Deep Learning Using CPU/GPU Architectures for Memory Optimization

Thesis of Alejandro Torres co-advising with Yves Denneulin



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Is it possible to optimize memory usage in training deep neural network models by distributing or parallelizing the Pipeline between the CPU and the GPU/TPU?

By distributing the Pipeline between the CPU and the GPU/TPU, can better results be obtained in training times while maintaining the accuracy of the model prediction?

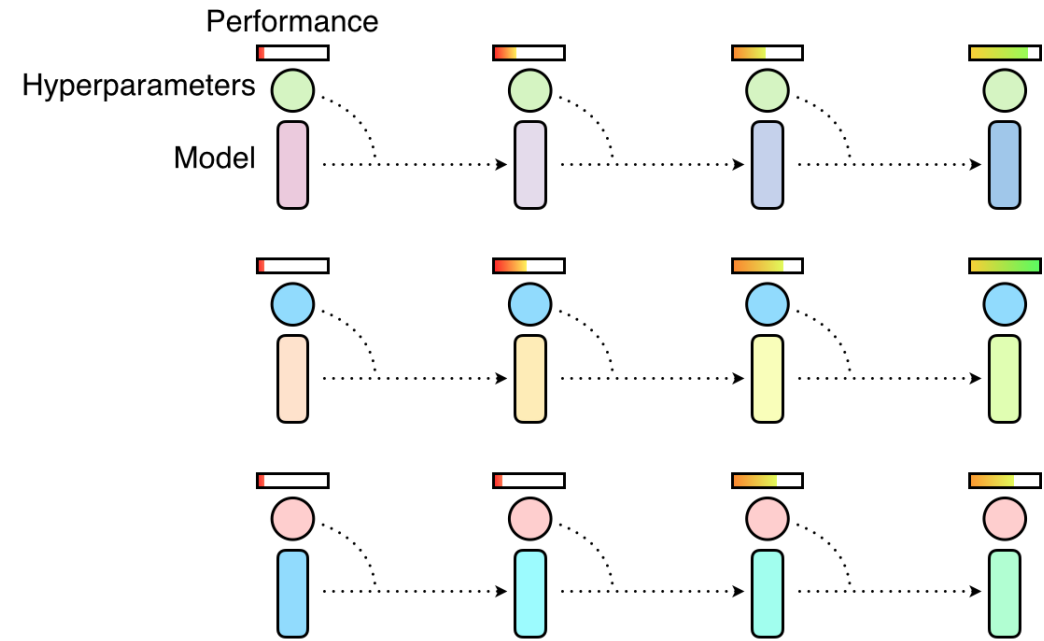
By having greater storage capacities in the CPU memory to use it as an active actor, is it possible to increase the size of the input batch and thus improve the efficiency of the training?

Does using the CPU and GPU/TPU simultaneously during training involve more or less energy expenditure when comparing training time Vs. Accuracy Vs. Power Consumption?

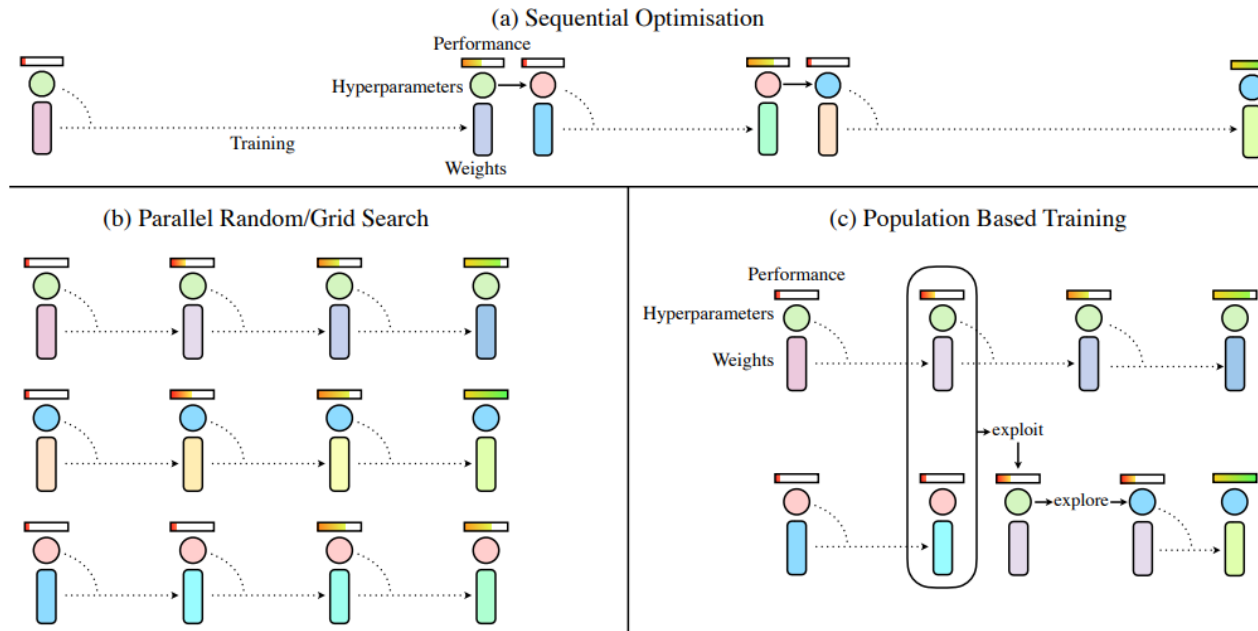
ALGORITHM APPROACH

Important Aspects:

- Complexity of deep learning models.
- Optimization of the search for hyperparameters in large-scale architectures.
- Population based training
- Generalized DL models
- Evolutionary algorithms in PBT
- Minimizing memory size in the produced model.
- Using AI to bring world-class specialist expertise to everyone's, at lower cost.
- Expert care, anywhere.



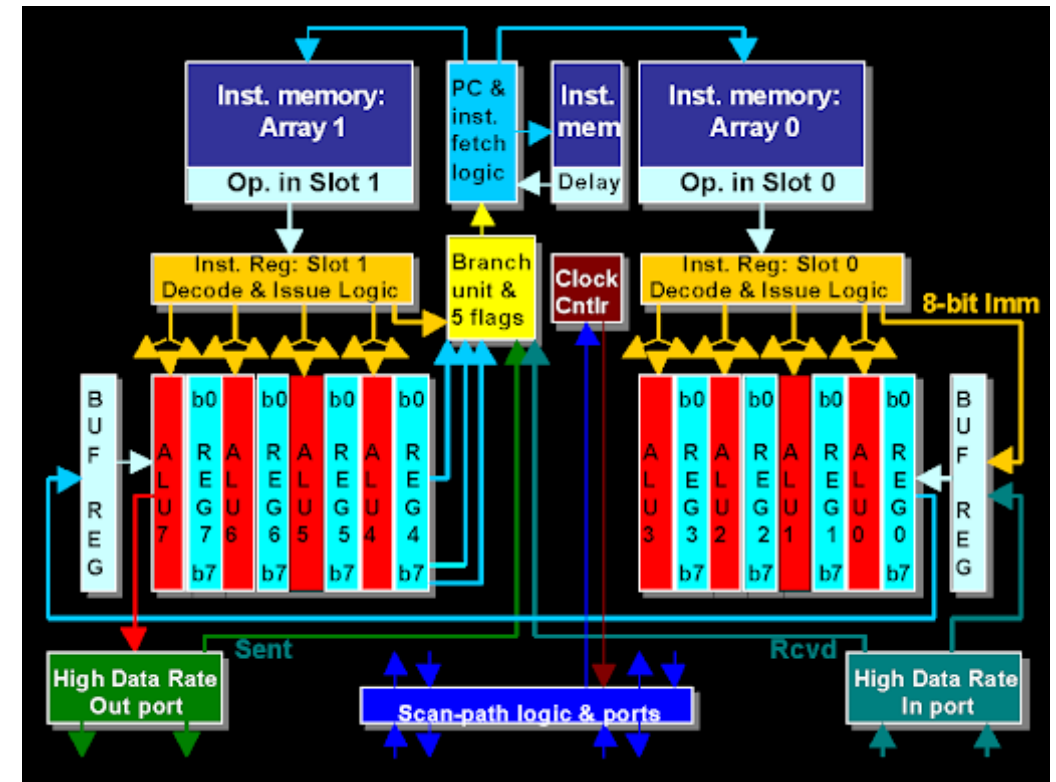
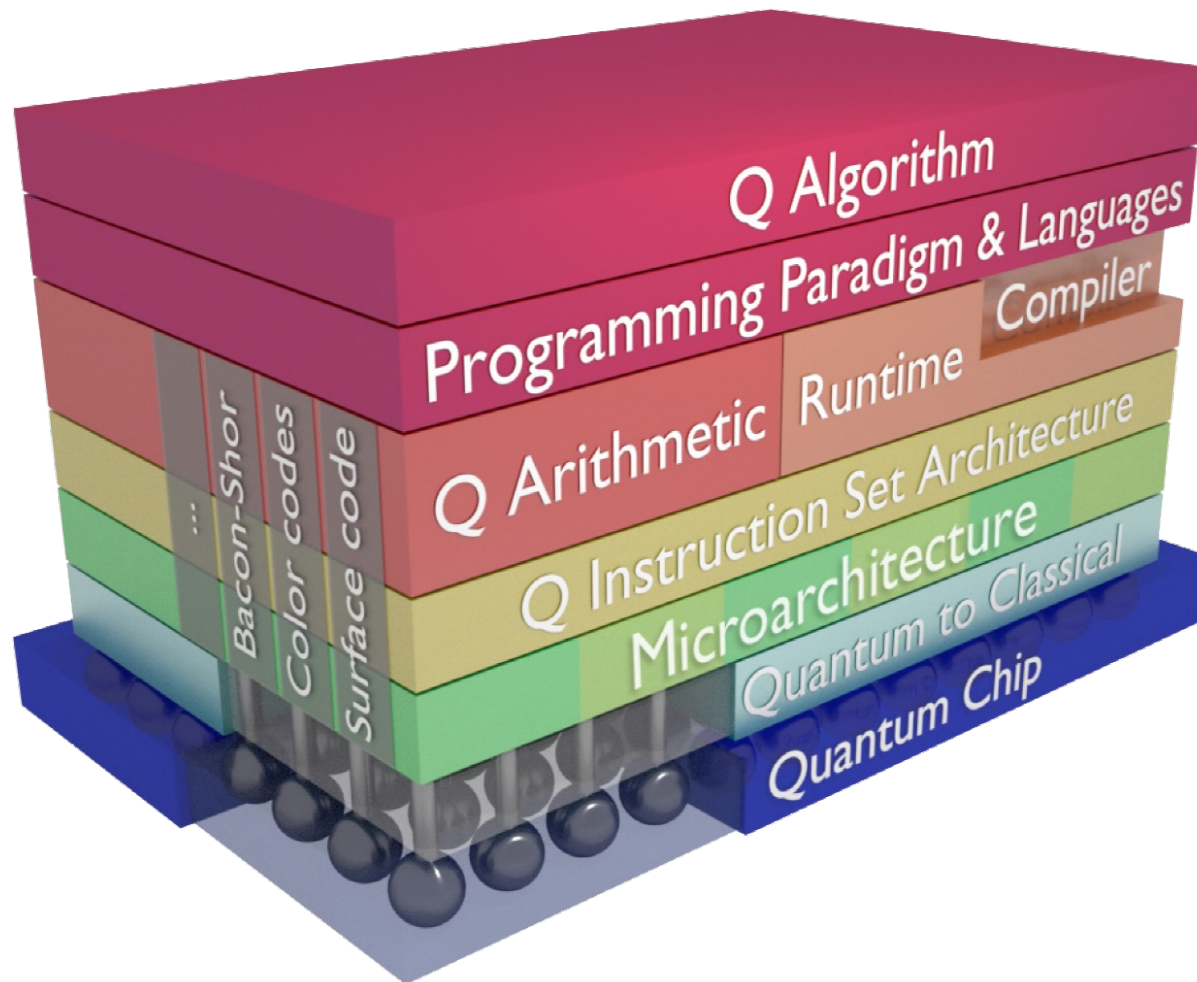
Our Contribution: Hyperparameters Approach



