

# Funcionamiento y usos de una Supercomputadora

Marcos Mazzini | CPA conicet / CCAD (UNC)

Lenovo

intel.

SMN  
Argentina



Instituto de Ciencia,  
Tecnología e Innovación  
Argentina

Clementina XXI



# Disclaimer:

- El centro de cómputo de Clementina XXI está en proceso de conformación.
- El equipo todavía está en fase de validación por parte Lenovo.
- Mis opiniones son mías, no representan una posición oficial.
- Los datos son datos 😊

## CUÁNDO ES HPC?

# High Performance Computing

- Realizar **miles de billones** de operaciones en punto flotante por segundo **FLOPS** (>1 PetaFLOP actualmente)
- **Almacenar** Petabytes de datos con acceso y disponibilidad continua y rendimiento cercano a un disco local.
- **Paralelizar** las tareas entre todos los procesadores/ GPUs comunicando en tiempo real los cambios de estado eficientemente en términos de **escalabilidad**.
- Opcionalmente, **visualizar** una representación tridimensional de los resultados obtenidos a partir de los cálculos efectuados

```
0[100.0] 4[100.0] 8[100.0] 12[100.0] 16[100.0] 20[100.0] 24[100.0] 28[100.0] 32[100.0] 36[100.0] 40[100.0] 44[100.0] 48[100.0] 52[100.0] 56[100.0] 60[100.0]
1[100.0] 5[100.0] 9[100.0] 13[100.0] 17[100.0] 21[100.0] 25[100.0] 29[100.0] 33[100.0] 37[100.0] 41[100.0] 45[100.0] 49[100.0] 53[100.0] 57[100.0] 61[100.0]
2[100.0] 6[100.0] 10[100.0] 14[100.0] 18[100.0] 22[100.0] 26[100.0] 30[100.0] 34[100.0] 38[100.0] 42[100.0] 46[100.0] 50[100.0] 54[100.0] 58[100.0] 62[100.0]
3[100.0] 7[100.0] 11[100.0] 15[100.0] 19[100.0] 23[100.0] 27[100.0] 31[100.0] 35[100.0] 39[100.0] 43[100.0] 47[100.0] 51[100.0] 55[100.0] 59[100.0] 63[100.0]
Mem[|||||] 55.8G/252G Tasks: 103, 311 thr, 692 kthr; 64 running
Swp[ 0K/16.0G] Load average: 65.01 64.73 64.65
Uptime: 28 days, 03:13:49
```

