

# ASE — The Atomic Simulation Environment

Minicourse in ASE, GPAW, and scripting with Python

Location: Universitat de Barcelona, May 29–31

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## Programme

### Monday, May 29

10:30 Introduction to Python and ASE  
11:00 Tutorial: Scripting with ASE, part I  
11:45 Break  
12:00 ASE: An overview  
12:45 Tutorial: Scripting with ASE, part II  
13:30 The end

### Tuesday, May 30

10:30 Scientific programming in Python:  
Numpy, SciPy, Matplotlib  
11:00 Tutorial: Computations in Python, part I  
11:45 Break  
12:00 More on scientific programming  
Python in parallel, C extensions  
12:30 Tutorial: Computations in Python, part II  
13:30 The end

### Wednesday, May 31

10:30 GPAW: Electronic structure code in Python and C  
11:30 Tutorial: ASE/GPAW exercises, part I  
12:15 Break  
12:30 Intermezzo on ASE/GPAW development:  
Web pages, mailing lists, Gitlab  
12:45 Tutorial: ASE/GPAW exercises, part II  
Python/ASE/GPAW install party  
13:30 The end

More information:

<https://wiki.fysik.dtu.dk/ase/>  
<https://wiki.fysik.dtu.dk/gpaw/>  
<https://www.python.org/>  
<http://www.numpy.org/>