

## Issues

| #    | Project         | Tracker | Status          | Priority | Subject  | Assignee       | Updated             | Target version   |
|------|-----------------|---------|-----------------|----------|--|----------------|---------------------|------------------|
| 1105 | Benchmark suite | Feature | New             | Normal   | produce a benchmark suite  |                | 09/13/2016 10:31 PM |                  |
| 1106 | Benchmark suite | Feature | New             | Normal   | publish benchmark numbers  |                | 06/19/2014 12:08 PM |                  |
| 3071 | GROMACS         | Bug     | Accepted        | Normal   | complex.nbnxn-ljpmc-LB-geometric failing with OpenCL timing debug mode assertions                  | Szilárd Páll   | 02/25/2020 03:39 PM | 2020.2           |
| 3266 | GROMACS         | Bug     | New             | High     | gmx density show wrong symmetrize density profile using -symm?                                     | Super duper    | 02/28/2020 08:24 AM | 2020.2           |
| 1964 | GROMACS         | Feature | Accepted        | Normal   | "pull=no" should not produce warnings about "unknown" pull keywords                                |                | 05/20/2016 02:37 PM |                  |
| 3309 | GROMACS         | Bug     | New             | Normal   | -reprod: checkpoint reading bug and general considerations   |                | 02/27/2020 10:45 PM |                  |
| 2902 | GROMACS         | Bug     | New             | Normal   | 2019.1 equilibration issue? (Intel 2018u3)   |                | 04/30/2019 08:17 AM |                  |
| 2876 | GROMACS         | Bug     | New             | Normal   | 2019.1 make check fails on AVX and AVX2 (Intel 2018u3)   | Erik Lindahl   | 03/08/2019 10:32 AM |                  |
| 2035 | GROMACS         | Task    | New             | Normal   | A common trajectory analysis data exchange format  |                | 03/15/2017 05:46 PM | future           |
| 2218 | GROMACS         | Feature | Feedback wanted | Normal   | A tiny feature: damping for umbrella pull  |                | 08/16/2017 07:20 PM |                  |
| 3300 | GROMACS         | Task    | New             | Normal   | Abandon docs/OpenCLTODOList.txt?   |                | 01/15/2020 02:46 PM |                  |
| 2068 | GROMACS         | Feature | New             | Normal   | Access to low level classes  |                | 03/02/2019 01:37 AM | future           |
| 2905 | GROMACS         | Task    | New             | Normal   | Add a Jenkins configuration with std library assert  |                | 08/24/2019 05:22 PM |                  |
| 2456 | GROMACS         | Task    | New             | Normal   | Add a pull module external potential tests   |                | 03/15/2018 03:02 PM |                  |
| 2603 | GROMACS         | Task    | New             | Normal   | Add ability to properly check coordinate files during testing                                      | Paul Bauer     | 10/15/2018 01:16 PM | future           |
| 2928 | GROMACS         | Feature | New             | Normal   | Add ability to use expression "count of ATOM_EXPR" in selection statements.                        |                | 04/16/2019 04:52 PM |                  |
| 3321 | GROMACS         | Task    | Accepted        | Normal   | Add D2D wrapper  | Artem Zhmurov  | 01/22/2020 09:50 AM | 2021-refactoring |
| 2579 | GROMACS         | Feature | New             | Normal   | Add dimensionality option to gmx trjconv -center   |                | 07/19/2018 04:53 PM | future           |
| 2185 | GROMACS         | Task    | New             | Normal   | add docs on MPI + CUDA w/wo MPS  |                | 05/24/2017 05:17 PM |                  |
| 1902 | GROMACS         | Feature | Accepted        | Low      | Add grompp check that non-excluded atoms are not too close to each other in the starting structure |                | 02/15/2016 01:34 PM |                  |
| 2080 | GROMACS         | Feature | New             | Normal   | add grompp warning for suitability for domain decomposition  |                | 11/23/2016 03:03 PM |                  |
| 2383 | GROMACS         | Task    | New             | Normal   | Add JSON interface to write and read files   | Paul Bauer     | 01/16/2018 02:01 PM | future           |
| 1523 | GROMACS         | Task    | New             | Normal   | add missing code-paths to CUDA emulation kernel  |                | 07/11/2016 08:09 PM |                  |
| 1373 | GROMACS         | Task    | New             | Low      | Add missing nbnxn tests  | Mark Abraham   | 06/09/2014 08:36 PM |                  |
| 2546 | GROMACS         | Task    | New             | Normal   | Add more assertions to AWH code  | Viveca Lindahl | 06/06/2018 11:20 AM | future           |
| 3268 | GROMACS         | Task    | New             | Normal   | add more Intel driver recommendations  |                | 12/26/2019 04:39 PM |                  |
| 2001 | GROMACS         | Feature | New             | Normal   | add MPI info to the mdrun log header   |                | 07/06/2016 05:21 PM |                  |
| 2682 | GROMACS         | Task    | New             | Normal   | Add MSAN configuration   |                | 10/09/2018 06:28 PM |                  |

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|------|---------|---------|--------------|----------|--|------------------|---------------------|----------------------------|
| 2547 | GROMACS | Feature | New          | Low      | Add option of averaging and obtaining error bars for AWH PMFs  | Viveca Lindahl   | 06/06/2018 11:31 AM | future                     |
| 2429 | GROMACS | Feature | New          | Normal   | Add option of periodic chain topology to pdb2gmx   |                  | 03/10/2018 01:01 PM |                            |
| 1511 | GROMACS | Feature | Accepted     | Normal   | add PDBx (ie mmCIF) support  |                  | 10/05/2018 07:14 PM |                            |
| 3369 | GROMACS | Feature | New          | Normal   | Add quote about "the truth"  |                  | 02/05/2020 05:08 PM |                            |
| 3322 | GROMACS | Task    | Accepted     | Normal   | Add reallocate(...) function that does not care about the contents of the buffer   | Artem Zhmurov    | 01/22/2020 09:50 AM | 2021-refactoring           |
| 3224 | GROMACS | Task    | New          | Normal   | add regression test case large enough to miscalculated GPU grid launch cases   |                  | 12/20/2019 01:18 PM | 2021                       |
| 1192 | GROMACS | Feature | Accepted     | Normal   | Add support for Verlet scheme with Buckingham  | Berk Hess        | 07/11/2016 08:19 PM |                            |
| 701  | GROMACS | Task    | New          | Normal   | Add symbol visibility macros   |                  | 03/02/2019 01:46 AM | future                     |
| 3064 | GROMACS | Task    | New          | Normal   | add test for perturbed bonded forces   |                  | 12/27/2019 04:22 PM | 2021                       |
| 920  | GROMACS | Task    | In Progress  | Normal   | Add test framework for trajectory analysis modules   | Teemu Murtola    | 07/11/2016 08:27 PM |                            |
| 2686 | GROMACS | Task    | New          | Normal   | add tests for gpu bonded interactions  |                  | 12/27/2019 04:40 PM | 2021                       |
| 907  | GROMACS | Feature | Accepted     | Normal   | Add tests for verifying installed headers  |                  | 03/11/2014 09:15 PM | future                     |
| 1641 | GROMACS | Feature | New          | Normal   | Add toolchain file for Cray systems  |                  | 06/06/2015 11:24 PM |                            |
| 3062 | GROMACS | Task    | New          | Normal   | add twin cut-off mdrun test  |                  | 12/27/2019 04:22 PM | 2021                       |
| 3162 | GROMACS | Task    | New          | Normal   | Add virtual site support to GPU version of update-constraints.   | Artem Zhmurov    | 01/23/2020 11:52 AM | 2021-infrastructure-stable |
| 1948 | GROMACS | Feature | New          | Low      | add warning when non-identical GPUs are used   |                  | 06/12/2017 08:45 PM |                            |
| 2428 | GROMACS | Feature | New          | Normal   | Add way of selecting interactive arguments of pdb2gmx by string rather than an index   |                  | 02/27/2018 06:28 PM |                            |
| 1030 | GROMACS | Feature | Fix uploaded | Low      | adding -tu option to some analysis tools   | Rossen Apostolov | 07/11/2016 08:22 PM |                            |
| 1303 | GROMACS | Feature | New          | Normal   | Adding lambda dependent distance for pull code   | Michael Shirts   | 07/11/2016 08:18 PM |                            |
| 1139 | GROMACS | Feature | New          | Normal   | Adding the possibility to arbitrarily evaluate different components in the energy/force term when the energy/force is calculated |                  | 07/11/2016 08:19 PM |                            |
| 3123 | GROMACS | Task    | New          | Normal   | address sanitizer coverage of parallelization code-paths   |                  | 10/05/2019 12:32 AM |                            |
| 3271 | GROMACS | Task    | Resolved     | Normal   | Adopt PEP-518 for Python package build system configuration.   |                  | 04/09/2020 10:15 PM | 2021-infrastructure-stable |
| 3326 | GROMACS | Task    | New          | Normal   | Allow changing task assignment   |                  | 01/22/2020 09:44 AM | 2021-refactoring           |
| 2855 | GROMACS | Task    | New          | Normal   | Allow compiling GROMACS without C compiler   |                  | 01/10/2020 12:06 PM |                            |
| 3325 | GROMACS | Task    | New          | Normal   | Allow complete re-initialization of a simulation   |                  | 01/29/2020 05:13 PM | 2021-refactoring           |
| 2491 | GROMACS | Feature | New          | Low      | Allow constant bias AWH simulations  | Viveca Lindahl   | 06/05/2018 10:38 PM | future                     |
| 3140 | GROMACS | Feature | New          | Normal   | Allow explicit input definition for gmxapi.operation function wrapper  | Eric Irrgang     | 12/10/2019 02:00 PM | 2021-infrastructure-stable |
| 3393 | GROMACS | Feature | Resolved     | Normal   | Allow gmxapi.commandline_operation to use STDIN  | Eric Irrgang     | 02/25/2020 05:15 PM | 2021-infrastructure-stable |
| 2735 | GROMACS | Task    | New          | Normal   | Allow gmx_genrestr to write correct position restraints for molecules after the first molecule                                   | Joe Jordan       | 12/11/2019 09:26 AM | future                     |

