
G 3
F 4
P 3
G 3
A 1
U 1

HPC: para la creación de medicamentos, explotación de GPUs y FPGAs

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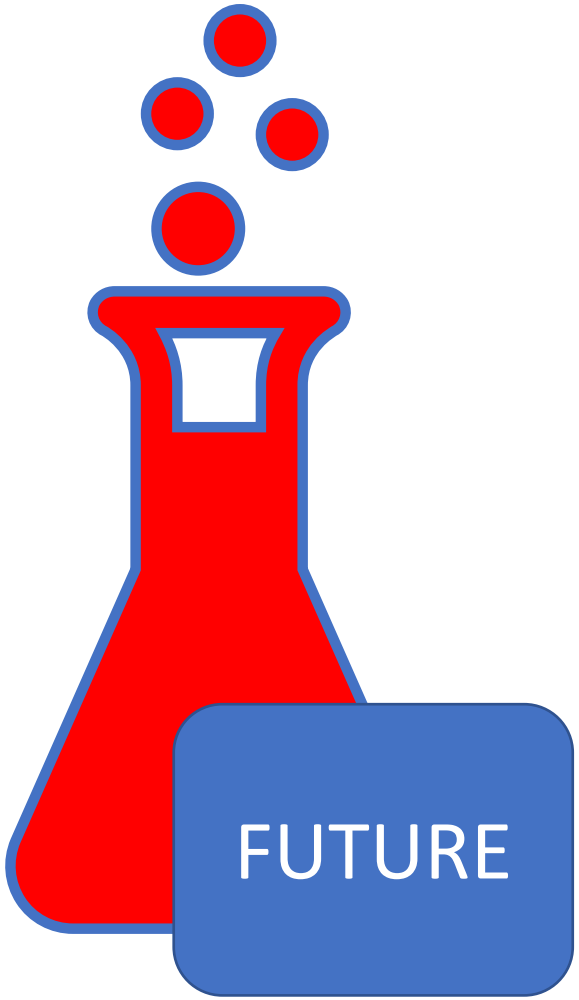
D0

The experiment

PAST

What we do?

PRESENT



FUTURE

ENLACE PARA VER EL VIDEO:

http://www.sie.es/wp-content/uploads/2021/05/multimedia1_KcXbZjuf.mp4

D4.1

What we do? Determining atomic structures

3GWH

Workgroup

https://www.nature.com/articles/nmeth.1365

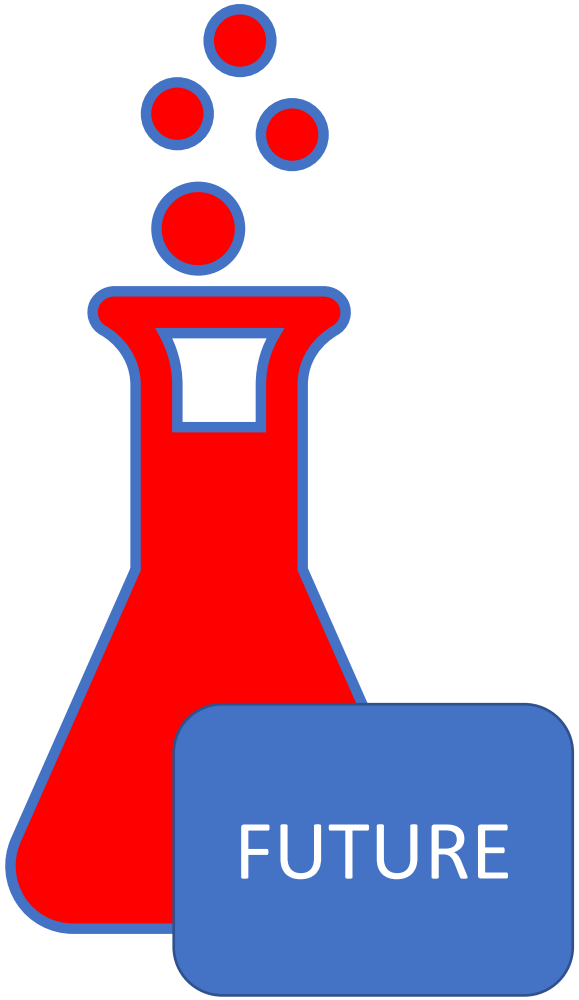
D2 …

The experiment

PAST

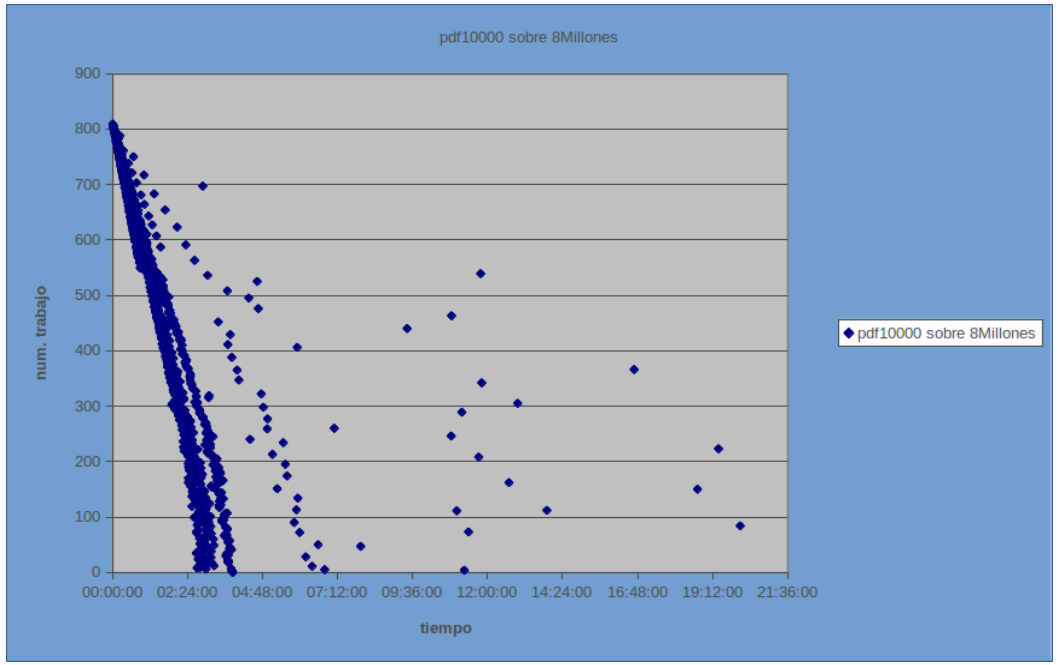
What we do?

