# QE on HPC and GPU systems

## Day-5: hands-on session

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2. CINECA, Casalecchio di Reno, Italy
3. SISSA, Trieste, Italy
4. Institute of Physics, Belgrade, Serbia
5. National Institute of Chemistry, Slovenia

# What is pw.x telling us...

```
Program PWSCF v.6.4.1 starts on  7Sep2019 at  9:45: 3

This program is part of the open-source Quantum ESPRESSO suite
for quantum simulation of materials; please cite
    "P. Giannozzi et al., J. Phys.:Condens. Matter 21 395502 (2009);
    "P. Giannozzi et al., J. Phys.:Condens. Matter 29 465901 (2017);
     URL http://www.quantum-espresso.org",
in publications or presentations arising from this work. More details at
http://www.quantum-espresso.org/quote

Parallel version (MPI), running on    24 processors

MPI processes distributed on     1 nodes
R & G space division:  proc/nbgrp/npool/nimage =      24
```

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```
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 for quantum simulation of
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     "P. Giannozzi et al.,
      URL http://www.quantu
 in publications or present
 http://www.quantum-espress

 Parallel version (MPI), ru

 MPI processes distributed
 R & G space division:  prc
```

```
Subspace diagonalization in iterative solution of the eigenvalue problem:
one sub-group per band group will be used
custom distributed-memory algorithm (size of sub-group:  4*  4 procs)

Message from routine setup:
DEPRECATED: symmetry with ibrav=0, use correct ibrav instead

Parallelization info
--------------------
sticks:   dense  smooth     PW     G-vecs:    dense   smooth      PW
Min        1199     640    159               383982   149548   18695
Max        1202     642    162               384004   149562   18714
Sum       28829   15389   3855              9215799  3589319  448895


Title:
DyOtBuClTHF_100K.cif


bravais-lattice index     =            0
lattice parameter (alat)  =      25.6474  a.u.
unit-cell volume          =   37134.3792 (a.u.)^3
number of atoms/cell      =          608
number of atomic types    =            6
number of electrons       =      1512.00
number of Kohn-Sham states=          756
kinetic-energy cutoff     =      80.0000  Ry
charge density cutoff     =     600.0000  Ry
convergence threshold     =      1.0E-09
mixing beta               =       0.5000
number of iterations used =            8  plain     mixing
Exchange-correlation      = SLA  PW   PBE  PBE ( 1  4  3  4 0 0)
nstep                     =          400
```

# How is time spent by pw.x

```
init_run     :     42.99s CPU     46.16s WALL (       1 calls)
electrons    :  60819.95s CPU  63107.94s WALL (      83 calls)
update_pot   :   1461.58s CPU   1522.64s WALL (      82 calls)
forces       :  17437.52s CPU  17714.01s WALL (      82 calls)

Called by init_run:
wfcinit      :     28.44s CPU     29.07s WALL (       1 calls)
potinit      :      0.79s CPU      2.21s WALL (       1 calls)
hinit0       :      8.50s CPU      8.60s WALL (       1 calls)

Called by electrons:
c_bands      :  37126.13s CPU  37854.42s WALL (     889 calls)
sum_band     :   9663.72s CPU  10448.81s WALL (     889 calls)
v_of_rho     :    501.54s CPU    536.25s WALL (     890 calls)
newd         :   2620.20s CPU   3367.58s WALL (     890 calls)
mix_rho      :    116.23s CPU    122.01s WALL (     889 calls)

Called by c_bands:
init_us_2    :    296.76s CPU    297.22s WALL (    1779 calls)
regterg      :  36350.79s CPU  36971.49s WALL (     889 calls)

Called by sum_band:
sum_band:bec :      6.01s CPU      6.08s WALL (     889 calls)
addusdens    :   3042.08s CPU   3745.04s WALL (     889 calls)

Called by *egterg:
h_psi        :  24521.86s CPU  24722.48s WALL (    3704 calls)
s_psi        :   3235.74s CPU   3235.97s WALL (    3704 calls)
g_psi        :     40.31s CPU     40.48s WALL (    2814 calls)
rdiaghg      :   2592.35s CPU   2678.62s WALL (    3540 calls)

Called by h_psi:
h_psi:pot    :  24426.82s CPU  24627.23s WALL (    3704 calls)
h_psi:calbec :   3349.63s CPU   3389.39s WALL (    3704 calls)
vloc_psi     :  17839.75s CPU  17998.35s WALL (    3704 calls)
add_vuspsi   :   3237.38s CPU   3239.45s WALL (    3704 calls)
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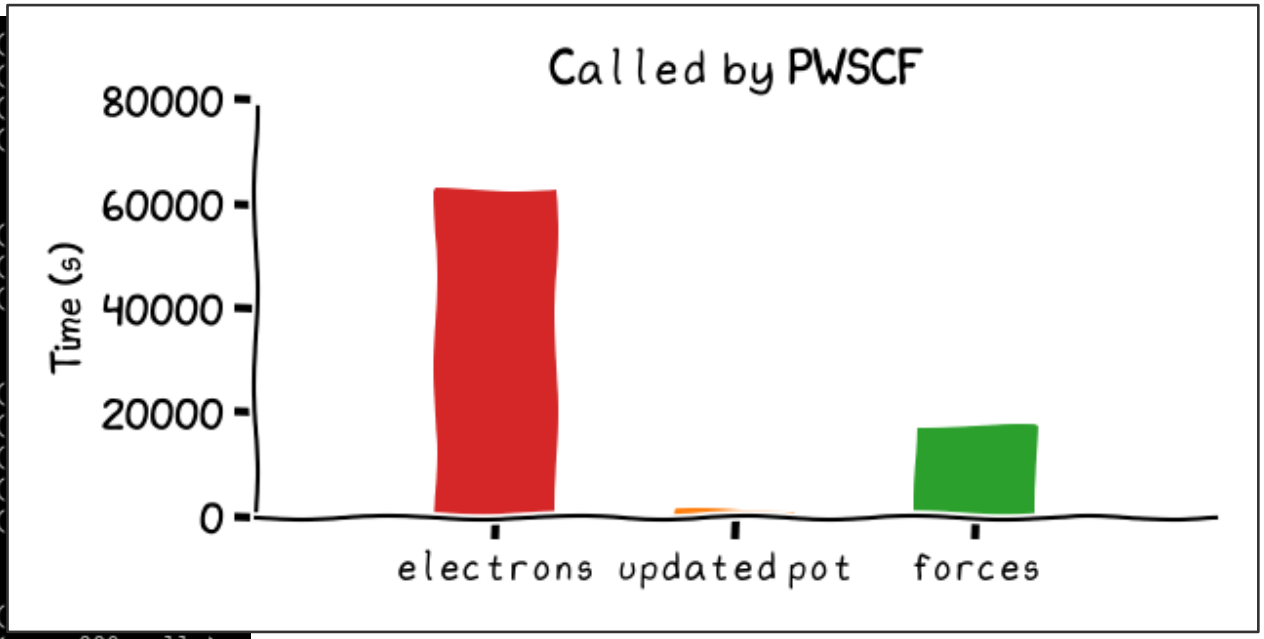

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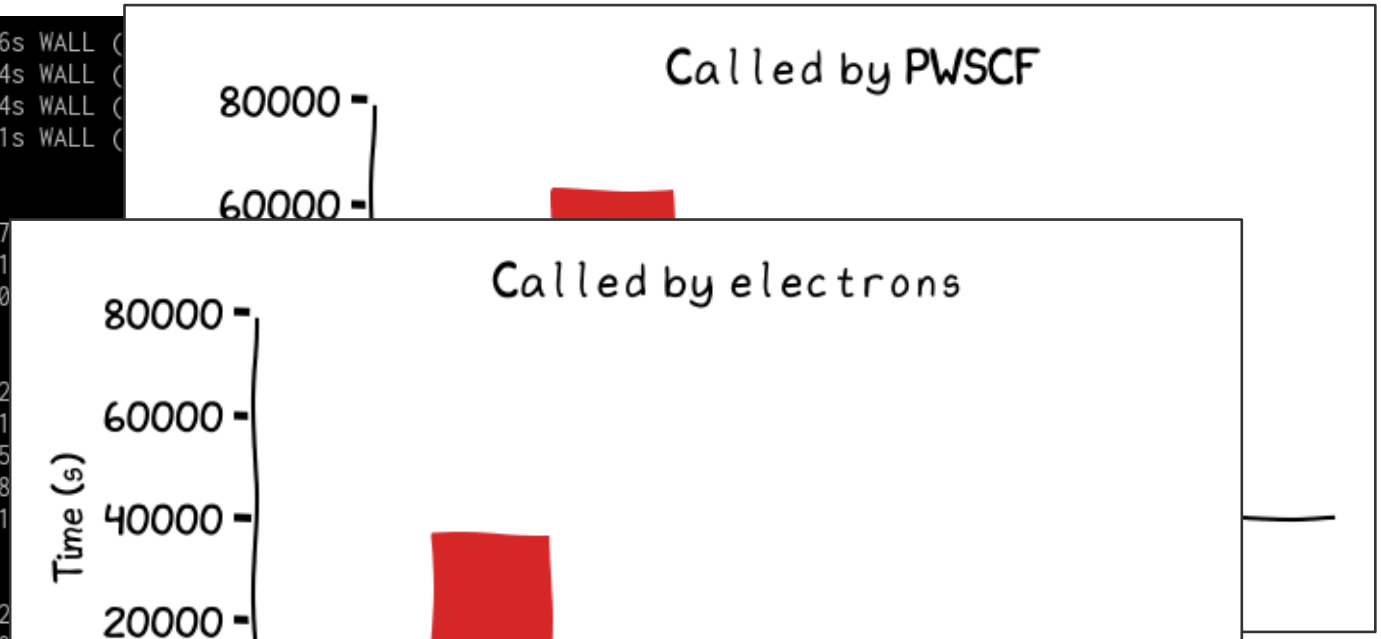

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Called by c_bands:
init_us_2    :
regterg      :  36

Called by sum_band
sum_band:bec :
addusdens    :   3

Called by *egterg:
h_psi        :  24
s_psi        :   3
g_psi        :
rdiaghg      :   2

Called by h_psi:
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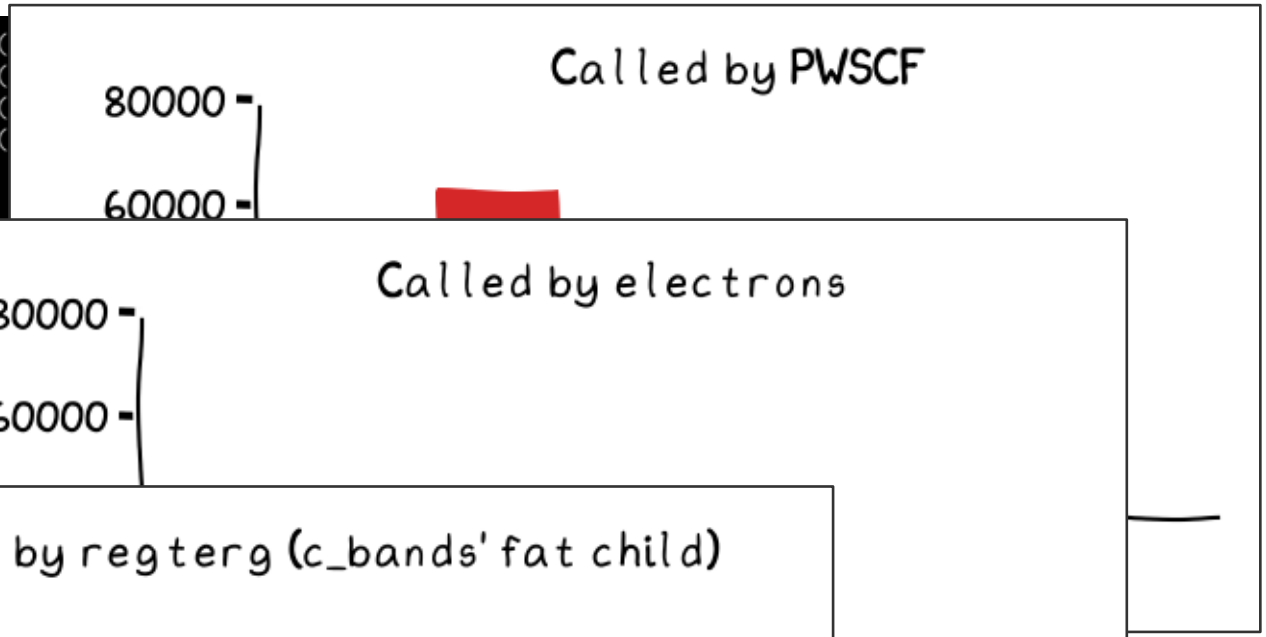
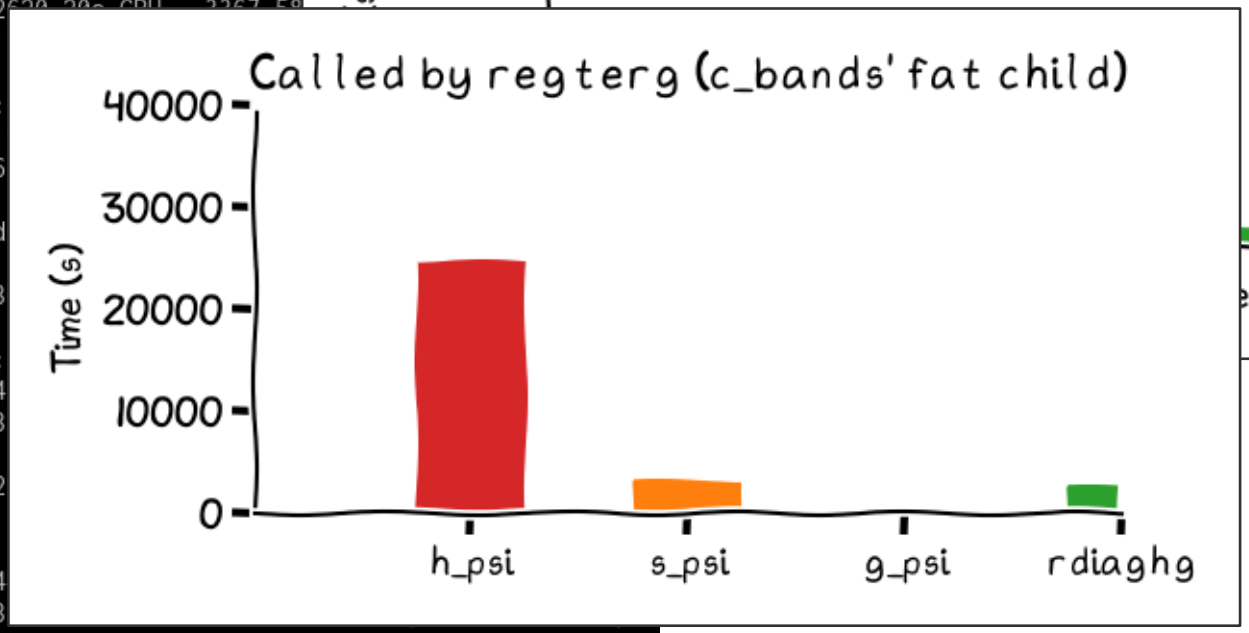