Main		I/O																							
PPID	PRI	NI	VIRT	RES	SHR	S	CPU%	MEM%	TIME+	Command															
91266	20	0	2214M	1015M	168M	R	100.3	0.4	14h25:41	/ccad/stack/23.09/env/apps/linux-rocky8-zen2/gcc-12.3.0/quantum-espresso-7.2-3qtnqojacrtgsojs5qptvtjn3txc7hpp/bin/															
91268	20	0	2175M	1002M	161M	R	100.3	0.4	14h13:28	/ccad/stack/23.09/env/apps/linux-rocky8-zen2/gcc-12.3.0/quantum-espresso-7.2-3qtnqojacrtgsojs5qptvtjn3txc7hpp/bin/															
91269	20	0	2168M	997M	159M	R	100.3	0.4	14h13:00	/ccad/stack/23.09/env/apps/linux-rocky8-zen2/gcc-12.3.0/quantum-espresso-7.2-3qtnqojacrtgsojs5qptvtjn3txc7hpp/bin/															
91281	20	0	2147M	996M	159M	R	100.3	0.4	14h46:52	/ccad/stack/23.09/env/apps/linux-rocky8-zen2/gcc-12.3.0/quantum-espresso-7.2-3qtnqojacrtgsojs5qptvtjn3txc7hpp/bin/															
91294	20	0	2173M	1006M	165M	R	100.3	0.4	15h01:27	/ccad/stack/23.09/env/apps/linux-rocky8-zen2/gcc-12.3.0/quantum-espresso-7.2-3qtnqojacrtgsojs5qptvtjn3txc7hpp/bin/															
91302	20	0	2174M	1011M	169M	R	100.3	0.4	14h48:10	/ccad/stack/23.09/env/apps/linux-rocky8-zen2/gcc-12.3.0/quantum-espresso-7.2-3qtnqojacrtgsojs5qptvtjn3txc7hpp/bin/															
91304	20	0	2187M	1008M	164M	R	100.3	0.4	14h34:51	/ccad/stack/23.09/env/apps/linux-rocky8-zen2/gcc-12.3.0/quantum-espresso-7.2-3qtnqojacrtgsojs5qptvtjn3txc7hpp/bin/															
91308	20	0	2163M	1008M	161M	R	100.3	0.4	14h22:50	/ccad/stack/23.09/env/apps/linux-rocky8-zen2/gcc-12.3.0/quantum-espresso-7.2-3qtnqojacrtgsojs5qptvtjn3txc7hpp/bin/															
91312	20	0	2167M	1015M	166M	R	100.3	0.4	14h52:05	/ccad/stack/23.09/env/apps/linux-rocky8-zen2/gcc-12.3.0/quantum-espresso-7.2-3qtnqojacrtgsojs5qptvtjn3txc7hpp/bin/															
91321	20	0	2164M	1016M	174M	R	100.3	0.4	14h42:43	/ccad/stack/23.09/env/apps/linux-rocky8-zen2/gcc-12.3.0/quantum-espresso-7.2-3qtnqojacrtgsojs5qptvtjn3txc7hpp/bin/															
91323	20	0	2182M	1008M	171M	R	100.3	0.4	14h55:08	/ccad/stack/23.09/env/apps/linux-rocky8-zen2/gcc-12.3.0/quantum-espresso-7.2-3qtnqojacrtgsojs5qptvtjn3txc7hpp/bin/															
91325	20	0	2165M	1013M	171M	R	100.3	0.4	14h47:04	/ccad/stack/23.09/env/apps/linux-rocky8-zen2/gcc-12.3.0/quantum-espresso-7.2-3qtnqojacrtgsojs5qptvtjn3txc7hpp/bin/															
91326	20	0	2173M	1024M	180M	R	100.3	0.4	14h59:41	/ccad/stack/23.09/env/apps/linux-rocky8-zen2/gcc-12.3.0/quantum-espresso-7.2-3qtnqojacrtgsojs5qptvtjn3txc7hpp/bin/															
91328	20	0	2148M	1014M	170M	R	100.3	0.4	14h52:01	/ccad/stack/23.09/env/apps/linux-rocky8-zen2/gcc-12.3.0/quantum-espresso-7.2-3qtnqojacrtgsojs5qptvtjn3txc7hpp/bin/															
91267	20	0	2219M	1009M	165M	R	99.6	0.4	14h27:31	/ccad/stack/23.09/env/apps/linux-rocky8-zen2/gcc-12.3.0/quantum-espresso-7.2-3qtnqojacrtgsojs5qptvtjn3txc7hpp/bin/															
91270	20	0	2182M	1003M	166M	R	99.6	0.4	14h46:16	/ccad/stack/23.09/env/apps/linux-rocky8-zen2/gcc-12.3.0/quantum-espresso-7.2-3qtnqojacrtgsojs5qptvtjn3txc7hpp/bin/															
91271	20	0	2178M	1000M	162M	R	99.6	0.4	14h42:53	/ccad/stack/23.09/env/apps/linux-rocky8-zen2/gcc-12.3.0/quantum-espresso-7.2-3qtnqojacrtgsojs5qptvtjn3txc7hpp/bin/															
91272	20	0	2170M	999M	160M	R	99.6	0.4	14h29:46	/ccad/stack/23.09/env/apps/linux-rocky8-zen2/gcc-12.3.0/quantum-espresso-7.2-3qtnqojacrtgsojs5qptvtjn3txc7hpp/bin/															
91273	20	0	2162M	1000M	161M	R	99.6	0.4	14h28:06	/ccad/stack/23.09/env/apps/linux-rocky8-zen2/gcc-12.3.0/quantum-espresso-7.2-3qtnqojacrtgsojs5qptvtjn3txc7hpp/bin/															
91274	20	0	2169M	999M	160M	R	99.6	0.4	14h42:35	/ccad/stack/23.09/env/apps/linux-rocky8-zen2/gcc-12.3.0/quantum-espresso-7.2-3qtnqojacrtgsojs5qptvtjn3txc7hpp/bin/															
91275	20	0	2154M	990M	156M	R	99.6	0.4	14h38:32	/ccad/stack/23.09/env/apps/linux-rocky8-zen2/gcc-12.3.0/quantum-espresso-7.2-3qtnqojacrtgsojs5qptvtjn3txc7hpp/bin/															
91276	20	0	2161M	993M	156M	R	99.6	0.4	14h27:35	/ccad/stack/23.09/env/apps/linux-rocky8-zen2/gcc-12.3.0/quantum-espresso-7.2-3qtnqojacrtgsojs5qptvtjn3txc7hpp/bin/															
91277	20	0	2147M	994M	157M	R	99.6	0.4	14h22:26	/ccad/stack/23.09/env/apps/linux-rocky8-zen2/gcc-12.3.0/quantum-espresso-7.2-3qtnqojacrtgsojs5qptvtjn3txc7hpp/bin/															
91279	20	0	2165M	997M	159M	R	99.6	0.4	14h56:43	/ccad/stack/23.09/env/apps/linux-rocky8-zen2/gcc-12.3.0/quantum-espresso-7.2-3qtnqojacrtgsojs5qptvtjn3txc7hpp/bin/															
91280	20	0	2150M	994M	158M	R	99.6	0.4	14h51:00	/ccad/stack/23.09/env/apps/linux-rocky8-zen2/gcc-12.3.0/quantum-espresso-7.2-3qtnqojacrtgsojs5qptvtjn3txc7hpp/bin/															
91283	20	0	2182M	1003M	159M	R	99.6	0.4	14h30:01	/ccad/stack/23.09/env/apps/linux-rocky8-zen2/gcc-12.3.0/quantum-espresso-7.2-3qtnqojacrtgsojs5qptvtjn3txc7hpp/bin/															
91284	20	0	2144M	990M	156M	R	99.6	0.4	14h21:07	/ccad/stack/23.09/env/apps/linux-rocky8-zen2/gcc-12.3.0/quantum-espresso-7.2-3qtnqojacrtgsojs5qptvtjn3txc7hpp/bin/															
91285	20	0	2164M	998M	157M	R	99.6	0.4	14h17:54	/ccad/stack/23.09/env/apps/linux-rocky8-zen2/gcc-12.3.0/quantum-espresso-7.2-3qtnqojacrtgsojs5qptvtjn3txc7hpp/bin/															
91286	20	0	2173M	998M	163M	R	99.6	0.4	14h48:42	/ccad/stack/23.09/env/apps/linux-rocky8-zen2/gcc-12.3.0/quantum-espresso-7.2-3qtnqojacrtgsojs5qptvtjn3txc7hpp/bin/															
91287	20	0	2163M	999M	161M	R	99.6	0.4	14h51:07	/ccad/stack/23.09/env/apps/linux-rocky8-zen2/gcc-12.3.0/quantum-espresso-7.2-3qtnqojacrtgsojs5qptvtjn3txc7hpp/bin/															
91288	20	0	2159M	1000M	161M	R	99.6	0.4	14h33:19	/ccad/stack/23.09/env/apps/linux-rocky8-zen2/gcc-12.3.0/quantum-espresso-7.2-3qtnqojacrtgsojs5qptvtjn3txc7hpp/bin/															
91290	20	0	2200M	1011M	166M	R	99.6	0.4	14h39:09	/ccad/stack/23.09/env/apps/linux-rocky8-zen2/gcc-12.3.0/quantum-espresso-7.2-3qtnqojacrtgsojs5qptvtjn3txc7hpp/bin/															

