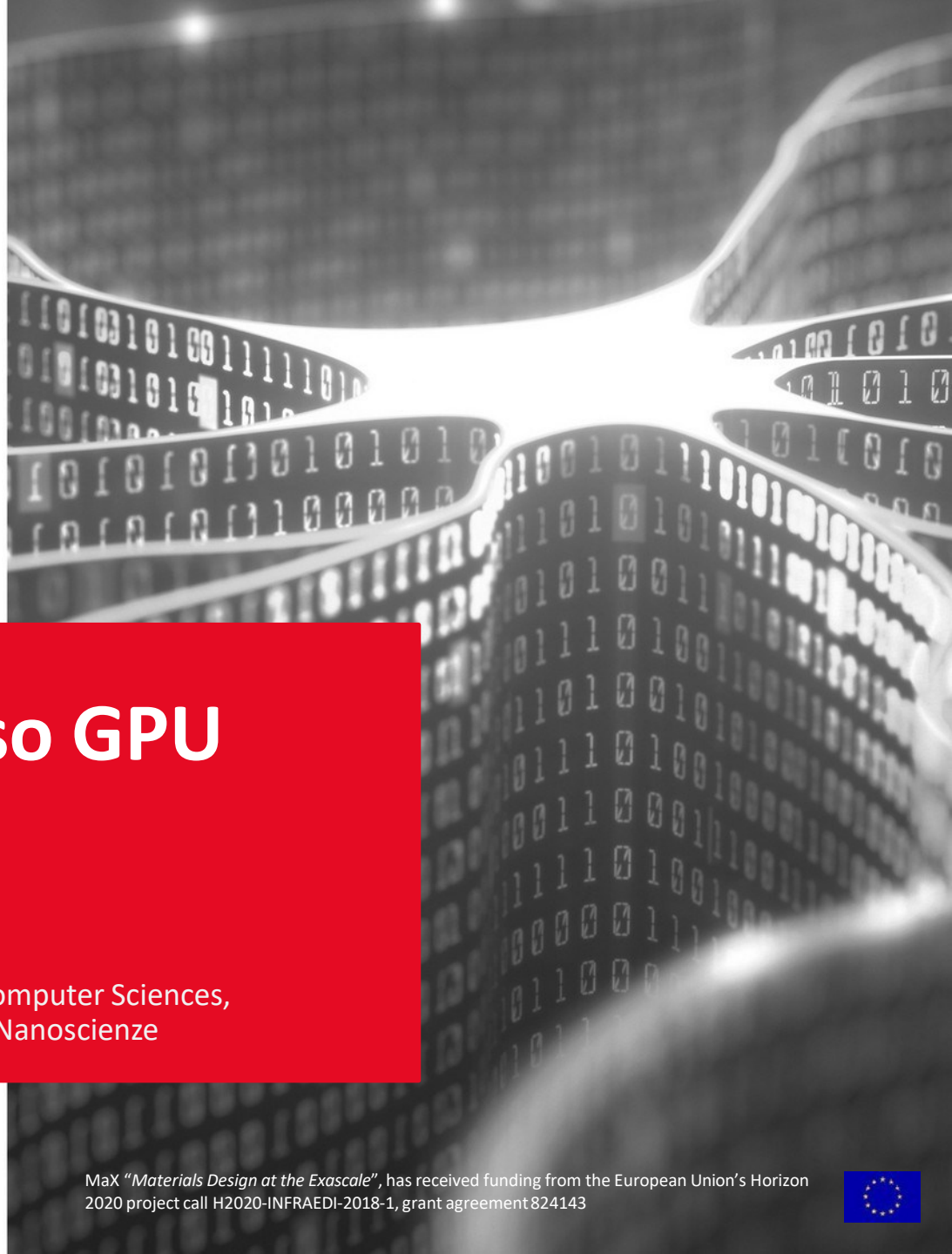
DRIVING THE EXASCALE TRANSITION



Quantum Espresso GPU on Marconi100

Pietro Bonfà

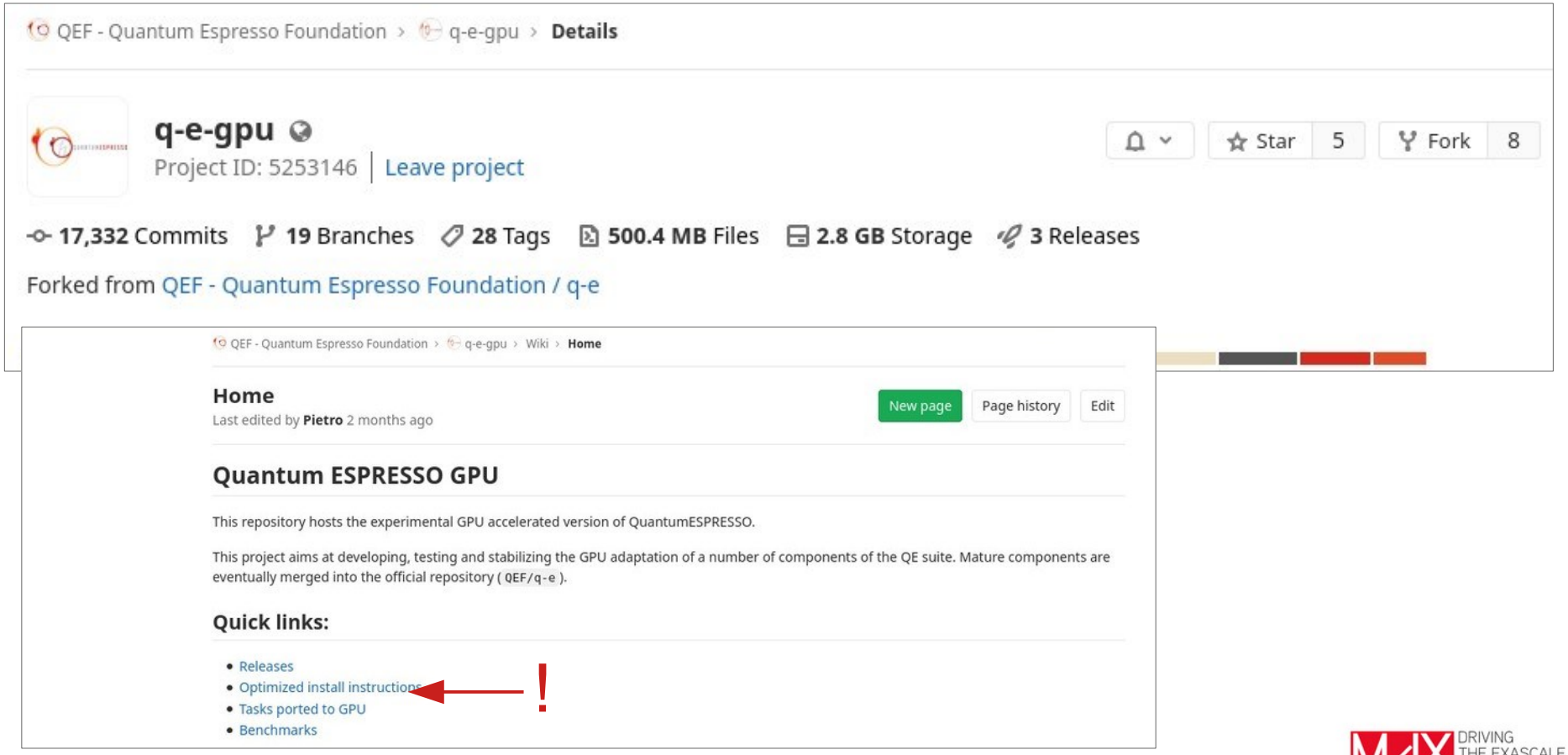
Department of Mathematical, Physical and Computer Sciences, University of Parma; Centro S3, CNR–Istituto Nanoscienze

