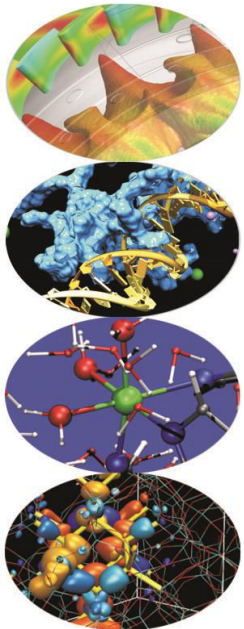
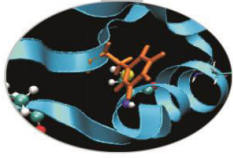


# Overview of applications performance on Marconi

*SCAI User Support team*



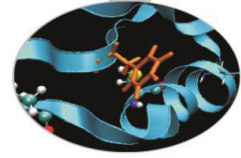


# We would like to:

- Try to “quantify” the technological trend via benchmarks...
- ...and use them to ***understand application performance issues, limitations and best practices on actual (Broadwell) and future architectures (KNL)***

## CAVEAT

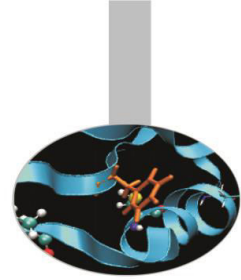
- ✓ All measurements was taken using HW at CINECA
- ✓ Sometimes there is an “unfair” comparison e.g.:
  - Sandy Bridge HW used was very “powerful”, HPC oriented
  - Ivy Bridge HW used was devoted to “data crunching”, not HPC oriented



# Tick/Tock

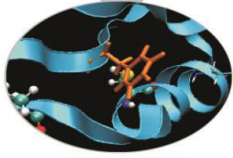
## Intel CPU roadmap: two step evolution

- Tock phase:
  - ✓ New architecture
  - ✓ New instructions (ISA)
  
- Tick phase:
  - ✓ Keep previous architecture
  - ✓ New technological step (e.g. Broadwell → 14nm)
  - ✓ Core “optimization”
  - ✓ Usually increasing core number, keeping Thermal Dissipation (TDP) constant



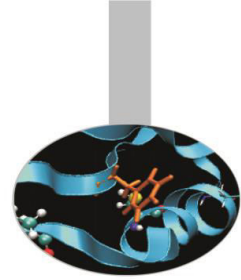
## Intel Xeon architectures evolution @ CINECA

- **Westmere (tick, a.k.a. plx.cineca.it)**
  - Intel(R) Xeon(R) CPU E5645 @2.40GHz, 6 Core per CPU
  - Only serial performance figure
- **Sandy Bridge (tock, a.k.a. eurora.cineca.it)**
  - Intel(R) Xeon(R) CPU E5-2687W 0 @3.10GHz, 8 core per CPU
  - Serial/Node performance figure
- **Ivy Bridge (tick, a.k.a. pico.cineca.it)**
  - Intel(R) Xeon(R) CPU E5-2670 v2 @2.50GHz, 10 core per CPU
  - Serial/Node/Cluster performance
  - Infiniband FDR
- **Haswell (tock, a.k.a. galileo.cineca.it)**
  - Intel(R) Xeon(R) CPU E5-2630 v3 @2.40GHz, 8 core per CPU
  - Serial/Node/Cluster performance
  - Infiniband QDR
- **Broadwell (tick) "real" Marconi A1: 2.3 GHz, 18 core per CPU**
  - Intel(R) Xeon(R) CPU E5-2699 v4 @ 2.20GHz, 22 core per CPU
  - Serial/Node performance figure



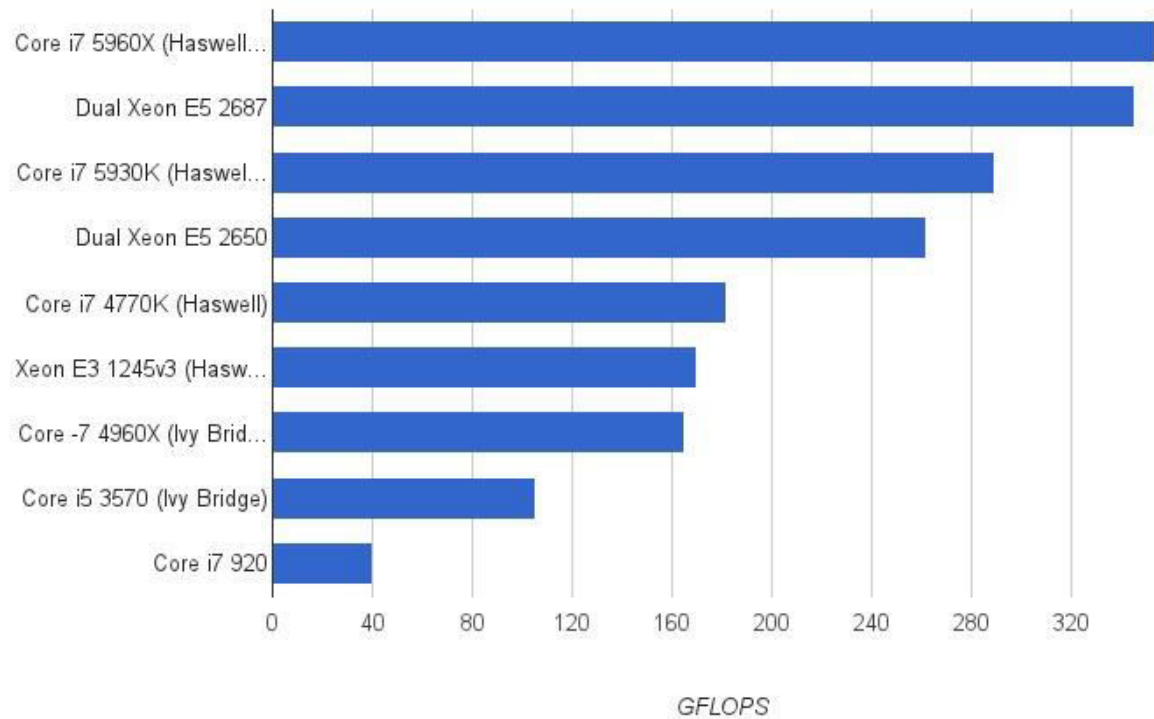
# Benchmark suites

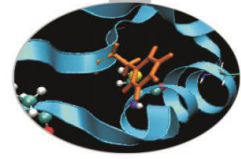
- Empirically tested on different HW at CINECA
  - **LINPACK**
    - Intel optimized benchmark, rel. 11.3
    - Stress Floating point performance, no Bandwidth limitation
  - **STREAM**
    - Rel. 3.6, OMP version
    - Bandwidth, no Floating point limitation
  - **HPCG**
    - Intel optimized benchmark, rel. 11.3
    - CFD oriented benchmark with Bandwidth Limitation



