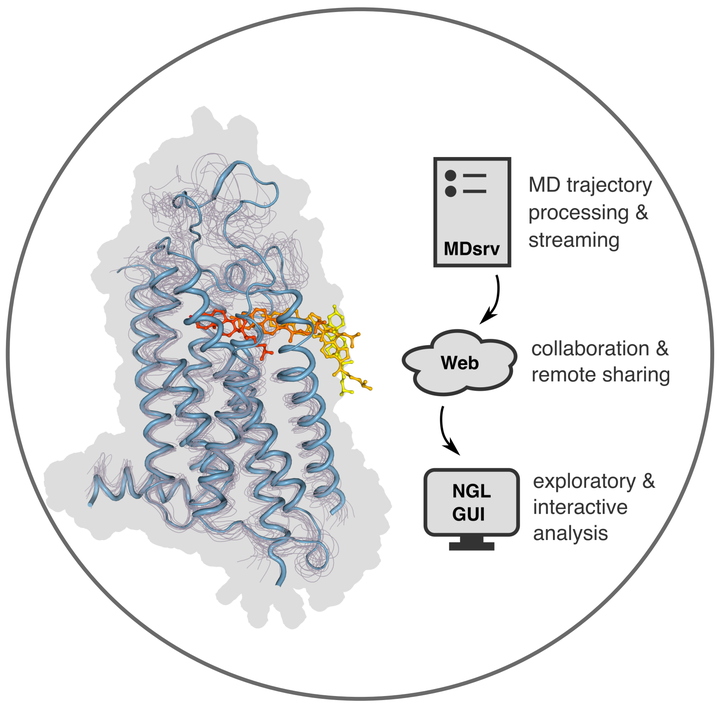
UNIVERSITÄT LEIPZIG
Medizinische Fakultät

Viewing and Sharing Molecular Dynamics Simulations on the Web using the MDsrv

Universitätsklinikum Leipzig
Medizin ist unsere Berufung.

Johanna K. S. Tiemann[*$], Ramon Guixà-González[$], Alexander S. Rose[$ #†], **Peter W. Hildebrand**[*$†]

* Institute of Medical Physics and Biophysics, University Leipzig
$ Institute of Medical Physics and Biophysics, Charité – Universitätsmedizin Berlin
# present address: RCSB Protein Data Bank, San Diego Supercomputer Center, University of California, San Diego
† To whom correspondance may be addressed: peter.hildebrand@charite.de, alexander.rose@weirdbyte.de



Abstract: Molecular dynamics (MD) simulations are widely used to **investigate time resolved motions** of G protein-coupled receptors (GPCR). Sharing of trajectories for visualization is complicated by their size (Gigabytes), the set-up and usage of specialized software. However, interdisciplinary research and collaborations necessitates **easy sharing of MD trajectories** facilitating discussions and further analyses. In contribution, we present **MDsrv** [1], a tool to serve trajectories and visualize them in a web browser by employing the NGL Viewer [2]. It supports structures, topologies and trajectories from common MD packages including **Amber, Gromacs, NAMD, Tinker or Desmond**. For interactive viewing of the MD simulations by co-workers or colleagues all over the world **no installation** - only a web browser is needed. MDsrv is available as a software package (via PyPi and conda), to be run locally or deployed to a dedicated web-server to make data from MD simulations **accessible to a wide audience of researchers & students.** This helps bridging the gap between computational and experimental researchers and even promotes concepts for publishing MD data along with publications of their analysis.

