

GROMACS - Feature #2194

xvg output requested as an output option in place of xpm files

05/30/2017 11:00 PM - Chris Neale

Status:	Accepted
Priority:	Low
Assignee:	
Category:	analysis tools
Target version:	
Difficulty:	simple
Description	
Some analysis tools have output options that would be useful as .xvg files with real numbers but are only provided as graphical .xpm files. For example, gmx rms has the -m matrix output available only as .xpm when giving the -f2 input. The only way to get an actual RMSD matrix in real numbers with high precision is to run the program many times, each with a different -s input. gmx cluster has similar issues with the matrix, as I imagine other tools do as well. It would be nice to be able to get either .xmp or .xvg output for all options that currently give output with .xpm.	

History

#1 - 05/31/2017 03:38 PM - Mark Abraham

- Category set to analysis tools
- Status changed from New to Accepted
- Difficulty simple added
- Difficulty deleted (uncategorized)

Agreed, this is a weakness of the analysis tools. One (historical) issue is that there was not really a widely accepted portable file format for a matrix file (text or binary). Do people have ideas on what would be good to use, e.g. to suit existing related workflows?

#2 - 05/31/2017 03:43 PM - Chris Neale

Not to disregard other formats, but the .xvg output if e.g. gmx pairdist can have an enormous number of columns for certain selections. I don't find that a problem at all... just parse it with a script.

#3 - 05/31/2017 04:26 PM - Mark Abraham

Chris Neale wrote:

Not to disregard other formats, but the .xvg output if e.g. gmx pairdist can have an enormous number of columns for certain selections. I don't find that a problem at all... just parse it with a script.

Yeah, there's definitely cases where xvg is good enough - particularly multiple-time-series data (or per-residue, etc). It's less obvious that e.g. a matrix of per-residue-pair distances is a good fit in the hands of a user who might xvgrace matrix.xvg :-D (But that still beats the heck out of only writing xpm!)