Lucia Coronel, PhD

Computational Biophysicist

@ lcor624@gmail.com +39 351 423 9924 lucia-coronel crnlcu publications

Biophysics researcher with 4 years of postdoctoral experience and a strong physics background, specialized in biopolymer simulations and molecular modeling. Skilled in data analysis and machine learning, with the ability to integrate quantitative modeling and biological insight to address complex problems, and a proven record of peer-reviewed publications, including 2 in *Nature Communications* and 2 in *Nucleic Acids Research*.

Experience

Computational Chemist and Biophysics

Temple University, Philadelphia, PA (USA)
2020 - 2024

- Deployed and optimized Molecular Dynamics (**MD**) and Metadynamics **simulations** on High-Performance Computing (**HPC**) systems.
- Managed GPU usage, software libraries, and parallelization for modeling proteins (ion channels) inhibition, **ligand–protein interactions**, and self-assembly metamaterials (DNA-origami).
- Developed workflows combining simulations, **Free Energy** calculations, and data-driven analysis (**python**), identifying *novel* inhibitor candidates and key mutation residues resulting in a Nat. Comm. publication.
- Applied structure-based **virtual screening** and **molecular docking** (Maestro), and applied **machine learning** (ML) clustering to cut 400M compounds down to 20 top candidates for experimental validation.
- Developed communication and collaboration skills by presenting results at conferences, seminars, and with cross-disciplinary teams
- Gained management experience by supervising student internships; conducted peer review for *Macromolecules*.

Researcher (Ph.D)

SISSA, Trieste (IT)
2015 - 2019

- Designed and operated **Monte Carlo** and MD simulations, generating novel insights into entanglement in biopolymers, published in peer-reviewed journals.
- Performed translocation simulations to model directional stress propagation and nonlinear mechanical responses, resulting in a Nat. Comm. publication.
- Developed a novel algorithm to automatically identify 3D supercoiled structures in 2kbp oxDNA rings.
- Collaborated on open source *GitHub* package twith a script converting SMOG inputs from GROMACS to LAMMPS, streamlining simulation workflows.
- Coordinated SBP-Group seminars, lessons, and workshops for two years.

Speaker & Volunteer

- Chaired sessions and staff for *Python Pescara* meetups, *PyCon DE & PyData*, and *GDG DevFest* conferences.
- *TUPA Committee Member*: coordinated events, including design, promotion, and logistics. *2023 - 2024*
- *Science Outreach*: promoted STEM as an invited radio speaker, reaching 100,000+ listeners (Ep. 31/07/2018).

Skills

Programming: Python, C++, Bash, Tcl, GitHub, HPC PBS & SLURM
Tools: VMD, Scikit-Learn, Numpy, Matplotlib, Seaborn, Pandas, MDAnalysis, Jupyter, PyTorch, pyMC
Others: LaTeX, Gnuplot, Unix/Linux, MS Office
Scientific: Molecular Dynamics, NAMD, GROMACS, PLUMED, LAMMPS, MonteCarlo, Schrödinger Suite
ML & DL: SVM, PCA, K-Means, Random Forests, XGBoost, Regression, VAE
Languages: Italian (N), English (F), Spanish (F)

Education

Ph.D *cum Laude* Physics and Chemistry of Biological Systems, fellowships, SISSA, Trieste, Italy *2019*
M.Sc. Physics of Complex Systems, Universita' degli Studi di Torino, Torino, Italy *2015*
B.Sc. Physics, Universita' degli Studi di Torino, Torino, Italy *2013*