

## Issues

| #    | Project | Tracker | Status      | Priority | Subject   | Assignee      | Updated             | Target version   |
|------|---------|---------|-------------|----------|---|---------------|---------------------|------------------|
| 3326 | GROMACS | Task    | New         | Normal   | Allow changing task assignment  |               | 01/22/2020 09:44 AM | 2021-refactoring |
| 3325 | GROMACS | Task    | New         | Normal   | Allow complete re-initialization of a simulation                                  |               | 01/29/2020 05:13 PM | 2021-refactoring |
| 3330 | GROMACS | Task    | New         | Normal   | Compile list of codepaths for testing task assignment                             |               | 01/22/2020 10:03 AM | 2021-refactoring |
| 3295 | GROMACS | Feature | New         | Normal   | Expand gmxapi.modify_input use cases.   | Eric Irrgang  | 01/16/2020 05:13 PM | 2021-refactoring |
| 3329 | GROMACS | Task    | New         | Normal   | Extend energy comparison testing framework  |               | 01/22/2020 09:51 AM | 2021-refactoring |
| 3307 | GROMACS | Feature | New         | Normal   | General interface for communication between simulation ranks                      |               | 01/22/2020 03:22 PM | 2021-refactoring |
| 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 |
| 2967 | GROMACS | Feature | New         | Normal   | GPU reallocateDeviceBuffer improvements   |               | 01/23/2020 12:15 PM | 2021-refactoring |
| 3416 | GROMACS | Task    | New         | Normal   | Port post-submit matrix to Gitlab CI  | Joe Jordan    | 03/16/2020 05:50 PM | 2021-refactoring |
| 3415 | GROMACS | Task    | New         | Normal   | Port Pre-submit matrix to Gitlab CI   | Szilárd Páll  | 03/23/2020 10:09 AM | 2021-refactoring |
| 3327 | GROMACS | Task    | New         | Normal   | Refactor workload flags   |               | 01/22/2020 09:45 AM | 2021-refactoring |
| 3324 | GROMACS | Task    | New         | Normal   | Rework CMake handling of GPU code   |               | 01/22/2020 09:52 AM | 2021-refactoring |
| 3374 | GROMACS | Feature | New         | Normal   | SimulationInput abstraction   |               | 03/03/2020 05:32 PM | 2021-refactoring |
| 3328 | GROMACS | Feature | New         | Normal   | Testing framework for task assignment   |               | 01/22/2020 09:48 AM | 2021-refactoring |
| 3321 | GROMACS | Task    | Accepted    | Normal   | Add D2D wrapper   | Artem Zhmurov | 01/22/2020 09:50 AM | 2021-refactoring |
| 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 |
| 3316 | GROMACS | Task    | Accepted    | Normal   | Context and Stream manager  | Artem Zhmurov | 01/22/2020 09:49 AM | 2021-refactoring |
| 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 |
| 3033 | GROMACS | Task    | In Progress | Normal   | Clean up and modernize googletest bundling and usage                              |               | 01/16/2020 04:50 PM | 2021-refactoring |
| 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 |
| 2756 | GROMACS | Task    | In Progress | Normal   | gmxapi integration testing  |               | 01/16/2020 05:12 PM | 2021-refactoring |
| 3311 | GROMACS | Feature | In Progress | Normal   | GPU infrastructure development  |               | 03/20/2020 09:54 AM | 2021-refactoring |
| 3320 | GROMACS | Task    | In Progress | Normal   | Remove duplicating D2H/H2D wrappers in NBNXM                                      | Artem Zhmurov | 01/22/2020 09:50 AM | 2021-refactoring |
| 3323 | GROMACS | Task    | In Progress | Normal   | Rework the StatePropagatorDataGpu   | Artem Zhmurov | 01/22/2020 09:50 AM | 2021-refactoring |
| 3319 | GROMACS | Task    | In Progress | Normal   | Use DeviceBuffer instead of native GPU types in NBNXM                             | Artem Zhmurov | 01/22/2020 09:49 AM | 2021-refactoring |
| 3318 | GROMACS | Feature | In Progress | