**Data-Enhanced Simulation for Solids – Fall 2024**

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*Plan of the lectures*

1. 29/8 Introduction to scientific computing: high-performance numerical computing with the JAX library.
2. 5/9 Simulation of multiple-degree-of-freedom (MDOF) systems.
3. 12/9 Recap on feedforward neural networks; creating and training neural networks in Flax/NNX.
4. 19/9 Physics-Informed Neural Networks (PINNs) for ODE- and PDE-based modeling.
5. 26/9 Introduction to Graph Neural Networks.
6. 3/10 GNN-based surrogate physical models.
7. 10/10 Introduction to reinforcement learning: basic concepts.
8. 24/10 Q-learning/deep Q-learning; catastrophic forgetting and experience replay.
9. 31/10 Improving stability with a target network; policy function using neural network; stochastic policy gradient; REINFORCE.
10. 7/11 Actor-critic methods. PPO/TRPO/SAC.
11. 14/11 Reinforcement Learning for PDE control problems. Assignment.
12. 21/11 Symbolic regression with Genetic Programming: introduction; the DEAP library.
13. 28/11 Q/A about the assignment. Course evaluation.
14. 5/12 Model-Based Reinforcement Learning with symbolic regression

*References*

Lecture notes and Jupyter notebooks are the study materials for this course. If you are interested in digging into the Reinforcement Learning literature, here are recommended books:

* Zai and Brown, “Deep Reinforcement Learning in Action”, Manning, 2020;
* Sutton and Barto, “Reinforcement Learning: An Introduction”, MIT Press, 2020.

*About the exam*

The exam consists of:

1. A take-home, individual assignment consisting of a coding problem based on the concepts, libraries and applications studied during the course. The statement of the assignment will be presented in class on 14/11 and then uploaded on Brightspace. Students must submit (via WISEFlow) a Jupyter notebook or a Python script appropriately commented that solves the task of the assignment within December 7th (ultimo teaching period). There are no other assignments during the course.
2. An oral exam (20 min): a discussion of the take-home assignment and questions about all the contents of the course, aimed at veryifing the course’s learning goals.

An overall grade is given composed of approximately 60% oral exam and 40% take-home assignment. For re-examination, a new take-home assignment can be submitted.

*Installing Python on your laptop*

For this course, we recommend creating a conda environment containing all the relevant libraries. Otherwise, you can rely on Google Colab to run the code contained in the notebooks. There is a link in each of the notebooks provided as course materials that allows to execute them using Google Colab.

We suggest to create a folder that you can easily access from the terminal (a short path that does not contain spaces, such as C:\data\_sim on Windows) to download the course notebooks in.

If you already have Anaconda installed on your computer:

* (Optional step) Open the Anaconda Prompt (Windows)/Terminal (MacOS/Linux) and execute the following commands:

conda install -n base conda-libmamba-solver

conda config --set solver libmamba

* Then, download the *environment.yml* from Brightspace and execute

conda env create -f environment.yml

to create the datasim environment and install all the Python libraries required for this course.

* Activate the new environment to start coding and running the Python scripts/notebooks:

conda activate datasim

(this step must be done every time you open a new Prompt/Terminal.)

If you DO NOT have Anaconda already installed on your computer, follow these instructions:

**Windows**

* Download the latest miniforge installer from [here](https://github.com/conda-forge/miniforge) (click on the link Miniforge-Windows-x86\_64).
* Run the installer and leave the default options during the installation procedure. **Warning**: you *cannot* use the default settings (in particular, the installation path) if your username contains spaces. In this case, open File Explorer and create a new directory *without spaces* (e.g. "mamba") under C:\. Then, run the installer and choose this path as a destination folder.
* From the *Start* menu, launch the **Miniforge Prompt**.
* Navigate (using the cd command) into the directory where you downloaded the *environment.yml* from Brightspace and execute

mamba env create -f environment.yml

to create the datasim environment and install all the Python libraries required for this course.

* Activate the new environment to start coding and running the Python scripts/notebooks:

mamba activate datasim

(this step must be done every time you open a new Prompt/Terminal.)

**MacOS / Linux**

* Open a terminal (e.g. Terminal under MacOS) and execute the following commands to download the installer using curl or wget and start the installation, e.g.

curl -L -O "https://github.com/conda-forge/miniforge/releases/latest/download/Miniforge3-$(uname)-$(uname -m).sh"

bash Miniforge3-$(uname)-$(uname -m).sh

or

wget "https://github.com/conda-forge/miniforge/releases/latest/download/Miniforge3-$(uname)-$(uname -m).sh"

bash Miniforge3-$(uname)-$(uname -m).sh

**Note**: answer “Yes” when asked whether you want to automatically configure your shell profile for mamba.

* Navigate (using the cd command) into the directory where you downloaded the *environment.yml* from Brightspace and execute

mamba env create -f environment.yml

to create the datasim environment and install all the Python libraries required for this course. If you get an error saying that the mamba command is not recognized, close and re-open the terminal.

* Activate the new environment to start coding and running the Python scripts/notebooks:

mamba activate datasim

(this step must be done every time you open a new Prompt/Terminal.)

**Using Jupyter notebooks**

To edit/run [jupyter](https://jupyter.org/) notebooks (\*.ipynb), start [JupyterLab](https://jupyter.org/) by executing the following command from the command prompt (remember to activate the datasim environment first!)

jupyter lab

and use the web interface to open notebooks. Press CTRL+C while on the prompt to terminate JupyterLab.