Data-Enhanced Simulation for Solids

MSc in Mechanical Engineering

Academic year 2024-2025

Course program:

1. Introduction to scientific computing: high-performance simulations and parallel hardware; the Python libraries ecosystem: JAX – accelerated array computing. Motivation: writing simulators that integrate well with ML/DL codes. Exercise/tutorial session: creating a conda environment for the course, using Google Colab, JAX basics. <https://github.com/gordicaleksa/get-started-with-JAX/blob/main/Tutorial_1_JAX_Zero2Hero_Colab.ipynb> Exercise: gradient descent optimization of a function; solving a non-linear system of equations using Newton’s method
2. Simulation of MDOF systems: mass-spring-damper systems, rigid spheres and elastic beam in a viscous fluid (Chapters 3 and 4 of “Discrete Simulation Notes”). Implicit and explicit time integration.

Exercise: implementation and assignments.

1. Recap on MLP. Exercise: Creating a NN in Flax and solving a simple regression problem <https://github.com/gordicaleksa/get-started-with-JAX/blob/main/Tutorial_4_Flax_Zero2Hero_Colab.ipynb>
2. Physics-Informed Neural Networks (PINNs): solving ODEs and PDEs. Exercise: compare PINN solution with finite difference approximation Poisson and wave equations (see Data Science nb).
3. Introduction to reinforcement learning: basic concepts; multi-arm bandit problem; exploration vs exploitation (epsilon-greedy strategy); value and policy.

Exercise: implement and solve multi-arm bandit

1. Q-learning/deep Q-learning; the Gridworld problem; catastrophic forgetting and experience replay. Exercise: Gridworld
2. Improving stability with a target network; policy function using neural network; stochastic policy gradient; REINFORCE. Introduction to Gym. Exercise: solving CartPole with REINFORCE.
3. Actor-critic methods. Application? Something more mechanical (Swimmer) or robot path planning; rocket control
4. PPO/TRPO/SAC – StableBaselines. Exercise: LunarLander with PPO. Inverted pendulum?
5. Assignment
6. Symbolic regression and Genetic Programming: introduction. Genetic operations. DEAP library. Exercise: a benchmark symbolic regression problem with DEAP.
7. MBRL with symbolic regression: recovering symbolic expressions from a custom environment (simulator written in JAX).
8. Q/A about the assignment. Course evaluation.