GABELLINI CRISTIAN

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www.cristiangabellini.com FNTwin • Italian: Native Speaker - English: Fluent

EXPERIENCE

Research - University of Trieste (UNITS)

Researcher

01/2021 - *Now* Trieste, Italy

- Developed and implemented routines to model nanomaterials by correctly simulating the pKa-influenced behaviour
- Development of computational models of a variety of SAM-AuNPs via the integration of many technique (QM, MD and CG dynamics) and use of classical and advanced molecular simulation approaches (e.g., enhanced sampling techniques) on a wide spatio-temporal scale.

Research - University of Jan Evangelista (UJEP)

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

- Researched machine learning models used for nanomaterials simulations
- Designed and implemented machine learning approaches to coarse-grain water solvents
- Implemented 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

- Designed and implemented the automatic creation of complex 2D and 3D objects from tabular data by using parametric modeling
- Developed a new internal procedure to apply the new modeling technique between different technical departments
- Led the implementation of a new interactive data visualization procedure by using GIS data and Microsoft PowerBI.

SKILLS

- **Technical:** Experience in Machine Learning, Data visualization, Data Analytics. 2+ Years experience in material modeling and simulations.
- **Programming:** Proficiency in Python, Jupyter Notebook, Bash and Git. Knowledge of C++(14, STL, Boost), Javascript, SQL and MongoDB.
- **Packages/Frameworks:** NumPy, SciPy, Pandas, Matplotlib, Scikit-learn, PyTorch, Flask, FastAPI, Vue.js
- **Software:** Microsoft Office (advanced excel user), Microstation Connect, Solidworks
- **Modeling:** Amber, LAMMPS, Quantum-Espresso, DigiMat, Material Studio, Avogadro, Packmol

CERTIFICATIONS

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

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 **modeling** of the gelation of a poly-aromatic LMOG chiral system

09/12 - 12/17 University of Trieste

AWARDS

- **JetBrains PyCharm**, Winner of the 10 Years of Coding together competition with my GPGO project

PROJECTS

GPGO | *Python*

- **Bayesian optimization and Gaussian Processes framework.** Hyperparameters tuning using gradient information and different numerical solvers. Implementation of various acquisition functions and different solvers to achieve convergence on high dimensional functions.

Classification of surface defects | *Python, Jupyter*

- Implementation of **CNNs to classify images** of surface defects on hot-rolled steel. High accuracy was achieved by cross-validating the hyperparameters and topology of the tested nets.

Dissipative Particle Dynamics | *Python, Bash*

- **Parametrization of a DPD potential** for a nanoparticle grafted by polymers (AuNPs) by using a **novel bayesian optimization approach** exploiting structural insights from atomistic simulations.

Calibration of Adenine spectra | *Python*

- Regression model for an Adenine spectra using **Gaussian Process, Supported Vector Machines and Artificial Neural Networks**. Cross-validation was used to compare the different models.

GANs | *Python, Jupyter*

- Implementation and training of a Generative Adversarial Network and a **Conditional Generative Adversial Network** from the corresponding scientific literature.

Personal site | *JS, Vue.Js, HTML/CSS*

- Implementation of my homepage from scratch.

Rendering engine | *C++*

- Small ray-tracing rendering engine developed in modern C++.

Gels rheological Analysis

- Rheological **analysis** of gel samples based on polyurethane and nanocellulose with stationary and oscillatory regime tests.