André Lanrezac

Scientific Software Developer

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lanzac.github.io

Skills

Programming: Python3, C++, C#, Bash, C, HTML, CSS
Technologies: Git, CI/CD (GitHub Actions), Docker, Unity, GDB, LLDB, CMake, MongoDB
Languages: French (native), English (proficient), Mandarin (beginner)

Experience

Research Assistant & Reseach engineer 2019 – 2024
Laboratory of Theoretical Biochemistry, IBPC · CNRS , Paris

- Developed a Python algorithm to estimate interaction parameters between a reduced-resolution particle system and an analytical field, allowing large-scale dynamic simulations [1]
- Standardized multi-threaded workflows (C++, C#) for real-time molecular simulation control and monitoring, ensuring seamless and extensible data exchange
- Enhanced a 3D visualization interface (Unity, C#) for real-time Human-computer interaction and visualization of the complex dynamics of molecular shapes and their spatial evolution [1, 2]
- Implemented a CI/CD pipeline (GitHub Actions, Docker), automating software releases, resolving dependency issues, and improving accessibility for end-users
- Led the writing of the first review article on interactive molecular simulations (IMS) [3], synthesizing decades of community research

Bioinformatics Drug Design Intern Feb 2019 – June 2019
Bioinformatics and biophysics team, IMPMC · Sorbonne université , Paris

- Developed a workflow combining molecular docking and sampling simulations using a national supercomputer, with results compared to alternative methods
- Designed cyclic peptides using molecular visualization and modeling tools

Bioinformatics Structural Analysis Intern July 2018
Bioinformatics Research Team, ISYEB · Sorbonne université , Paris

- Optimized a protein similarity search by re-implementing Bellman's algorithm (Python) to find the longest path through shared motifs, and developing heuristic algorithms for faster matching

Education

Université Paris Cité – Ph.D. in Bioinformatics 2023
Advisor: Dr Marc Baaden
Sorbonne Université, Paris – B.S. in Biology & M.S. in Bioinformatics 2019

Publications

[1] André Lanrezac and Marc Baaden. "UNILIPID, a Methodology for Energetically Accurate Prediction of Protein Insertion into Implicit Membranes of Arbitrary Shape". *Membranes* (Mar. 2023). DOI:10.3390/membranes13030362.

[2] André Lanrezac et al. "Fast and Interactive Positioning of Proteins within Membranes". *Algorithms* (Nov. 2022). DOI:10.3390/a15110415.

[3] André Lanrezac, Nicolas Férey, and Marc Baaden. "Wielding the power of interactive molecular simulations". *WIREs Computational Molecular Science* (July 2022). DOI:10.1002/wcms.1594.

[4] André Lanrezac, Nicolas Férey, and Marc Baaden. "Interactive Molecular Dynamics". *Reference Module in Chemistry, Molecular Sciences and Chemical Engineering*. Elsevier, 2023. DOI:10.1016/B978-0-12-821978-2.00115-X.