GROMACS

Project ID: 17679574

22,053 Commits **705** Branches **133** Tags **3 TiB** Project Storage **16** Releases

Topics: molecular dy... simulation

The GROMACS molecular simulation toolkit.

Project badge Project badge Project badge Latest Release v2023.2 Project badge

GROMACS GitLab and Version Control

Sebastian Wingbermühle

How to code for GROMACS (day 1)

Tonight

Up for dinner, chatting and some games?

Ugglan
Närkesgatan 6 (Södermalm)
T-bana: walk from Medborgarplatsen
7 pm

Agenda

1. Set up and manage your local git
2. Prepare for uploading a change
3. Upload an MR
4. Our review system
5. GROMACS on GitLab – an overview

Set up and manage your local git

- After cloning, you have one branch main
- However, at least one release branch is actively maintained (now release-2023). To add it:
  git fetch origin
  git checkout -b ’release-2023' 'origin/release-2023’
- GitLab identifies you by your mail address. Set it in your config file you edit by typing:
  git config --global --edit

Set up and manage your local git

- Keep your git up-to-date:
  git checkout main
  git pull origin main
  git checkout release-2023
  git pull origin release-2023

- These commands can be stored in a script you run daily or once a week

Set up and manage your local git

- For every change, create a new branch with a meaningful name (will be visible on GitLab):
  git checkout -b <name_of_new_branch>

- Helpful git commands while coding:
  git diff, git grep, …

- Once done, create a commit:
  git add .
  git commit -m “<title_of_MR>”

Prepare for uploading a change

- Make sure your branch is compatible with the current state of the repository:
  git checkout <my_branch>
  git pull --rebase origin main

- If your local git is up-to-date, you can use:
  git checkout <my_branch>
  git rebase main

- Reuse recorded resolution for merge conflicts:
  git config --global rerere.enabled true

Prepare for uploading a change

- Test compile your branch locally (the most relevant setup):

```
cmake <branch> -DGMX_DOUBLE=?\
               -DGMX_MPI=?\
               -DGMX_GPU=?\
               -DREGRESSIONTEST_DOWNLOAD=ON\
               -DCMAKE_BUILD_TYPE=Debug
make -j <processes> # build code
(make -j <processes> webpage # only if docs changed)
make -j <processes> tests
make check # pass this before uploading!
```

Prepare for uploading a change

- We use automatic code formatting by clang:
  git checkout <my_branch>
  # diff-index to preview, update-workdir to format
  bash admin/clang-format.sh update-workdir
  bash admin/clang-tidy.sh -B=<build_dir> update-workdir

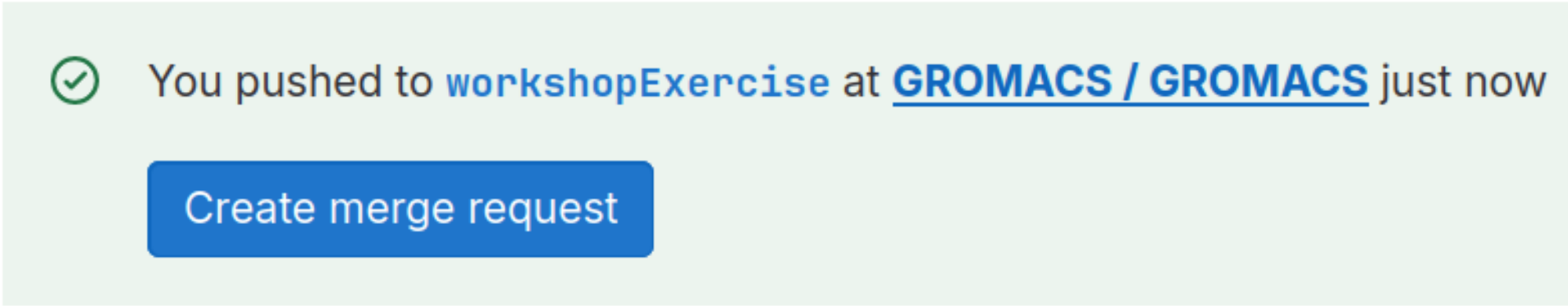
- Make sure the copyright is up-to-date:
  bash admin/copyright.sh --copyright=full update-workdir

