

# Interactive Molecular Simulations and Analyses for Everyone

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## 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

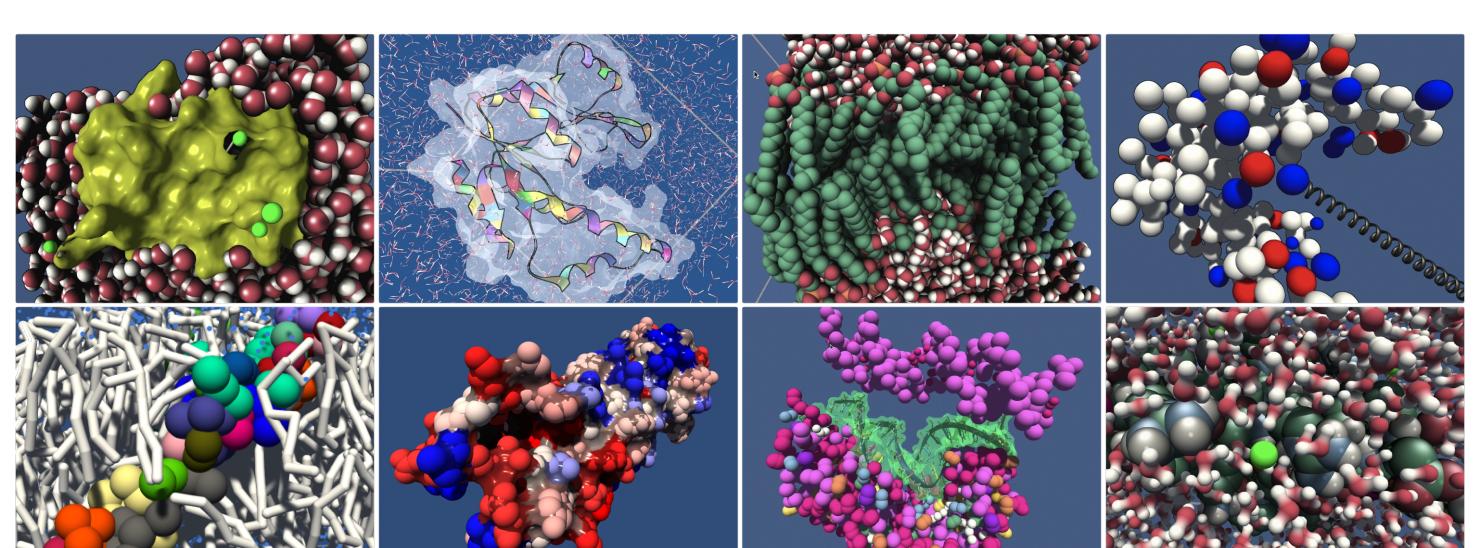


Figure 1: Interactive Molecular Simulation and Analysis examples.

