

# QE dev meeting

Trieste - January, 14th

# Summary

- Cineca as IPCC
  - Porting of QE in native mode
  - Implementation of libxphi – offload mode
  - Status and perspectives
- Cineca infrastructure
  - PICO: a data-centric infrastructure
  - GALILEO: the replacement for PLX

# Native mode

## PW (SCF)

## Quantum ESPRESSO\* for Intel® Xeon Phi™ Coprocessor

Wed, Jun 4, 2014

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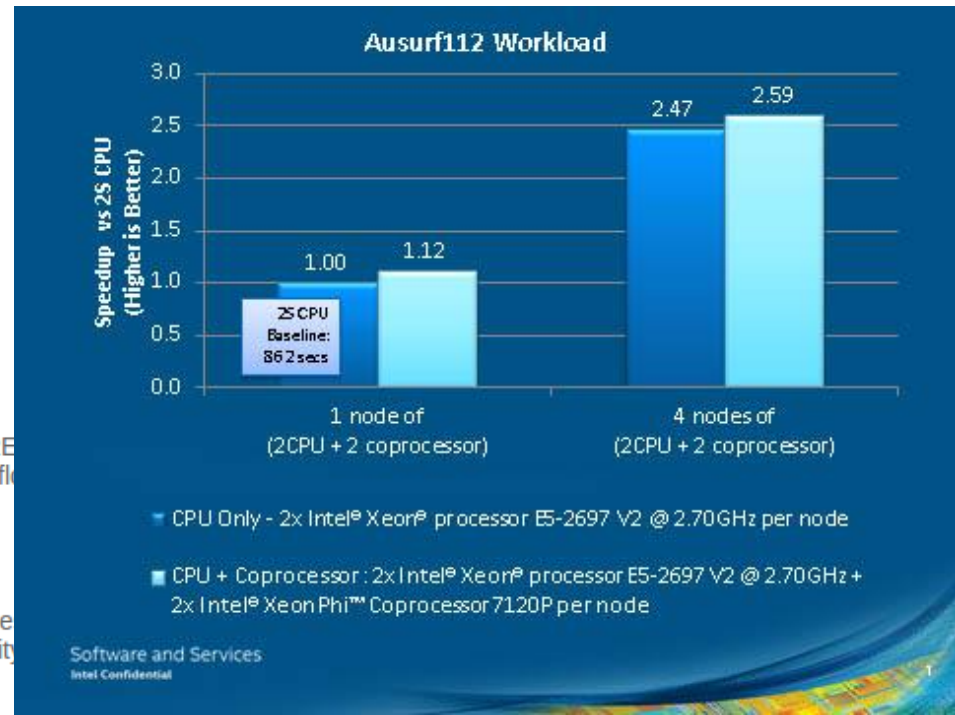


### Purpose

This code recipe describes how to get, build, and use the Quantum ESPRESSO Phi™ coprocessor using the Intel® Math Kernel Library with Automatic Offload.

