

How to contribute to the code and documentation

Where to find documentation and how to use it

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Outline

WHY?

HOW?

GROMACS
documenta-
tion

EXAMPLES

DO those
things

DON'T DO
this things

- 1 **WHY?**
- 2 **HOW?**
- 3 **GROMACS documentation**
- 4 **EXAMPLES**
- 5 **DO those things**
- 6 **DON'T DO this things**

Why contribute to the code?

WHY?

HOW?

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tion

EXAMPLES

DO those
things

DON'T DO
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- Why contribute, other people are working on it.
- Feeling that there is not enough expertise.
- Harsh review on initial changes.
- Feeling of wasted effort when changes rot in review for years.

Good reasons to contribute

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HOW?

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- Fix small issue that is annoying you.
- You have a great idea what could improve performance and can prove it.
- Update to analysis methods.
- Improve the documentation where you think it needs improving.

What to do first when you decide to contribute

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things

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- Have a good idea what you want to do.
- Work out the requirements for what you want.
- Reduce scope of your change as much as possible.
- Test that it does what it should and nothing else.

Resources to get information

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- `gerrit.gromacs.org`
- `redmine.gromacs.org`
- `gmx-users@gromacs.org`
- `gmx-developers@gromacs.org`

Where to continue after the first steps

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- Contact one of the developers on the mailing list.
- Open a Redmine issue to discuss the issue.
- Set up local repository to build the binary.
- Prepare testing for what will be touched by your change.

Prepare for frustration

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HOW?

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things

DON'T DO
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- Once you upload a reasonable change, people will see and review it.
- Review can and will be on point to keep up our software standards.
- Be prepared to go through a large number of rounds of review.
- Depending on the state of the change, it may be rejected and you need to reconsider.

How to reduce your frustration and that of the developers

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HOW?

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DO those
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- More on this later in the Does and Don't.
- Do not upload large changes without context.
- Test your changes beforehand.
- Read the style guide and get updated on new coding standards.

What is the GROMACS documentation

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HOW?

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- Your source for everything that you need to start.
- Recently reworked to be more accessible.
- Info on how to build and what parts of the code do.
- Always has and will be work in progress.

What to find where

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HOW?

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DO those
thingsDON'T DO
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- User guide
(<http://manual.gromacs.org/documentation/2019-beta1/user-guide/index.html>): How to run the program.
- Reference manual
(<http://manual.gromacs.org/documentation/2019-beta1/reference-manual/index.html>): The physics behind it.

What to find where - cont.

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HOW?

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EXAMPLES

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- Developer guide
(<http://manual.gromacs.org/documentation/2019-beta1/dev-manual/index.html>): What you need to read before coding.
- Doxygen documentation
(<http://manual.gromacs.org/documentation/2019-beta1/doxygen/html-full/index.xhtml>): What every (documented) bit does and how.

Documentation rework

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HOW?

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- My first project related to GROMACS.
- Documentation build was split between on-line html and PDF manual.
- Made it difficult to related sections from both with each other.
- Split over different webpages.

Process to change things

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HOW?

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things

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- Learn how Gerrit works.
- Set up local build environment.
- See how the automated testing works.
- Prepare change and upload it.

Result of rework

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HOW?

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- One format for documentation: RST markup.
- Better cross-referencing between sections.
- Further deprecation of ancient webpages.
- Making it possible to have DOI for manual.

Update to gmx cluster

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HOW?

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- External contributor wanted to contribute changes to tool.
- Started discussion on mailing list and Redmine.
- Uploaded patch to Gerrit.
- Helped in clean up and review.

Get involved in the community

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- Try to help with code review for other changes.
- Help people with questions on using or developing the program.
- Fix small things, learn more about the codebase.

Be active on Gerrit and Redmine

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- Care about the state of the program.
- Read more code to help in finding errors in other peoples work.
- Be thorough, but stay civil and kind in pointing out issues.

Be inconsiderate with your changes

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HOW?

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- Time is finite each day.
- Developers cannot spend all day reviewing your change.
- Testing infrastructure has limited resources.
- Listen to advise, don't brush away comments.

20000+ line changes are a bad idea

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HOW?

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- Large changes scare away even the hardened dev.
- Bugs will be hidden in your change and hard to find.
- If main parts are touched, it becomes more and more difficult to understand and validate.

Acknowledgements

WHY?

HOW?

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Erik Lindahl, Berk Hess, Mark Abraham

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All developers and contributors to GROMACS

Thanks for your attention/patience

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HOW?

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Questions? Comments? Suggestions?