QUANTUM ESPRESSO FOUNDATION

QUANTUMESPRESSO

Efficient materials modelling on HPC
with QUANTUM ESPRESSO, Yambo and BigDFT

Hands-on session – Day 2

PHONONS FOR HPC AND GPUs

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MAX

CINECA

ENCCS
EuroCC National Competence Centre Sweden

PAUL SCHERRER INSTITUT
PSI

MARVEL
NATIONAL CENTRE OF COMPETENCE IN RESEARCH

Swiss National Science Foundation

INTERATOMIC FORCE CONSTANTS

Let us consider a unit cell with *Nat* atoms:

$s = 1 \ldots N_{at}$	index of an atom in the unit cell
$\alpha = x, y, z$	is the cartesian index
$\mathbf{R}$	is the point in the Bravais lattice, identifying the position of a given cell
$N_{\mathbf{R}}$	is the number of unit cells in the crystal
$\mathbf{u}_{s\alpha}(\mathbf{R})$ ↓ $3 \times N_{at}$	is the α component of the displacement of the s-th atom

Matrix of Interatomic Force Constants :

$$C_{s\alpha,s'\beta}(\mathbf{R},\mathbf{R}') = C_{s\alpha,s'\beta}(\mathbf{R}-\mathbf{R}') = \frac{\partial^2 E_{tot}}{\partial \mathbf{u}_{s\alpha}(\mathbf{R}) \partial \mathbf{u}_{s'\beta}(\mathbf{R}')}$$

SECULAR EQUATION

Normal mode frequencies, ω, and eigenvectors, $\tilde{\mathbf{u}}_{s\alpha}$ are determined by the secular equation:

$$\sum_{s',\beta} \tilde{D}_{s\alpha,s'\beta}(\mathbf{q})\, \tilde{\mathbf{u}}_{s'\beta}(\mathbf{q}) = \omega_{\mathbf{q}}^2\, \tilde{\mathbf{u}}_{s\alpha}(\mathbf{q})$$

Interatomic Force Constants (IFC)

where

$$\tilde{D}_{s\alpha,s'\beta}(\mathbf{q}) = \frac{1}{\sqrt{M_s M_{s'}}} \sum_{\mathbf{R},\mathbf{R}'} \frac{\partial^2 E_{tot}}{\partial \mathbf{u}_{s\alpha}(\mathbf{R}) \partial \mathbf{u}_{s'\beta}(\mathbf{R}')} e^{i\mathbf{q}(\mathbf{R}'-\mathbf{R})}$$

is the ***dynamical matrix***.

Diagonalization of the dynamical matrix gives phonon modes at **q**.

DENSITY FUNCTIONAL PERTURBATION THEORY

Sternheimer equation (solve_linter):

$$(H_{SCF}^{\mathbf{k}+\mathbf{q}} + \alpha P_v^{\mathbf{k}+\mathbf{q}} - \epsilon_v^{\mathbf{k}})\,|\Delta\psi_v^{\mathbf{k}+\mathbf{q}}\rangle = -P_c^{\mathbf{k}+\mathbf{q}}\,\Delta v_{SCF}^{\mathbf{q}}(\mathbf{r})\,|\psi_v^{\mathbf{k}}\rangle$$

h_psi — orthogonalize — apply_dpot

$$\Delta v_{SCF}^{\mathbf{q}}(\mathbf{r}) = \Delta v^{\mathbf{q}}(\mathbf{r}) + e^2 \int \frac{\Delta n^{\mathbf{q}}(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} e^{-i\mathbf{q}\cdot(\mathbf{r}-\mathbf{r}')} d\mathbf{r}' + \left.\frac{dv_{xc}(n)}{dn}\right|_{n=n(\mathbf{r})} \Delta n^{\mathbf{q}}(\mathbf{r}).$$

$$\Delta n_v^{\mathbf{q}}(\mathbf{r}) = 4 \sum_{\mathbf{k}v} u_v^{\mathbf{k}*}(\mathbf{r}) \Delta u_v^{\mathbf{k}+\mathbf{q}}(\mathbf{r})$$

incdrhoscf

DENSITY FUNCTIONAL PERTURBATION THEORY

Sternheimer equation:

$$(H_{SCF}^{\mathbf{k}+\mathbf{q}} + \alpha P_v^{\mathbf{k}+\mathbf{q}} - \epsilon_v^{\mathbf{k}}) \left| \Delta \psi_v^{\mathbf{k}+\mathbf{q}} \right\rangle = - P_c^{\mathbf{k}+\mathbf{q}} \Delta v_{SCF}^{\mathbf{q}}(\mathbf{r}) \left| \psi_v^{\mathbf{k}} \right\rangle$$

$$C_{s\alpha,s'\beta}(\mathbf{R}, \mathbf{R}')$$

$$\tilde{D}_{s\alpha,s'\beta}(\mathbf{q})$$

PHONONS

Rev. Mod. Phys.
73, 515 (2001).

Phys. Rev. B
43, 7231 (1991).

CALCULATIONS AVAILABLE FROM ph.x

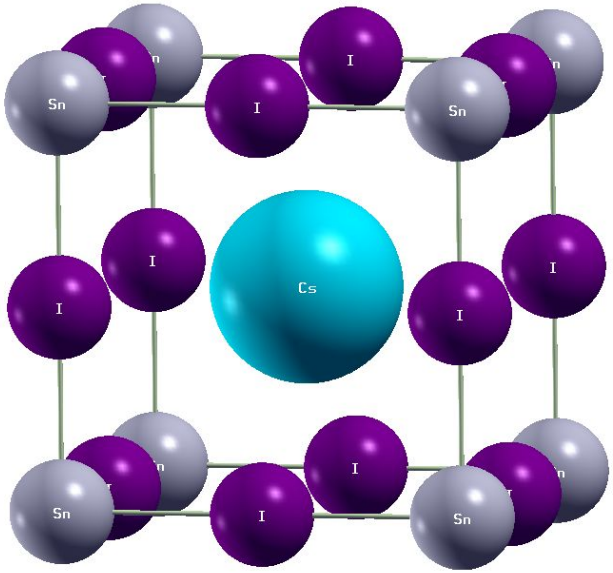
The phonon code works for a rather wide variety of systems and methods:

- ✓ Insulators (also polar insulators, with LO-TO splitting)
- ✓ Metals
- ✓ Magnetic systems at the scalar relativistic collinear level
- ✓ Spin-orbit coupling (fully relativistic approach)
- ✓ Electric field calculations: Born effective charges, dielectric tensor

Recent developments:

- ! Phonons for magnetic systems in the fully relativistic non-collinear approach
- ! Phonons within the DFT+U approach