MaX "*Materials Design at the Exascale*", has received funding from the European Union's Horizon 2020 project call H2020-INFRAEDI-2018-1, grant agreement 824143

GPU enabled version of QuantumESPRESSO

The last release of QE-GPU is available at

https://gitlab.com/QEF/q-e-gpu



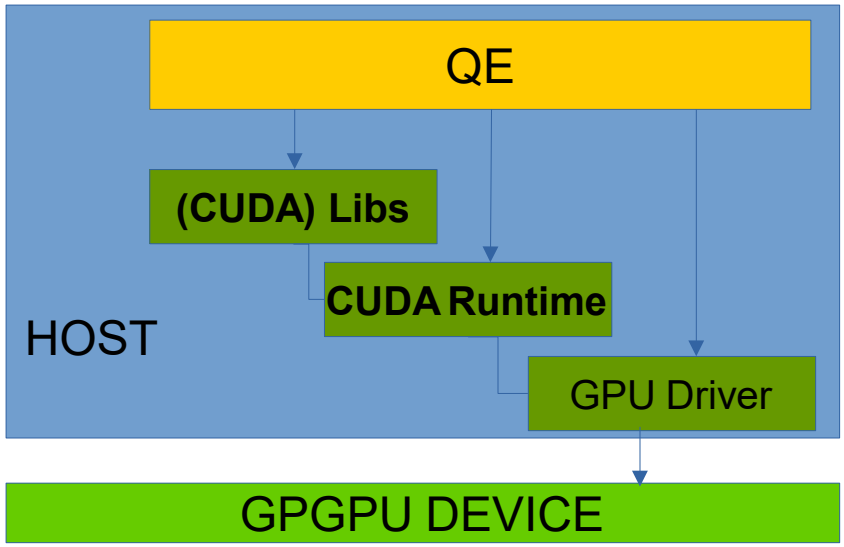
Compiling QE GPU

Compiling is as simple as...

```
./configure --with-cuda=XX --with-cuda-runtime=Y.y --with-cuda-cc=ZZ --enable-openmp [ --with-scalapack=no ]
```

where `XX` is the location of the CUDA Toolkit (in HPC environments it is generally `$CUDA_HOME`, be sure that this variable is not empty with a simple `echo $CUDA_HOME`), `Y.y` is the version of the CUDA Toolkit (`Y` and `y` are the two numbers identifying major and minor release, e.g. `9.0`) and `ZZ` is the compute capability (cc) of the card. This information can be found on the internet using the model name of the GPU card or by using `pgaccelinfo` command.

Openmp is required in order to successfully compile the accelerated version.

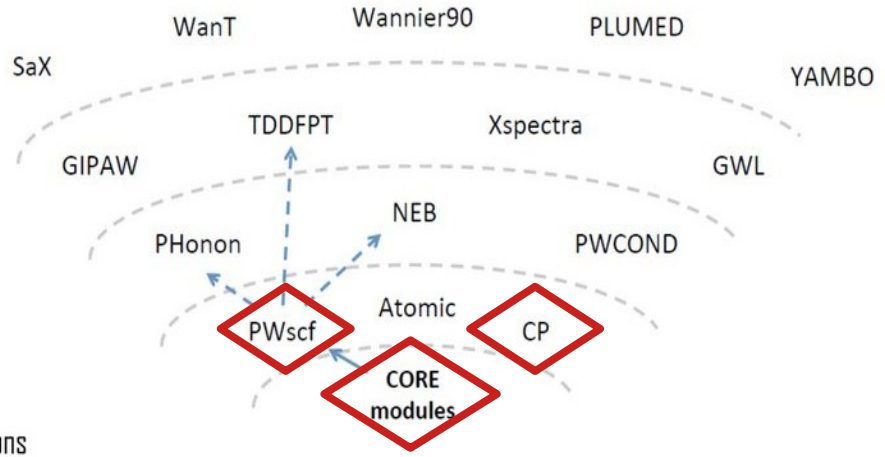


Cuda Toolkit is generally in $CUDA_HOME.

The *compute capabilities* codify the features and specifications of the target device.

```
[pbonfa00@login02 scf]$ pgaccelinfo | grep cc
PGI Default Target:             -ta=tesla:cc70
PGI Default Target:             -ta=tesla:cc70
PGI Default Target:             -ta=tesla:cc70
PGI Default Target:             -ta=tesla:cc70
```

What does QE GPU provide



Programming model | Objective

Applications — Directive based programming — Optimize memory duplication, allocation and syncronization.

Domain Specific Libraries

LAXLib

$$A\mathbf{v} = \lambda B\mathbf{v}$$

TASK: parallel linear algebra
LIBS: ELPA, MKL, cuBLAS, cuSOLVER, ESSL, ...

FFTXlib

TASK: Parallel distributed FFT
LIBS: FFTW, MKL, ESSL, cuFFT, ...

KS_Solvers

$$|\delta\psi_i\rangle = \frac{1}{D-\epsilon_i}(H-\epsilon_i)|\psi_i\rangle$$

TASK: Iterative solvers
LIBS: LAXLib, MKL, cuBLAS, ...

Explicit accelerator programming — Optimize computational efficiency and concurrency

What does QE GPU provide

What can be done with the accelerated version of pw.x

GPU version	Total Energy (K points)	Forces	Stress	Collinear Magnetism	Non-collinear magnetism	Gamma trick	US PP	PAW PP	DFT+U	All other functions
v5.4	A	W	W	B (?)	U	A	A	?	W (?)	W (?)
v6.1	A	A	A	A	U	W (*)	A	A (*)	U (?)	U (?)
v6.4	A	W	W	A	A	A	A	A (*)	W	W
V6.5a1	A	A	W	A	A	A	A	A	W	W
V6.5a2	A	A	A	A	A	A	A	A	W	W

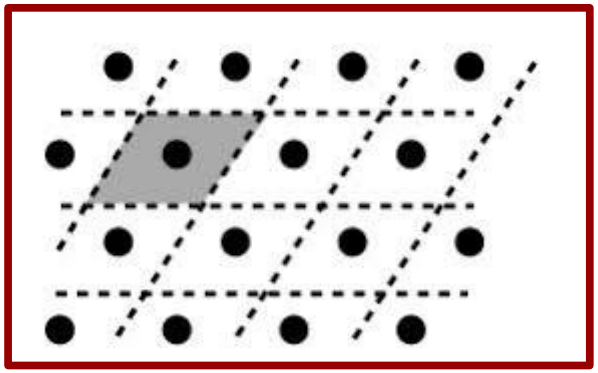
Accelerated, **W**orking, **U**navailable, **B**roken

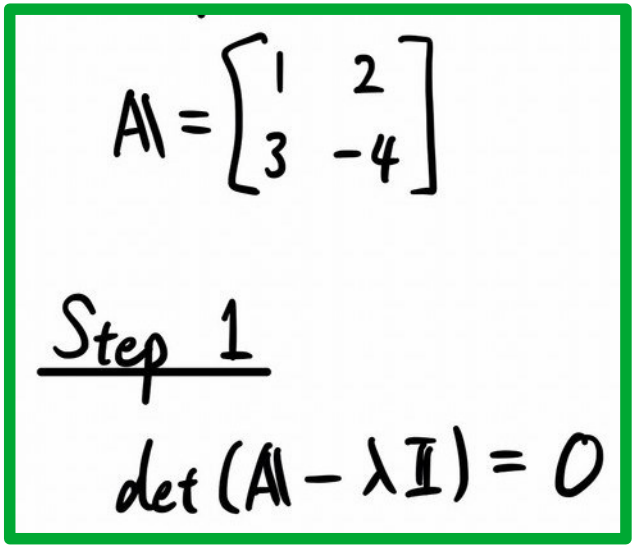
* Acceleration obtained from other parts of the code.