- If you change the docs:
  docs/doxygen/includesorter.py -S . -B <build_dir>

Upload an MR

- Push your branch to our online repository (origin, sometimes remote in GitLab docs)
  git push origin <name_of_local_branch>

- When logging in to GitLab, you'll be asked to create a merge request (MR)



New merge request

From `workshopExercise` into `main` Change branches

Title (required) Meaningful title (Gitlab suggests your commit message)

Rename check_atom_names to checkAtomNames

☐ Mark as draft
Drafts cannot be merged until marked ready.

Description Documentation for the future: concise and intelligible

Preview

This MR renames a function internal to grompp such that it meets the recent GROMACS naming conventions.

Switch to rich text editing

Add description templates to help your contributors to communicate effectively!

Assignees

Unassigned ⌄ Assign to me

Reviewers

Unassigned ⌄

2 approval rules require eligible members to approve before merging.

› Approval rules

Milestone

Select milestone ⌄

Labels

Select label ⌄

Merge request dependencies

List the merge requests that must be merged before this one. Learn more.

Enter merge request URLs or references

References should be in the form of path/to/project!merge_request_id

Merge options

- [x] Delete source branch when merge request is accepted.
- [x] Squash commits when merge request is accepted. ⓘ

Create merge request | Cancel

Upload an MR

- After pressing “Create merge request”, you’ll be re-directed to the overview page of your new MR

Draft: Rename check_atom_names to checkAtomNames

Open **Sebastian Wingbermühle** requested to merge `workshopExercise` into `main` 1 minute ago

Overview 0 | Commits 2 | Pipelines 1 | Changes 1

This MR renames a function internal to grompp such that it meets the recent GROMACS naming conventions.

0 0

Merge request pipeline #994457522 running

Merge request pipeline running for 129552b7

Requires 3 approvals from GMX Core Main and GMX Developer Main.

Merge blocked: the source branch must be rebased onto the target branch. Rebase

Merge details

- The source branch is 2 commits behind the target branch
- 1 commit will be added to `main`.
- Source branch will be deleted.

Activity

All activity

Preview

Write a comment or drag your files here…

Switch to rich text editing

Comment | Close merge request

Upload an MR

- After pressing “Create merge request”, you’ll be re-directed to the overview page of your new MR
- You can inspect the contents of your MR
  - The commits

Upload an MR

Draft: Rename check_atom_names to checkAtomNames

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Overview 0 | **Commits 2** | Pipelines 1 | Changes 1

Sep 06, 2023

fixClangTidy
Sebastian Wingbermühle authored 11 minutes ago

Rename check_atom_names to checkAtomNames
Sebastian Wingbermühle authored 14 minutes ago

Add previously merged commits

Please squash commits to not pollute the history!

Upload an MR

- After pressing “Create merge request”, you’ll be re-directed to the overview page of your new MR
- You can inspect the contents of your MR
  - The commits
  - The modified files (“glorified diff”)