EXERCISE ON LEONARDO : SIMULATION OF CnSnI3



- Experimentally metallic due to self-doping
- In DFT it is a semiconductor (polar material)
- 5 atoms in the primitive unit cell
- 3 x 5 = 15 phonon modes

EXERCISE ON LEONARDO : PHONON MODES AT Γ

```
cd  /leonardo_work/EUHPC_TD02_030/$USER/max-coe-workshop/day2/example_ph/
```

- `step*/` — folder for exercise
  - `README.md` — exercise description
  - submit.job — job file for Leonardo
- inputs/ — folder containing the input files
  - `pw.CnSnI3.in`: — vc-relax/SCF calculation input
  - `ph.CnSnI3.in`: — phonon calculation input
  - `dyn.CnSnI3.in` : — acoustic sum rule input
- `solution/` — directory with the reference results

PWSCF SIMULATION, STEP 1

The Phonon workflow for modes at a single q point

PWSCF SIMULATION, STEP 1

1. `cd day2/exercise_ph/step1/`

   Perform a vc-relax calculation for CnSnI3 using the `pw.x` *program.*

- Copy `../inputs/pw.CnSnI3.in` in the current folder and modify `&CONTROL` namelist to do a `vc-relax`
- Open `submit.job` and modify *npw* to use R&G on 4 MPIs : GPUs
- Submit the job file
- Copy the `output` directory `out/` in the folder of the next step

```
$ cat pw.CnSnI3.in
&CONTROL
        calculation = 'vc-relax'
        prefix = 'pwscf'
        outdir = './out'
/
&SYSTEM
   ecutwfc          = 80
   ecutrho          = 320
   occupations      = 'fixed'
   ntyp             = 3
   nat              = 5
   ibrav            = 0
/
&ELECTRONS
   conv_thr         = 1e-14
/
&IONS
/
&CELL
        press = 0
        press_conv_thr = 0.05
/

ATOMIC_SPECIES
Cs 132.90545196 Cs-nc-pbesol.upf
Sn 118.71 Sn-nc-pbesol.upf
I 126.90447 I-nc-pbesol.upf

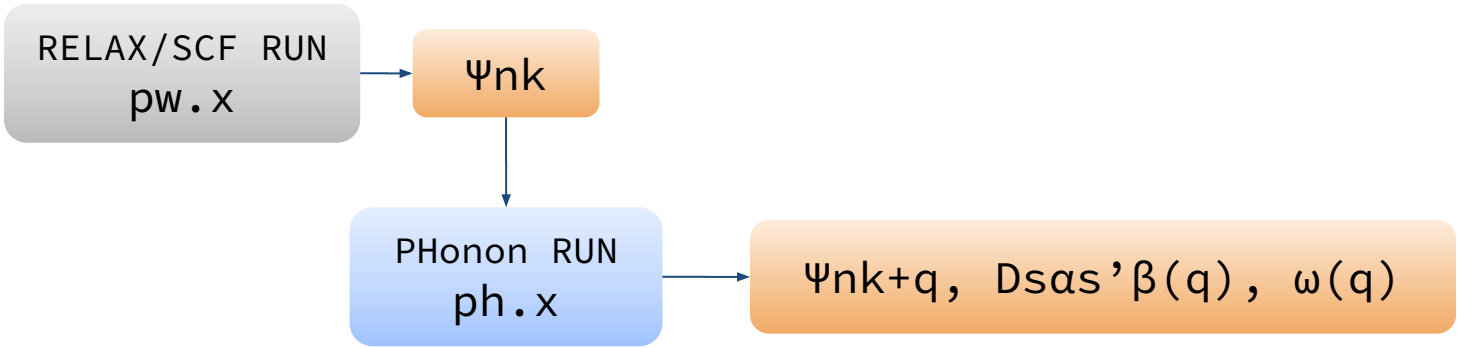
K_POINTS automatic
8 8 8  1 1 1

CELL_PARAMETERS angstrom
6.1821206415142775  0.0000000000000000  0.0000000000000000
0.0000000000000000  6.1821206415142775  0.0000000000000000
0.0000000000000000  0.0000000000000000  6.1821206415142775

ATOMIC_POSITIONS angstrom
Cs     3.0910603207571383  3.0910603207571383  3.0910603207571383
Sn     0.0000000000000000  0.0000000000000000  0.0000000000000000
I      3.0910603207571383  0.0000000000000000  0.0000000000000000
I      0.0000000000000000  0.0000000000000000  3.0910603207571383
I      0.0000000000000000  3.0910603207571383  0.0000000000000000
```

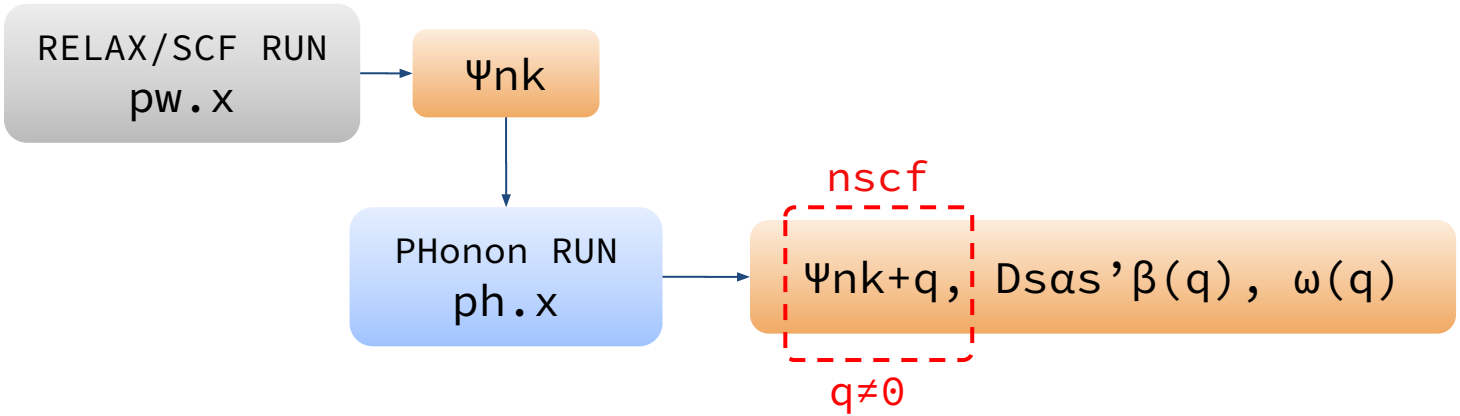
PHONON CALCULATION, STEP 2

The Phonon workflow for modes at a single q point



PHONON CALCULATION, STEP 2

The Phonon workflow for modes at a single q point



PHONON CALCULATION, STEP 2

2. `cd day2/exercise_ph/step2/`

QE/INPUT_PH

Perform a phonon calculation at Γ using the `ph.x` *program.*

- Copy `../inputs/ph.CnSnI3.in` in the current folder and modify the `&inputph` namelist ; add coordinates of the Gamma point

```
$ cat ph.CnSnI3.in
&inputph
        prefix = 'pwscf'
        fildyn = 'harmdyn_support'
        amass(1) = 132.90545196
        amass(2) = 118.71
        amass(3) = 126.90447
        tr2_ph = 1d-16
        outdir = './out'
/
0.0 0.0 0.0
```