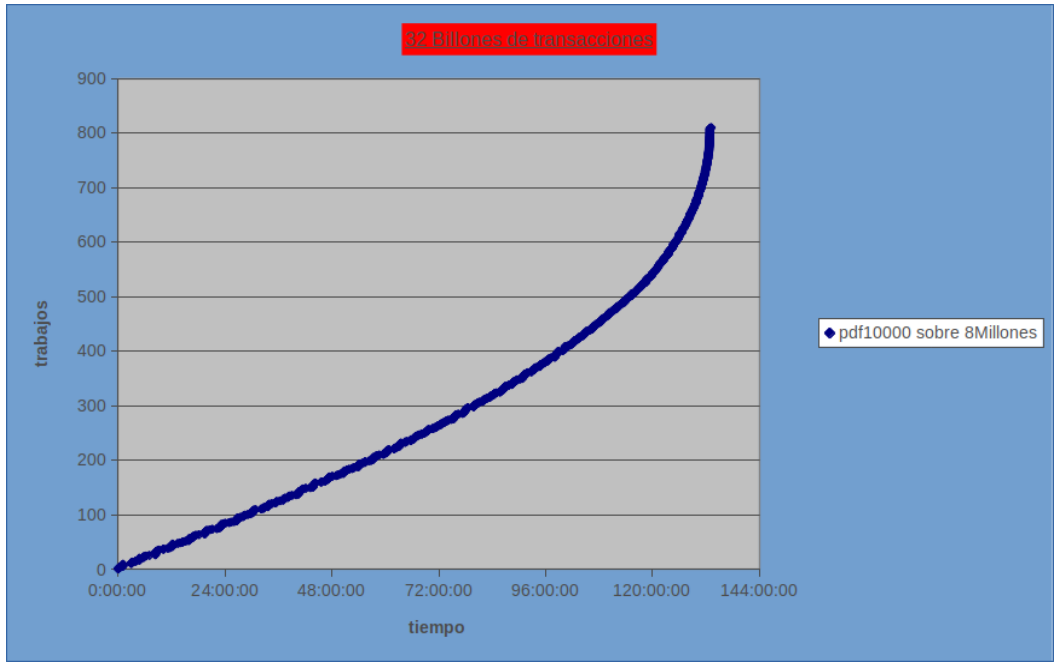
PRESENT



FUTURE

Where we came from? Year 2001, grid





Year 2011, GPUs

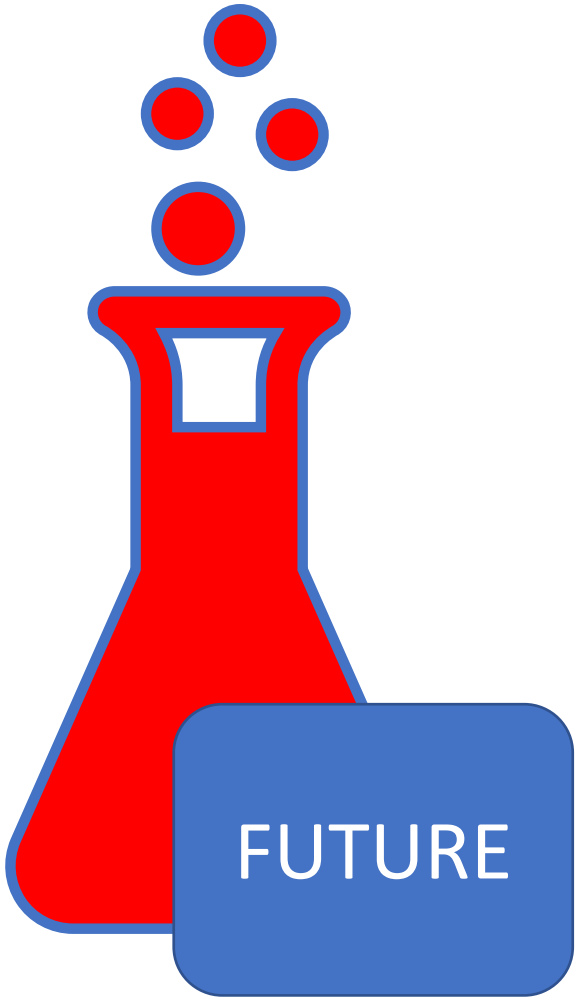
```
__global__ void VecAdd(int* A, float*AP, const float* B1, const float* B2,
const float* B3, const float* B4, const int N, const int ii)
{
    int i = blockDim.x * blockIdx.x + threadIdx.x;
    if ((ii < i) && (i < N))
        A[i] = 0; AP[i] =0;
        A[i] = int(sqrt((B1[ii]-B1[i])*(B1[ii]-B1[i]) +
                        (B2[ii]-B2[i])*(B2[ii]-B2[i]) +
                        (B3[ii]-B3[i])*(B3[ii]-B3[i])));
    AP[i] = B4[ii]*B4[i];
}
```

The experiment

PAST

What we do?