Sino está así,  
está mal.

```
Help F2Setup F3Search F4Filter F5Tree F6SortBy F7Nice -F8Nice +F9Kill F10Quit
```



```

NVIDIA-SMI 510.47.03   Driver Version: 510.47.03   CUDA Version: 11.0
-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+
GPU  Name          Persistence-M| Bus-Id          Disp.A | Volatile Uncorr. ECC
Fan  Temp    Perf  Pwr:Usage/Cap|      Memory-Usage | GPU-Util  Compute M.
                               MIG M.
-----+-----+-----+-----+-----+-----+-----+-----+
  0   NVIDIA A30           On          | 00000000:03:00.0 Off  |      0
N/A   42C    P0      80W / 165W | 271MiB / 24576MiB |    61%      Default
                               Disabled
-----+-----+-----+-----+-----+-----+-----+
  1   NVIDIA A30           On          | 00000000:85:00.0 Off  |      0
N/A   41C    P0     113W / 165W | 271MiB / 24576MiB |    60%      Default
                               Disabled
-----+-----+-----+-----+-----+-----+-----+

```

# También las GPUs.

Processes:

```

GPU  GI  CI          PID  Type  Process name          GPU Memory
    ID ID          |      |      |                    Usage
-----+-----+-----+-----+-----+-----+-----+
  0   N/A N/A    341013  C    ...qqup77pmb6cjf/bin/gmx_mpi  269MiB
  1   N/A N/A    341666  C    qqup77pmb6cjf/bin/gmx_mpi    269MiB

