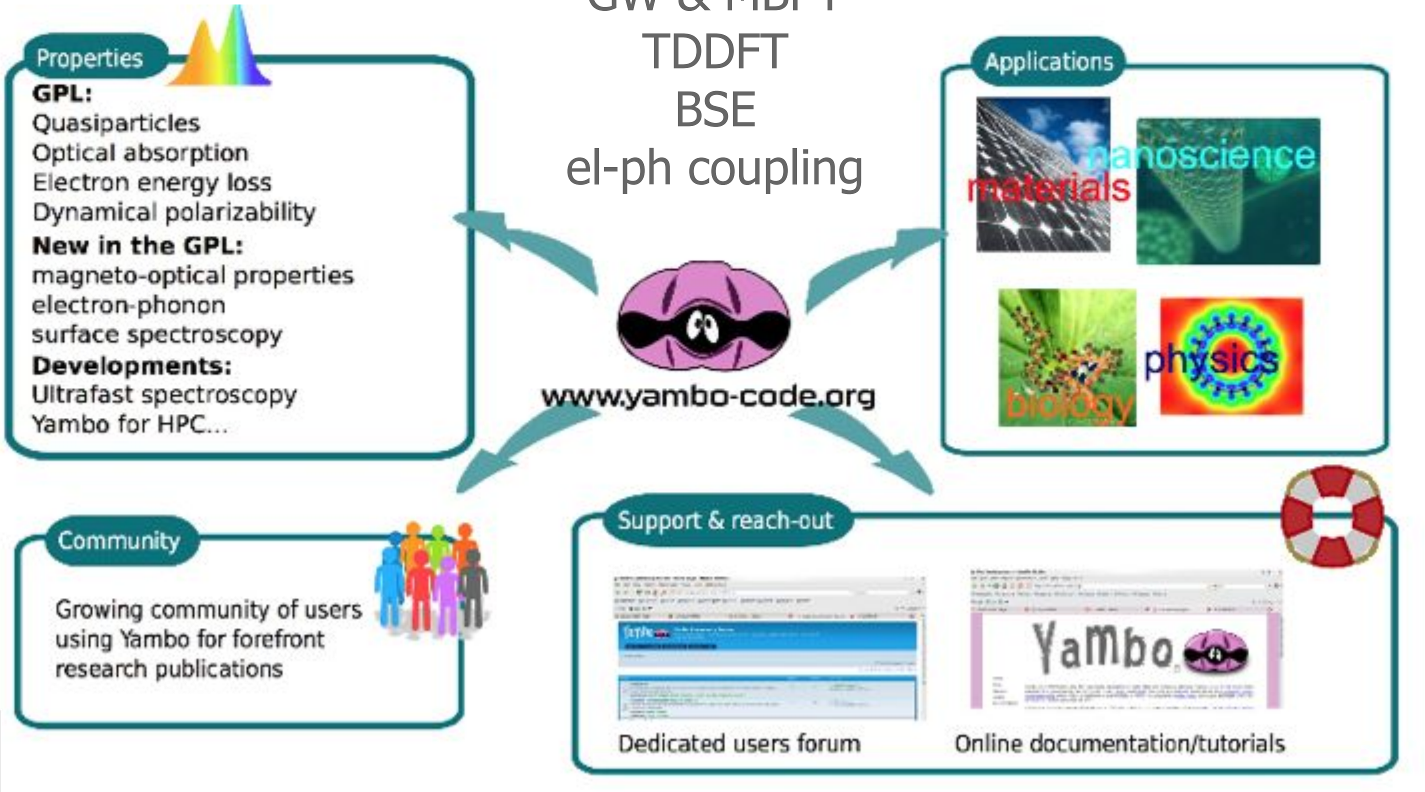
YOGA: Yambo on GPU Accelerators

Pietro Bonfà, Massimiliano Fatica, Andrea Ferretti,
Anton Kozhevnikov, Ivan Marri, Everett Phillips, Josh Romero

Eurohack 2018

Yambo Project

GW & MBPT
TDDFT
BSE
el-ph coupling



Properties

GPL:
Quasiparticles
Optical absorption
Electron energy loss
Dynamical polarizability

New in the GPL:
magneto-optical properties
electron-phonon
surface spectroscopy

Developments:
Ultrafast spectroscopy
Yambo for HPC...