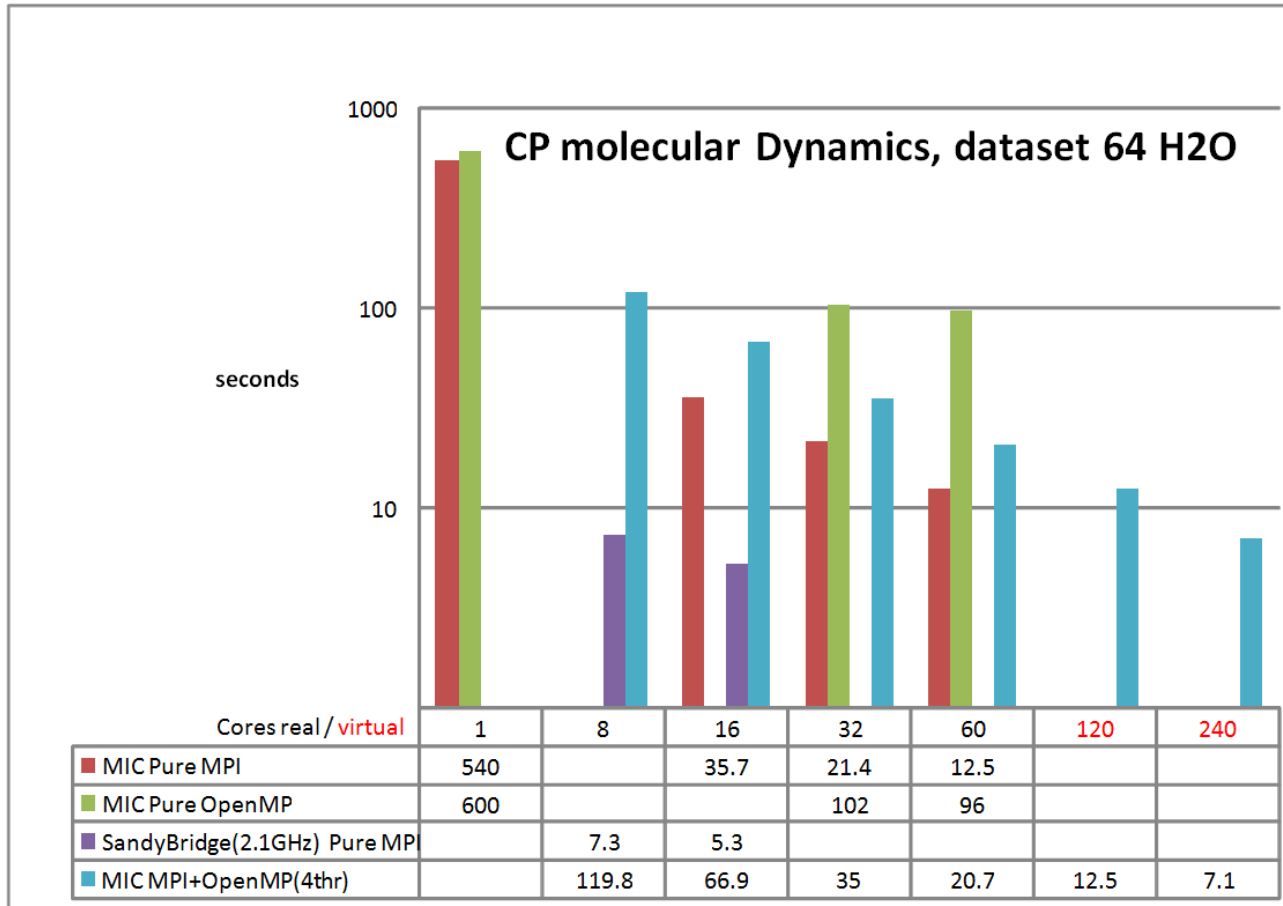
### Introduction<sup>1</sup>

Quantum ESPRESSO is an integrated suite of open source computer code calculations and materials modeling at the nanoscale. It is based on density functional theory, plane waves, and pseudo potentials.



# Native mode

## CP (Car-Parrinello)



In native mode it is also possible to use more than one Xeon PHI coprocessor at the same time, like if the parallel system were built using Xeon PHI alone. The good news is that the code works and it is really possible to run the application on more than one coprocessor, the bad news is that the performance are very bad due to communication latency and bandwidth limitation of the low level protocol used to communicate between coprocessor.

# DGEMM: Xlibphi

## Strategy:

- Implementation of a “double-buffer” technique to hide the latency between host and coprocessor
- Implemented through a dynamic library (plugin) that wraps the MKL function.

## Status:

- Currently available on github (<https://github.com/cdahnken/libxphi>)
- Currently working to the documentation and how-tos (submitting scripts, etc.)

Host: Xeon Sandy Bridge E2670

(2 sockets ->16 cores)

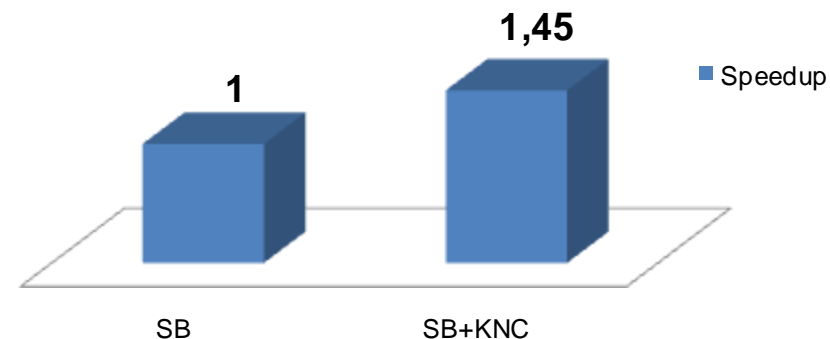
Coprocessor: KNC 7120

(2 cards -> 2x61 cores)

Ausurf 112:

Au complex 2,158,312 G-vectors, 2  
k-points, FFT dimensions =  
(180,90,288)

