GROMACS

Groningen Machine for Chemical Simulations

USER MANUAL

Version 5.0.2

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More information can be found on our website: www.gromacs.org.

Preface & Disclaimer

This manual is not complete and has no pretention to be so due to lack of time of the contributors – our first priority is to improve the software. It is worked on continuously, which in some cases might mean the information is not entirely correct.

Comments on form and content are welcome, please send them to one of the mailing lists (see www.gromacs.org), or open an issue at redmine.gromacs.org. Corrections can also be made in the GROMACS git source repository and uploaded to gerrit.gromacs.org.

We release an updated version of the manual whenever we release a new version of the software, so in general it is a good idea to use a manual with the same major and minor release number as your GROMACS installation.

On-line Resources

You can find more documentation and other material at our homepage www.gromacs.org. Among other things there is an on-line reference, several GROMACS mailing lists with archives and contributed topologies/force fields.

Citation information

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However, we prefer that you cite (some of) the GROMACS papers [1, 2, 3, 4, 5, 6] when you publish your results. Any future development depends on academic research grants, since the package is distributed as free software!

GROMACS is *Free Software*

The GROMACS source code and and selected set of binary packages are available on our homepage, www.gromacs.org. Have fun.

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