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|------|---------|---------|-----------------|----------|---|---------------------|---------------------|----------------------------|
| 2460 | GROMACS | Bug     | New             | Normal   | Allow inclusion of user libraries through CMake cache variables   |                     | 03/28/2018 08:47 PM |                            |
| 3078 | GROMACS | Task    | New             | Normal   | Allow MD modules to register energy output fields themselves  |                     | 09/06/2019 11:36 AM |                            |
| 2787 | GROMACS | Task    | New             | Normal   | allow passing flags to allocateDeviceBuffer   |                     | 12/03/2018 01:54 PM |                            |
| 3277 | GROMACS | Feature | New             | Normal   | Allow testing feature that is partly implemented  |                     | 12/31/2019 12:44 PM | 2021                       |
| 2866 | GROMACS | Feature | New             | Normal   | Alternative non-bonded potentials   | David van der Spoel | 03/05/2019 03:50 PM | future                     |
| 2045 | GROMACS | Task    | New             | Normal   | API design and language bindings  | Peter Kasson        | 01/29/2020 03:59 PM |                            |
| 3446 | GROMACS | Task    | New             | Normal   | apply maintainability updates across all GPU kernels  | Jonathan Vincent    | 03/19/2020 03:31 PM |                            |
| 3333 | GROMACS | Bug     | New             | Normal   | Assertion failure when trying to get unit test help   | Paul Bauer          | 02/25/2020 10:16 AM | 2021-infrastructure-stable |
| 2850 | GROMACS | Task    | In Progress     | Normal   | assess Raptor Talos for testing   | Szilárd Páll        | 02/12/2019 01:14 PM |                            |
| 2987 | GROMACS | Bug     | New             | Normal   | assess the bonded GPU task assignment default   |                     | 12/20/2019 01:06 PM | 2021                       |
| 2341 | GROMACS | Task    | New             | Low      | assess the state of building and using GROMACS on Windows   |                     | 07/29/2019 11:09 PM | future                     |
| 1648 | GROMACS | Bug     | Feedback wanted | Normal   | Atoms with zero LJ parameters but partial charges appear to cause crashes in free energy calculations when perturbed in the presence of other charges | Michael Shirts      | 06/25/2015 06:07 AM |                            |
| 2482 | GROMACS | Bug     | Feedback wanted | Normal   | Atoms/molecules in freezegrps move and system crashes   |                     | 05/18/2018 07:13 PM |                            |
| 2412 | GROMACS | Task    | New             | Normal   | attempt to do better FFTW planning  |                     | 03/15/2018 05:01 PM |                            |
| 2015 | GROMACS | Feature | New             | Normal   | Auto recovery from dd communication error   |                     | 07/28/2016 03:17 PM |                            |
| 2221 | GROMACS | Task    | New             | Normal   | Avoid preprocessor for SIMD functions   |                     | 02/21/2018 01:43 PM |                            |
| 2715 | GROMACS | Feature | New             | Normal   | Avoid requesting the user to recompile gromacs for Intel OpenCL support   |                     | 12/27/2019 04:06 PM | future                     |
| 2351 | GROMACS | Task    | New             | Normal   | Avoid the SIMD module depending on non-trivial parts of Gromacs   |                     | 12/14/2017 02:47 AM | future                     |
| 2478 | GROMACS | Task    | New             | Low      | avoid use of getenv in static initialization  |                     | 04/13/2018 11:57 AM |                            |
| 2976 | GROMACS | Task    | New             | Normal   | Basic math for Multidimensional arrays  |                     | 12/27/2019 04:37 PM | 2021                       |
| 2925 | GROMACS | Task    | New             | Normal   | BasicVector addition operator yields unexpected result when adding scalar   | Christian Blau      | 12/17/2019 10:04 AM | 2021-infrastructure-stable |
| 2570 | GROMACS | Feature | New             | Normal   | Better string formatting and printing   |                     | 05/02/2019 12:20 PM |                            |
| 2983 | GROMACS | Task    | New             | Normal   | better suited data-types for bonded GPU kernels   |                     | 07/11/2019 04:32 PM |                            |
| 1010 | GROMACS | Task    | In Progress     | Normal   | Better support for multiple AnalysisData datasets   | Teemu Murtola       | 07/11/2016 08:23 PM |                            |
| 2657 | GROMACS | Bug     | New             | Normal   | Biphasic tutorial   |                     | 09/28/2018 10:02 AM |                            |
| 2675 | GROMACS | Task    | In Progress     | Normal   | bonded CUDA offload task  |                     | 02/12/2020 05:54 PM | 2021                       |
| 2818 | GROMACS | Task    | In Progress     | Normal   | bonded GPU kernel fusion  | Magnus Lundborg     | 07/03/2019 09:01 PM |                            |
| 3443 | GROMACS | Bug     | New             | Normal   | Bonded GPU kernel performance regression with 2020  |                     | 03/15/2020 08:15 PM |                            |

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| 2695 | GROMACS | Task    | New                   | Low      | bonded GPU module timing   |                | 12/27/2019 04:40 PM | 2021                       |
| 1634 | GROMACS | Feature | New                   | Normal   | Boxed Molecular Dynamics   |                | 11/04/2014 04:40 PM |                            |
| 2395 | GROMACS | Task    | In Progress           | Normal   | break up commrec   | Mark Abraham   | 12/15/2019 11:51 AM | 2021-infrastructure-stable |
| 3264 | GROMACS | Task    | New                   | Normal   | Break up MdrunMpiTests   | Paul Bauer     | 12/23/2019 11:44 AM | 2021-infrastructure-stable |
| 2526 | GROMACS | Bug     | New                   | Normal   | Bug of gmx hbond   |                | 05/30/2018 03:12 PM |                            |
| 2602 | GROMACS | Bug     | New                   | Low      | build information gets outdated if build tree is reused                      |                | 08/13/2018 09:04 PM |                            |
| 2555 | GROMACS | Bug     | New                   | Low      | building GROMACS 2018.2  |                | 07/03/2018 11:41 PM |                            |
| 2864 | GROMACS | Task    | New                   | Normal   | Building incompatibilities   | Benson Muite   | 02/19/2019 02:00 PM |                            |
| 3379 | GROMACS | Feature | New                   | Normal   | C++ API for simulation input and output                                      |                | 02/28/2020 10:38 AM | 2021-infrastructure-stable |
| 2834 | GROMACS | Task    | In Progress           | Normal   | C++ matrix classes   | Christian Blau | 12/29/2019 10:32 AM | 2021                       |
| 996  | GROMACS | Task    | New                   | Normal   | C++ MPI Framework  | Roland Schulz  | 07/14/2014 11:53 AM | future                     |
| 2919 | GROMACS | Task    | New                   | Normal   | C++ style guidelines for namespace use                                       |                | 04/15/2019 01:21 PM |                            |
| 948  | GROMACS | Task    | New                   | Normal   | C++ thread synchronization primitives  | Sander Pronk   | 07/11/2016 08:24 PM |                            |
| 1017 | GROMACS | Task    | New                   | Normal   | C++ Vector/Matrix classes  |                | 07/11/2016 08:23 PM |                            |
| 2048 | GROMACS | Task    | New                   | Normal   | C++11: CUDA dependency on general headers                                    |                | 09/07/2016 10:30 PM |                            |
| 3305 | GROMACS | Bug     | New                   | Normal   | Case gives FPE with Debug build when GPU update is enabled                   |                | 01/21/2020 05:44 PM |                            |
| 1339 | GROMACS | Bug     | New                   | Normal   | Center of mass drift with Nose-Hoover, MTTK and md-vv                        | Michael Shirts | 06/18/2015 08:53 PM | future                     |
| 3244 | GROMACS | Bug     | In Progress           | Normal   | center of mass motion removal with position restraints can lead to artifacts | Berk Hess      | 12/27/2019 10:40 AM | 2021                       |
| 2859 | GROMACS | Task    | Resolved              | Normal   | Change ArrayRef iterator type from pointer to std::iterator                  |                | 06/26/2020 06:15 PM |                            |
| 2770 | GROMACS | Task    | New                   | Normal   | change branch maintenance policy   |                | 01/16/2020 05:09 PM | 2021                       |
| 3220 | GROMACS | Task    | New                   | Normal   | change rolling pruning scheduling with GPU update                            |                | 02/25/2020 03:41 PM | 2021-infrastructure-stable |
| 652  | GROMACS | Task    | Blocked,<br>need info | Normal   | Change selection method implementation to use C++                            |                | 04/23/2017 08:05 PM | future                     |
| 2672 | GROMACS | Task    | New                   | Normal   | check & document execution width requirements in OpenCL                      |                | 12/31/2018 11:20 AM | future                     |
| 3334 | GROMACS | Bug     | New                   | Normal   | Check for DD when increasing rlist is broken                                 | Berk Hess      | 02/25/2020 03:28 PM | 2020.2                     |
| 2379 | GROMACS | Task    | New                   | Normal   | check leftover FIXMEs in r2018   | Szilárd Páll   | 12/31/2018 11:16 AM | future                     |
| 3233 | GROMACS | Bug     | New                   | Normal   | clang-format incorrectly aligning altered function arguments                 |                | 12/13/2019 12:41 PM |                            |
| 3119 | GROMACS | Task    | New                   | Normal   | clang-tidy coverage of parallelizaton codepaths                              |                | 12/27/2019 04:20 PM | 2021                       |
| 3179 | GROMACS | Feature | New                   | Normal   | Clarify access to parallel data outputs                                      | Eric Irgang    | 10/26/2019 12:23 PM |                            |
| 3402 | GROMACS | Feature | New                   | Normal   | Clarify distinction between public API documentation and developer docs.     |                | 02/26/2020 04:16 PM | 2021-infrastructure-stable |
| 2375 | GROMACS | Task    | New                   | Normal   | Clarify execution phases for MD simulation                                   |                | 04/30/2019 12:59 PM |                            |

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|------|---------|---------|--------------------|----------|--|--------------|---------------------|----------------------------|
| 2857 | GROMACS | Task    | New                | Normal   | Clarify recommended function specifies (constexpr, noexcept, pure)                         |              | 02/04/2019 04:48 AM |                            |
| 2796 | GROMACS | Task    | New                | Low      | clarify what mdrun -cpt means  |              | 01/03/2019 02:09 PM |                            |
| 1140 | GROMACS | Task    | New                | Normal   | Class design for passing options and data  |              | 07/11/2016 08:19 PM |                            |
| 3033 | GROMACS | Task    | In Progress        | Normal   | Clean up and modernize googletest bundling and usage                                       |              | 01/16/2020 04:50 PM | 2021-refactoring           |
| 2988 | GROMACS | Task    | In Progress        | Low      | clean up and refactor code to modern standards   |              | 12/27/2019 04:37 PM | future                     |
| 3032 | GROMACS | Feature | Feedback wanted    | Normal   | Clean up dev-manual structure  |              | 12/11/2019 11:27 AM | 2021-infrastructure-stable |
| 1793 | GROMACS | Task    | New                | Normal   | cleanup of integration loop  | Mark Abraham | 10/31/2018 10:49 PM | future                     |
| 3000 | GROMACS | Bug     | New                | Normal   | CMake "webpage" target does not fail when it should  |              | 06/25/2019 02:43 PM |                            |
| 3249 | GROMACS | Bug     | In Progress        | Low      | cmake bad tests for avx512 on AMD  | Erik Lindahl | 02/26/2020 05:00 PM |                            |
| 2949 | GROMACS | Bug     | New                | Normal   | cmake fails when building mdrun only   |              | 07/08/2019 10:04 AM |                            |
| 1827 | GROMACS | Bug     | New                | Low      | cmake multi-configuration generator support partly broken                                  |              | 12/11/2017 05:20 PM | future                     |
| 1963 | GROMACS | Task    | New                | Low      | collect examples of systems where users tried to do something that performed badly         | Mark Abraham | 08/09/2016 07:30 AM |                            |
| 3413 | GROMACS | Bug     | Feedback wanted    | Normal   | COMM Removal Failure in GROMACS 2020.1   |              | 03/12/2020 02:31 PM |                            |
| 3166 | GROMACS | Bug     | New                | Normal   | Compilation failing on Ubuntu 19.04 with Cuda 10.1   |              | 10/19/2019 09:13 PM |                            |
| 2582 | GROMACS | Bug     | Blocked, need info | Normal   | Compilation issues with CUDA V9.1.85 and both gcc5 and gcc6                                | Szilárd Páll | 07/23/2018 07:46 PM |                            |
| 3330 | GROMACS | Task    | New                | Normal   | Compile list of codepaths for testing task assignment                                      |              | 01/22/2020 10:03 AM | 2021-refactoring           |
| 2958 | GROMACS | Bug     | New                | Normal   | Compiling master (to become 2020) using CUDA 9.0   |              | 03/02/2020 03:57 PM | 2020.2                     |
| 3021 | GROMACS | Feature | Feedback wanted    | Normal   | Completion of docs for GPU developments  |              | 03/02/2020 03:58 PM | 2020.2                     |
| 2158 | GROMACS | Task    | New                | Normal   | consider adding post-submit test that runs PME with 2xNN kernels                           |              | 04/19/2017 08:04 PM |                            |
| 2462 | GROMACS | Task    | New                | Normal   | consider adding STL misuse tests   |              | 03/23/2018 01:23 AM |                            |
| 2535 | GROMACS | Task    | New                | Normal   | consider compiling opencl fft kernels once   |              | 05/31/2018 01:33 PM |                            |
| 1947 | GROMACS | Task    | New                | Normal   | Consider fixing corner case in TinyXML2  | Mark Abraham | 04/19/2016 01:40 AM |                            |
| 2909 | GROMACS | Task    | New                | Normal   | consider implementing mechanisms to ensure pair lists are not used past their max lifetime |              | 04/03/2019 05:14 PM |                            |
| 3365 | GROMACS | Task    | New                | Low      | consider making GPU bonded work independent from nonbonded                                 |              | 03/01/2020 01:11 PM |                            |
| 2531 | GROMACS | Task    | New                | Low      | Consider optimizing tabulated data access on GPU   |              | 07/30/2018 12:31 PM |                            |
| 3194 | GROMACS | Task    | New                | Normal   | consider passing GPU dependency list to both dependency producers and consumers            |              | 11/01/2019 07:10 PM |                            |
| 3395 | GROMACS | Feature | Feedback wanted    | Normal   | Consider scripted composition of Dockerfiles   |              | 03/16/2020 12:16 PM |                            |