- Better understanding of PBT-based training mechanisms using distributed computational architectures
- Framework that implements efficient and scalable PBT mechanisms that, through evolutionary algorithms, allows finding generalizable models that minimize memory consumption.
- PBT techniques allow obtaining more optimal generalized models that consume less memory.

Felix Mejia Thesis, Computational efficiency of the implementation of algorithms in Deep Learning applications for health in large-scale architectures in co-advising with M. Riveill and Collaboration with J. A. Garcia.

Quantum Processor Unit Architecture*



*Simplest Approach

Quantum Computing Over HPC

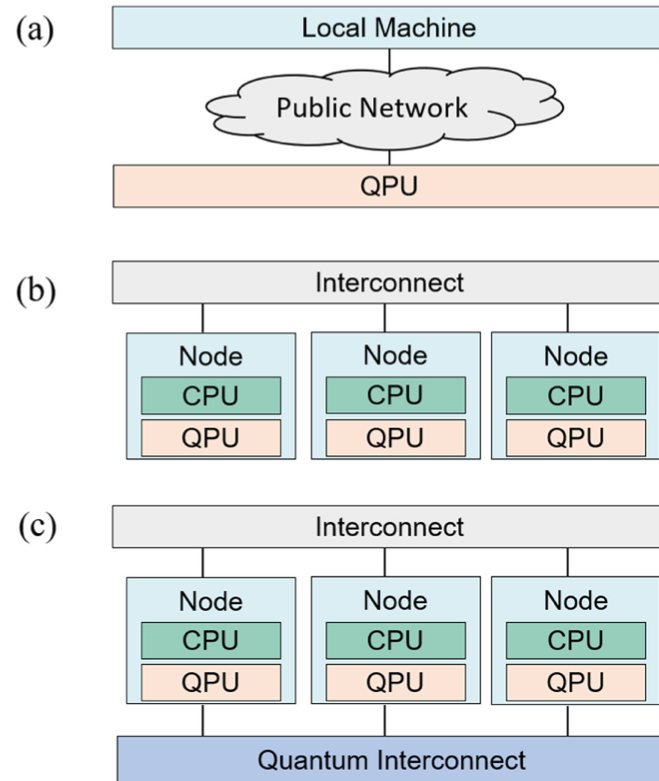


FIGURE 2. Three macroarchitectures for integrating quantum computing with conventional computing. (a) A local machine remotely accesses a QPU through public cloud network. (b) A network of quantum-accelerated nodes communicate through a common interconnect. (c) A network of quantum-accelerated nodes communicate through both conventional and quantum networks.