### 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

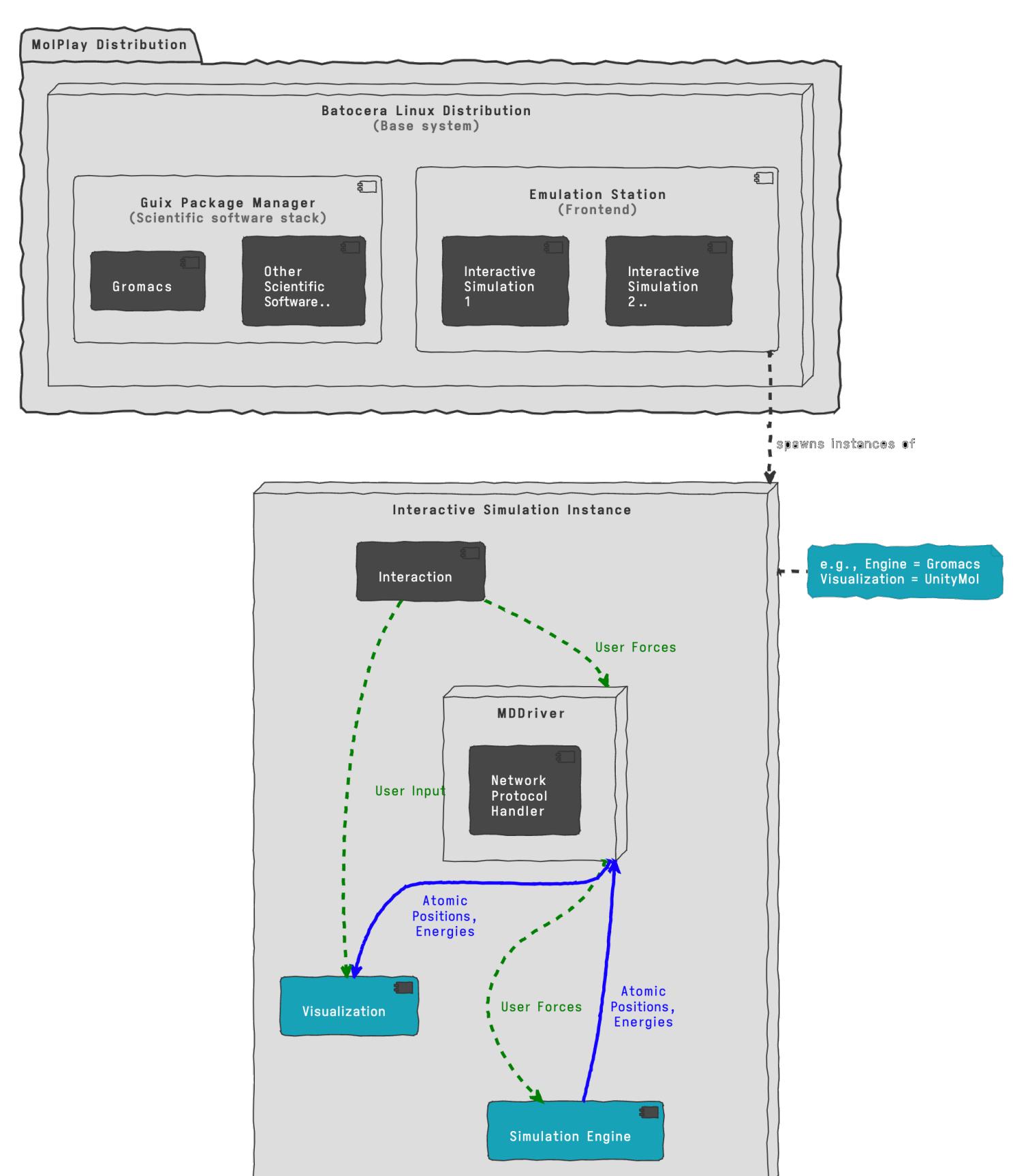


Figure 2: An overview of MolPlay's architecture.