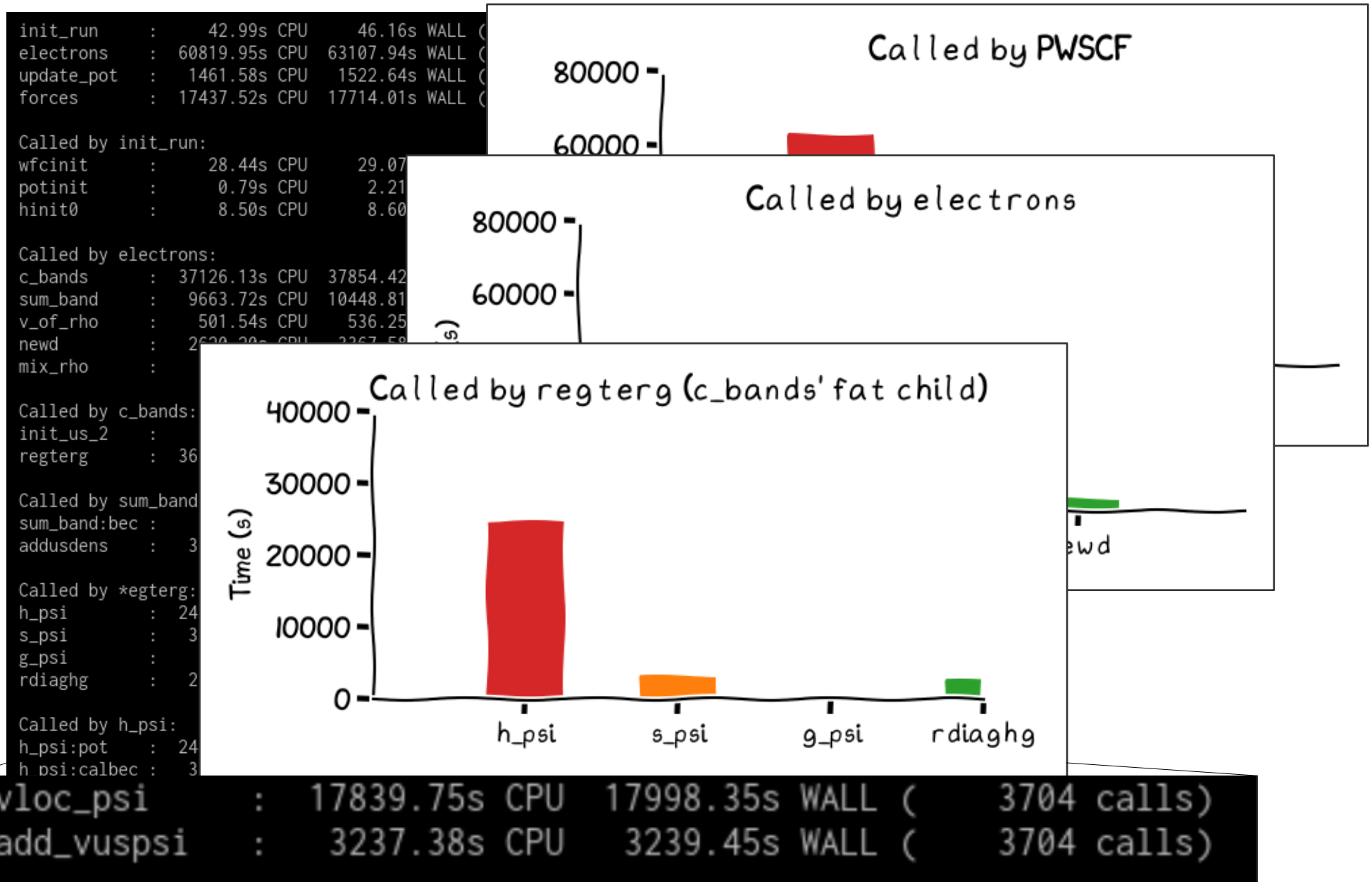




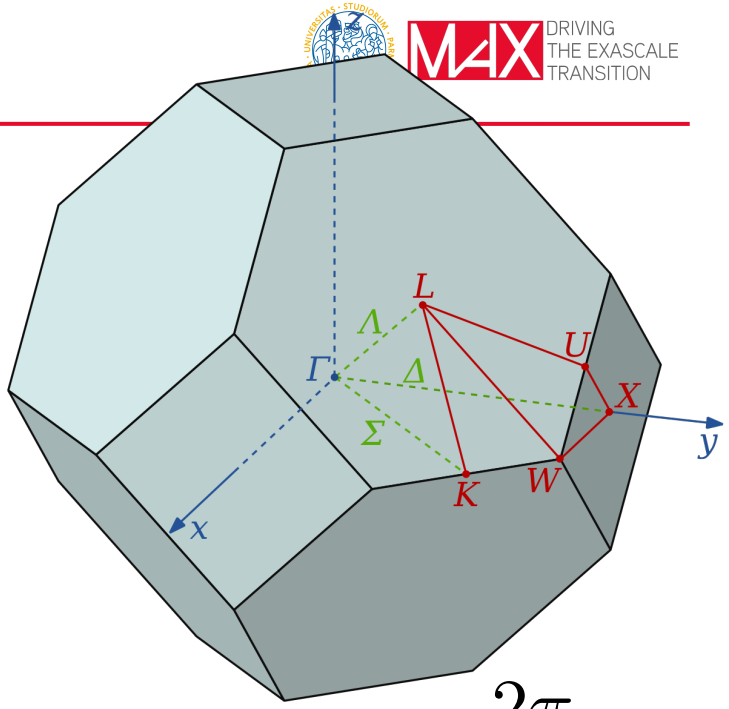



(real|complex) eigen iterative generalized
(real|complex) diagonalization Hermitean generalized

# How is time spent by pw.x



# Plane waves




## Orbitals in Fourier space

$$\phi_i(\boldsymbol{r}) = \int \phi_i(\boldsymbol{g}) e^{i\boldsymbol{g}\boldsymbol{r}} d^3\boldsymbol{g}$$

$$\mathbf{G}_m = m_1 \cdot \mathbf{a}^* + m_2 \cdot \mathbf{b}^* + m_3 \cdot \mathbf{c}^*$$

$$\boldsymbol{a}^* = \frac{2\pi}{\Omega} \boldsymbol{b} \times \boldsymbol{c}$$

## For a periodic system (Bloch's Theorem)

$$\phi_i(\boldsymbol{r}) = u_{ik}(\boldsymbol{r}) e^{i\boldsymbol{k}\boldsymbol{r}}$$

$$\phi_{i,\boldsymbol{k}}(\boldsymbol{r}) = \sum_{\boldsymbol{G}} c_{\boldsymbol{k},\boldsymbol{G}} \frac{1}{\sqrt{\Omega}} e^{i(\boldsymbol{G}+\boldsymbol{k})\boldsymbol{r}}$$

## Complete basis set!

$\boldsymbol{k}$ is in FBZ

# Plane waves

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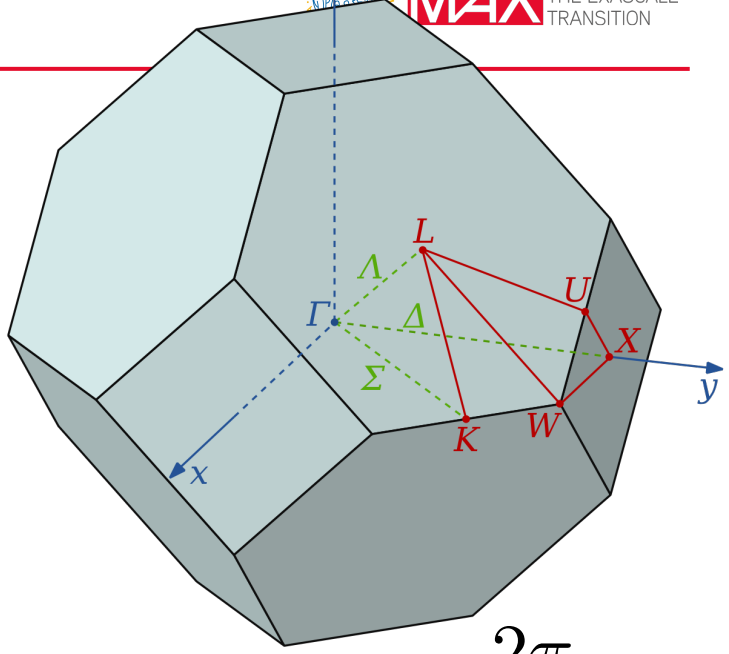



$$\boldsymbol{a}^* = \frac{2\pi}{\Omega} \boldsymbol{b} \times \boldsymbol{c}$$

## For a periodic system (Bloch's Theorem)

$$\phi_{i,\boldsymbol{k}}(\boldsymbol{r}) = \sum_{\boldsymbol{G}}^{|\boldsymbol{G}|<G_{max}} c_{\boldsymbol{k},\boldsymbol{G}} \frac{1}{\sqrt{\Omega}} e^{i(\boldsymbol{G}+\boldsymbol{k})\boldsymbol{r}}$$

$$E_c = \frac{\hbar^2 |\boldsymbol{G}_{max} + \boldsymbol{k}|^2}{2m_e}$$

$\boldsymbol{k}$ is in FBZ

# Plane waves

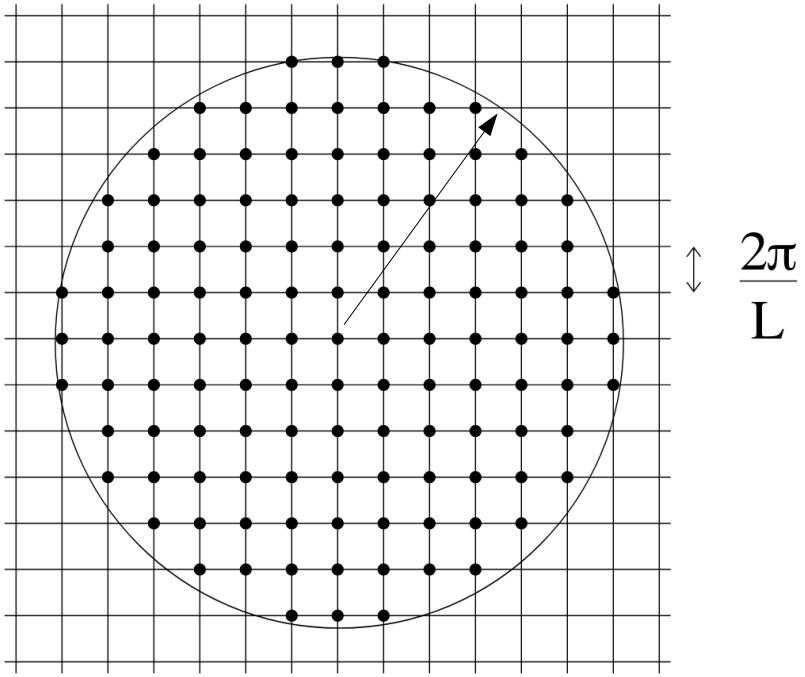
$$E_c = \frac{\hbar^2 G_{max}^2}{2m_e}$$

$$V_{sphere} = \frac{4}{3}\pi G_{max}^3$$

$$V_{PW} = \frac{(2\pi)^3}{\Omega}$$

Cell volume

$$N_{G_{max}} \propto \Omega E_c^{3/2}$$



# Computation and data

$$\sum_{m'} H_{m,m'}(\boldsymbol{k}) c_{i,m'}(\boldsymbol{k}) = \epsilon_i(\boldsymbol{k}) c_{i,m}(\boldsymbol{k})$$

$$\phi_{\boldsymbol{i},\boldsymbol{k}}(\boldsymbol{r}) \propto \sum_{\boldsymbol{G}} c_{i,\boldsymbol{G}}(\boldsymbol{k}) e^{i(\boldsymbol{G}+\boldsymbol{k})\boldsymbol{r}}$$

How to split tasks and data among many workers
(not necessarily close to each others)

# Computation and data

$$\sum_{m'} H_{m,m'}(\boldsymbol{k}) c_{i,m'}(\boldsymbol{k}) = \epsilon_i(\boldsymbol{k}) c_{i,m}(\boldsymbol{k})$$

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Multiple k points:
pools of processors

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Multiple k points:
pools of processors

G domain decomposition: band group

# Computation and data

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Multiple k points:
pools of processors

Multiple KS states

G domain decomposition: band group

# Solving the eigenvalue problem

$$\sum_{m'} H_{m,m'}(\boldsymbol{k}) c_{i,m'}(\boldsymbol{k}) = \epsilon_i(\boldsymbol{k}) c_{i,m}(\boldsymbol{k})$$

Diagonalize → $\{\phi_i, \epsilon_i\}, i = 1 \ldots N_G$

What is actually needed are $\sim \frac{1}{2} N_e$ orbitals

Guess $|\phi_j\rangle \; j = 1 \ldots N_b$ prepare $H(\rho)$ $h_{\phi_i \phi_j} = \langle \phi_i | H | \phi_j \rangle$

# Solving the eigenvalue problem

$$\sum_{m'} H_{m,m'}(\boldsymbol{k}) c_{i,m'}(\boldsymbol{k}) = \epsilon_i(\boldsymbol{k}) c_{i,m}(\boldsymbol{k})$$

Diagonalize

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$$h_{\phi_i \phi_j} = \langle \phi_i | H | \phi_j \rangle$$

$$\boldsymbol{h}\boldsymbol{v}_k = \tilde{\epsilon}_k \boldsymbol{v}_k$$

$$|\tilde{\phi}_k\rangle = \sum_j v_{jk} |\phi_j\rangle$$

# Solving the eigenvalue problem

$$\sum_{m'} H_{m,m'}(\boldsymbol{k}) c_{i,m'}(\boldsymbol{k}) = \epsilon_i(\boldsymbol{k}) c_{i,m}(\boldsymbol{k})$$

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What is actually needed are $\sim \frac{1}{2} N_e$ orbitals

Guess $|\phi_j\rangle \; j = 1 \ldots N_b$ prepare $H(\rho)$ → $h_{\phi_i \phi_j} = \langle \phi_i | H | \phi_j \rangle$

Now use $|\phi_j\rangle |\delta_j\rangle \quad j = 1 \ldots N_b$ to build

$$\boldsymbol{h}\boldsymbol{v}_k = \tilde{\epsilon}_k \boldsymbol{v}_k$$

$$\delta_k = \left(H_{diag} - \epsilon_k S_{diag}\right)^{-1} \left(H - \epsilon_k S\right) |\phi_k\rangle$$

$$|\tilde{\phi}_k\rangle = \sum_j v_{jk} |\phi_j\rangle$$

# Solving the eigenvalue problem

$$\sum_{m'} H_{m,m'}(\boldsymbol{k}) c_{i,m'}(\boldsymbol{k}) = \epsilon_i(\boldsymbol{k}) c_{i,m}(\boldsymbol{k})$$

Diagonalize → $\{\phi_i, \epsilon_i\}, i = 1 \ldots N_G$

What is actually needed are $\sim \frac{1}{2} N_e$ orbitals

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$$|\tilde{\phi}_k\rangle = \sum_j v_{jk} |\phi_j\rangle$$

Really small?