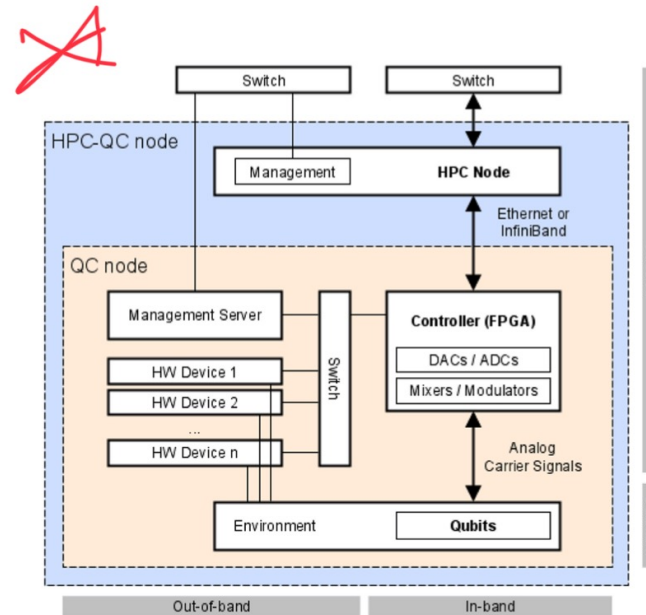


FIGURE 3. A component diagram representing the microarchitecture of a HPC-QC node with a common interconnect as depicted in Figure 2(b). The diagram shows the major components needed for the operation of a QPU within the HPC node infrastructure. Individual components are grouped into so-called out-of-band and in-band scopes and are placed on the left-hand and right-hand side of the figure, respectively. The components of these future computational nodes must be tightly integrated to balance data movement with processing power and workload in order to optimize overall system performance.

DEPARTMENT: EXPERT OPINION

Quantum Computers for High-Performance Computing

Trevor S. Humble, Alexander McCaskey, Dmitry I. Lyakh, and Meenambika Gowrishankar, Quantum Computing Institute, Oak Ridge National Laboratory, Oak Ridge, TN, 37830, USA
Albert Frisch, Alpine Quantum Technologies, Innsbruck, 6020, Austria
Thomas Monz, Alpine Quantum Technologies, Innsbruck, 6020, Austria and also Institut für Experimentalphysik, Universität Innsbruck, Innsbruck, 6020, Austria

Quantum computing systems are developing rapidly as powerful solvers for a variety of real-world calculations. Traditionally, many of these same applications are solved using conventional high-performance computing (HPC) systems, which have progressed sharply through decades of hardware and software improvements. Here, we present a perspective on the motivations and challenges of pairing quantum computing systems with modern HPC infrastructure. We outline considerations and requirements for the use cases, macroarchitecture, microarchitecture, and programming models needed to integrate near-term quantum computers with HPC system, and we conclude with the expectation that such efforts are well within reach of current technology.

High-performance computing (HPC) systems define the pinnacle of modern computing by drawing on massively parallel processing. This leading paradigm for HPC often relies on specialized accelerators and highly tuned networks to optimize data movement and application performance, whereby many computational nodes are connected by high-bandwidth networks to support shared information processing tasks. Existing computational nodes also support highly concurrent execution with multi-threaded processing, and technology trends indicate that future node designs will integrate heterogeneous processing paradigms that include conventional central processing units (CPUs), graphics processing units (GPUs), field-programmable gate arrays (FPGAs), and other specialized processors.¹ The components of these future computational nodes must be tightly integrated to balance data movement with processing

power and workload in order to optimize overall system performance.

By comparison, quantum computers (QCs) represent a young yet remarkable advance in the science and technology of computation that are often cited as rivals or successors to state-of-the-art conventional high-performance computing (HPC) systems. The source of this proposed advantage of QCs derives from quantum information processing in which information is encoded in the quantum state of physical systems such as atoms, electrons, and photons.² These quantum physical systems present the unique features of quantum coherence and quantum entanglement that permit quantum computing to reduce exponentially the computational time and memory needed to solve many problems from chemistry, materials science, finance, and cryptanalysis among other application domains. The advantage afforded to quantum computing is therefore aptly named the “quantum computational advantage,” and there is now a fervent effort to realize quantum computing systems that demonstrate this advantage. Notably, recent efforts have focused on besting the world’s leading HPC systems to great effect.^{3,4,5}

Many of the most promising applications of quantum computing overlap strongly with existing applications of HPC,⁶ which begs the question of how QCs may be integrated with modern HPC to accelerate these

Please see the Acknowledgements section at the end of the article for a special statement regarding the copyright.

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Date of current version 14 September 2021.