```

## INFRAESTRUCTURA

# Datacenter



### Refrigeracion

Aire / Agua / Inmersión



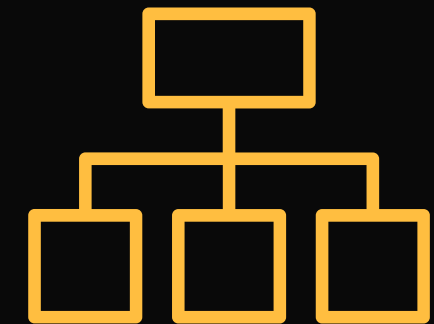
### Alimentación Eléctrica

Consumo eléctrico



### Storage

Filesystem Paralelo



### Interconexión

Infiniband

Slingshot

Ethernet + RDMA



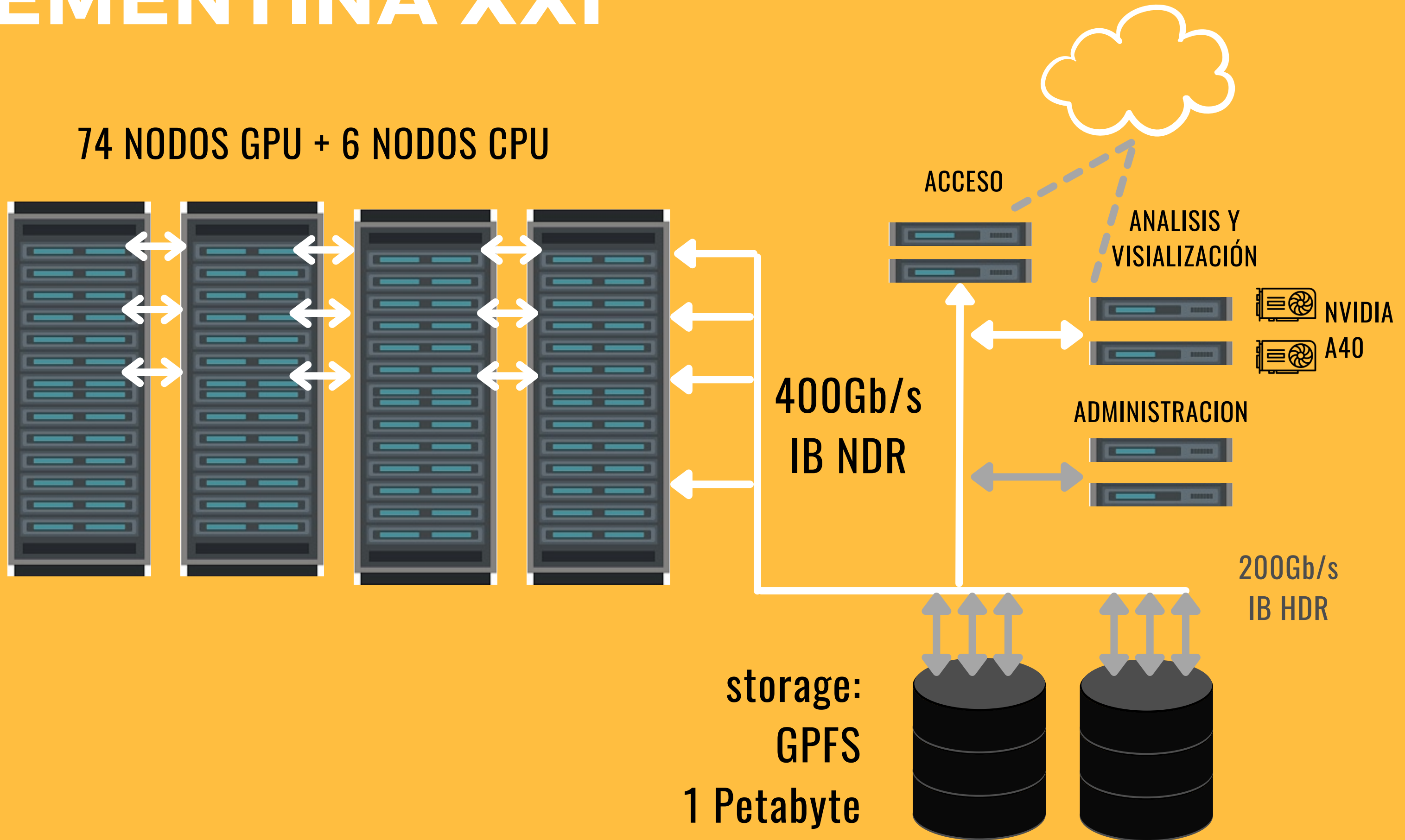
# Refrigeración Direct Water Cooling

**99% heat capture  
at 40°C**

**CPU's | GPU's | DIMMs | Fuentes**

# CLEMENTINA XXI

74 NODOS GPU + 6 NODOS CPU



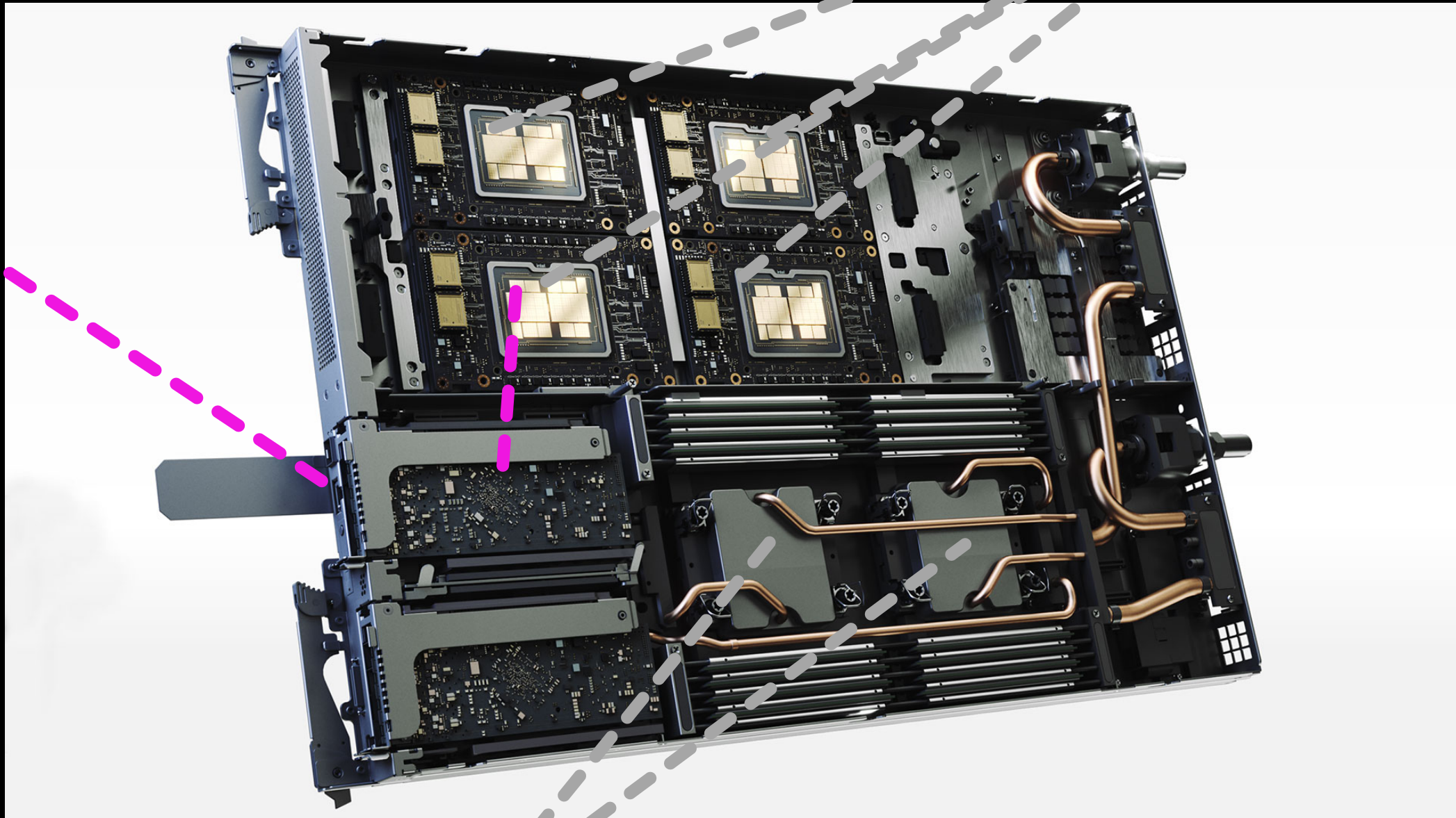


# NODO

RED INFINIBAND  
CONNECTX-7 NDR  
QSFP400

