

Anaconda, GPAW/ASE, Jupyter, and OVITO Installation Guide

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Purpose: This guide provides the setup for running the GPAW-based DFT tutorial notebooks and optional atomistic visualization in OVITO.

Component	Purpose
Anaconda or Miniconda	Provides conda, the environment manager used to create an isolated Python/GPAW environment.
GPAW and ASE	GPAW performs DFT calculations; ASE builds structures, manages calculators, and handles input/output.
Jupyter Notebook/Lab	Runs the tutorial notebooks interactively.
OVITO	Optional visualization tool for atomic structures, trajectories in LAMMPS-style dump files.

1. Prerequisites

Before starting, make sure you have a working terminal or command prompt and internet access on your personal computer.

Useful official resources:

- [Anaconda installation documentation](#)
- [conda getting started guide](#)
- [GPAW documentation](#)
- [OVITO website](#)
- [OVITO installation manual](#)

2. Install Anaconda or Miniconda

Install Anaconda Distribution or Miniconda using the official installer for your operating system. Anaconda includes many packages by default; Miniconda is smaller and installs only conda plus a minimal Python stack. Either option works for this guide.

```
conda --version
```

If conda is installed correctly, this command prints the installed conda version.

3. Create the GPAW/ASE Conda Environment

Place the provided environment file in your working folder. The recommended file is:

```
cms_gpaw_environment.yml
```

Create the environment with:

```
conda env create -f cms_gpaw_environment.yml
```

This creates an environment named:

```
cms-gpaw
```

If your course folder instead provides a file named `cms_gpaw_environment.yml`, run the same command with that filename:

```
conda env create -f cms_gpaw_environment.yml
```

4. Activate the Environment

Activate the environment before running GPAW scripts or opening the tutorial notebooks:

```
conda activate cms-gpaw
```

Tip: If the command fails, confirm that Anaconda or Miniconda was initialized for your shell and restart the terminal.

5. Verify the Installation

Check that GPAW and ASE import correctly:

```
python -c "import gpaw, ase; print('GPAW:', gpaw.__version__); print('ASE:', ase.__version__)"
```

Expected output will look like:

```
GPAW: 25.7.0  
ASE: 3.28.0
```

The exact ASE version may vary slightly depending on the package resolver, but GPAW and ASE should both import without errors.

6. Open the Tutorial Notebooks

Start Jupyter from within the activated environment:

```
jupyter notebook
```

or, if you prefer JupyterLab:

```
jupyter lab
```

7. Install OVITO Optional Visualization Software

OVITO is optional. It is useful for visualizing atomic structures, trajectories, and LAMMPS dump files produced by the GPAW/ASE workflows. The free version called OVITO Basic is sufficient for this tutorial and use the official instructions for your operating system.

ASE also includes simple structure visualization tools, but OVITO is more convenient for trajectory and particle-property visualization.

10. Troubleshooting

Problem	Suggested fix
conda command not found	Restart the terminal, initialize conda for your shell, or reinstall Anaconda/Miniconda.
GPAW import fails	Confirm that the cms-gpaw environment is active, then recreate the environment if needed.
GPAW setup files missing	Run gpaw info and confirm that gpaw-data is installed.
Jupyter does not show cms-gpaw	Register the kernel using <code>python -m ipykernel install -user --name cms-gpaw --display-name "Python (cms-gpaw)"</code> .

11. Updating or Removing the Environment

To update the environment after changes to the YAML file:

```
conda env update -f cms_gpaw_environment.yml --prune
```

To remove the environment completely:

```
conda env remove -n cms-gpaw
```

12. Installation Checklist

- ☐ Anaconda or Miniconda is installed.
- ☐ The cms-gpaw conda environment was created successfully.
- ☐ The cms-gpaw environment activates without errors.
- ☐ GPAW and ASE import correctly.
- ☐ Jupyter opens and shows the Python (cms-gpaw) kernel.
- ☐ OVITO is installed if visualization beyond ASE is needed.