## 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:

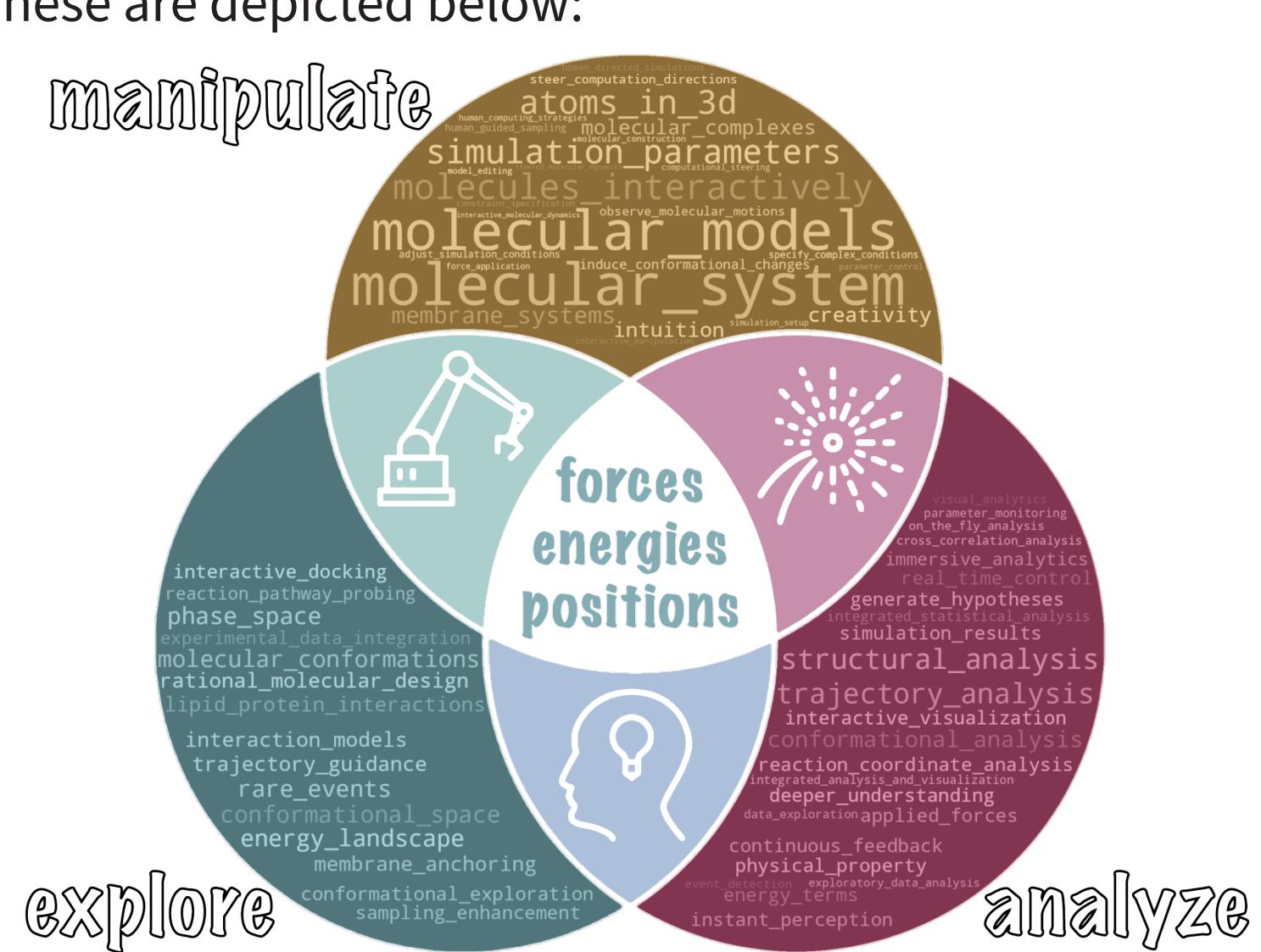


Figure 3: Task categories for interactive approaches.