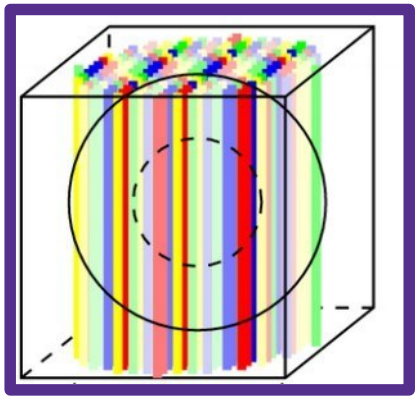
QE in the homogeneous HPC world

You know how to run QE efficiently on a HPC machine:

```
mpirun pw.x -npool X -ndiag Y -ntg Z -inp pw.in
```



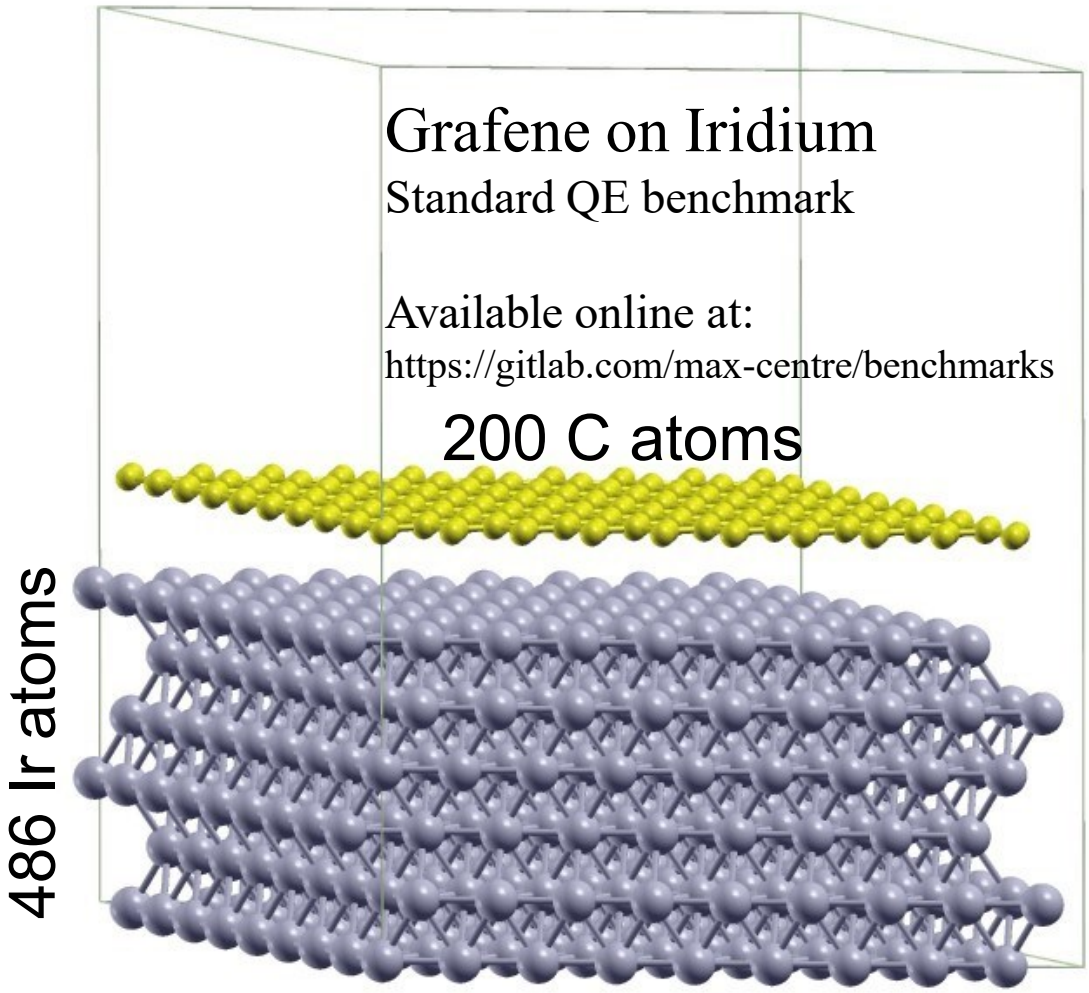




QE in the homogeneous HPC world

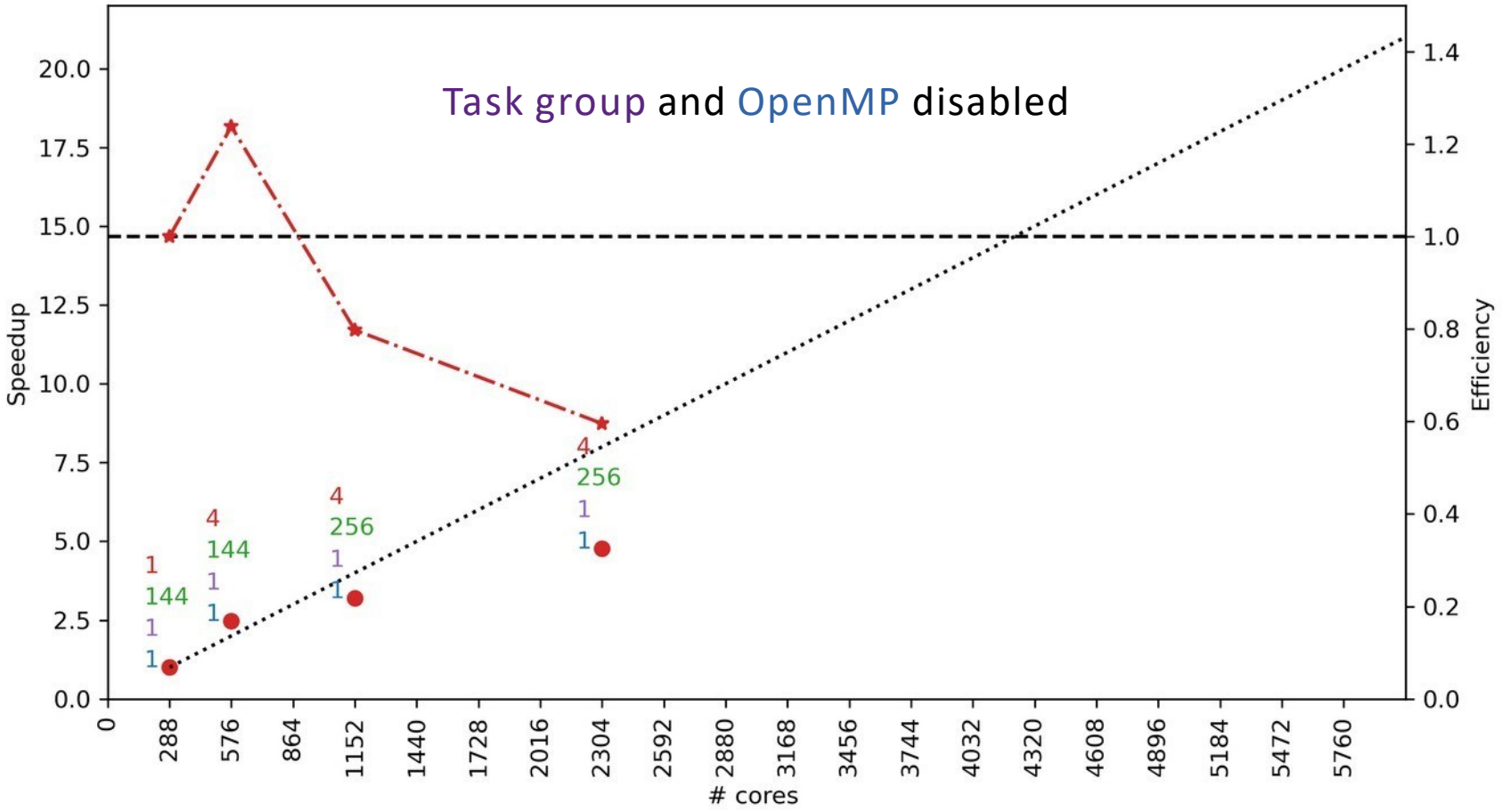
```
mpirun pw.x -npool X -ndiag Y -ntg Z -inp pw.in
```

```
 &control
    calculation = 'scf'
    prefix='GRIR'
    restart_mode='from_scratch'
    pseudo_dir='./',
 /
 &system
    ibrav=  4
    celldm(1) = 46.5334237988185d0
    celldm(3) =  1.274596
     nat=686
    ntyp= 2,
