HPC Ecosystems

Carlos J. Barrios H., PhD.

@carlosjaimebh

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CAGE

camp

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

SCA RISC2

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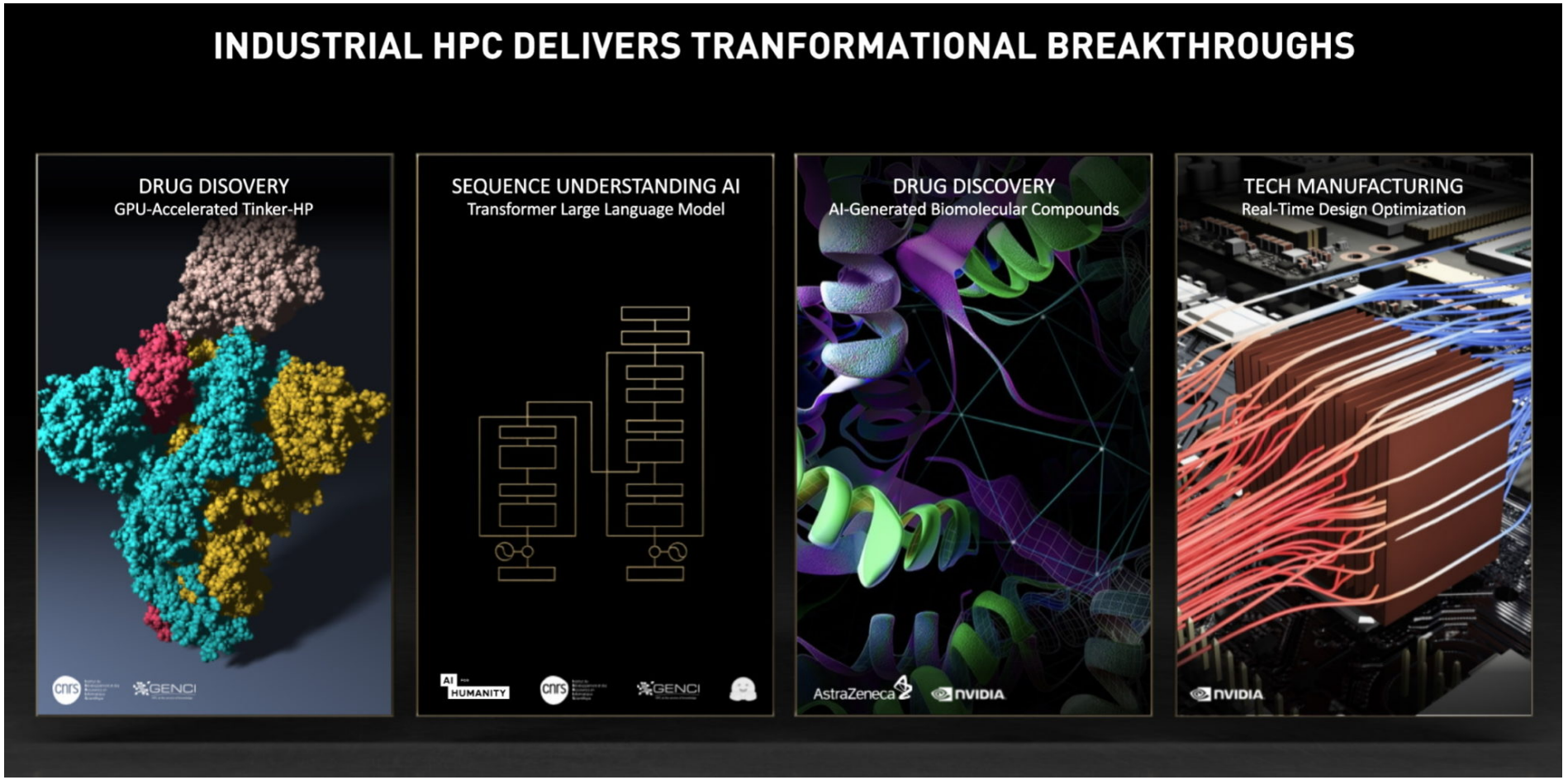
HPC BREAKTHROUGHS



From NVIDIA BLOG

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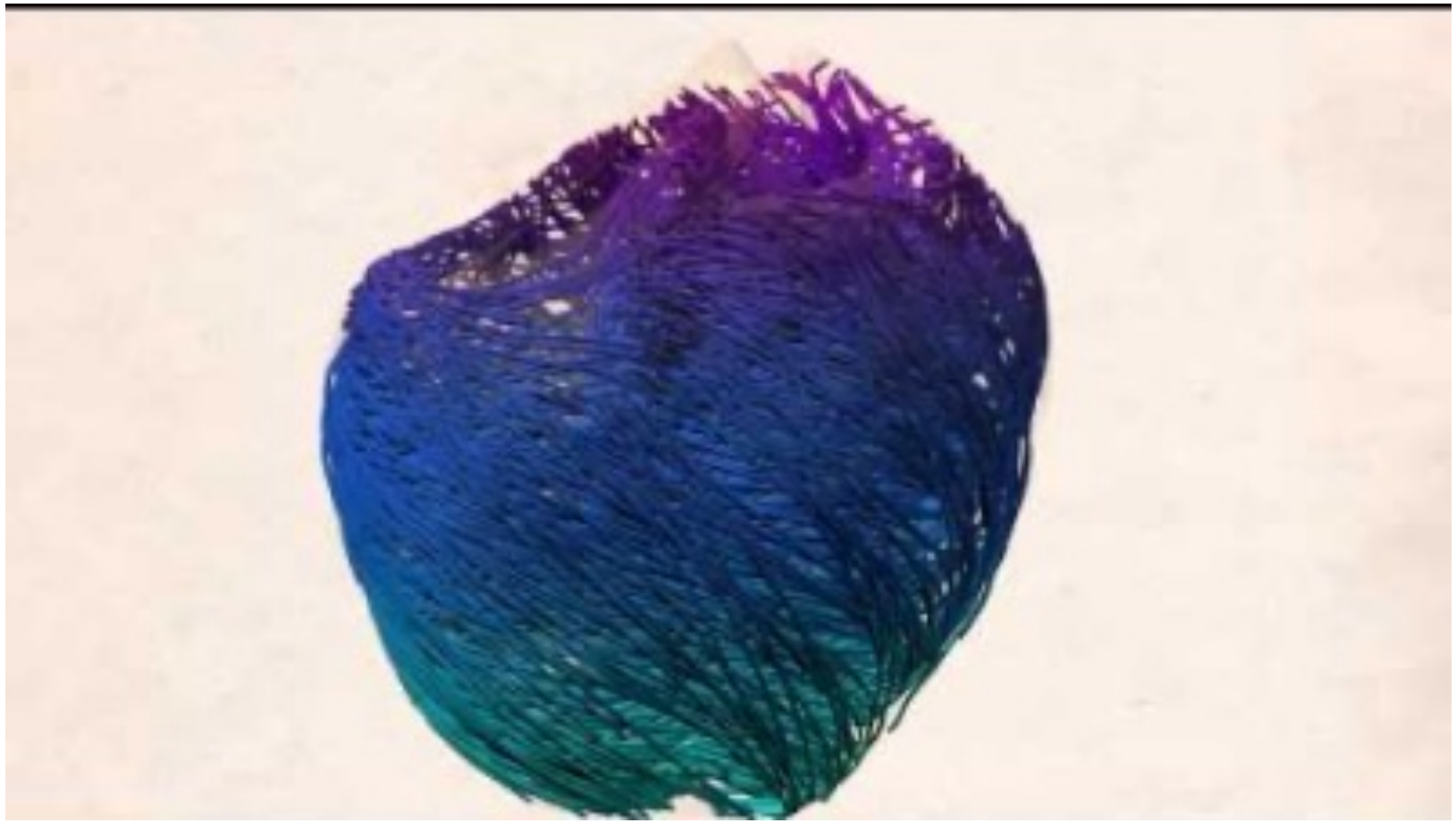
HPC + LIFE SCIENCES



https://youtu.be/tKD2hfF27rM

From www.bsc.es

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HPC + HEALTHCARE

Precision medicine is based on a better knowledge of phenotype-genotype relationships. That is the knowledge od **disease** and **drug action mechanisms**