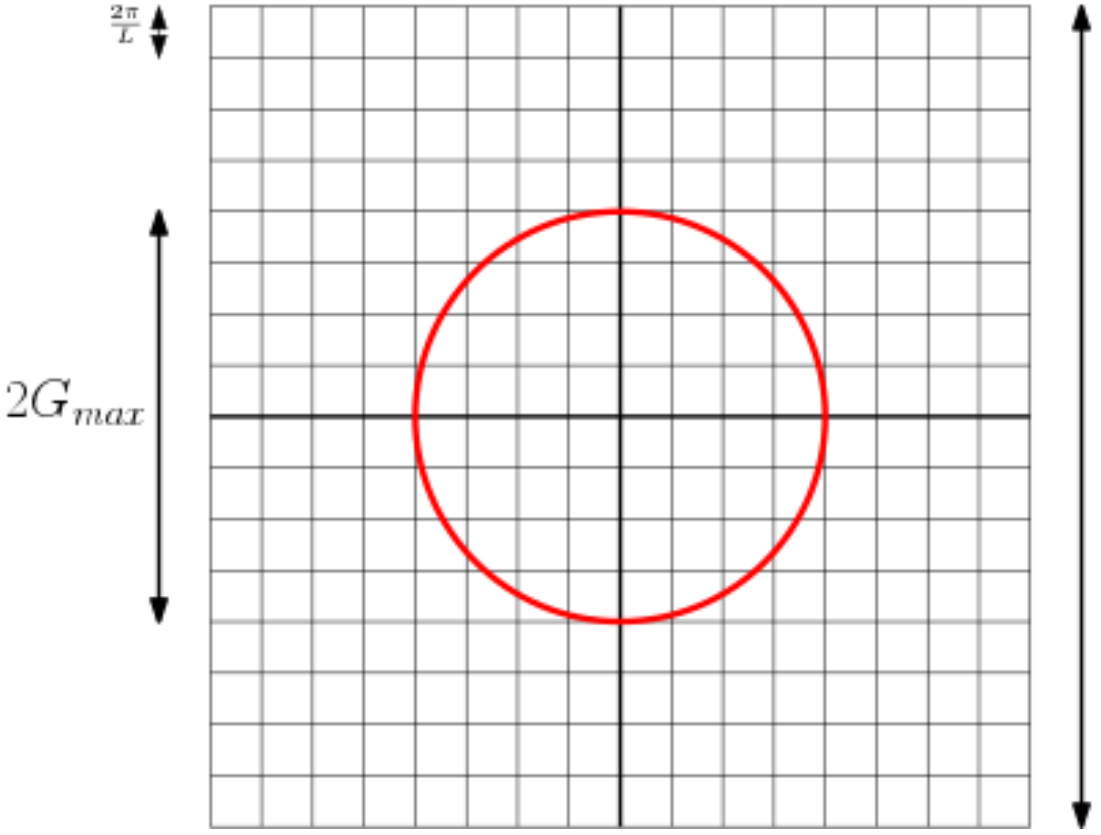
# Wave-function & density

$$\rho(\boldsymbol{r}) = \sum_i \sum_{\boldsymbol{k}} w_{\boldsymbol{k}} f_{i\boldsymbol{k}} |\phi_{i\boldsymbol{k}}(r)|^2$$

$$\rho(\boldsymbol{r}) \propto \sum_i \sum_{\boldsymbol{k}} w_{\boldsymbol{k}} f_{i\boldsymbol{k}} \sum_{G_{max}} \sum_{G'_{max}} c_{i\boldsymbol{k}}(\boldsymbol{G'})^* c_{i\boldsymbol{k}}(\boldsymbol{G}) e^{i(\boldsymbol{G}-\boldsymbol{G'})\boldsymbol{r}}$$

$$\rho(\boldsymbol{r}) \propto \sum_{\boldsymbol{G} \leq 2G_{max}} \rho(\boldsymbol{G}) e^{i\boldsymbol{G}\boldsymbol{r}}$$

# Real and reciprocal space

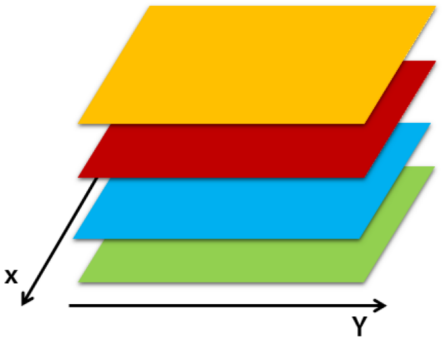


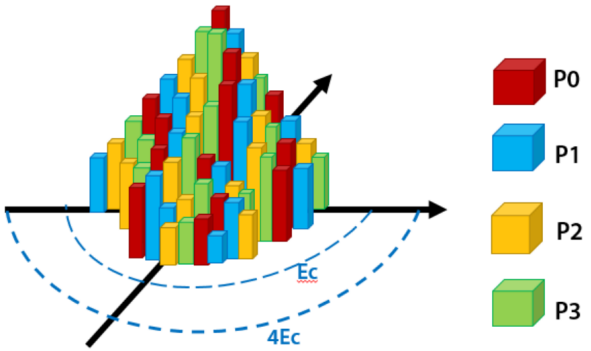

$$c_{i\boldsymbol{k}}(\boldsymbol{r}) = \sum_{\boldsymbol{G}} c_{i\boldsymbol{k}}(\boldsymbol{G}) e^{i\boldsymbol{G}\boldsymbol{r}}$$

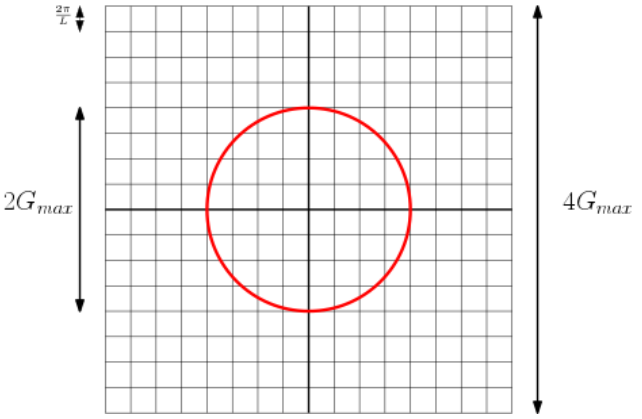
FFT

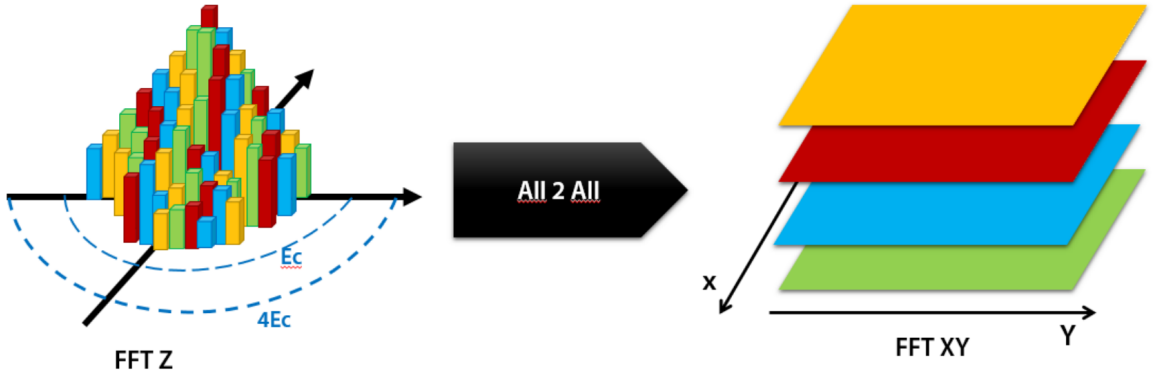
$$c_{i\boldsymbol{k}}(\boldsymbol{G}) = \frac{1}{N} \sum_{\boldsymbol{r}} c_{i\boldsymbol{k}}(\boldsymbol{r}) e^{-i\boldsymbol{G}\boldsymbol{r}}$$

# Real and reciprocal space




F(Gx, Gy, Gz)

F(Gx, Gy, Rz)

1D FFT

fft_scatter

F(Gx, Gy, Rz)

F(Rx, Ry, Rz)

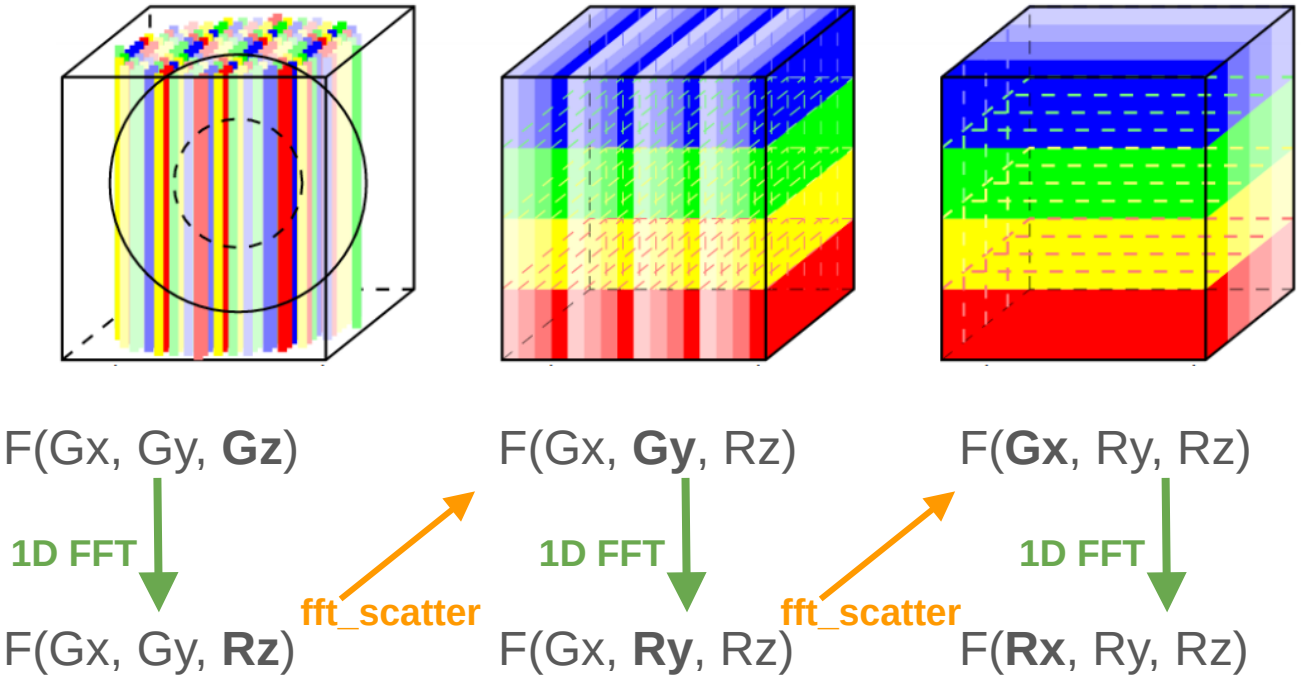
2D FFT

Eric Pascolo, master thesis

# Distribute FFT?

- In real space, distributed as slices
- In reciprocal space, distributed as sticks
- How to scale above nz planes?
  - Distribute the other dimension(s)
  - Split processors and compute multiple FFT

# Multiple 1D FFTs



# Local potential

The local potential contribution is computed more efficiently in real space:

$$\psi_{ik}(\boldsymbol{G}) \xrightarrow{FFT} \psi_{ik}(\boldsymbol{r})$$

$$[v_{KS}\psi_{ik}](\boldsymbol{r}) = v_{KS}(\boldsymbol{r})\psi_{ik}(\boldsymbol{r})$$

$$[v_{KS}\psi_{ik}](\boldsymbol{r}) \xrightarrow{FFT} [v_{KS}\psi_{ik}](\boldsymbol{G})$$

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$$[v_{KS}\psi_{ik}](\boldsymbol{r}) = v_{KS}(\boldsymbol{r})\psi_{ik}(\boldsymbol{r})$$

$$[v_{KS}\psi_{ik}](\boldsymbol{r}) \xrightarrow{FFT} [v_{KS}\psi_{ik}](\boldsymbol{G})$$

# Task groups

## vloc_psi

```
  IF( use_tg ) THEN
  ELSE
     DO ibnd = 1, m
        !
        psic(:) = (0.d0, 0.d0)
        psic (nls (igk_k(1:n,current_k))) = psi(1:n, ibnd)
        !
        CALL invfft ('Wave', psic, dffts)
        !
!$omp parallel do
        DO j = 1, dffts%nnr
           psic (j) = psic (j) * v(j)
        ENDDO
!$omp end parallel do
        !
        CALL fwfft ('Wave', psic, dffts)
        !
        !   addition to the total product
        !
!$omp parallel do
        DO j = 1, n
           hpsi (j, ibnd)   = hpsi (j, ibnd)   + psic (nls(igk_k(j,current_k)))
        ENDDO
!$omp end parallel do
        !
     ENDDO
  ENDIF
```

Orbitals

Wave-function

Compute G-space to R-space

Compute R-space to G-space

Add to hpsi

# Task groups

```
IF( use_tg ) THEN

   CALL tg_get_nnr( dffts, right_nnr )

   DO ibnd = 1, m, fftx_ntgrp(dffts)
      !
      tg_psic = (0.d0, 0.d0)
      ioff   = 0
      !
      DO idx = 1, fftx_ntgrp(dffts)
      !
      CALL  invfft ('tgWave', tg_psic, dffts )
      !
      CALL tg_get_group_nr3( dffts, right_nr3 )
      !
!$omp parallel do
      DO j = 1, dffts%nr1x*dffts%nr2x* right_nr3
         tg_psic (j) = tg_psic (j) * tg_v(j)
      ENDDO
!$omp end parallel do
      !
      CALL fwfft ('tgWave',  tg_psic, dffts )
      !
      !   addition to the total product
      !
      ioff   = 0
      !
      CALL tg_get_recip_inc( dffts, right_inc )
      !
      DO idx = 1, fftx_ntgrp(dffts)
      !
   ENDDO
ELSE
```

More than one band at a time

```
      DO idx = 1, fftx_ntgrp(dffts)

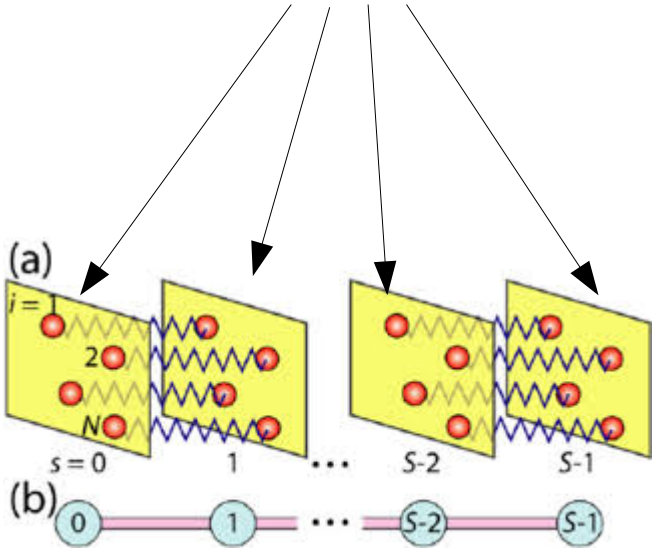
         IF( idx + ibnd - 1 <= m ) THEN
!$omp parallel do
            DO j = 1, n
               tg_psic(nls (igk_k(j,current_k))+ioff) =  psi(j,idx+ibnd-1)
            ENDDO
!$omp end parallel do
         ENDIF

         ioff = ioff + right_nnr
      ENDDO
```

# Other options for parallelism

## Nudged Elastic Band

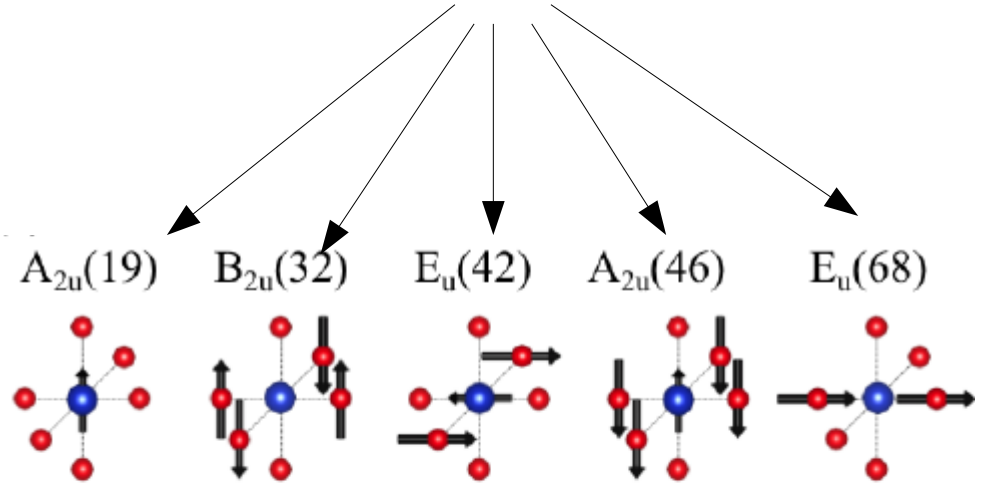
Images




DOI: 10.1016/j.cpc.2007.09.011

## PHonon (linear response)

Irreducible modes




DOI: 10.1103/PhysRevB.93.174419

# Other options for parallelism

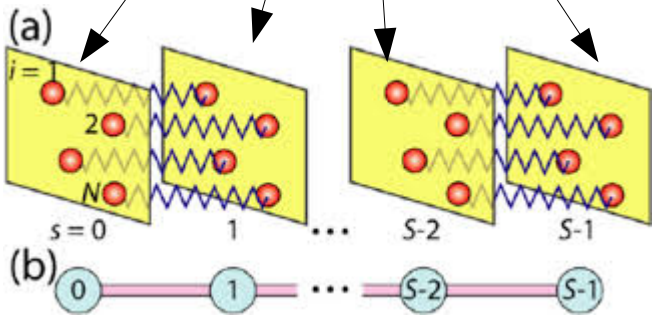
## Nudged Elastic Band

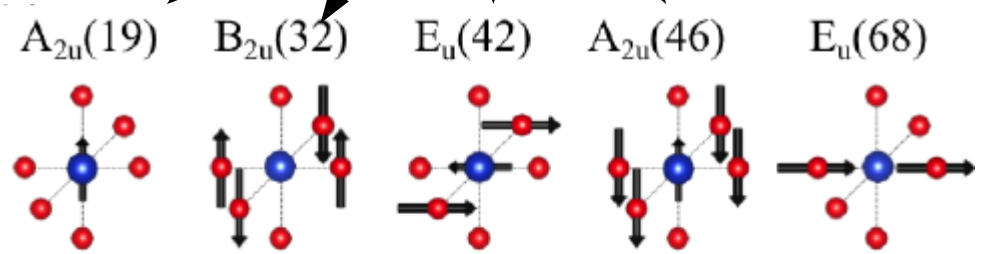
## PHonon (linear response)