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|------|---------|---------|-----------------|----------|---|---------------------|---------------------|----------------------------|
| 3002 | GROMACS | Task    | New             | Normal   | consider splitting bonded work into local/nonlocal  |                     | 06/25/2019 04:06 PM |                            |
| 2530 | GROMACS | Task    | New             | Normal   | consider using CUDA Driver API  |                     | 09/23/2018 11:47 PM | future                     |
| 3181 | GROMACS | Task    | New             | Normal   | consolidate task assignment and workload data initialization  |                     | 10/28/2019 02:53 PM |                            |
| 1354 | GROMACS | Bug     | New             | Normal   | Constant acceleration NEMD is broken.   | David van der Spoel | 01/09/2019 04:42 PM |                            |
| 2713 | GROMACS | Feature | New             | Normal   | Constant offset for external electric fields  |                     | 10/28/2018 12:57 AM |                            |
| 2596 | GROMACS | Feature | New             | Normal   | Constant potential method   | Benson Muite        | 05/10/2019 09:54 AM |                            |
| 2367 | GROMACS | Task    | New             | Normal   | construct pbc_simd less often   |                     | 09/24/2018 11:02 PM | future                     |
| 3316 | GROMACS | Task    | Accepted        | Normal   | Context and Stream manager  | Artem Zhmurov       | 01/22/2020 09:49 AM | 2021-refactoring           |
| 3442 | GROMACS | Bug     | Accepted        | Normal   | continuing mdrun with -deffnm and pulling does not work   |                     | 03/15/2020 08:33 AM |                            |
| 3371 | GROMACS | Feature | New             | Normal   | Control FEP using AWH   | Magnus Lundborg     | 02/06/2020 02:20 PM | 2021                       |
| 2060 | GROMACS | Feature | New             | Normal   | Convert enum to enum class  |                     | 10/17/2016 05:27 PM |                            |
| 3243 | GROMACS | Bug     | Feedback wanted | Normal   | Convert GROMACS 1 OpenMP thread per rank fatal error into a warning   |                     | 12/27/2019 10:31 AM |                            |
| 3201 | GROMACS | Task    | In Progress     | Normal   | Convert mdp parameters to key value tree  |                     | 11/06/2019 06:06 PM |                            |
| 1855 | GROMACS | Task    | New             | Normal   | Convert preprocessor use so that symbols are always defined   |                     | 06/28/2016 02:17 PM |                            |
| 2933 | GROMACS | Task    | New             | Normal   | Convert walls to a ForceProvider  |                     | 04/25/2019 02:43 PM |                            |
| 2231 | GROMACS | Bug     | New             | Normal   | convert-tpz aborts when saving subset of the system   |                     | 01/12/2018 03:52 PM |                            |
| 3133 | GROMACS | Task    | In Progress     | Normal   | Cookiecutter for sample_restraint   | Eric Irrgang        | 12/10/2019 01:59 PM | 2021-infrastructure-stable |
| 3042 | GROMACS | Bug     | New             | Normal   | core dump error in grompp command   |                     | 10/09/2019 07:30 PM |                            |
| 2600 | GROMACS | Bug     | New             | High     | coul-lambdas turns off all coulombic interactions in system instead of the molecule specified in the couple-moltype |                     | 08/07/2018 06:50 PM |                            |
| 3117 | GROMACS | Feature | New             | Normal   | Coulomb FEP PME on GPU  | Magnus Lundborg     | 02/17/2020 03:58 PM | 2021-infrastructure-stable |
| 3015 | GROMACS | Task    | New             | Normal   | Create central log handle for calls to gm_x_fatal   |                     | 09/06/2019 02:34 PM | 2021-infrastructure-stable |
| 3445 | GROMACS | Task    | New             | Normal   | create heuristic for c_skipNeutralAtoms   | Jonathan Vincent    | 03/17/2020 12:12 PM |                            |
| 1670 | GROMACS | Feature | New             | Normal   | create mdrun option checking mini-tool  |                     | 06/23/2016 04:06 PM |                            |
| 1422 | GROMACS | Feature | New             | Normal   | CSH angle incorrect with GROMOS force field and virtual sites   | David van der Spoel | 06/12/2014 12:01 AM |                            |
| 1985 | GROMACS | Bug     | Fix uploaded    | Low      | CUDA build system refactoring awaiting review   |                     | 12/20/2019 12:07 PM | 2021                       |
| 2208 | GROMACS | Bug     | New             | Normal   | cuFFT linking   |                     | 06/30/2017 01:58 PM |                            |
| 2380 | GROMACS | Bug     | New             | Low      | cycle counter issues with separate PME rank + GPUs  |                     | 01/16/2018 10:21 PM |                            |
| 2994 | GROMACS | Feature | New             | Normal   | Data flow topology in gm_xapi 2020  |                     | 12/11/2019 11:33 AM | 2021-infrastructure-stable |

| #    | Project | Tracker | Status             | Priority | Subject   | Assignee            | Updated             | Target version             |
|------|---------|---------|--------------------|----------|---|---------------------|---------------------|----------------------------|
| 3312 | GROMACS | Task    | In Progress        | Normal   | Data type for coordinates, xyzq data, LJ parameters data to use for GPU buffers   | Artem Zhmurov       | 03/20/2020 09:54 AM | 2021-refactoring           |
| 2182 | GROMACS | Task    | New                | Low      | de-duplicate code in densorder and hydorder   |                     | 05/16/2017 11:29 AM |                            |
| 3387 | GROMACS | Bug     | New                | Normal   | Death test bug  |                     | 02/20/2020 05:39 PM |                            |
| 1768 | GROMACS | Task    | New                | Normal   | decide future of command-line options vs env vars   |                     | 11/03/2016 05:51 PM | future                     |
| 2916 | GROMACS | Task    | New                | Normal   | Decide future of symtab   | Paul Bauer          | 09/06/2019 02:35 PM | 2021-infrastructure-stable |
| 3433 | GROMACS | Feature | New                | Normal   | Decide how to handle multisim with modular simulator  | Pascal Merz         | 03/11/2020 06:42 AM | 2021-infrastructure-stable |
| 1653 | GROMACS | Feature | New                | Normal   | Decide how to represent multiple lambda states in the .top file and how to parse them   | Michael Shirts      | 06/05/2018 03:58 PM |                            |
| 1652 | GROMACS | Feature | New                | Normal   | Decide how to represent multiple lambda states internally   | Michael Shirts      | 06/05/2018 03:58 PM |                            |
| 2445 | GROMACS | Task    | New                | Normal   | Decide if/how to check for incompatible user input to mdrun for bonds and vsites  |                     | 03/13/2018 02:02 PM |                            |
| 921  | GROMACS | Feature | Blocked, need info | Normal   | Default index groups and selections   |                     | 07/11/2016 08:27 PM |                            |
| 988  | GROMACS | Task    | New                | Normal   | Definition of "public API"  |                     | 08/28/2019 02:50 PM | future                     |
| 2282 | GROMACS | Feature | New                | Normal   | Density map toolset   | Christian Blau      | 03/21/2019 06:08 PM | future                     |
| 3287 | GROMACS | Task    | New                | Normal   | Deprecate make_ndx, use select instead  |                     | 01/23/2020 01:16 PM |                            |
| 2168 | GROMACS | Task    | Feedback wanted    | Normal   | Design for multiple comparisons against same test reference data  |                     | 05/08/2017 02:45 PM | future                     |
| 3101 | GROMACS | Bug     | Blocked, need info | Normal   | detect compilation failed   | Erik Lindahl        | 12/27/2019 10:52 AM |                            |
| 1102 | GROMACS | Feature | New                | Normal   | Detect incompletely written itp files   |                     | 06/19/2014 03:23 PM |                            |
| 1323 | GROMACS | Task    | New                | Normal   | determine future of existing tools for  | David van der Spoel | 12/04/2018 11:53 AM |                            |
| 2354 | GROMACS | Feature | New                | Normal   | develop configuration file support for control of task layout   |                     | 09/19/2018 03:01 PM | future                     |
| 3115 | GROMACS | Feature | New                | Normal   | Device stream manager   |                     | 10/04/2019 09:00 AM |                            |
| 2573 | GROMACS | Bug     | New                | High     | Different mdp files describing the same change yield different free energy on the same trajectory   |                     | 07/19/2018 06:52 PM |                            |
| 3048 | GROMACS | Bug     | New                | Normal   | Dihedral parameters for N-terminal in gromos53a6 force field in the aminoacids.n.tdb file with different values in versions 4.6.7 and gromacs 2019/2016/5.1.5 |                     | 07/29/2019 10:41 AM |                            |
| 3289 | GROMACS | Task    | New                | Normal   | Distinguish identifying and non-identifying inputs to API operations.   | Eric Irrgang        | 01/10/2020 11:30 AM |                            |
| 2304 | GROMACS | Task    | New                | Normal   | Document and propose tracking mdrun heuristics  |                     | 10/03/2018 09:39 PM | future                     |
| 3275 | GROMACS | Task    | New                | Normal   | Document Gitlab CI instead of Jenkins and releng  | Paul Bauer          | 03/09/2020 05:55 PM | 2021-infrastructure-stable |
| 3353 | GROMACS | Task    | New                | Normal   | Document gmx densmap output   |                     | 01/23/2020 12:52 PM |                            |
| 3306 | GROMACS | Task    | New                | Normal   | Document gmx dos tool more clearly  | Christian Blau      | 01/20/2020 02:31 PM | future                     |