# Benchmarks

Linpack Benchmark from Intel MKL

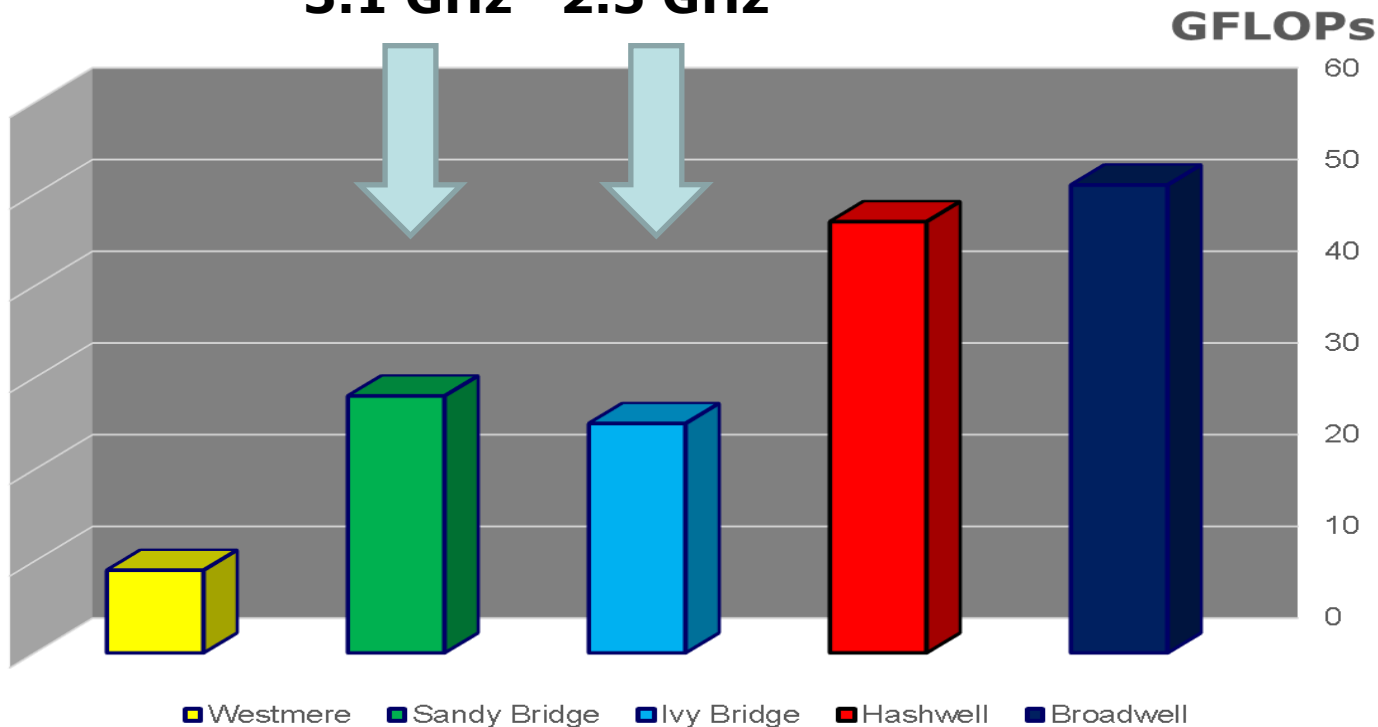


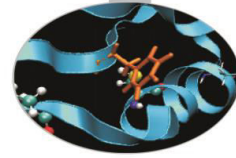


# LINPACK

- Best result obtained, single core
- ✓ 5.6x increase in 6 years (Q1-2010, Q1-2016)