     ecutwfc=30
    occupations = 'smearing'
    smearing='mv'
    degauss=0.025d0
    nspin = 2
    starting_magnetization(1) = +.00
    starting_magnetization(2) = +.00
 /
 &electrons
    conv_thr =  1.0d-5
    mixing_beta=0.3d0
    mixing_mode='local-TF'
    startingwfc='atomic'
    diagonalization='david'
    electron_maxstep = 1
  /
ATOMIC_SPECIES
 C    12.010   C.pbe-paw_kj-x.UPF
 Ir  192.22   Ir.pbe-paw_kj.UPF
K_POINTS {automatic}
2 2 2 0 0 0
```



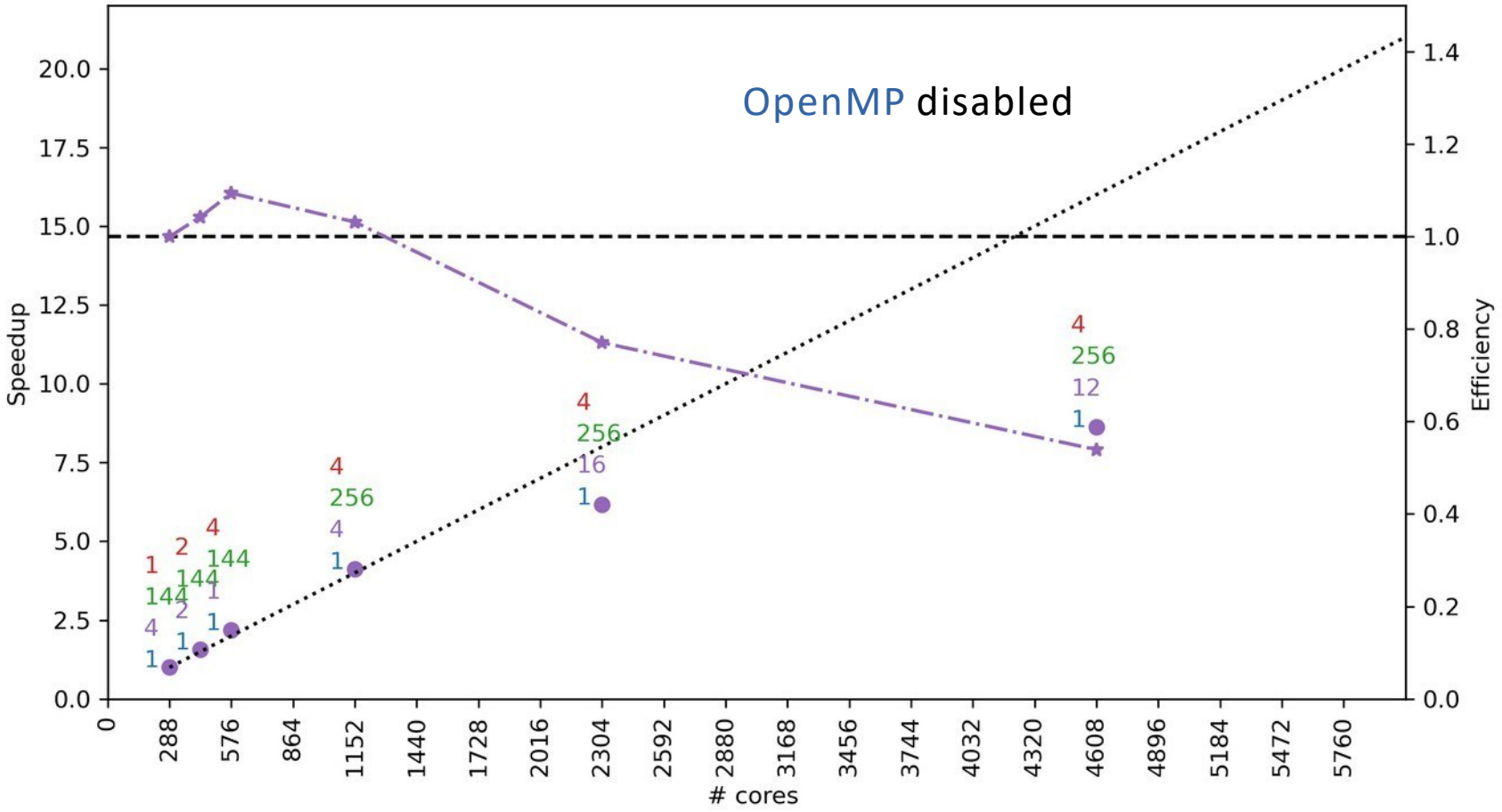
QE in the homogeneous HPC world

```
mpirun pw.x -npool X -ndiag Y -ntg Z -inp pw.in
```



