GABELLINI CRISTIAN

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www.cristiangabellini.com • Italian: Native Speaker - English: 8 IELTS Academic

EXPERIENCE

Software Engineer - R&D Modeling and Digitalization, SMS Group

10/2021 - *Now* Udine, Italy

- Performed signal processing and implemented a bayesian updated exponential degradation model for the predictive maintenance of bearing machinery.
- Time-Series forecasting using Theta, ARIMA and LSTM models.
- Visualization of models data (thresholds, RUL, alarms) on Grafana with InfluxDB.
- Development of finite element thermoelastic linear models for continuos casting.

Researcher - University of Trieste

01/2021 - *12/2021* Trieste, Italy

- Created a framework (BayGPGO) to perform global multi-objective optimization of Coarse-Grainded force fields by using bayesian optimization (derivative-free method) on a gaussian process regression model.
- Developed and implemented routines to model AuNPs by correctly simulating the pKa-influenced behaviour in explicit solvents. Replica Exchange used to improve the Monte-Carlo protonation.
- Created machine learning approaches to analyze and predict the similarity between local environments of different AuNPs by exploiting SOAP fingerprints, dimensionality reduction (PCA), Gaussian Mixtures clustering, kernels product and ESR measurements.
- Development of computational models of a variety of SAM-AuNPs via the integration of many technique (QM, MD and CG dynamics). Free energy calculations via Umbrella sampling and Free energy perturbation.
- Researched Generative models (Variational Autoencoders) for molecules optimization and properties predictions.

Researcher - University of Jan Evangelista

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

- Researched Behler-Parrinello neural networks used for nanomaterials simulations.
- Implemented k-nearest neighbors and autoencoder techniques to coarse-grain different solvents
- Usage of frameworks for simulating CG and atomistic dynamics.

SKILLS

- **Technical:** 2+ Experience in Machine Learning, Data visualization. 3+ Years experience in material modeling and simulations.
- **Programming:** Proficiency in Python and Bash. Familiar with C#, Fortran, C++(14, Boost), Javascript, HTML/CSS, SQL, HPC.
- **Packages/Frameworks:** NumPy, SciPy, Pandas, Matplotlib, Scikit-learn, PyTorch, ASE, Dscribe, DeepChem, FLARE, Flask, FastAPI, VueJs.
- **Modeling:** Amber, LAMMPS, Gromacs, Quantum-Espresso, Material Studio, Avogadro, Packmol
- **Tools:** Git, Jupyter, Jira

EDUCATION

Master's Degree in Materials Engineering

Thesis: Development of **Machine-Learning** based approaches for coarse-grained simulations *107/110*

Graduated 10/2020 University of Trieste

Bachelor's Degree in Industrial Engineering

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

Graduated 12/2017 University of Trieste

AWARDS & PAPERS

- **JetBrains PyCharm**, 2020 - Winner of the 10 Years of Coding together competition with the BayGPGO project
- **oxo-Graphene as a new efficient platform for gene silencing** – Manuscript in preparation
- **Surface accessibility of AuNPs** – Manuscript in preparation
- **Solvent-mediated interactions at the interface of AuNPs** – Manuscript in reparation
- **Brownian Dynamics Optimization** – Manuscript in preparation

PROJECTS

BayGPGO | *Python*

- **Multi Objective Bayesian optimization and Gaussian Processes framework**. Derivative-free Multi Objective Bayesian Optimization is implemented by using a genetic solver and hypervolume maximization.

Brownian Dynamics Optimization | *Python, Fortran*

- Multi Objective Brownian Dynamics force field optimization of a Polyethylene glycol polymer by exploiting different structural insights and the Jensen-Shannon divergence.

GANs | *Python, Jupyter*

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

Dissipative Particle Dynamics | *Python, Bash*

- **Parametrization of a DPD potential** for a nanoparticle grafted by polymers (AuNPs) by using a **custom bayesian optimization single objective approach** exploiting the structural distributions from atomistic simulations.

Classification of surface defects | *Python, Jupyter*

- Implementation of **CNNs to classify images** of surface defects on hot-rolled steel. Different nets were tested (Custom ones, ResNet) to increase the accuracy on the multi-class classification (90%).

Targeted therapy simulation

- All-atom simulation of targeted therapy medication for leukemia. Modelling and searching of a docking site for a Dasatinib molecule. Atomistic simulation of the protein-ligand complex and analysis of the energies.