The same prefix as in the `pw.x` calculation

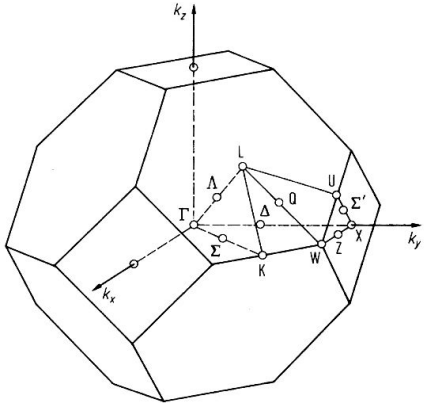
File storing the dynamical matrix

Atomic masses

Threshold for self consistency

Directory for temporary files

Coordinates of the q point **q** = 2*pi/a (0.0, 0.0, 0.0)



- Submit the job file `submit.job` to run on 1 MPI : GPU

DYNMAT MATRIX, STEP 2

- Check the number of k points

  `awk '/number of k/' ph.CnSnI3.out`

- Check the number of **irreducible representations**

  `awk '/irreducible/' ph.CnSnI3.out`

- Check the dynamical matrix in `harmdyn_`

  `tail -n 97 harmdyn_support`

Acoustic modes

Optical modes

```
$ tail -n 97 harmdyn_support
 ***************************************************************
     freq (    1) =      -0.154619 [THz] =      -5.157525 [cm-1]
 (  0.302230  0.000000 -0.378303  0.000000  0.000822  0.000000 )
 (  0.284598  0.000000 -0.356232  0.000000  0.000774  0.000000 )
 (  0.275368  0.000000 -0.332855  0.000000  0.000723  0.000000 )
 (  0.265921  0.000000 -0.332855  0.000000  0.000749  0.000000 )
 (  0.265921  0.000000 -0.344679  0.000000  0.000723  0.000000 )
     freq (    2) =      -0.154619 [THz] =      -5.157525 [cm-1]
 ( -0.378274  0.000000 -0.302192  0.000000  0.006755 -0.000000 )
 ( -0.356205  0.000000 -0.284562  0.000000  0.006361 -0.000000 )
 ( -0.344653  0.000000 -0.265888  0.000000  0.005943 -0.000000 )
 ( -0.332829  0.000000 -0.265888  0.000000  0.006154 -0.000000 )
 ( -0.332829  0.000000 -0.275333  0.000000  0.005943  0.000000 )
     freq (    3) =      -0.154619 [THz] =      -5.157525 [cm-1]
 (  0.004764  0.000000  0.004858  0.000000  0.484160  0.000000 )
 (  0.004486  0.000000  0.004575  0.000000  0.455913  0.000000 )
 (  0.004341  0.000000  0.004274  0.000000  0.425994  0.000000 )
 (  0.004192  0.000000  0.004274  0.000000  0.441128  0.000000 )
 (  0.004192  0.000000  0.004426  0.000000  0.425994 -0.000000 )
     freq (    4) =       0.242591 [THz] =       8.091968 [cm-1]
 (  0.050786 -0.000000 -0.087553  0.000000  0.844718 -0.000000 )
 ( -0.009193  0.000000  0.015848 -0.000000 -0.152903  0.000000 )
 ( -0.011864  0.000000  0.033584 -0.000000 -0.324021  0.000000 )
 ( -0.019481  0.000000  0.033584 -0.000000 -0.197328  0.000000 )
 ( -0.019481  0.000000  0.020453 -0.000000 -0.324021  0.000000 )
     freq (    5) =       0.242591 [THz] =       8.091968 [cm-1]
 (  0.258416  0.000000 -0.804506  0.000000 -0.098921  0.000000 )
 ( -0.046776  0.000000  0.145624  0.000000  0.017906  0.000000 )
 ( -0.060367  0.000000  0.308596  0.000000  0.037945  0.000000 )
 ( -0.099124  0.000000  0.308596  0.000000  0.023108  0.000000 )
 ( -0.099124  0.000000  0.187934  0.000000  0.037945  0.000000 )
     freq (    6) =       0.242591 [THz] =       8.091968 [cm-1]
 (  0.808972  0.000000  0.262486  0.000000 -0.021431  0.000000 )
 ( -0.146432  0.000000 -0.047513  0.000000  0.003879  0.000000 )
 ( -0.188978  0.000000 -0.100685  0.000000  0.008221  0.000000 )
 ( -0.310309  0.000000 -0.100685  0.000000  0.005006  0.000000 )
 ( -0.310309  0.000000 -0.061317  0.000000  0.008221  0.000000 )
```