www.yambo-code.org

Applications

Community

Growing community of users using Yambo for forefront research publications

Support & reach-out

Dedicated users forum

Online documentation/tutorials

Yambo Parallelization

- yambo implements a **hybrid MPI+OpenMP** paradigm

- **MPI** works over several (3 to 5) **different levels**, according to the run level

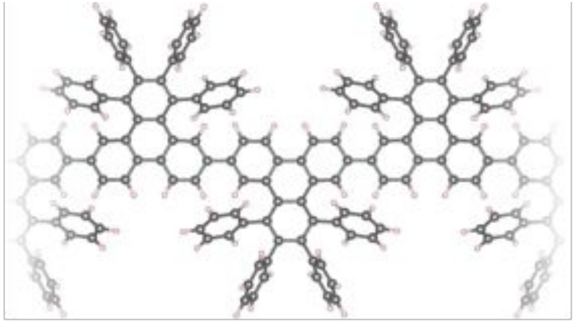
- **OpenMP** works at a **lower level**, usually on space degrees of freedom (not always the case, though),
- reaching very different levels of efficiency

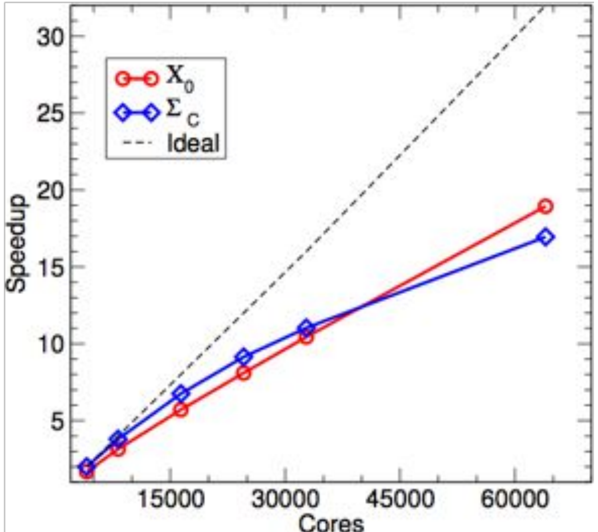
- **parallel linear algebra** is supported (ScaLapack, SLEPC, PETSC)