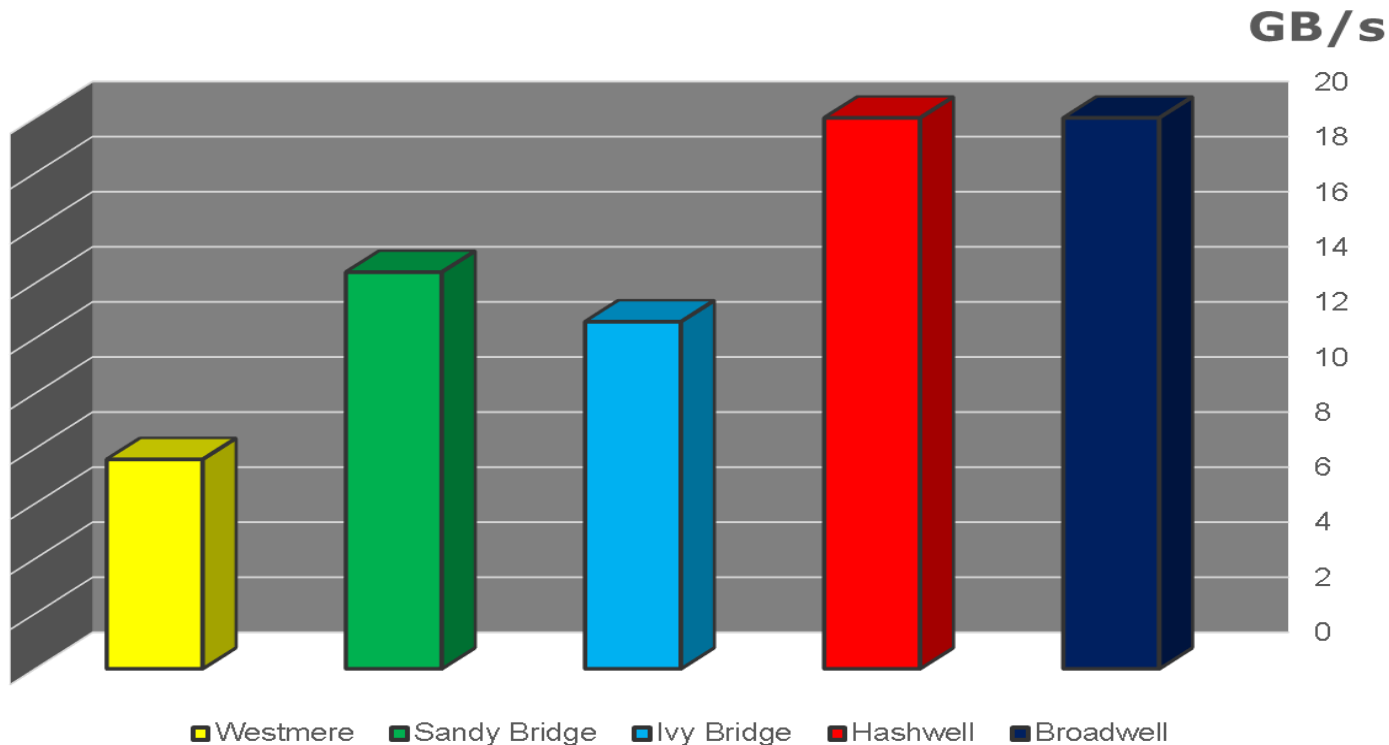
**3.1 GHz    2.5 GHz**



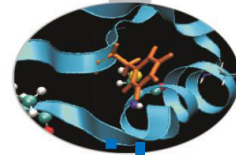


# STREAM

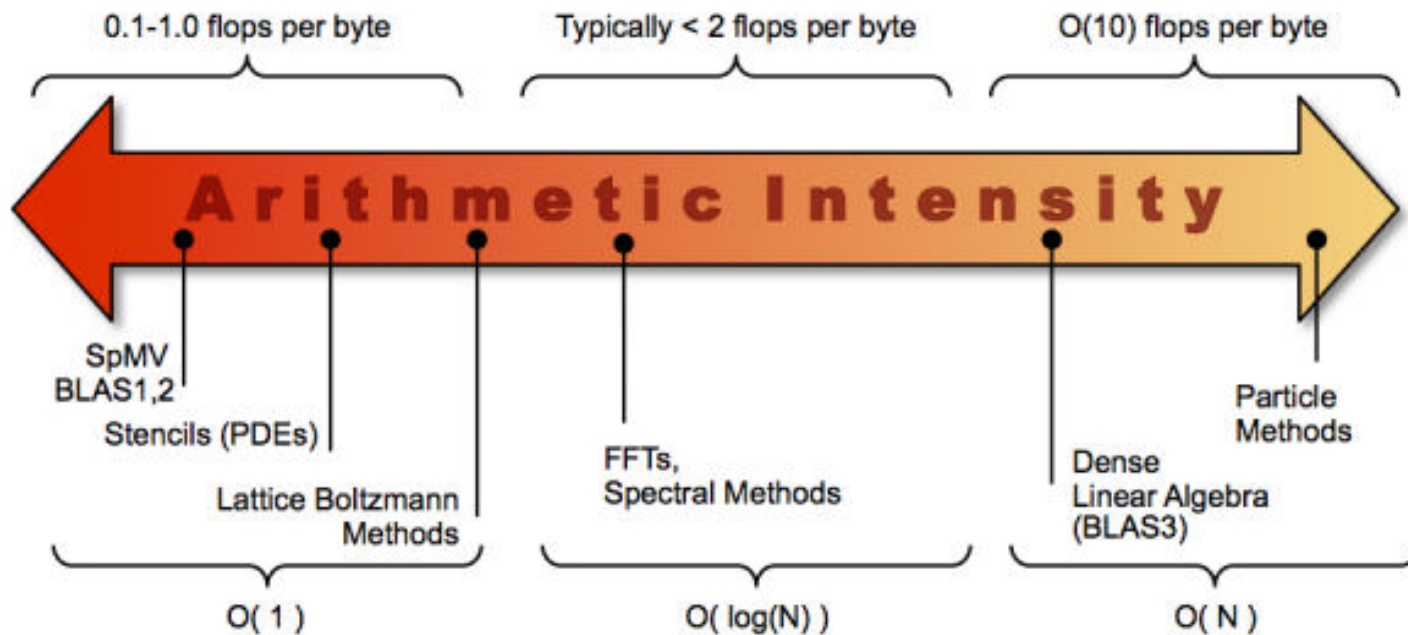
- Best result obtained (using intel/gnu), single core
- 2.6x speed-up in 6 years



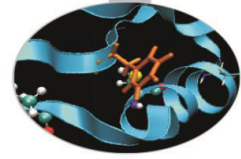




# Roofline Model: Arithmetic Intensity



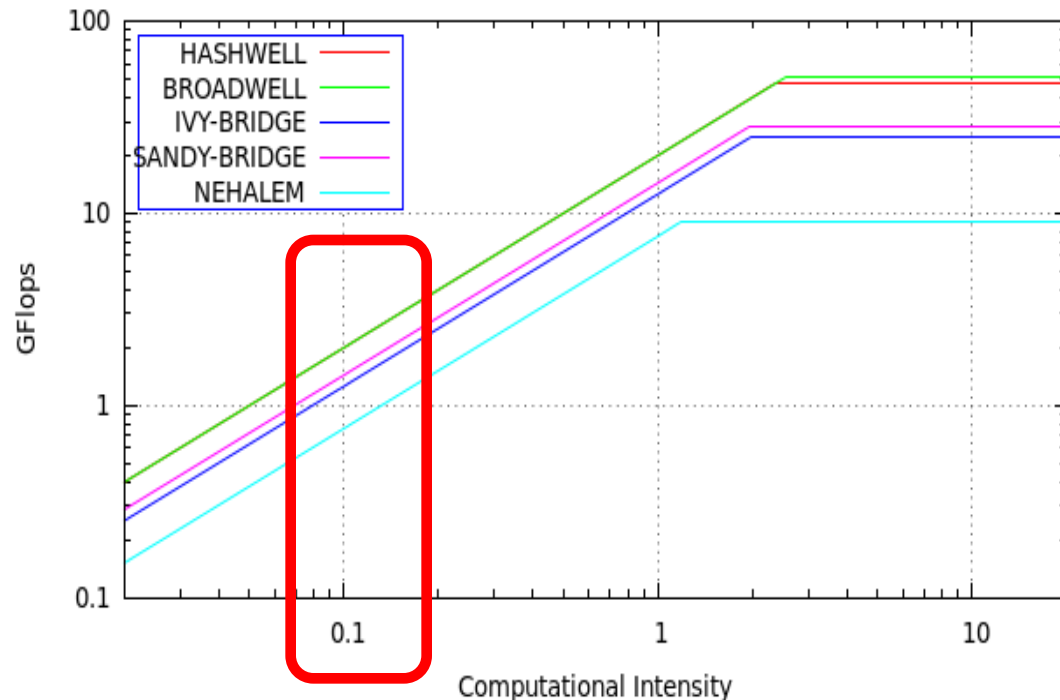
- Which is the typical application arithmetic intensity?
- About 0.1, may be less...
- It depends on application domain, solver, method,...

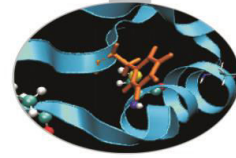


# Roofline Mode: serial case

- Using the results obtained on different HW (LINPACK, STREAM)

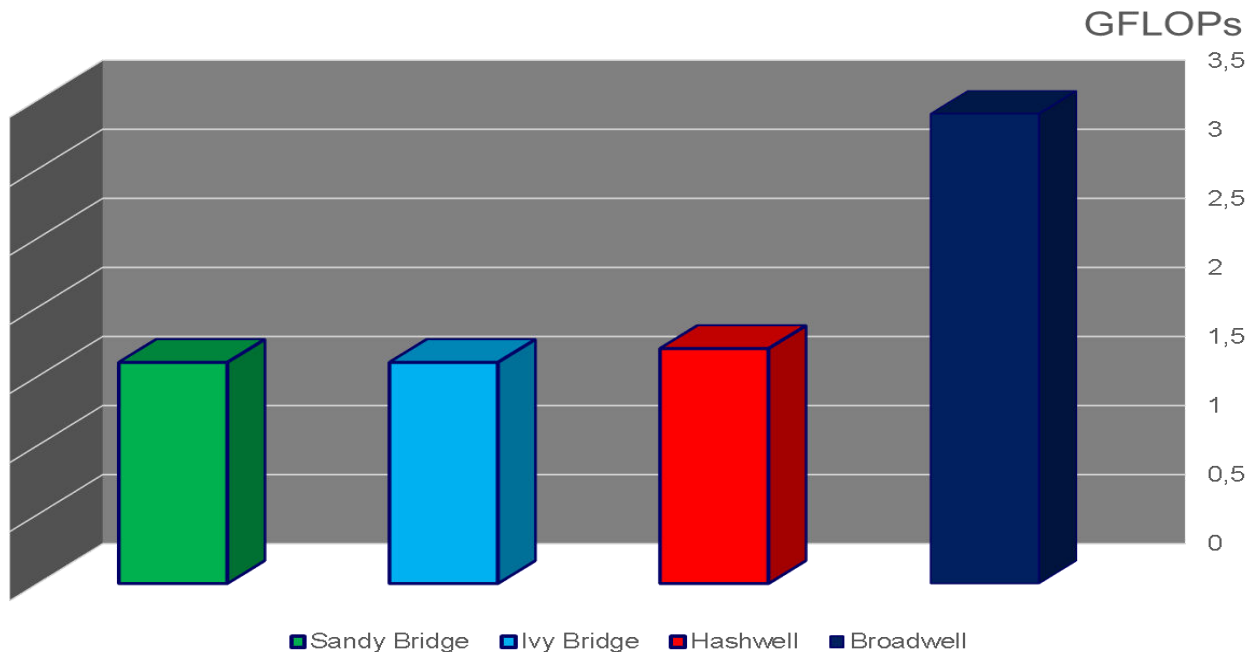
GFLOP vs Computational Intensity (single core)