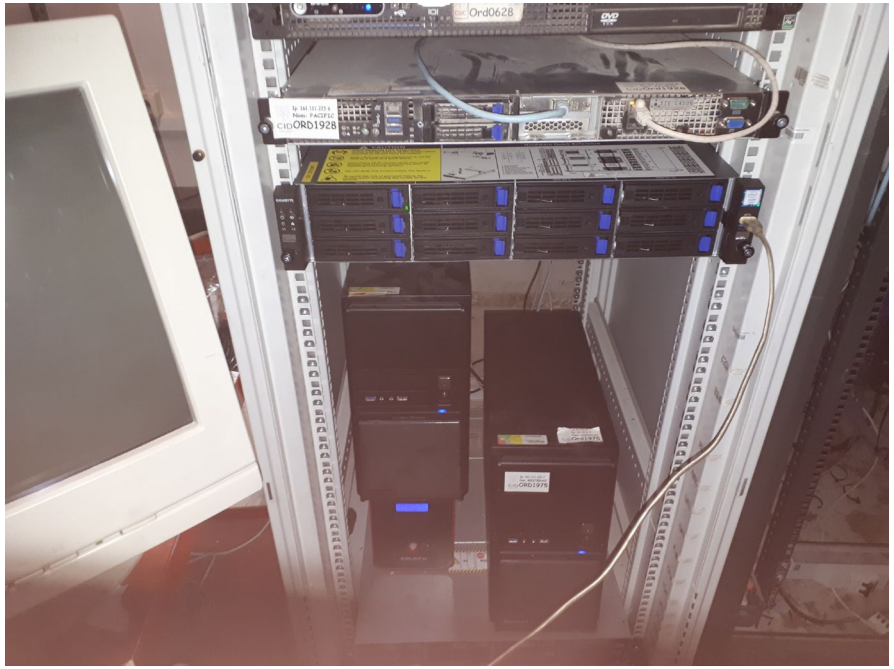
PRESENT

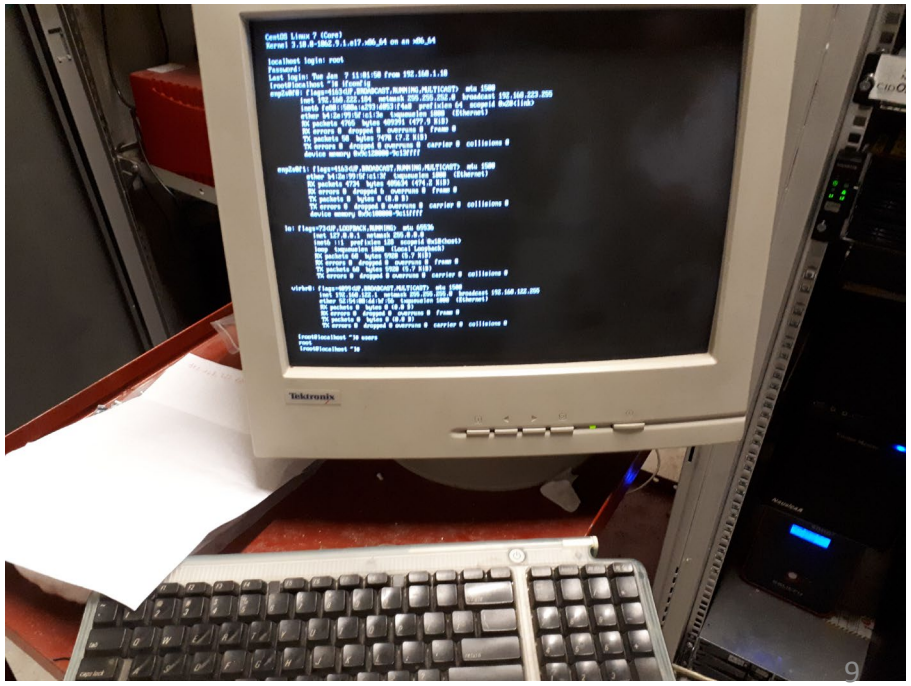


FUTURE

The equipment

- 1 Intel FPGA STRATIX 10 Model GX2800
- 1 GPU NVidia RTX 2070 SUPER™ Blower, 8 GB RAM GDDR6 2.560 cores
- 2 Processors Xeon Cascade-lake Bronze 3204 de 1,9 GHz, six cores each



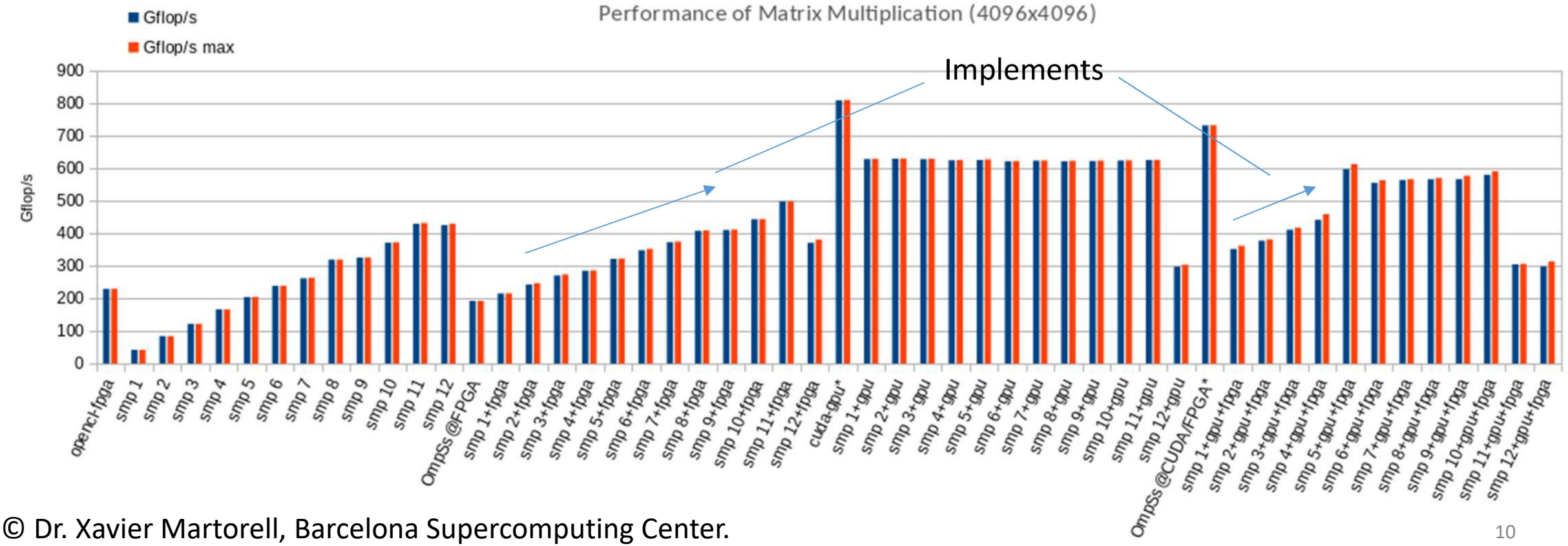


Runtimes– OmpSs@CUDA & OpenCL

D3

- Evaluation on Intel CPUs, Nvidia GPU and Intel Stratix 10 FPGA
  - Lesson learned: devices similar in performance contribute better to overall performance

