### Lab 1 - Tiny MD

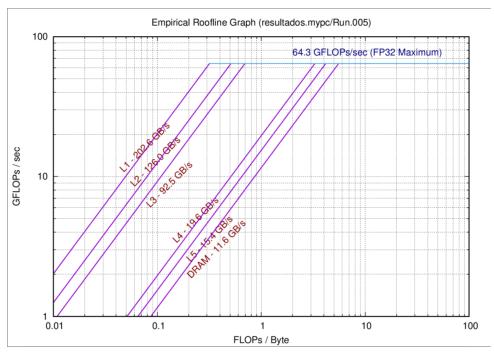
Fernando Blanco Ignacio J. Chevallier-Boutell

# Detalles Computacionales

Se utilizó un procesador Intel Core i5-4460:

- Microarquitectura Haswell.
- Disponibilidad de 4 núcleos.
- Frecuencia de 3,20 GHz.
- Caché de 6 MB.
- RAM de 8GB, 1600 MT/s
- Ubuntu 20.04.1 LTS, kernel 5.4.0-72-generic.

# Medidas Empiricas

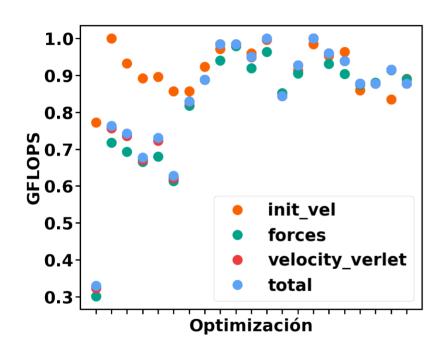


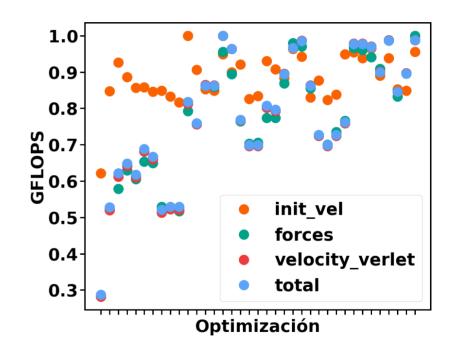
- Poder de computo de un core: 64.3 GFLOPs/sec
- Ancho de banda para un core: 11.6GB/s

# Profiling

```
Samples: 75K of event 'cycles', Event count (approx.): 61223703386
Overhead Command Shared Object
                                Symbol
        tiny md tiny md
                          [.] forces
 67,88%
 29,44%
        tiny md tiny md
                         [.] minimum image
                                [.] velocity verlet
  0.90%
        tiny md tiny md
        tiny md libc-2.31.so [.] GI printf fp l
  0,54%
  0,23% tiny md tiny md
                                [.] main
        tiny md
                [unknown]
                                 [k] 0xfffffffffab9167fe
  0,18%
```

### Clang - Gcc





## Optimizaciones usadas

- Optimizaciones
- -O1
- -02
- -O3
- Ofast

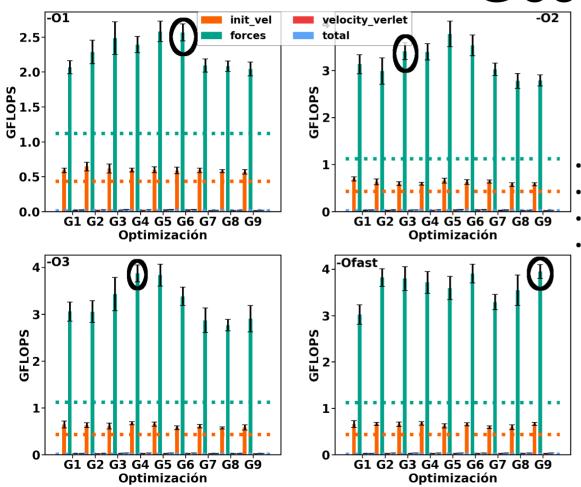
- Flags
- -march=native
- -ffast-math
- -funroll-loops
- -floop-block