With the introduction of **molecular biomarkers** we are living now the **transition** from **intuitive** to **empirical** medicine (From J. Dopazo Slides 2016)

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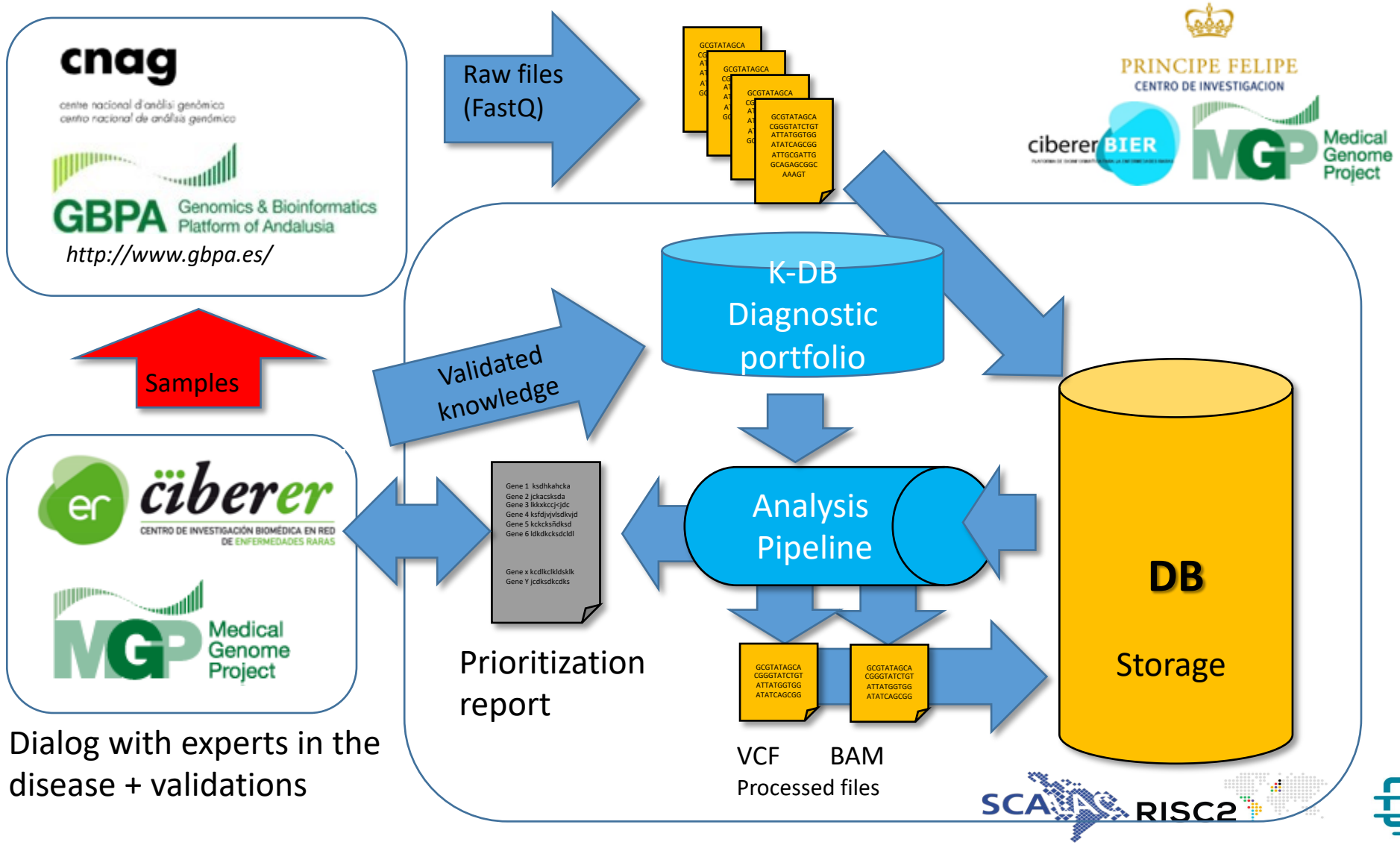
HPC + HEALTHCARE

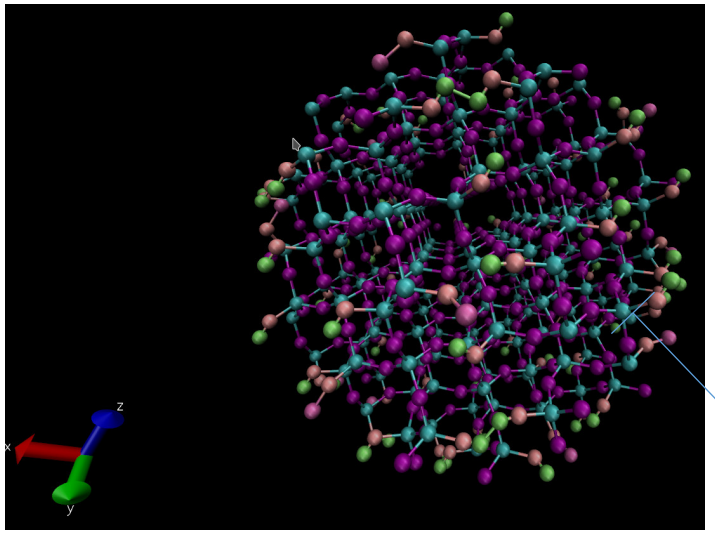
An Example: Ciberetech Project. (to observe in detail after)

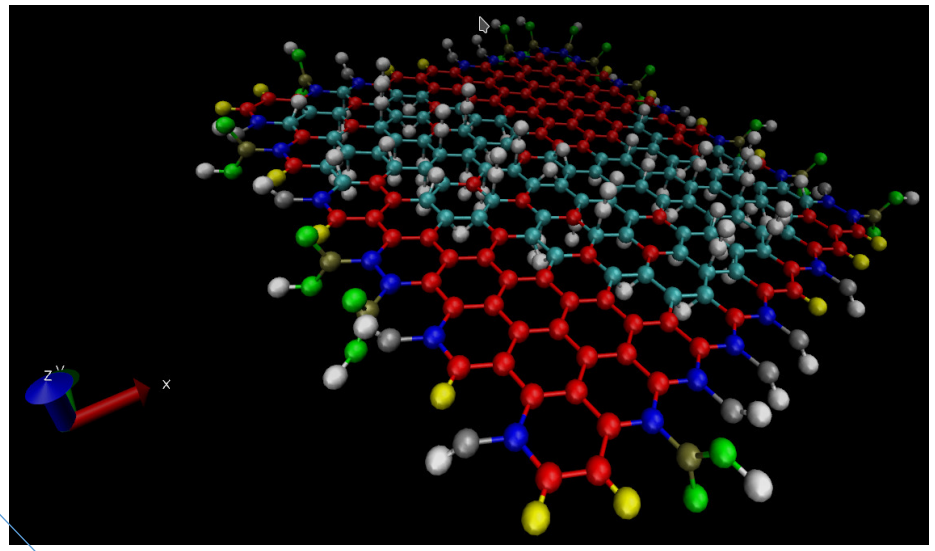


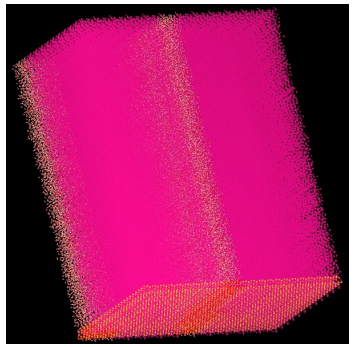
HPC + Molecular Dynamics

Molecular Dynamics Simulations of the Nanomaterials Effect on Reducing Mud Loss and Swelling of Clays

Juan S. Avila Parra, Eng; Zuly H., PhD; Carlos J. Barrios, PhD and Adán Y. León, PhD.

