



TERATEC Campus, Bruyères-le-châtel  
February 2-6 2026

# Welcome to the ABINIT school 2026



- Most lessons and all tutorials will be held in this room
- Coffee breaks will be in the room next door
- Please don't bring coffee or food in this room !
- Also don't plug anything (phones, USB keys..) in the computer USB ports. Even for charging !
- There is a water fountain next to the toilet in the hall
- Lunch will be at the cafeteria in this building (ground floor)
- If you want a coffee after lunch you should ask for a coffee pod at the cafeteria when getting your lunch
- *The poster session is today after the tutorials in the room next door*
- There will be a shuttle going from the center to the hotel (Belambra in Dourdan) every evening **15 min** after the last session

**So at 18:45 today**

- There will be a shuttle going to the TERATEC Campus from the hotel at **8:15** every morning
- On Wednesday afternoon there will be an excursion to visit the Castle of Dourdan followed by the social Dinner at the restaurant "La Table de Blache" also in Dourdan *You have to choose your meal now !*



## Tuesday morning

Choose between:

- Plane wave DFT
- PSP & PAW (more advanced)

## From Thursday afternoon

Choose between:

- Response: DFPT – X.Gonze
- Excited states: GW – F. Bruneval
- Correlations: DFT+ U & DMFT – B. Amadon

### ABINIT SCHOOL 2026 – Bruyères-le-Châtel

	Monday 2 Feb.	Tuesday 3 Feb.	Wednesday 4 Feb.	Thursday 5 Feb.	Friday 6 Feb.
09:00					
09:30		Plane-wave DFT or Pseudopotential & PAW			
10:00					
10:30		Break	Break	Break	Break
11:00					
11:30		Basic usage of ABINIT 2	ABINIT and parallelism	Post-processing and analysis	Advanced features 2 Optional labs: Response, Excited states, Correlations
12:00					
12:30	Arrival and Lunch	Lunch	Lunch	Lunch	Lunch and departure
14:00	Introduction to the school & the ABINIT project	Basic usage of ABINIT 3	Molecular dynamics and geometry optimization	Tuning ABINIT for HPC	
14:30					
15:00	Compiling ABINIT	Magnetism		Tuning ABINIT for HPC	
15:30	Break			Break	
16:00	Compiling ABINIT	Break		Advanced features 1 Optional labs: Response, Excited states, Correlations	
16:30					
17:00	Basic usage of ABINIT 1	Magnetism		Advanced features 1 Optional labs: Response, Excited states, Correlations	
17:30	Poster session				
18:00					
18:30					
19:30	Dinner (hotel)	Dinner (hotel)	Social Dinner (Dourdan)	Dinner (hotel)	

Lectures
Hands-on
Breaks
Others (social activities)

## The workstation

- To connect enter the login that was given to you « **stagXX** » (XX from 01 to 38) and type the associated password
- Once logged, you are on a network called « OCRE ». You should have access to the Internet.
- Typical use of the workstation: Visualize the ABINIT documentation, browse the Internet, use a webmail,  
**Open a terminal and log on the INTI cluster**
- There is only a minimal disk space on the workstation so please don't download large files

## The *INTI* cluster

- To access *INTI* : Open a terminal and enter **ssh -Y username@inti.ocre.cea.fr**
- username and password: same as your workstation login **stagXX** (XX: from 01 to 38)
- You should only use the workdir filesystem (which has a big disk quota) : **cd \$CCCWORKDIR**
- The files for the tutorials are located in the directory **\$ABISCHOOL**
- There are some information on how to use *INTI* in **\$ABISCHOOL/docs/howto\_inti.pdf**
- The sources of ABINIT are accessible in **\$ABISCHOOL/abinit-10.4.7.tar.gz**
- You can get information on the supercomputer environment and how to use it at any time by typing **machine.info** or **man inti**
- We have access to two partitions for the school :
  - A CPU partition with nodes composed of 128 AMD Rome CPUs
  - A GPU partition with nodes containing 288 ARM Neoverse CPUs + 4 Nvidia GH200 GPUs