ACOUSTIC SUM RULE (ASR) RULE, STEP 3

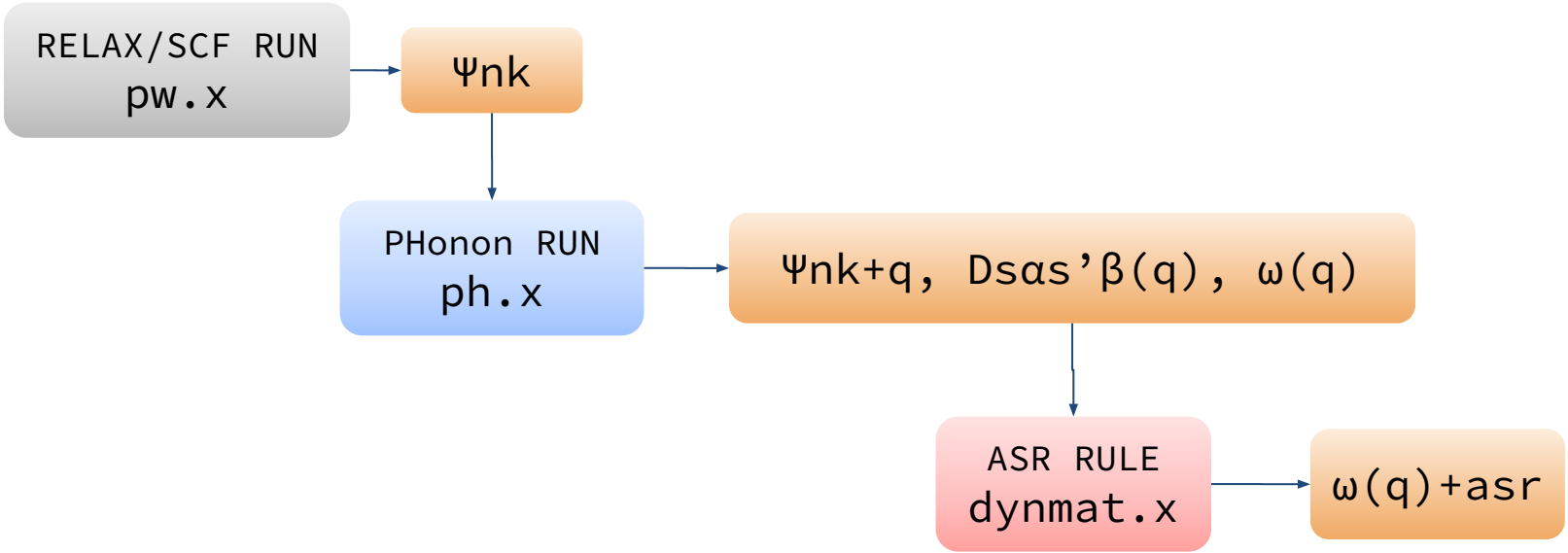
Because of the numerical inaccuracies the interatomic force constants do not strictly satisfy the acoustic sum rule (ASR). ASR comes directly from the continuous translational invariance of the crystal. If we translate the whole solid by a uniform displacement, the forces acting on the atoms must be zero.

$$\text{For each } \alpha, \beta \text{ and } i \ : \ \sum_{\mathbf{L},\mathbf{j}} C_{\alpha i,\beta j}(\mathbf{R_L}) = 0$$

As a consequence, the frequencies of the acoustic modes must be zero. ASR can be imposed with `dynmat.x`

ACOUSTIC SUM RULE (ASR) RULE, STEP 3

The Phonon workflow for modes at a single q point



ACOUSTIC SUM RULE (ASR) RULE, STEP 3

3. `cd day2/exercise_ph/step3/`

*Apply the **Acoustic Sum Rule (ASR)** with* `dynmat.x`

Because of the numerical inaccuracies the interatomic force constants do not strictly satisfy the acoustic sum rule (ASR). ASR comes directly from the continuous translational invariance of the crystal. If we translate the whole solid by a uniform displacement, the forces acting on the atoms must be zero.

$$\text{For each } \alpha, \beta \text{ and } i \ : \ \sum_{\mathbf{L},\mathbf{j}} C_{\alpha i,\beta j}(\mathbf{R_L}) = 0$$

As a consequence, the frequencies of the acoustic modes must be zero. ASR can be imposed with `dynmat.x`

ACOUSTIC SUM RULE (ASR) RULE, STEP 3

3. `cd day2/exercise_ph/step3/`

QE/INPUT_DYNMAT

*Apply the **Acoustic Sum Rule (ASR)** with* `dynmat.x`

- Copy `../inputs/dyn.CnSnI3.in` and add the 'crystal' ASR rule
- Copy `../step2/harmdyn_support` in the current folder
- Submit the job
- Check phonon modes with ASR rule applied in `dyn.CnSnI3.out`

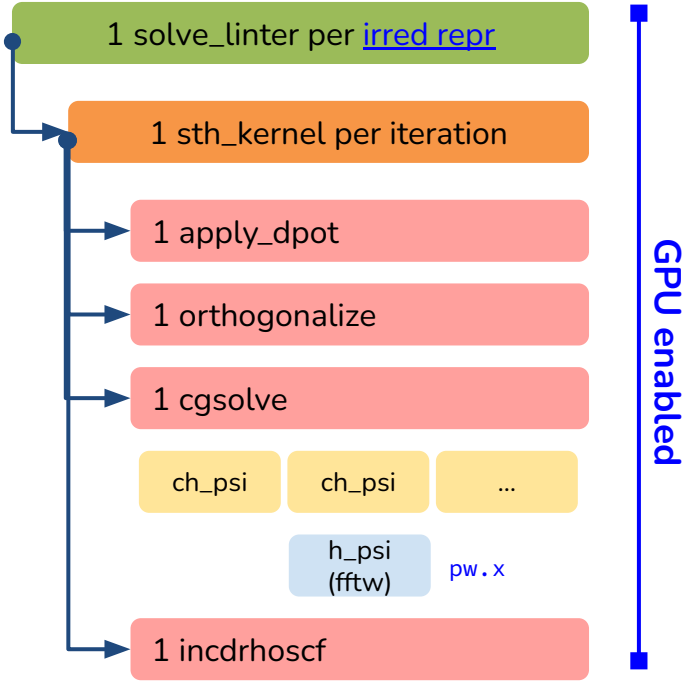
```
$ cat dyn.CnSnI3.in
&input
  fildyn = 'harmdyn_support',
  asr = 'crystal'
 /
```