September/October 2021

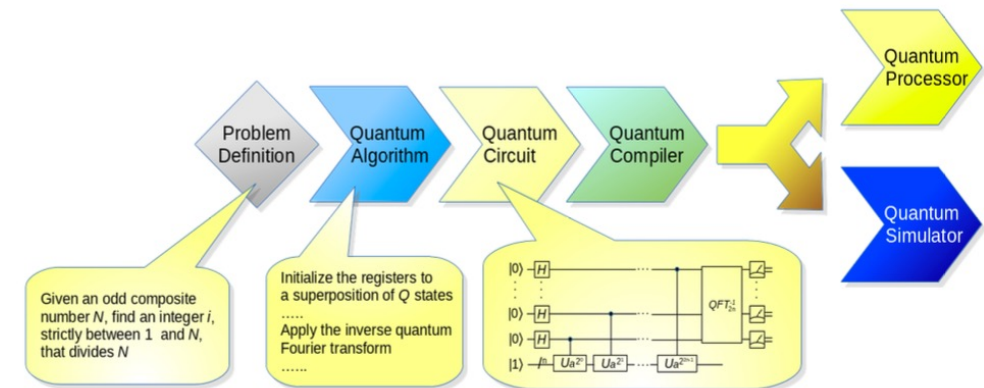
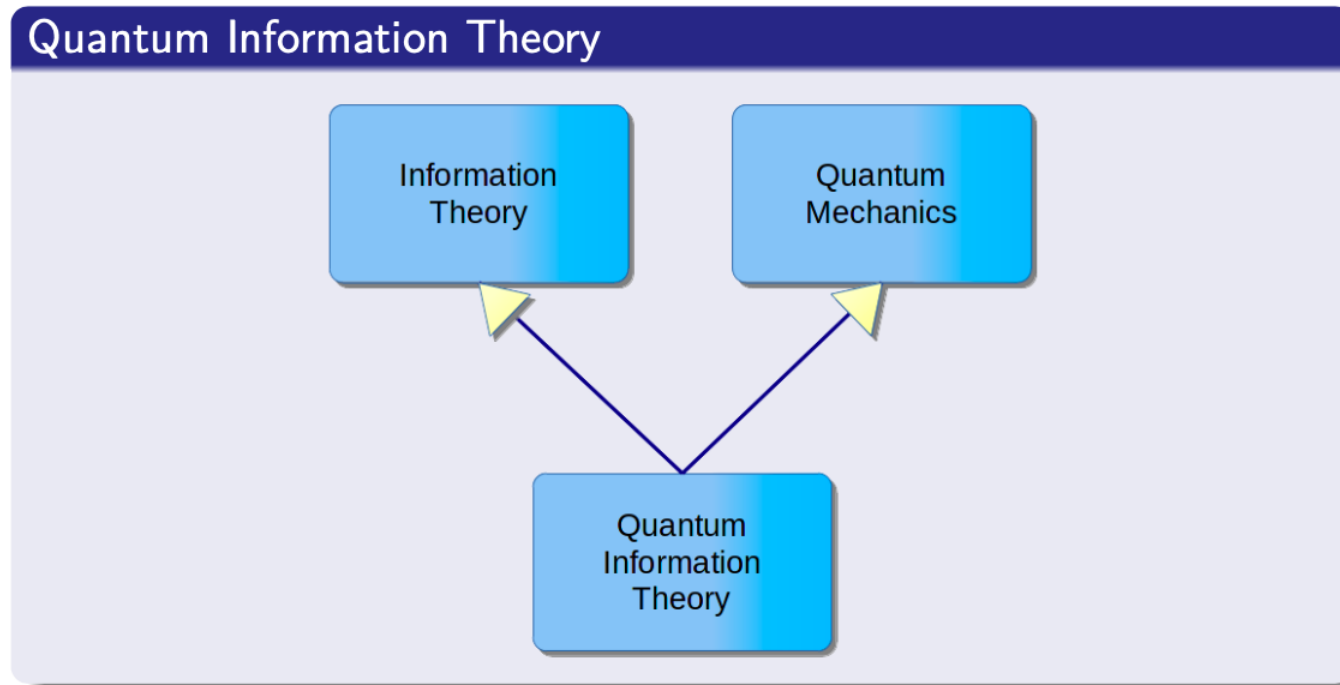
Published by the IEEE Computer Society

IEEE Micro

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Open Question 4: And Quantum Computing?

