Supplementary Information for *MDAnalysis: A Toolkit for the Analysis of Molecular Dynamics Trajectories*

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Table S1: Comparison of various computational software packages that are used to analyze molecular dynamics trajectories.

package	version	license [1]	open source [2]	languages (code)	command language [3]	modularity [4]	object-oriented [5]	volumetric data [6]	atom selection [7]	geometric transformation [8]	visualization	simulation setup [9]	molecular simulations [10]	interactive use [11]
MDAnalysis	0.7	GPL v2	x	Python, C	Python	library	x	x	x	x	-	-	-	x
CHARMM[1]	35b1	non-free	-	FORTRAN	CHARMM	monolithic	-	x	x	x	-	x	x	-
ptraj (AmberTools) [2]	1.4	GPL	x	C	ptraj	monolithic	-	x	x	x	-	-	-	-
Gromacs [3]	4.5.3	GPL	x	C	-	tools	-	x	-	-	-	x	x	-
LOOS [4]	1.5.5	GPL	x	C++	C++	library	x	x	x	x	-	-	-	-
MMTK [5]	2.7.3	CeCILL	x	Python, C	Python	library	x	x	-	x	(external viewer or VRML)	x	x	x
WORDOM [6]	0.22	GPL v2	x	C	-/Python	monolithic/ library (simple SWIG)	-	-	-	-	-	-	-	-
MD-TRACKS [7]	0.004	GPL v3	x	Python	-	tools	-	-	-	-	-	-	-	-
Simulaid [8]		non-free	-	FORTRAN	-	monolithic	-	-	-	-	x (only Irix)	x	-	x
MMTSB [9]	Aug 2008	non-free	-	Perl, FORTRAN, C	-	tools	-	-	-	-	-	x	x	-
pymacs [10]	0.4	GPL v2	x	Python, C	Python	library	x	-	-	x	-	x	-	x
VMD [11]	1.8.7	UIUC Open	x	C, tcl	tcl, Python	monolithic	-	x	x	x	x	x	-	x
PyMOL [12]	1.3	MIT	x	C	PyMOL, Python	monolithic	-	x	x	x	x	-	-	x
Chimera [13]	1.5	non-free	-	C++	Chimera, Python	monolithic	x	x	x	x	x	x	-	x
Adun [14]	0.81	GPL	x	Objective-C	SmallTalk	framework	x	-	-	x	-	x	x	x
OpenStructure [15]	1.0.1	LGPL v3	x	C++, Python	Python	monolithic/library	x	x	x	-	x	-	-	x
Python Macromolecular Library (mmLib) [16]	1.0.0	Artistic Licence	x	Python, C	Python	library	x	-	-	x	x	-	-	-
Atomic Simulation Environment [17]	3.4.1	LGPL v2.1	x	Python	Python	library	x	x	-	x	x	x	x	x

[1] license: *GPL* is the open source GNU Public License; *LGPL* is the GNU Lesser General Public License; CeCILL (Cea Cnrs Inria Logiciel Libre) is an open source license used by French research institutions; *MIT* is a free software license originating from the Massachusetts Institute of Technology; for details on open source licenses see http://www.opensource.org/licenses/index.html . *non-free* is a specific license for the package that can be different for academic and commercial use but it always restricts the way in which the code can be used, modified, and republished
[2] open source means that source code is publicly available under a license in the spirit of the Open Source Definition http://www.opensource.org/osd.html
[3] computer language that is primarily used to carry out analysis tasks; often a scripting language. Not all packages contain a full-fledged "language" but a set of actions. Shell-scripting to join separate command line tools is not listed.
[4] modularity: How the packages is used typically: as a *library*, as a *framework* to build other tools, as a set of command line *tools*, or as a (effectively) *monolithic* program that controls all aspects of operation
[5] object-oriented: design focused on treating atoms/molecules/systems as objects
[6] volumetric data: capability to generate, process and/or read volumetric data such as densities or general fields
[7] atom selections: syntax to select atoms with descriptors and boolean combinations thereof (not just simple index files)
[8] geometric transformations: broad category that captures if it is possible to manipulate individual atoms and thus edit the system; many packages contain additional sophisticated model building capabilities
[9] simulation setiup: Does the package contain special functionality to support the setting up of MD simulations?
[10] molecular simulations: Is it possible to run particle-based simulations with the package?
[11] interactive use: Does the package contain special functionality to support the interactive analysis of MD trajectories?

Table S2: Comparison of analysis software package input/output capabilities. Basic reading (R) and writing (W) is listed for a number of frequently encountered file formats. *molfile* indicates that the program relies on the VMD molfile plugin [11] to support I/O.

package	version	PDB	PSF (CHARMM, NAMD,XPLOR)	PARMTOP (Amber)	TPR (Gromacs)	DCD (CHARMM/NAMD/ LAMMPS)	Amber (trj, netCDF)	XTC/TRR (Gromacs)	CRD (CHARMM/ XPLOR)	GRO (Gromacs, GROMOS)	PQR (electro-statics)	XYZ trajectory
MDAnalysis	0.7	R/W	R	R	-	R/W	R (trj)	R/W	R/W	R/W (single frame)	R	R
CHARMM [1]	35b1	R/W	R/W	-	-	R/W	-	-	R/W	-	-	-
ptraj (AmberTools) [2]	1.4	R/W	R	R	-	R/W	R/W	-	-	-	-	-
Gromacs [3]	4.5.3	R/W	-	-	R/W	R (*molfile*)	R (*molfile*)	R/W	R (*molfile*)	R/W	R (*molfile*)	R (*molfile*)
LOOS [4]	1.5.5	R/W	R	R	-	R/W	R	R	R	R	-	R
MMTK [5]	2.7.3	R/W	-	-	-	R/W	-	-	-	-	-	-
WORDOM [6]	0.22	R/W	-	-	-	R/W	-	R/W	R/W	R/W	-	R/W
MD-TRACKS [7]	0.004	-	R	-	-	-	-	-	-	R	-	R
Simulaid [8]	Dec 2010	R/W	R	R	-	R/W	R/W	-	R/W	R/W	-	-
MMTSB [9]	Aug 2008	R/W	R	-	-	R/W	-	-	-	-	-	-
pymacs [10]	0.4	R/W	-	-	R/W	-	-	R/W (xtc)	-	R/W	-	-
VMD [11]	1.8.7	R/W	R/W	R	-	R/W	R/W	R, R/W	R	R	R	R
PyMOL [12]	1.3	R/W	R (*molfile*)	-	-	R (*molfile*)	R (*molfile*)	R (*molfile*)	R (*molfile*)	R (*molfile*)	R	R (*molfile*)
Chimera [13]	1.5	R/W	-	R/W	-	-	R/W	-	-	R	R	R
Adun [14]	0.81	R/W	-	-	-	-	-	-	-	-	-	-
OpenStructure [15]	1.0.1	R/W	-	-	-	-	-	-	R (traj)	-	-	-
Python Macromolecular Library (mmLib) [16]	1.0.0	R/W	-	-	-	-	-	-	-	-	-	-
Atomic Simulation Environment [17]	3.4.1	R/W	-	-	-	-	-	-	-	-	-	R/W

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