Compare **main** and **latest version**

src/gromacs/gmxpreprocess/grompp.cpp

```
@@ -264,11 +264,11 @@ static int rm_interactions(int ifunc, gmx::ArrayRef<MoleculeInformation> mols)
264 264     return n;
265 265  }
266 266
267     - static int check_atom_names(const char*          fn1,
268     -                             const char*          fn2,
269     -                             gmx_mtop_t*          mtop,
270     -                             const t_atoms*       at,
271     -                             const gmx::MDLogger& logger)
    267 + static int checkAtomNames(const char*          fn1,
    268 +                           const char*          fn2,
    269 +                           gmx_mtop_t*          mtop,
    270 +                           const t_atoms*       at,
    271 +                           const gmx::MDLogger& logger)
272 272  {
273 273      int      m, i, j, nmismatch;
274 274      t_atoms* tat;

@@ -730,7 +730,7 @@ static void new_status(const char* topfile,
730 730      /* This call fixes the box shape for runs with pressure scaling */
731 731      set_box_rel(ir, state);
732 732
733     -     nmismatch = check_atom_names(topfile, confin, sys, &conftop->atoms, logger);
    733 +     nmismatch = checkAtomNames(topfile, confin, sys, &conftop->atoms, logger);
734 734      done_top(conftop);
735 735      sfree(conftop);
736 736
```

Upload an MR

- After pressing “Create merge request”, you’ll be re-directed to the overview page of your new MR
- You can inspect the contents of your MR
  - The commits
  - The modified files (“glorified diff”)
- A pipeline will start whenever you modify the MR. It has to pass before you can merge the MR. There are also post-merge pipelines.

Draft: Rename check_atom_names to checkAtomNames

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Activity

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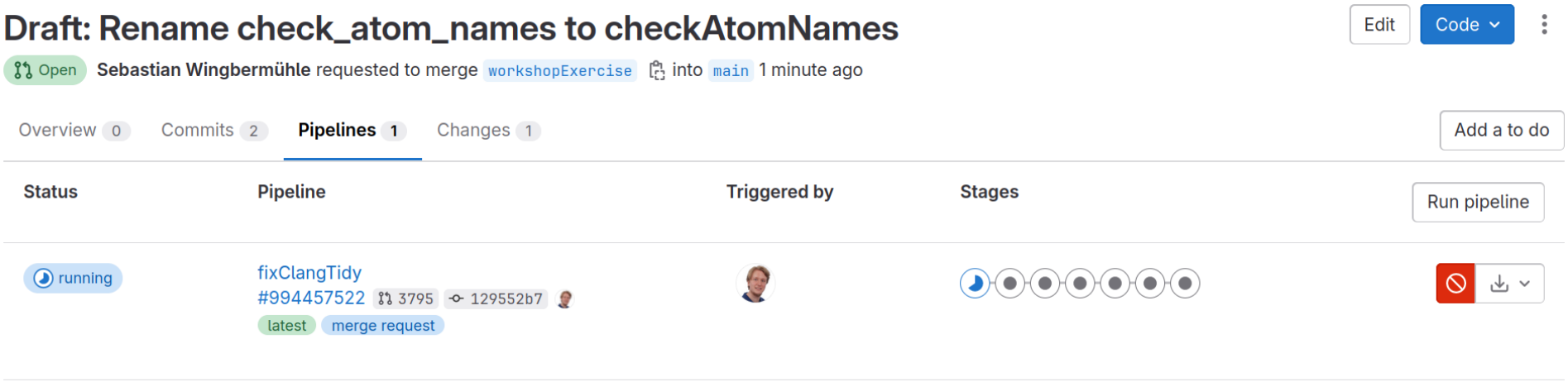
Preview