Our Contribution: Quantum Computing Theory for Quantum Computing Applications

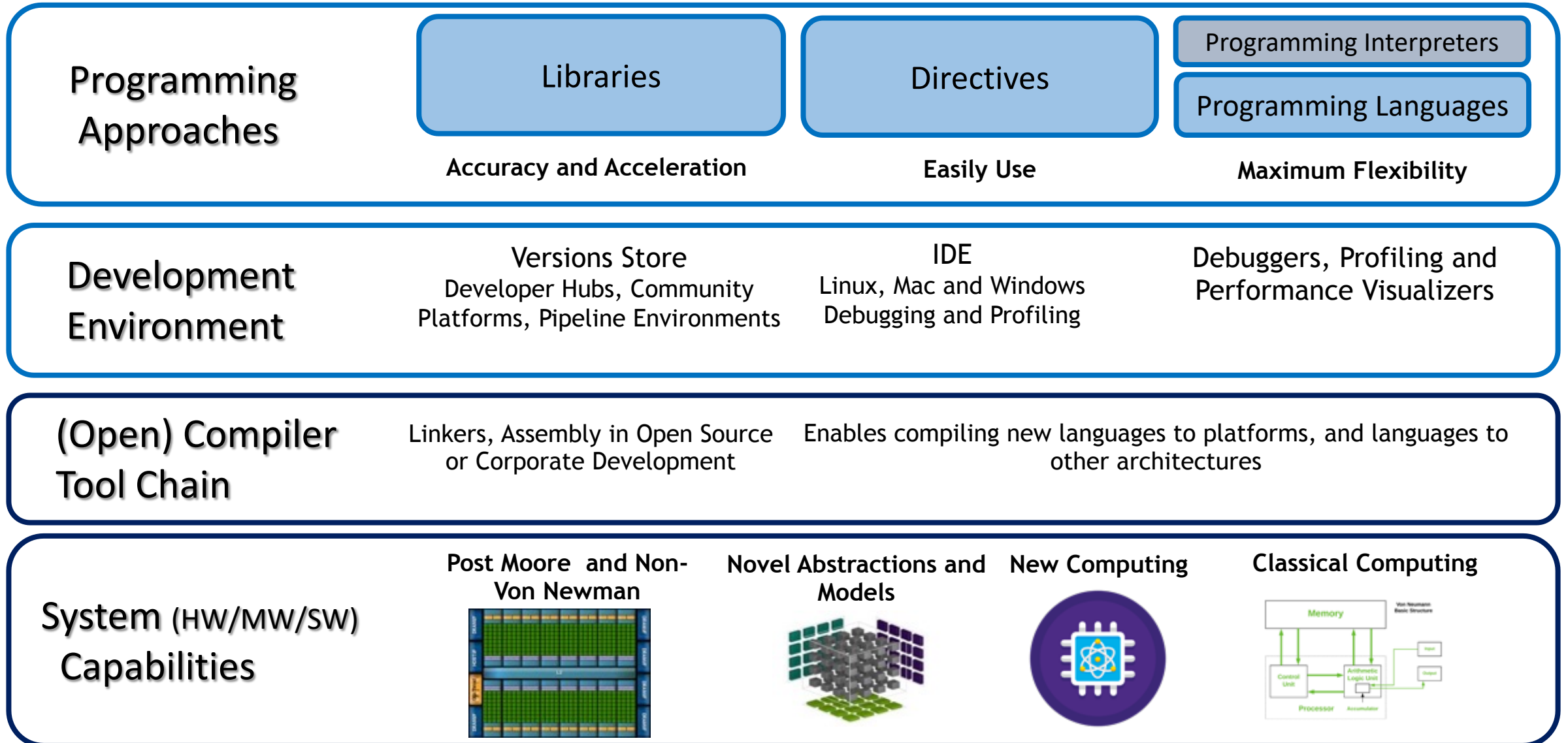


The term **quantum algorithm** is generally used for those algorithms that incorporate some essential feature of **quantum computing**, such as superposition or entanglement. By using this special features, we can speed up significantly the calculation, that is called **quantum parallelism**.

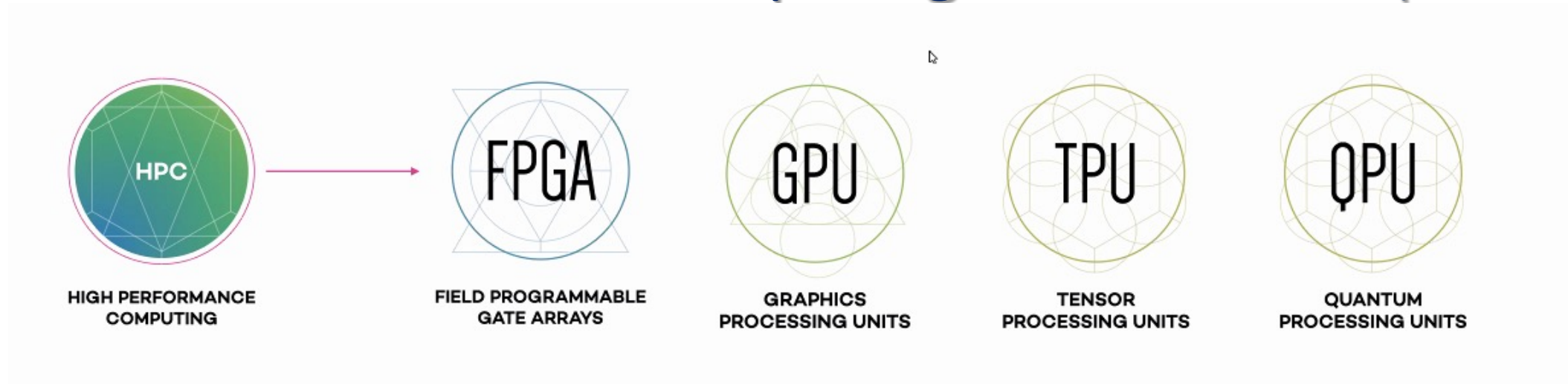
**Final Note: A New Approach of the
HPC/HPDA Platforms for Unified
Advanced Computing Support (! Or ?)**

Why an Advanced Computing Platform Vision (and Not Only HPC)?