| #    | Project | Tracker | Status          | Priority | Subject  | Assignee               | Updated             | Target version             |
|------|---------|---------|-----------------|----------|--|------------------------|---------------------|----------------------------|
| 3267 | GROMACS | Task    | New             | Normal   | Document tools   |                        | 12/26/2019 03:20 PM | future                     |
| 2501 | GROMACS | Task    | New             | Normal   | Documentation section on log file contents   | Kevin Boyd             | 10/03/2018 09:48 PM | future                     |
| 3412 | GROMACS | Bug     | New             | Normal   | Domain decomposition problems with Gromacs >2018   |                        | 03/06/2020 04:10 PM |                            |
| 1489 | GROMACS | Feature | New             | Normal   | Don't solely rely on filename extension  |                        | 04/30/2014 05:23 AM |                            |
| 3444 | GROMACS | Bug     | Resolved        | Normal   | do_dssp does not work(gmx 2020 and 2020.1)   | Christian Blau         | 06/10/2020 02:45 PM | 2020.2                     |
| 1627 | GROMACS | Feature | In Progress     | Normal   | DPD integrator   |                        | 07/11/2016 08:08 PM |                            |
| 1885 | GROMACS | Feature | New             | Normal   | DPD Thermostat   |                        | 01/26/2016 10:17 AM |                            |
| 1658 | GROMACS | Feature | New             | Normal   | Electrostatics treatment for multiple lambda sites   | Berk Hess              | 07/11/2016 08:05 PM |                            |
| 1518 | GROMACS | Feature | New             | Low      | Enable automatic build checking for newer versions   | Mark Abraham           | 06/04/2014 04:13 PM | future                     |
| 3183 | GROMACS | Task    | Accepted        | Normal   | enable bonded interactions on GPU  |                        | 12/20/2019 08:32 AM | 2021-infrastructure-stable |
| 2532 | GROMACS | Task    | New             | Normal   | enable queue priorities in OpenCL  |                        | 05/29/2018 02:29 PM |                            |
| 2089 | GROMACS | Task    | New             | Normal   | Encourage code review  |                        | 01/10/2017 12:03 AM |                            |
| 3366 | GROMACS | Task    | New             | Normal   | Enforce compability of MdModules   |                        | 02/28/2020 11:20 AM |                            |
| 742  | GROMACS | Feature | New             | Normal   | Enhancing the performance of the free energy code  |                        | 08/26/2019 04:55 PM | future                     |
| 2696 | GROMACS | Task    | In Progress     | Normal   | ensure PME queue is flushed  | Szilárd Páll           | 12/31/2018 11:21 AM | future                     |
| 3368 | GROMACS | Bug     | New             | Normal   | Erroneous interplay between gmx rms command and atommass.dat: Can not find mass in database for atom MG in residue | Vedat Durmaz           | 02/05/2020 04:51 PM | future                     |
| 2360 | GROMACS | Bug     | New             | Low      | error at counter reset with PME-only rank  |                        | 01/05/2018 12:43 PM | future                     |
| 3055 | GROMACS | Bug     | Feedback wanted | Normal   | Error in gmx xpm2ps  |                        | 08/22/2019 03:27 PM |                            |
| 3058 | GROMACS | Bug     | Feedback wanted | Normal   | Error when using a large PME grid on a GPU   |                        | 09/04/2019 07:26 PM |                            |
| 2590 | GROMACS | Task    | New             | Normal   | Essential Dynamics as module providing forces  | Christian Blau         | 08/22/2018 05:03 PM | future                     |
| 2883 | GROMACS | Bug     | New             | Normal   | essentialdynamics fail with Intel MPI  |                        | 03/08/2019 03:10 AM |                            |
| 2882 | GROMACS | Task    | New             | Normal   | evaluate different storage layouts for GPU coordinates/changes/forces  | Szilárd Páll           | 03/07/2019 06:21 PM |                            |
| 3031 | GROMACS | Task    | New             | Normal   | evaluate the impact of particle order on PME   |                        | 12/27/2019 04:29 PM | 2021                       |
| 2490 | GROMACS | Task    | New             | Normal   | evaluate two-step communicators  | Szilárd Páll           | 10/03/2018 09:47 PM | future                     |
| 3441 | GROMACS | Bug     | Resolved        | Normal   | Ewald surface-epsilon is incorrect   | Berk Hess              | 03/18/2020 11:15 PM | 2020.2                     |
| 2853 | GROMACS | Bug     | New             | Normal   | EwaldUnitTests segfault on armv7hl with gcc-9.0.1  | Paul Bauer             | 02/04/2019 05:34 PM |                            |
| 1828 | GROMACS | Task    | New             | Normal   | Exception handling in mdrun  |                        | 10/07/2015 11:36 AM |                            |
| 3295 | GROMACS | Feature | New             | Normal   | Expand gmxapi.modify_input use cases.  | Eric Irrgang           | 01/16/2020 05:13 PM | 2021-refactoring           |
| 1849 | GROMACS | Feature | New             | Normal   | expanded ensemble -- Adaptive Integration Method   | Christopher Mirabzadeh | 07/11/2016 08:01 PM |                            |



| #    | Project | Tracker | Status | Priority | Subject   | Assignee          | Updated             | Target version             |
|------|---------|---------|--------|----------|---|-------------------|---------------------|----------------------------|
| 1246 | GROMACS | Task    | New    | Normal   | expanded ensemble .tpr cannot be rerun  | Michael Shirts    | 06/19/2015 01:56 PM |                            |
| 3001 | GROMACS | Task    | New    | Normal   | explore simplifying virial and shift force reduction  |                   | 12/27/2019 04:30 PM | 2021                       |
| 1994 | GROMACS | Feature | New    | Low      | explore using JIT for CUDA  |                   | 07/11/2016 10:20 PM | future                     |
| 3196 | GROMACS | Bug     | New    | Normal   | ExponentialMovingAverage.DeterminesCorrectlyIfIncreasing failing  |                   | 11/01/2019 11:28 PM |                            |
| 3356 | GROMACS | Task    | New    | Normal   | Expose setting of random seed to API  |                   | 01/29/2020 06:16 PM | 2021                       |
| 3329 | GROMACS | Task    | New    | Normal   | Extend energy comparison testing framework  |                   | 01/22/2020 09:51 AM | 2021-refactoring           |
| 3013 | GROMACS | Task    | New    | Normal   | Extend logging levels in MDLogger   |                   | 09/06/2019 02:34 PM | 2021-infrastructure-stable |
| 1972 | GROMACS | Feature | New    | Normal   | external potential modules for refinement against experimental data   |                   | 08/22/2018 05:03 PM | future                     |
| 1811 | GROMACS | Bug     | New    | Normal   | Extrae build issues   |                   | 12/13/2017 03:43 AM |                            |
| 2924 | GROMACS | Bug     | New    | Normal   | Failing version check when reading new tpr file with older gromacs version  |                   | 04/12/2019 10:52 AM |                            |
| 3198 | GROMACS | Bug     | New    | Normal   | Fails to build on FreeBSD with Clang since f7940fa01e8b6ef0703236b53721cca2d81b40d3 Use gmock and gtest targets from googletest-release-1.8.0 |                   | 11/06/2019 12:20 PM |                            |
| 3304 | GROMACS | Bug     | New    | Normal   | Failure in Log Output for Expanded Ensemble Weights using Simulated Tempering in GROMACS 2019.5   | Michael Shirts    | 03/01/2020 03:23 PM | 2020.2                     |
| 2496 | GROMACS | Task    | New    | Low      | find system xdr properly  |                   | 05/02/2018 02:19 PM |                            |
| 3385 | GROMACS | Bug     | New    | Normal   | FindLibStdCpp.cmake - wrong sanity check for clang  |                   | 03/04/2020 06:59 PM |                            |
| 2621 | GROMACS | Task    | New    | Normal   | Fine-Grained API to Describe Force Calculation and Neighbourhood Search   | Prashanth Kanduri | 08/22/2018 11:36 AM | future                     |
| 1247 | GROMACS | Feature | New    | Normal   | fix hardcoded references to atom names in analysis tools  | Mark Abraham      | 06/12/2014 01:20 AM | future                     |
| 3050 | GROMACS | Bug     | New    | Low      | Fix tests on Solaris  | Vedran Miletic    | 02/27/2020 11:05 AM | 2020.2                     |
| 2283 | GROMACS | Feature | New    | Normal   | Force distribution analysis   | Bernd Doser       | 10/27/2017 11:44 AM |                            |
| 2606 | GROMACS | Bug     | New    | Normal   | Free Energy Calculation -- Function type Fourier Dih. Not implemented in ip_pert  |                   | 08/10/2018 01:48 AM |                            |
| 2601 | GROMACS | Feature | New    | Normal   | Free energy calculations, soft-core potential   | Vytautas Gapsys   | 02/10/2020 11:29 AM | future                     |
| 3075 | GROMACS | Bug     | New    | Normal   | Frozen atoms are moving   | Erik Lindahl      | 12/27/2019 10:51 AM |                            |
| 2005 | GROMACS | Feature | New    | Normal   | Full Correlation Analysis (FCA) as Trajectory Analysis Module   | Christian Blau    | 02/07/2018 02:19 PM | future                     |
| 2229 | GROMACS | Feature | New    | High     | Full Object Oriented Modularization of GROMACS MDRUN Codebase   | Mark Abraham      | 08/22/2018 05:03 PM | future                     |
| 1862 | GROMACS | Task    | New    | Normal   | Fully replace t_topology by gmx_mtop_t  |                   | 02/13/2019 04:53 PM |                            |
| 3370 | GROMACS | Task    | New    | High     | Further improvements to GPU Buffer Ops and Comms  |                   | 03/04/2020 01:38 PM |                            |
| 1347 | GROMACS | Feature | New    | Normal   | future of tables  | Berk Hess         | 01/09/2020 02:37 PM | future                     |
| 1829 | GROMACS | Task    | New    | Normal   | Future of thread level parallelism  |                   | 11/18/2016 05:29 PM |                            |