Write a comment or drag your files here…

Switch to rich text editing

Comment | Close merge request

Upload an MR

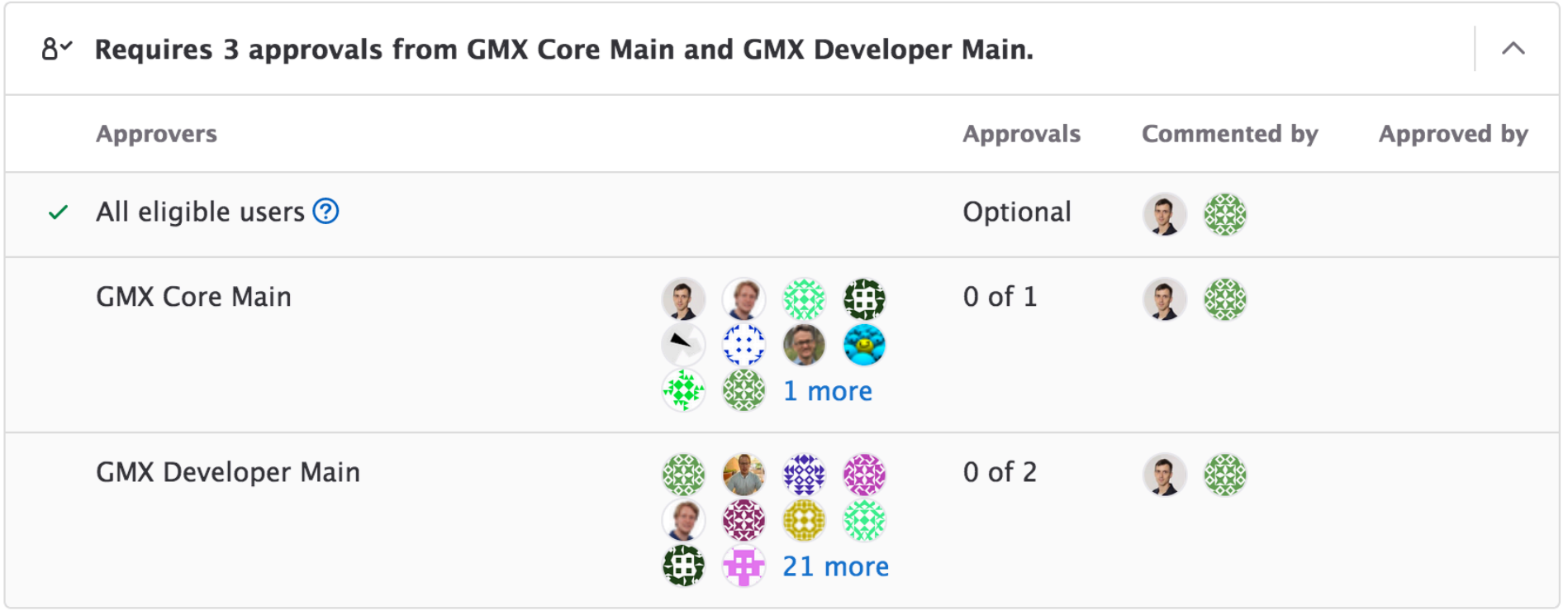


If you already know that you will soon modify the MR, please cancel this pipeline to save resources!

Our review system

- Goals:
  - Can the MR be understood?
  - Is the MR scientifically correct?
  - Does it conform to our coding standards?
  - Is the implementation efficient?
- 2 approvals (1 from each group) needed