(Inspired by the Accelerated/Hybrid Computing World)

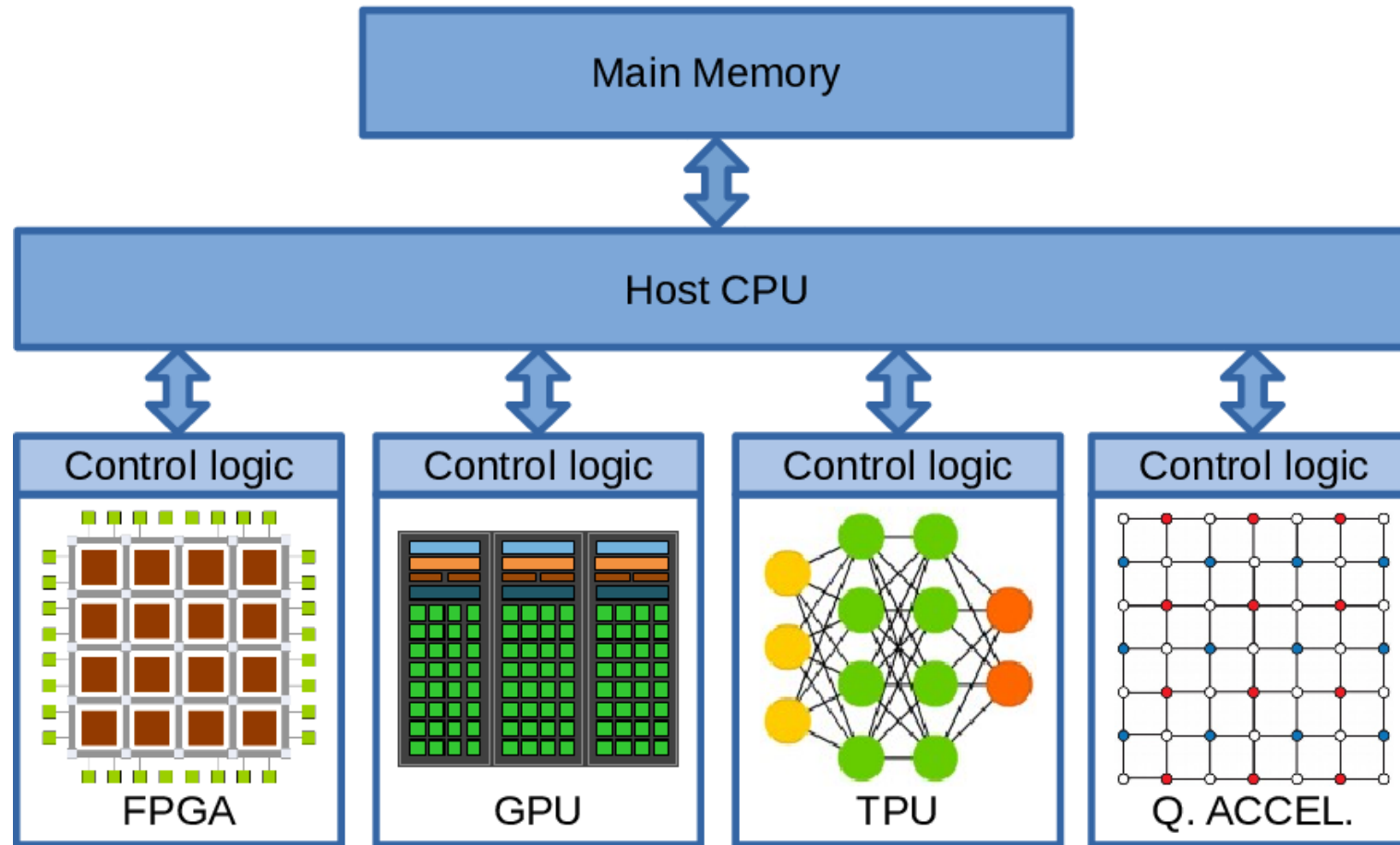


The Many-Architectures Challenge: How to exploit better Advanced Computing Architectures (for All)?



From Why Quantum Computing is Integral to the Future of HPC'. By William "Whurley" Hurley, CEO of Strangeworks

Conclusion: HPC/Advanced Computing Systems



From : Bertels, K., Sarkar, A., Hubregtsen, T., Serrao, M., Mouedenne, A.A., Yadav, A., Krol, A.M., Ashraf, I., & Almudever, C.G. (2020). Quantum Computer Architecture Toward Full-Stack Quantum Accelerators. IEEE Transactions on Quantum Engineering, 1, 1-17.

Questions?

CARLA 2023

LATIN AMERICA HIGH PERFORMANCE
COMPUTING CONFERENCE



Cartagena de Indias, Colombia
September 18-22

What is SC3UIS?

**R+D+i
National
Strategic
Areas**

**.com and
.org**

**.gov and
.co**

**International
R+D+i**

.edu



Application
Deployment



Scientific Software
Development



SCI- IT Management and
Support



Strategic Mediation
and Training



Research and
Innovation

Where is SC3UIS?