| #    | Project | Tracker | Status   | Priority | Subject   | Assignee            | Updated             | Target version             |
|------|---------|---------|----------|----------|---|---------------------|---------------------|----------------------------|
| 1411 | GROMACS | Task    | New      | Normal   | Future of thread_mpi  | Mark Abraham        | 02/26/2018 04:56 PM | future                     |
| 3066 | GROMACS | Bug     | New      | Normal   | Gauss transform and density fit classes should operate on real values instead of float        | Christian Blau      | 08/26/2019 11:53 AM |                            |
| 3307 | GROMACS | Feature | New      | Normal   | General interface for communication between simulation ranks                                  |                     | 01/22/2020 03:22 PM | 2021-refactoring           |
| 2954 | GROMACS | Bug     | New      | Normal   | genion changes residue numbering  |                     | 05/26/2019 12:08 AM |                            |
| 3378 | GROMACS | Feature | New      | Normal   | genion usage without stdin (facilitates use in gmx python api)                                |                     | 02/13/2020 12:04 PM |                            |
| 3361 | GROMACS | Task    | New      | Normal   | Gitlab source archive contains files from build directory                                     | Paul Bauer          | 02/25/2020 10:13 AM | 2020.2                     |
| 2373 | GROMACS | Bug     | New      | Low      | gmx -nice can't work  |                     | 01/04/2018 11:17 AM |                            |
| 3448 | GROMACS | Bug     | New      | Normal   | GMX 2020.1 - Multidir simulations can stop at different times when killed by job manager      |                     | 03/23/2020 02:50 PM |                            |
| 1730 | GROMACS | Bug     | New      | Normal   | gmx compare does not compare all fields of a .tpr   |                     | 06/12/2015 09:33 PM | future                     |
| 1667 | GROMACS | Bug     | New      | Normal   | gmx convert-tpr writes wrong number of mol in output tpr                                      | David van der Spoel | 06/27/2016 08:29 PM |                            |
| 2483 | GROMACS | Bug     | New      | Low      | gmx dump writes mdp files that can not be parsed by grompp                                    | Paul Bauer          | 10/08/2018 10:50 AM | future                     |
| 2568 | GROMACS | Bug     | New      | Low      | gmx editconf -rotate does not rotate the box  |                     | 07/10/2018 10:27 AM | future                     |
| 1397 | GROMACS | Feature | New      | Normal   | gmx eneconv -offset 1.998 -dt 2 is broken for large times                                     | Mark Abraham        | 06/12/2014 01:31 AM | future                     |
| 3332 | GROMACS | Feature | New      | Normal   | gmx helixorient doesn't have a -tu option to change time unit                                 |                     | 01/22/2020 11:57 AM |                            |
| 2848 | GROMACS | Bug     | New      | Normal   | gmx make_ndx ignores last residue in case only CA's are present in GRO file                   |                     | 01/30/2019 06:16 AM |                            |
| 3284 | GROMACS | Bug     | New      | Normal   | gmx msd cannot output two xvg files as suggested by command line option                       | Christian Blau      | 01/08/2020 04:50 PM | 2021-infrastructure-stable |
| 2288 | GROMACS | Feature | Accepted | Low      | gmx msd doesn't optimally handle missing input trajectory frames                              |                     | 11/10/2017 11:03 AM |                            |
| 1583 | GROMACS | Bug     | New      | Normal   | gmx msd with mol flag requires excessive memory   |                     | 12/18/2017 03:34 PM |                            |
| 3049 | GROMACS | Bug     | New      | Low      | gmx nmeig should plot a real infrared spectrum  | David van der Spoel | 09/24/2019 03:25 PM | future                     |
| 1602 | GROMACS | Feature | New      | Low      | gmx order S per slice along all 3 axes  |                     | 09/22/2014 07:25 AM |                            |
| 2576 | GROMACS | Bug     | New      | Normal   | gmx potential -correct outputs the wrong potential  |                     | 07/25/2018 02:58 PM |                            |
| 2544 | GROMACS | Bug     | New      | Normal   | gmx rmsf does not fix periodicity in reference structure                                      | David van der Spoel | 08/21/2018 10:36 AM | future                     |
| 2427 | GROMACS | Bug     | New      | Normal   | gmx select gives syntax error for selection involving evaluating simple arithmetic expression |                     | 02/27/2018 05:15 PM |                            |
| 2872 | GROMACS | Bug     | New      | Normal   | gmx solvate and genion topology update  |                     | 02/27/2019 10:18 AM |                            |
| 3202 | GROMACS | Bug     | New      | Low      | gmx solvate fails to overwrite topology file  |                     | 11/13/2019 02:44 PM |                            |
| 2637 | GROMACS | Bug     | New      | High     | gmx solvate tears apart molecules   |                     | 09/11/2018 07:43 PM |                            |
| 2289 | GROMACS | Feature | New      | Normal   | gmx spatial add ability to perform over multiple reference structures                         |                     | 11/08/2017 12:31 AM |                            |
| 2133 | GROMACS | Task    | New      | Low      | gmx traj needs reform   |                     | 03/07/2017 02:02 PM |                            |

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|------|---------|---------|-----------------|----------|---|---------------|---------------------|----------------------------|
| 3362 | GROMACS | Feature | New             | Normal   | gmx traj: add an option to plot each component in a separate file                               |               | 01/29/2020 06:18 PM |                            |
| 2166 | GROMACS | Task    | Accepted        | Normal   | gmx trjconv functionality should check for mismatch between the tpr and the trajectory          |               | 05/05/2017 04:32 PM |                            |
| 2211 | GROMACS | Bug     | New             | Low      | gmx writes normal output to stderr  |               | 03/05/2018 02:00 PM | future                     |
| 3150 | GROMACS | Bug     | New             | Normal   | gmxapi data type annotations are confusing and inadequate                                       | Eric Irrgang  | 10/22/2019 03:08 PM | 2021-infrastructure-stable |
| 2698 | GROMACS | Task    | In Progress     | Normal   | gmxapi documentation integration  |               | 01/29/2020 03:59 PM | 2021-infrastructure-stable |
| 3014 | GROMACS | Task    | In Progress     | Normal   | gmxapi example Python scripts   |               | 01/03/2020 11:00 AM | 2021-infrastructure-stable |
| 2996 | GROMACS | Feature | In Progress     | Normal   | gmxapi execution model  | Eric Irrgang  | 12/10/2019 01:57 PM | 2021-infrastructure-stable |
| 3086 | GROMACS | Bug     | New             | Normal   | gmxapi fails with MPI build of GROMACS 2020   |               | 09/25/2019 04:18 PM |                            |
| 3141 | GROMACS | Bug     | New             | Normal   | gmxapi File placeholders missing from beta release  | Eric Irrgang  | 12/10/2019 02:02 PM | 2021-infrastructure-stable |
| 3139 | GROMACS | Task    | New             | Normal   | gmxapi Futures should be subscribable   | Eric Irrgang  | 10/15/2019 03:56 PM |                            |
| 2756 | GROMACS | Task    | In Progress     | Normal   | gmxapi integration testing  |               | 01/16/2020 05:12 PM | 2021-refactoring           |
| 2763 | GROMACS | Bug     | New             | Normal   | GMXAPI layout / grouping in development docs "modules" page                                     |               | 12/14/2018 12:49 PM | future                     |
| 3134 | GROMACS | Feature | Feedback wanted | Normal   | gmxapi Python exception names may need improvement  | Eric Irrgang  | 10/13/2019 01:50 PM |                            |
| 3273 | GROMACS | Bug     | New             | Normal   | gmxapi setup.py complains too much  |               | 12/27/2019 06:42 PM | 2021-infrastructure-stable |
| 3132 | GROMACS | Task    | New             | Normal   | gmxapi testing support tools  |               | 10/31/2019 03:35 PM |                            |
| 2764 | GROMACS | Task    | New             | Normal   | gmxapi version updates for post release-2019  | Eric Irrgang  | 11/21/2018 12:53 PM |                            |
| 3147 | GROMACS | Feature | New             | Normal   | gmxapi workflow checkpointing   | Eric Irrgang  | 10/15/2019 06:18 PM | 2021-infrastructure-stable |
| 3408 | GROMACS | Bug     | Fix uploaded    | Normal   | Gmxapi* tests segfault in rpmbuild  | Eric Irrgang  | 03/23/2020 01:27 PM | 2020.2                     |
| 3228 | GROMACS | Bug     | New             | Normal   | gmxapi.commandline_operation should gracefully handle input/output file arguments               | Eric Irrgang  | 12/04/2019 03:27 PM | 2021-infrastructure-stable |
| 3145 | GROMACS | Task    | New             | Normal   | gmxapi.mdrun needs improved (and public) interface for attaching an MD extension.               | Eric Irrgang  | 01/16/2020 04:31 PM | 2021-refactoring           |
| 3136 | GROMACS | Bug     | New             | Normal   | gmxapi.operation data flow topology unclear or incomplete                                       | Eric Irrgang  | 12/11/2019 11:25 AM | 2021-infrastructure-stable |
| 2628 | GROMACS | Bug     | Fix uploaded    | Normal   | GMXRC removes trailing colon from existing MANPATH  |               | 08/28/2018 03:13 PM |                            |
| 2113 | GROMACS | Bug     | New             | Normal   | Google tests and execution order  |               | 03/05/2018 02:05 PM |                            |
| 2624 | GROMACS | Bug     | New             | Normal   | GPU build system not robust enough  |               | 09/05/2018 02:00 AM |                            |
| 3246 | GROMACS | Bug     | Accepted        | Normal   | GPU code misses settle error check, simulation crashes with segfault without any further output | Artem Zhmurov | 12/20/2019 09:52 AM | 2021-infrastructure-stable |
| 3239 | GROMACS | Bug     | New             | Normal   | GPU DD direct communication with GPU update error with RF                                       |               | 12/14/2019 05:15 PM |                            |
| 2870 | GROMACS | Bug     | New             | Normal   | GPU detection error message missing from the output   |               | 03/05/2019 03:55 PM |                            |
| 2869 | GROMACS | Bug     | New             | Normal   | GPU detection error only issued as a note to the log  |               | 03/05/2019 04:09 PM |                            |
| 2915 | GROMACS | Feature | In Progress     | High     | GPU direct communications   |               | 02/14/2020 12:48 PM |                            |
| 2217 | GROMACS | Bug     | New             | Low      | GPU emulation and separate PME ranks doesn't work properly                                      |               | 12/12/2017 11:50 AM |                            |

