**Onboarding - Computational Materials L&D**

Welcome to the Computational Materials L&D Team. It’s a very broad area so we have to narrow it down to what’s most accessible the moment. Each semester the group is going to follow one of these topics, finish the one announced.

Check your access to our GitHub, Google Drive and text us in Slack!

**Materials Informatics**

To understand Machine Learning, it’s fundamental to know your data and how to manipulate it. While most of it is learned on the go, it’s important to be aware of the importance of Statistics and Linear Algebra in this field.

The answers should be obtained using **Python** (with Numpy, Pandas, Matplotlib, Scikit-learn and SciPy Libraries) and your knowledge of Materials Science. Please, use the internet as a supporting resource, but do not get full answers.

1. Install Python and the libraries listed above using pip or anaconda (recommended for easiness of use)

2. Develop a simple program that determine the highest and lowest Ultimate Tensile strength of the metals that were heat treated as rolled [here](https://github.com/Computational-Materials-L-D/polymer-mech-prop-model/blob/e57b82f433d81a0c0e29d8a5a03da737bc0ce978/MechanicalPropertiesMetals.csv)

3. Using the same data, plot the Ultimate Tensile Strength vs Yield Strength with appropriate units and labels. Make an appropriate linear fit and print on the plot the angular coeff.

3.1 Can you infer any relationship?

3.2 Propose a scientific model that can describe such similar/dissimilar behavior

4. [Watch the first four videos of this playlist from 3Blue1Brown](https://youtube.com/playlist?list=PLZHQObOWTQDNU6R1_67000Dx_ZCJB-3pi&si=j7SAjGL7Haggmbn0)

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On Construction…

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**Density Functional Theory**

1. Install ORCA
2. Access this archive and explain the entries
3. Simulate and give the water ground state energy

**Molecular Dynamics**

1. Install LAMMPS
2. Prepare a small simulation with following parameters (Use this as references):
   1. Simulation time = 100ns
3. Now, using the following formulas and your own knowledge, estimate the specific heat of water

**Finite-Elements Method and CAD**

1. Get access to ANSYS and Solid Works
2. Create a simple cylinder with a small
3. Put it under some stress with the following boundary conditions
4. Starting with Granta EduPack, select 5 different polymers
   1. Make an Ashby Plot relating two of its Thermal properties
   2. Propose a theory or use a mathematical law to explain this relationship
   3. Export this data (copy and paste, because EduPack doesn’t allow us to do what we would need)
   4. In Excel, use a statistical measure to describe this relationship
5. In Python, from [this link](https://github.com/Computational-Materials-L-D/polymer-mech-prop-model/blob/dcaa0d03fa2f279ebde9cc16ff80b2283f6aa8a4/MechanicalPropertiesMetals.csv), graph the ultimate tensile strength vs yield strength data
   1. What kind of relationship can you infer? Use statistics to support your claim
   2. Propose a theory or use a mathematical law to explain this relationship
6. Now do the same with yield strength vs density, but just for the annealed alloys
   1. Can you infer the same as 1.?
   2. Propose a theory or use a mathematical law to explain this relationship