Images

Irreducible modes

Abstract layer for embarassingly parallel tasks



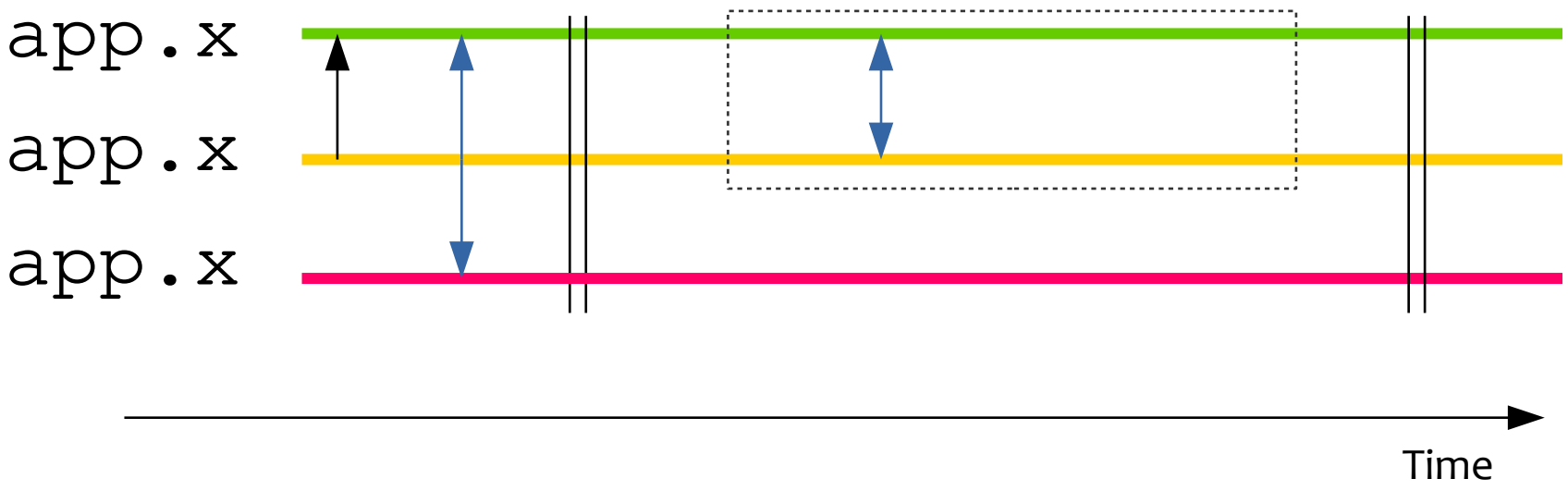

DOI: 10.1016/j.cpc.2007.09.011

DOI: 10.1103/PhysRevB.93.174419

# MPI

## Message Passing Interface:

```
mpirun -np 3 app.x
```

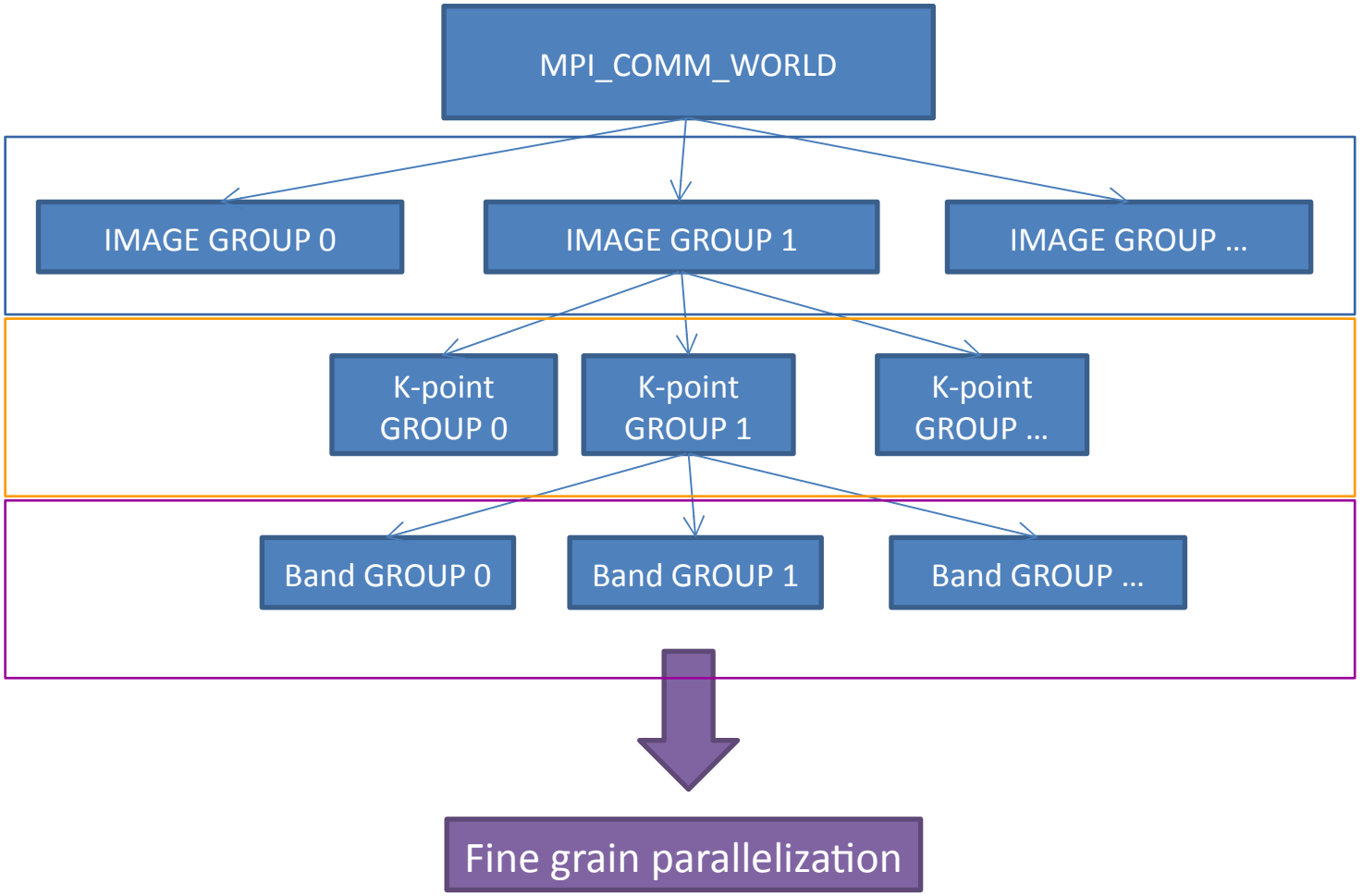


# QE parallelization layout

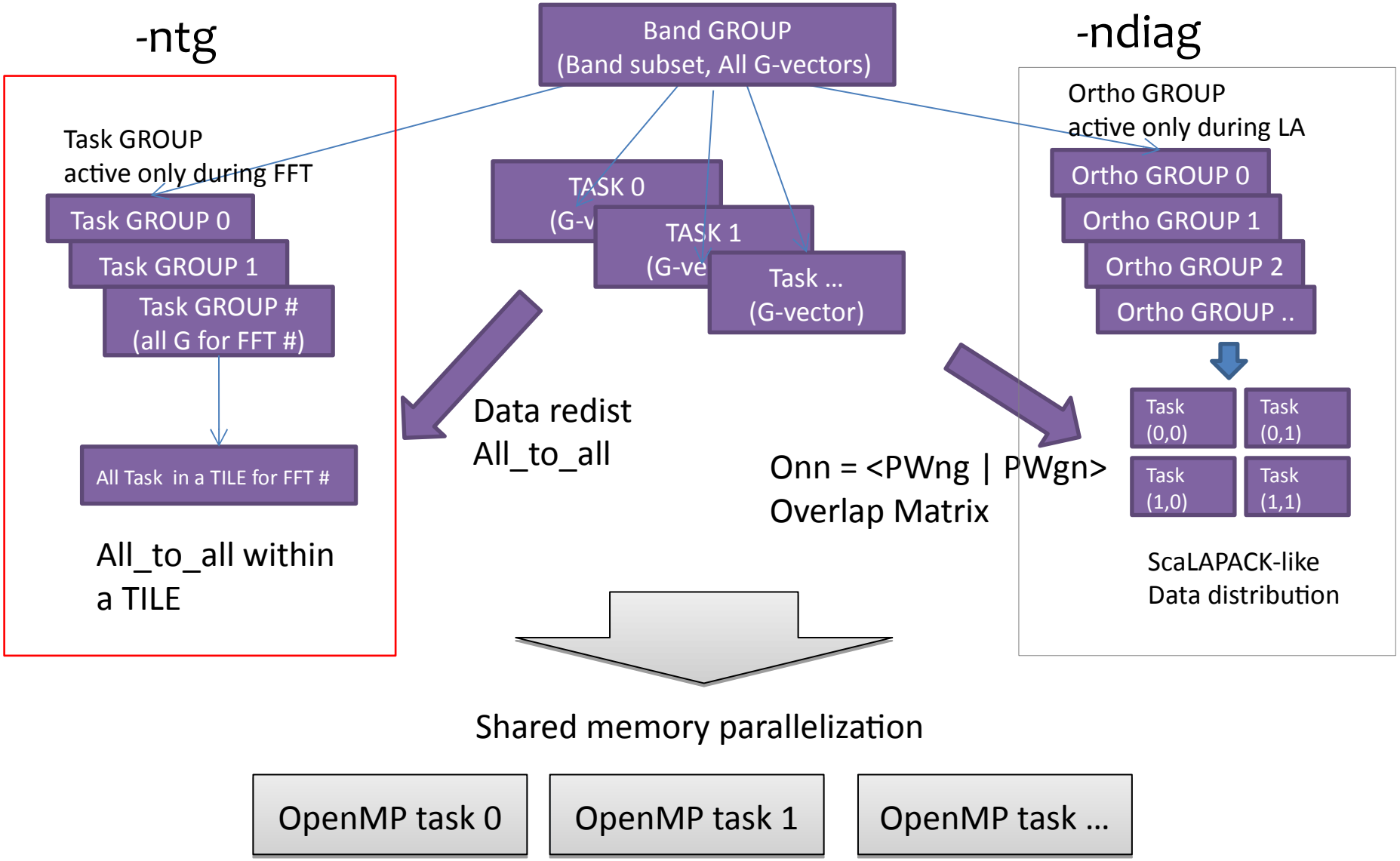
-nimage

-npool

what remains

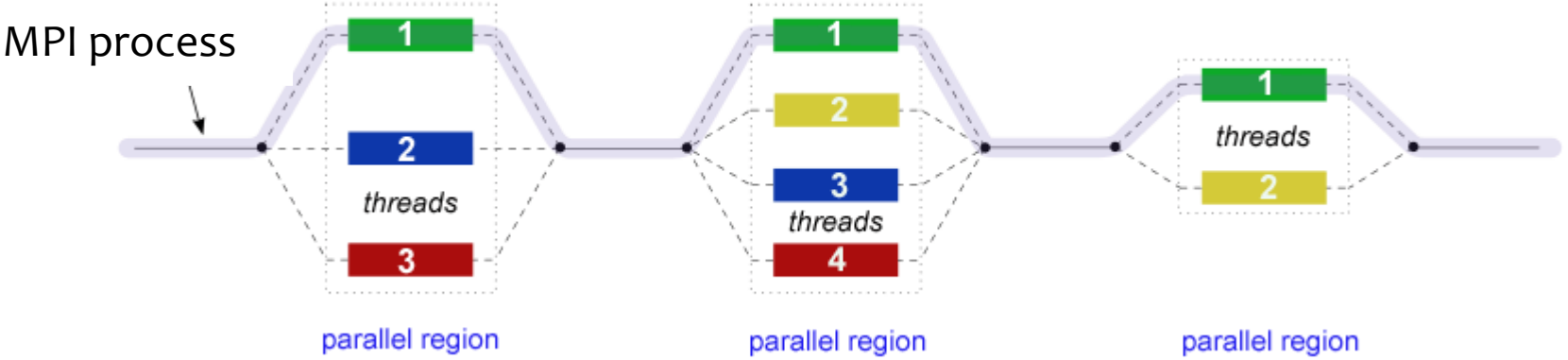


# QE parallelization layout



# What is OpenMP

Multi-platform *shared memory* multiprocessing programming.




Used in:

* BLAS and LAPACK libraries (example, MKL)
* FFT library
* Explicit in QE, still mainly fork & join paradigm

# Parallelization, in practice

## Distribution of images

```
mpirun neb.x -nimage I -inp neb.in > neb.out
```

Output:

```
     path-images division:  nimage    =     I
```

Max value: total number of images in the simulation.

Constraints:
- Depend on code using this "abstract" parallelism

Tentative optimal value: `nimage` = max possible value

# Parallelization, in practice

## Distribution of k points

```
mpirun pw.x -npool X -inp pw.in > pw.out
```

Output:

```
     K-points division:     npool     =       X
```

Distribute k points among `X` pools of MPI procs.
Max value: n(k)

Constraints:
- at least 1 k point per MPI process
- Must be a divisor of the total number of processes

Tentative optimal value: npool = max(n(k))

# Parallelization, in practice

## Parallel diagonalization

```
mpirun pw.x -npool X -ndiag Y -inp pw.in > pw.out
```

Output

```
Subspace diagonalization (size of sub-group: sqrt(Y)*sqrt(Y) procs)
```

Distribute and parallelize matrix diagonalization and matrix-matrix multiplications needed in iterative diagonalization (pw.x) or orthonormalization(cp.x).

Max value: n(MPI)/X
Constraints:

- Must be square
- Must be smaller than band-group size

Tentative optimal value:

- Use it for inputs with more than 100 KS;
- depends on many architectural parameters

# Parallelization, in practice

## FFT task groups

```
mpirun pw.x -npool X -ntg Y -inp pw.in > pw.out
```

Output

```
     R & G space division:  proc/nbgrp/npool/nimage =    1152
     wavefunctions fft division:  Y-proc x Z-proc =      Y     96
     wavefunctions fft division:  task group distribution
                                  #TG    x Z-proc =      Y     96
```

Each plane-wave group of processors is split into `ntg` task groups of nFFT processors, with ntg×nFFT= nBGRP; each task group takes care of the FFT over $N_{KS}$/ntg states.

Max value: n(MPI)/X

Constraints:

- Must be divisor of nBGRP (for nyfft)

Tentative optimal value: use when nBGRP~nr3 or larger, depends on the HPC system.

# Parallelization, in practice

- OpenMP
  - In the code and **in the libraries**.
  - Only when MPI is saturated.
  - Generally no more than 8 threads.
  - Don't forget it!
- Multithreading
  - Generally not useful (not memory bound)

# Parallelization, recap

- Pools:
  - Very effective, small communication
  - A lot of memory duplication!
- G vectors:
  - Lower memory duplication
  - More communication
- OpenMP:
  - Practically no memory duplication
  - When MPI is saturated
- Diagonalization method:
  - Davidson: faster, more memory
  - CG: slower, less memory

# Compile QE

- Get & compile ELPA (already done for you today)
- Load/use machine specific math libs. (eg. Intel® MKL)
- Configure QE with scalapack, ELPA and OpenMP:

```
$ ./configure --enable-openmp --with-scalapack=intel \
--with-elpa-include=/path/to/elpa-2016.11.001.pre/modules \
--with-elpa-lib=/path/to/elpa-2016.11.001.pre/.libs/
libelpa_openmp.a
```

```
The following libraries have been found:
  BLAS_LIBS=  -lmkl_intel_lp64  -lmkl_intel_thread -lmkl_core
  LAPACK_LIBS=
  SCALAPACK_LIBS=-lmkl_scalapack_lp64 -lmkl_blacs_intelmpi_lp64
  ELPA_LIBS=/marconi_scratch/userinternal/pbonfa01/school/pw-elpa-bdw/
elpa-2016.11.001.pre/.libs/libelpa_openmp.a
  FFT_LIBS=
```

# Advanced compilation options

- Check make.inc
- Add optimization flags, eg.
  - KNL → AVX512MIC
  - SKL → AVX512CORE
- Possibly add profiling libraries
  - Gperftools → memory profiling
  - GPTL → accurate timing

# Check flags

How make.inc should look like on an Intel based platform...

```
MANUAL_DFLAGS  =
DFLAGS         =  -D__DFTI -D__MPI -D__SCALAPACK -D__ELPA_2016
FDFLAGS        = $(DFLAGS) $(MANUAL_DFLAGS)

[…]

MPIF90         = mpiifort
F90            = ifort
CC             = icc
F77            = ifort

# C preprocessor and preprocessing flags - for explicit
preprocessing,
# if needed (see the compilation rules above)
# preprocessing flags must include DFLAGS and IFLAGS

CPP            = cpp
CPPFLAGS       = -P -traditional $(DFLAGS) $(IFLAGS)
```

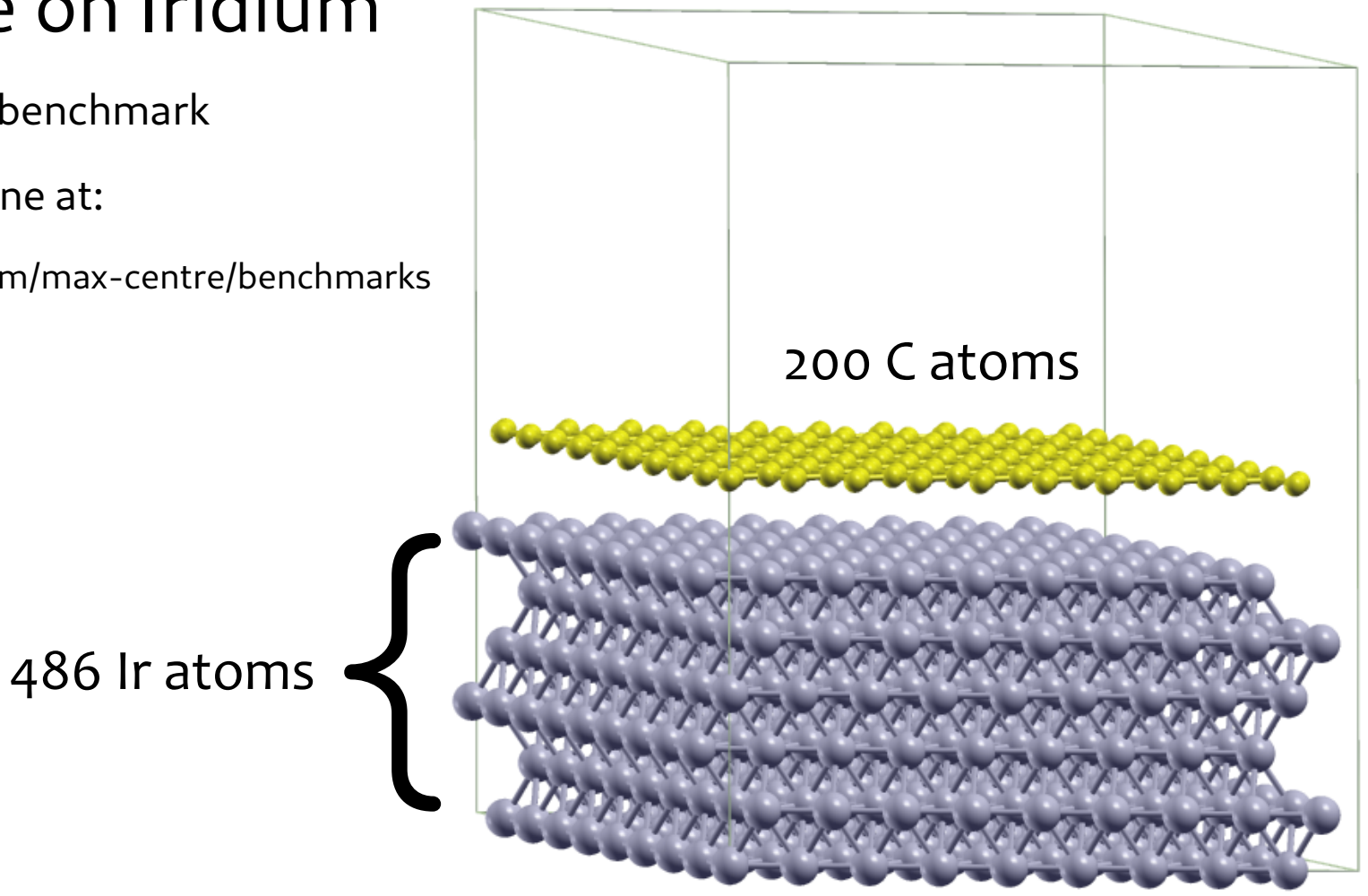
# A real case

## Grafene on Iridium

Standard QE benchmark

Available online at:

https://gitlab.com/max-centre/benchmarks



# Input

```
 &control
    calculation = 'scf'
    prefix='GRIR'
    restart_mode='from_scratch'
    pseudo_dir='./',
    outdir='/path/to/scratch'
 /
 &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
```

How many k points?

How many states?

How many G vectors?

How would you run it?

# Naive run output

```
Program PWSCF v.6.2 starts on  1Dec2017 at  9:56:26

This program is part of the open-source Quantum ESPRESSO suite
for quantum simulation of materials; please cite
    "P. Giannozzi et al., J. Phys.:Condens. Matter 21 395502 (2009);
    "P. Giannozzi et al., J. Phys.:Condens. Matter 29 465901 (2017);
     URL http://www.quantum-espresso.org",
in publications or presentations arising from this work. More details at
http://www.quantum-espresso.org/quote

Parallel version (MPI & OpenMP), running on     144 processor cores
Number of MPI processes:                144
Threads/MPI process:                      1

MPI processes distributed on     4 nodes
K-points division:     npool     =       4
R & G space division:  proc/nbgrp/npool/nimage =      36
Reading input from grir686.in

Current dimensions of program PWSCF are:
Max number of different atomic species (ntypx) = 10
Max number of k-points (npk) =  40000
Max angular momentum in pseudopotentials (lmaxx) =  3
          file Ir.pbe-paw_kj.UPF: wavefunction(s)  5D renormalized

Subspace diagonalization in iterative solution of the eigenvalue problem:
a serial algorithm will be used


Parallelization info
--------------------
sticks:   dense  smooth     PW     G-vecs:    dense   smooth      PW
Min         497     497    128                68583    68583    9018
Max         498     498    129                68592    68592    9025
Sum       17917   17917   4639              2469147  2469147  324807
```

# Memory

```
Dynamical RAM for                 wfc:     406.00 MB
Dynamical RAM for     wfc (w. buffer):    1217.99 MB
Dynamical RAM for           str. fact:       2.09 MB
Dynamical RAM for           local pot:       0.00 MB
Dynamical RAM for          nlocal pot:    1353.50 MB
Dynamical RAM for                qrad:      13.00 MB
Dynamical RAM for          rho,v,vnew:      15.18 MB
Dynamical RAM for               rhoin:       5.06 MB
Dynamical RAM for            rho*nmix:      33.49 MB
Dynamical RAM for           G-vectors:       4.45 MB
Dynamical RAM for          h,s,v(r/c):    7056.75 MB
Dynamical RAM for          <psi|beta>:     490.12 MB
Dynamical RAM for                 psi:    1623.99 MB
Dynamical RAM for                hpsi:    1623.99 MB
Dynamical RAM for                spsi:    1623.99 MB
Dynamical RAM for      wfcinit/wfcrot:    1966.26 MB
Dynamical RAM for           addusdens:     704.31 MB
Estimated static dynamical RAM per process >       2.59 GB
Estimated max dynamical RAM per process >      14.72 GB
Estimated total dynamical RAM >    2120.01 GB
```

1) This is a lower estimate!
2) MPI itself requires memory
3) Rule of thumb: crash without error message.