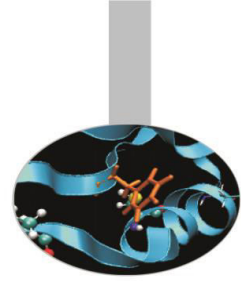




# HPCG

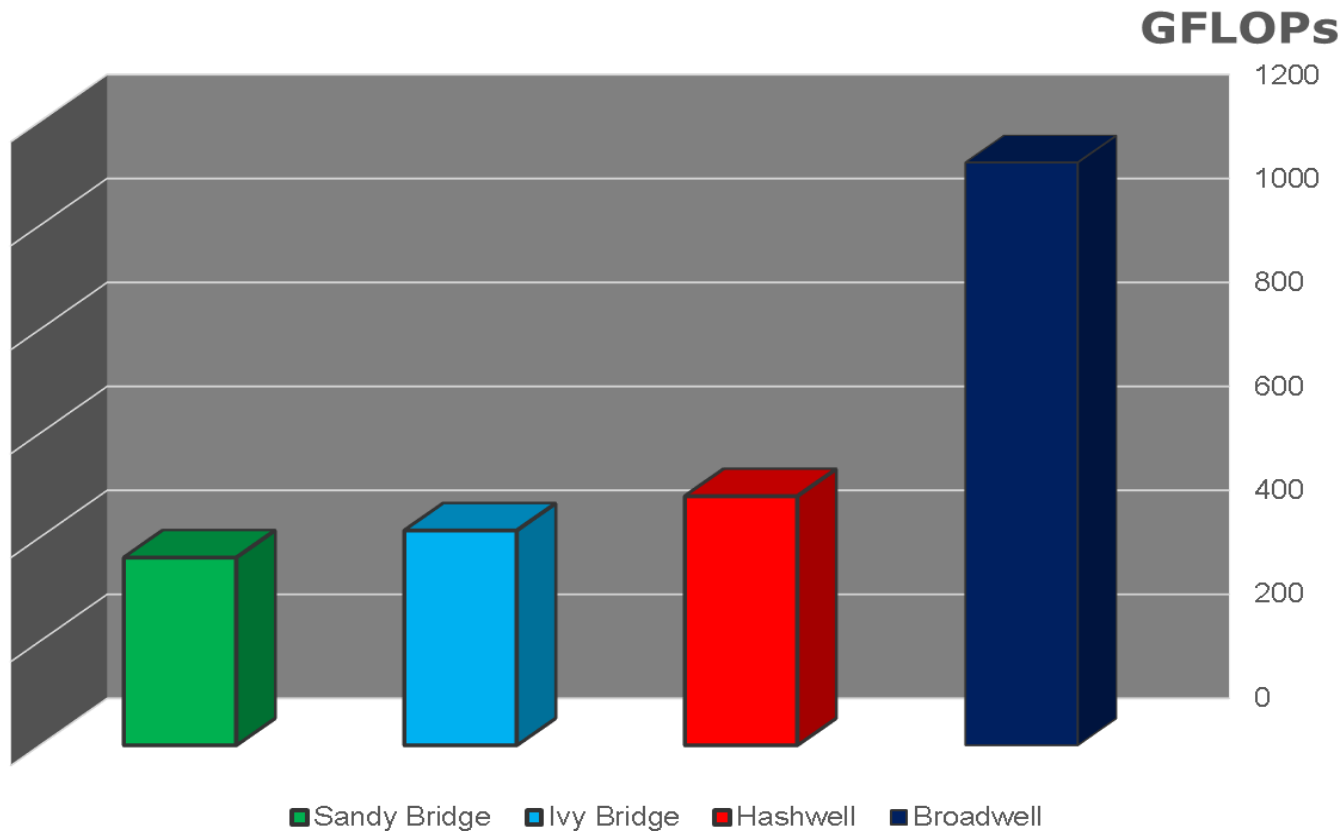
- Conjugate Gradient Benchmark (<http://hpcg-benchmark.org/>)
- Intel benchmark: Westmere not supported
- 2x speed-up for Broadwell