- overall, yambo is quite **parallel oriented**

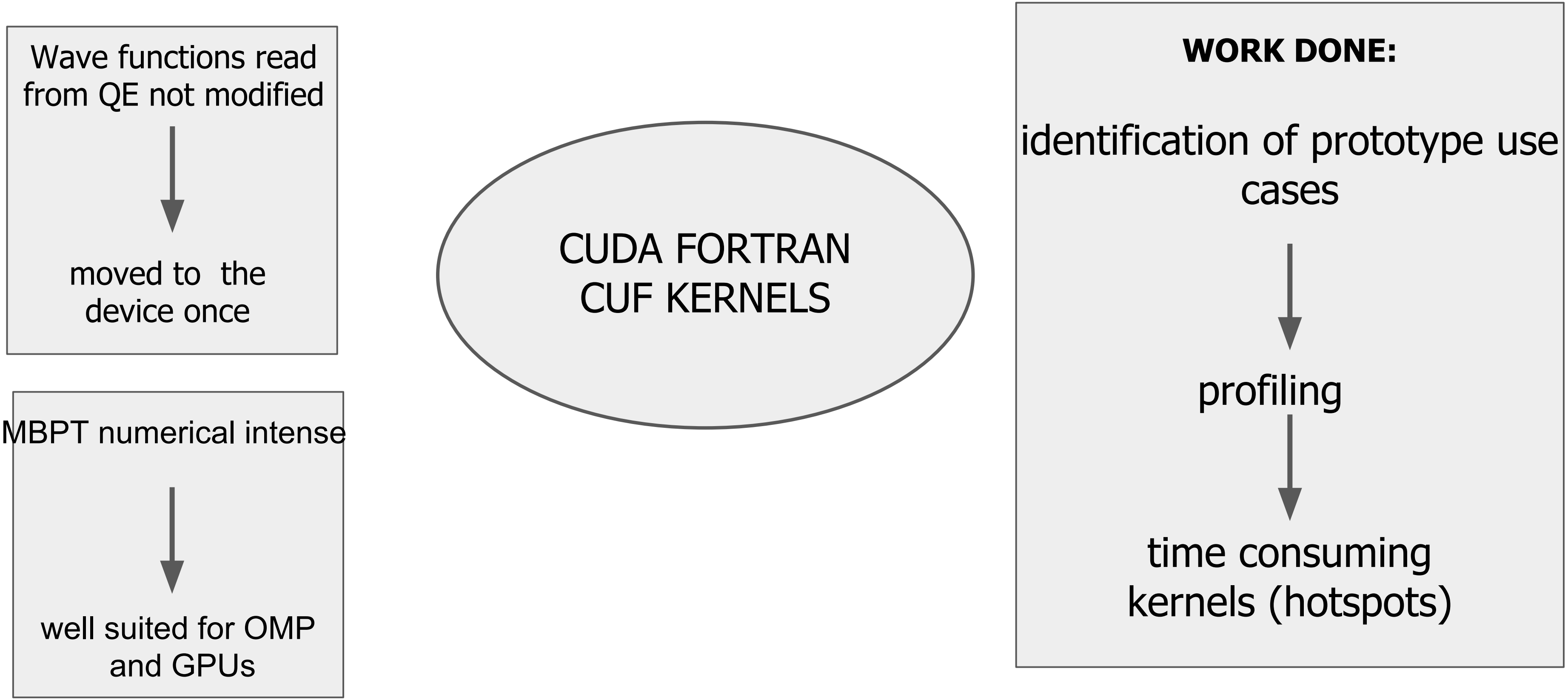
Yambo Performance

- Yambo **single GW calculation** scaling up to 1000 KNL nodes (~ 3 PFl/s)
- hybrid **MPI+OpenMP** +scaLapack
- Calculations relevant for an **active research field** (graphene nanoribbons)
- Performed on the recently deployed **KNL** partition of Marconi @ CINECA





Porting Strategy



Wave functions read from QE not modified

moved to the device once

MBPT numerical intense

well suited for OMP and GPUs

CUDA FORTRAN
CUF KERNELS

WORK DONE:

identification of prototype use cases

profiling

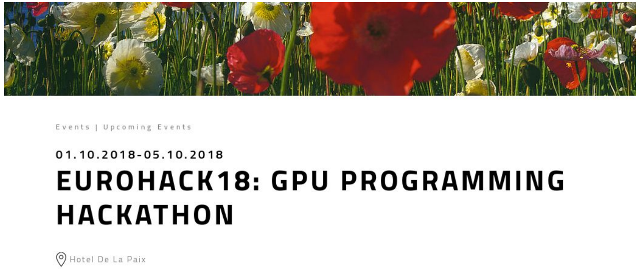
time consuming kernels (hotspots)