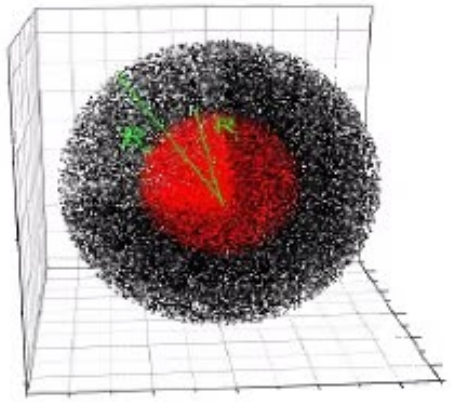
6-core Intel Xeon® Bronze 3204 @1.9GHz, no ht
Nvidia GeForce RTX 2070 SUPER
Intel Stratix 10 FPGA

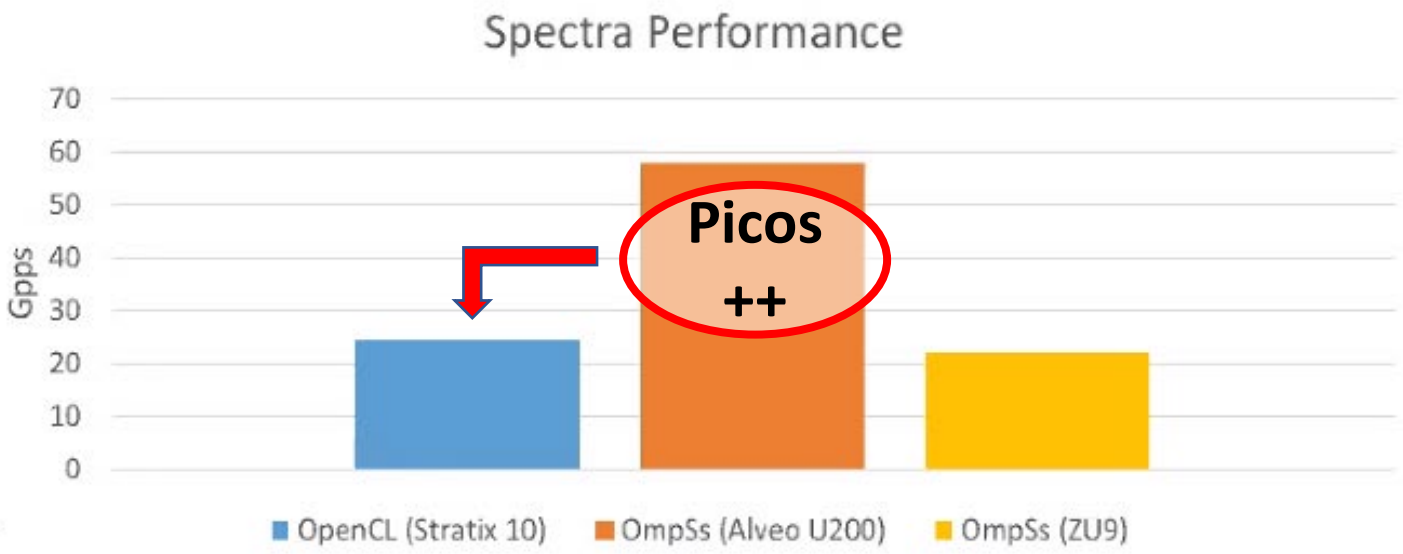


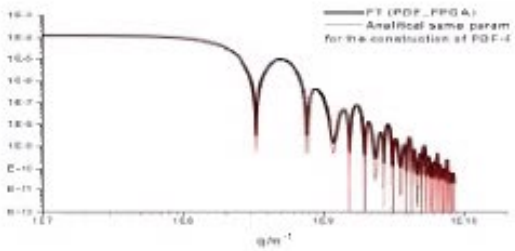
Electrons

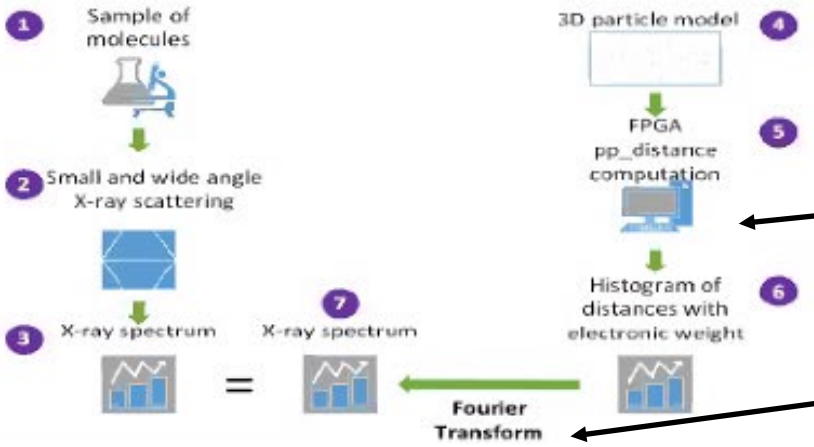
Spectra results (OpenCL comparison)

D2 ...









