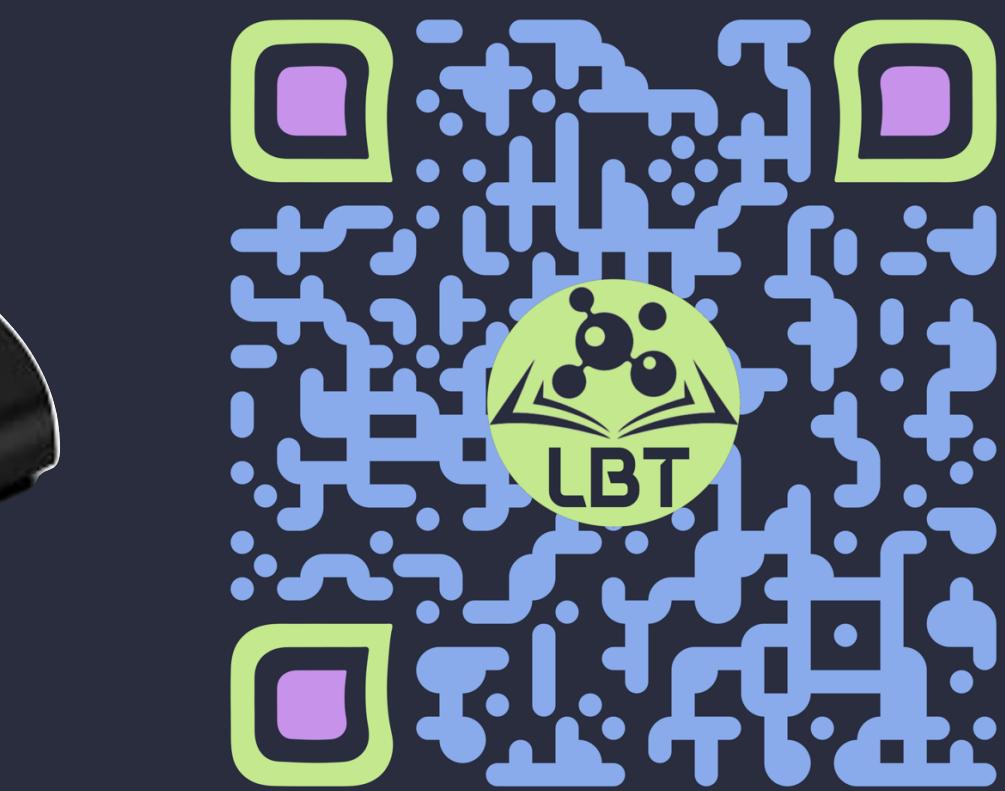


Interactive Molecular Simulations and Analyses for Everyone

Marc Baaden¹

¹Université Paris Cité, CNRS, Laboratoire de Biochimie Théorique, 13 rue Pierre et Marie Curie, 75005, Paris, France



🏁 Introduction

The Challenge

- **Interactive Molecular Simulations & Analyses (IMSA)** are powerful but underutilized
- High technical barriers limit adoption
- Complex installations discourage exploration
- Limited access to specialized hardware

