GABELLINI CRISTIAN

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EXPERIENCE

Research - University of Jan Evangelista (UJEP)

02/2020 - 05/2020 Ústí nad Labem, Czech Republic

- Parallel Computing using the MPI protocol
- Worked on implementing novel machine learning approaches to coarse-grain a water solvent
- Researching machine learning models used for nanomaterials simulations
- Setup of different atomistic and Coarse-Grained simulations to build datasets for testing different machine learning approaches

Internship - Fincantieri S.p.A.

Technical System Engineer

09/2019 - 12/2019 Trieste, Italy

- Implemented the parametric modelling to automate the creation of complex 2D and 3D objects
- Successfully developed a new internal process to apply the new modelling technique between different technical departments
- Corrosion problems on different types of plumbing pipes
- Solved the topology problems with .topoJSON files in Microsoft PowerBI

TECHNICAL SKILLS

- **Languages:** Python, C++, HTML/CSS, Javascript, SQL
- **Machine Learning:** Focus on Gaussian Process, Deep Learning, Bayesian Optimization
- **Frameworks:** NumPy, SciPy, Pandas, Matplotlib, Tensorflow, scikit-learn, OpenCV, MDanalysis, Flask, FastAPI, Vue.js
- **Software:** Microsoft Office (advanced excel user), Microstation v8i, Microstation Connect, Solidworks, Packmol, Avogadro
- **Simulations:** LAMMPS, Quantum-Espresso, Amber, DigiMat
- **Miscellaneous:** Git, Unit testing, RESTful, Bash

CERTIFICATIONS

- **Certificate of Completion** Summer School on Energy Giacomo Ciamician, 2018 Sesto, Italy
- **Certificate of Attendance** Summer English courses, 2011 Anglia Ruskin University, Cambridge, UK

AWARDS

- **JetBrains PyCharm** 10 Years of Coding together competition winner for the GPGO project

EDUCATION

Master's Degree in Materials Engineering

Thesis: Development of Machine-Learning based approaches for coarse-grained simulations

01/18 - 10/20 University of Trieste

Bachelor's Degree in Industrial Engineering

Thesis: Theorical modelling of the gelation of a poly-aromatic LMOG chiral system

09/12 - 12/17 University of Trieste

PROJECTS

GPGO

- Framework for Bayesian optimization with Gaussian Processes. Hyperparameters tuning using gradient information and numerical solvers. Implementation of various acquisition functions and different solvers to achieve an convergence on high dimensional function.

Dissipative Particle Dynamics Optimization

- Derivation of the DPD interaction parameters for a coarse-grained simulation of a nanoparticle grafted by polymers by using a novel bayesian optimization approach exploiting structural insights from atomistic simulations.

Gels rheological Analysis

- Rheological analysis of gel samples based on polyurethane and nanocellulose. Stationary and oscillatory regime tests have been conducted and the data was analyzed to extract the correct rheological behaviour.

Targeted therapy simulation

- A Dasatinib molecule and a protein were used to search a docking site. A box of solvatation for the complex was created and the system was simulated to study the binding energy.

Classification of surface defects

- Utilized a CNN to classify images of surface defects on hot-rolled steel. High accuracy was achieved by changing the hyperparameters and topology.

Spectrometer

- Built a DIY spectrometer and a calibration tool in excel. They were used to extract and analyze the spectra from different materials.

Calibration of Adenine spectra

- Regression model for an Adenine spectra using Gaussian Process and SVM