$\forall i\ \forall j$, histogram[dij]+= ei·ej

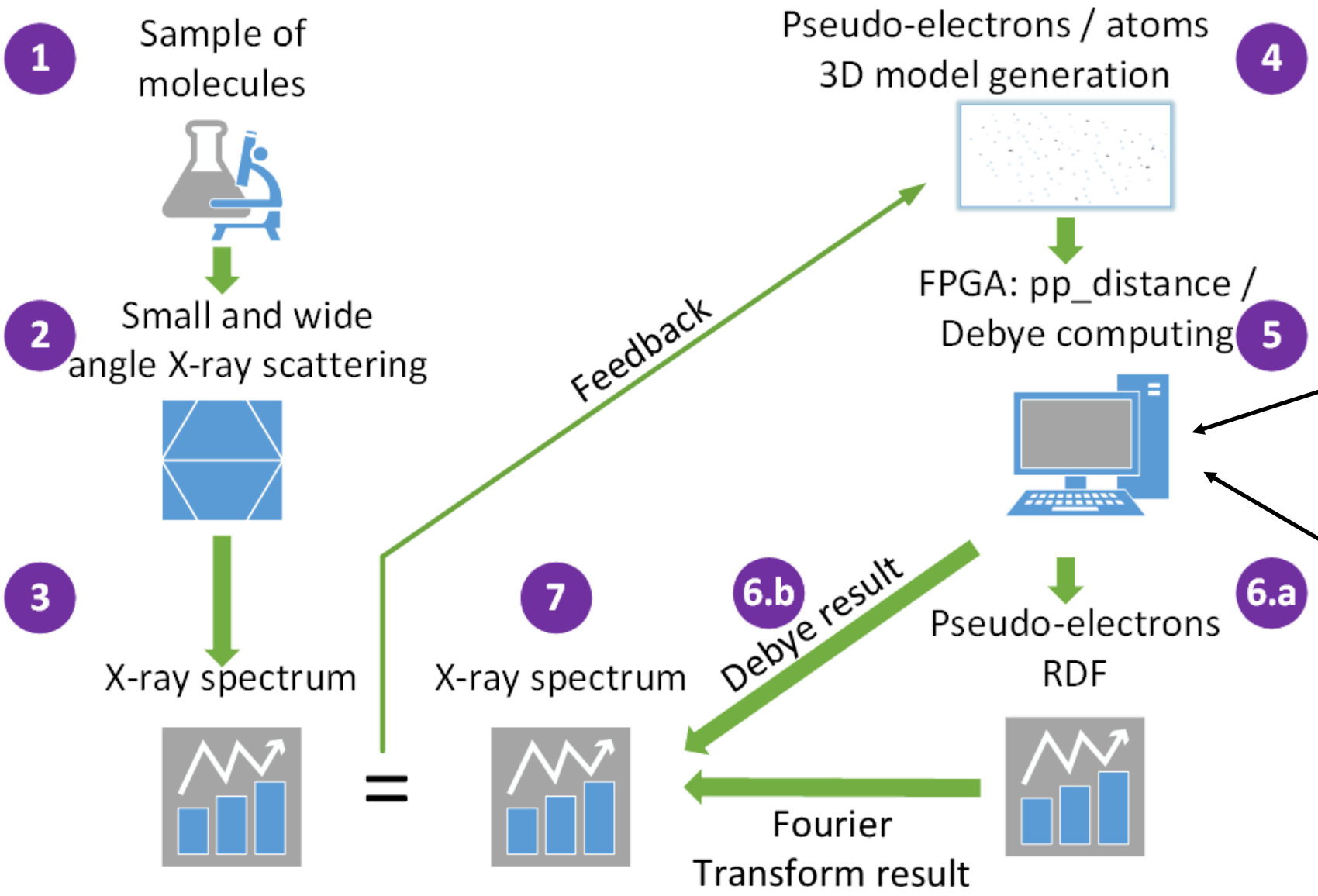
$$P(q) = 4\pi \int_0^{\infty} (p)\, r \frac{\sin(qr)}{qr}\, dr$$

Fourier transform in the sine

Results submitted for publication, under review.

Atoms

D2 ...



Atomic Form Factors

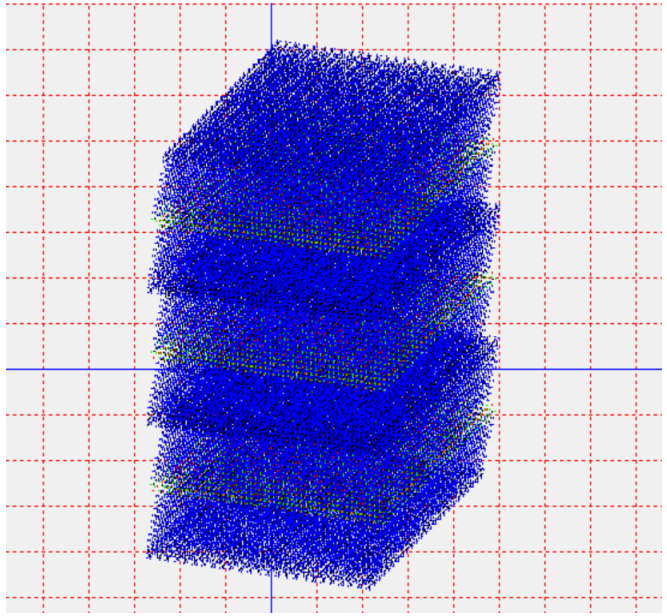
$$f(q) = \left(\sum_{i=1}^{4} a_i \, e^{\left(-b_i \left(\frac{q}{4\pi}\right)^2\right)} \right) + c$$