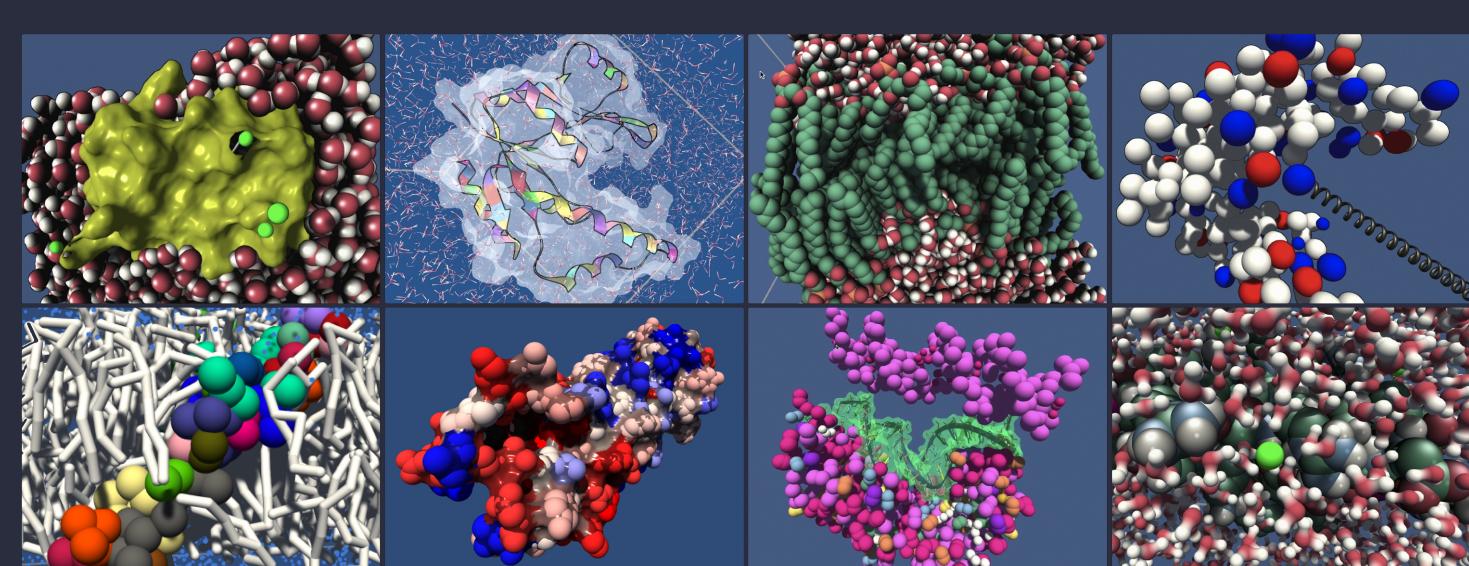


Figure 1: Interactive Molecular Simulation and Analysis examples.

One Possible Solution: MolPlay [1, 4]

MolPlay is a *bootable USB platform* providing turnkey access to IMSA.

Key Features:

- No installation required
- Works on standard hardware
- User-friendly interface
- Curated examples included
- Portable and self-contained