4 X

INTEL GPU MAX 1550  
(PONTE VECCHIO)  
128 GB POR GPU, 600W TDP



2 X

INTEL XEON MAX 9462 @ 2,7GHZ (SAPHIRE RAPIDS)  
64 GB HBM + 256 GB RAM DDR5 4800 MT/S



# Intel GPU MAX 1550 (PVC)

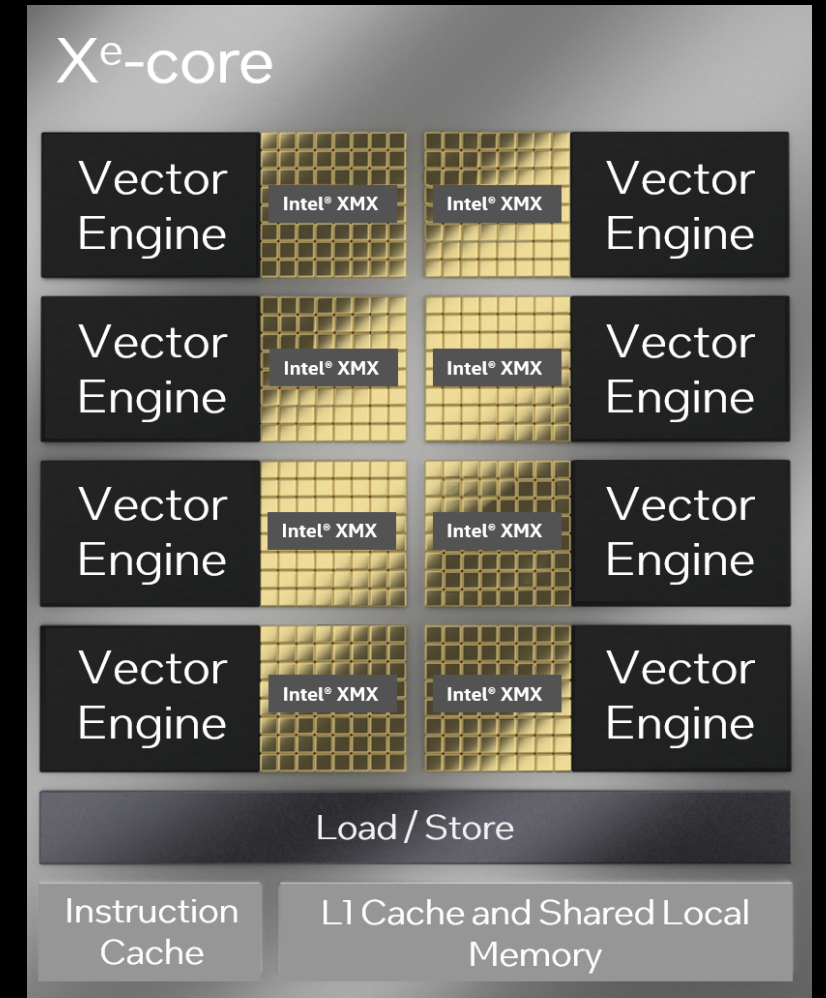
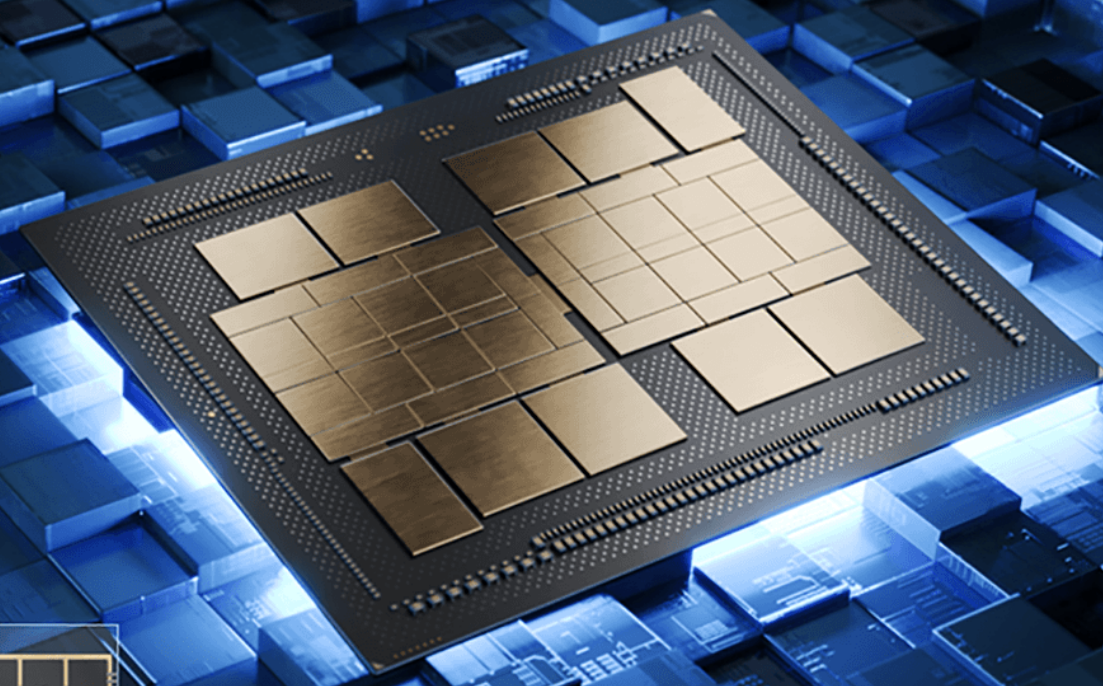