**Ausurf 112 workload  
112 atoms – 2 k-points**



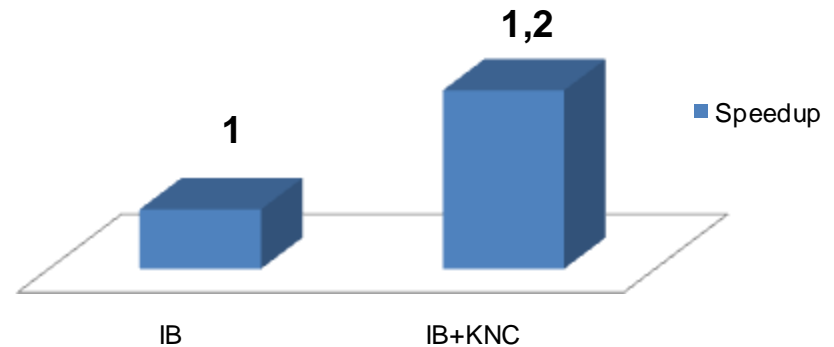
# Xlibphi – benchmarks

Host: Xeon Ivy Bridge E5-2697  
(2 x 12 cores)  
Coprocessor: KNC 7120 (2  
cards)

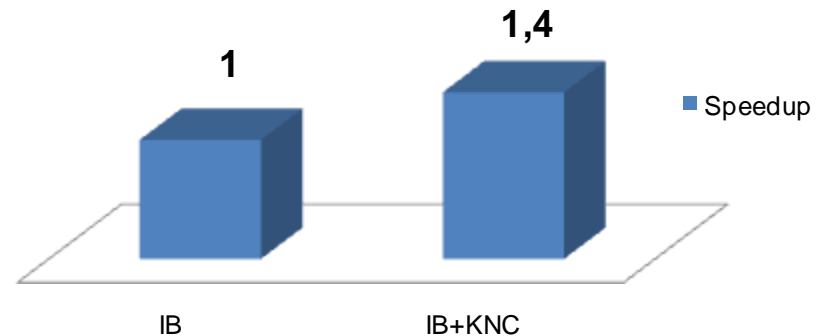
8 nodes equipped with:  
Host: Xeon Ivy Bridge E5-2697  
(2 x 12 cores)  
Coprocessor: KNC 7120 (2  
cards)

GRIR443:  
Carbon-Iridium complex (C<sub>200</sub>Ir<sub>243</sub>),  
2,233,063 G-vectors, 8 k-points, FFT  
dimensions: (180, 180, 192)

**Ausurf 112 workload**  
112 atoms – 2 k-points



**GRIR443 workload**  
443 atoms – 8 k-points



# Offloading FFT

FFT loop:

QE require to compute a 3D FFT for each electron of the system  
-> thousands of parallel 3D FFT are computed at each iteration

Strategy:

decompose the parallel 3D FFT in sequence of 1D FFTs  
explicitly manage (outside the FFT) the communication for data reshuffling  
offload the 1D FFTs to MIC  
implement software pipelining to mask data transfer latency

Status:

first working implementation completed

```
do ib=1,nbands
  3D fft
enddo
```



```
do ib=1,nbands
  fft along z
end do
mpi transpose
do ib=1,nbands
  fft along xy
enddo
```

Parallel 3D FFT driver  
fft along z  
Internal mpi transpose  
fft along xy



Parallel 1D driver  
Global Transpose driver  
Parallel 2D driver

(More memory requirements: 30% more)



## Next steps:

- To complete the FFT offload. Then testing and preparing docs
- Address the diagonalization part
- Look at the multinode scaling

# New Cineca infrastructure: PICO

A machine for data-analytics and post-processing.  
Already in production.



	Total Nodes	CPU	Cores per Nodes	Memory (RAM)	Notes
<b>Compute/login node</b>	66	Intel Xeon E5 2670 v2 @2.5Ghz	20	128 GB	
<b>Visualization node</b>	2	Intel Xeon E5 2670 v2 @ 2.5Ghz	20	128 GB	2 GPU Nvidia K40
<b>Big Mem node</b>	2	Intel Xeon E5 2650 v2 @ 2.6 Ghz	16	512 GB	1 GPU Nvidia K20
<b>BigInsight node</b>	4	Intel Xeon E5 2650 v2 @ 2.6 Ghz	16	64 GB	32TB of local disk

## New Cineca infrastructure: GALILEO

- Double socket Intel Xeon 2630 v3@2.4GHz, 8 cores each (“Haswell”)
- 524 nodes for a total number of 8384 cores
- 128 GB of RAM memory per node
- 768 Xeon Phi co-processor model 7120p
- 8 nodes for visualization
- Expected peak performance around 1PF

It replaces PLX and EURORA.

It will start production from early 2015 (February)