🔍 Architecture

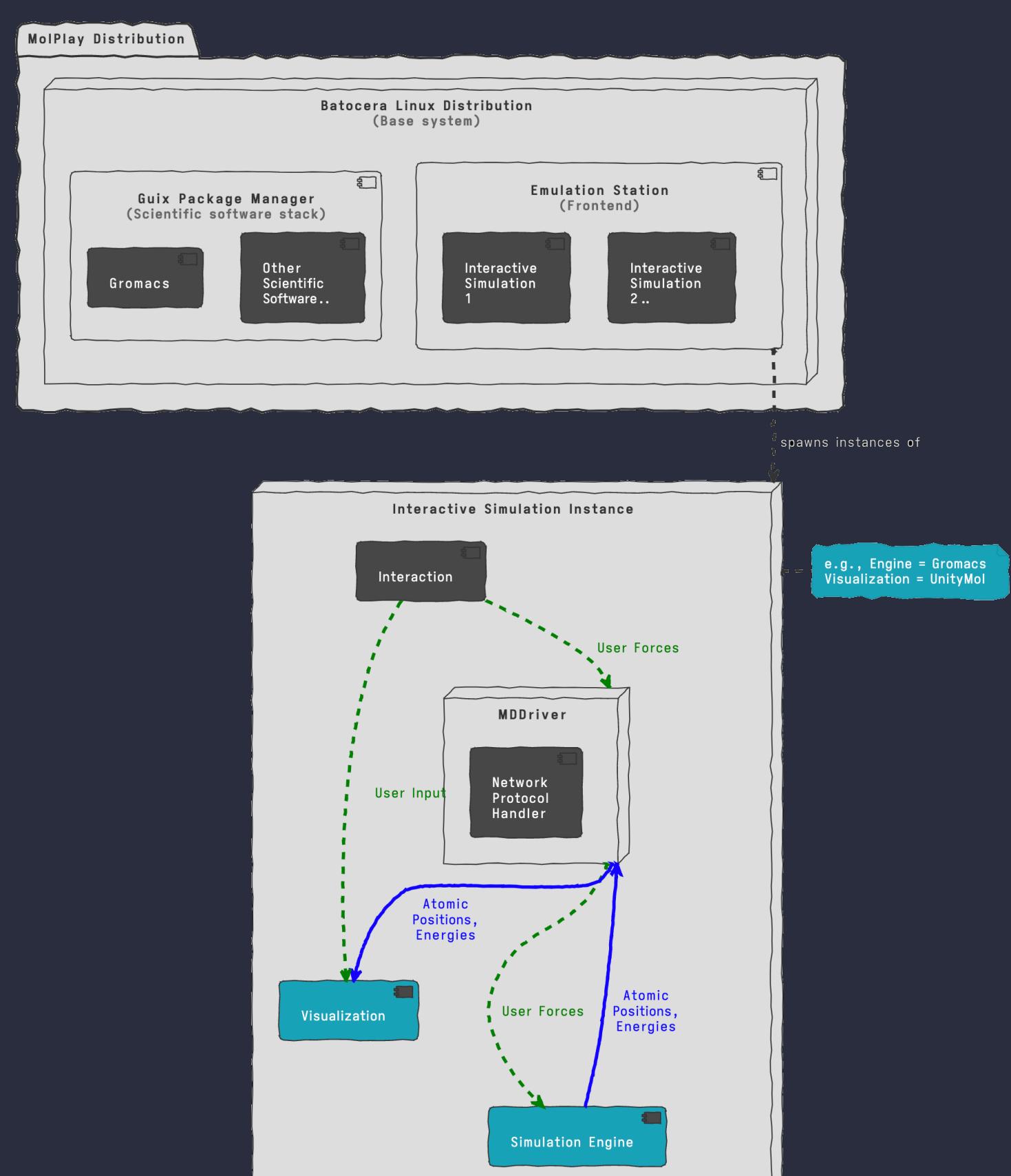


Figure 2: An overview of MolPlay's architecture.

Components

- **Batocera Linux**: Lightweight base OS
- **Guix Package Manager**: Scientific software distribution
- **Emulation Station**: Intuitive menu interface
- **MDDriver Protocol**: Connects simulation components

Task Taxonomy

We identified three **main IMSA task categories**:

- **Manipulate**: Model construction, deformation, force application
- **Explore**: Conformational sampling, rare event investigation
- **Analyze**: Real-time visualization, interaction scrutiny

These are depicted below:

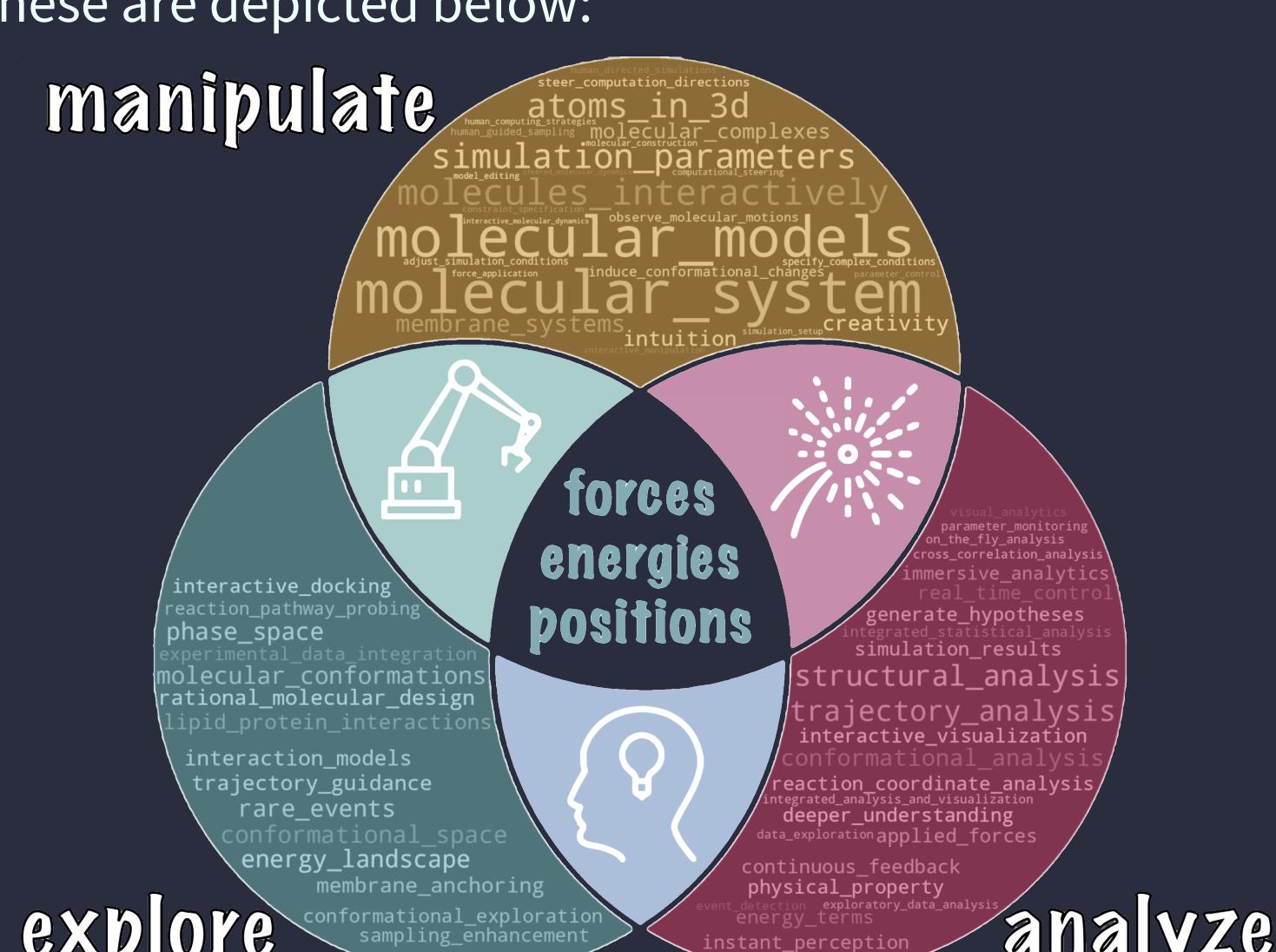


Figure 3: Task categories for interactive approaches.