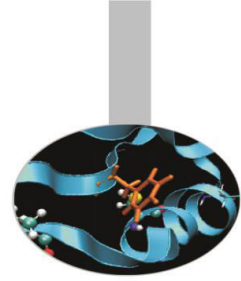




# LINPACK parallel results

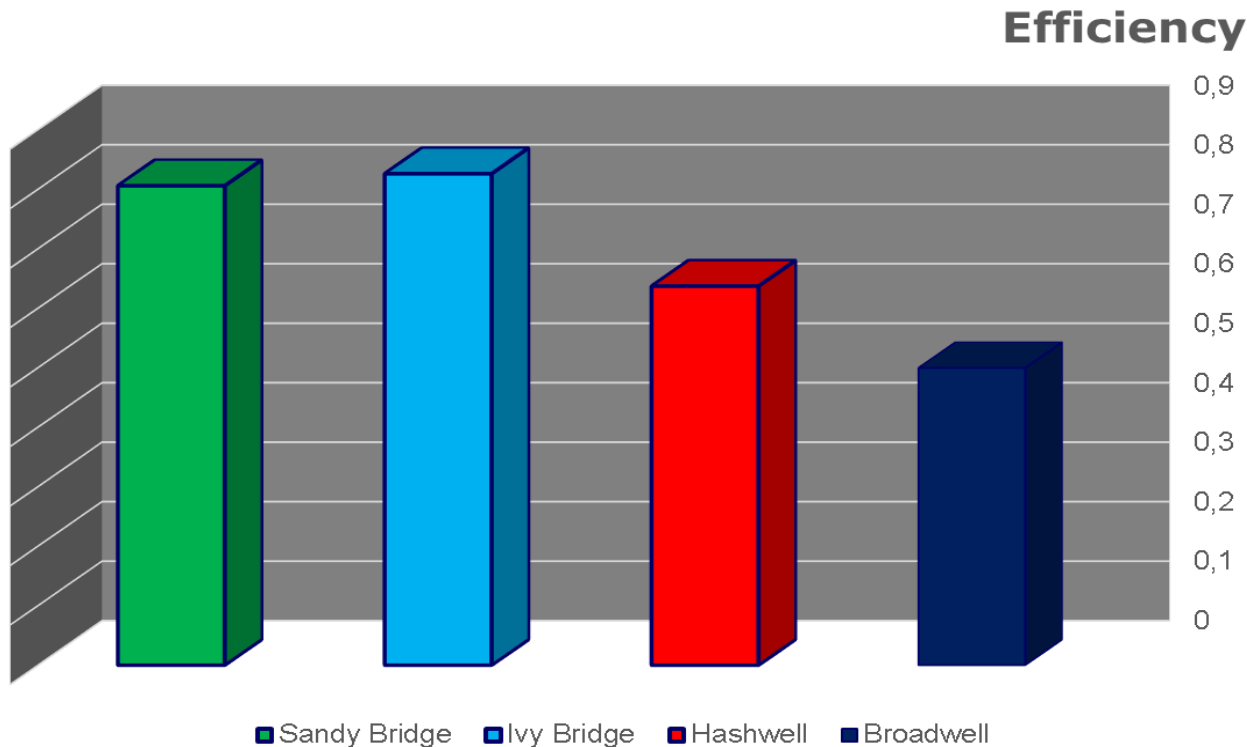
- Best result obtained

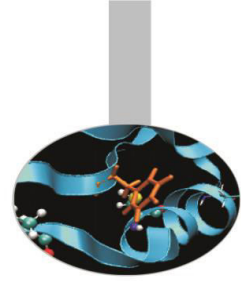




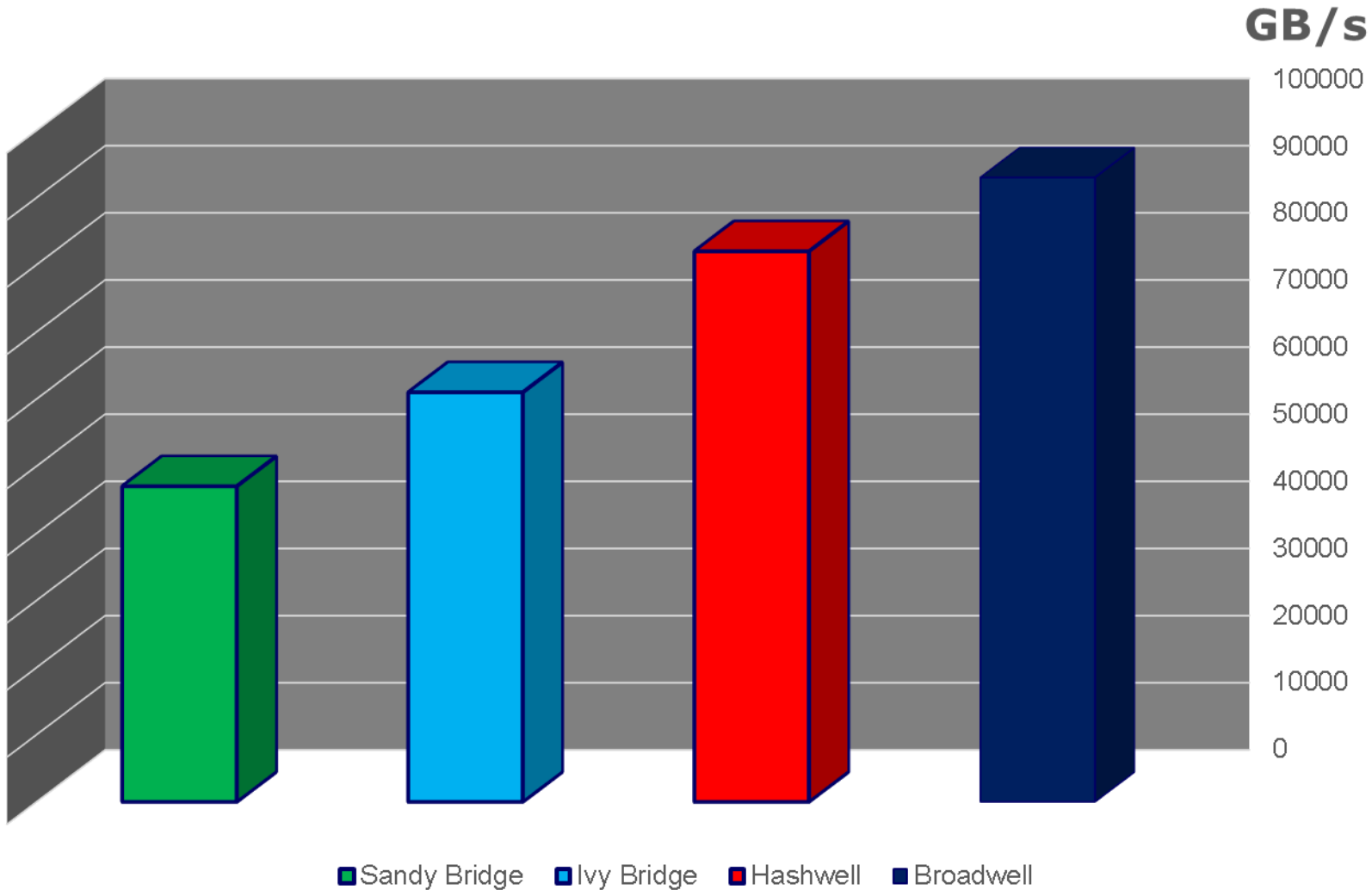
# LINPACK parallel results/2

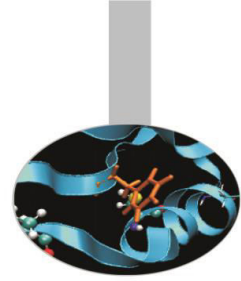
- Best result obtained
- Efficiency =  $\text{Parallel\_Flops} / (\# \text{core} * \text{Serial\_Flops})$ 
  - 1  $\rightarrow$  Linear speed-up