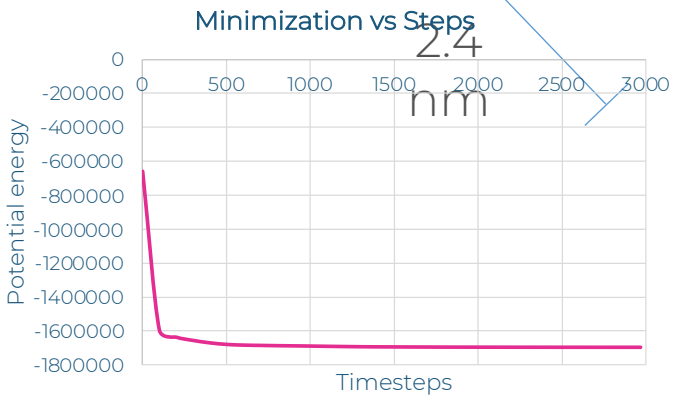


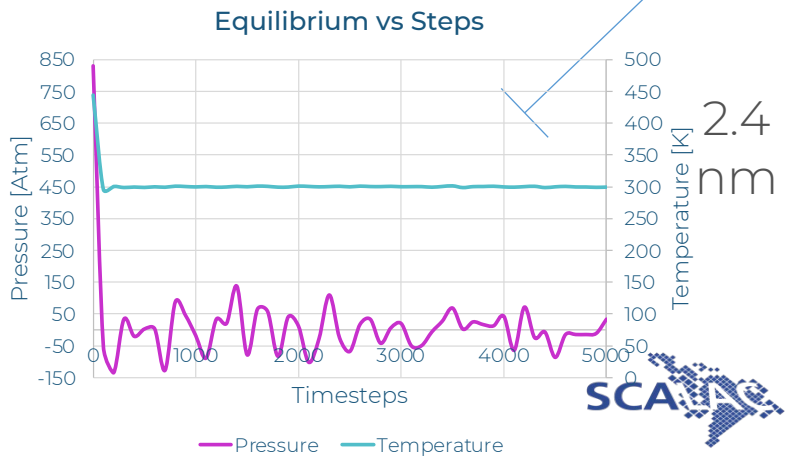




Graphene Nanomaterial

2.4 nm





2.4 nm

HPC Industry Offer

Training

- Strengthening of Formal Courses in Undergraduate, Postgraduate and Specialized Formations
  - Data Analytics
  - HPC and Scientific Computing
- Non – Formal Seminars

Infrastructure and HPC Resources

- Specialized Data Storage
- Large Scale Systems
- New Generation of HPC/EIP Systems

Collaborative Research

- Formalization of Specific Research Lines in the at SC3UIS for Sciences
- Support for External Proposals (i.e. EU 9 Framework Program, National Calls) and Internal Projects (i.e. Software Development, Data Analytics)

Support and Development

- HPC-Advanced Computing Platform and Frameworks Engagement of a Specific Support Engineer for Sciences Faculty
- Assistant (Students) for projects or research lines
- Development of Libraries, Science Portals and Frameworks

From www.sc3.uis.edu.co

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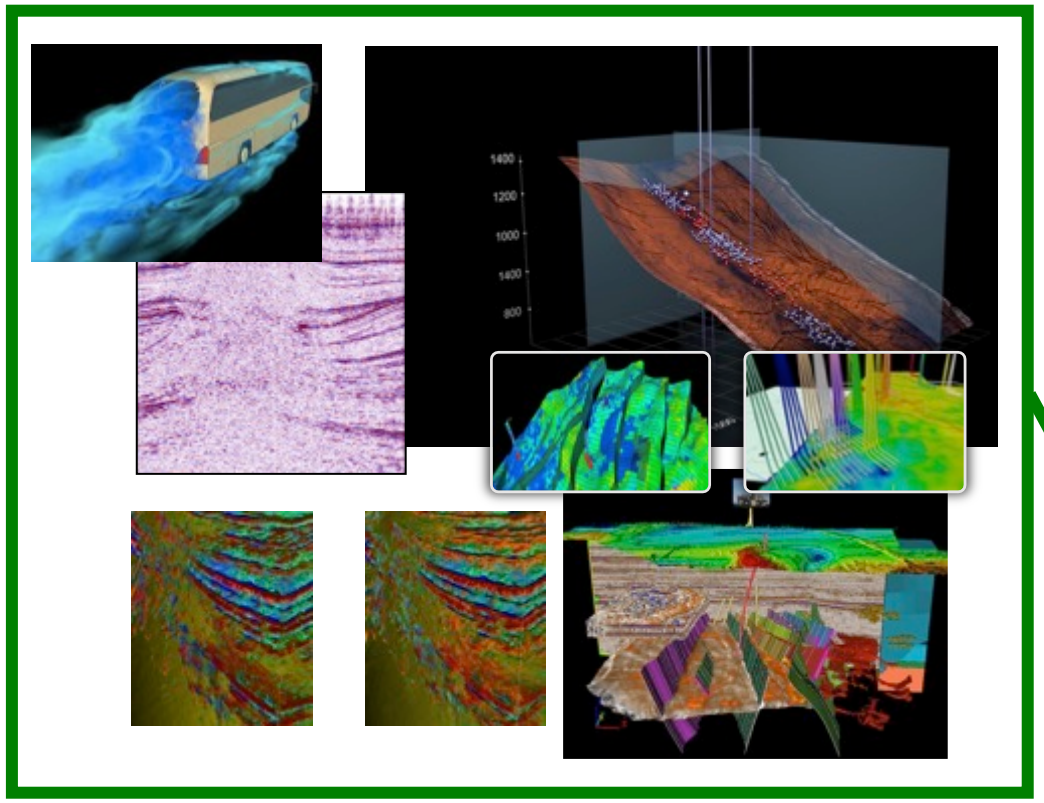
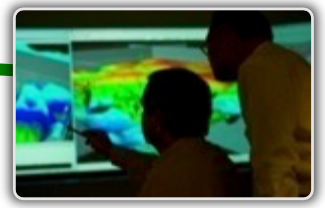
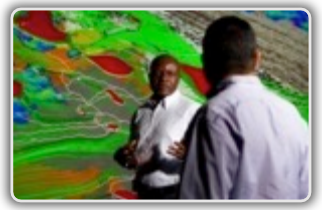
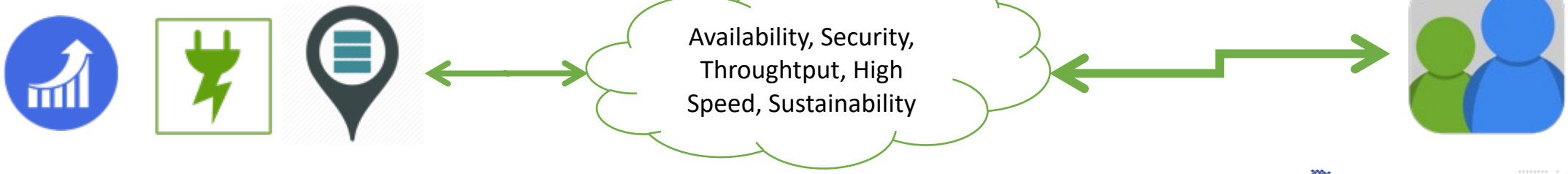
Why HPC?