Motivation

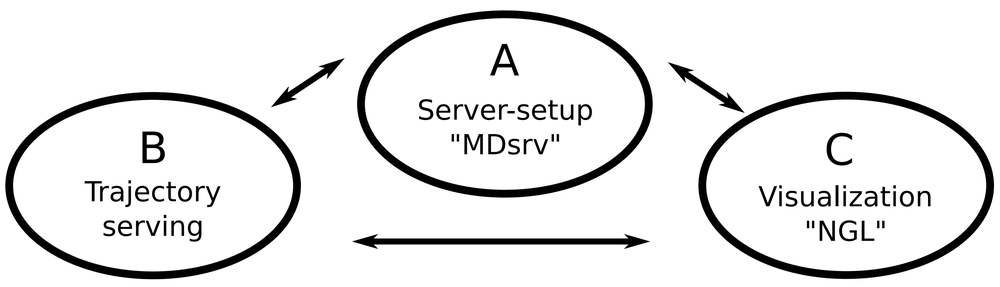
sharing & collaboration
- remotely access trajectories
- prepare data for collaborative visual analysis
- create an interactive figure

browser
- no additional software required
- spontaneous access

server
- large datasets accessible via web
- no need to transfer

chances
- attain wider audience
- enhance transparency & impact of MDs

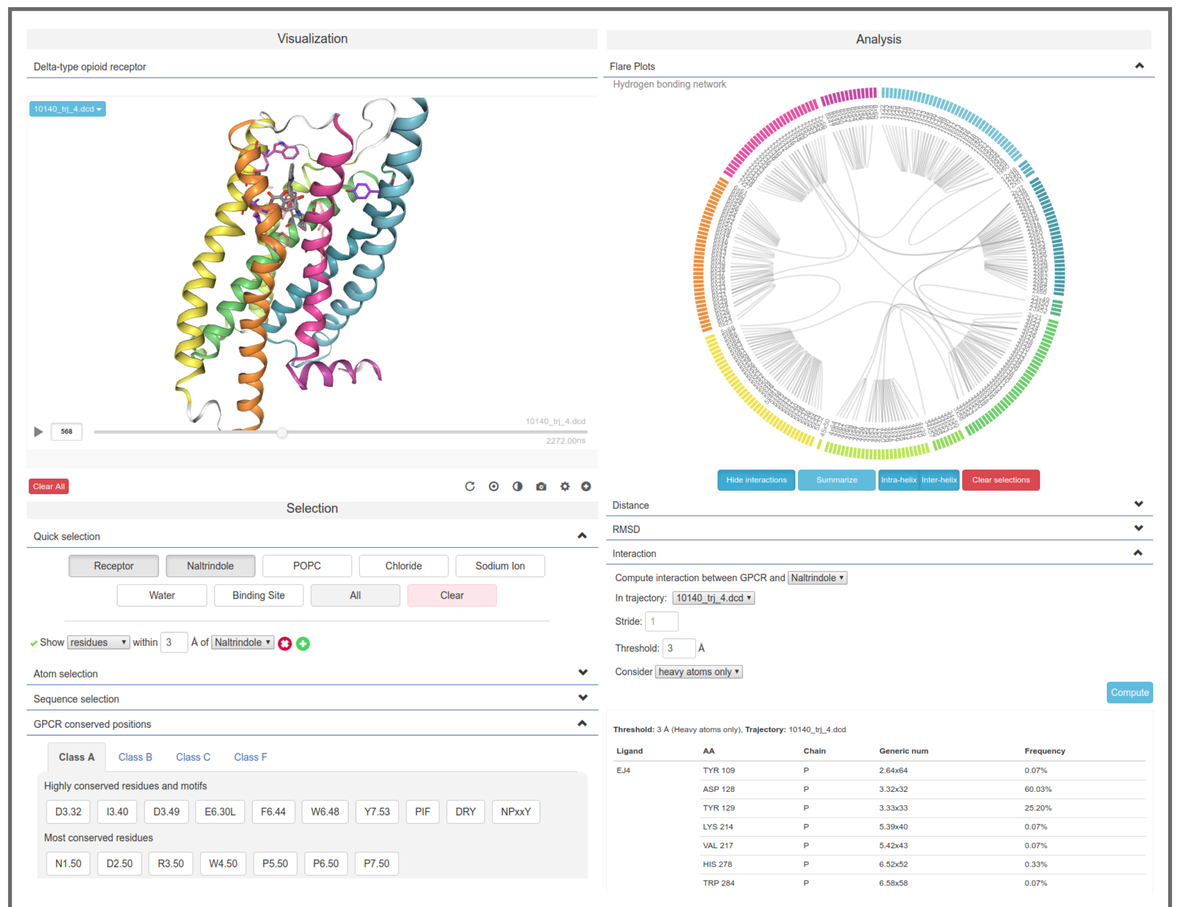
http://nglviewer.org/mdsrv



Implementation:
(A) Server component:
Written in Python & uses Flask framework to create WSGI compliant web server
(1) Serve static JavaScript, HTML, CSS, GLSL, font and image files
(2) Provide data files (trajectory, molecular-coordinate and NGL script files)
(3) Handle requests for trajectory frames
(4) Ensure basic access control to server, specific data directories or none

(B) Trajectory serving:
Provides access to vast amounts of trajectory data (for most common fromats) by using function derived from the MDTraj [3] and MDAnalysis [4].

(C) Visualization via NGL [2]:
Written in JavaScript, including a GUI (HTML, CSS)
(1) Reading, processing and updating of molecular structures
(2) Transforming molecular structures into display representations
(3) Rendering of display representations on the GPU using WebGL
(4) Creating an interactive user interface, GUI and scripting support



MDsrv used by the simulation database GPCRmd:
In collaboration with Jana Selent laboratory and Stanford University (GPCRviz) the MDsrv was incorporated in GPCRmd to visulaize basic analysis (using Flareplot) of deposited GPCR-related MDs. Providing this, the GPCRmd community aims to generate a platform for sharing MDs and their protocols, including citable IDs for referencing in publications.

Projects & examples:

