HPC Ecosystems

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SC Camp
computo Avanzado y a Gran Escala
Advanced and Large Scale Computing
Research group
INDUSTRIAL HPC DELIVERS TRANSFORMATIONAL BREAKTHROUGHS

From NVIDIA BLOG
Precision medicine is based on a better knowledge of phenotype-genotype relationships. That is the knowledge of 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)
An Example: Ciberetech Project. (to observe in detail after)

Raw files (FastQ)

Validated knowledge

Samples

K-DB
Diagnostic portfolio

Analysis Pipeline

Prioritization report

DB
Storage

VCF   BAM
Processed files

Dialog with experts in the disease + validations

HPC + HEALTHCARE
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.
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](http://www.sc3.uis.edu.co)
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

Availability, Security, Throughput, High Speed, Sustainability
Remember Monday Talk: HPC/Advanced Computing Systems

HPC Ecosystem Elements

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

Resources Centers

Software and Data

People
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
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 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
About Software

- 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

Massively Parallel Computing - HPC

- **Strict HPC**
  - High Speed network
  - High Speed interconnection between cores

- **High Performance Data Analysis**
  - No High Speed network

- Data Analytics

- Deep Learning

- Scientific Simulations

From [https://www.hpcwire.com/](https://www.hpcwire.com/)
## About Software Stack

**Software To Deliver Acceleration For HPC & AI Apps; 500+ New Updates**

|----------------------------------|----------------------------------|-----------------------------|--------------------------------|----------------------|------------------|-------------------------------|-------------------|-------------------------------|

**600+ Apps**

- Linear Algebra
- Parallel Algorithms
- Signal Processing
- Deep Learning
- Machine Learning
- Visualization

**CUDA-X HPC & AI**

40+ GPU Acceleration Libraries

**CUDA**

- Desktop Development
- Data Center
- Supercomputers
- GPU-Accelerated Cloud

[www.nvidia.com](http://www.nvidia.com)
Some HPC Skills (in Software)

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<tr>
<th>Performance Monitoring</th>
<th>HPCC</th>
<th>Perfctr</th>
<th>IOR</th>
<th>PAPI/PM</th>
<th>netperf</th>
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<tbody>
<tr>
<td>Development Tools</td>
<td>Cray® Compiler Environment (CCE)</td>
<td>Intel® Cluster Studio</td>
<td>PGI (PGI CDK)</td>
<td>GNU</td>
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<tr>
<td>Application Libraries</td>
<td>Cray® LibSci, LibSci_ACC</td>
<td>MVAPICH2</td>
<td>OpenMPI</td>
<td>Intel® MPI- (Cluster Studio)</td>
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<tr>
<th>Resource Management / Job Scheduling</th>
<th>SLURM</th>
<th>Grid Engine</th>
<th>MOAB</th>
<th>Altair PBS Pro</th>
<th>IBM Platform LSF</th>
<th>Torque/Maui</th>
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<tbody>
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<td>File System</td>
<td>NFS</td>
<td>Local FS (ext3, ext4, XFS)</td>
<td>PanFS</td>
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<td>Provisioning</td>
<td>Cray® Advanced Cluster Engine (ACE) management software</td>
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<td>Cluster Monitoring</td>
<td>Cray ACE (ISCB and OpenIPMI)</td>
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<td>Remote Power Mgmt</td>
<td>Cray ACE</td>
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| Operating System | Linux (Red Hat, CentOS, SUSE) |
Valuable Knowledge

- 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
Challenges and Open Questions

1. Use 70% - 90% of Installed Resources
2. Improve Skills in all the Ecosystem/Community
3. Thinking about the value and not just monetize
4. Collaborate and Join Communities (Partnerships)
5. Sustainable life cycle (long term)
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
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
HPC for Relevance and Survival

Before 2020

« Quien no computa, no compite »

After 2021

« Quien no colabora no sobrevive »
HPC for Relevance and Survival

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

CARLA 2023
LATIN AMERICA HIGH PERFORMANCE COMPUTING CONFERENCE
Cartagena de Indias, Colombia
September 18-22