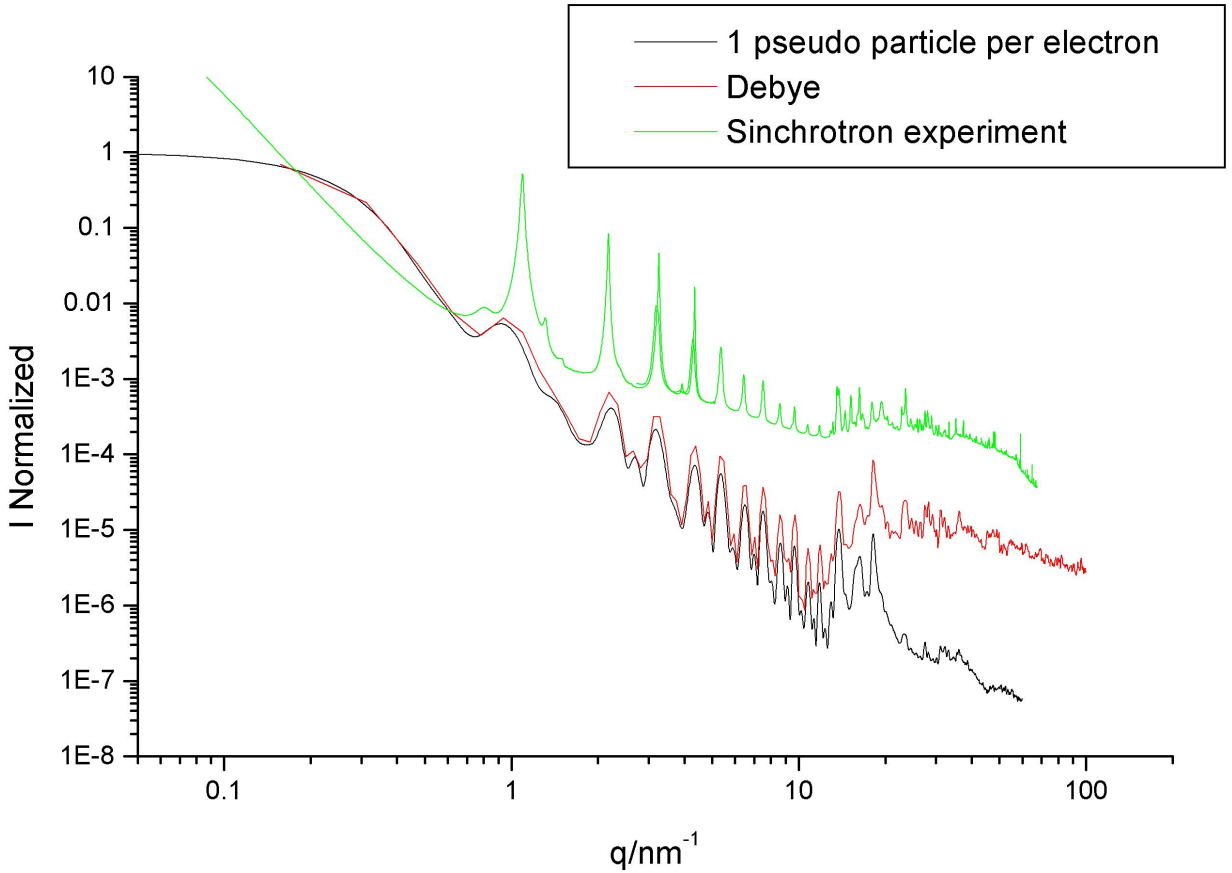
$$I(q) = \sum_{i=1}^{N} \sum_{j=1}^{N} f_i f_j \frac{\sin(q \cdot r_{ij})}{q \cdot r_{ij}}$$

Debye formula

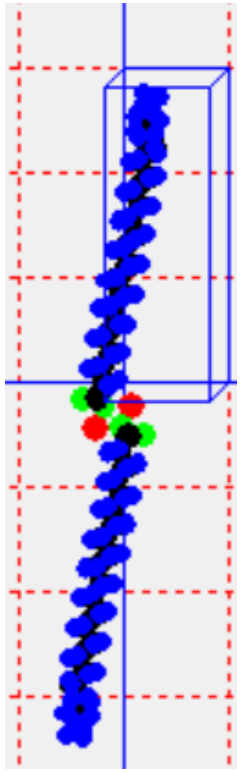
Comparison pseudo-electrons/atoms/experimental