- Large Data Sets
- Complex Mathematics
- Complex Models
- Real Time
- Interaction and Confrontation
- Large Scale Visualization
- High Resolution
- High Performance and Capacity
  - VR Needs
  - Big Data and Deep Learning







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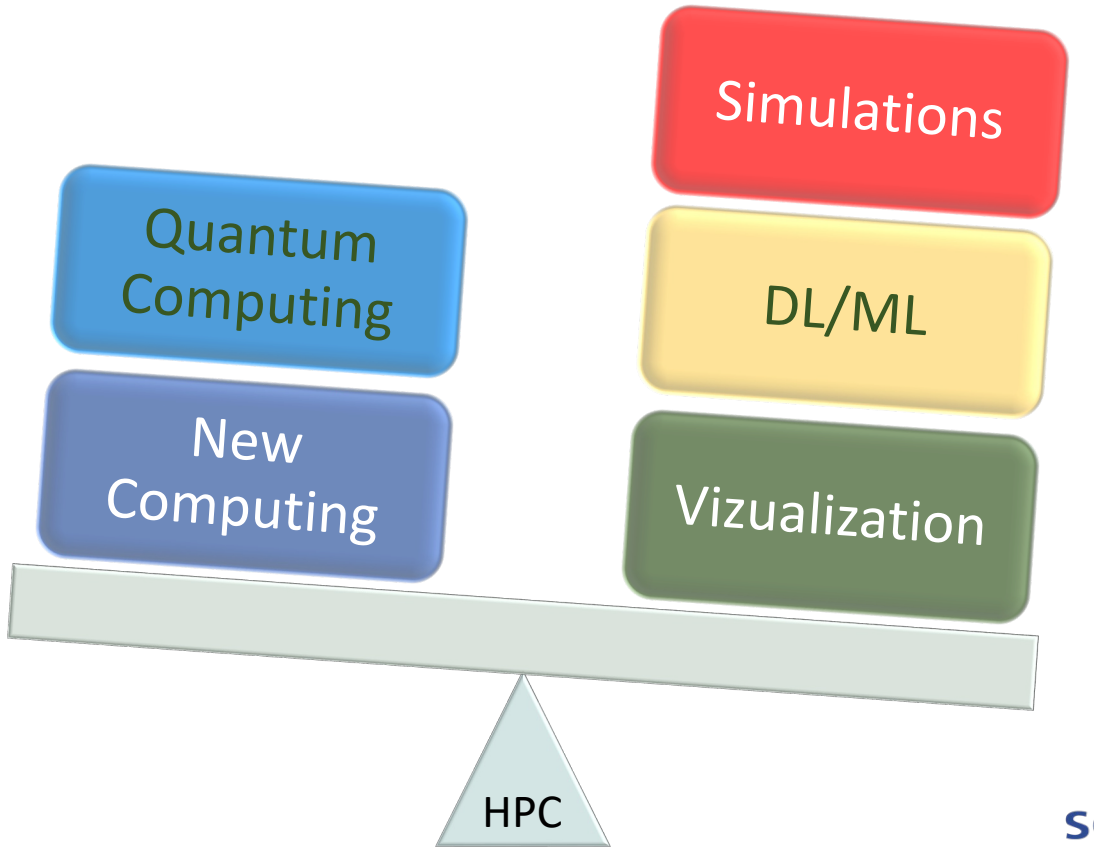
HPC SUPPORT ADVANCED COMPUTING

Non-Classical Computing

Classical Computing



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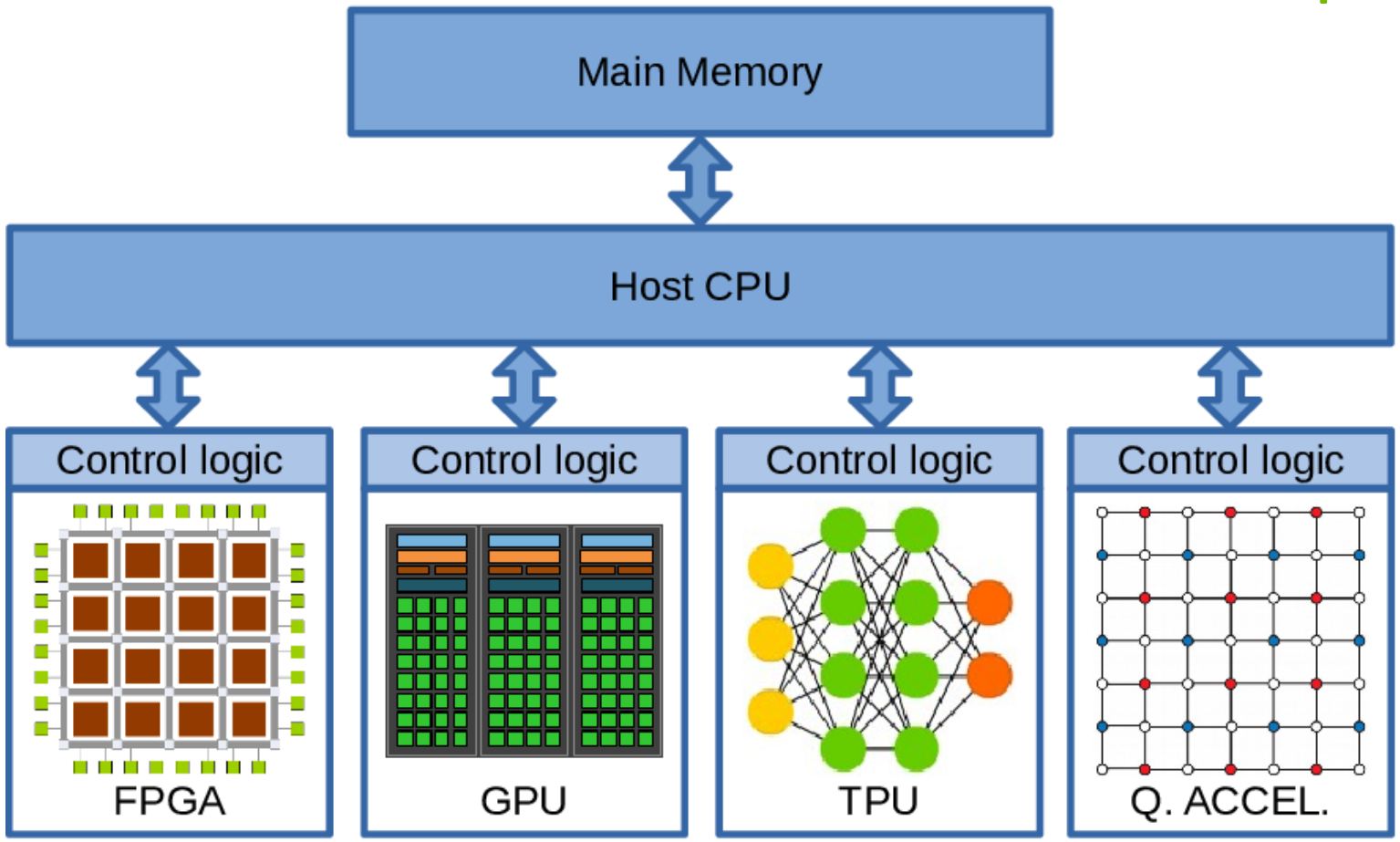
Remember Monday Talk: HPC/Advanced Computing Systems



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.