| #    | Project | Tracker | Status          | Priority | Subject  | Assignee      | Updated             | Target version             |
|------|---------|---------|-----------------|----------|--|---------------|---------------------|----------------------------|
| 2240 | GROMACS | Task    | Accepted        | Low      | GPU emulation mode support for PME missing   |               | 09/16/2017 10:02 PM |                            |
| 2238 | GROMACS | Task    | In Progress     | Normal   | GPU emulation mode support for rolling pruning missing   | Berk Hess     | 12/21/2017 03:21 PM |                            |
| 2254 | GROMACS | Feature | Resolved        | Normal   | GPU extensions for Google Tests  |               | 10/06/2020 12:15 PM |                            |
| 2890 | GROMACS | Feature | In Progress     | Normal   | GPU Halo Exchange  |               | 02/14/2020 12:41 PM | 2021                       |
| 3311 | GROMACS | Feature | In Progress     | Normal   | GPU infrastructure development   |               | 03/20/2020 09:54 AM | 2021-refactoring           |
| 3348 | GROMACS | Task    | New             | Normal   | GPU LINCS and SETTLE: unify virial reduction   | Artem Zhmurov | 01/23/2020 11:58 AM | 2021-infrastructure-stable |
| 3340 | GROMACS | Task    | New             | Normal   | GPU LINCS: Move more data to local/shared memory   | Artem Zhmurov | 01/23/2020 11:56 AM | 2021-infrastructure-stable |
| 3341 | GROMACS | Task    | New             | Normal   | GPU LINCS: Use analytical solution for the matrix A inversion.                                       | Artem Zhmurov | 01/23/2020 11:56 AM | 2021-infrastructure-stable |
| 3339 | GROMACS | Task    | New             | Normal   | GPU LINCS: Warp-level synchronization for coupled constraints  | Artem Zhmurov | 01/23/2020 11:55 AM | 2021-infrastructure-stable |
| 2464 | GROMACS | Task    | New             | Normal   | GPU performance goals overview   |               | 03/26/2018 10:42 AM |                            |
| 2967 | GROMACS | Feature | New             | Normal   | GPU reallocateDeviceBuffer improvements  |               | 01/23/2020 12:15 PM | 2021-refactoring           |
| 3342 | GROMACS | Task    | New             | Normal   | GPU SETTLE: Read only one index per water molecule.  | Artem Zhmurov | 01/23/2020 11:56 AM | 2021-infrastructure-stable |
| 3343 | GROMACS | Task    | New             | Normal   | GPU SETTLE: Use different ordering for matrices.   | Artem Zhmurov | 01/23/2020 11:57 AM | 2021-infrastructure-stable |
| 3346 | GROMACS | Task    | New             | Normal   | GPU SETTLE: Use the same parameters and parameters initialization in GPU and CPU versions of SETTLE. | Artem Zhmurov | 01/23/2020 11:58 AM | 2021-infrastructure-stable |
| 3351 | GROMACS | Feature | New             | Normal   | GPU update-constraints code organization and integration   | Artem Zhmurov | 01/23/2020 11:59 AM | 2021                       |
| 3352 | GROMACS | Feature | New             | Normal   | GPU update-constraints feature support   | Artem Zhmurov | 01/23/2020 11:59 AM | 2021                       |
| 3350 | GROMACS | Feature | New             | Normal   | GPU update-constraints performance   | Artem Zhmurov | 01/23/2020 11:59 AM | 2021                       |
| 3344 | GROMACS | Task    | New             | Normal   | GPU update-constraints: Better virial reduction.   | Artem Zhmurov | 01/23/2020 11:57 AM | 2021-infrastructure-stable |
| 3308 | GROMACS | Task    | New             | Normal   | GPU update-constraints: Cycle counting for GPU launches  |               | 01/23/2020 11:54 AM | 2021-infrastructure-stable |
| 3338 | GROMACS | Task    | New             | Normal   | GPU update-constraints: Do not save intermediate coordinates if there is no constraints              | Artem Zhmurov | 01/23/2020 11:55 AM | 2021-infrastructure-stable |
| 3258 | GROMACS | Task    | New             | Normal   | GPU update-constraints: Enable free energy perturbation  | Artem Zhmurov | 01/23/2020 11:54 AM | 2021-infrastructure-stable |
| 3337 | GROMACS | Task    | New             | Normal   | GPU update-constraints: Merge Leap-Frog, LINCS and SETTLE kernels.                                   | Artem Zhmurov | 01/23/2020 11:55 AM | 2021-infrastructure-stable |
| 3236 | GROMACS | Task    | New             | Normal   | GPU update-constraints: Pulling support  | Artem Zhmurov | 01/23/2020 11:53 AM | 2021-infrastructure-stable |
| 3345 | GROMACS | Task    | New             | Normal   | GPU update-constraints: Reconsider the naming of coordinates buffer in constraints.                  | Artem Zhmurov | 01/23/2020 11:57 AM | 2021-infrastructure-stable |
| 2907 | GROMACS | Bug     | New             | Normal   | Gromacs autocompletion appears to be broken with ZSH   |               | 07/16/2019 04:46 AM |                            |
| 2390 | GROMACS | Bug     | Feedback wanted | Normal   | GROMACS build system should check for valid nvcc flags before use                                    |               | 12/20/2019 12:13 PM | 2021                       |
| 1625 | GROMACS | Feature | New             | Normal   | Gromacs Python API   |               | 03/02/2019 01:44 AM | future                     |
| 2216 | GROMACS | Task    | New             | Normal   | GROMACS SIMD acceleration: generation 3  | Erik Lindahl  | 07/17/2017 06:57 PM | future                     |
| 2607 | GROMACS | Bug     | New             | Normal   | Grompp becomes extremely slow when many pull groups are present                                      |               | 08/11/2018 08:54 AM |                            |

| #    | Project | Tracker | Status       | Priority | Subject  | Assignee            | Updated             | Target version             |
|------|---------|---------|--------------|----------|--|---------------------|---------------------|----------------------------|
| 2192 | GROMACS | Bug     | Accepted     | Low      | grompp should read floats (e.g charge) from data files to double, to avoid accumulating round-off error                            | Berk Hess           | 12/20/2019 12:11 PM | 2021                       |
| 1481 | GROMACS | Bug     | New          | Low      | g_chi output file chi.log reports atomic definitions for phi and psi that do not correspond to the angles output in the .xvg files | David van der Spoel | 06/12/2014 01:37 PM |                            |
| 1688 | GROMACS | Feature | New          | Low      | g_cluster "middle" is not exactly the same as the definition in the cited paper  |                     | 04/01/2015 05:53 AM |                            |
| 1168 | GROMACS | Feature | In Progress  | Low      | g_density does not do what users think it does, given PBC over z and constant pressure simulation                                  | Erik Lindahl        | 10/20/2018 12:49 AM | future                     |
| 1498 | GROMACS | Feature | New          | Low      | g_dipoles does not work properly with ionic systems  | David van der Spoel | 07/11/2016 08:11 PM |                            |
| 843  | GROMACS | Feature | New          | Low      | g_helixorient could benefit from more documentation  | Erik Lindahl        | 05/23/2014 02:02 PM |                            |
| 1655 | GROMACS | Bug     | New          | Normal   | g_membed and box type  |                     | 12/09/2014 01:33 PM |                            |
| 1166 | GROMACS | Bug     | New          | Low      | g_order is incorrect for unsaturated carbons   | David van der Spoel | 02/06/2020 02:32 PM | future                     |
| 1618 | GROMACS | Bug     | In Progress  | Normal   | g_protonate segfaults unconditionally  | Erik Lindahl        | 08/17/2015 02:10 PM |                            |
| 895  | GROMACS | Feature | In Progress  | Normal   | g_rmsf previous frame as reference   |                     | 04/29/2013 07:39 PM | future                     |
| 986  | GROMACS | Task    | New          | Normal   | Handling C++ out-of-memory errors  |                     | 12/24/2014 08:42 PM | future                     |
| 2226 | GROMACS | Feature | New          | Normal   | Harmonise commands for exit in make_ndx and distance   |                     | 08/04/2017 12:24 PM |                            |
| 3213 | GROMACS | Bug     | New          | Normal   | Having a local residuetypes.dat for custom force field   |                     | 11/21/2019 09:18 PM |                            |
| 2961 | GROMACS | Feature | New          | Normal   | How should Python package find GROMACS resources under various circumstances?  |                     | 12/09/2019 10:47 AM |                            |
| 1654 | GROMACS | Feature | New          | Normal   | How to carry out movement between chemical end states in a multiple end state framework?   | Michael Shirts      | 07/11/2016 08:05 PM |                            |
| 1966 | GROMACS | Feature | New          | Low      | Hydrogen mass repartiniog  |                     | 05/25/2016 06:04 PM | future                     |
| 3380 | GROMACS | Bug     | Resolved     | Low      | IBM VSX checks fail with gcc-10  | Erik Lindahl        | 04/30/2020 01:30 PM | 2020.2                     |
| 2435 | GROMACS | Task    | New          | Normal   | identify and note about/tune task offload in GPU-bound runs  |                     | 03/02/2018 04:08 PM |                            |
| 2574 | GROMACS | Feature | New          | Normal   | iForceSchedule Abstraction   | Prashanth Kanduri   | 03/29/2019 05:20 PM | future                     |
| 2791 | GROMACS | Feature | In Progress  | Normal   | Implement a module for lambda-dynamics simulations (lambda_site module)  | Thomas Ullmann      | 03/01/2019 01:36 AM | future                     |
| 3423 | GROMACS | Feature | New          | Normal   | Implement additional temperature and pressure control algorithms for modular simulator   | Pascal Merz         | 03/10/2020 11:22 PM | 2021-infrastructure-stable |
| 2521 | GROMACS | Task    | New          | Normal   | Implement alternating PME/NB wait for OpenCL   |                     | 10/15/2018 12:39 PM |                            |
| 3436 | GROMACS | Feature | New          | Normal   | Implement AWH for modular simulator  | Pascal Merz         | 03/11/2020 06:32 AM | 2021-infrastructure-stable |
| 3421 | GROMACS | Task    | New          | Normal   | Implement client system for global reduction   | Pascal Merz         | 03/11/2020 03:31 PM | 2021-infrastructure-stable |
| 1104 | GROMACS | Feature | New          | Low      | Implement dihedral restraints  |                     | 02/06/2013 07:04 PM | future                     |
| 3160 | GROMACS | Feature | Fix uploaded | High     | implement direct comm for different src/target memory spaces   | Alan Gray           | 02/14/2020 11:28 AM | 2021-infrastructure-stable |

