Molmil: A versatile WebGL based molecular viewer

Gert-Jan Bekker
Java on the web; the end of an age

• jV & Jmol applets were used on the web

• Oracle bought Sun (developer of Java) in 2009

• WebGL: prototypes in 2006 (Canvas 3D), WebGL Working Group (Khronos) in 2009, v1.0 specs released in 2011

• First draft implementation in Chrome in 2010, Firefox soon after, IE in 2013 and finally Safari in 2014

• 2015: Chrome drops Java support, Edge (IE12) never supported it; 2017: Firefox
• 2016: Oracle deprecates applets from JDK 9
Molmil: the start of a new one

- Work on a molecular viewer for tablets started in 2012

- A new viewer for only tablets isn’t worthwhile; we wanted wide support

- WebGL was a new, but unproven technology with the potential for very wide support

- Beta version released in 2013; v0.9 in 2014, source (v1.0) published on GitHub in 2016 (along with J. Chem. Inf. paper)
Molmil Beta

- Released in 2013
- Part of PDBj website; not a standalone web app
- Only Mine PDB entry viewer
- Could only read PDBx/mmJSON format
PDBx/mmJSON format

- Only a few programming languages have a PDBx/mmCIF parser
  - However many have a JSON parser (some have multiple)

  "Jsonified" version of PDBx/mmCIF format
  - Data structure of PDBx/mmJSON is very similar to that of PDBx/mmCIF

- Includes some optimizations for improved gzip compression
  - Gzipped ~40% smaller than PDBx/mmCIF
  - Simple typing (integer/float) is included in the format

- Metadata-only version used on PDBj website for displaying entries
Molmil 0.9

• Revolutionary update
  • Standalone version (no longer requires the PDBj website to function)
  • Support for multiple file formats ➔ even USER specified files could be loaded
• Molmil UI
Molmil 1.0

- Evolutionary update
- Many improvements and bugfixes
- Support for additional PDBj services
Beyond PDBj

• Rudimentary command line
  • Subset of Pymol commands
  • Molmil JavaScript API
  • Future: jV commands
  • Future: jmol commands

• Load Molmil script (e.g. from DropBox)

• Integrating Molmil & loading scripts/data from your local machine

Local scripts & files

• Many programs with command lines support loading files by commands

• Molmil, which runs inside a web browser, is limited due to security issues

• You don’t want your browser to give any random website access to your files!

• Thus using Molmil in such a way is limited
Local scripting using Mozilla Firefox

• Mozilla Firefox allows running scripts locally, while having access to files in the same folder as where it was started from

• Files stored locally for easy reproducibility

• Perfect for making images for publication
  • Especially if you have to remake your images
  • Used extensively for my own paper:
Load MD trajectories

• Currently supported:
  • PDB models (not recommended)
  • Presto COD
  • Gromacs TRR
  • Gromacs XTC (compressed)

• Molmil can play MD trajectories using various representations

• Molmil can also be used to make MP4 movies
Movies

- Molmil can use the browser to generate PNG images.
- Requires a “server-side” component to stitch the PNG images together to build a MP4 file.
- This “server-side” component is just a script which runs on your local machine:
  - [https://github.com/gjbekker/molmil/wiki/Load-MD-trajectory-files](https://github.com/gjbekker/molmil/wiki/Load-MD-trajectory-files)
- Combined with local scripting can produce very nice movies.

New features (currently in testing stage)

• New UI (menu)

• Show H-bonds function (if the structure includes hydrogens)

• Show nearby residues function
Future features

• Scripting: jV (rasmol-like) & jmol

• Superposition of structures (like Chimera’s MatchMaker)

• Improved rendering
  • VR/AR (first need a device for testing)
  • Improved graphics
  • More versatile render pipeline
Demos

• PDBj Services

• Basic usage of Molmil (standalone version)

• Custom local scripts examples
Questions, etc

• https://pdbj.org/contact

• https://github.com/gjbekker/molmil/issues

• gertjan.bekker@protein.osaka-u.ac.jp

Reference: Gert-Jan Bekker et al. J. Cheminf. 2016, 8, 42