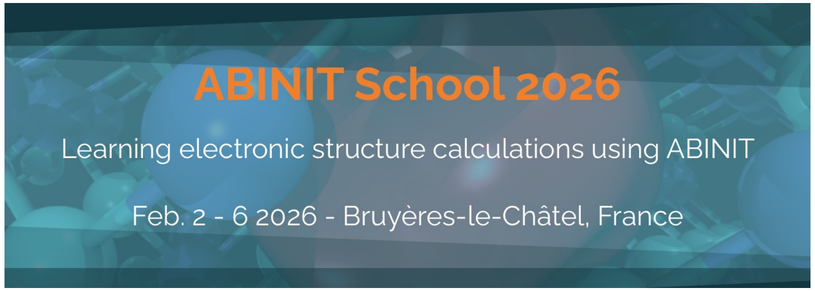


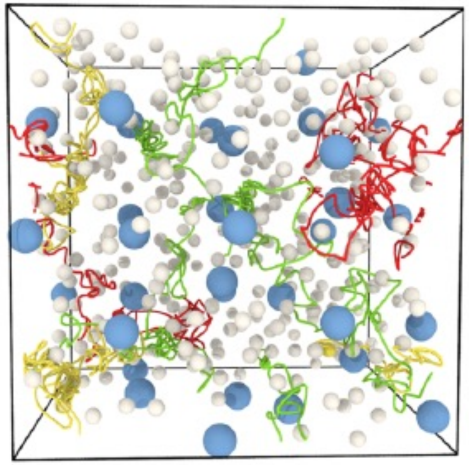
ABINIT School 2026

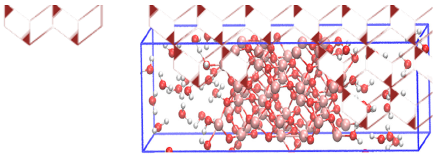
Learning electronic structure calculations using ABINIT

Feb. 2 - 6 2026 - Bruyères-le-Châtel, France

Ab Initio Molecular Dynamics

Hands-on session



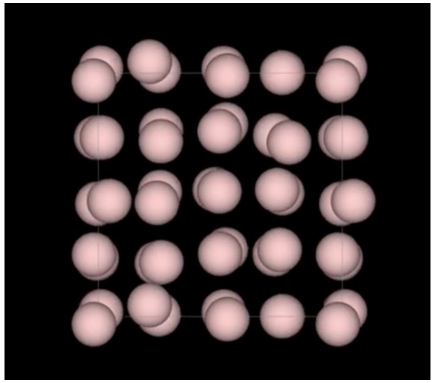


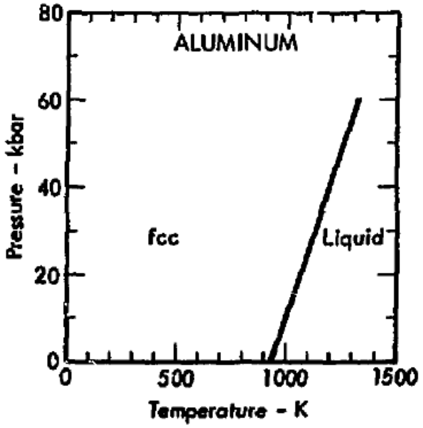
Aluminium melting temperature

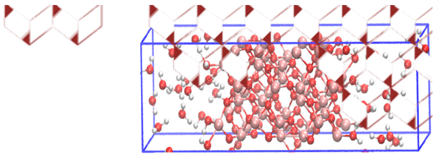
A first application of Ab Initio Molecular Dynamics (AIMD)

- **Objectives**
  - Learn how to perform molecular dynamics with ABINIT using a parallel computer
  - Learn what are the main input variables that govern convergence and numerical efficiency of a molecular dynamics simulation
  - Learn how to use post-processing tools

- **Material: Aluminium**
  - Compute the melting temperature using the « Heat Until it Melts » (HUM) method
  - 2x2x2 fcc supercell containing 32 atoms
    Isokinetic ensemble







Preliminary information

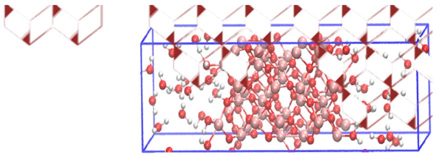
- All the necessary files can be found in the **ABISCHOOL/handson_dynamics/** directory.

- To run the examples in parallel with e.g. X MPI processes and Y openMP threads, use the attached `job.sub` file and edit it as follows:

```
#MSUB -E '--reservation=Formation-Abinit-gpu-20260205’
#MSUB --n=X              # Number of MPI processes
#MSUB --c=Y       # Number of openMP threads
ccc_msub job.sub
```

- The standard output of the application will be redirected to `abinit.log`.

- Don’t hesitate to activate the use of GPUs
  (for that you must use `gh200-bxi` partition).

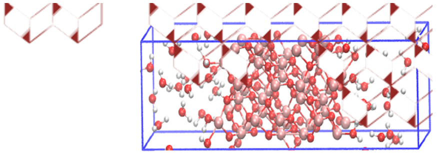


Basics of AIMD with ABINIT

What are the main input variables for AIMD?

- There are **different algorithms** to perform molecular dynamics, depending on the statistical ensemble. See the variables `moldyn` and `geoopt` (or `ionmov`).
- `dtion` controls the ion **time step** in atomic units of time. You should try several values in order to establish the stable and efficient choice.
- `ntime` controls the max. **number of time steps**. Usually you can set it to a large value, since there is no end to a MD simulation. You can always stop a calculation and restart.
- The input variable `restartxf=-1` is used to **restart** a calculation from a previous one with the same file names.
- The `xxxx_HIST.nc` file contains the **trajectories** from the very beginning (binary format). It can be explored with the **qAgate** (or **agate**) tool.
- Except for the isothermal/isenthalpic ensemble, the input variable `optcell` must be 0 (default value), i.e. the cell is not changed during the simulation.
- `mdtemp` is used to set the initial and final **temperatures** (in Kelvin). At constant temperature, use the same value for both.

1- First MD simulation



- Use the `dynamics.abi` file to run a calculation in parallel with 32 CPU cores (8MPI x 4threads). Look at the output file. For each iteration you will see the coordinates, the forces, the velocities, the kinetic energy and the total energy.
- ABINIT should have generated a **`_HIST.nc`** file (in the `TMP` directory), which contains the whole history of the molecular dynamics simulation.
- In `dynamics.abi` add the keyword `restartxf` and set it to -1. Run the calculation again, in the same directory.

Since we performed twice 50 steps of molecular dynamics, the total number of time steps is now 100. So the first 50 iterations are from the previous calculation. There is only one `_HIST.nc` file and it contains the history of the two calculations.

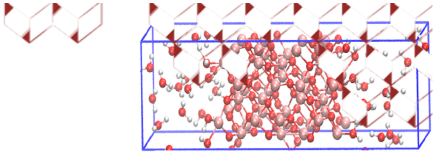
- Now you can calculate and plot several quantities. For that, use the **`atb_md`** Python script:

```
atm_md.py TMP/XXX_HIST.nc
```

- The script plots different quantities as functions of time (pressure, temperature, etc.)…

<u>Tip</u>: to see the average value of a thermodynamic quantities, close the window and look at the terminal.

2- Convergence on k-points and cell size



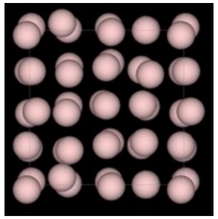
- **K-points convergence**
  Now change the input file and use a 2x2x2 k-point grid (8 k-points in irreducible Brillouin zone).
  Run 50 MD steps.
  Repeat with a 3x3x3 k-point grid (14 k-points in irreducible Brillouin zone).
  Use the appropriate number of processors and the GPUs!!!... if they are available.

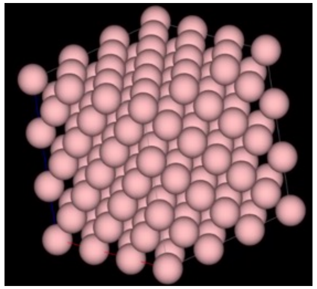
  Since the parallelisation is the most efficient over the k-point level you should always put np_spkpt to the largest possible value before increasing npband and #MSUB -c.

  Use **atb_md** script to visualize the trajectories and compare the average values of pressure.

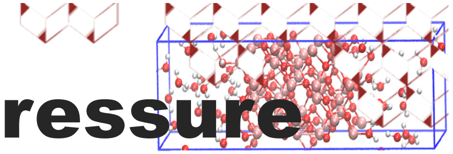
- **[OPTIONAL] - Supercell size convergence**
  For this test we use a 108 atom supercell file: dynamics_108at.abi.
  Run the trajectory with this file (112x4 CPUs should be OK, or 4 GPUs)
  Compare the result with the 32 atom supercell (1 kpoint).

Without GPUs, this run is a bit long
You can directly look at the provided
*.abo and *_HIST.nc files



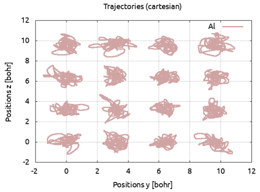


3- Melting temperature of Al at a given pressure



*You are going to calculate the melting temperature of aluminum using the so-called **Heat Until it Melts** (HUM) method. In this method the solid phase is heated gradually until melting occurs.*

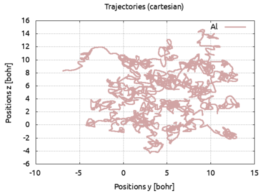
- First start with a temperature of 4500 K.
  To work fast, we use the 32 atoms supercell and 1 k-point.
  Run 100 MD steps with ABINIT.



- Then Look at the mean square displacements (MSD) with the **atb_msd** Python script:

```
atm_msd.py TMP/XXX_HIST.nc
```

What should be the evolution of Mean Square Displacements if the material is liquid?

