

Tiny MD

Laboratorio 2

Vectorización

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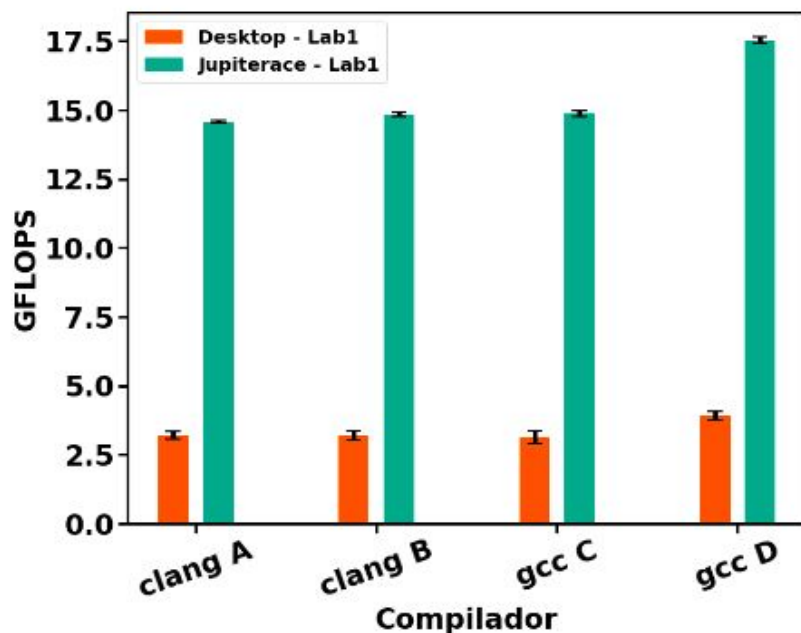
Detalles computacionales

| Computadora | ID | Microarq. | Cores | Base | Turbo | Cache |
|-------------|-----------------------|-----------|-------|----------|----------|-------|
| Desktop | Intel Core i5-4460 | Haswell | 4 | 3.20 GHz | 3.40 GHz | 6 MB |
| Jupiterace | Intel Xeon E5-2680 v4 | Broadwell | 14 | 2.40 GHz | 3.30 GHz | 35 MB |



Nuevo punto cero

- **A:** -O2 -march=native -funroll-loops.
- **B:** -O3 -march=native -funroll-loops.
- **C:** -O3 -march=native -funroll-loops.
- **D:** -Ofast -march=native -ffast-math -funroll-loops -floop-block