3D model



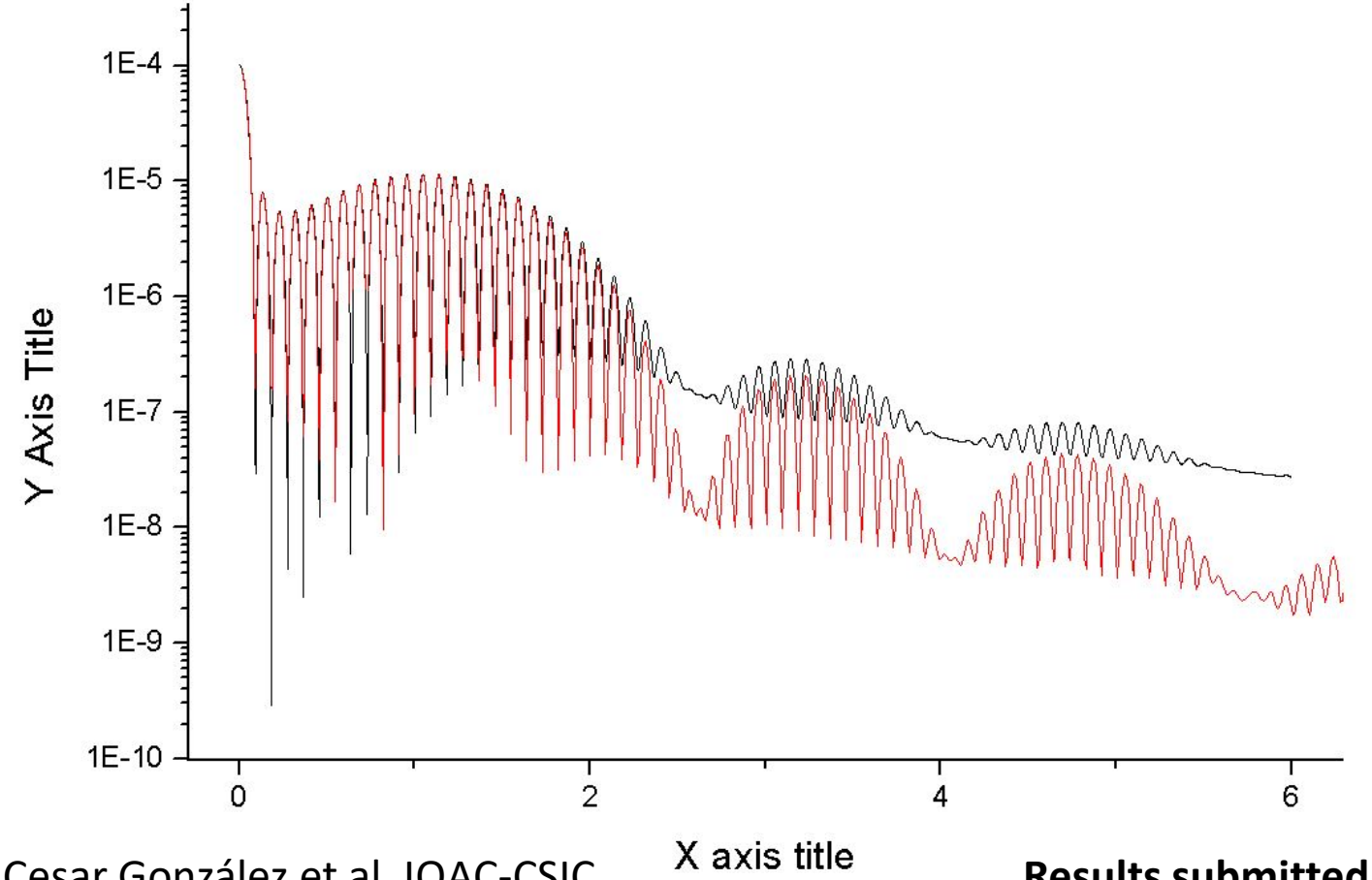


$AgC_{22}H_{43}O_2$



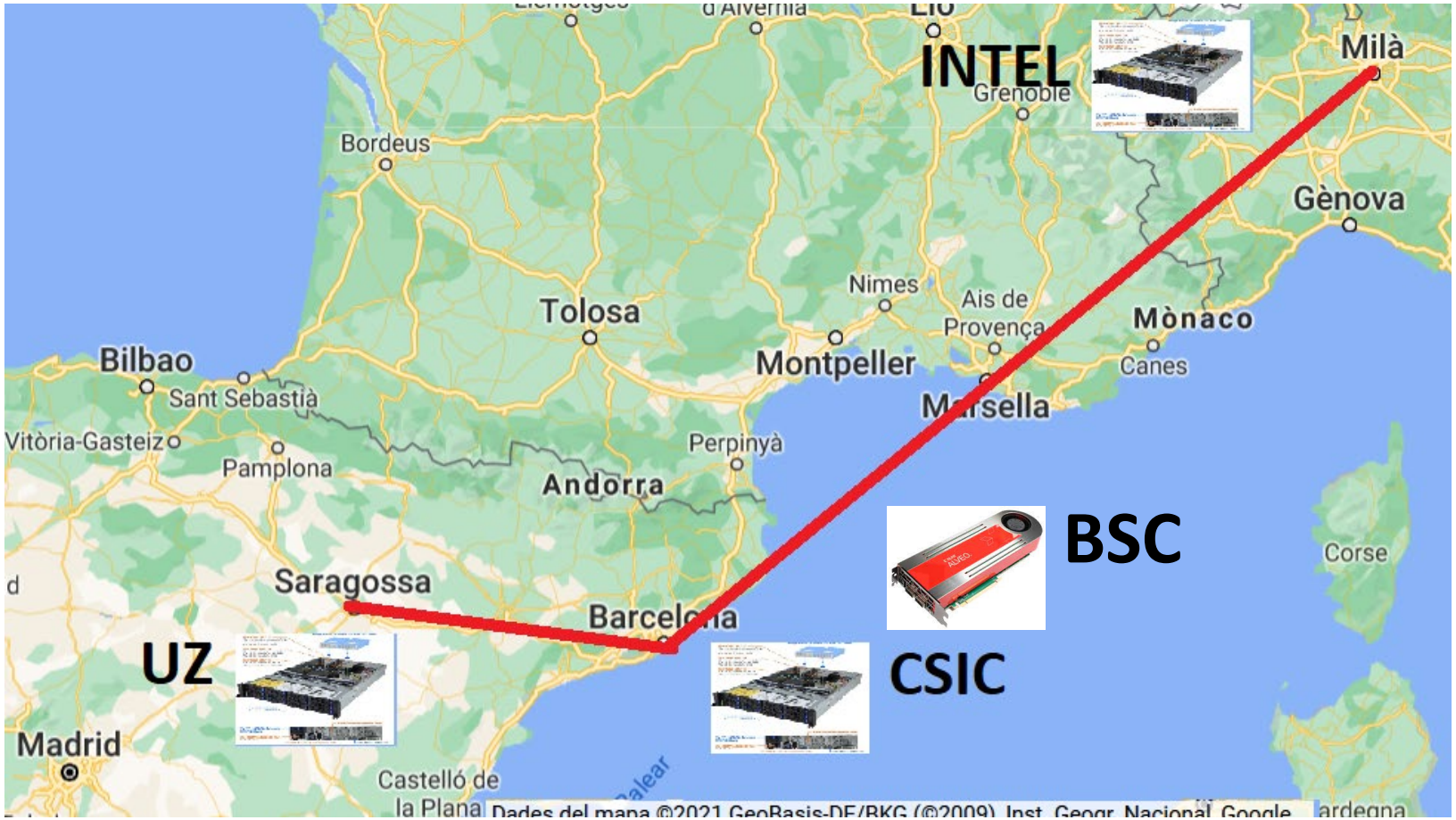
D5

Comparison and more …



Results submitted for publication, under review.

Explainning the results



Latency, 80 sec.

Picos ++, 34 sec.

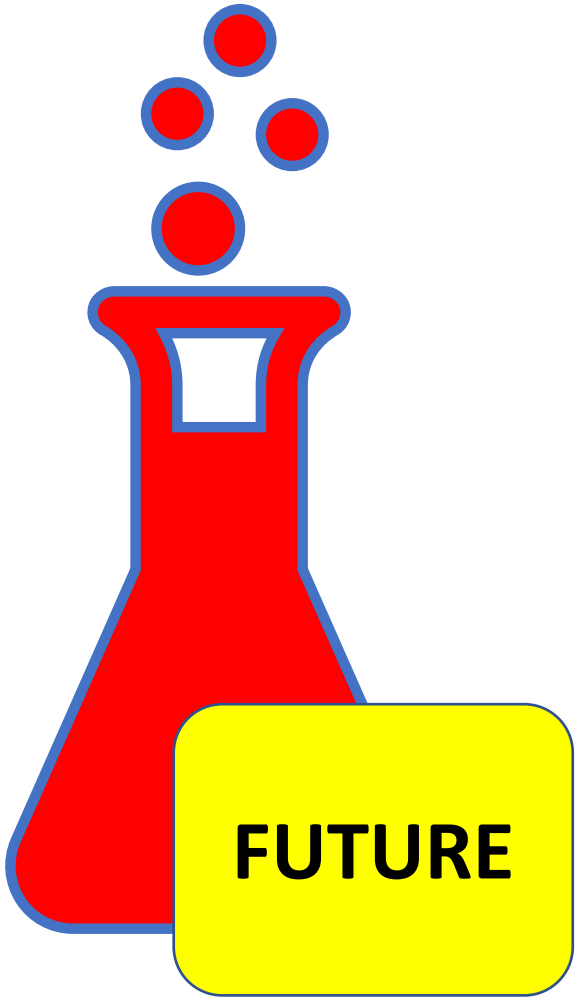
D1

The experiment

PAST

What we do?