Our review system

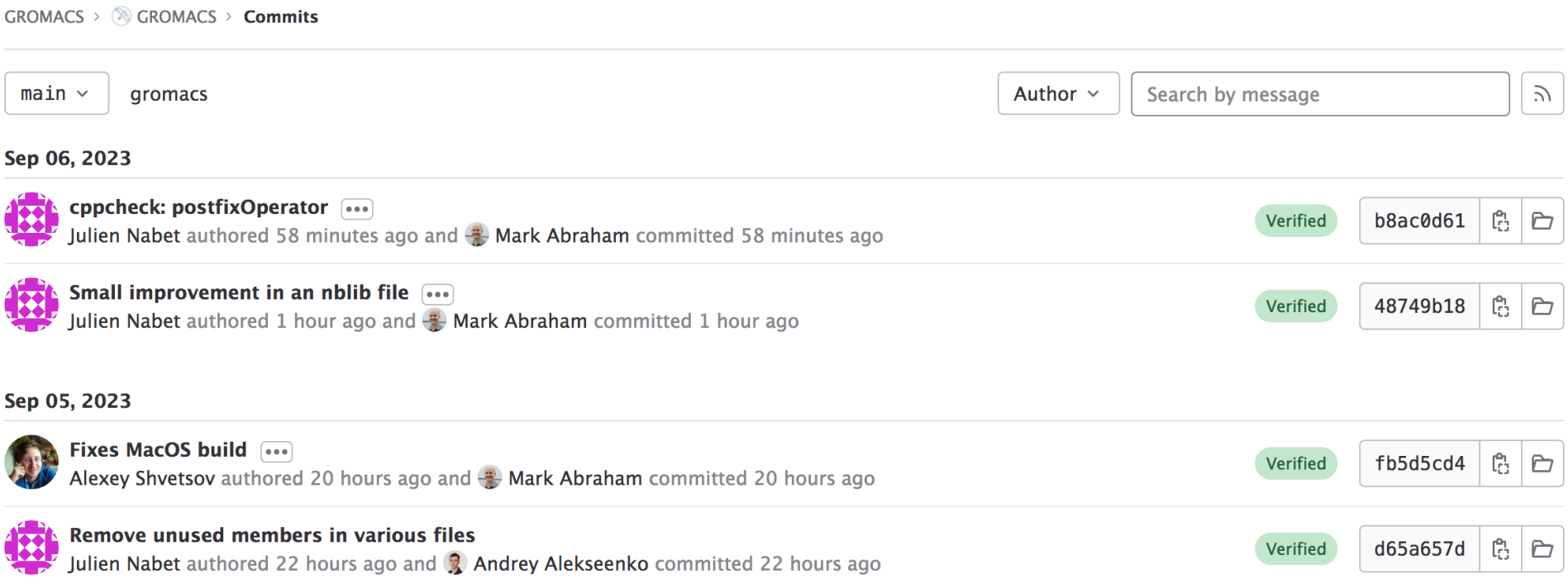


Our review system

- Review is needed to ensure code quality, but it is nearly always the bottleneck when trying to get code in!
- Be an active reviewer and build trust to get approval permissions!
- Trade reviews (with both core developers as well as other workshop participants)!
- Engage in design discussions early!

