GROMACS - Task #2009

improve command-line reporting of useful things

07/18/2016 12:21 AM - Mark Abraham

Status:	New
Priority:	Normal
Assignee:	
Category:	
Target version:	
Difficulty:	uncategorized

Description

Some ideas from recent gmx-users threads:

- People struggle with -DPOSRE vs -DPOSRES etc. so it would probably be useful for grompp to report the number of active restraints to the terminal
- People think constraints = none might make water flexible so we should check that there's some explicit statement about the number of constraints+settles used and number of bonds/angles converted (along with the check that the timestep is likely to be stable)
- Further, even though constraints is documented to be about automatic conversion, we could change the name to something like convert-to-constraints = none|h-bonds|all-bonds with the usual backwards-compatibility things. That we made an unfortunate choice that can be misunderstood isn't a reason to avoid improving it. Or we could replace the -DFLEXIBLE mechanism.
- New people don't know how to interpret their EM result. The warnings about final step size being too large don't help noobs. Some people don't even know that +1e6 kj/mol is terrible, so we should find some heuristic that pats them on the back if the final energy is less than some suitable negative number of kJ/mol per atom (or dof). Someone needing a tight EM for NMA already knows how to interpret what they need to know.

History

#1 - 07/26/2016 12:54 PM - Mark Abraham

The use of vdwradii.dat isn't made explicit enough in some docs and command line reporting, eg
https://mailman-1.sys.kth.se/pipermail/gromacs.org_gmx-users/2016-July/107500.html