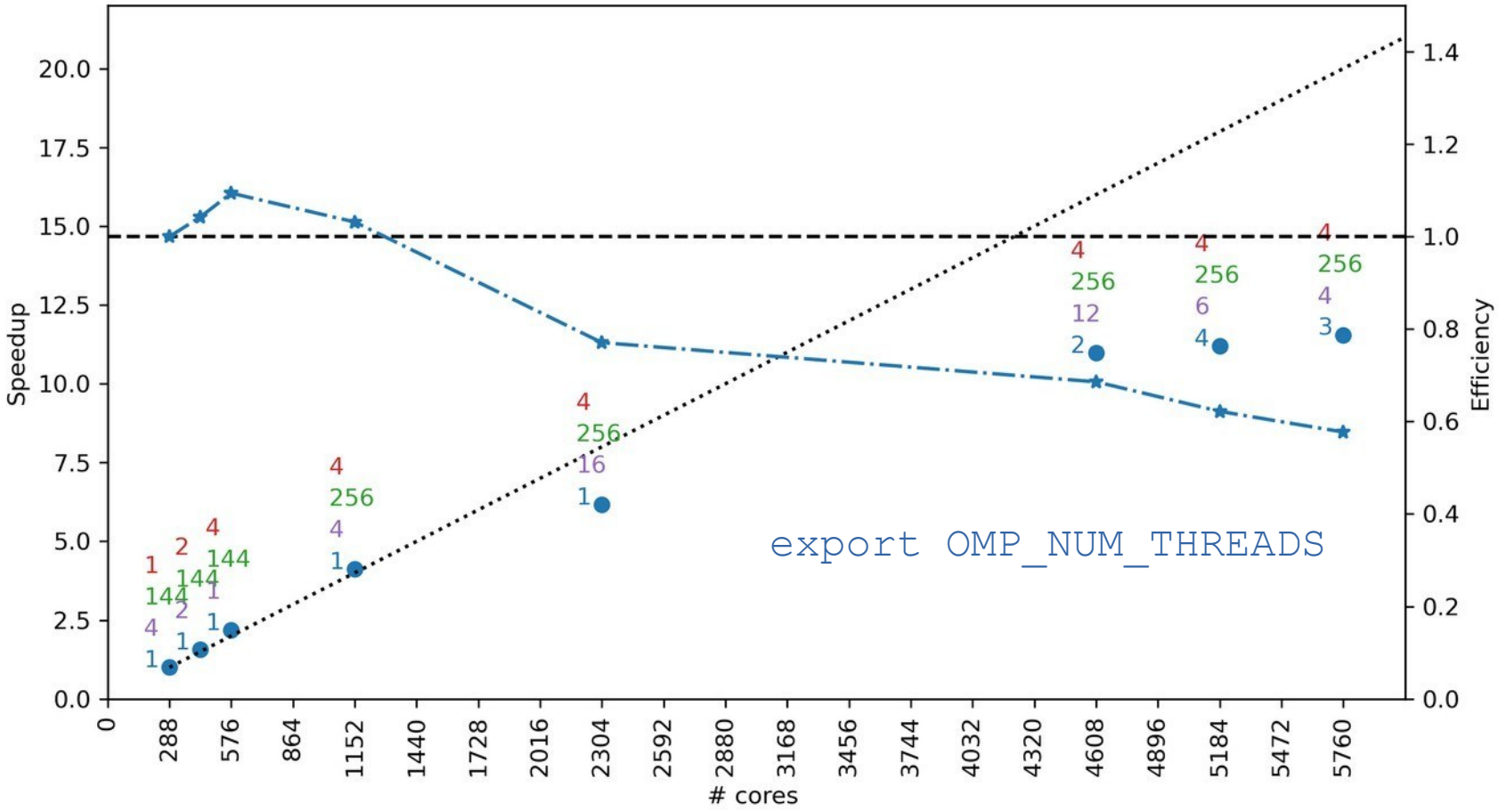
QE in the homogeneous HPC world

```
mpirun pw.x -npool X -ndiag Y -ntg Z -inp pw.in
```



QE in the homogeneous HPC world

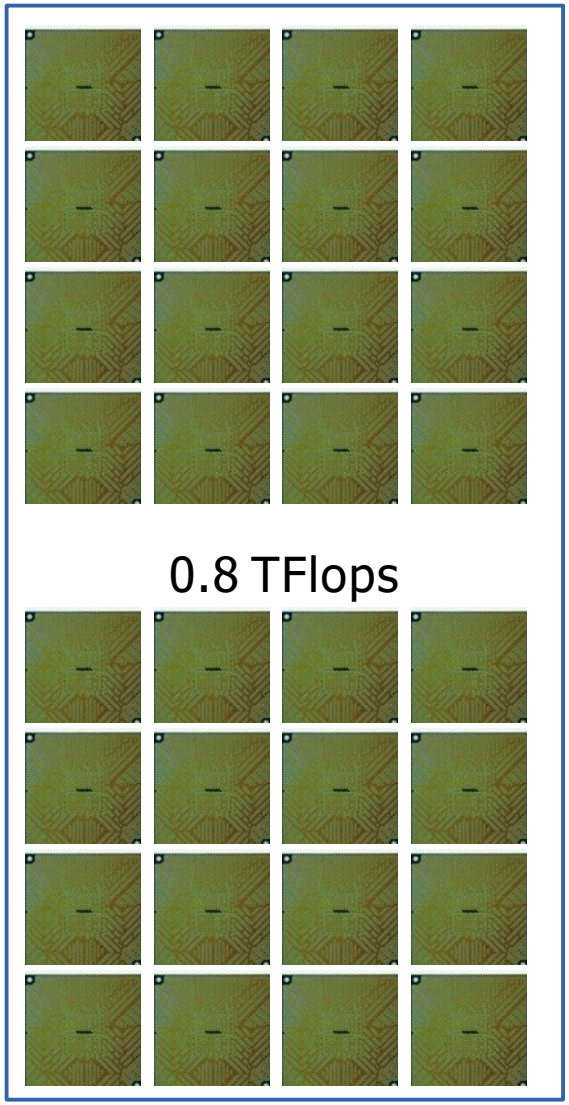
```
mpirun pw.x -npool X -ndiag Y -ntg Z -inp pw.in
```



QE in the heterogeneous HPC world

7.8 TFlops

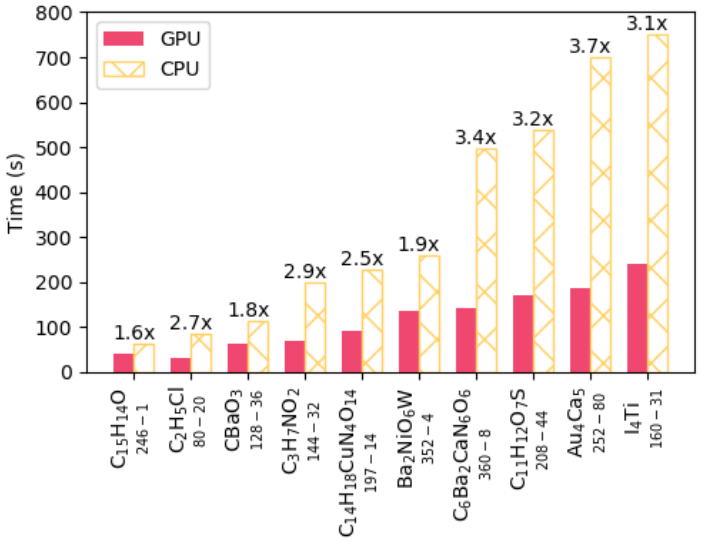
About ten times more powerful!

