Gromacs - Bug #312

xdrfile bugs

04/08/2009 12:30 PM - Jussi Lehtola

Status: Closed
Priority: Normal
Assignee: David van der Spoel
Category:
Target version: CVS
Affected version -
extra info:

Affected version:

Description

First and foremost: xdrfile license is incorrect.

output of Debian's licensecheck.pl:
./include/xdrfile.h: MIT/X11 (BSD like)
./include/xdrfile_trr.h: GPL (v2 or later)
./include/xdrfile_xtc.h: GPL (v2 or later)
./src/xdrfile_trr.c: MIT/X11 (BSD like)
./src/trr2xtc.c: MIT/X11 (BSD like)
./src/xdrfile_xtc.c: MIT/X11 (BSD like)
./src/xdrfile.c: MIT/X11 (BSD like)
./src/xdrfile_c_test.c: MIT/X11 (BSD like)
./config/lmain.sh: GPL (v2 or later) GENERATED FILE

Also, no declaration of license is included in the package. Please put the correct license in COPYING, which is now empty.

2. Empty files: aforementioned COPYING, also AUTHORS, INSTALL, NEWS and README.

3. Upon compilation, 'make tests' is suggested. No such object exists in makefile.

4. IMHO the include files should be installed in /usr/include, not /usr/include/xdrfile, since there are just 3 files and they don't have general names that could conflict with other software..

History

#1 - 04/08/2009 12:34 PM - Jussi Lehtola
Also, I couldn't find a section on the GROMACS homepage dedicated to xdrfile. Having one would be nice, since the one would be able to refer to it in rpm packages.

#2 - 04/08/2009 12:35 PM - Jussi Lehtola
ChangeLog is empty, too.

#3 - 05/18/2009 11:10 AM - David van der Spoel
Hi Jussi,

please check the version I'm linking to from http://wiki.gromacs.org/index.php/XTC_Library

I think this resolves most problems, except the location of the include files.
It seems to be default to put stuff in subdirectories now, just to prevent any mixing with the OS.

#4 - 05/18/2009 08:54 PM - Jussi Lehtola
(In reply to comment #3)
Hi Jussi,

please check the version I'm linking to from http://wiki.gromacs.org/index.php/XTC_Library

I think this resolves most problems, except the location of the include files.

Hi David,

thanks a lot. Now everything seems to be fixed.

It seems to be default to put stuff in subdirectories now, just to prevent any mixing with the OS.

Hmm, as a distribution maintainer I don't think so.

For GROMACS it's logical since it has quite a few include files, some of which have generic names, but xdrfile on the other hand has only two headers which have very specific names. In this case using an own directory is IMHO a bit of an overkill, it just means that the users have to specify -I/usr/include/xdrfile when compiling apps.

It's not a problem per se, just an inconvenience to the user.

#5 - 05/18/2009 09:06 PM - David van der Spoel
Problem is I couldn't find out how to change it in configure.ac. You can however override it with --includedir

#6 - 05/18/2009 09:16 PM - Jussi Lehtola
(In reply to comment #5)
Problem is I couldn't find out how to change it in configure.ac. You can however override it with --includedir

Okay. I'm not going to change it in the Fedora package, though, since then codes that
#include <xdrfile/xdrfile.h>

will not work.