💡 Use Cases

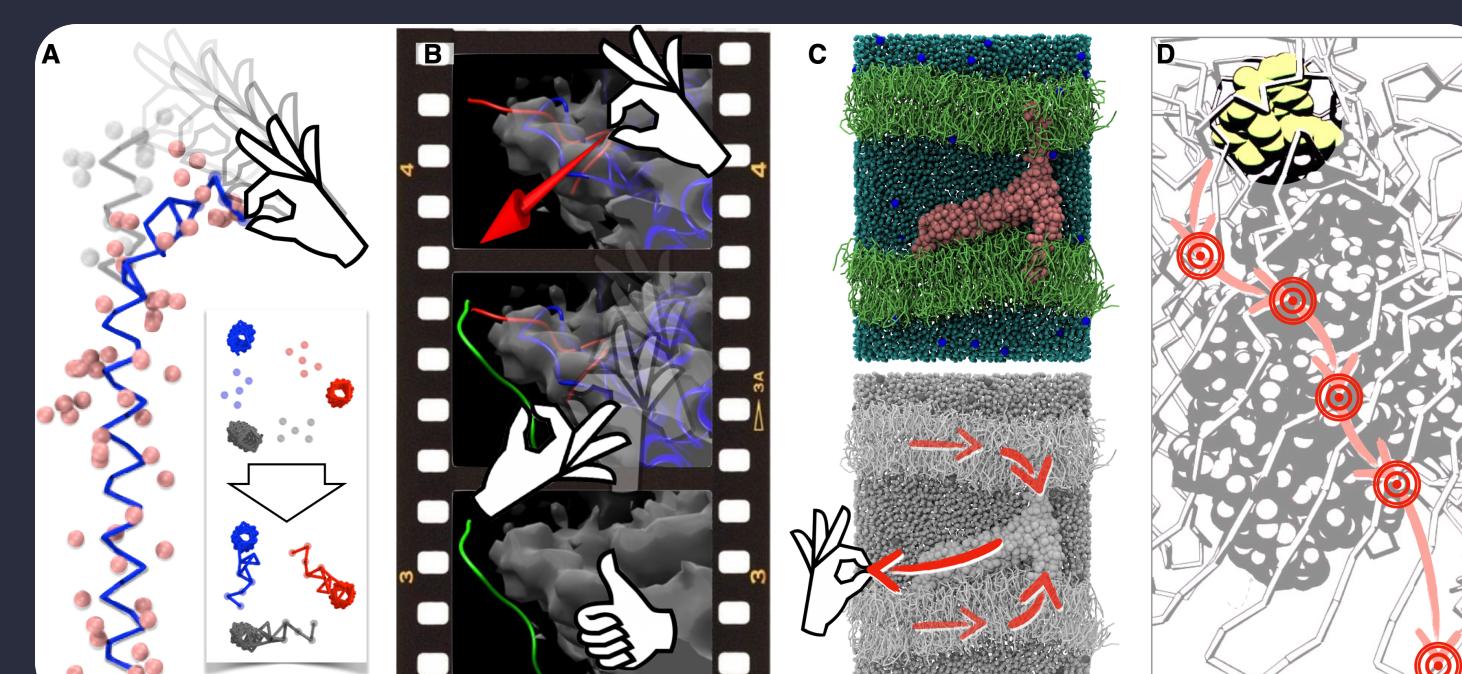


Figure 4: Four use cases for interactive simulations.

The examples above represent:

- **A**: Preparing simulations - bending transmembrane helices
- **B**: Integrative modeling - ryanodine receptor reconstruction
- **C**: Mechanical properties - SNARE complex investigation
- **D**: Guided exploration - siderophore transport pathway