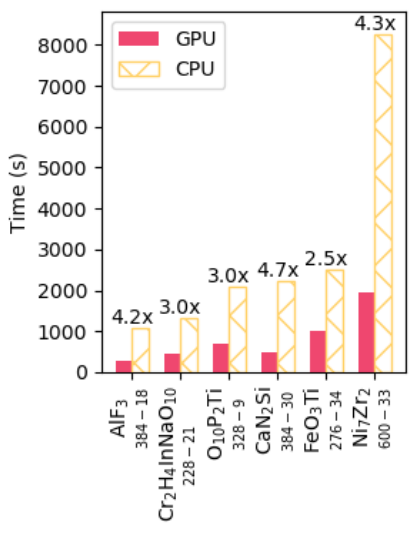


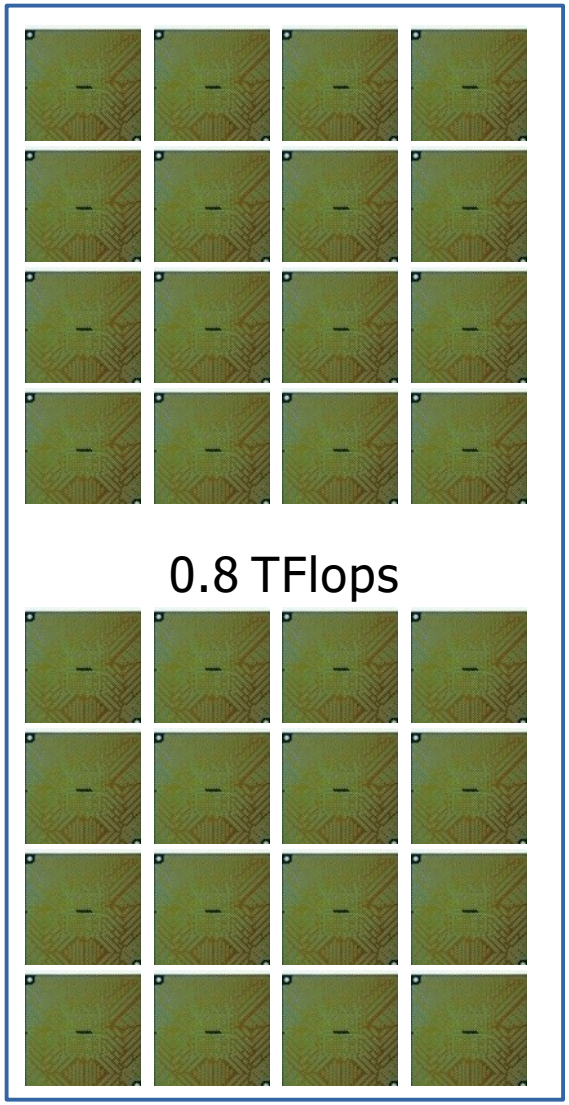
QE in the heterogeneous HPC world

7.8 TFlops

About ten times more powerful!







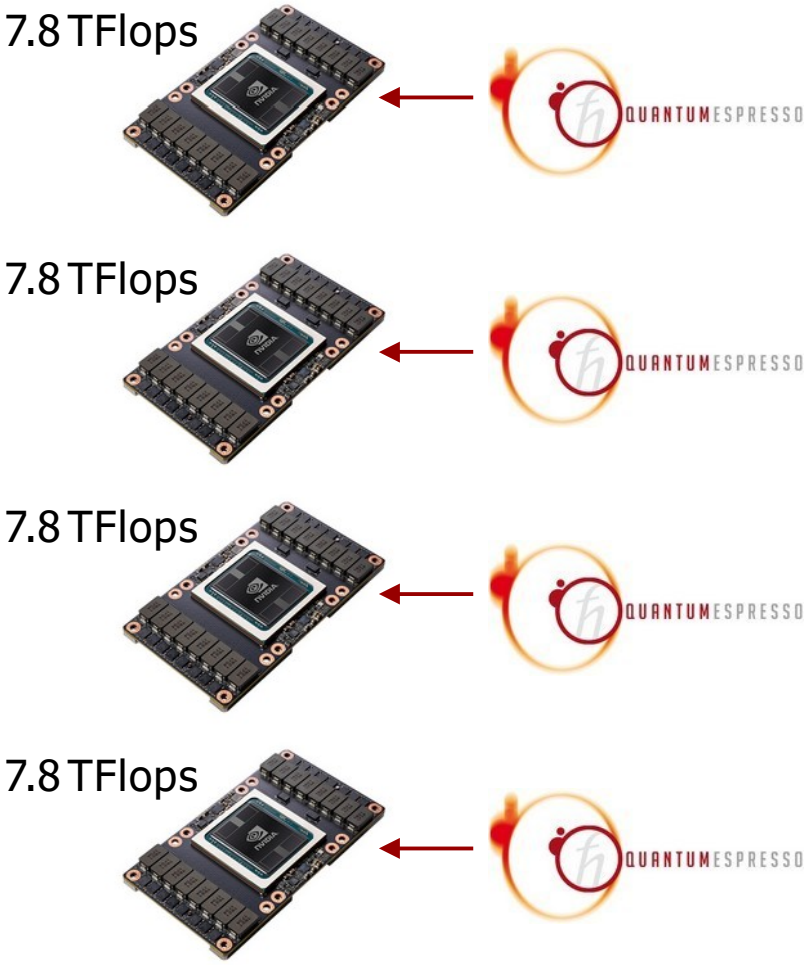
Quantum ESPRESSO toward the exascale
P. Giannozzi *et al.*
J. Chem. Phys. 152, 154105 (2020); DOI: 10.1063/5.0005082