Porting Steps

Trieste 2017: Cuda Fortran for Materials Scientists, Feb 27- Mar 1

Barcelona 2018: MaX Hackathon, July 16 - 20

Lugano 2018: EuroHack, October 1-5



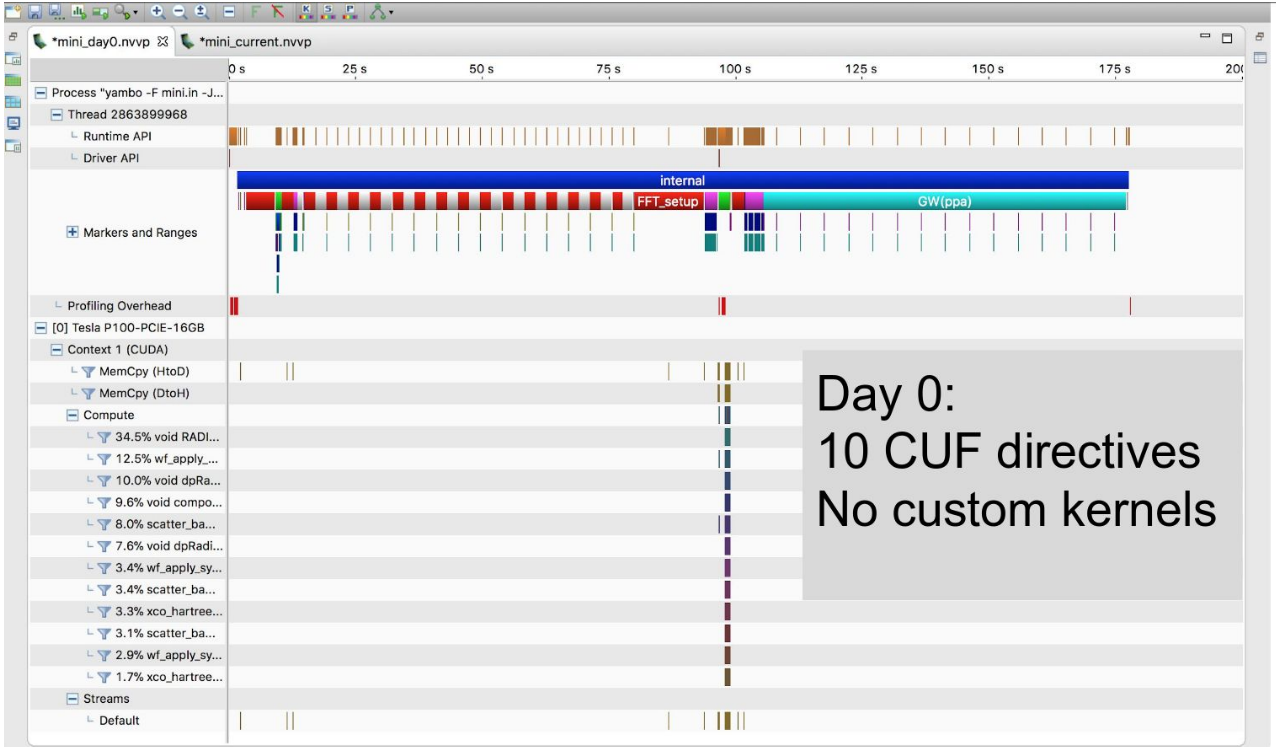
Events | Upcoming Events