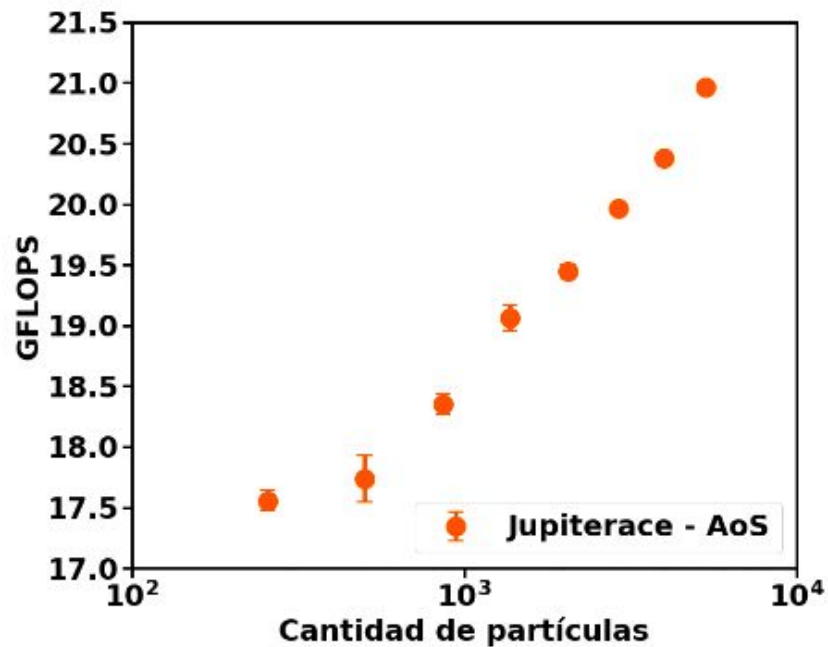
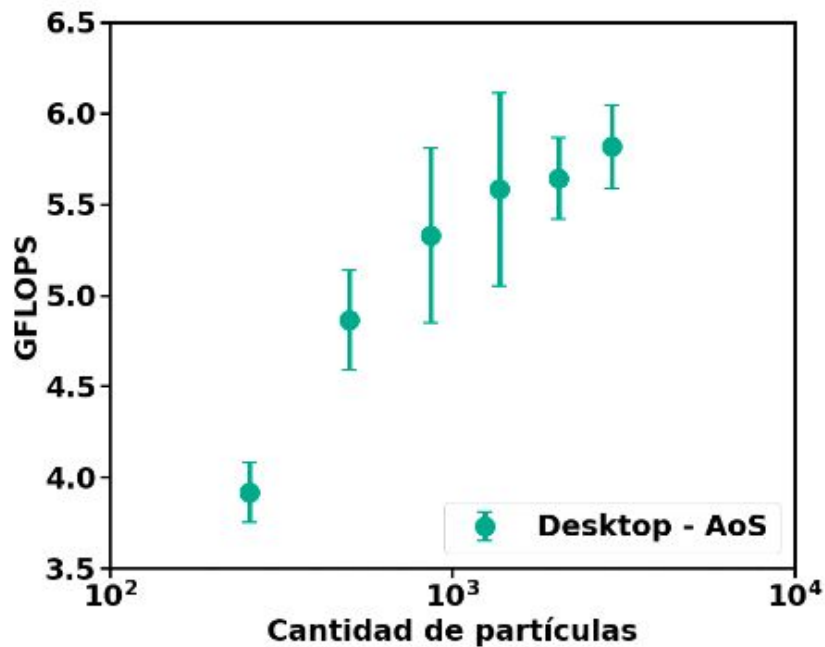
| Función | Desktop (-O0) | Jupiterace (-O0) | Jupiterace (D) |
|-----------------|---------------|------------------|----------------|
| Forces | 67.88 % | 68.19 % | 96.12 % |
| Minimum image | 29.44 % | 29.50 % | — |
| Velocity verlet | 0.90 % | 0.86 % | 0.35 % |




Nuevo punto cero

Cantidad de partículas:

2916 → 5324





AoS \rightarrow SoA

```
fxyz[i + 0] += fr * rx;  
fxyz[i + 1] += fr * ry;  
fxyz[i + 2] += fr * rz;
```

```
fxyz[j + 0] -= fr * rx;  
fxyz[j + 1] -= fr * ry;  
fxyz[j + 2] -= fr * rz;
```

AoS

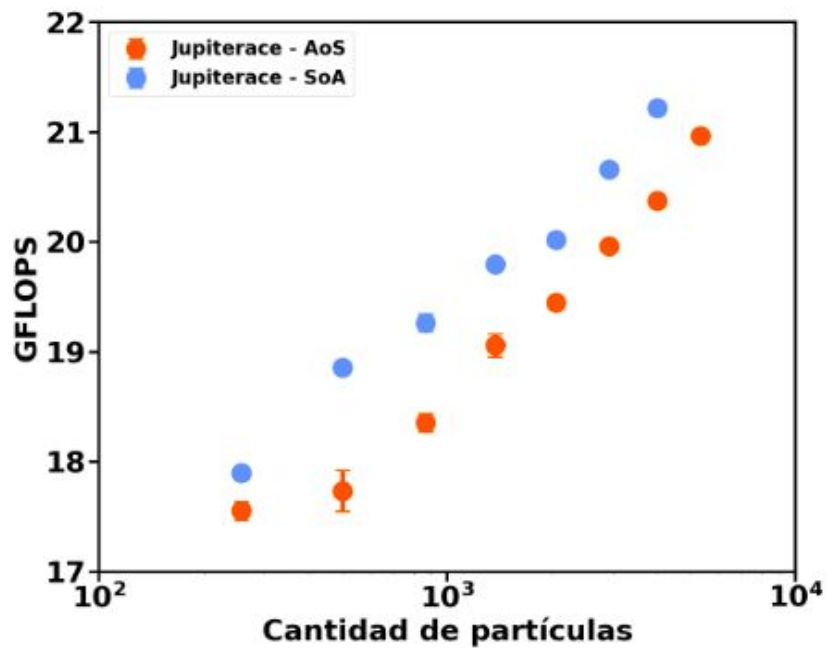
```
fxyz[i] += fr * rx;  
fxyz[i + N] += fr * ry;  
fxyz[i + 2*N] += fr * rz;
```

```
fxyz[j] -= fr * rx;  
fxyz[j + N] -= fr * ry;  
fxyz[j + 2*N] -= fr * rz;
```