# Happens more often than not

```
$ salloc --nodes=12 --ntasks-per-node=36
```

# Happens more often than not

```
$ salloc --nodes=12 --ntasks-per-node=36
```

```
Program PWSCF v.6.2 starts on 29Nov2017 at 15:22:59

This program is part of the open-source Quantum ESPRESSO suite
for quantum simulation of materials; please cite
    "P. Giannozzi et al., J. Phys.:Condens. Matter 21 395502 (2009);
    "P. Giannozzi et al., J. Phys.:Condens. Matter 29 465901 (2017);
     URL http://www.quantum-espresso.org",
in publications or presentations arising from this work. More details at
http://www.quantum-espresso.org/quote

Parallel version (MPI & OpenMP), running on   15552 processor cores
Number of MPI processes:               432
Threads/MPI process:                    36

MPI processes distributed on    12 nodes
K-points division:     npool     =       2
R & G space division:  proc/nbgrp/npool/nimage =     216
Reading input from grir686.in

Current dimensions of program PWSCF are:
Max number of different atomic species (ntypx) = 10
Max number of k-points (npk) =  40000
Max angular momentum in pseudopotentials (lmaxx) =  3
```

# Minimal jobscript

```
$ salloc --nodes=4 --ntasks-per-node=36 --ncpus-per-task=1 --
mem=100G -t 0:25:00

Waiting for job to start...

$ export OMP_NUM_THREADS=1
$ export MKL_NUM_THREADS=1
$ export KMP_AFFINITY=scatter,granularity=fine,1


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

# Running on CINECA's BDW…

```
#!/bin/bash
#SBATCH -N 4
#SBATCH --tasks-per-node=36
#SBATCH --partition=bdw_usr_prod
#SBATCH --time=23:55:00

$ export OMP_NUM_THREADS=1
$ export MKL_NUM_THREADS=1
$ export KMP_AFFINITY=scatter,granularity=fine,1


mpirun pw.x -npool 1 -ndiag 144 -ntg 1 -inp pw.in > pw.out
```

Estimated max dynamical RAM per process > 2.97 GB

# Running on CINECA's BDW…

```
&control
   calculation = 'scf'
   prefix='GRIR'
   max_seconds=20000 !42000
   restart_mode='from_scratch'
   pseudo_dir='./',
   outdir='./tmp',
   disk_io = 'high'
/
&system
   ibrav=  4
       celldm(1) = 46.5334237988185d0
       celldm(3) =  1.274596
   nat=  686
   ntyp= 2,
   ecutwfc=30
   !nbnd=3300
   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='cg'
   electron_maxstep = 1
 /
```

```
d

ranularity=fine,1

-ntg 1 -inp pw.in > pw.out
```

RAM per process > **2.97 GB**

Estimated max dynamical RAM per process > **1.38 GB**

# Running on CINECA's BDW…

```
&control
   calculation = 'scf'
   prefix='GRIR'
   max_seconds=20000 !42000
   restart_mode='from_scratch'
   pseudo_dir='./',
   outdir='./tmp',
   disk_io = 'high'
/
&system
   ibrav=  4
       celldm(1) = 46.5334237988185d0
       celldm(3) =  1.274596
   nat=  686
   ntyp= 2,
   ecutwfc=30
   !nbnd=3300
   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'
   diago_david_ndim='2'
   electron_maxstep = 1
 /
```

```
                                    l
                                    ranularity=fine,1
                                    -ntg 1 -inp pw.in > pw.out
```

RAM per process > **2.97 GB**

# Running on CINECA's BDW…

```
#!/bin/bash
#SBATCH -N 8
#SBATCH --tasks-per-node=36
#SBATCH -mem=115G

$ export OMP_NUM_THREADS=1
$ export MKL_NUM_THREADS=1
$ export KMP_AFFINITY=scatter,granularity=fine,1


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

X: 1 Y: 36 Z: 1

```
R & G space division:  proc/nbgrp/npool/nimage =     288

Subspace diagonalization in iterative solution of the eigenvalue problem:
ELPA distributed-memory algorithm (size of sub-group:  6*  6 procs)

sticks:   dense  smooth     PW     G-vecs:    dense   smooth      PW
Min          62      62     16                 8568     8568    1120
Max          63      63     17                 8578     8578    1132
Sum       17917   17917   4639              2469147  2469147  324807

Dense  grid:  2469147 G-vectors     FFT dimensions: ( 180, 180, 216)
```

# Running on CINECA's BDW…

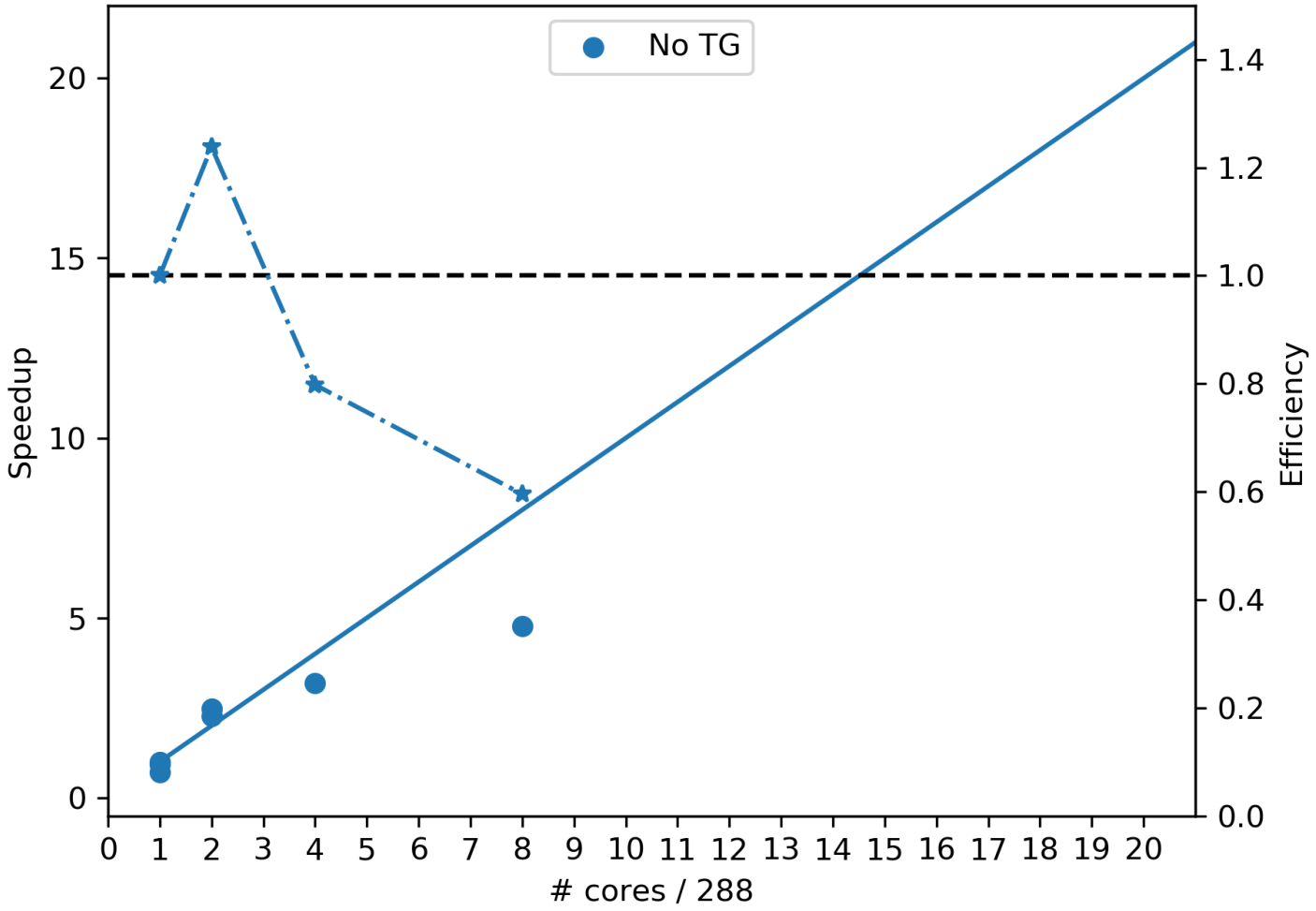
```
#!/bin/bash
#SBATCH -N 8
#SBATCH --tasks-per-node=36
#SBATCH -mem=115G

$ export OMP_NUM_THREADS=1
$ export MKL_NUM_THREADS=1
$ export KMP_AFFINITY=scatter,granularity=fine,1

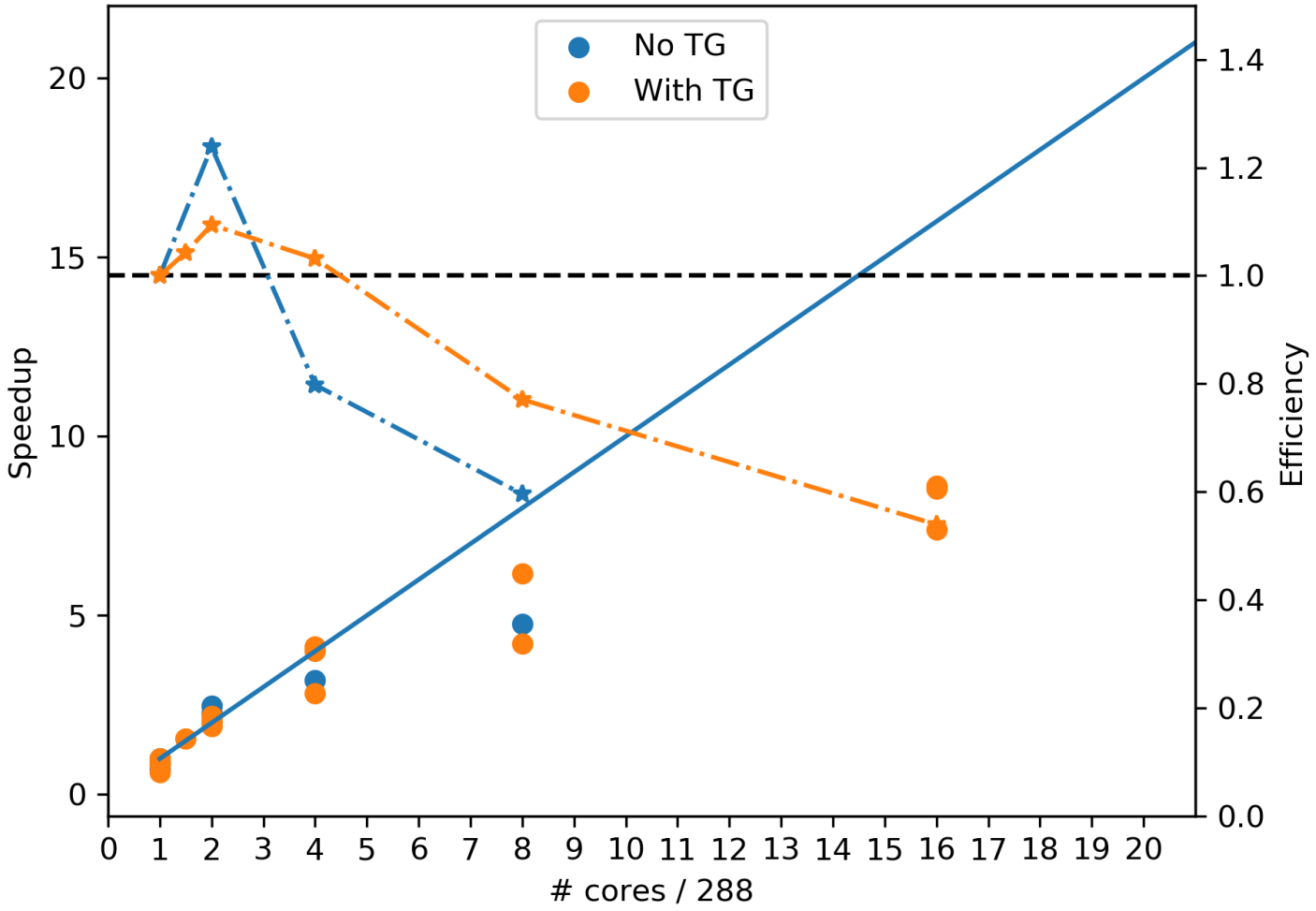

mpirun pw.x -npool X -ndiag Y -ntg Z -inp pw.in > pw.out
```

| X | Y | Z | Time CPU | Time Wall |
|---|---|---|---|---|
| 1 | 36 | 1 | 2071.28s | 2108.70s |
| 1 | 144 | 1 | 1442.97s | 1470.78s |
| 1 | 256 | 1 | 1544.03s | 1576.22s |
| 1 | 144 | 2 | 1286.43s | 1312.28s |
| 1 | 144 | 4 | 1274.49s | 1299.47s |