HPC Ecosystem Elements

Resources Centers

Software and Data

People

- Depreciable Hardware
- Appreciable Software
- Valuable Knowledge
- Friendly Partnerships

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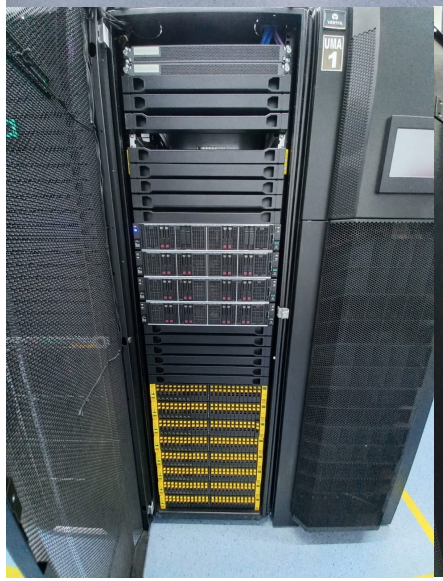
System Specs



The Good :

- Loosely-coupled Linux Supercomputer (Beowulf systems)
- Efficient for a number of use-cases
  - Embarrassingly parallel / single-threaded jobs
  - SMP / multi-threaded, single-node jobs (OpenMP)
  - Massive Parallel Processing
  - MPI / parallel multi-node jobs (Or Hybrid Computing)
- Very cost-effective HPC solution
  - Commodity X86_64 server hardware and storage
  - Linux based operating system
  - Specialist high-performance interconnect and software.
  - Flexible and Scalable Hardware

The Bad :

- 3-5 Years of Technology “Pertinence”
- Noise and Heat
- Important Energy Power Consumption
- SLAs and QoS Compromised in the time
- Technology (Fabric) Dependence

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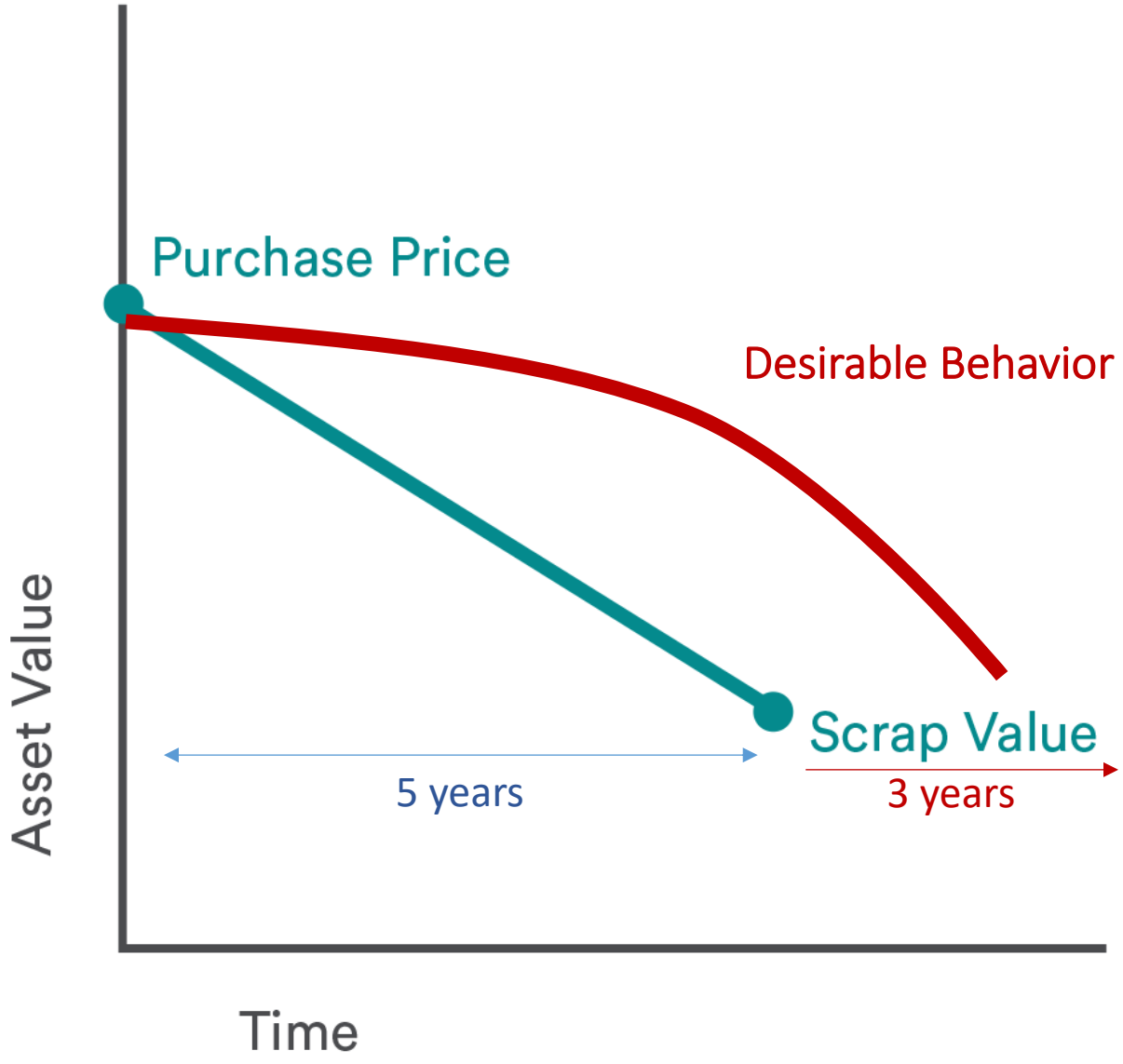
The Awful Thru



- Hardware value depreciation by year
  - Technology evolution
  - Market
- Hardware Degradation
  - Use
  - Faults
  - Environment

- However…
  - See Trends
  - Take Measured Risks
  - Do not be manipulated by sellers
  - Minimal 70% of Use
  - Good Maintenance
  - Good Environment
  - Add Updates and New Platforms in the Schedule

HPC Platform

Programming Approaches

- **Libraries** — Accuracy and Acceleration
- **Directives** — Easily Use
- **Programming Interpreters**, **Programming Languages** — Maximum Flexibility

Development Environment

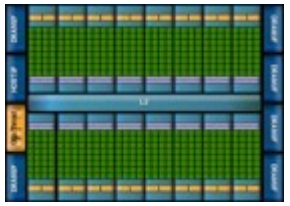
- Versions Store
  Developer Hubs, Community Platforms, Pipeline Environments
- IDE
  Linux, Mac and Windows Debugging and Profiling
- Debuggers, Profiling and Performance Visualizers

(Open) Compiler Tool Chain

- Linkers, Assembly in Open Source or Corporate Development
- Enables compiling new languages to platforms, and languages to other architectures