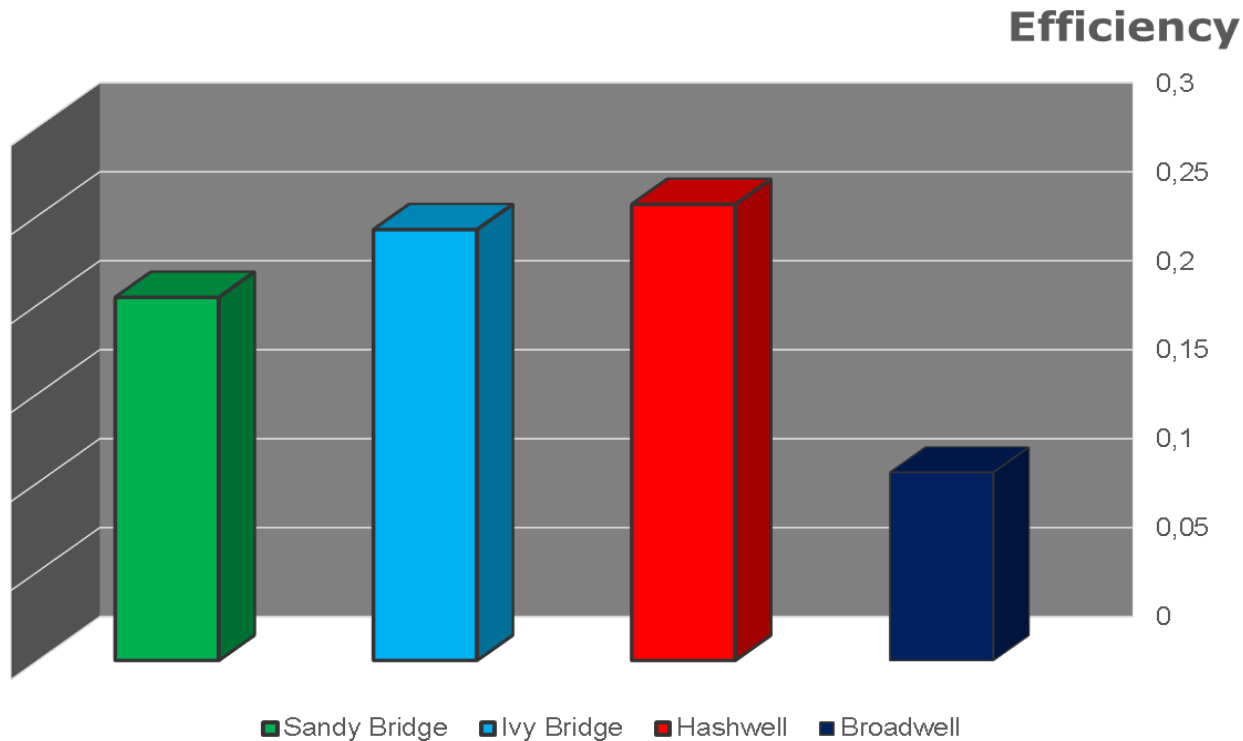
# STREAM parallel results

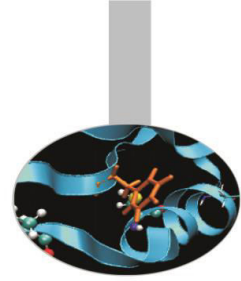




# STREAM parallel results/2

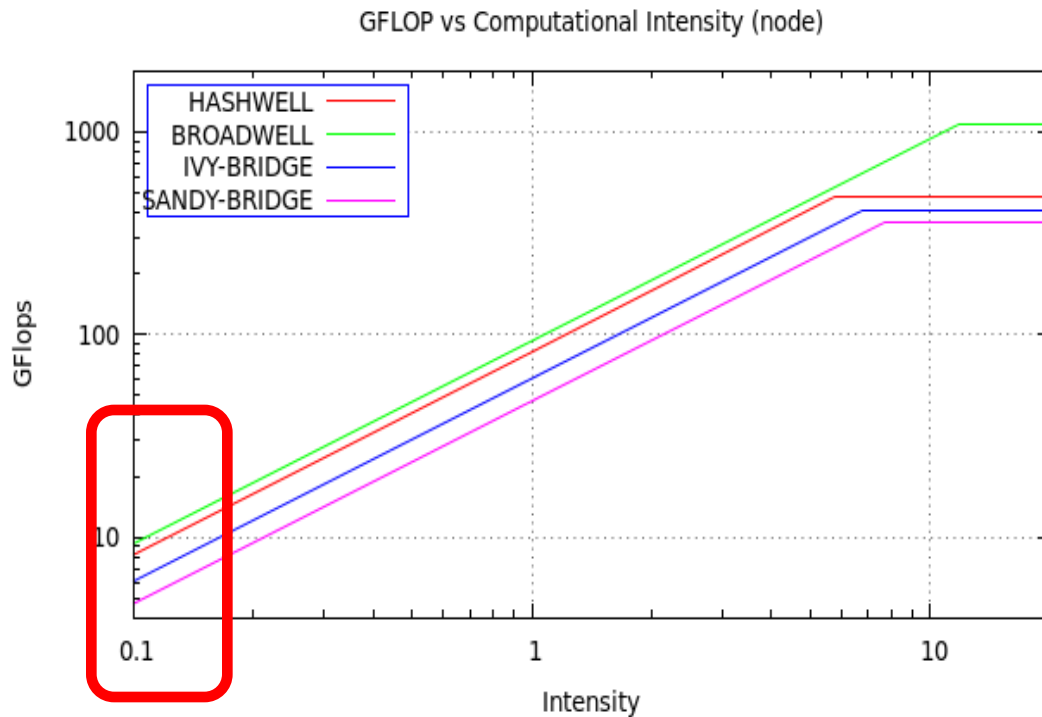
- Best result obtained (intel/gnu compiler)
- Efficiency =  $\text{Parallel\_BW} / (\# \text{core} * \text{Serial\_BW})$ 
  - 1  $\rightarrow$  Linear Speed-up



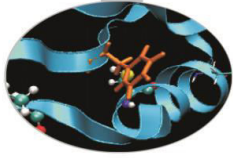


# Roofline: parallel graph

- Using the results obtained on different HW (LINPACK, STREAM)

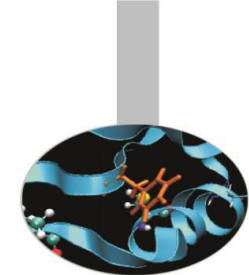




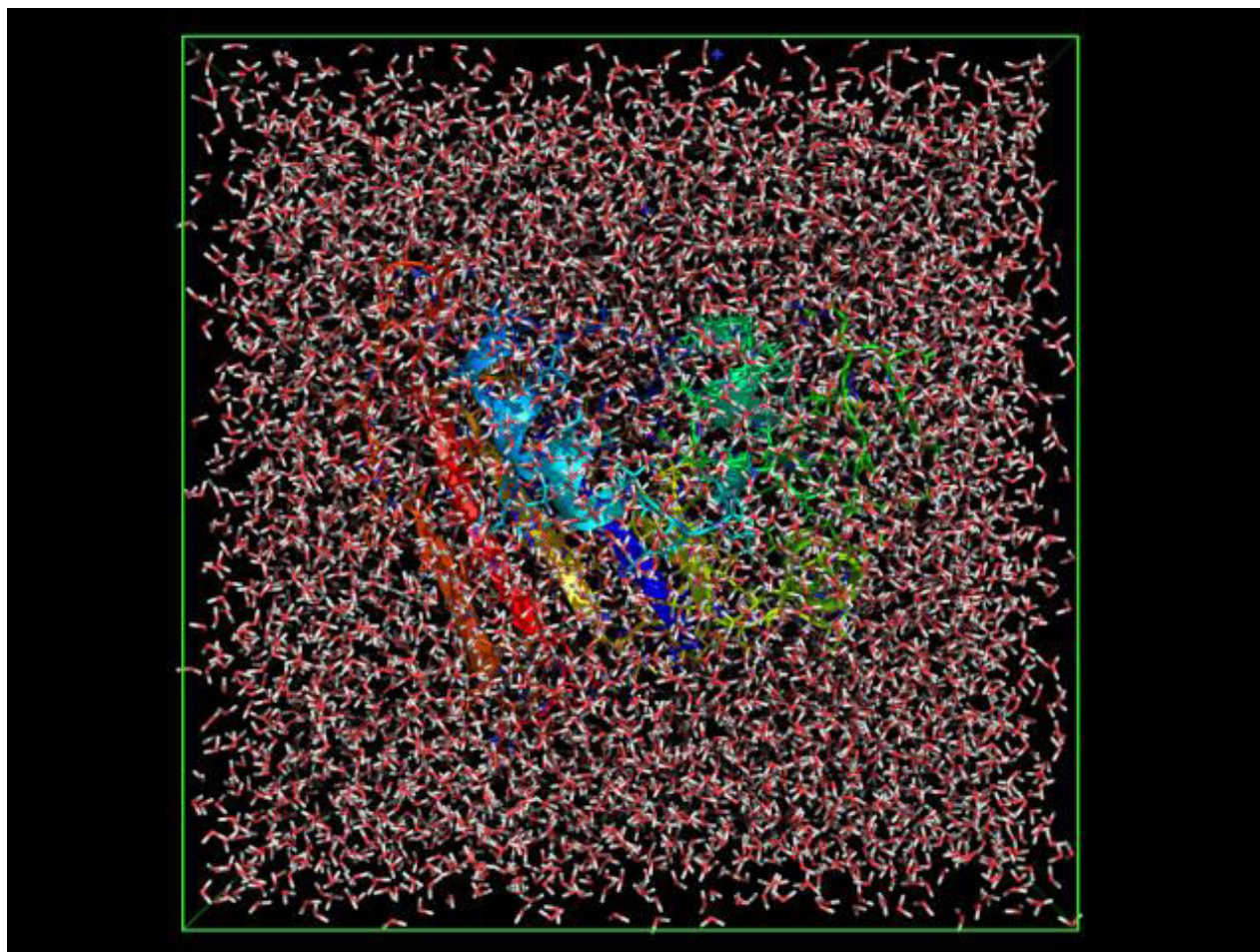


# Intel Turbo mode

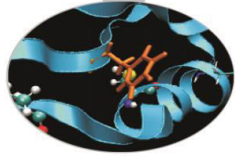
- i.e. Clock increase
- From Haswell the increase depends on the number of the core involved
- For CINECA Haswell:
  - ✓ Core 1,2: 3.2 GHz
  - ✓ Core 3: 3.0 GHz
  - ✓ Core 4: 2.9 GHz
  - ✓ Core 5: 2.8 GHz
  - ✓ Core 6: 2.7 GHz
  - ✓ Core 7: 2.6 GHz
  - ✓ Core 8: 2.6 GHz