Intel® Data Center  
GPU Max Series

Up to  
**128**  
Xe  
Cores

**52TF**  
Peak FP64  
Throughput

**16**  
Xe Links for GPU-  
to-GPU  
communication



**128 Xe cores**

128GB HBM2E  
PCI-EXPRESS 5.0 X16  
TDP/TBP 600 W

**4 X**





# Intel Xeon Scalable 9462 (SPR)



## First & only x86 CPU with HBM

Choose the right memory configuration for your needs

<b>64GB</b> HBM2e 4 stacks of 16GB	<b>~1TB/s</b> Memory Bandwidth	<b>&gt;1GB</b> HBM per Core	<b>Memory Modes</b>		
			<b>HBM Only</b> Bootable from HBM No code change  	<b>HBM Flat</b> 2 Memory Regions SW Optimization Needed  	<b>HBM Caching</b> HBM as cache for DDR No code change  

Under Embargo until November 9th, 2022, 6am PT

32 CORES GOLDEN COVE  
64 GB HBM  
256 GB DE RAM (8 MODULOS)  
TDP/TBP 350 W

# 2 X



# Cómo se usa?

EL USO ES NO INTERACTIVO

01

## Conexion SSH

Consola remota modo texto

02

## Sistema de colas

Scripts no intetractivos con:

- Software propio
- Aplicaciones específicas

03

## Análisis de resulatados

Visualización y transferencia de archivos

# Top500: FLOPS

- **Rpeak:**
  - Máxima performance pico teórica
- **Rmax:**
  - Máxima performance efectiva
    - Mejor resultado ejecutando HPL

OPs en FP64 (double de C)

# Top 5

Rank	System	Cores	Rmax (PFlop/s)	Rpeak (PFlop/s)	Power (kW)
1	<b>Frontier</b> - HPE Cray EX235a, AMD Optimized 3rd Generation EPYC 64C 2GHz, AMD Instinct MI250X, Slingshot-11, HPE DOE/SC/Oak Ridge National Laboratory United States	8,699,904	1,194.00	1,679.82	22,703
2	<b>Supercomputer Fugaku</b> - Supercomputer Fugaku, A64FX 48C 2.2GHz, Tofu interconnect D, Fujitsu RIKEN Center for Computational Science Japan	7,630,848	442.01	537.21	29,899
3	<b>LUMI</b> - HPE Cray EX235a, AMD Optimized 3rd Generation EPYC 64C 2GHz, AMD Instinct MI250X, Slingshot-11, HPE EuroHPC/CSC Finland	2,220,288	309.10	428.70	6,016
4	<b>Leonardo</b> - BullSequana XH2000, Xeon Platinum 8358 32C 2.6GHz, NVIDIA A100 SXM4 64 GB, Quad-rail NVIDIA HDR100 Infiniband, Atos EuroHPC/CINECA Italy	1,824,768	238.70	304.47	7,404
5	<b>Summit</b> - IBM Power System AC922, IBM POWER9 22C 3.07GHz, NVIDIA Volta GV100, Dual-rail Mellanox EDR Infiniband, IBM DOE/SC/Oak Ridge National Laboratory United States	2,414,592	148.60	200.79	10,096