PRESENT



Road map to the structures

1. **Model the real structure of ??? with atoms and try to converge a random model to its spectrum with pseudo-electons.**

2. **Try to converge a random model to the BSA real spectrum.**

3. **Try to converge a random model to an unknown structure.**

D4.2

THE END: Performance summary

YEAR	Technologies	Time	Place
Before 2001	CPU	Week	IQAC-CSIC lab
2001	Grid	Weekend	CID-CSIC
2011	GPU	10,000 seconds	CID-CSIC lab
2021	FPGA	30 seconds	BSC

Breaking news !

C-CUDA	Bpps	seg.
K40	14	142,86
GTX 1060	50	40,00
GTX 1670	116	17,24
GTX 1080	188	10,64
RTX 2070	218	9,17

GPU (*pseudo-electrons*)

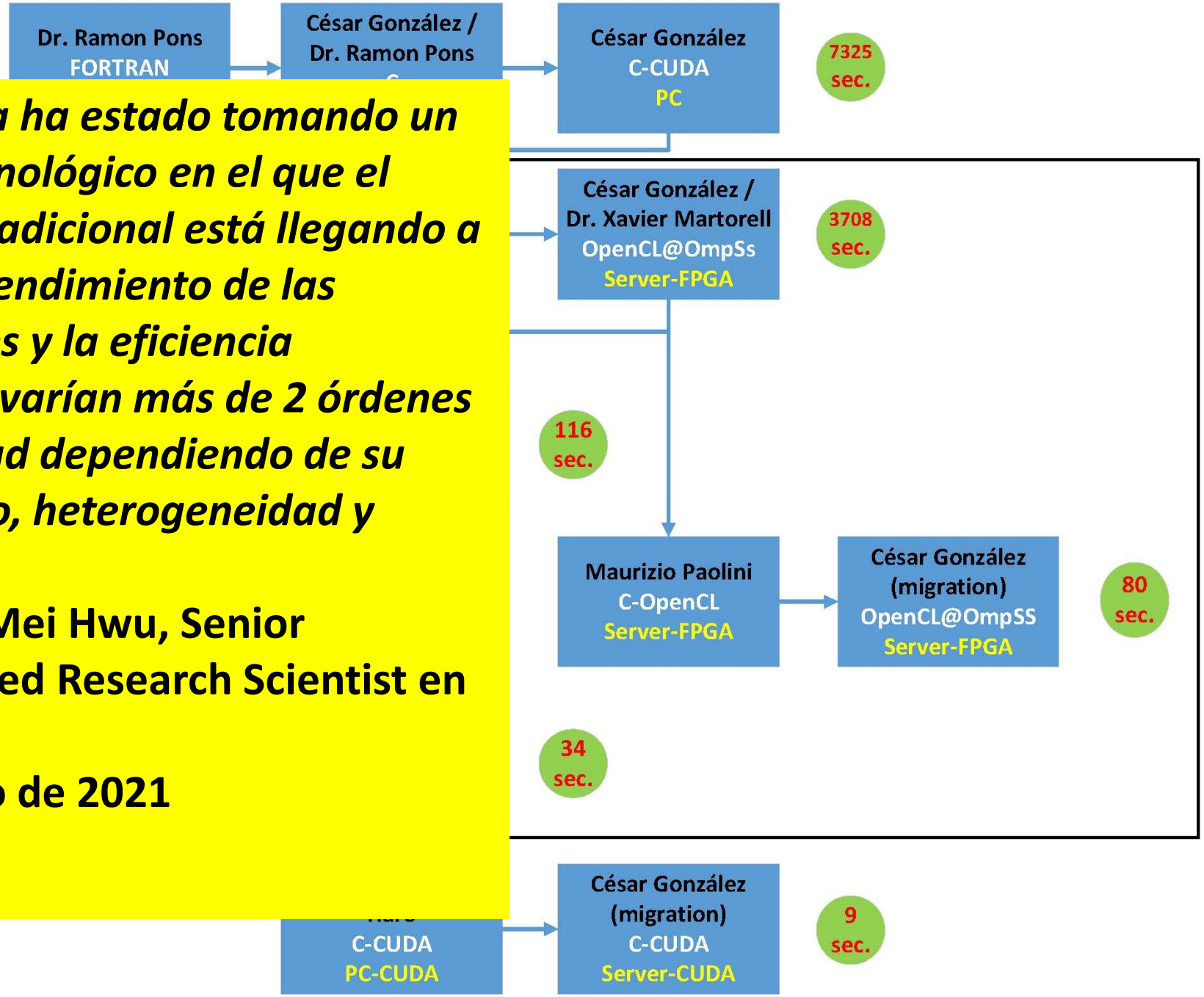
RDF F vector affect performance: x10 → time x2

Results submitted for publication, under review.

La industria ha estado tomando un camino tecnológico en el que el escalado tradicional está llegando a su fin y el rendimiento de las aplicaciones y la eficiencia energética varían más de 2 órdenes de magnitud dependiendo de su paralelismo, heterogeneidad y localidad.

Dr. Wen – Mei Hwu, Senior Distinguished Research Scientist en NVIDIA ...

11 de mayo de 2021



Moore's law

D2

“You can dream, but you can never go back the way you came.”

Jackson Browne, 9-JUN-1977