| #    | Project | Tracker | Status      | Priority | Subject   | Assignee         | Updated             | Target version             |
|------|---------|---------|-------------|----------|---|------------------|---------------------|----------------------------|
| 3432 | GROMACS | Feature | New         | Normal   | Implement essential dynamics for modular simulator                                      | Pascal Merz      | 03/11/2020 12:38 AM | 2021-infrastructure-stable |
| 2492 | GROMACS | Task    | New         | Normal   | implement force calculation via ForceProviders containing collections of IForceProvider | Mark Abraham     | 09/19/2018 03:13 PM | future                     |
| 2111 | GROMACS | Feature | In Progress | Normal   | Implement Gaussian screening of electrostatics  |                  | 02/23/2019 12:33 PM |                            |
| 1162 | GROMACS | Feature | New         | Normal   | Implement gb_saltconc   | Berk Hess        | 02/26/2013 05:33 PM | future                     |
| 3104 | GROMACS | Task    | New         | Normal   | implement GPU DD cycle counting   |                  | 12/27/2019 04:21 PM | 2021                       |
| 3105 | GROMACS | Task    | New         | Normal   | implement GPU PME/PP comm cycle counting  |                  | 12/27/2019 04:20 PM | 2021                       |
| 2469 | GROMACS | Task    | New         | Normal   | implement GPU timer reduction for reporting   |                  | 03/27/2018 05:08 PM |                            |
| 3003 | GROMACS | Task    | New         | Normal   | implement heuristic fallback to CPU when there is too little work for GPU offload       |                  | 06/25/2019 04:10 PM |                            |
| 3189 | GROMACS | Task    | In Progress | High     | implement heuristics for switching between different spread/gather kernel layouts       | Jonathan Vincent | 01/29/2020 04:18 PM | 2021-infrastructure-stable |
| 3422 | GROMACS | Task    | Resolved    | Normal   | Implement modular checkpointing for modular simulator                                   | Pascal Merz      | 09/16/2020 09:45 AM | 2021-infrastructure-stable |
| 2126 | GROMACS | Feature | New         | Normal   | implement native CUDA support in CMake  |                  | 10/29/2019 09:03 PM |                            |
| 3430 | GROMACS | Feature | New         | Normal   | Implement NMR restraints for modular simulator  | Pascal Merz      | 03/11/2020 12:28 AM | 2021-infrastructure-stable |
| 868  | GROMACS | Feature | In Progress | Normal   | Implement parallelization support to analysis framework                                 | Kevin Boyd       | 12/20/2019 11:59 AM | 2021                       |
| 1464 | GROMACS | Feature | New         | Normal   | implement PP-PME re-balancing   | Szilárd Páll     | 10/16/2015 08:34 AM | future                     |
| 3435 | GROMACS | Feature | New         | Normal   | Implement pull for modular simulator  | Pascal Merz      | 03/11/2020 06:31 AM | 2021-infrastructure-stable |
| 3425 | GROMACS | Feature | New         | Normal   | Implement rerun for the modular simulator   | Pascal Merz      | 03/10/2020 11:57 PM | 2021-infrastructure-stable |
| 760  | GROMACS | Feature | New         | Low      | Implement rigid body groups   | Berk Hess        | 12/30/2012 06:04 AM | future                     |
| 3428 | GROMACS | Feature | New         | Normal   | Implement SIMD version of modular simulator propagators                                 | Pascal Merz      | 03/11/2020 12:12 AM | 2021-infrastructure-stable |
| 1900 | GROMACS | Feature | New         | Normal   | Implement some new errors in grompp   |                  | 06/22/2016 05:20 PM |                            |
| 3424 | GROMACS | Feature | New         | Normal   | Implement stochastic dynamics / langevin integrator in modular simulator                | Pascal Merz      | 03/10/2020 11:48 PM | 2021-infrastructure-stable |
| 3431 | GROMACS | Feature | New         | Normal   | Implement virtual sites for modular simulator   | Pascal Merz      | 03/11/2020 12:33 AM | 2021-infrastructure-stable |
| 2175 | GROMACS | Task    | New         | Normal   | improve clang static analyzer docs further  |                  | 01/04/2018 04:13 PM | future                     |
| 1083 | GROMACS | Feature | In Progress | Normal   | Improve collective error/warning/note handling in mdrun                                 |                  | 07/11/2016 08:21 PM |                            |
| 2009 | GROMACS | Task    | New         | Normal   | improve command-line reporting of useful things   |                  | 07/26/2016 12:54 PM |                            |
| 3216 | GROMACS | Task    | New         | Normal   | improve CPU force reductions  | Szilárd Páll     | 12/04/2019 09:24 PM |                            |
| 1715 | GROMACS | Feature | New         | Low      | improve cycle counting GPU sharing and multi-sim  |                  | 08/03/2016 12:32 PM | future                     |
| 2674 | GROMACS | Task    | Accepted    | Normal   | Improve domain decomposition for bilayer systems  |                  | 12/07/2018 04:03 PM | future                     |
| 3138 | GROMACS | Feature | New         | Normal   | Improve ensemble support in Context specification.                                      |                  | 10/15/2019 03:56 PM |                            |
| 3363 | GROMACS | Feature | New         | Normal   | Improve FEP testing   | Pascal Merz      | 03/01/2020 03:22 PM | 2021-infrastructure-stable |
| 2697 | GROMACS | Task    | New         | Normal   | improve FFT library flavor/version reporting  |                  | 12/27/2019 04:40 PM | future                     |

| #    | Project | Tracker | Status             | Priority | Subject  | Assignee       | Updated             | Target version             |
|------|---------|---------|--------------------|----------|--|----------------|---------------------|----------------------------|
| 1665 | GROMACS | Feature | New                | Normal   | improve free energy non-bonded kernel performance  |                | 08/26/2019 03:47 PM | future                     |
| 838  | GROMACS | Task    | New                | Normal   | Improve generic error reporting routines   |                | 07/11/2016 08:29 PM |                            |
| 3394 | GROMACS | Feature | New                | Normal   | improve gmxapi error handling  | Eric Irrgang   | 02/24/2020 11:45 AM | 2021-infrastructure-stable |
| 2773 | GROMACS | Task    | New                | Normal   | improve GPU error handling and make such handling uniform across modules   |                | 12/20/2019 01:09 PM | 2021                       |
| 3114 | GROMACS | Feature | New                | Normal   | Improve GPU update-constraints module  | Artem Zhmurov  | 02/10/2020 04:30 PM | 2021                       |
| 1515 | GROMACS | Task    | New                | Normal   | improve g_bar output   | Szilárd Páll   | 07/11/2016 08:10 PM |                            |
| 1505 | GROMACS | Task    | New                | Normal   | improve handling of logging  | Mark Abraham   | 01/02/2019 06:06 PM |                            |
| 2766 | GROMACS | Task    | In Progress        | Normal   | Improve hardware option selection  | Kevin Boyd     | 12/20/2019 02:34 PM | 2021                       |
| 2353 | GROMACS | Task    | New                | Normal   | improve on relative tolerance for constructing tables  |                | 12/20/2019 12:12 PM | 2021                       |
| 2863 | GROMACS | Task    | New                | Normal   | improve PBC handling   |                | 03/11/2019 04:28 PM |                            |
| 2997 | GROMACS | Task    | New                | Normal   | improve performance of alchemical free energy calculations   |                | 12/27/2019 04:31 PM | 2021                       |
| 3317 | GROMACS | Task    | Resolved           | Normal   | Improve testing of the GPU code  | Artem Zhmurov  | 10/06/2020 12:15 PM | 2021-refactoring           |
| 1587 | GROMACS | Task    | New                | Normal   | improve the configurability of regression tests  |                | 12/20/2019 12:02 PM | 2021                       |
| 1182 | GROMACS | Feature | New                | Normal   | improve trajectory writing to support parallel I/O   |                | 05/13/2014 10:42 AM | future                     |
| 1211 | GROMACS | Task    | New                | Low      | improve use of preprocessor macros in CUDA kernels   | Szilárd Páll   | 01/12/2015 06:42 PM | future                     |
| 2519 | GROMACS | Task    | New                | High     | Improve/remove PME OpenCL kernel barriers  |                | 02/15/2019 06:34 PM |                            |
| 1335 | GROMACS | Feature | New                | Normal   | Improved interaction of free energies with pull code to better support Hamiltonian replica exchange with umbrella sampling | Michael Shirts | 05/13/2014 10:38 AM | future                     |
| 2792 | GROMACS | Task    | New                | High     | Improvement of PME gather and spread CUDA kernels  |                | 03/18/2020 03:57 PM |                            |
| 3038 | GROMACS | Feature | New                | Normal   | Improvements to MD plugin development environment  | Eric Irrgang   | 12/10/2019 01:58 PM | 2021-infrastructure-stable |
| 765  | GROMACS | Task    | New                | Normal   | Improving serialization of data structures prior to communication  | Mark Abraham   | 05/13/2014 10:04 AM | future                     |
| 2785 | GROMACS | Bug     | New                | Normal   | Inconsistent and erroneous behaviour of trjconv when writing a partial TNG   |                | 11/30/2018 02:36 PM |                            |
| 1568 | GROMACS | Bug     | New                | Low      | inconsistent/incorrect threading checks and reporting in mdrun   |                | 05/25/2016 02:01 AM |                            |
| 2795 | GROMACS | Task    | New                | Normal   | Incorporate regressiontests into core gromacs  |                | 12/02/2019 01:44 PM | 2021-infrastructure-stable |
| 2393 | GROMACS | Bug     | New                | Normal   | incorrect error message with omitted command line flag before its argument   |                | 01/24/2018 11:24 PM |                            |
| 2468 | GROMACS | Bug     | New                | Low      | incorrect GPU timing reported with OpenCL and domain decomposition   |                | 12/17/2018 01:28 PM | future                     |
| 2762 | GROMACS | Bug     | Blocked, need info | Normal   | incorrect results with Ubuntu 18.04 / glibc 2.27 (?) and >20 threads   |                | 07/01/2019 11:26 PM |                            |
| 3152 | GROMACS | Feature | New                | Normal   | Infrastructure and patterns for expressing public interfaces   |                | 01/09/2020 05:19 PM | 2021-infrastructure-stable |
| 3418 | GROMACS | Task    | New                | Normal   | Infrastructure improvements for modular simulator  | Pascal Merz    | 03/10/2020 10:24 PM | 2021-infrastructure-stable |
| 2585 | GROMACS | Feature | Resolved           | Normal   | Infrastructure supporting external API   |                | 12/11/2019 12:39 PM |                            |

| #    | Project | Tracker | Status          | Priority | Subject  | Assignee            | Updated             | Target version             |
|------|---------|---------|-----------------|----------|--|---------------------|---------------------|----------------------------|
| 3028 | GROMACS | Bug     | Feedback wanted | Normal   | install fail on Centos 6   |                     | 07/15/2019 12:32 PM |                            |
| 2828 | GROMACS | Bug     | Feedback wanted | Normal   | Installation issue on Power 9 system with SIMD support                               |                     | 01/18/2019 11:54 AM |                            |
| 2707 | GROMACS | Bug     | New             | Normal   | Installed OpenCL files include clh file from gpu_utils directory                     |                     | 10/30/2018 04:02 AM |                            |
| 3209 | GROMACS | Bug     | New             | Normal   | Interactive molecular dynamics with VMD becomes stuttering after reconnecting        |                     | 11/19/2019 11:36 AM |                            |
| 3130 | GROMACS | Task    | New             | Normal   | Interim handling of gmxapi data references.  | Eric Irrgang        | 12/11/2019 11:26 AM | 2021-infrastructure-stable |
| 2132 | GROMACS | Feature | New             | Normal   | Intermediate code for xvg handling   |                     | 03/08/2017 05:12 PM | future                     |
| 3405 | GROMACS | Bug     | Accepted        | Normal   | intermittent OpenCL regressiontest failures  |                     | 03/02/2020 11:01 AM |                            |
| 3016 | GROMACS | Task    | New             | Normal   | intermittent failure of essentialdynamics test                                       |                     | 07/18/2019 05:23 PM |                            |
| 3398 | GROMACS | Bug     | New             | Normal   | Intermittent failure of non-bonded kernels when run using nvprof                     |                     | 02/25/2020 12:14 PM |                            |
| 3313 | GROMACS | Feature | Accepted        | Normal   | Introduce and use opaque types for the DeviceStream and DeviceContext                | Artem Zhmurov       | 01/23/2020 12:00 PM | 2021-refactoring           |
| 2936 | GROMACS | Task    | New             | Normal   | introduce check that CPU-GPU transfers/assignments are made between compatible types |                     | 02/05/2020 03:57 PM | 2021                       |
| 1562 | GROMACS | Feature | New             | Normal   | introducing a Monte Carlo framework (first application: MC barostat)                 | Michael Shirts      | 07/11/2016 08:08 PM |                            |
| 1826 | GROMACS | Task    | New             | Normal   | investigate non-optimal results with CPU-GPU balancing on AMD                        | Szilárd Páll        | 12/20/2019 12:04 PM | future                     |
| 3360 | GROMACS | Task    | New             | Normal   | investigate the future of DD dynamic load balancing with GPU offload                 |                     | 01/29/2020 11:23 AM |                            |
| 2611 | GROMACS | Bug     | New             | Normal   | issues with gpu_utils-test with GMX_BUILD_UNITTESTS=OFF and on OSX                   |                     | 08/14/2018 07:03 PM |                            |
| 3069 | GROMACS | Feature | New             | Low      | Iterator over span and indices into this span (zip-style iterator)                   | Christian Blau      | 08/29/2019 11:11 AM | future                     |
| 1214 | GROMACS | Task    | New             | Normal   | Keep track of important changes for Changelog  | Mark Abraham        | 06/26/2013 11:24 AM |                            |
| 3260 | GROMACS | Task    | New             | Low      | keep up to with mdspan reference implementation                                      | Christian Blau      | 12/20/2019 01:16 PM | 2021-infrastructure-stable |
| 1907 | GROMACS | Task    | Accepted        | Low      | keeping compile- and run-time CPU/arch detection consistent                          |                     | 08/01/2016 10:09 PM |                            |
| 1053 | GROMACS | Feature | In Progress     | Normal   | L-BFGS doesn't use constraints or call do_em_step                                    | Berk Hess           | 01/18/2013 11:00 AM | future                     |
| 2248 | GROMACS | Feature | New             | Normal   | Label all SIMD functions as pure/nodiscard   |                     | 02/04/2019 04:49 AM |                            |
| 3153 | GROMACS | Task    | New             | Low      | Let CMake process module directories earlier to support more modern CMake idioms.    |                     | 10/17/2019 10:40 AM | 2021-infrastructure-stable |
| 2310 | GROMACS | Feature | Accepted        | Low      | Let mdrun dump coordinates with non-finite energy                                    |                     | 10/03/2018 09:47 PM | future                     |
| 2930 | GROMACS | Feature | New             | Normal   | Limited range for reference group detection in cylinder pulling                      |                     | 04/26/2019 05:17 PM |                            |
| 2761 | GROMACS | Feature | New             | Low      | lincs-order 4 is too conservative for some force fields                              |                     | 11/16/2018 09:55 AM |                            |
| 2451 | GROMACS | Feature | Resolved        | Normal   | Linear virtual sites with fixed distance   | David van der Spoel | 09/16/2019 01:15 PM |                            |