01.10.2018-05.10.2018

EUROHACK18: GPU PROGRAMMING HACKATHON

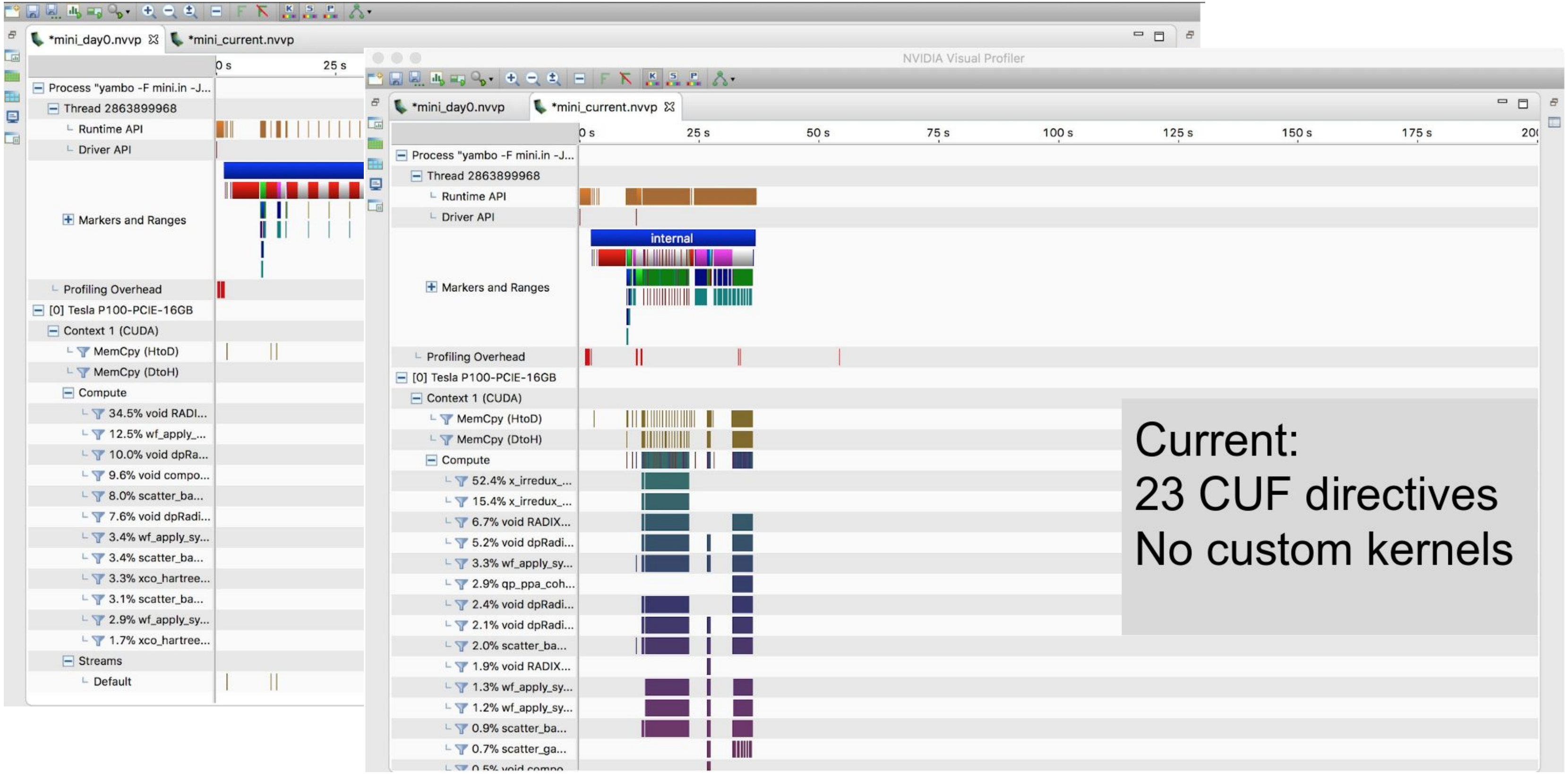
Hotel De La Paix

Profiling



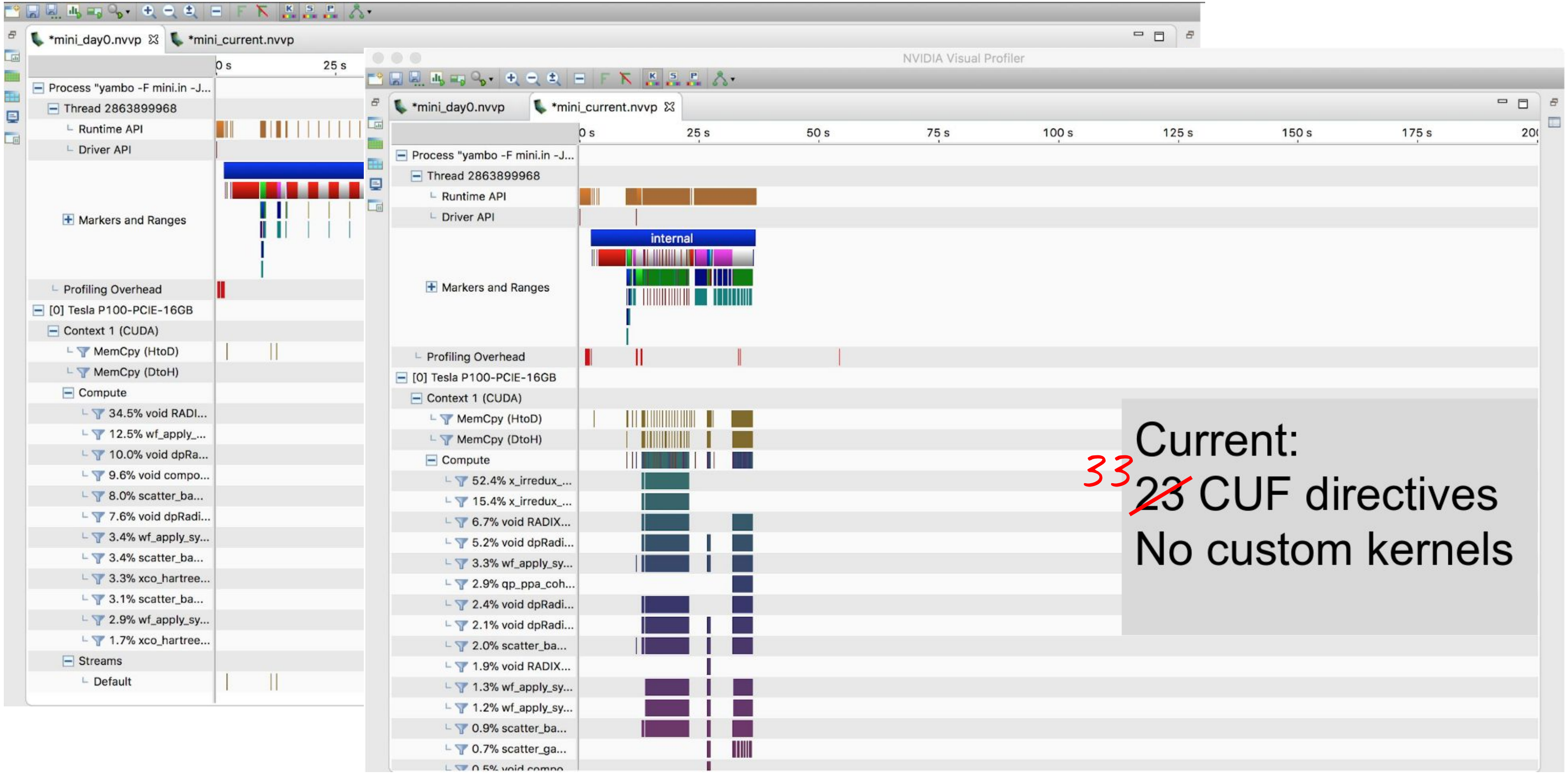
Day 0:
10 CUF directives
No custom kernels