SoA



AoS \rightarrow SoA

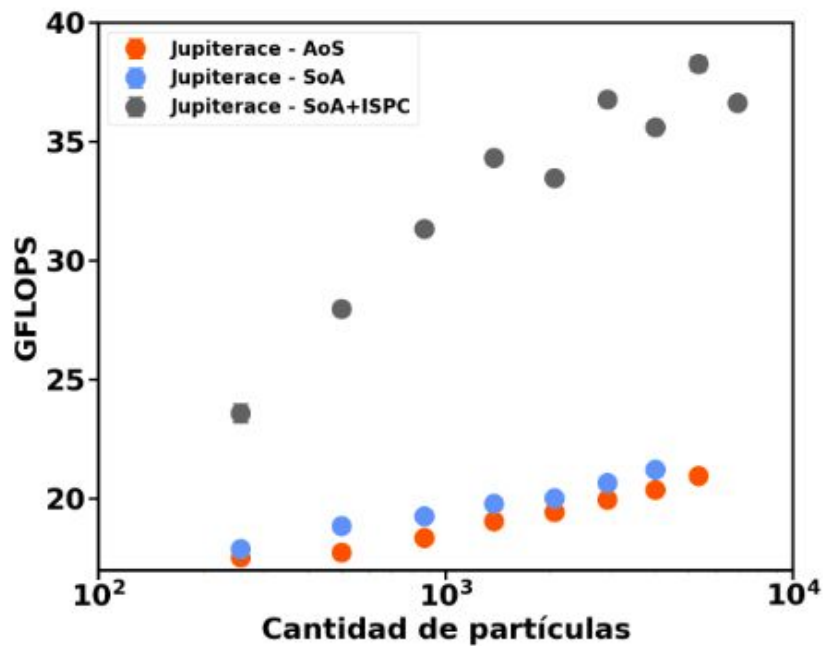




Vectorización con ISPC

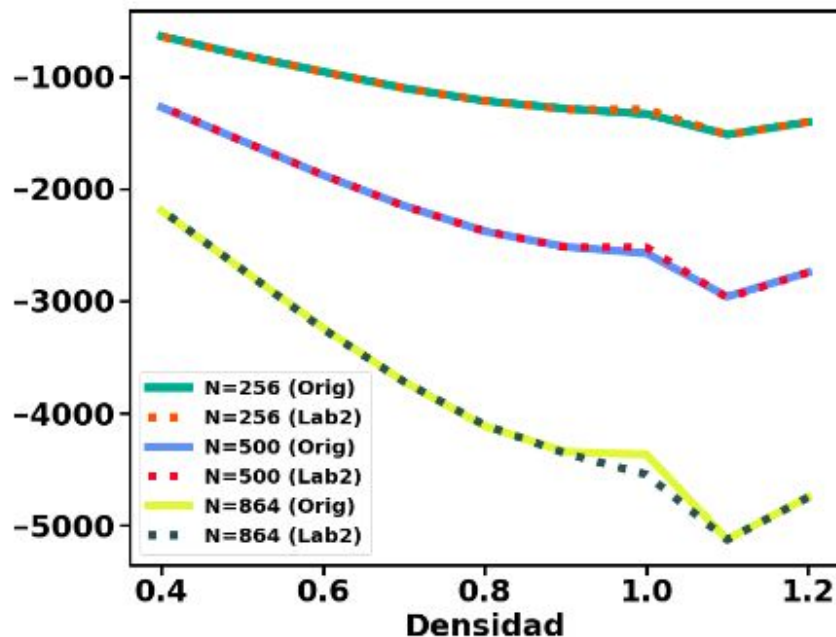
Cantidad de partículas:

5324 → 6912





Energía potencial: una segunda métrica



- **SoA ayuda a la autovectorización del compilador.**
- **SoA+ISPC mejoran en más de un 50 % los GFLOPS respecto a AoS**
- **2916 → 5324 → 6912**
- **El código no se ha roto**