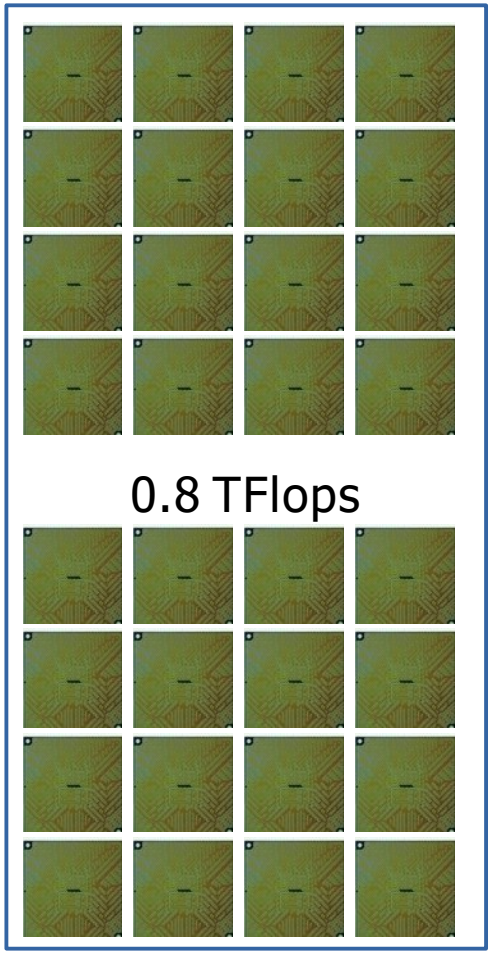
MAX DRIVING THE EXASCALE TRANSITION

QE in the heterogeneous HPC world

There are 4 GPUs per node on Marconi100!

```
mpirun -np 4 pw.x
```

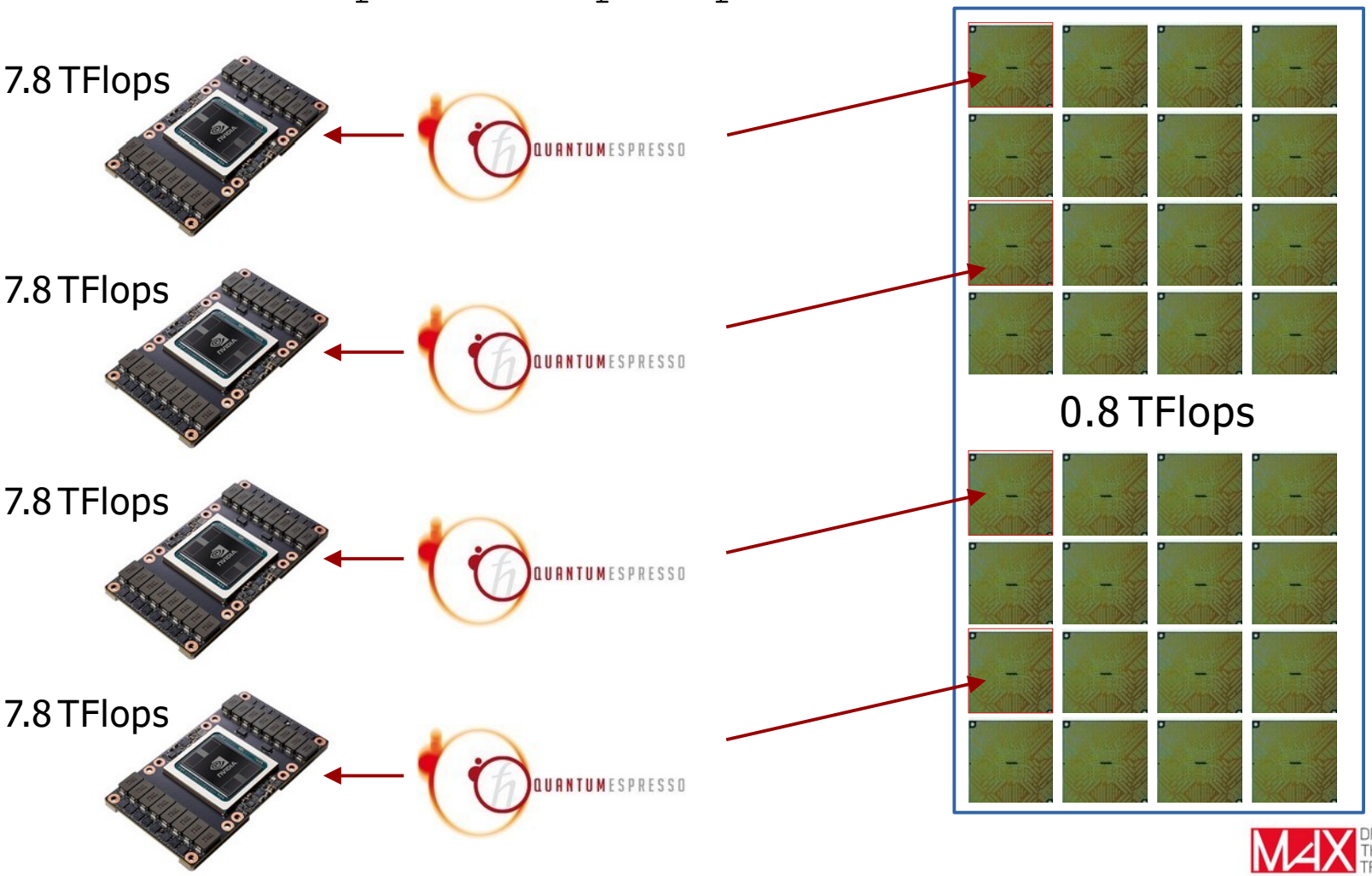




QE in the heterogeneous HPC world

There are 4 GPUs per node on Marconi100!

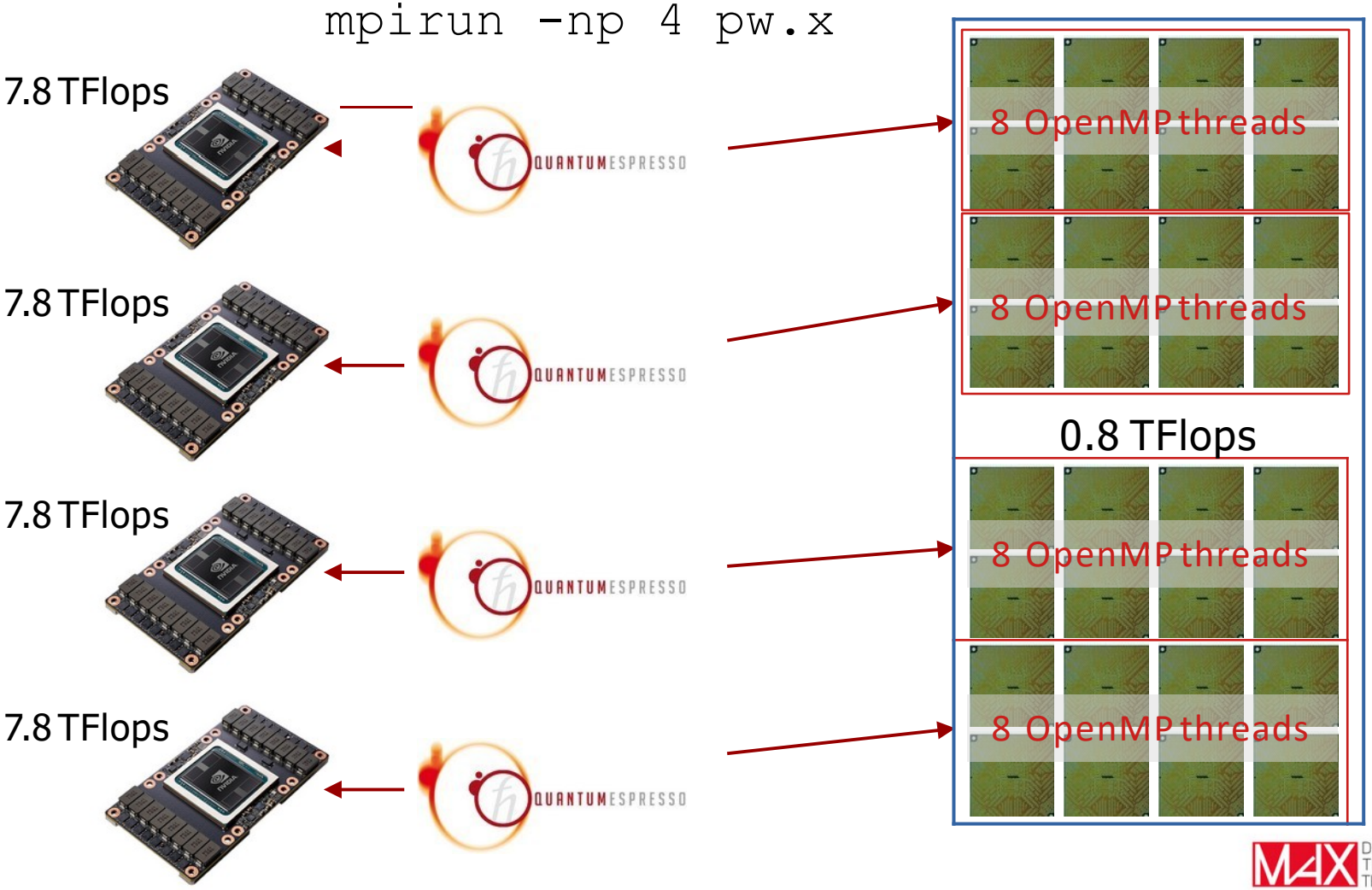
```
mpirun -np 4 pw.x
```



QE in the heterogeneous HPC world

There are 4 GPUs per node on Marconi100!

```
OMP_NUM_THREADS=8
mpirun -np 4 pw.x
```



QE in the heterogeneous HPC world

One MPI process per GPU! `mpirun -np nGPU pw.x …`

What about parallelism?