The ASR rule to impose

File storing the dynamical matrix

The phonon workflow

PHONON RUNNING ON GPUs



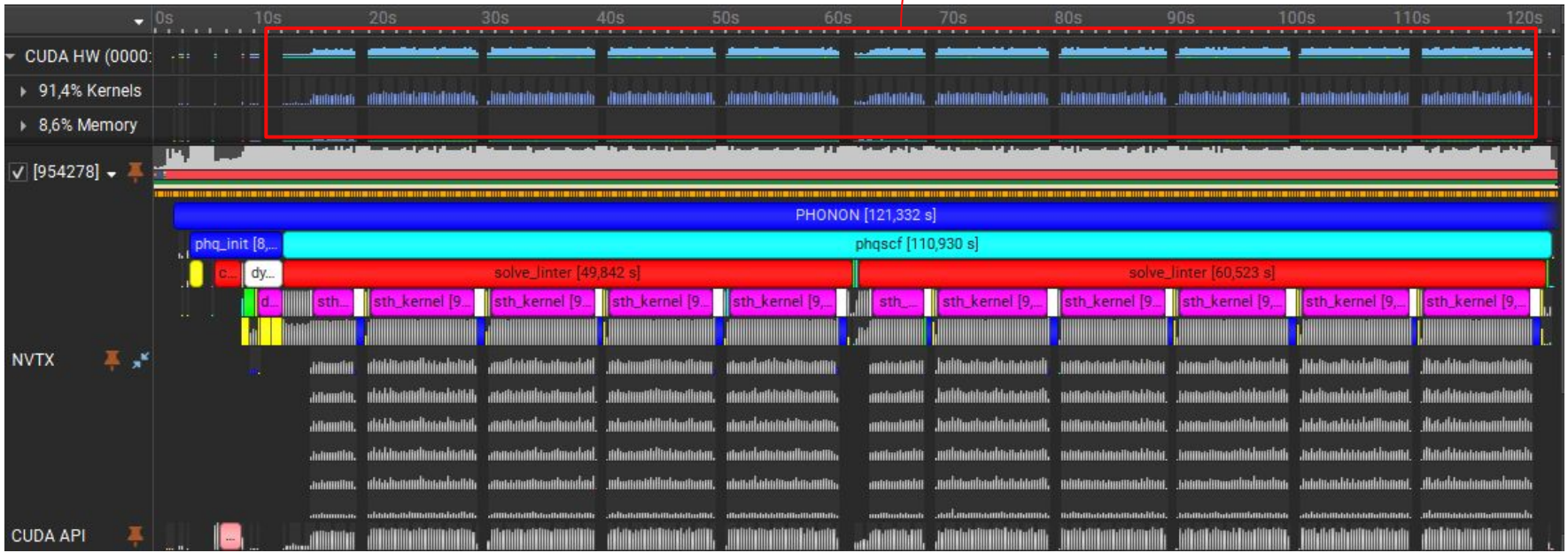
- GPU offloaded version currently available **since 7.2**
- Most of the routines in the call path for NC pseudopotentials are GPU-enabled
- GPU offload based on **OpenACC + CUDAFortran**
- h_psi offload inherited from PWscf
- Offload of routines from **LR_Modules/** exploited also in TDDFPT
- Check with tracing tools ;-)

GPU implementation

NSIGHT SYSTEM TRACE OF PHONON

Kernels in `phqscf` offloaded to GPUs

GPU enabled



`phqscf` is the main driver for phonon mode calculation (`trans=true`)

PARALLELIZATION HIERARCHIES FOR MULTI-GPU

- R&G to distribute memory

  ! distributed FFTs entail communications

- **pools** to distribute calculations on different k-points

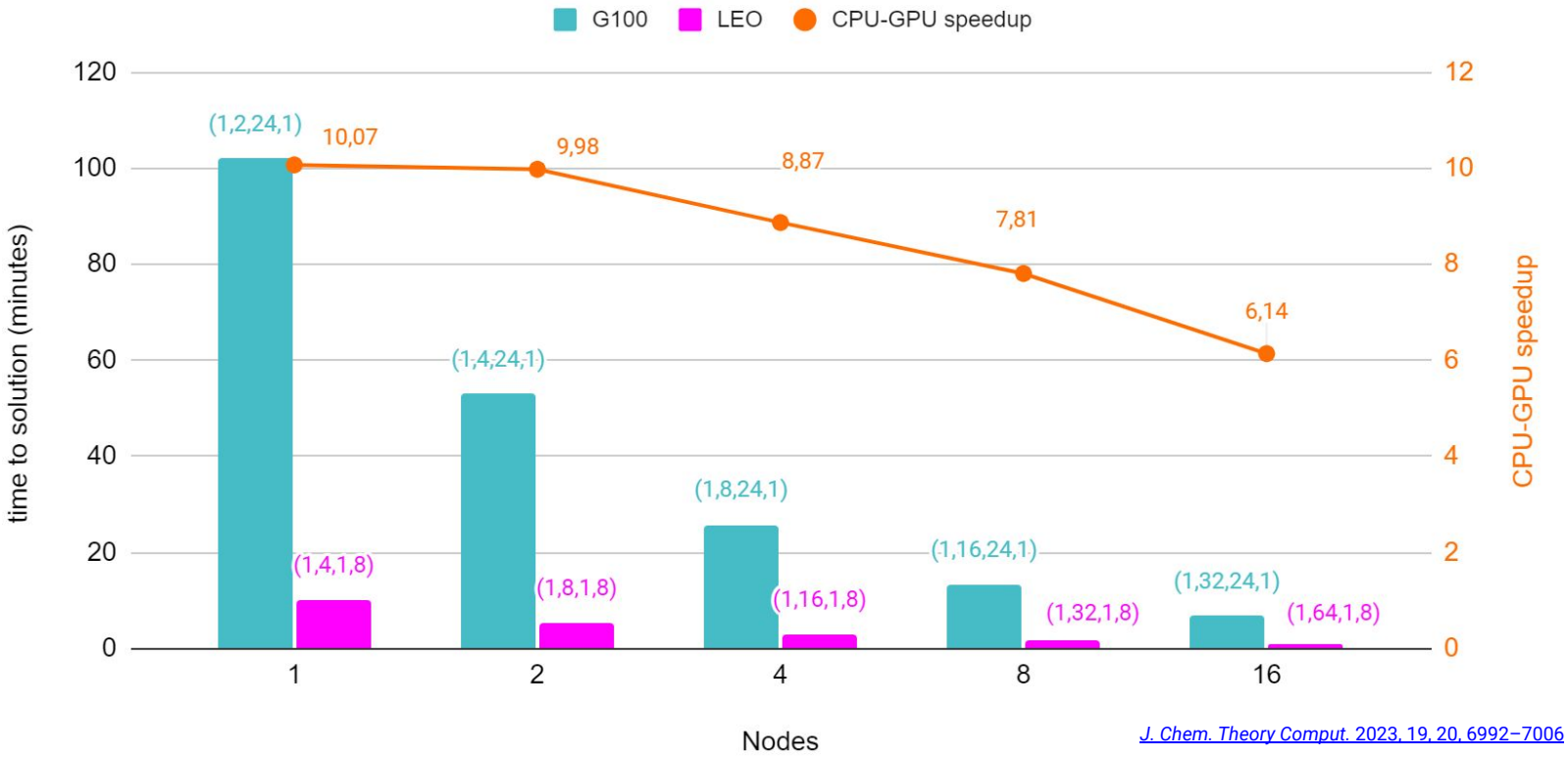
```
IF ( lgamma  ) THEN
   kunit = 1
   IF (noncolin.AND.domag) kunit = 2
ELSE
   kunit = 2
   IF (noncolin.AND.domag) kunit = 4
ENDIF
```

- **images** to distribute
  - irreducible representations (trans=true)
  - q-points (ldisp=true)