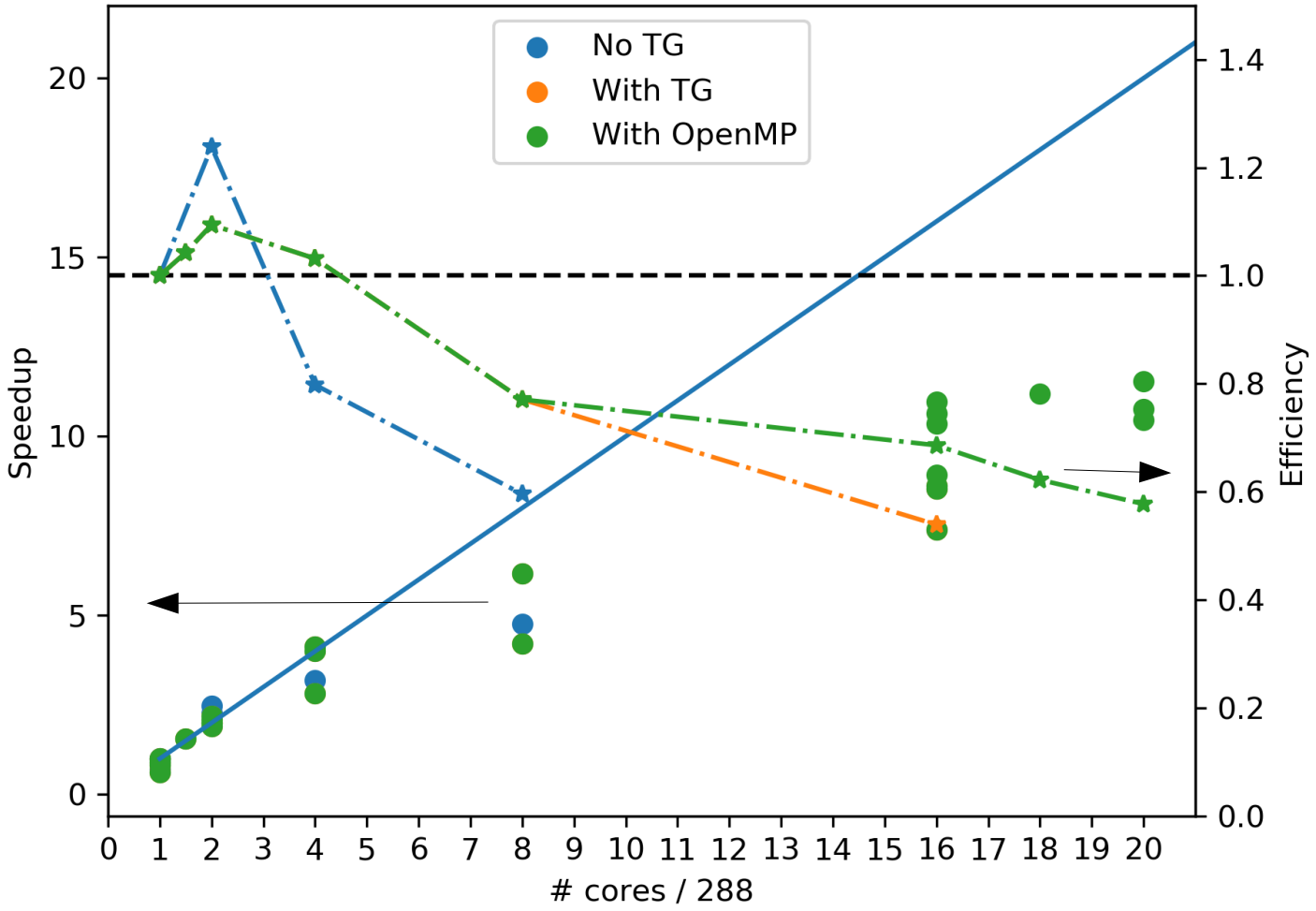
# Running on CINECA's BDW…



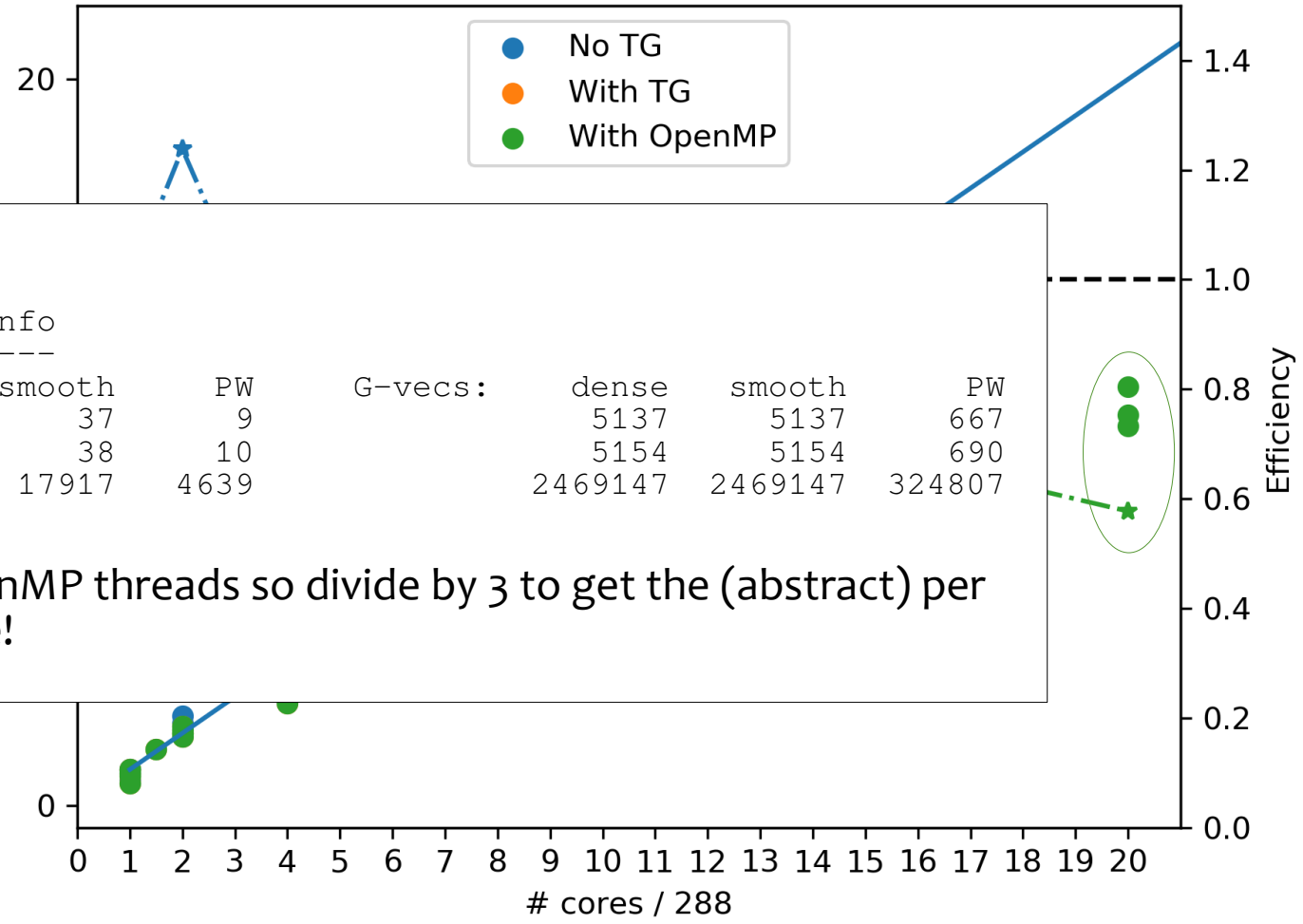
# Running on CINECA's BDW...



# Running on CINECA's BDW...



# Running on CINECA's BDW...




But...

```
Parallelization info
--------------------
sticks:   dense  smooth     PW     G-vecs:    dense   smooth      PW
Min          37      37      9                5137     5137     667
Max          38      38     10                5154     5154     690
Sum       17917   17917   4639             2469147  2469147  324807
```

I was using 3 OpenMP threads so divide by 3 to get the (abstract) per core problem size!

# During the hands-on…

- You will be working in 16 teams.
- You'll have access to 16 nodes equipped with:
  - 2 x 8 cores Intel Hashwell @ 2.60 GHz
  - 60 GB memory
  - 2 NVIDIA Tesla K40 (discussed later)
- You will be guided towards the setup of an optimized version of QE.
  - You are welcome to *try it at home,* we will help (with lower priority though)
- You will experiment with parallel options, but you will not see amazing speedups.
- Exercises are not just copy/paste, you will have to sort out some problems by yourself.

# Slurm scheduler

Optimize resource allocation on clusters

Cheat sheet:

```
sbatch job.sh          # Submit a job
squeue -u $USER        # Check status
scancel jobid          # Cancel a job
```

# Slurm jobfile

```
#!/bin/bash
#SBATCH --nodes=1
#SBATCH --ntasks=X                  # Number of MPI tasks
#SBATCH --ntasks-per-node=X         # Number of MPI tasks per node
#SBATCH --cpus-per-task=Y           # Number of CPUs/per MPI process
#SBATCH --ntasks-per-core=1         # Used for hyperthreading
#SBATCH --reservation=qe2019
#SBATCH --gres=gpu:2                 # make 2 GPUs visible

module load mpi/openmpi-x86_64 MKL/mkl_2019.4.243

export OMP_NUM_THREADS=$SLURM_CPUS_PER_TASK

srun --mpi=pmix /path/to/executable -inp file.in > file.out
```

# Input/output

- A parallel filesystem is basically a parallel application.
- Different performance have different cost:
  - Home directory
  - Long term storage
  - *Scratch space*

**Always set** the `outdir` folder in input to a fast scratch space.

(in our case `/data0/QE/YOURUSERNAME`)

# Your turn…

Open

https://gitlab.com/QEF/material-for-ljubljana-qe-summer-school/tree/master/Day-5

Open a terminal in the VM…

# GPU accelerated QE


Collaboration and support from: J. Romero, M. Marić, M. Fatica, E. Phillips (NVIDIA)
F. Spiga (ARM), A. Chandran (FZJ), I. Girotto (ICTP), Y. Luo (ANL), T. Kurth (NERSC), B. Cook (NERSC),
P. Giannozzi (Univ. Udine), P. Delugas, S. De Gironcoli (SISSA).

# Heterogenous Computing

Gain performance or energy efficiency not just by adding the same type of processors, but by adding dissimilar coprocessors, usually incorporating specialized processing capabilities to handle particular tasks.

# GPGPU

**G**eneral **P**urpose **G**raphical **P**rocessing **U**nits


# The trick...

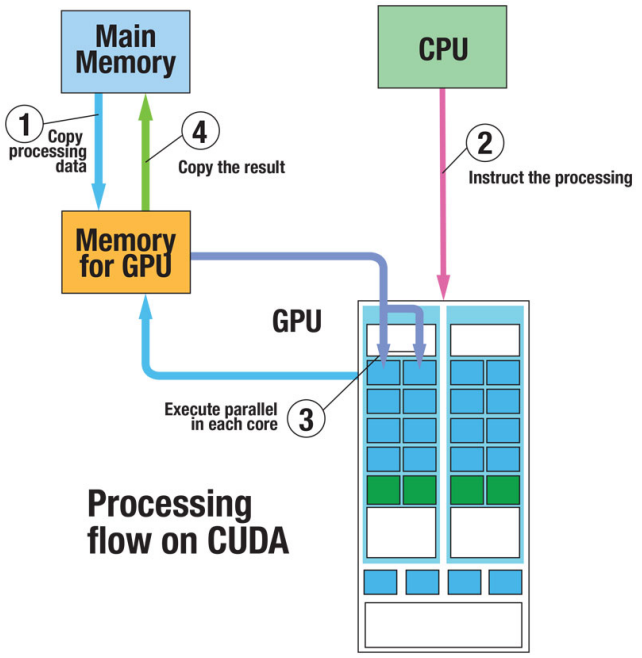
## Difference between GPU and CPU hardware


More transistors devoted to data processing
(but less optimized memory access and speculative execution)

# GPU programming

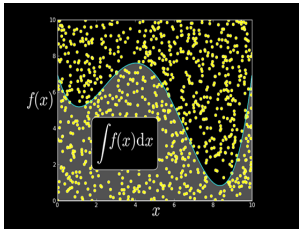
Typical code progression

1)Memory allocated on host and device
2)Data is transferred **from** the *Host* **to** the *Device*
3)Kernel is lunched by the Host on the Device
4)Data is transferred **from** the *Device* **to** the *Host*.
5)Memory is deallocated.

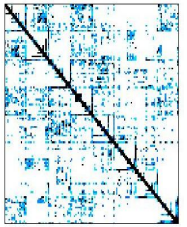


# Libraries

NVIDIA cuBLAS




NVIDIA cuRAND

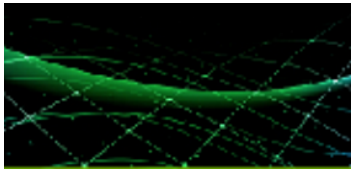


NVIDIA cuSPARSE

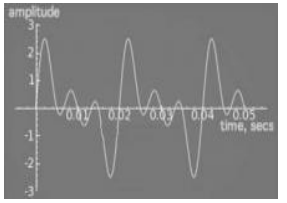
NVIDIA NPP

Vector Signal Image Processing

Matrix Algebra on GPU and Multicore



NVIDIA cuSolver




NVIDIA cuFFT

IMSL Library

**ArrayFire Matrix Computations**

Sparse Linear Algebra

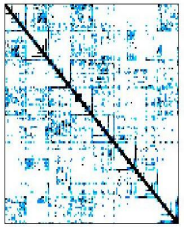
C++ STL Features for CUDA

# Libraries


NVIDIA cuBLAS




NVIDIA cuRAND



NVIDIA cuSPARSE

NVIDIA NPP

GPU VSIPL

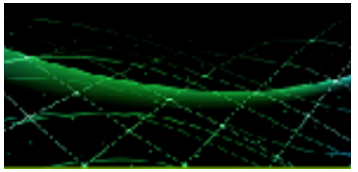
Vector Signal Image Processing

MAGMA

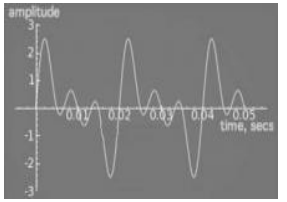
ICL UT

open source initiative

Matrix Algebra on GPU and Multicore



NVIDIA cuSolver




NVIDIA cuFFT

ROGUE WAVE SOFTWARE

IMSL Library

**ArrayFire Matrix Computations**

CUSP

Sparse Linear Algebra

Thrust

C++ STL Features for CUDA

# GPU Hardware details

- NVIDIA Tesla K40

Released: 10/2013

One GPUs (GK110B) per device
**12GB RAM per GPU**

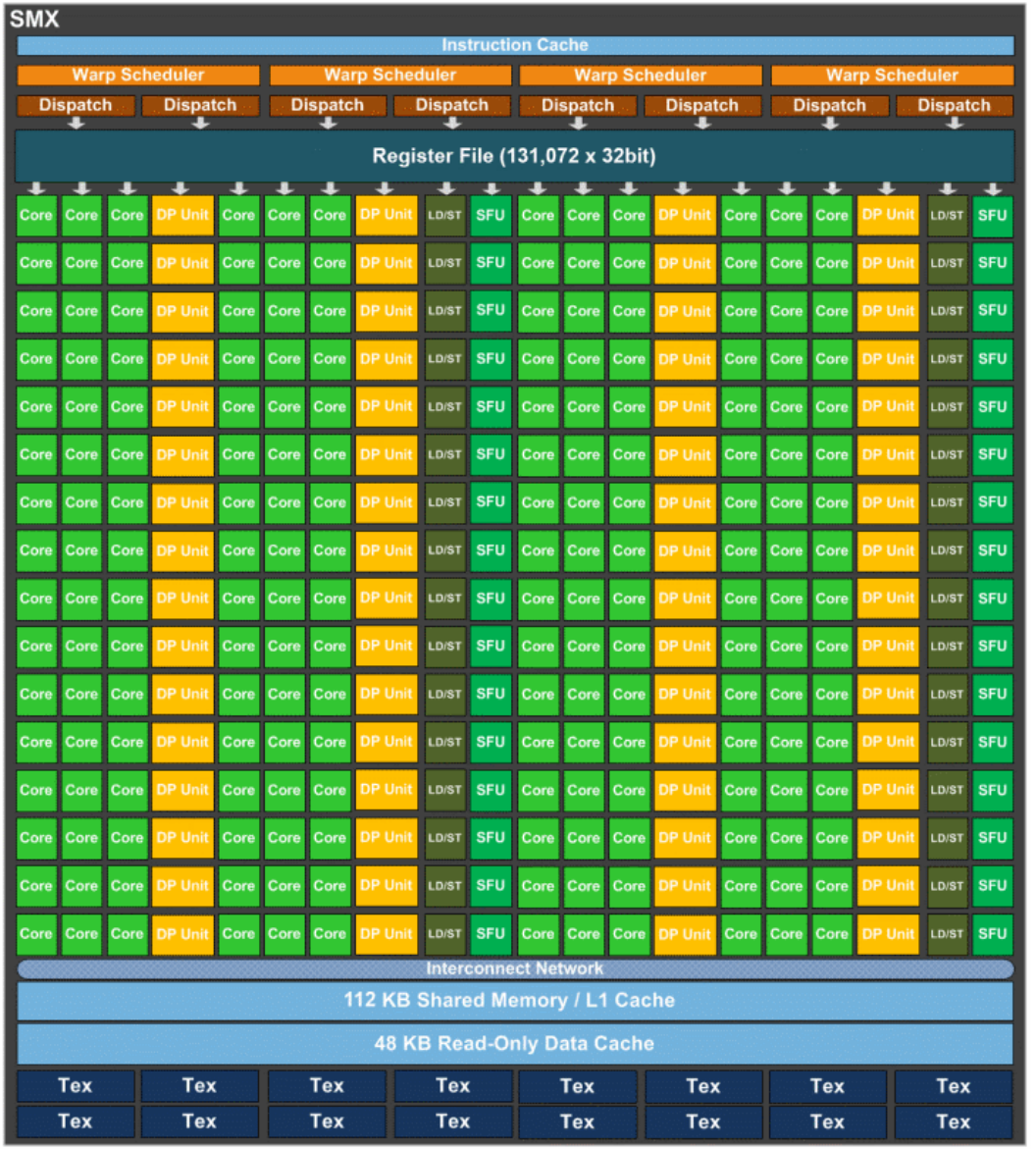
15 **Multiprocessors** (MP),
192 **CUDA Cores**/MP = 2880 CUDA Cores
Running at 500-800 Mhz