Profiling



Current:
23 CUF directives
No custom kernels

Profiling



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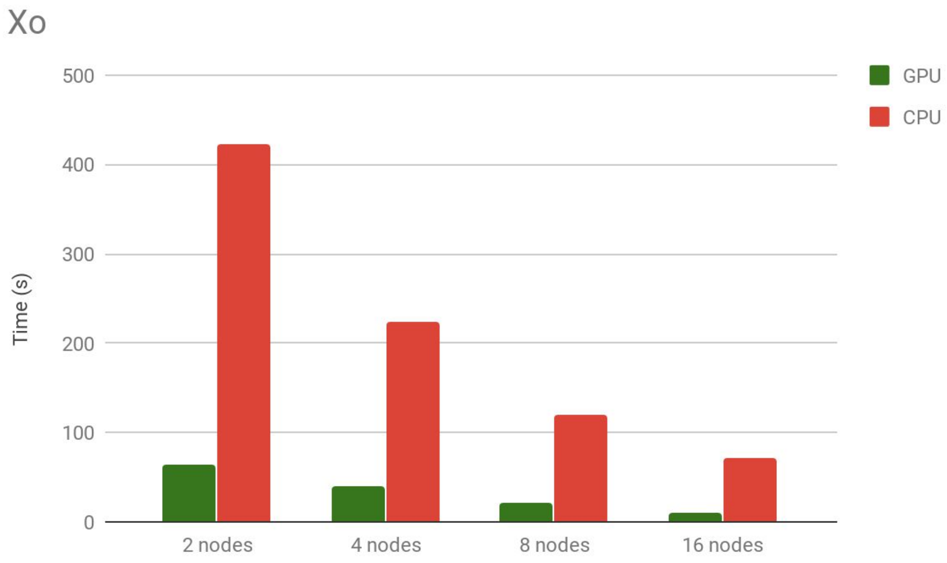
33 ~~23~~ CUF directives

No custom kernels

Performance

Full socket vs GPU on PizDaint XC50 partition.



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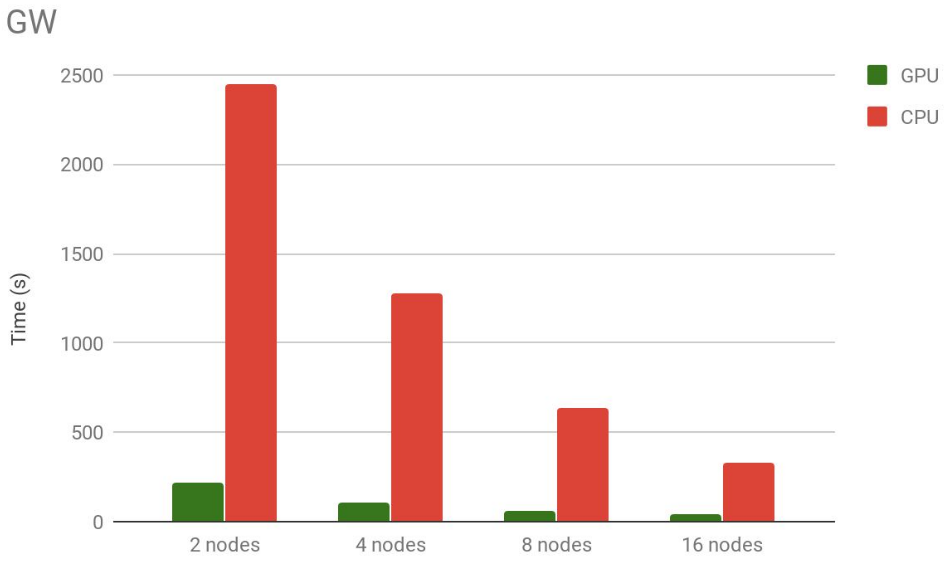