GPU implementation

PHONON AT LARGE SCALE

Excellent speed up with pool parallelism

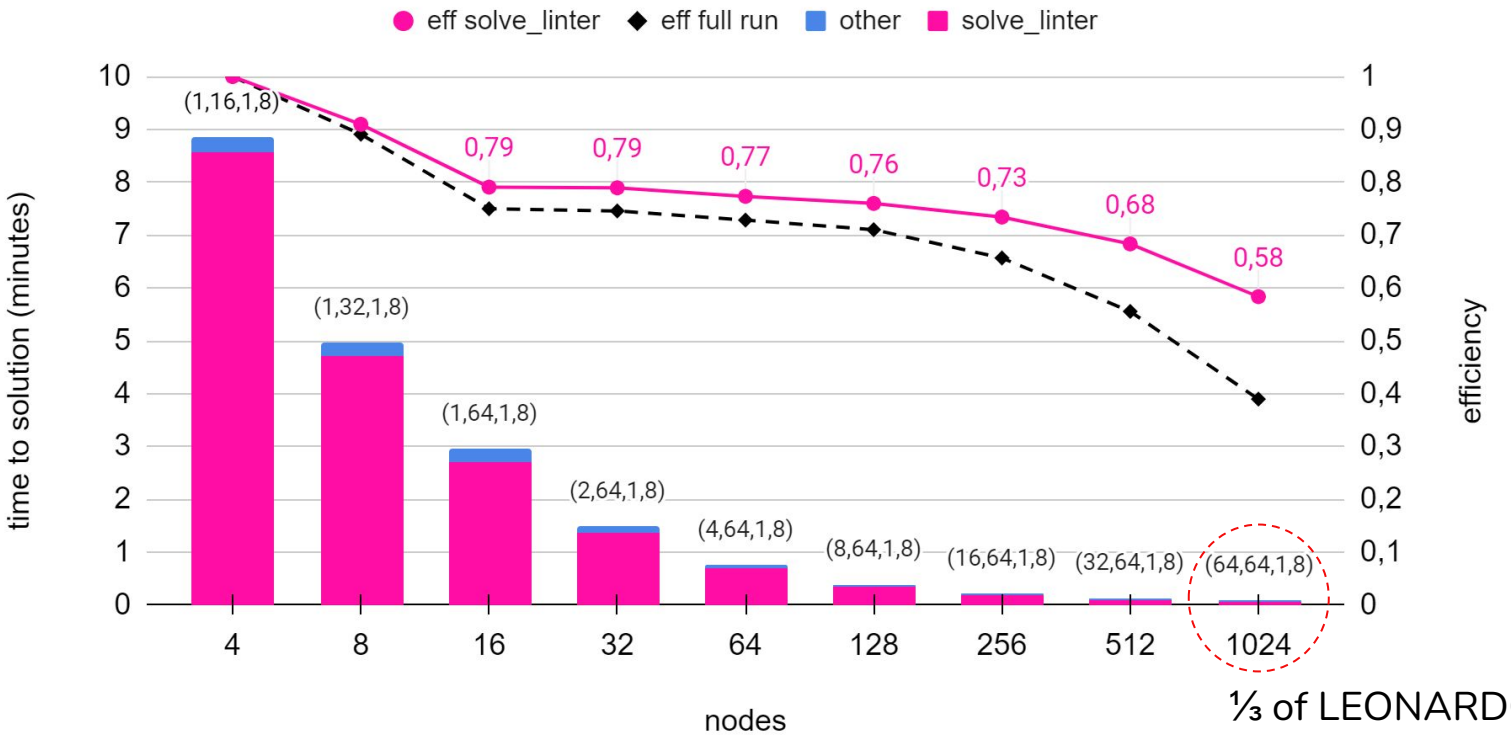


J. Chem. Theory Comput. 2023, 19, 20, 6992−7006

GPU implementation

PHONON AT LARGE SCALE

Large scale with pools + image distribution



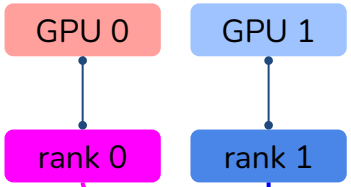
⅓ of LEONARDO!

MULTI-GPU EXECUTION WITH POOLS, STEP 4

4. `cd day2/exercise_ph/step4/`

With pool parallelism we distribute k-points among MPI ranks : GPU devices.

`mpirun -np N ph.x` **`-nk npools`** `ph.CnSnI3.in`




```
number of k points=    20
                  cart. coord. in units 2pi/alat
   k(    1) = (   0.0630215   0.0630215   0.0630215), wk =   0.0312500
   k(    2) = (   0.0630215   0.0630215   0.1890645), wk =   0.0937500
   k(    3) = (   0.0630215   0.0630215   0.3151076), wk =   0.0937500
   k(    4) = (   0.0630215   0.0630215   0.4411506), wk =   0.0937500
   k(    5) = (   0.0630215   0.1890645   0.1890645), wk =   0.0937500
   k(    6) = (   0.0630215   0.1890645   0.3151076), wk =   0.1875000
   k(    7) = (   0.0630215   0.1890645   0.4411506), wk =   0.1875000
   k(    8) = (   0.0630215   0.3151076   0.3151076), wk =   0.0937500
   k(    9) = (   0.0630215   0.3151076   0.4411506), wk =   0.1875000
   k(   10) = (   0.0630215   0.4411506   0.4411506), wk =   0.0937500
   k(   11) = (   0.1890645   0.1890645   0.1890645), wk =   0.0312500
   k(   12) = (   0.1890645   0.1890645   0.3151076), wk =   0.0937500
   k(   13) = (   0.1890645   0.1890645   0.4411506), wk =   0.0937500
   k(   14) = (   0.1890645   0.3151076   0.3151076), wk =   0.0937500
   k(   15) = (   0.1890645   0.3151076   0.4411506), wk =   0.1875000
   k(   16) = (   0.1890645   0.4411506   0.4411506), wk =   0.0937500
   k(   17) = (   0.3151076   0.3151076   0.3151076), wk =   0.0312500
   k(   18) = (   0.3151076   0.3151076   0.4411506), wk =   0.0937500
   k(   19) = (   0.3151076   0.4411506   0.4411506), wk =   0.0937500
   k(   20) = (   0.4411506   0.4411506   0.4411506), wk =   0.0312500
```

MULTI-GPU EXECUTION WITH POOLS, STEP 4

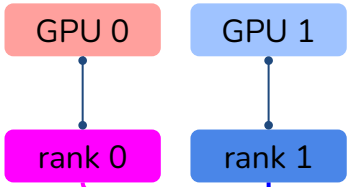
4. `cd day2/exercise_ph/step4/`

With pool parallelism we distribute k-points among MPI ranks : GPU devices.