PCI Express 3.0 Host Interface
GigaThread Engine
Memory Controller
Memory Controller
Memory Controller
Memory Controller
Memory Controller
Memory Controller
SMX
SMX
SMX
SMX
SMX
SMX
SMX
SMX
L2 Cache
SMX
SMX
SMX
SMX
SMX
SMX
SMX

# K40 chipset

- **Core/DP Units**: SP and DP arithmetic logic units.
- **Special Functions Units (SFUs)**: Execute transcendental instructions such as *sin, cosine, reciprocal, and square root*. Each SFU executes one instruction per thread, per clock.

**Take home message:**
*GPUs have different SP/DP ratios*, you may not get the speedup you expect.



# QE-GPU

Comparison of double precision performance for a single card and a single node:

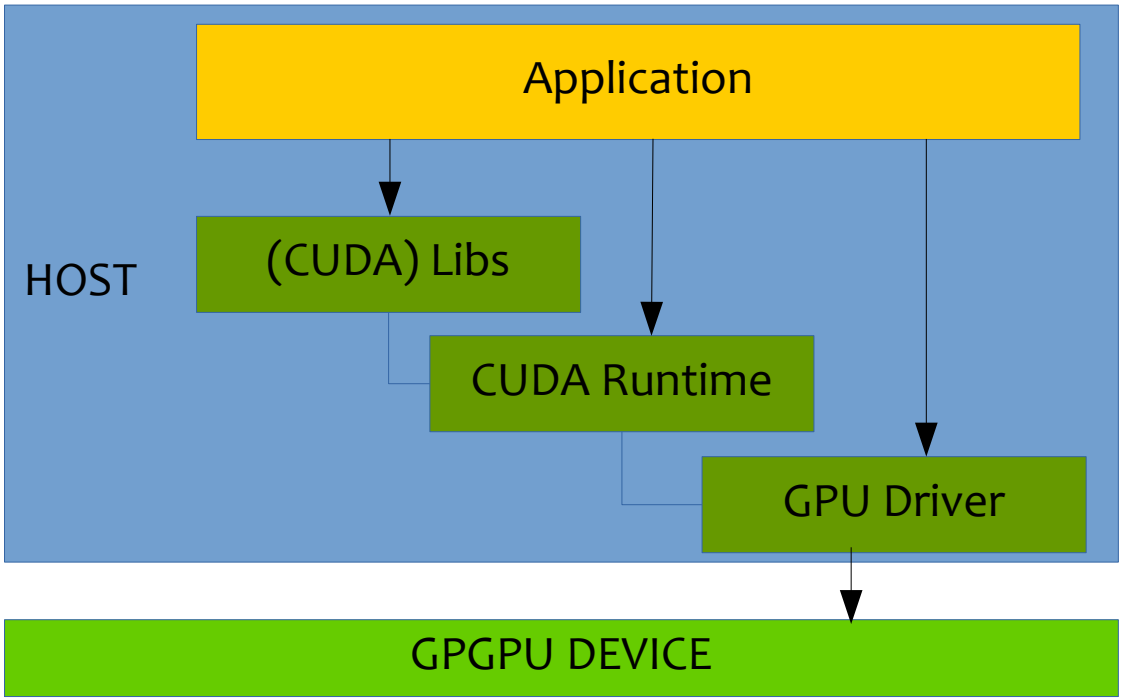
K40 : ~ 1400 GFLOP/s

Intel Haswell: ~ 665 GFLOP/s

(https://ark.intel.com/content/www/us/en/ark/products/83359/intel-xeon-processor-e5-2640-v3-20m-cache-2-60-ghz.html)

# CUDA Runtime

- In order to compile QE-GPU you'll need to know a bit about *CUDA* …



# CUDA Compute Capabilities

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

- Tesla K40: 3.5
- Tesla K80: 3.7
- Tesla P100: 6.0
- Tesla V100: 7.0

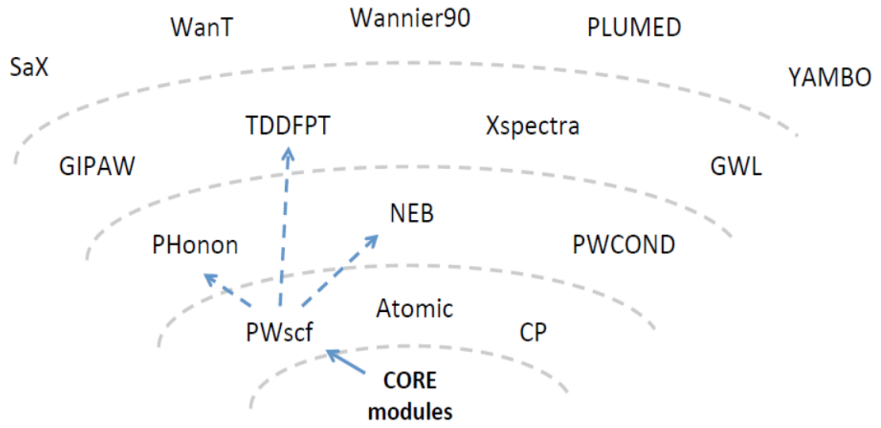
| Feature Support | Compute Capability | | | | | |
|---|---|---|---|---|---|---|
| (Unlisted features are supported for all compute capabilities) | 3.0 | 3.2 | 3.5, 3.7, 5.0, 5.2 | 5.3 | 6.x | 7.x |
| Atomic addition operating on 32-bit floating point values in global and shared memory (atomicAdd()) | Yes | | | | | |
| Atomic addition operating on 64-bit floating point values in global memory and shared memory (atomicAdd()) | No | | | | Yes | |
| Warp vote and ballot functions (Warp Vote Functions) | Yes | | | | | |
| __threadfence_system() (Memory Fence Functions) | | | | | | |
| __syncthreads_count(), __syncthreads_and(), __syncthreads_or() (Synchronization Functions) | | | | | | |
| Surface functions (Surface Functions) | | | | | | |
| 3D grid of thread blocks | | | | | | |
| Unified Memory Programming | | | | | | |
| Funnel shift (see reference manual) | No | Yes | | | | |
| Dynamic Parallelism | No | | Yes | | | |
| Half-precision floating-point operations: addition, subtraction, multiplication, comparison, warp shuffle functions, conversion | No | | | Yes | | |
| Tensor Core | No | | | | | Yes |



From CUDA C Programming guide v10

# GPU accelerated QE

Programming model | Objective




Applications

Directive based programming

Optimize memory duplication, allocation and syncronization.

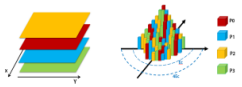
Domain Specific Libraries

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

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

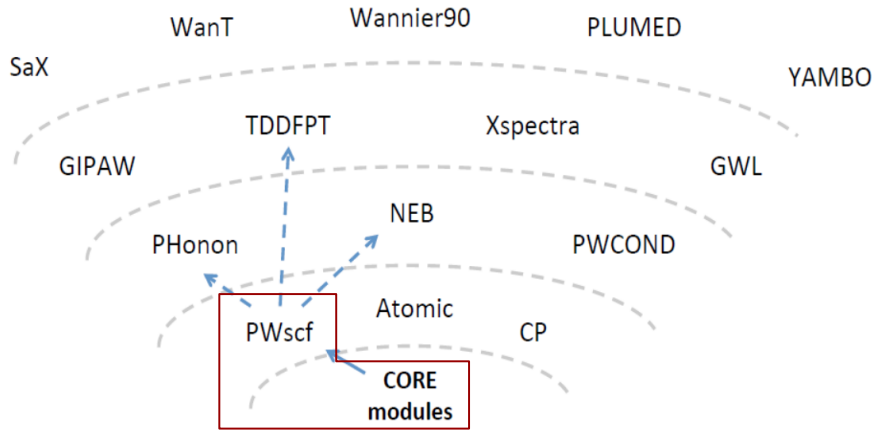
TASK: Iterative solvers
LIBS: LAXLib, MKL, cuBLAS, ...

Explicit accelerator programming

Optimize computational efficiency and concurrency

# GPU accelerated QE

Programming model | Objective

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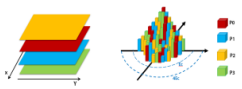

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Explicit accelerator programming

Optimize computational efficiency and concurrency

# Some details about pw.x

A number of different accelerated versions of pw.x have been released over the last years:

| 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 |

Accelerated, Working, Unavailable, Broken

* Acceleration obtained from other parts of the code.

# How fast?

- Strongly depends on your hardware, both Host and Device(s)
- On HPC systems ~3x speedup


9216 POWER9 22-core CPUs (2x node)
&
27,648 Nvidia Tesla V100 GPUs (6xnode)

# How fast?

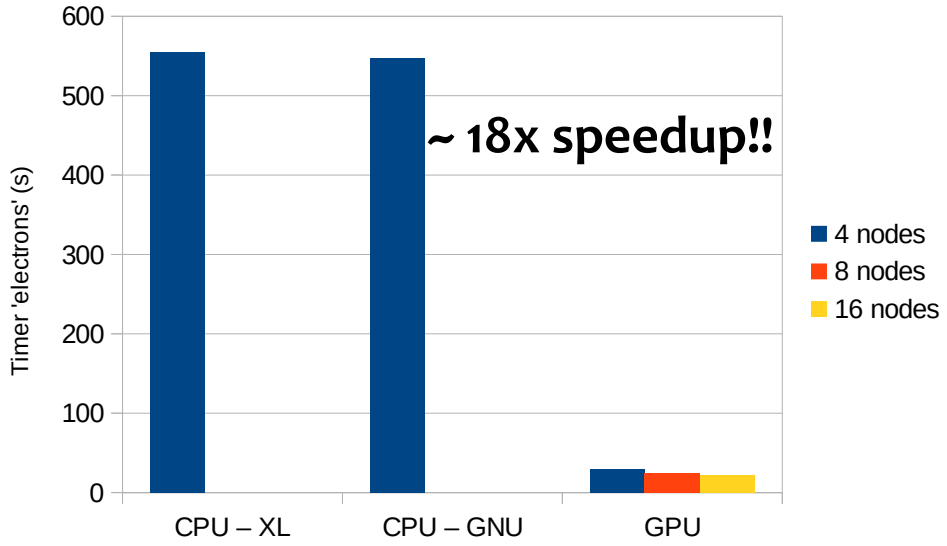
- Strongly depends on your hardware, both Host and Device(s)
- On HPC systems ~3x speedup

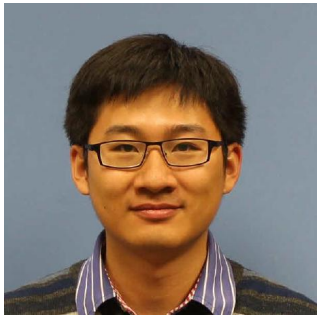
**Top 10 positions of the 53nd TOP500 in June 2019**[21]

| Rank | Rmax Rpeak (PFLOPS) | Name | Model | Processor | Interconnect | Vendor | Site country, year |
|---|---|---|---|---|---|---|---|
| 1 — | 148.600 200.795 | Summit | IBM Power System AC922 | POWER9, Tesla V100 | InfiniBand EDR | IBM | Oak Ridge National Laboratory United States, 2018 |
| 2 — | 94.640 125.712 | Sierra | IBM Power System S922LC | POWER9, Tesla V100 | InfiniBand EDR | IBM | Lawrence Livermore National Laboratory United States, 2018 |
| 3 — | 93.015 125.436 | Sunway TaihuLight | Sunway MPP | SW26010 | Sunway[22] | NRCPC | National Supercomputing Center in Wuxi China, 2016[22] |

# How fast?

- Strongly depends on your hardware, both Host and Device(s)
- On HPC systems ~3x speedup, but…



Courtesy of Dr. Ye Luo

| | Components | |
|---|---|---|
| Processor | CPU | GPU |
| Type | POWER9 | V100 |
| Count | 9,216<br>2 × 18 x 256 | 27,648<br>6 × 18 x 256 |
| Peak FLOPS | 9.96 PF | 215.7 PF |
| Peak AI FLOPS | | 3.456 EF |

From https://en.wikichip.org/wiki/supercomputers/summit

# Where to get the code

- Current development repository:

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

- Last release: 6.4.1a1
- Compile requirements:
  - PGI compilers
    https://www.pgroup.com/products/community.htm
  - CUDA Runtime and Libraries

# How to compile the code

- Same as standard QE distribution, but three new options must be provided:

```
--with-cuda=/path/to/cuda/ or yes
--with-cuda-cc=target-compute-capabilities (x 10 )
--with-cuda-runtime=runtime-version
```

- OpenMP is mandatory (and no scalapack unless you no what you are doing)
- You can find detailed instructions on the wiki:

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

# How to run the code

The rules:

1 GPU ↔ 1 MPI

Fill the CPU with OpenMP threads

No task grous (-ntg 1)

No parallel eigensolver (-ndiag 1)

K-point pools are great™, but device memory is limited.

# How to run the code

You may get additional speedup by *breaking the rules:*

more GPUs ↔ 1 MPI

Don't fill the CPU with OpenMP threads

# Thank you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