### Clang 2.5-01 init vel velocity verlet forces total 2.0 2.5 S 1.5 GFLOPS 1.5 1.0 0.5 0.5 0.0 0.0 C1 C<sub>2</sub> **C3** C4 C<sub>2</sub> **C**3 C4 C5 Optimización Optimización 3.5 -Ofast -03 3.5 3.0 3.0 2.5 2.5 SHOPS 2.0-1.5-Second 2.0 1.0 0.5 0.5 0.0 0.0 **C3** C4 C5 **C**3 **C**5 C2 C2 C4 Optimización Optimización

Mejores resultados con clang

- -O1 -march=native -funroll-loops
- -O2 -march=native -funroll-loops
- -O3 -march=native -funroll-loops
- -Ofast -march=native -ffast-math -funroll-loops

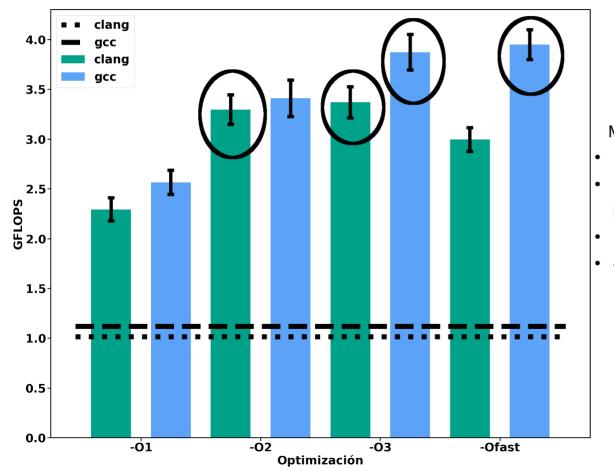




Mejores resultados con gcc

- -O1 -march=native -ffast-math -funroll-loops
- -O2 -march=native -ffast-math
- -O3 -march=native -funroll-loops
- -Ofast -march=native -ffast-math -funroll-loops -floop-block

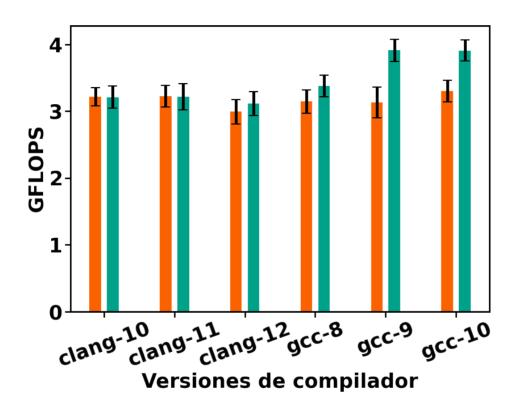
# Comparaciones de mejores flags



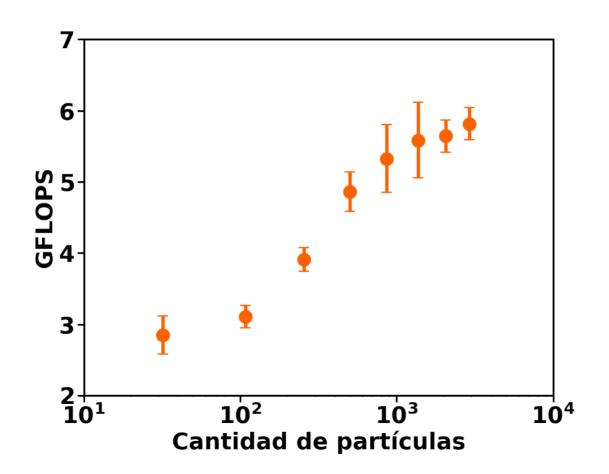
Mejores resultados con clang

- -O2 -march=native -funroll-loops
- -O3 -march=native -funroll-loops
   Mejores resultados con gcc
- -O3 -march=native -funroll-loops
  - -Ofast -march=native -ffast-math -funroll-loops -floop-block

## Distintas versiones de compiladores



## Distintos números de particulas



### Conclusiones

- Gcc nos dio mejores resultados
- Las versiones 9 y 10 de este no da mejores performance
- GFLOPS resultó ser una buena metrica