Supporting information for: MDANSE : an Interactive Analysis Environment for Molecular Dynamics Simulations

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Trajectory converters currently implemented in MDANSE

Table S1: List of the trajectory converters currently implemented in MDANSE.

dmol	from Materials Studio[S1] DMOL package
castep	from CASTEP[S2]
charmm	from CHARMM[S3]
dlpoly	from DL_POLY[S4]
discover	from Materials Studio[S1] Discover package
forcite	from Materials Studio[S1] Forcite package
lammps	from LAMMPS[S5,S6]
namd	from NAMD[S7]
pdb	from a set of PDB[S8] snapshots
vasp	from VASP[S9]
xplor	from X-PLOR[S10]

Analyses currently implemented in MDANSE

Table S2: List of the analyses currently implemented in MDANSE.

	Dynamics
ac	autocorrelation of a vector defined with respect to a molecule
dos	vibrational density of states
gacf	autocorrelation function for a user defined property
msd	mean square displacement of a set of atoms
op	order parameter
pacf	autocorrelation of the coordinates of a set of atoms
vacf	autocorrelation of the velocities of a set of atoms
	Scattering
ccf	transversal and longitudinal current correlation function
dcsf	dynamic coherent scattering function and structure factor
disf	dynamic incoherent scattering function and structure factor
eisf	elastic incoherent structure factor
gdisf	dynamic coherent structure factor using gaussian approximation
sffsf	dynamic (inc)coherent structure factors from intermediate scattering functions
	Structure
apm	area covered per lipid in a membrane
cn	coordination number
dp	density profile along a cartesian axis
ecc	eccentricity of a set of atoms
mt	framewise 3D map of the spatial occurence of a set of atoms
pdf	pair distribution function
rog	radius of gyration
rmsd	root mean square deviation
rmsf	root mean square fluctuation of atomic coordinates
sas	solvent accessible surface
sd	spatial density around a molecule
ssf	static structure factor
vo	volume of Voronoi cells for a set of atoms
xssf	static structure factor using X-ray atomic form factors
	Thermodynamics
den	atomic and mass densities of the system
temp	temperature of the system
	Trajectory handling
btt	centers the trajectory around the center of a set of atoms
com	generates a new trajectory from the center of masses of a set of atoms
ct	generates a new trajectory from a subset of the atoms of the original one
gmft	filters the trajectory from the rotational and translational global motions
rmt	rebuilds the trajectory correctly folded of a membrane
ut	rebuilds a contiguous trajectory for a given molecule

Technical Description

As a python application, MDANSE has several dependencies

- NumPy[S11] for working on N-dimensional arrays
- Matplotlib[S12] for producing 1D/2D plots
- VTK[S13] for visualising trajectory and producing 3D plots
- wxPython[S14] for designing the GUI
- MMTK[S15] for molecular structure representation and trajectory handling
- NetCDF[S16] file format for storing trajectories and output of the analyses
- Cython[S17] to build extensions for time-critical algorithms

MDANSE has been implemented using the Oriented Object Programming (OOP) paradigm. It is based on a set of interfaces designed to make easier the development and the integration of the components necessary for implementing easily new analyses. The different types of interfaces available in MDANSE framework are listed in table S3.

Table S3: List of the interfaces that build the MDANSE framework

Interfaces	Description	Scope*
Configurator	Check and configure an individual entry of an analysis	L
Iormat	Handle the ouput of the analysis	L
Handler	Manage the application loggers	L
InputData	Define behaviour common to all input data	L
Resolution	Define models for instrument resolution functions	L
Job	Implements the running engine common to all analysis	L
OutputVariable	Defines MDANSE output variables	L
Plugin	Describes generically a draggable and droppable window	G
Projector	Abstract definition of coordinates projection models	L
QVectors	Generates the reciprocal vectors for scattering analysis	L
Selector	Manages the different ways to select atoms of the system	L
Widget	Graphical representation of the IConfigurator objects	G

*Scope of the interfaces : (L)ibrary or (G)raphical User Interface

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