🎬 Ask for a Demo! ⭐



🎮 User Experience

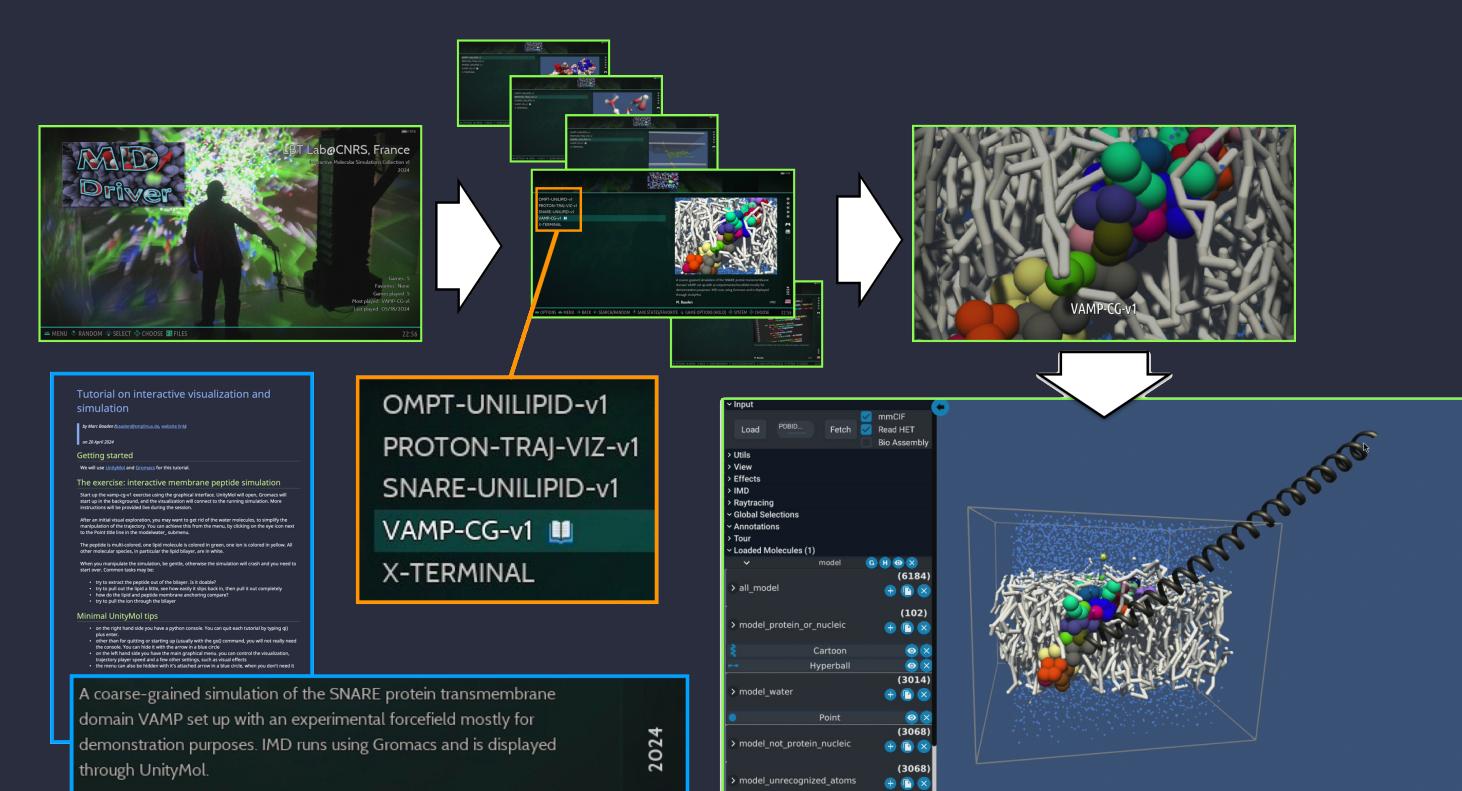


Figure 5: MolPlay's user interface is simple and user friendly.

Features:

- Simple boot from USB
- Intuitive navigation
- Built-in tutorials and documentation
- Multiple levels of expertise

🎯 Target Applications

Education & Outreach

- Science fairs and museums
- Classroom demonstrations
- Hands-on learning experiences

Research

- Hypothesis validation
- Preliminary investigations
- Collaborative analysis

🎲 Featured Simulation Engine [2, 6]