System (HW/MW/SW) Capabilities

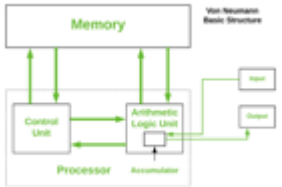
- **Post Moore and Non-Von Newman**



- **Novel Abstractions and Models**

- **New Computing**

- **Classical Computing**



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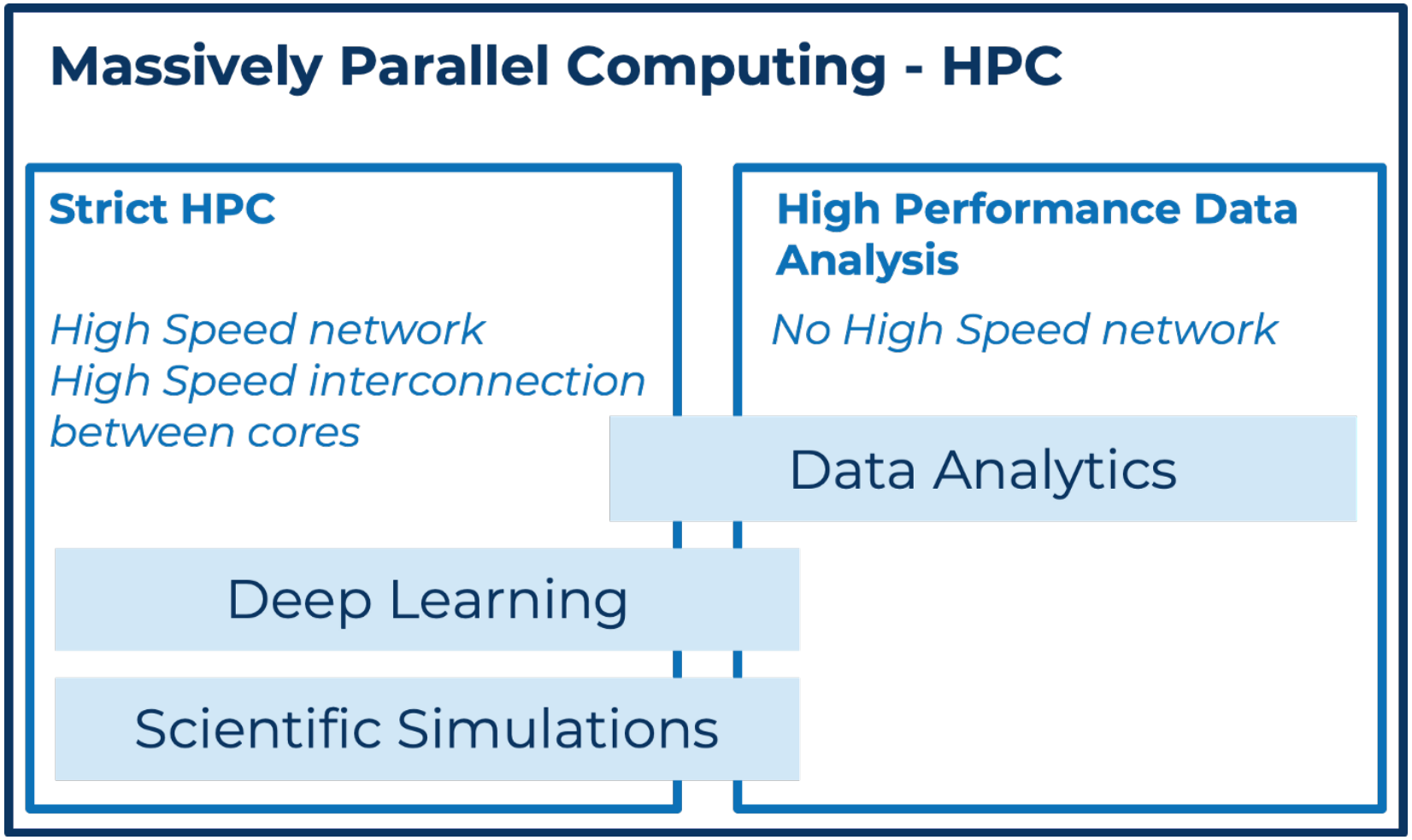
About Software



From https://www.hpcwire.com/

- Computer Science, Artificial Intelligence and Data Science.
- Critical Infrastructure.
- Cyberpsychology.
- Engineering.
- Engineering Technologies.
- Intelligence and Security Studies.
- Occupational Safety and Health.
- Unmanned Systems.
- Digital Twins

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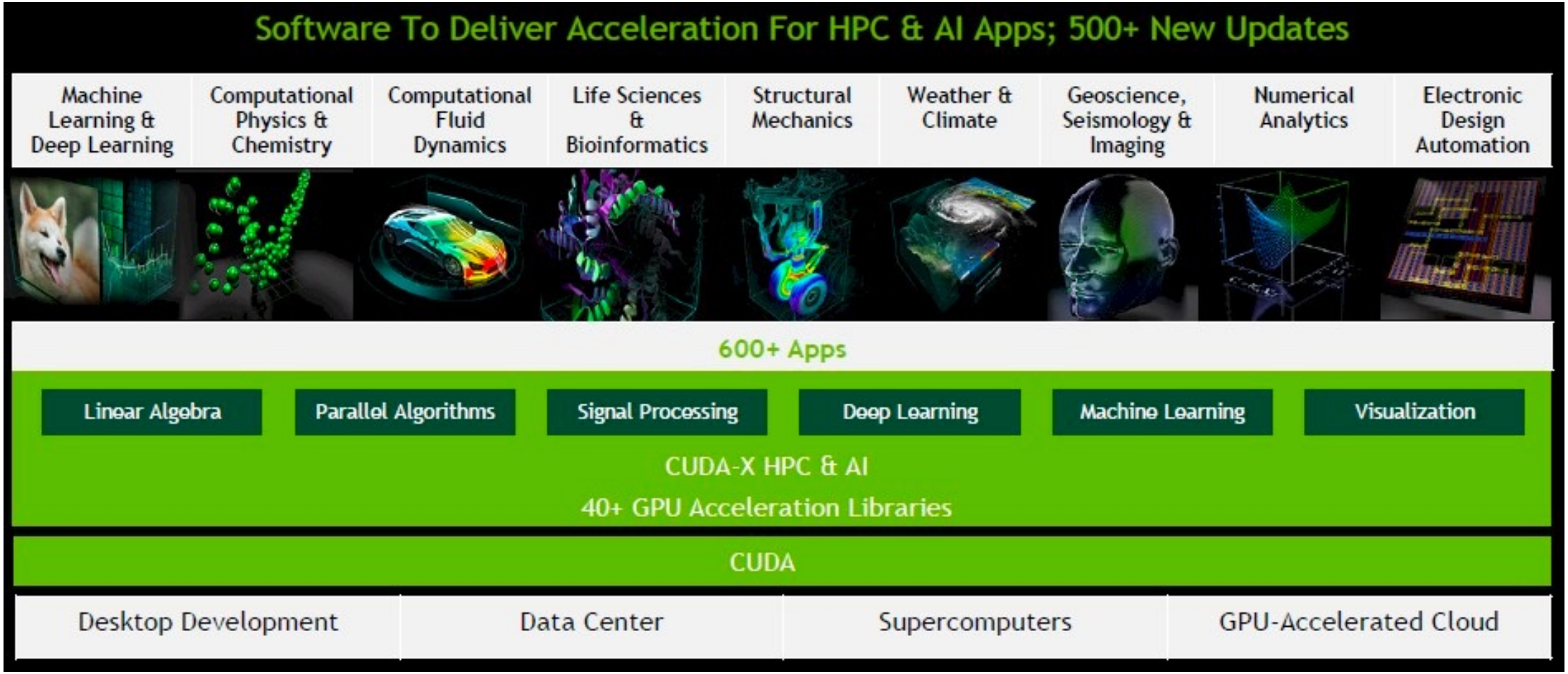
About Software Stack



www.nvidia.com

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Some HPC Skills (in Software)

HPC Programming Tools

Performance Monitoring	HPCC	Perfctr	IOR	PAPI/IPM	netperf
Development Tools	Cray® Compiler Environment (CCE)	Intel® Cluster Studio	PGI (PGI CDK)	GNU	
Application Libraries	Cray® LibSci, LibSci_ACC	MVAPICH2	OpenMPI	Intel® MPI- (Cluster Studio)	

Middleware Applications and Management

Resource Management / Job Scheduling	SLURM	Grid Engine	MOAB	Altair PBS Pro	IBM Platform LSF	Torque/Maui
File System	NFS	Local FS (ext3, ext4, XFS)	PanFS	Lustre		
Provisioning	Cray® Advanced Cluster Engine (ACE) management software					
Cluster Monitoring	Cray ACE (iSCB and OpenIPMI)					
Remote Power Mgmt	Cray ACE					
Remote Console Mgmt	Cray ACE					

Operating Systems

Operating System	Linux (Red Hat, CentOS, SUSE)