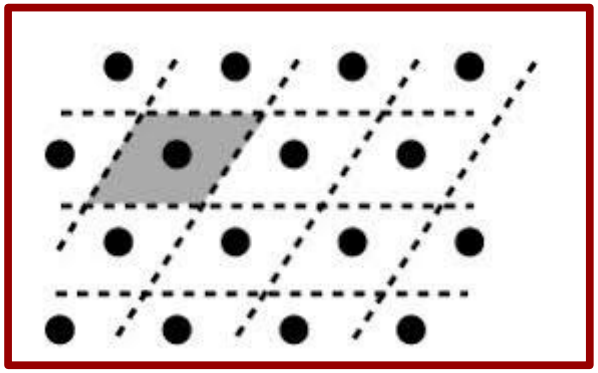
```
mpirun -np nGPU pw.x -npool X -ndiag Y -ntg Z
```

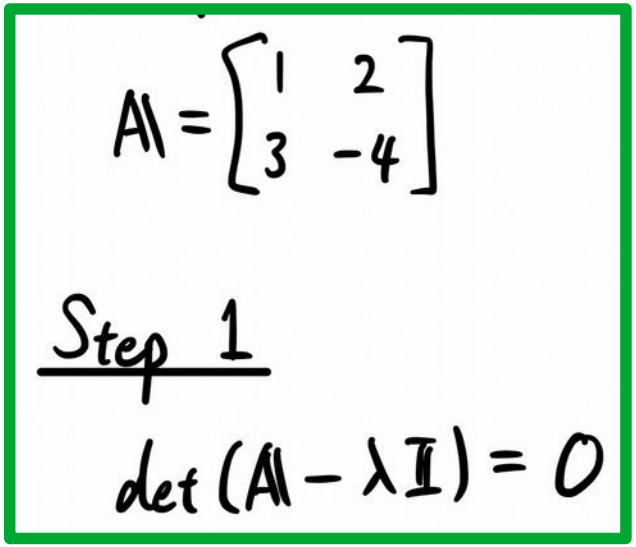
QE in the heterogeneous HPC world

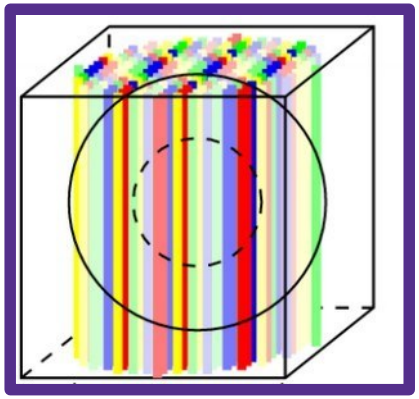
One MPI process per GPU! `mpirun -np nGPU pw.x …`

What about parallelism?

`mpirun -np nGPU pw.x -npool X -ndiag Y -ntg Z`





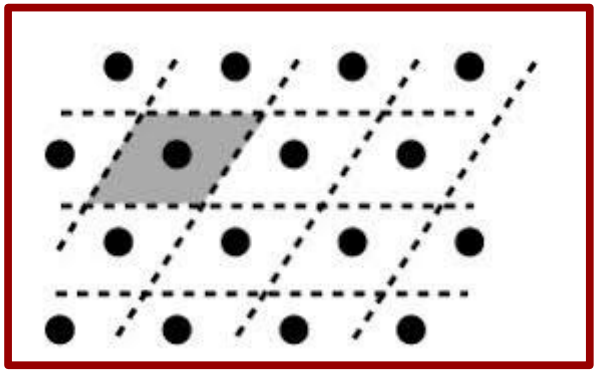


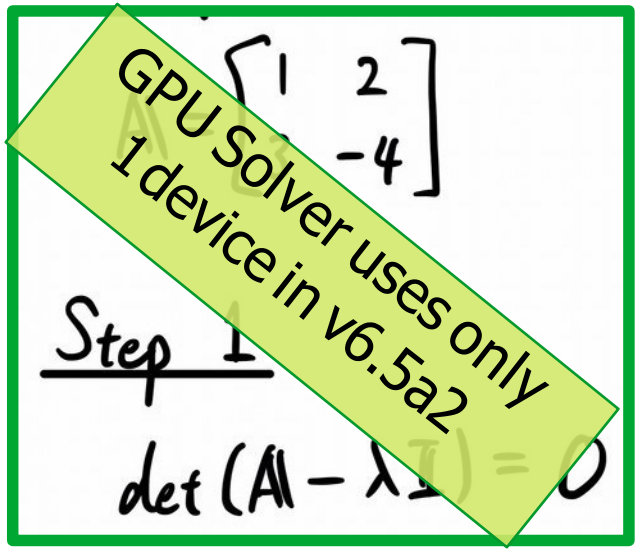
QE in the heterogeneous HPC world

One MPI process per GPU! `mpirun -np nGPU pw.x …`

What about parallelism?

`mpirun -np nGPU pw.x -npool X -ndiag Y -ntg Z`





QE in the heterogeneous HPC world

One MPI process per GPU! `mpirun -np nGPU pw.x …`

What about parallelism?

`mpirun -np nGPU pw.x -npool X -ndiag 1 -ntg 1`

```
     Subspace diagonalization in iterative solution of the eigenvalue problem:
     a serial algorithm will be used                         ✔
[…]
     GPU acceleration is ACTIVE.                             ✔
```

QE in the heterogeneous HPC world

What about memory…

Only 16GB!

```
mpirun -np nGPU pw.x -npool X -ndiag 1 -ntg 1
```

Check memory estimator!

```
X=4     Estimated max dynamical RAM per process > 14.72 GB
X=1     Estimated max dynamical RAM per process > 2.97 GB
```

Choose the largest value for X that can fit available memory.

Tips & Tricks

You run out of memory … what to do?

- use more GPUs…
- reduce subspace dimension in Davidson algorithm
- Change diagonalization method

```
&electrons
   conv_thr =  1.0d-9
   mixing_beta=0.3d0
   startingwfc='atomic'
   diago_david_ndim='2'
 /
```

```
&electrons
   conv_thr =  1.0d-9
   mixing_beta=0.3d0
   startingwfc='atomic'
   diagonalization='cg'
 /
```

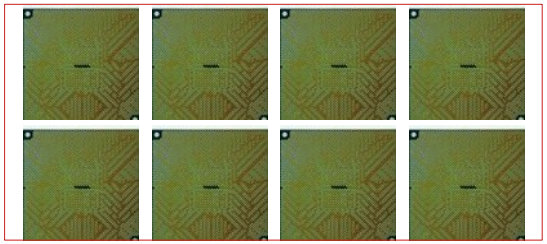
Feature X is slow!

→Open an issue at https://gitlab.com/QEF/q-e-gpu/-/issues

Take home message

A few things you should remember when running the GPU version of the code:

- *1 MPI process per GPU,*
- CPU cores can (must!) be exploited with *OpenMP parallelism*
- Pool parallelism is very effective, but requires memory
- The dense eigenvalue problem is (as of v6.5a2) solved on 1 GPU, *use the serial eigensolver*.
- Check the Wiki, it's updated with a collaborative effort!
- More details: P. Giannozzi *et al.* J. Chem. Phys. 152, 154105 (2020)



DRIVING THE EXASCALE TRANSITION

THANKS

Follow us on:

company/max-centre/

@max_center2

http://www.max-centre.eu/