-
-

- Lead writing the first known advanced review of interactive molecular simulations (IMS) [1]
- interaction [2,3]:

  Development in \(\verb!C#!\) of UnityMol visualization software:
  - Automatic generation of Unity UIs from personal XML parameter files
  - Algorithms for curved membrane mesh generation
  - Graphical and controls features dedicated for preparing and interact with simulations
  -

    HADDOCK

    experiments (1).

  Development in C++ of BioSpring molecular simulation engine:
  -

    take account of the calculation constraint on a local machine
  - Integration of a dynamic SASA calculation method for protein complex assembly
  - Automating sampling algorithm of protein positions within membrane

  Development in Python3 of analysis scripts of molecular simulations data:
  -

    representation)
  - Reactive plot for interactive trajectories analysis using a linking and brushing approach.
  -

    generate dynamic plot

    Data communication:
  -

\(\verb!C!\))

- Application to a double membrane system and to a curved viral membrane of arbitrary shape

Master internship with Dr. Dirk Stratmann

Institute of Mineralogy, Physics of Materials and Cosmochemistry, Sorbonne Université - CNRS, France • 2019

- GROMACS.
- Comparison with HADDOCK. Manual design of cyclic peptides with UCSF-Chimera.

Master internship with Dr. Mathilde Carpentier

Institute of Systematics, Evolution and Biodiversity, Sorbonne Université - CNRS, France • 2018

- bank.

Peer-reviewed publications & scientific production

Publications:

[4] Lanrezac A, Férey N, Baaden M. "*Interactive Molecular Dynamics*" Reference Module in Chemistry, Molecular Sciences and Chemical Engineering (2023) DOI: 10.1016/B978-0-12-821978-2.00115-X

[3] Lanrezac A, Baaden M. "*UNILIPID, a Methodology for Energetically Accurate Prediction of Protein Insertion into Implicit Membranes of Arbitrary Shape*" Membranes (2023) DOI: 10.3390/membranes13030362

[2] Lanrezac A, Laurent B, Santuz H, Férey N, Baaden M. "*Fast and Interactive Positioning of Proteins within Membranes* " Algorithms (2022) DOI: 10.3390/a15110415

[1] Lanrezac A, Férey N, Baaden M. "*Wielding the power of interactive molecular simulations* " WIREs Comput Mol Sci (2021) DOI: 10.1002/wcms.1594

Poster:

(1) Lanrezac A, Férey N, Baaden M. "*Combining human interaction and empirical data using interactive elastic network models*" EMBO Workshop: Advances and Challenges in Biomolecular Simulations (2021) : Poster, Abstract

Education

Laboratory of Theoretical Biochemistry - CNRS, France

Ph.D in Chemistry Physics • Nov, 2019 — Apr, 2023

"Interpretation of experimental data through interactive simulation and molecular visualization"

Sorbonne Université, Paris

Master in Bioinformatics and Modelisation • 2017 — 2019

Major in structural bioinformatics and modelisation

Université Pierre et Marie Curie, Paris

Bachelor in Molecular and cellular biology • 2014 — 2017

Major in Biology, minors in bioinformatics, modelling, thermodynamics of living systems

Professional skills

Languages : French (native), English (proficient)

Scientific software
HADDOCK

Communication : Apple/Microsoft office suites, Website design (HTML/CSS), Authorea, \(\LaTeX\)

Programming : Python3, \(\verb!C++11!\), \(\verb!C#!\), Bash, \(\verb!C!\), Unix

Development tools : git, lldb, CMake, Unity, Docker, Pixlr E

Softwares & Tools

Laboratory.

`BioSpring` : Interactive simulation engine based on an extended elastic network model
Developer • 2019 — Present • \(\verb!C++11!\)

`UnityMol` : Molecular viewer
Developer • 2019 — Present • \(\verb!C#!\)

`MDDriver` : Socket for data communication
Developer • 2019 — Present • \(\verb!C!\)

`LIPTUNE` : *Leveraging IMPALA Parameterization Technique Using New Energies* [4]

IMPALA
atomic to coarse-grained scales.
Designer & Developper • 2023 • Python3

Outside Interests

Sport : Climbing (boudering), badminton, cycling

Miscellaneous
computer science (qualified in Google CodeJam 2022), coffee enthusiast, chess.