OpenMP

NVIDIA CUDA

BASH THE BOURNE-AGAIN SHELL

Ganglia

```
[~]$ gprof
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Valuable Knowledge

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CATAI Collaboration France-Colombia

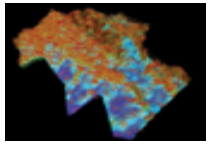
INSA · CPE Lyon · citi Lab · Inria · Université Côte d'Azur · i3S · UGA Université Grenoble Alpes · LIG · Grenoble INP · Super Computación y Cálculo Científico UIS · Universidad de los Andes · COMIT · IMAGINE

CoviData

Sustainable Cities

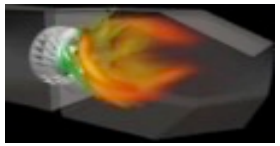
Health Genomics

Energy

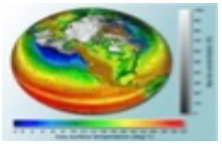


IoT

Industry



Climatology



Agriculture

Develop Skills & Competencies related to High Performance Computing (HPC) and AI (Big Data, ML/DL)

Foster cooperations (Industries, SME's and Universities)

Facilitate Access to Ecosystem for Private companies & PyMES

Share Secured Computing Resources. Guaranteed Sovereignty

Accelerate Innovation, Competitivity, Collaboration with Advanced IT

- Simulation, HPC & Bigdata to support the national initiatives following the peace process
- Accelerate integration of production-economy in the global added value chain and **human wellness**
- Facilitate cooperation (scientific, research, industry & international …)
- Boost key segments: Agriculture, Health, Energy, Human Science… through innovative Advanced IT

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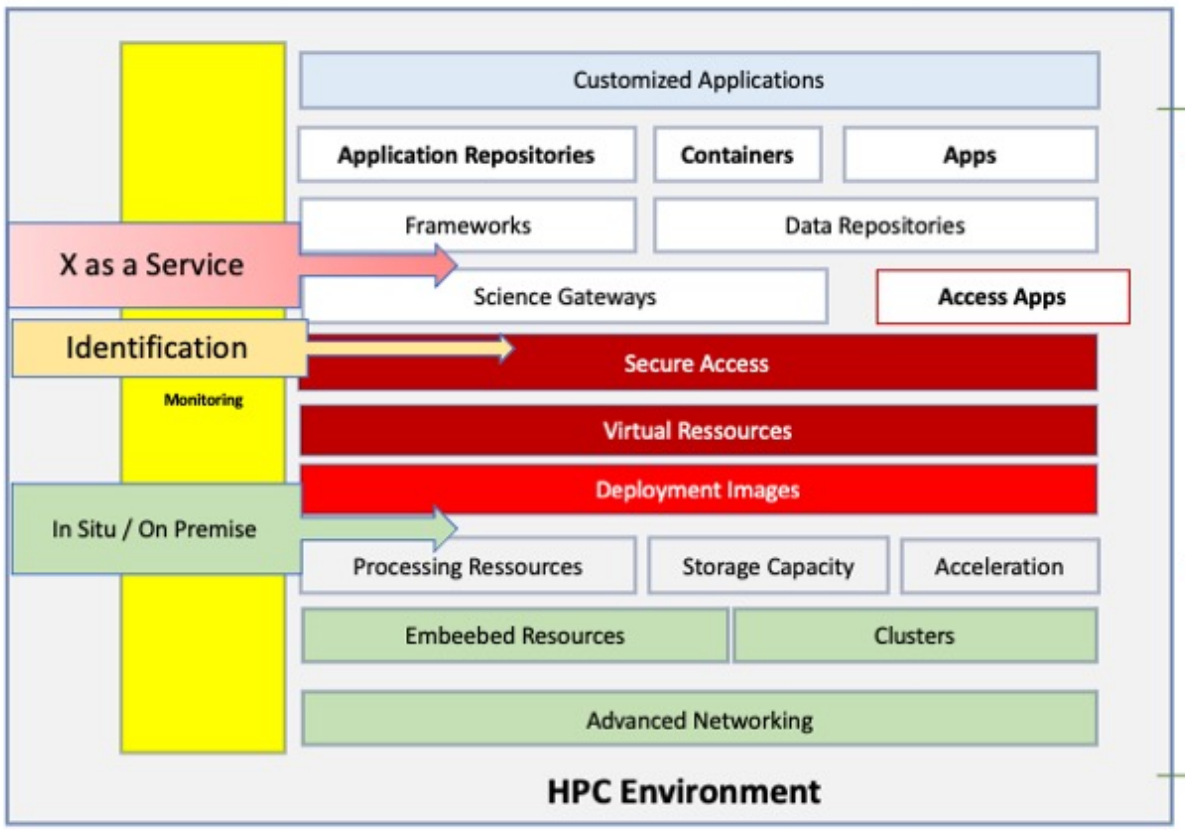
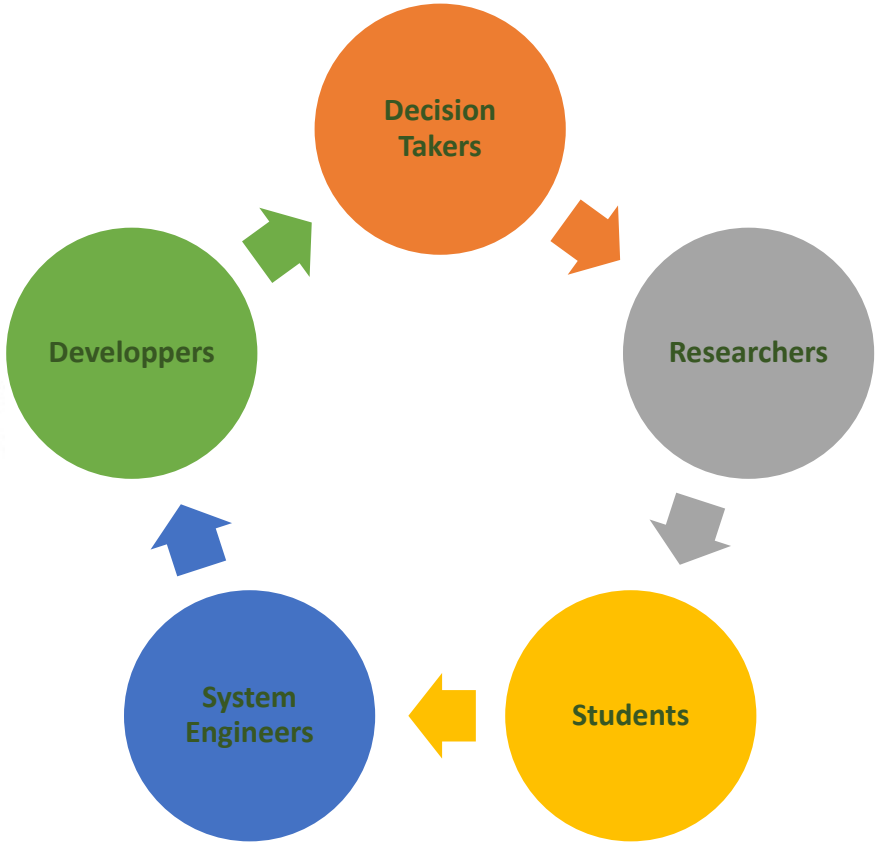
(In)valuable People



HPC Applications and Uses

HPC Software Development

HPC Operations and Technology Support



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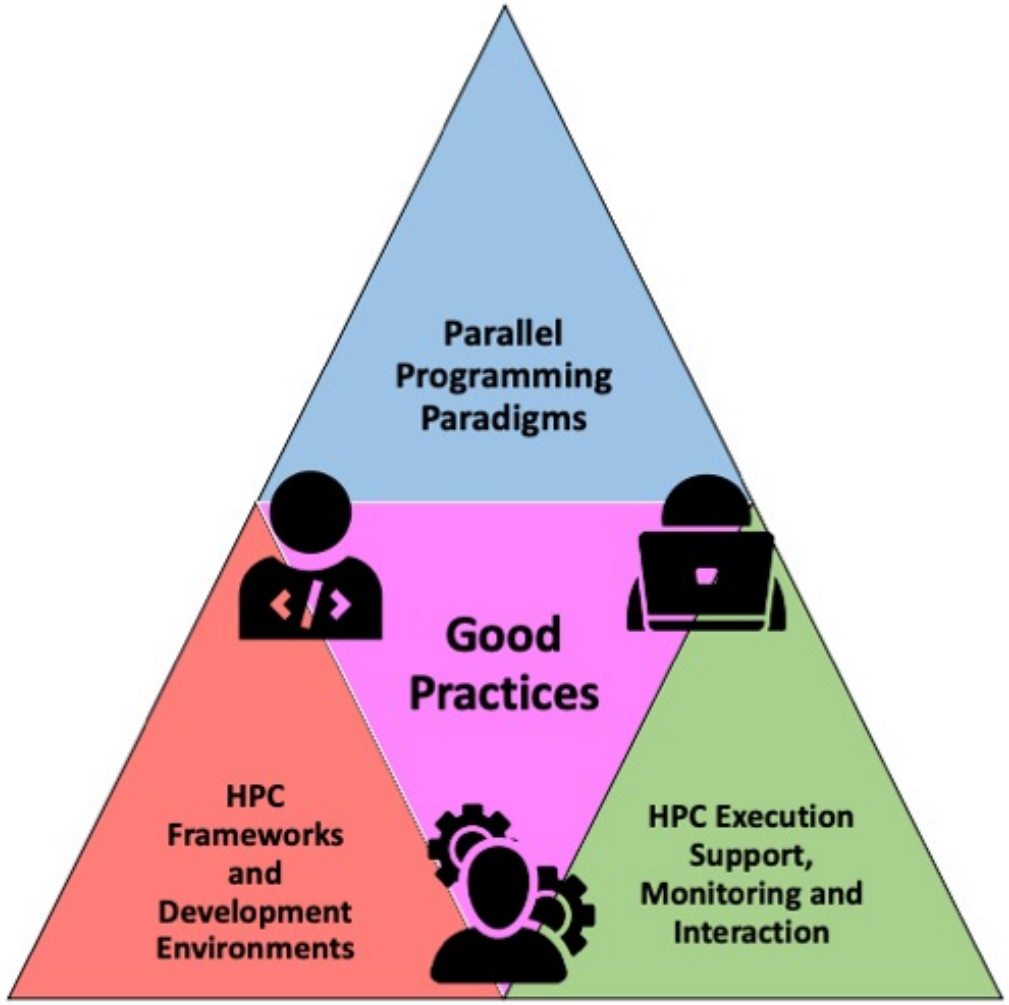
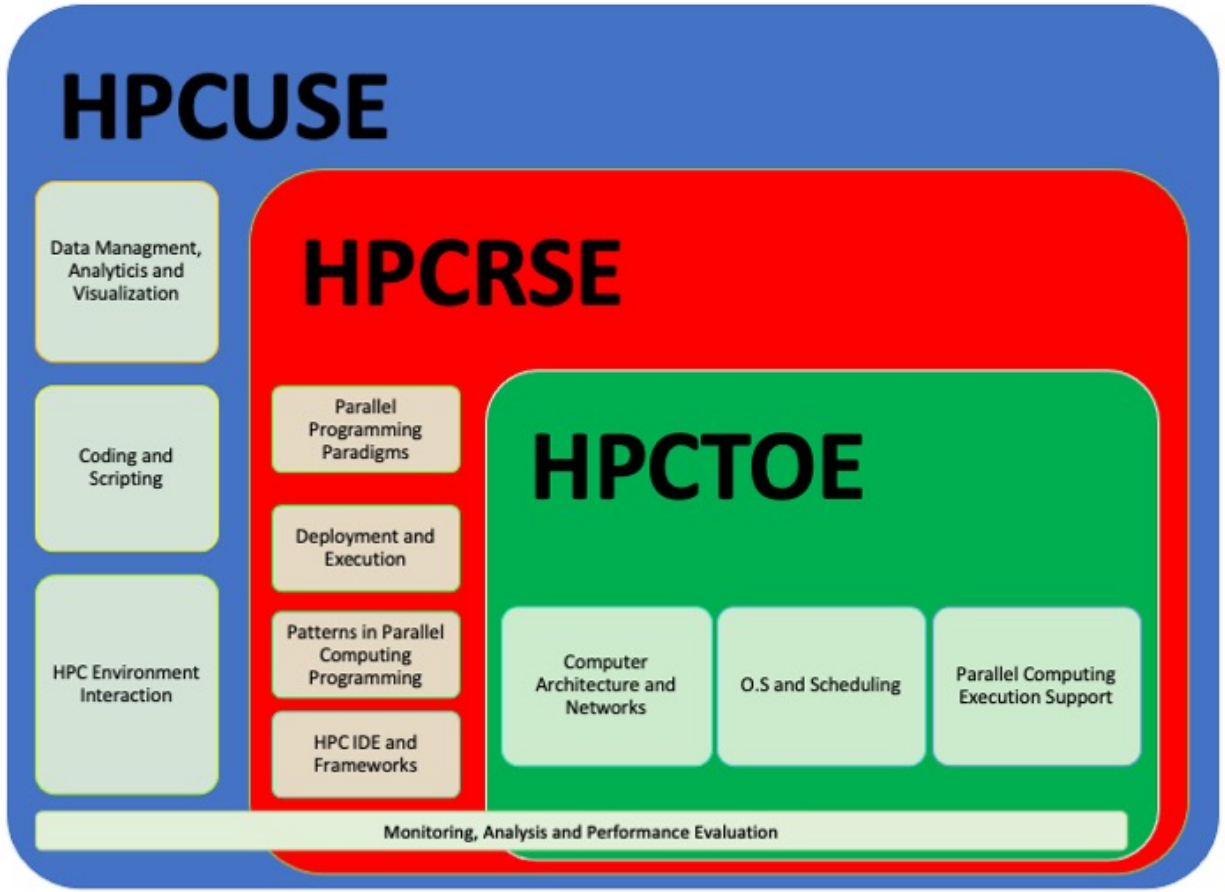
Humanware





From www.sc-camp.org

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Challenges and Open Questions

- Use 70% - 90% of Installed Resources
- Improve Skills in all the Ecosystem/Community
- Thinking about the value and not just monetize
- Collaborate and Join Communities (Partnerships)