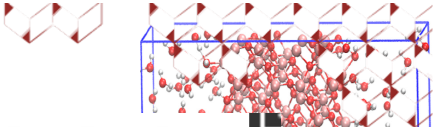


- If not sufficient to conclude, run 100 additional steps…
- Then increase the temperature and repeat the procedure… until it melts.
  A liquid can be identified with the MSD, the trajectories or the « pair distribution function ».
- When you have found a liquid phase, then you can try to refine the melting temperature by choosing a temperature between the solid and the liquid phases…

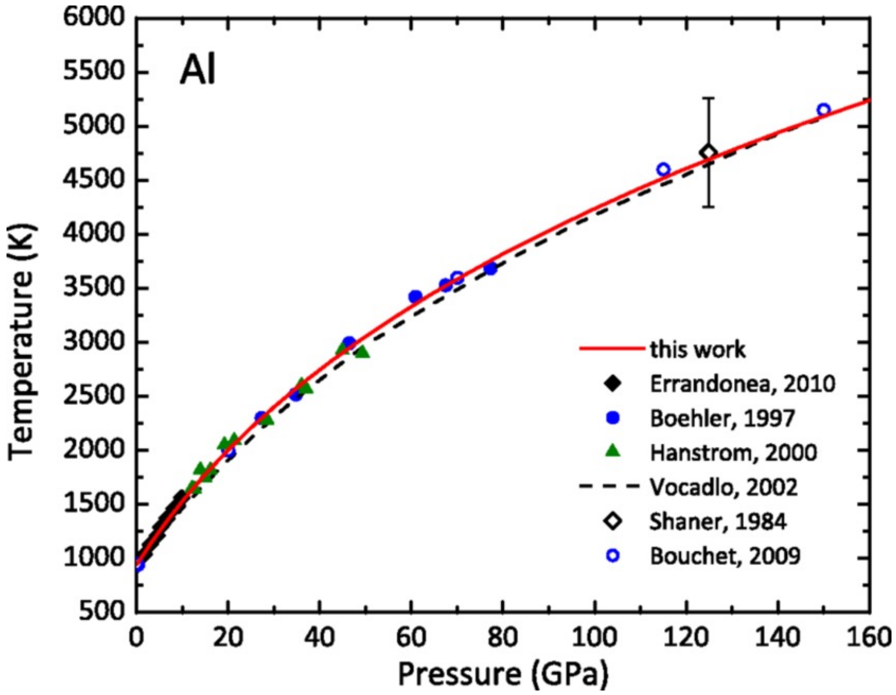
Tip: you can use a very practical procedure in ABINIT input files : several datasets in the same input file.

```
ndtset 3
mdtemp1 4500 4500 K tsmear1 4500 K
mdtemp2 5000 5000 K tsmear2 5000 K
mdtemp3 5500 5500 K tsmear3 5500 K
```

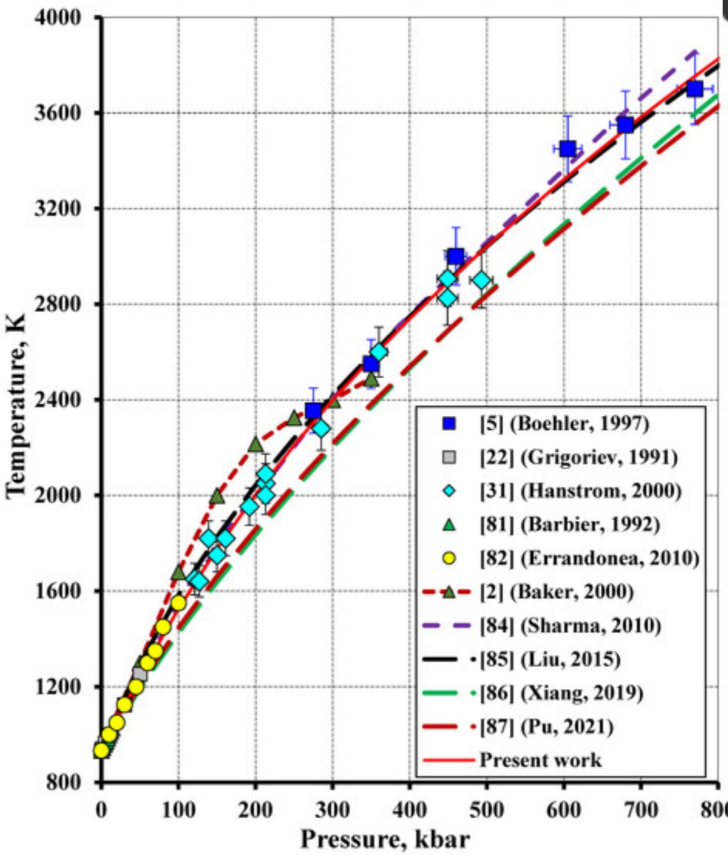
- **Is the melting temperature obtained by this method correct? Why?**



From the literature



Minakov, Levashov, *Melting curves of metals with excited electrons in the quasiharmonic approximation*, Physical Review B **92**, 101103 (2015)



Kozyrev, Gordeev, *Thermodynamic Properties and Equation of State for Solid and Liquid Aluminum*, Metals **12**, 1346 (2022)