# Molecular Dynamics



# Using MD on Marconi – Phase I



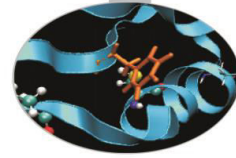
## Phase 1: Broadwell nodes

- Similar to Haswell cores present on Galileo.
- Expect only a small difference in single core performance wrt Galileo, but a big difference compared to Fermi.
- More cores/node (36) should mean better OpenMP performance (e.g. for Gromacs) , but also MPI performance will improve (faster network).
- Life much easier for MD programmers and users.



cores/node	36
Memory/node	128 GB

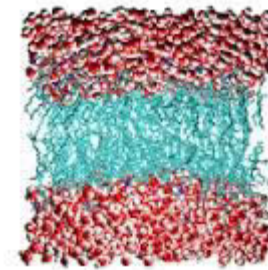
# MD Broadwell benchmarks



## *Gromacs DPPC (1 core)*

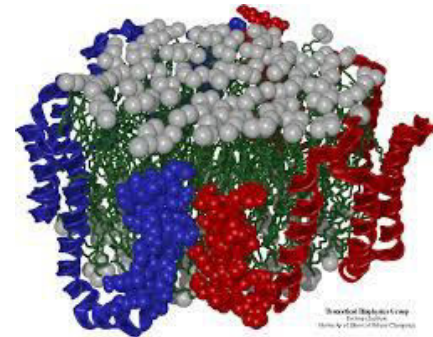
Computer system	ns/day	Speedup wrt Fermi
Haswell (5.0.4, Galileo)	1.364	13.64
Fermi (5.0.4)	0.100	1.00
Broadwell (5.1.2)	1.977	19.77

Based on a 1-node Broadwell partition (40 cores, hyperthreading on).

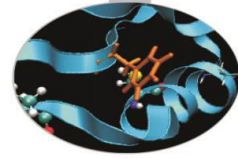


## *NAMD APOA1 (16 tasks)*

Computer System	ns/day	Speedup wrt Fermi
Haswell (2.10, Galileo)	1.425	7.27
Fermi (2.10)	0.196	1.00
Broadwell (2.11)	1.516	7.73



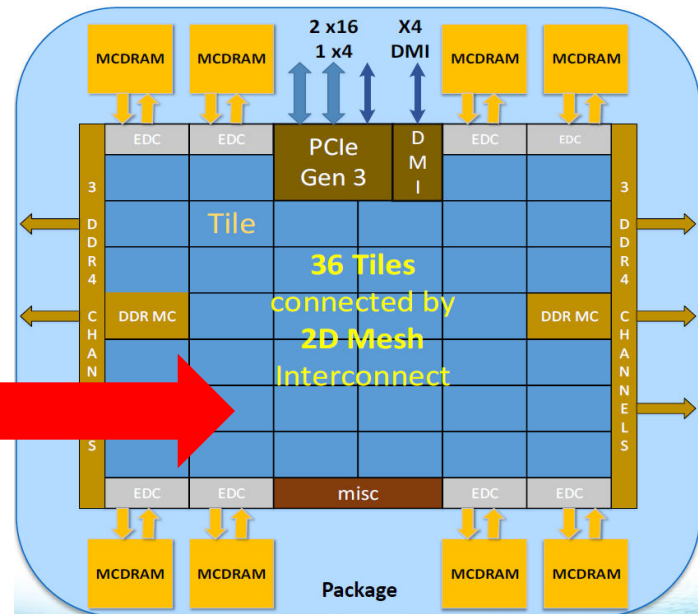
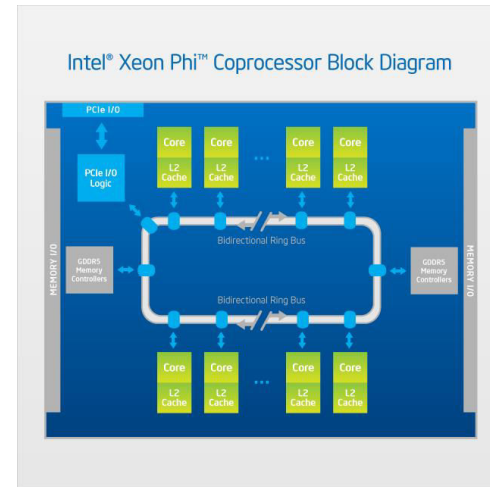
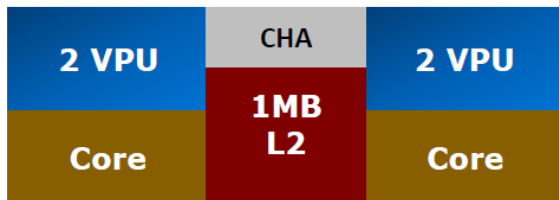
# Using MD on Marconi – Phase II



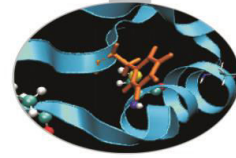
## Phase 2: Knights Landing (KNL)

- A big unknown because very few people currently have access to KNL.
- But we know the architecture of KNL and the differences and similarities with respect to KNC.
- The main differences are:

- KNL will be a **standalone** processor not an accelerator (unlike KNC)
- KNL has more powerful cores and faster internal network.
- On package high performance, memory (16Gb, MCDRAM).



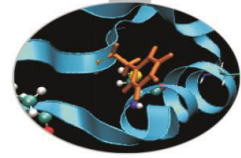
# Xeon Phi KNC-KNL comparision



	KNC (Galileo)	KNL (Marconi)
#cores	61 (pentium)	68 (Atom )
Core frequency	1.238 GHz	1.4 Ghz
Memory	16Gb GDDR5	96Gb DDR4 +16Gb MCDRAM
Internal network	Bi-directional Ring	Mesh
Vectorisation	512 bit /core	2xAVX-512 /core
Usage	Co-processor	Standalone
Performance (Gflops)	1208 (dp)/2416 (sp)	~3000 (dp)
Power	~300W	~200W

A KNC core can be 10x slower than a Haswell core. A KNL core is expected to be 2-3X slower. Big differences also in memory bandwidth.

# Using MD on Marconi-Phase II



🔧 Programmers must utilise vectorisation (SIMD) and OpenMP threads, and possibly the fast memory of KNL.

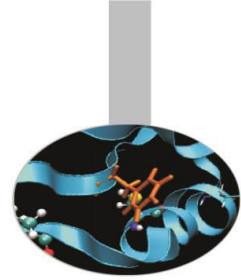
🔧 For the user, MD performances will depend on how software developers are able to exploit the KNL architecture:

🔧 **NAMD**. Already reasonable results with KNC. According to NAMD mailing list much effort being devoted to KNL version.

