



Faculty IT & Research Support Team

The Faculty of Science and Environments dedicated IT Research Support Team.

FIRST work as an independent specialist engineers supporting and providing IT solutions needed for the delivery of teaching and research in FSE.

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Introduction: Why We Run KF6003 Module in a Container

Why a container?

This module relies on GPAW, a Density Functional Theory (DFT) package used for materials simulation. GPAW's build and its supporting scientific libraries are only supported on Linux, there is no native Windows build.

As most student devices (and lab machines) run Windows, we need a way to run a genuine Linux environment on top of Windows, with GPAW and its dependencies pre-installed exactly once, so every student gets an identical, working setup without needing to compile anything themselves.

How the technology stack links up on Windows

Four layers sit on top of each other, each solving one part of the problem:

1. Windows : Installed on your physical machine, (Windows 10/11 supported).
2. WSL2 (Windows Subsystem for Linux) : A Microsoft feature that runs a real Linux kernel inside Windows. This is what makes a Linux-only tool like GPAW runnable at all.
3. Podman: A container engine that uses WSL2's Linux VM to build and run containers. Podman packages GPAW and everything it needs into a single container image, so it never has to be installed or compiled by hand.
4. The container instance: a running copy of that image. It hosts a Jupyter Lab server, reachable from your normal Windows browser via a mapped port (e.g. localhost:8888), so day-to-day work feels like using a regular web app.

What this means for you

You do not install GPAW, Linux, or any scientific libraries yourself. You enable WSL once, install Podman Desktop once, build the provided container image once, and then simply start/stop that same container instance whenever you work, all through a graphical interface, with your files saved in a normal Windows folder. **The remaining guides in this series (Steps 1–4) walk through each layer in turn: enabling WSL, installing Podman Desktop, building the image, and running the container.**