Python Basics

Arrays and plotting

Welcome to Python Basics!

This presentation will introduce you to fundamental concepts in Python, focusing on working with data. Today, we'll learn:

- **Loading Data from a File:** How to bring your data into Python, specifically from a `.dat` file.
- **Plotting Data:** Visualizing your insights, focusing on `Etot` vs. `alat` from the loaded data.
- We'll primarily use the powerful libraries **NumPy** and **Matplotlib**.

Your First Python Code

Let’s begin with a classic: printing “Hello, Python!” to the console. This simple step demonstrates how to execute basic code and view its output.

```
# This is a comment - it's ignored by Python when the code runs.
print("Hello, Python!")
```

What’s happening here?

- `print()` is a built-in **function** in Python used to display values to the standard output (usually your terminal or console).
- `"Hello, Python!"` is a **string**, which is a sequence of characters enclosed within single or double quotes.

Reading Data from a File: `Etot-vs-alat.dat`

First, we import the necessary libraries:

```
1 import numpy as np
```

Then, we read the data from the file, using comma as the delimiter:

```
1 data = np.loadtxt('Etot-vs-alat.dat', delimiter=',')
```

Next, we extract the `alat` and `Etot` columns:

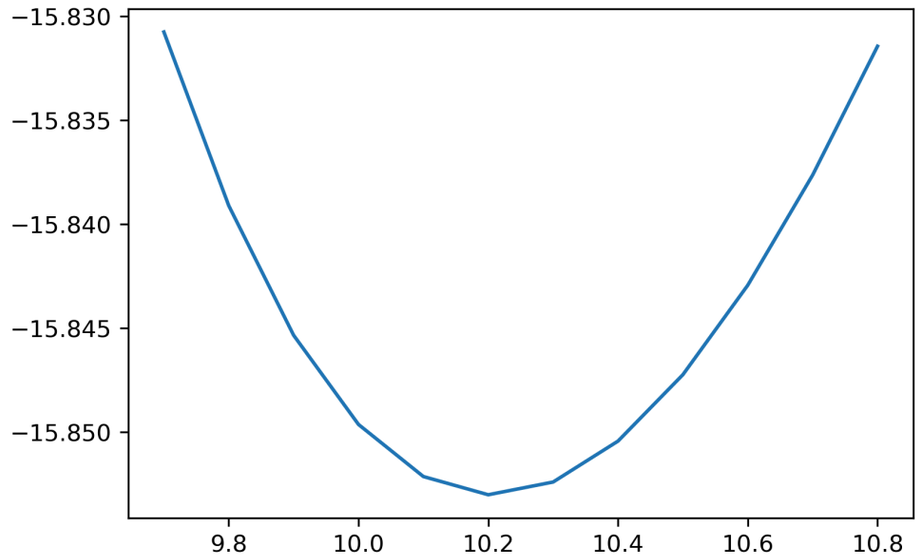
```
1 alat = data[:, 0]
2 Etot = data[:, 1]
```

Plotting Data: Basics

```
1 import matplotlib.pyplot as plt
2 plt.plot(alat, Etot)
3 plt.show()
```

`matplotlib` is the biggest plotting library in python and the one we will use at ASESMA

`plt.plot` graphs the data

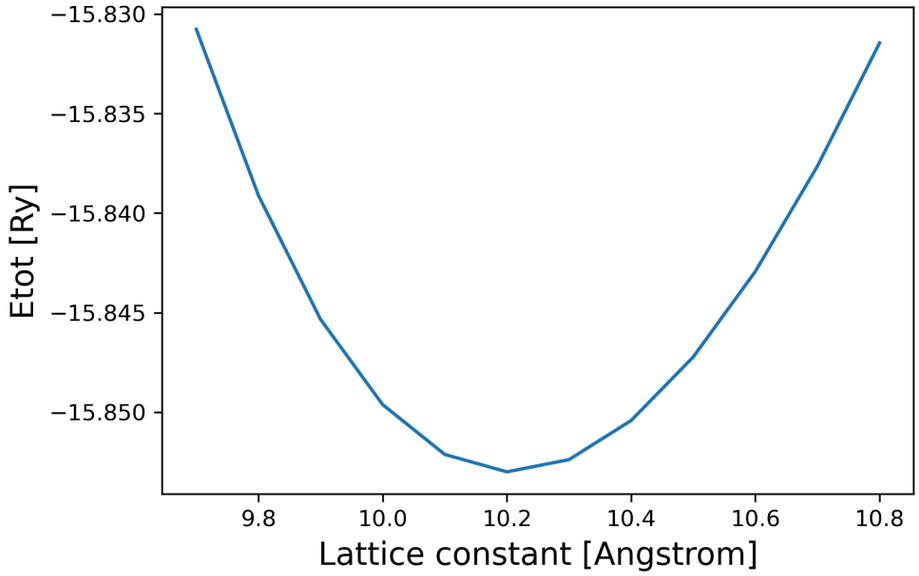


Plotting Data: Add Labels

```
1 import matplotlib.pyplot as plt
2 plt.plot(alat, Etot)
3 plt.xlabel("Lattice constant [Angstrom]", size=14)
4 plt.ylabel("Etot [Ry]", size=14)
5 plt.show()
```