| #    | Project | Tracker | Status      | Priority | Subject  | Assignee      | Updated             | Target version             |
|------|---------|---------|-------------|----------|--|---------------|---------------------|----------------------------|
| 3083 | GROMACS | Bug     | New         | Normal   | Listed forces tests failing on ICC19 with AVX2_256 nightly build               |               | 09/10/2019 11:56 AM |                            |
| 2975 | GROMACS | Feature | New         | Normal   | LJ PME calculations on GPUs  |               | 06/12/2019 01:17 PM |                            |
| 2071 | GROMACS | Task    | In Progress | High     | Low accuracy default settings yield incorrect liquid densities                 | Berk Hess     | 01/05/2018 03:32 PM |                            |
| 2947 | GROMACS | Task    | Accepted    | Normal   | make an end to end test for membed   |               | 09/24/2019 03:22 PM | future                     |
| 869  | GROMACS | Task    | In Progress | Normal   | Make analysis data histogramming and multipoint data easier to use in parallel | Teemu Murtola | 07/11/2016 08:28 PM |                            |
| 1120 | GROMACS | Feature | New         | Low      | Make build work with multi-cogfiguration generators                            |               | 06/03/2014 03:04 PM | future                     |
| 2567 | GROMACS | Bug     | New         | Normal   | make check fails at test 23 SIMD errors  |               | 07/10/2018 09:35 AM |                            |
| 1867 | GROMACS | Feature | New         | Normal   | make coupling implementations reversible                                       |               | 12/02/2015 07:43 AM |                            |
| 2556 | GROMACS | Feature | New         | Normal   | make default selections suitable for DNA and RNA                               | Mark Abraham  | 06/20/2018 01:48 PM |                            |
| 3135 | GROMACS | Feature | New         | Normal   | Make GPU traits ino opaque types   |               | 10/14/2019 10:24 AM |                            |
| 3417 | GROMACS | Feature | New         | Normal   | Make modular simulator feature-complete  | Pascal Merz   | 03/23/2020 03:57 AM | 2021-infrastructure-stable |
| 2839 | GROMACS | Task    | New         | Normal   | make module and file naming consistent   |               | 01/16/2020 05:11 PM | 2021                       |
| 2822 | GROMACS | Task    | Accepted    | Normal   | Make nbxn a module   | Berk Hess     | 12/18/2019 10:49 AM | future                     |
| 2475 | GROMACS | Task    | New         | Normal   | make OpenCL 1st class-citizen in the build system                              |               | 12/20/2019 12:14 PM | 2021                       |
| 3357 | GROMACS | Task    | New         | Normal   | Make sure "colvars" interoperates stably and smoothly with gromacs             |               | 03/04/2020 11:25 AM |                            |
| 2632 | GROMACS | Task    | New         | Low      | make sure cmake defines proper hwloc versionc with cross-compilation enabled   |               | 12/03/2018 01:35 PM | future                     |
| 677  | GROMACS | Task    | New         | Normal   | Make sure manual uses consistent style throughout                              |               | 06/19/2014 11:49 AM |                            |
| 1943 | GROMACS | Task    | Accepted    | Low      | make sure releases are submitted early for Debian Experimental                 | Szilárd Páll  | 12/20/2019 12:05 PM | 2021                       |
| 1879 | GROMACS | Task    | In Progress | Low      | make the GROMACS OpenCL kernel work on Gallium                                 |               | 11/30/2018 05:46 PM | future                     |
| 3219 | GROMACS | Bug     | New         | Normal   | MANPATH setting is fragile   |               | 11/29/2019 12:44 PM |                            |
| 2835 | GROMACS | Task    | New         | Normal   | Matrix class constraint to upper or lower triangle                             |               | 02/07/2019 02:44 PM |                            |
| 2376 | GROMACS | Task    | New         | Normal   | max_mpi_ranks has wrong name   |               | 02/10/2018 11:03 AM |                            |
| 2755 | GROMACS | Feature | New         | Low      | md5 sums and sha256, sha512 hashes   | Benson Muite  | 02/19/2019 11:00 PM |                            |
| 1170 | GROMACS | Task    | New         | Normal   | mdlib reorganization   |               | 11/17/2016 03:47 PM | future                     |
| 2643 | GROMACS | Feature | New         | Low      | mdp options and/or docs for anisotropic aspects of implementations             |               | 09/12/2018 02:23 PM |                            |
| 2039 | GROMACS | Bug     | New         | Normal   | mdrun -pinstride defaults are too confusing                                    |               | 12/13/2017 04:14 AM |                            |
| 2740 | GROMACS | Bug     | New         | Normal   | mdrun reports incorrect error with -bonded gpu without gpu                     | Mark Abraham  | 11/07/2018 01:59 PM |                            |
| 2473 | GROMACS | Bug     | New         | Normal   | mdrun sometimes stalls due to large coordinates with no constraints            |               | 04/04/2018 10:15 PM |                            |
| 3127 | GROMACS | Bug     | New         | Normal   | mdrun-mpi-test -ntmpi 2 runs out of memory with OpenCL on Nvidia               |               | 10/09/2019 05:33 PM |                            |

| #    | Project | Tracker | Status                | Priority | Subject  | Assignee       | Updated             | Target version             |
|------|---------|---------|-----------------------|----------|--|----------------|---------------------|----------------------------|
| 2733 | GROMACS | Bug     | Blocked,<br>need info | Normal   | MdrunUtilityMpiUnitTests timeout on i686 and armv7hl with OpenMPI 2.1.5              | Paul Bauer     | 01/17/2020 08:40 AM |                            |
| 2252 | GROMACS | Bug     | New                   | Low      | Memory allocation failures with large page sizes during PME tuning                   |                | 12/14/2017 04:27 AM |                            |
| 3068 | GROMACS | Bug     | New                   | Normal   | Misleading warning on rerun  |                | 08/26/2019 03:44 PM |                            |
| 3054 | GROMACS | Bug     | New                   | Normal   | Missing dihedral define  |                | 08/02/2019 05:47 PM |                            |
| 2910 | GROMACS | Feature | New                   | Normal   | Mixed scaling for 1-4 interactions   |                | 04/10/2019 10:13 PM |                            |
| 2616 | GROMACS | Task    | New                   | Normal   | Model for MD state   |                | 09/14/2018 05:12 PM |                            |
| 2423 | GROMACS | Task    | New                   | Normal   | modernize constraints code   | Mark Abraham   | 09/19/2018 03:01 PM | future                     |
| 3020 | GROMACS | Feature | New                   | Low      | modernize DeviceBuffer and GPU memory management                                     |                | 08/13/2019 06:01 PM |                            |
| 2758 | GROMACS | Task    | New                   | Low      | Modernize genconf  |                | 11/15/2018 07:38 AM | future                     |
| 2017 | GROMACS | Task    | In Progress           | Normal   | Modularize simulation option storage and reading from mdp files                      | Christian Blau | 04/06/2018 06:07 PM | future                     |
| 2984 | GROMACS | Feature | New                   | Normal   | More Extensive Selections Examples   | Dallas Warren  | 06/18/2019 11:50 PM |                            |
| 1221 | GROMACS | Feature | Accepted              | Normal   | More generic position mapping for selections   |                | 06/10/2014 02:58 PM | future                     |
| 2139 | GROMACS | Feature | New                   | Normal   | More precise/explicit documentation conventions                                      |                | 01/07/2018 11:54 PM |                            |
| 2118 | GROMACS | Feature | New                   | Low      | More verbose comments requested in header of gmx distance -xyz                       |                | 02/08/2017 05:46 AM |                            |
| 2999 | GROMACS | Task    | New                   | Normal   | Move all logging in core library and tools to use MDLogger                           |                | 09/06/2019 02:36 PM | 2021-infrastructure-stable |
| 3255 | GROMACS | Task    | New                   | Normal   | Move benchmarking options from mdrun to a dedicated tool                             |                | 12/19/2019 01:21 PM |                            |
| 3229 | GROMACS | Task    | New                   | Normal   | Move checkpointing to the beginning of the MD step                                   |                | 01/16/2020 04:31 PM | 2021-infrastructure-stable |
| 2178 | GROMACS | Task    | New                   | Normal   | Move checks for specific warnings to source repo                                     |                | 05/12/2017 03:57 PM |                            |
| 3082 | GROMACS | Task    | New                   | High     | move launch/synchronization points to clarify task dependencies                      |                | 12/27/2019 04:21 PM | 2021                       |
| 3005 | GROMACS | Task    | New                   | Normal   | Move logging in gmx preprocess to MDLogger   |                | 06/26/2019 10:01 AM |                            |
| 2097 | GROMACS | Feature | New                   | Low      | Move output of dhd file entirely to edr, rather than having a separate text dhd file |                | 01/05/2017 05:21 PM | future                     |

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