## Use Cases

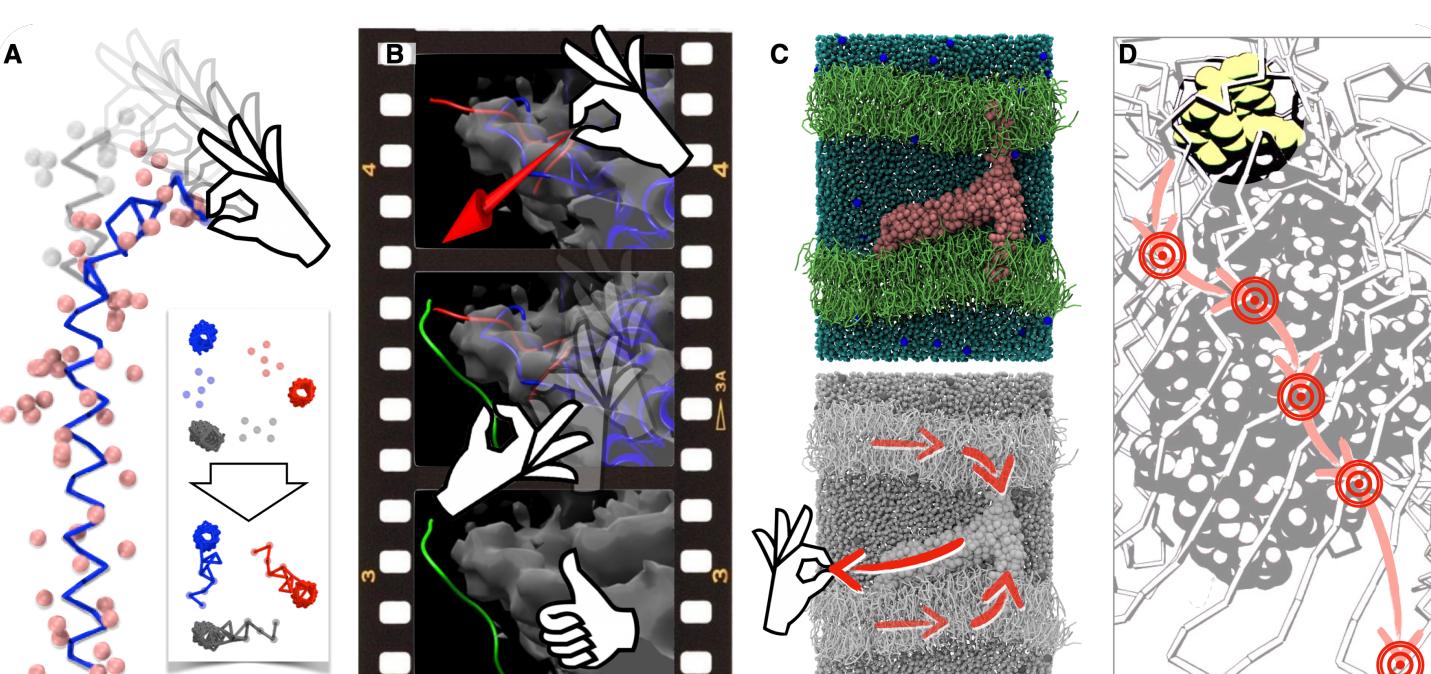


Figure 4: Four use cases for interactive simulations.