SC3UIS at UIS (@UIS) and Guatiguara Technology Park (@PTGuatiguara)

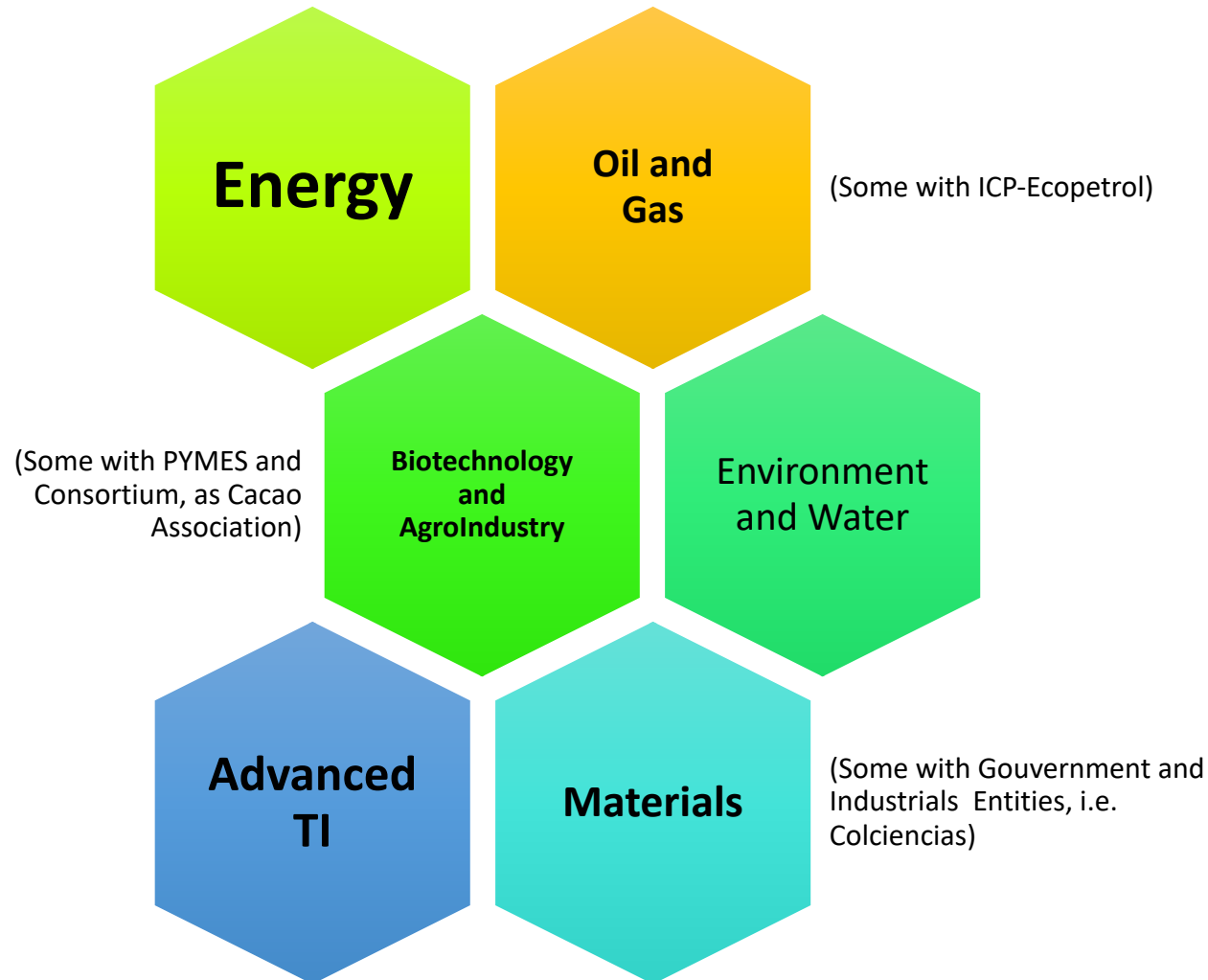


- Founded in 1948 (Following the German /French Polytechnic Model)
- Public State University
- 8 Campus in the Department
 - 4 at Metropolitan Zone of Bucaramanga
 - 4 in Other Regional Cities (Barrancabermeja, Socorro, Malaga, Barbosa)
- 25000 Students (2300 Postgraduate Students)
- 530 Faculty (4 at SC3UIS)
- Support and R+D+I and General Training of SC3UIS



- Guatiguara Site was created in 1989 (New Foundation at 2007 as Technology Park)
- 8 Industrial Corporations
- 3 National Labs
- National Core Repository and ANR Site
- 5 Centers
- High Performance Computing Data Center
 - GUANE-1 and CHAMAN are here!
- R+D+I and Specialized Training Site of SC3UIS

R+D+i Axes (@PTGuatiguara)



2017 Important Numbers

4 Patents

5 Spin Off in Incubation Process
(Potentially for 2018 more than 10)

3 Big International Collaborations (more than 5M USD)

2018 New Axes:

Healthcare

New Generation of Automotive Motors
Human and Social Development



Gracias...
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