`mpirun -np N ph.x -nk npools ph.CnSnI3.in`

- Copy the input file `../step2/ph.CnSnI3.in`
- Copy the folder `../step1/out`
- Modify *npools* in `submit.slurm` to use 2 pools : GPUs
- Submit the jobfile
- Check PHONON wall time

  `tail ph.CnSnI3.out`




```
number of k points=    20
                  cart. coord. in units 2pi/alat
   k(    1) = (   0.0630215   0.0630215   0.0630215), wk =   0.0312500
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   k(   12) = (   0.1890645   0.1890645   0.3151076), wk =   0.0937500
   k(   13) = (   0.1890645   0.1890645   0.4411506), wk =   0.0937500
   k(   14) = (   0.1890645   0.3151076   0.3151076), wk =   0.0937500
   k(   15) = (   0.1890645   0.3151076   0.4411506), wk =   0.1875000
   k(   16) = (   0.1890645   0.4411506   0.4411506), wk =   0.0937500
   k(   17) = (   0.3151076   0.3151076   0.3151076), wk =   0.0312500
   k(   18) = (   0.3151076   0.3151076   0.4411506), wk =   0.0937500
   k(   19) = (   0.3151076   0.4411506   0.4411506), wk =   0.0937500
   k(   20) = (   0.4411506   0.4411506   0.4411506), wk =   0.0312500
```

MULTI-GPU EXECUTION WITH IMAGES, STEP 5

5. `cd day2/exercise_ph/step5/`

With image parallelism at q point we distribute irreducible representations among MPI ranks : GPU devices.

```
mpirun -np N ph.x -ni nimages ph.CnSnI3.in
```

```
$awk '/There are / {x=NR+10} (NR<=x) {print $0} ' ph.CnSnI3.out
There are    5 irreducible representations

Representation     1      3 modes -  To be done

Representation     2      3 modes -  To be done

Representation     3      3 modes -  To be done

Representation     4      3 modes -  To be done

Representation     5      3 modes -  To be done
```

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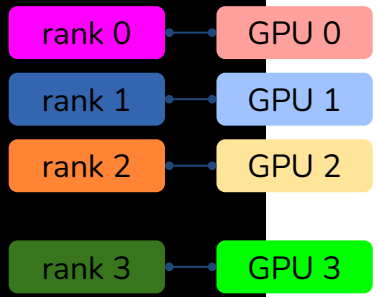
There are    5 irreducible representations
Representation     1      3 modes -  To be done
Representation     2      3 modes -  To be done
Representation     3      3 modes -  To be done
Representation     4      3 modes -  To be done
Representation     5      3 modes -  To be done
```



MULTI-GPU EXECUTION WITH IMAGES, STEP 5

5. `cd day2/exercise_ph/step5/`

With image parallelism at q point we distribute irreducible representations among MPI ranks : GPU devices.

```
mpirun -np N ph.x -ni nimages ph.CnSnI3.in
mpirun -np 1 ph.x -ni 1 ph.CnSnI3.recover.in
```

! A **recover run** is needed to collect the IFCs and diagonalize the dynamical matrix

- Copy the input file `../step2/ph.CnSnI3.in`
- Copy `ph.CnSnI3.in` as `ph.CnSnI3.recover.in` and add `recover=.true.` in `&inputph` of the latter
- Copy the `../step1/out` directory in the current folder
- Modify *nimages* in submit.slurm to distribute on 4 MPIs : GPUs
- Submit the jobfile

  ! *With image parallelism there is 1 output file for each image*

```
$ cat ph.CnSnI3.recover.in
&inputph
        fildyn = 'harmdyn_support'
        tr2_ph = 1d-16
        outdir = './out'
       recover = .true.
/
0.0 0.0 0.0
```

MULTI-GPU EXECUTION WITH IMAGES, STEP 5

5. `cd day2/exercise_ph/step5/`

With image parallelism at q point we distribute irreducible representations among MPI ranks : GPU devices.

```
mpirun -np N ph.x -ni nimages ph.CnSnI3.in
mpirun -np 1 ph.x -ni 1 ph.CnSnI3.recover.in
```

- Check the workfload for each image

  ! *image 0 has an extra scf run to compute the part of the dyn matrix not depending upon the change of Bloch functions*

- Compare the wall times. Which image takes longer? Why ?

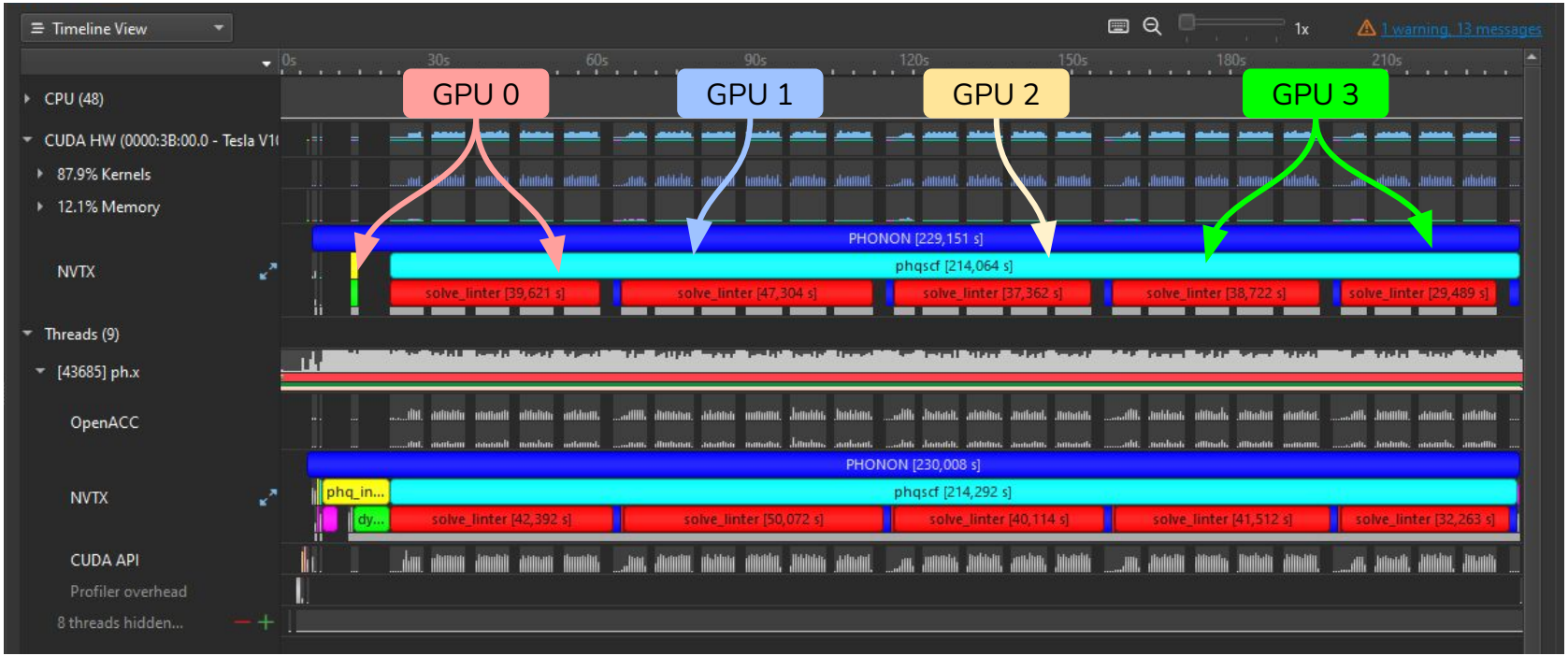
```
$ awk '/I am image/ {x=NR+3} (NR<=x) {print $0} ' out.*_0
I am image number     0 and my work is about    4 scf runs. I calculate:
q point number     1, representations:
0 1

