NAME

AMBERDASH − Dash interface for Amber trajectories

SYNOPSIS

amberdash [options] *seed* [−− *dash_options*]

Run **dash** on trajectories generated by the Amber molecular dynamics package (http://ambermd.org/).

OPTIONS

−help
Print help message and exit.

−version
Print version number and exit.

−debug
Print progress messages on **stderr**.

−keep
Keep all the intermediate files that are normally deleted when the program exits.

−keep−dash−input
Keep the **dash** input file *seed*.dash.in which is normally deleted when the program exits.

−keep−ptraj−input
Keep the **ptraj** input file *seed*.ptraj.in which is normally deleted when the program exits.

−no−dash
Generate (and keep) the **dash** input file *seed*.dash.in but do not run **dash**.

−progress
Print output from the **ptraj** command on **stdout**. Useful for monitoring progress when reading large trajectories.

−snap
Write PDB files containing snapshots representing the **dash** states.

−backbone *r1*:*r2*
Analyze the sequence of backbone torsion angles from residue *r1* to residue *r2*.

DASH OPTIONS

The *dash_options* are described in the **dash** documentation. The **dash** flags *−N* (number of frames) and *−T* (number of torsions) are not required; they are supplied automatically by **amberdash**.

INPUT FILES

Several input files are required, specified by the *seed* prefix, in order to identify the topology, the torsion angles and the trajectory.

The topology is always specified by an Amber topology file *seed*.top.

The torsion angles may be specified either by the **−backbone** option or by a file *seed*.tor. The **−backbone** option takes precedence.

The trajectory may be specified either as a single Amber trajectory file *seed*.trj, or by a sequence of **trajin** commands in a text file *seed*.trajin. If *seed*.trajin exists, it is used and *seed*.trj is ignored; otherwise *seed*.trj is used. The *seed*.trajin approach is necessary if the trajectory spans several files or a subset of the trajectory is required via *start*, *stop* and *offset* arguments to **trajin**.

If snapshots are required (**−snap**) and the trajectory is specified in *seed*.trajin, the trajin commands in *seed*.trajin must include start, stop and offset fields. Otherwise the script is unable to locate the representative **dash** states in the trajectory and the snapshots are omitted.

seed.top
An Amber topology file corresponding to the trajectory to be analyzed.

seed.trajin
: A text file containing **trajin** commands to extract the trajectory to be analyzed. Any lines not containing **trajin** commands are ignored.

seed.trj
: An Amber trajectory file.

seed.tor
: A text file defining the torsion angles to be analyzed. Each torsion angle is specified by a whitespace-separated line with five fields:

```
name mask1 mask2 mask3 mask4
```

Here *name* is an identifier and *mask1*, ..., *mask4* are Amber atom masks defining the torsion angle. Lines starting with '#' are treated as comments and ignored. This file must be prepared manually by the user.

OUTPUT FILES

seed.dash.out
: The **dash** output file.

seed.ptraj.out
: The output from the **ptraj** command to extract the torsions.

If **−snap** is specified, the following files are written for each **dash** state:

seed.state*N*.*frame*
: The PDB file containing the representative frame *frame* for **dash** state *N*.

seed.ptraj.state*N*.out
: The output from the ptraj command to generate the PDB file for **dash** state *N*.

If **−keep** is specified, the following intermediate files are retained:

seed.ptraj.in
: The input file for the **ptraj** command to extract the torsions.

seed.*name*
: The torsion angles for each torsion *name*.

seed.dash.in
: The dash input file obtained by joining the torsion angle files.

If **−keep−ptraj** and **−snap** are specified, the following files are retained:

seed.ptraj.state*N*.in
: The input file for the ptraj command to generate the PDB file for **dash** state *N*.

INSTALLATION

The programs **dash** and either **ptraj** or **cpptraj** are required. If they are not on the **PATH** their full pathnames must be specified at the top of the **amberdash** script. **cpptraj** reads large trajectories faster than **ptraj**, while **ptraj** calculates statistics for the torsion angles.

NOTE

All the output files will be clobbered by the next run of the script for the same *seed*.

REFERENCE

D. W. Salt, B. D. Hudson, L. Banting, M. J. Ellis and M. G. Ford
DASH: A novel analysis method for molecular dynamics simulation data.
Analysis of ligands of PPAR−gamma, J. Med. Chem., 48, 3214−3220, 2005.

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