👀 Visual Analysis

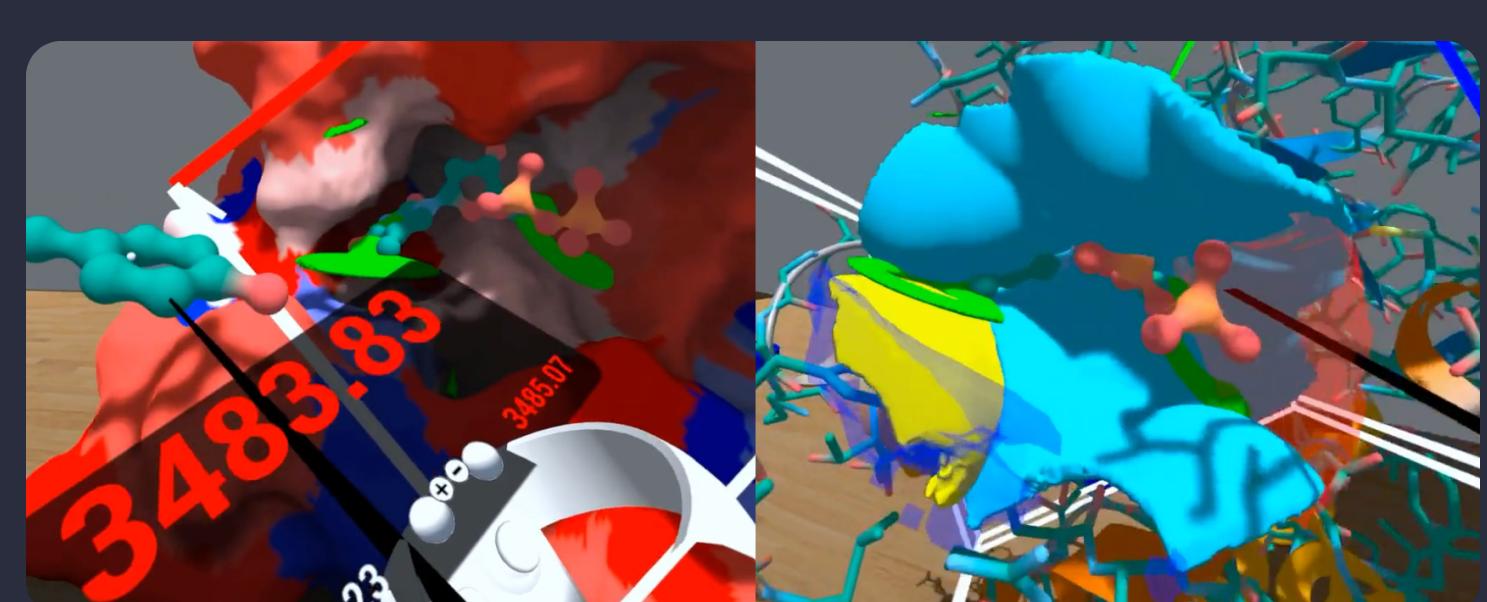


Figure 6: Visual analysis of statistical molecular interaction fields [3, 5].

↗ Impact & Future

- **Tested** at international workshop (~30 participants)
- **Positive feedback** from diverse user groups
- **Expandable** catalog of examples
- **Modular design** for future integrations

❗ Conclusions

MolPlay bridges the gap between advanced IMSA techniques and accessible education/research tools. By consolidating expertise into a portable platform, it promotes broader adoption of interactive molecular simulations across disciplines.

🎭 Acknowledgments

M.B. thanks past (Sébastien Doutreligne, André Lanrezac, Xavier Martinez, Joao Rodriguez, Alex Tek) and present (Olivier Delalande, Nicolas Férey, Benoît Laurent, Hubert Santuz) collaborators who were essential in laying the foundations for the work described on this poster.

💶 Funding

This research was funded by the “Initiative d’Excellence” program from the French State, grants “DYNAMO,” ANR-11-LABX-0011, and “CACSICE,” ANR-11-EQPX-0008. I thank ANR for support of grants “PIRATE,” ANR-21-CE45-0014 and “MINOMICS,” ANR-19-CE45-0017. Many thanks to Sesame Ile-de-France for co-funding the display wall used for testing some of the interactive use cases described on the poster.

🔗 References and links

- [1] <https://molplay.mol3d.tech>.
- [2] <https://biospring.mol3d.tech>.
- [3] <https://smiffer.mol3d.tech>.
- [4] M Baaden. “MolPlay: Democratizing Interactive Molecular Simulations and Analyses with a Portable, Turnkey Platform”. *inJ Phys Chem B*: 128 (2024), 9132.
- [5] D Barquero Morera **and others**. “Statistical Molecular Interaction Fields: A Fast and Informative Tool for Characterizing RNA and Protein Binding Pockets”. *inbioRxiv*: (2025).
- [6] B Laurent **and others**. “BioSpring: An elastic network framework for interactive exploration of macromolecular mechanics”. *inProt Sci*: 34 (2025), e70130.

📞 Contact

- ✉ Email: baaden@smplinux.de
- 🌐 Website: www.baaden.ibpc.fr
- linkedin: [baaden](https://www.linkedin.com/in/baaden/)
- Mastodon: [@baam93@mastodon.social](https://baam93.mastodon.social)
- Bluesky: [@baam93.bluesky](https://baam93.bluesky.social)
- Twitter/X: [@baam93](https://twitter.com/baam93)