- Sustainable life cycle (long term)

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Cooperation Opportunities

- Collaborative Projects in STEM (National and International)
- Formal Programs (in Co-Advising), Seminars, Workshops and Outreach activities
- Achieve an identity and speciality (Visibility)
- Join Networks and Partnerships (LaRedCCA, SCALAC and Others)
- Collaboration for Sustainable life cycle (long term) with strategic mediation

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Cooperation Opportunities (In Concrete)

Collaborative Projects in STEM (National and International)

- Advanced Computing Materials Research
- Micro-Weather Simulation and Extreme Climate Events
- HPC as a Service Research
- UltraScale and Circular and Sustainable Computer Architecture Research

Achieve an identity and speciality (Visibility)

Join Networks and Partnerships (LaRedCCA, SCALAC and Others)

- Collaboration in Productive and Government Projects
- Think Tank in Advanced Computing Prospective
- Node of the Caribbean Supercomputing Collaboration (via SCALAC/RedCLARA to Caribbean Interests)

Collaboration for Sustainable life cycle (long term) with strategic mediation

- Continuous Advising and Support (Non-profit but with a specific agreement as part of the advisory council)
- Technology Industries and Advanced Computing Mediation

Formal Programs (in Co-Advising), Seminars, Workshops and Outreach activities

- PhD in Computer Science and Master Degree (Via UIS but in co-advising and in UdC Interests
- Events (CARLA, SCCAMP)
- Support in development of formal courses for undergraduate students

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HPC for Relevance and Survival

Before 2020

« Quien no computa, no compite »

After 2021

« Quien no colabora no sobrevive »

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HPC for Relevance and Survival

https://www.youtube.com/watch?v=REDuvjuTVbU

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Questions?

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@carlosjaimebh