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

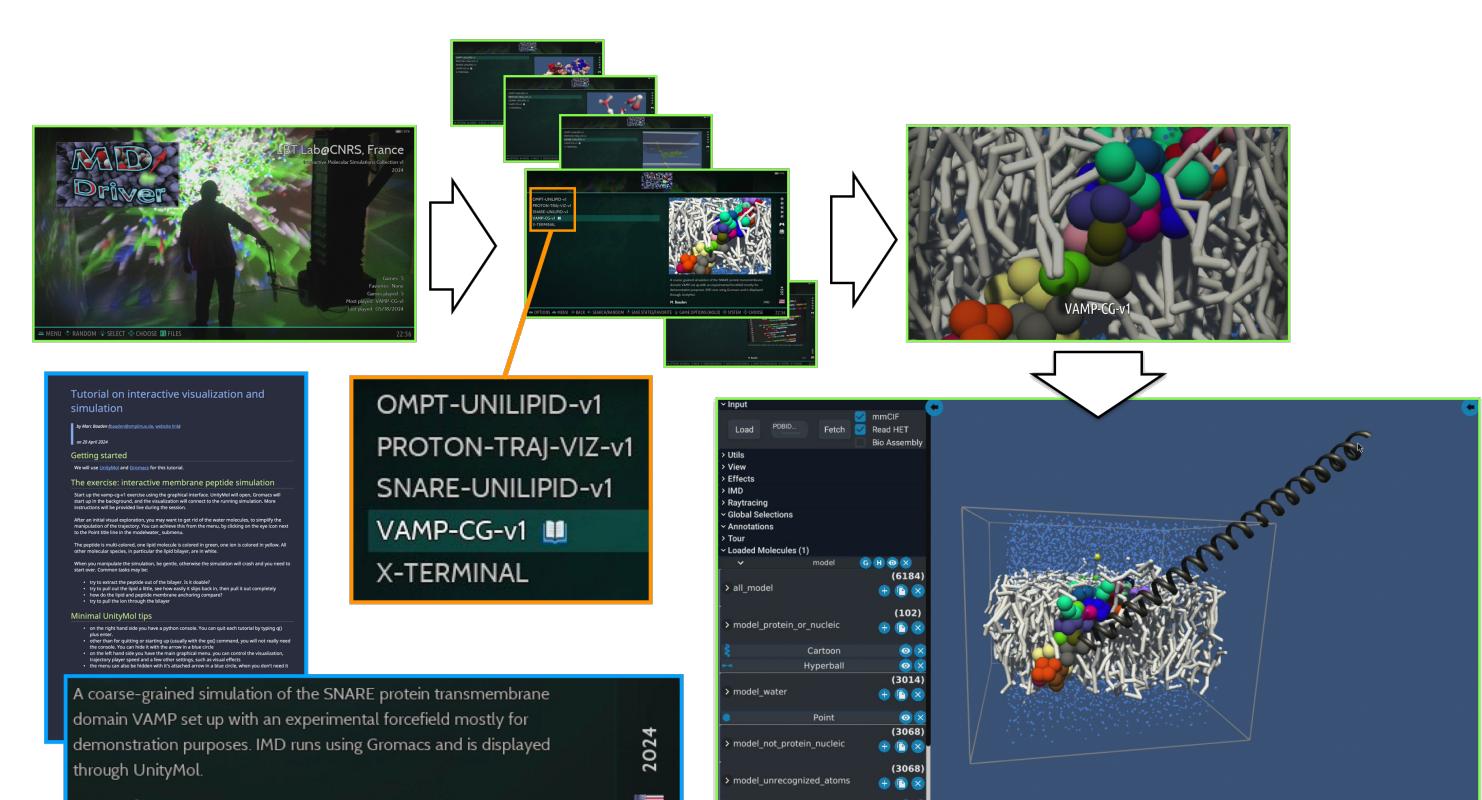


Figure 5: MolPlay's user interface is simple and user friendly.

#### 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

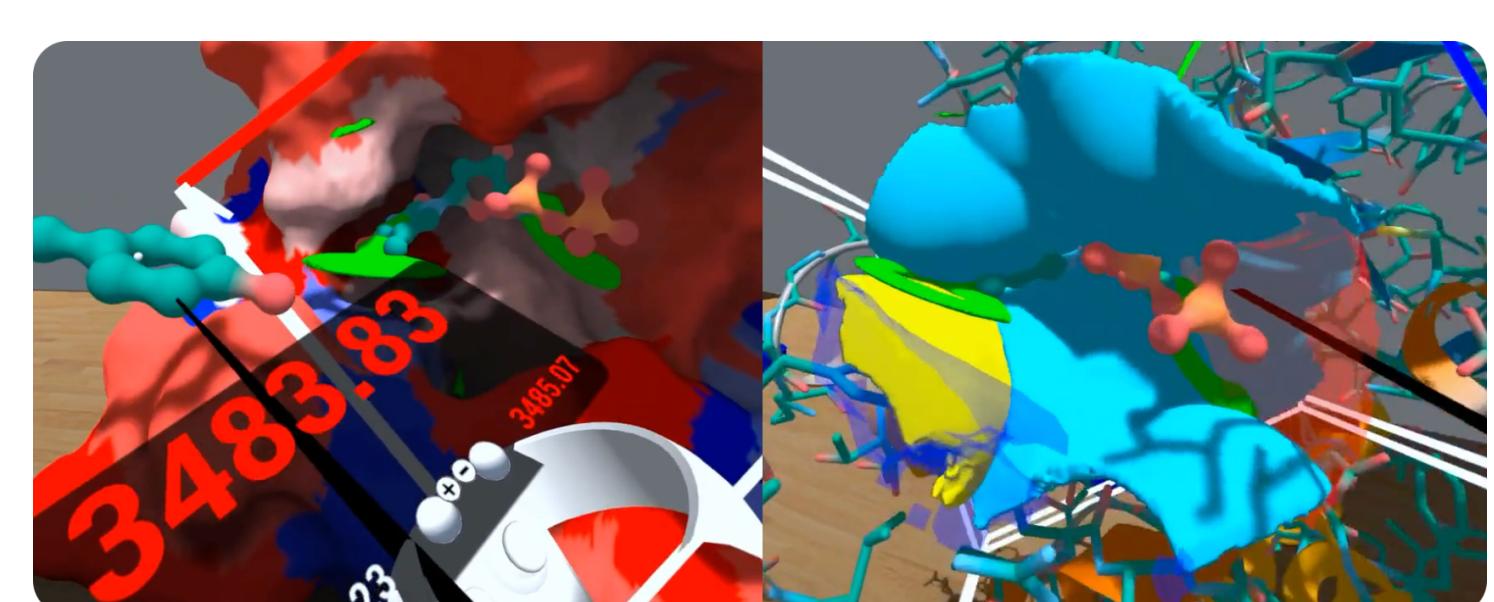


Figure 6: Visual analysis of statistical molecular interaction fields [3, 5].

## 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

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## 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”. *J. Phys. Chem. B*: 128 (2024), page 9132.
- [5] D Barqueró Morera *et al.*. “Statistical Molecular Interaction Fields: A Fast and Informative Tool for Characterizing RNA and Protein Binding Pockets”. *bioRxiv*: (2025).
- [6] B Laurent *et al.*. “BioSpring: An elastic network framework for interactive exploration of macromolecular mechanics”. *Int. J. Prot. Sci.* 34 (2025), e70130.

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