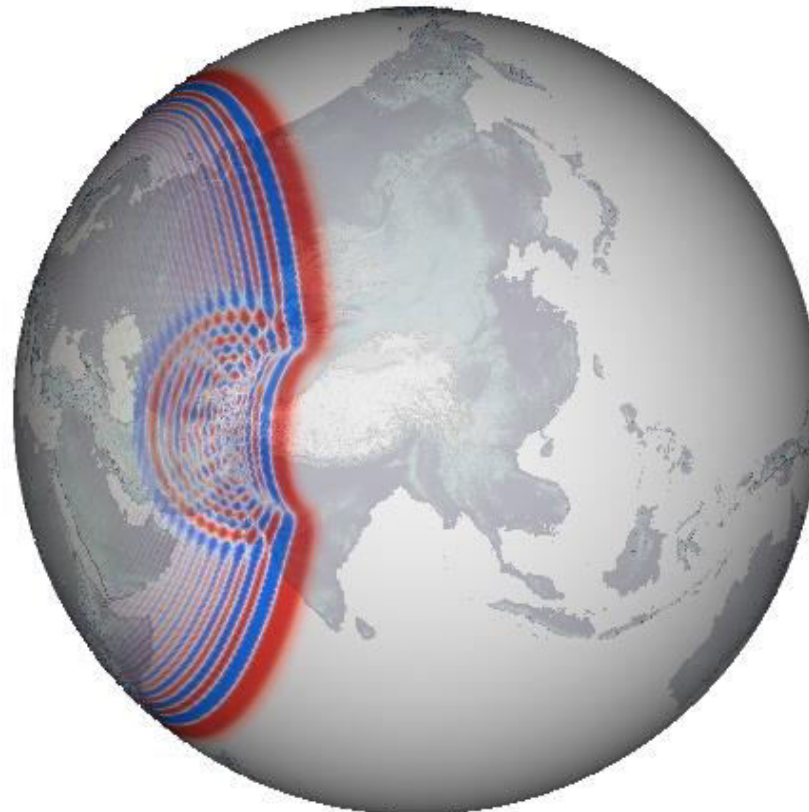
🔧 **GROMACS**. Developers didn't really bother with KNC Xeon Phi's (no offload version and poor symmetric mode). But since KNL is standalone and Gromacs can use OpenMP threads (which are advisable on KNL) should run well on KNL. Also GROMACS has good SIMD optimisation.

🔧 **Amber**. Already support for KNC and with OpenMP probably should be ok for KNL.

Worth noting that up to now KNC MICs haven't been widely supported by software developers. But this should change for KNL.

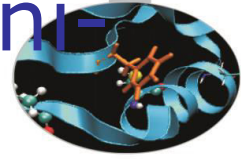


# Global Seismology



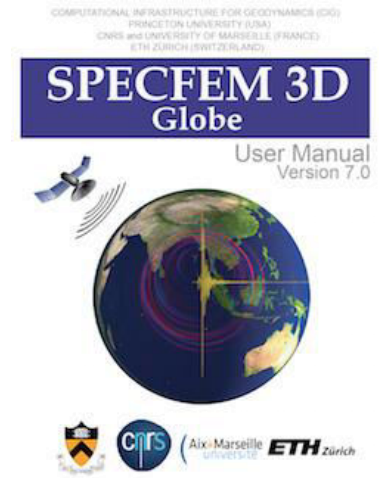


# Global seismology activity on Marconi- Phase II



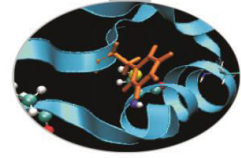
- Global seismology developers must utilise vectorisation (SIMD) and OpenMP threads, and possibly the fast memory of KNL.
- For the user, global seismology experience will depend on how software developers are able to exploit the KNL architecture:

- SPECFEM3D\_GLOBE**. Already reasonable results with KNC (“native” and “offload” version in the framework of the IPCC@CINECA activity). Good amount of vectorisation (FORCE\_VECTORIZATION preprocessing enabling ) and SIMD optimization suitable for KNC and future KNL. High number of OpenMP threads scaling (up to more than 60 on KNC)



Worth noting that up to now KNC MICs haven't been widely supported by Global seismology software developers and users. A remarkable exception is SPECFEM3D\_GLOBE software CIG repo where the “native” version is maintained and tested. Again, this should be fine for KNL startup.

# Global seismology benchmarks



*SPECFEM3D\_GLOBE Regional\_MiddleEast test case: forward simulation*

Computer system	e.t. (sec.)	Speedup wrt Haswell
Haswell (Galileo)	570.20	1.00
KNC (Galileo)	430.35	1.32

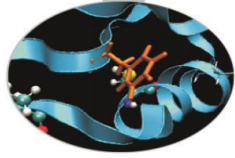
Based on a 4-node Galileo partition (16 MPI processes, 4 and 60 OpenMP threads on Haswell and KNC respectively).

*SPECFEM3D\_GLOBE Regional\_MiddleEast test case: no vectorisation*

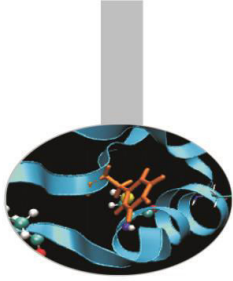
Computer System	e.t. (sec.)	Slowdown factor wrt vectorised
Haswell (Galileo)	687.14	1.20
KNC (Galileo)	848.12	1.97 <b>&lt;- 2x Slowdown factor</b>

The impact of vectorisation: on Haswell and KNC respectively).

# Conclusions



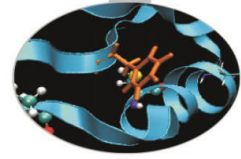
- Marconi A1 Broadwell
- “Standard” increase of performances wrt the chip evolution phase
- Bandwidth grows more slowly
  
- High expectations of Marconi A2 KNL performances
- KNC paves the way for increasing performances...
- ....try to manage domain parallelism, increase threading, exploit data parallelism (vectorisation) and improve data locality (new: use on package memory)



# Credits

- Giorgio Amati, Ivan Spisso (Benchmarks, CFD)
- Andrew Emerson (Molecular Dynamics)
- Vittorio Ruggiero (Global Seismology)

# Some Links



- TICK-TOCK: <http://www.intel.com/content/www/us/en/silicon-innovations/intel-tick-tock-model-general.html>
- WESTMERE: <http://ark.intel.com/it/products/family/28144/Intel-Xeon-Processor-5000-Sequence#@Server>
- SANDY BRIDGE: <http://ark.intel.com/it/products/family/59138/Intel-Xeon-Processor-E5-Family#@Server>
- IVY BRIDGE: <http://ark.intel.com/it/products/family/78582/Intel-Xeon-Processor-E5-v2-Family#@Server>
- HASHWELL: <http://ark.intel.com/it/products/family/78583/Intel-Xeon-Processor-E5-v3-Family#@Server>
- BROADWELL: <http://ark.intel.com/it/products/family/91287/Intel-Xeon-Processor-E5-v4-Family#@Server>
- LINPACK: <https://en.wikipedia.org/wiki/LINPACK>
- STREAM: <https://www.cs.virginia.edu/stream/ref.html>
- HPCG: <http://hpcg-benchmark.org/>
- ROOFLINE: <http://crd.lbl.gov/departments/computer-science/PAR/research/roofline/>
- TURBO MODE: [http://cdn.wccftech.com/wp-content/uploads/2016/03/Intel-Broadwell-EP-Xeon-E5-2600-V4\\_Non\\_AVX.png](http://cdn.wccftech.com/wp-content/uploads/2016/03/Intel-Broadwell-EP-Xeon-E5-2600-V4_Non_AVX.png)