# Top500: Ilegaremos?

**74 nodos**

**x 4 GPUs**

**x 52 TFLOPS peak**

**= 15.329 TFLOPS**

**15.329 TFLOPS x 0,50%**

**+ 400 TFLOPS CPU**

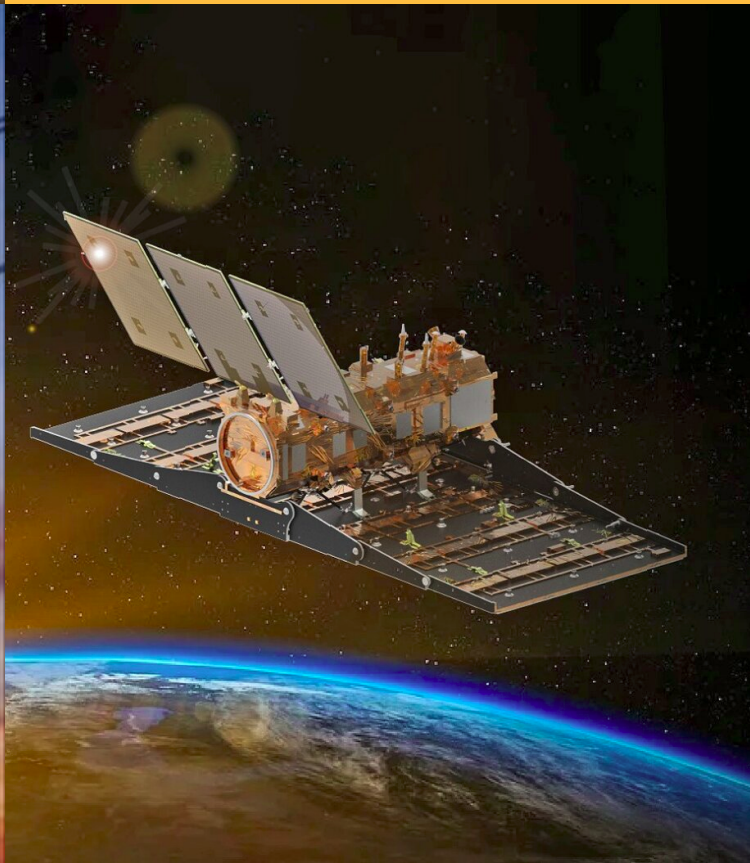
**= ~8,06 PFLOPS**

79	<b>LANTA</b> - HPE Cray EX235n, AMD EPYC 7713 64C 2GHz, NVIDIA A100 40GB, Slingshot-11, HPE NSTDA Supercomputer Center (ThaiSC) Thailand	87,296	8.15	13.77	310
80	<b>TSUBAME3.0</b> - SGI ICE XA, IP139-SXM2, Xeon E5-2680v4 14C 2.4GHz, Intel Omni-Path, NVIDIA Tesla P100 SXM2, HPE GSIC Center, Tokyo Institute of Technology Japan	135,828	8.12	12.13	792
81	<b>Roxy</b> - Apollo 2000, Xeon Gold 6248 20C 2.5GHz, Infiniband EDR, HPE Government United States	174,720	8.12	13.98	
82	<b>HoreKa-Green</b> - ThinkSystem SD650 V2, Xeon Platinum 8368 38C 2.4GHz, NVIDIA A100 40GB, Mellanox HDR Infiniband, Lenovo Karlsruhe Institut für Technologie (KIT) Germany	90,932	8.03	15.01	359
83	<b>Narwhal</b> - HPE Cray EX, AMD EPYC 7H12 64C 2.6GHz, Slingshot-10, HPE Navy DSRC United States	276,480	8.02	11.50	
84	<b>Plasma Simulator</b> - SX-Aurora TSUBASA A412-8, Vector Engine Type10AE 8C 1.58GHz, Infiniband HDR 200, NEC National Institute for Fusion Science (NIFS) Japan	34,560	7.89	10.51	1,550





**Recurso  
+ Modelado numérico  
+ Optimización  
= Valor agregado + ROI**





# Qué esperar en los próximos años?

- Tener equipos ES soberanía.
- Los equipos pasan, la gente queda.
- El HPC va a seguir creciendo.
- Demanda global de personal capacitado.
- Academia e Industria.

**Más de 60 años para recuperar  
potencia de cálculo competitiva  
en Argentina.**

**Clementina ... clusters ... Clementina XXI ...**



**Preguntas?**

**Marcos Mazzini | CPA conicet / CCAD (UNC)**