

XDRIO: A library for accessing GROMACS files

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GROMACS

- * Classical Molecular Dynamics code
- * Extremely efficient on modern hardware
- * User base estimated > 3000 (+ 1 million in Folding at Home)
- * GNU General Public License (GPL)

Gmx Highlights

- * The need for speed...
- * Portability due to use of modern free software tools (autoconf/automake)
- * Great manual, user support through very active mailing lists
- * Relatively easy to use
- * Support from third parties: VMD, gOpenMol and more.

XDRIO: Portability

- * Based on the code used in the networking file system (NFS)
- * Portable binary files
- * Programming interface agnostic to single/double issues
- * C / Fortran / Python interfaces
- * Documentation with doxygen

XDRIO: Files

- * Trajectory (trr) containing coordinates, velocities, forces
- * Compressed trajectory (xtc)
- * Energy (edr) containing all energy terms, temperature, pressure etc.

eXtAcY files

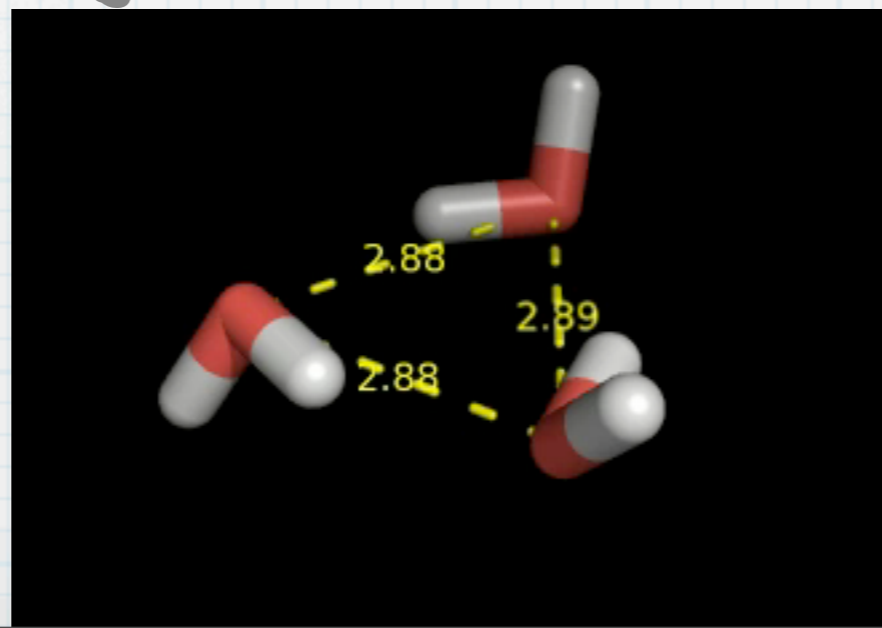
- * File format designed by Frans van Hoesel (Groningen) using lossy compression
- * User defined precision
- * Stores one coordinate (x,y,z) in roughly 32 bits (at default 1 pm precision)

eXTaCy files

- * Round coordinates to integers
- * Use spatial information: assume the next coordinate is close to the previous one and store the distance in as few bits as possible: frames have different size
- * Special magic for molecules with three atoms

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XDRIO: API

- * `XDRFILE *xdrfile_open (const char *path, const char * mode);`
- * `int xdrfile_read_int(int *ptr, int ndata, XDRFILE *xfp);`
- * `int xdrfile_compress_coord_float(float *ptr, int ncoord, float precision, XDRFILE *xfp);`
- * ... and so on ...

XDRIO: When, how?

- * Under development for GROMACS 4.0
- * Will be released separately, probably under BSD license

Related Ideas

- * Use XML for static data files, e.g. force fields - moving target
- * What about HDF5?
- * Collaboration with other groups (anyone patent the wheel recently?)
- * XDRIO could be foundation for a Babel for trajectory files

Questions

- * Is there an open source DCD reader?
- * Other "proprietary" trajectory files?