`xlabel` and `ylabel` label the axes

`size` determines the fontsize

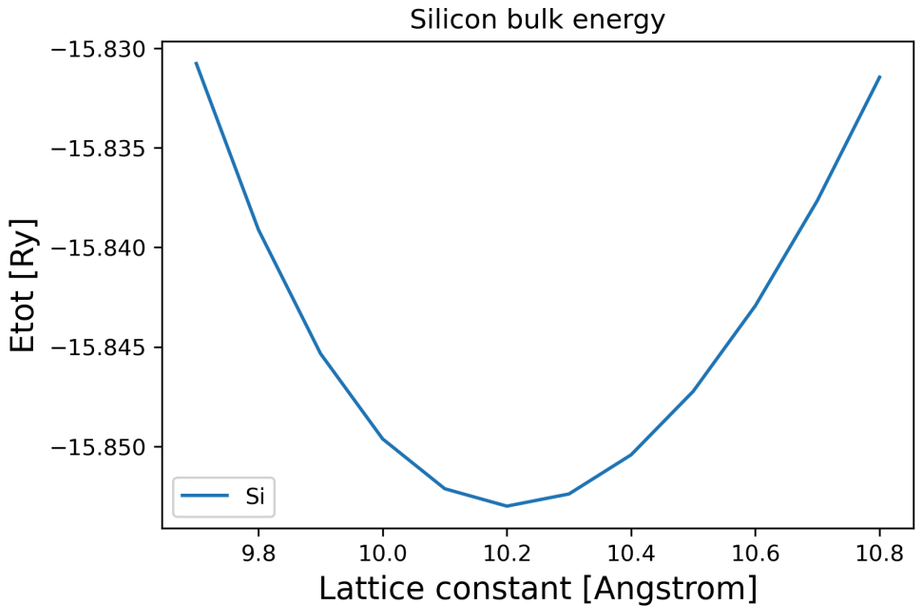


Plotting Data: Add legend and title

```
1 import matplotlib.pyplot as plt
2 plt.plot(alat, Etot, label="Si")
3 plt.xlabel("Lattice constant [Angstrom]", size=14)
4 plt.ylabel("Etot [Ry]", size=14)
5 plt.legend()
6 plt.show()
```

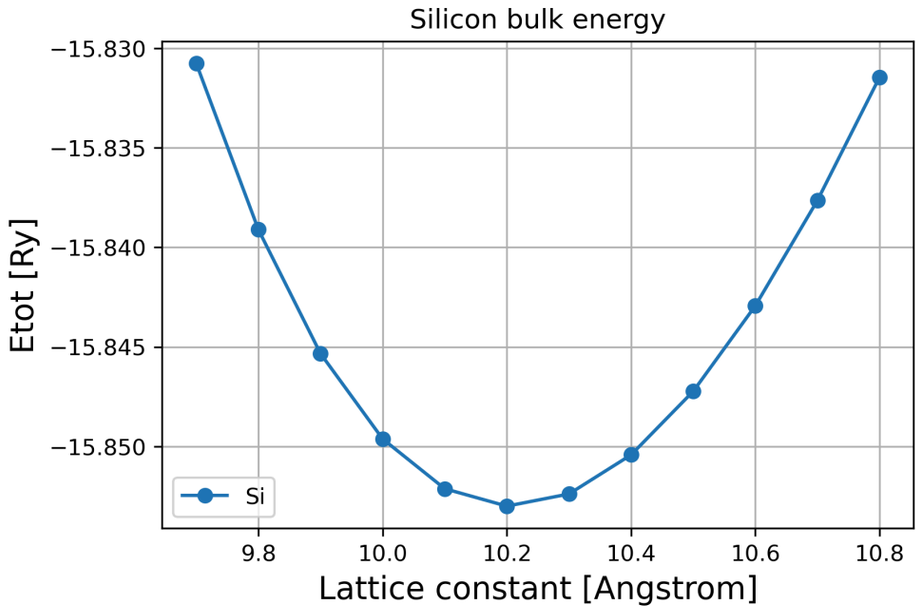
The `label` key in the `plt.plot` method allows

You also need `plt.legend()`



Plotting Data: final touches

```
1 import matplotlib.pyplot as plt
2 plt.plot(alat, Etot, label="Si", marker='o')
3 plt.xlabel("Lattice constant [Angstrom]", size=14)
4 plt.ylabel("Etot [Ry]", size=14)
5 plt.legend()
6 plt.title("Silicon bulk energy")
7 plt.grid(True)
```



Questions?