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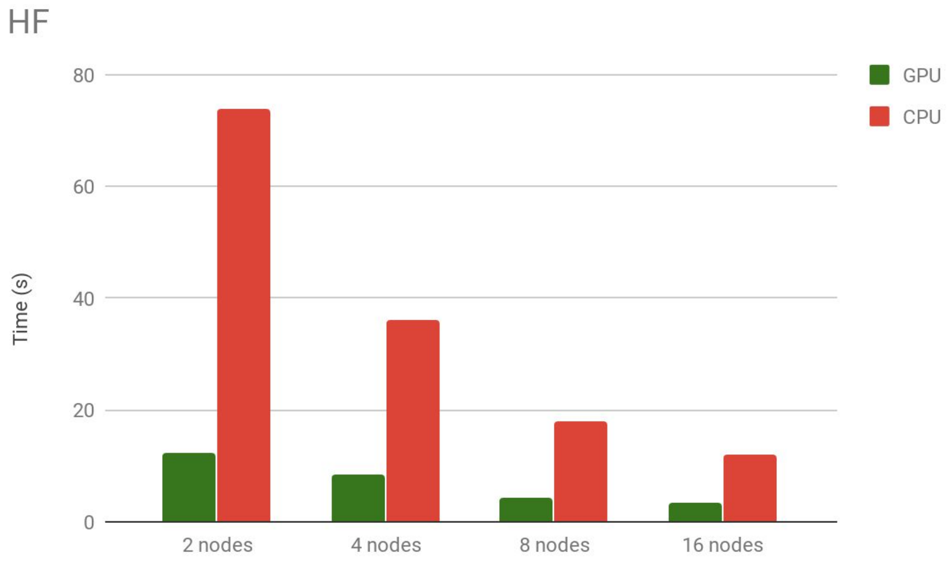

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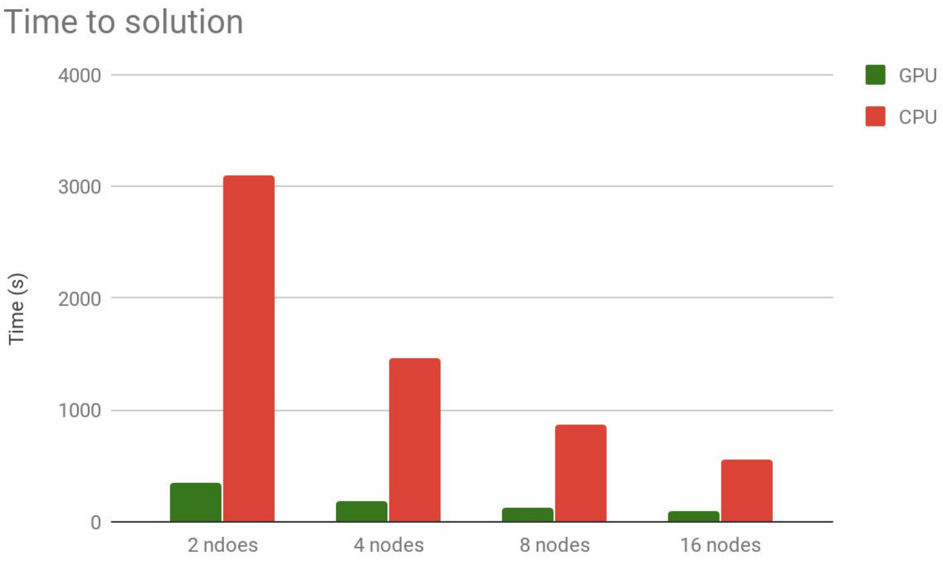

Conclusions

- CUDA Fortran based porting based on **cuf kernel directives** and cuda libraries (FFT)
- Profiling allowed us to spot room also for some CPU optimizations.
- 5 to 10x speedup in optimized subroutines, **5 to 10x speedup** in time to solution.
- Small impact on the code, accelerated part localized in a few subroutines.

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Thank you!