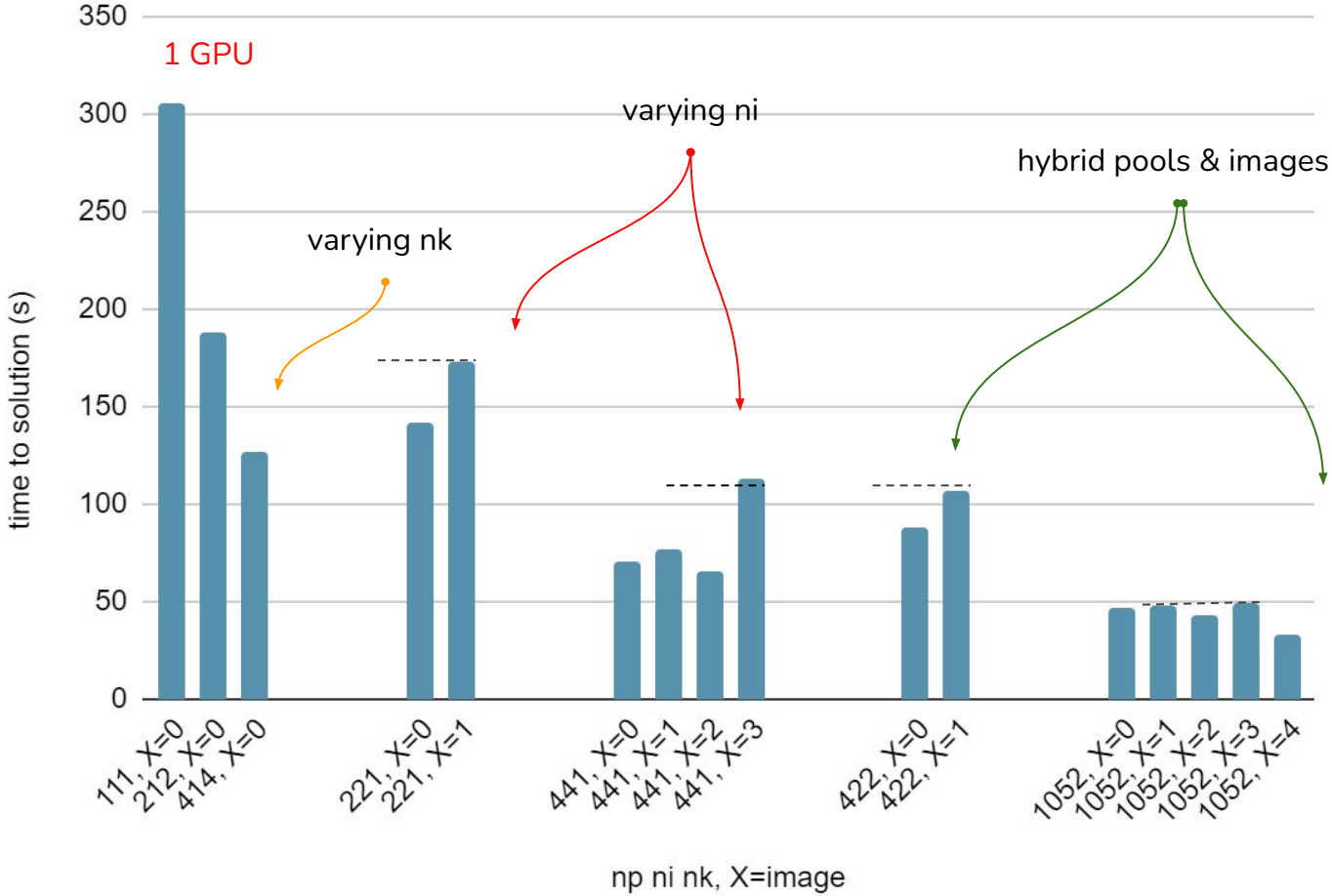
I am image number     1 and my work is about    3 scf runs. I calculate:
q point number     1, representations:
2

I am image number     2 and my work is about    3 scf runs. I calculate:
q point number     1, representations:
3

I am image number     3 and my work is about    6 scf runs. I calculate:
q point number     1, representations:
4 5
```

MULTI-GPU EXECUTION WITH IMAGES, STEP 5




1 GPU
varying nk
varying ni
hybrid pools & images
time to solution (s)
350
300
250
200
150
100
50
0
111, X=0
212, X=0
414, X=0
221, X=0
221, X=1
441, X=0
441, X=1
441, X=2
441, X=3
422, X=0
422, X=1
1052, X=0
1052, X=1
1052, X=2
1052, X=3
1052, X=4
np ni nk, X=image

HOW TO EXPLOIT GPUs

- Prioritize image and pool distribution if available
- Ensure the workload is balanced among MPI processes
- R&G is available, but good efficiency is limited to intra-node communications
- Use a GPU-aware version of the code to minimize the cost of H2D-D2H data movements

CALCULATIONS AVAILABLE FROM ph.x

Find the input option for your calculation at QE/INPUT_PH

→ Single q calculation (trans = .true.) + ASR (TODAY)

✳ Dielectric constant (`epsil = .true.`), effective charges (`zeu = .true.`)

✳ LO-TO splitting in insulators and IR cross sections (`dynmat.x`)

✳ Raman cross sections (`lraman=.true.`)

✳ Phonon mode dispersion (`ldisp = .true.` , `ph.x` + `q2r.x` + `matdyn.x`)

✳ Electron-phonon interaction coefficients (`electron_phonon='simple','interpolated',...`)