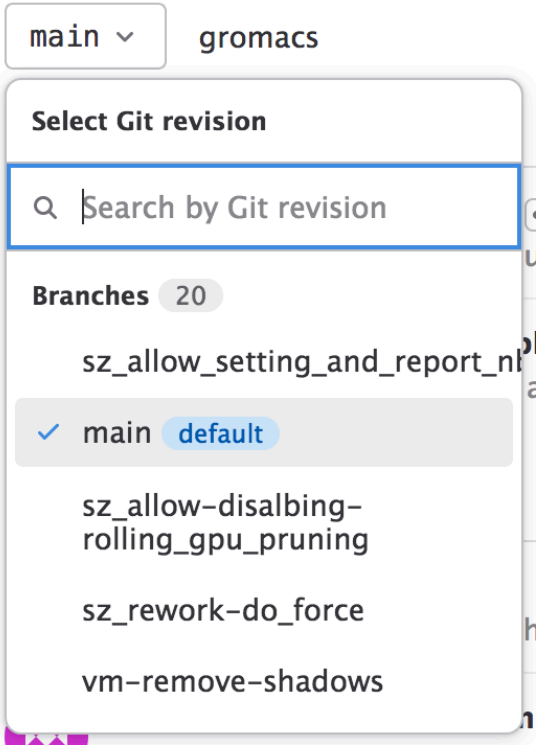
GROMACS on GitLab – an overview

- We squash commits to keep our history clean



GROMACS on GitLab – an overview

- We delete source branches after merging to save space

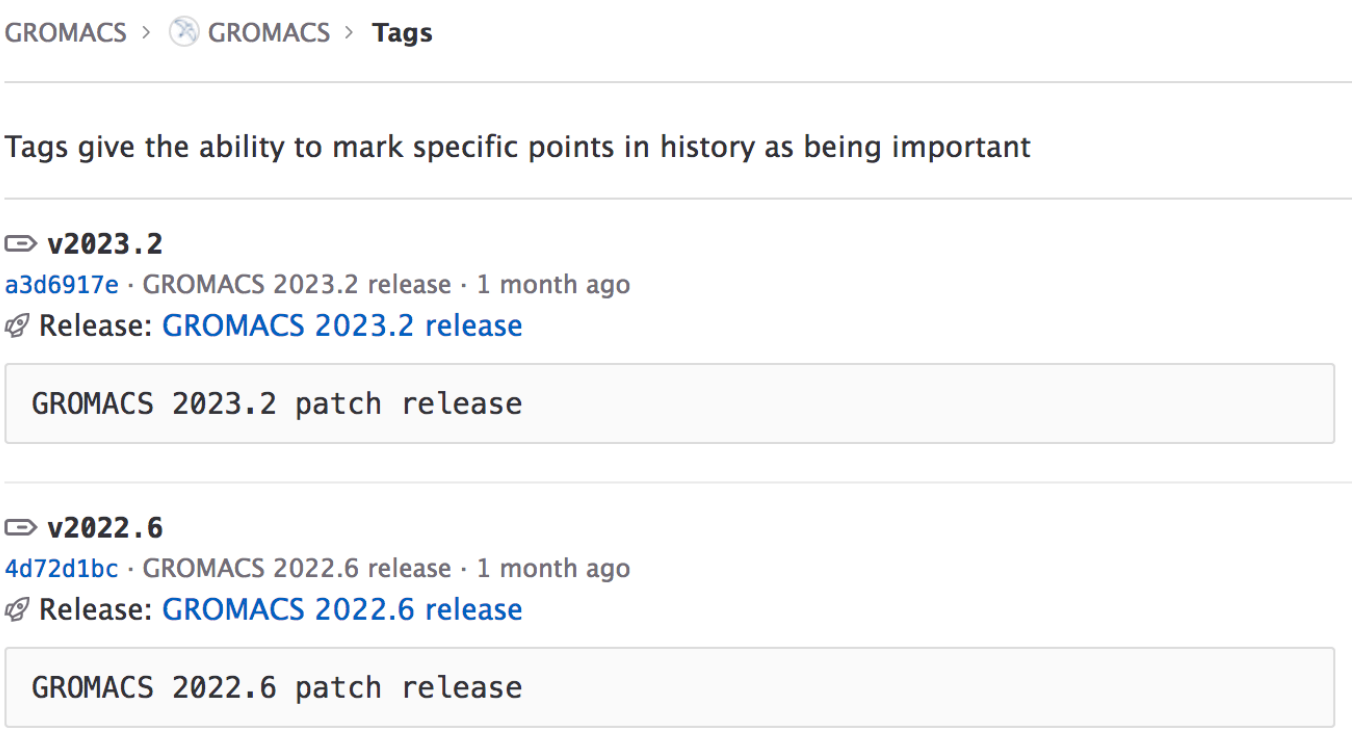


GROMACS on GitLab – an overview

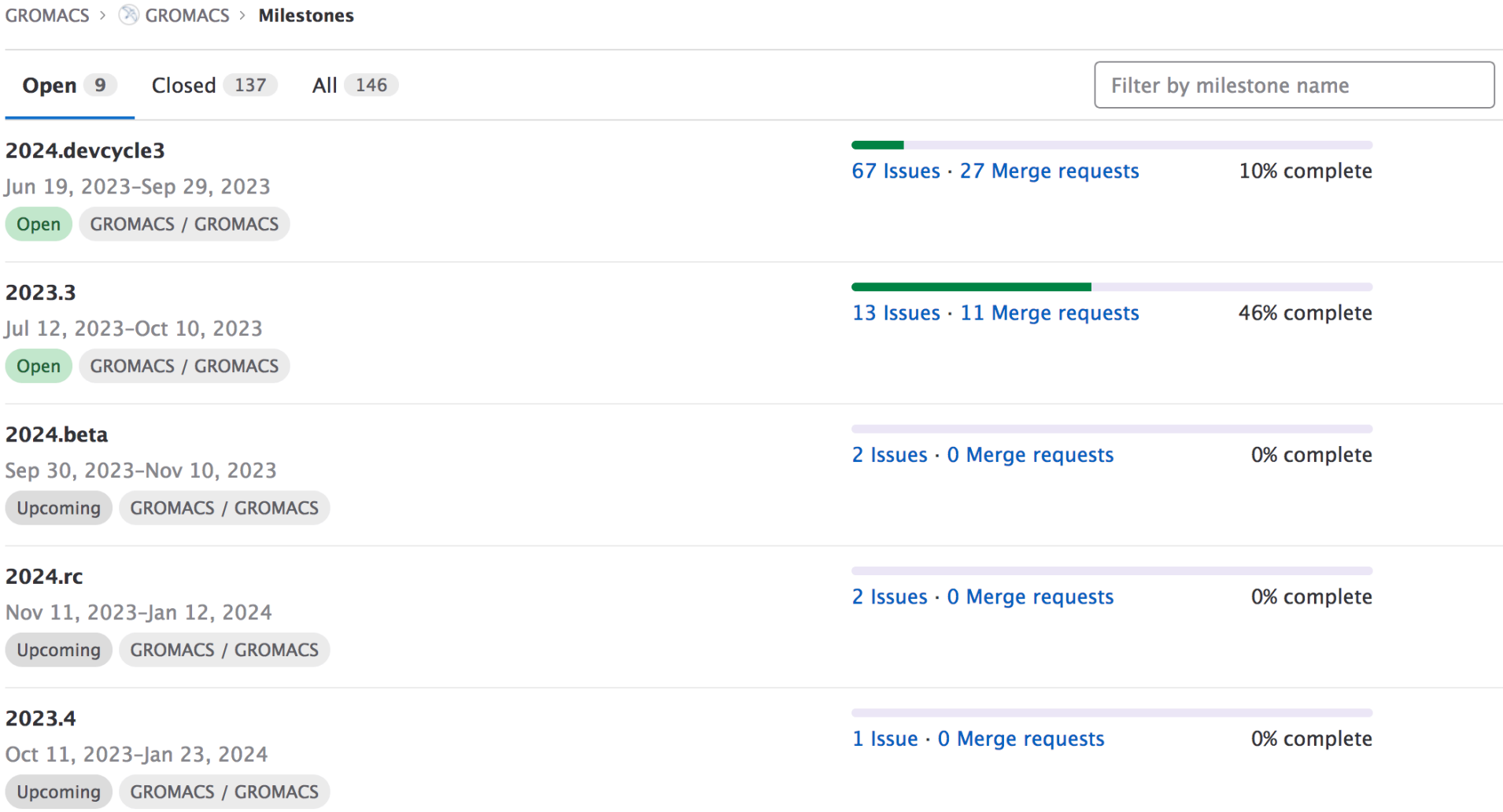
- Every MR is a branch of the GROMACS repository on GitLab
- The official GROMACS versions are stored in protected branches: main (the next major release) and release-*
- We frequently merge from the oldest release up to main to make sure bug fixes are propagated
  - Always fix bugs in the first maintained release they were found in

GROMACS on GitLab – an overview

- We document the contents of a release with the help of tags and GitLab releases



GROMACS on GitLab – an overview



GROMACS on GitLab – an overview

- We document our plans in issues linked to milestones
- The milestones are the actual deadlines enforced during our release cycle!
- If you want the Stockholm team to be aware of a larger code contribution, write an issue and link it to the correct milestone!

Questions?

Exercise

Change the name of the function
check_atom_names to **checkAtomNames**
everywhere in the GROMACS source code!