TRY IT OUT!

GPCRmd:
http://gpcrmd.org/

Wiki-like article with embedded MDs:
http://proteinformatics.charite.de/MDsrv-embedded-example2

Published article embedded next to the reference:
http://proteinformatics.charite.de/MDsrv-embedded-example1

(Published) Simulation sets within the NGL gui:
http://proteinformatics.charite.de/MDsrv-example1
...
http://proteinformatics.charite.de/MDsrv-example6

NGL/MDsrv features:
- *Viewer environments:* web browser (no installation)
- *File formats:*
  - *Structure:* mmCIF, PDB, PQR, GRO, SDF, MOL2, MMTF, PSF, PRMTOP, TOP
  - *Trajectory:* DCD, NCTRAJ/NetCDF, TRR, XTC, LAMMPSTRJ, XYZ, BINPOS, HDF5, DTR, ARC, TNG
  - *Volume:* MRC/MAP/CCP4, DX/DSN6, XPLOR/CNS
- *Rendering:* depth cueing/fog, front/back cutting planes, anti aliasing (MSAA,SSAA), material parameters
- *Representations:* cartoon, ball+stick, spacefill, surface, line, isosurface, slice, hyperBall, rope, ...
- *On-the-fly trajectory processing:* interpolation (linear, spline), centering, approximate PBC, removal, superpositioning
- *Analysis tools:* distance measurements, info about picked atoms

BERLINER INSTITUT FÜR GESUNDHEITS FORSCHUNG
Charité & Max-Delbrück-Centrum

CHARITÉ
UNIVERSITÄTSMEDIZIN BERLIN

DFG

HLRN

References.
[1] Tiemann JKS, Guixà-González R, Hildebrand PW, Rose AS. MDsrv: viewing and sharing molecular dynamics simulations on the web. Nat. Methods 2017
[2] Rose AS, Hildebrand PW. NGL Viewer: a web application for molecular visulaization. NAR 2015.
[3] McGibbon RT et al. MDTraj: A Modern Open Library for the Analysis of Molecular Dynamics Trajectories. BPJ 2015
[4] Michaud-Agrawal N, Denning EJ, Woolf TB, Beckstein O. MDAnalysis: a toolkit for the analysis of molecular dynamics simulations. J Comp Chem 2011.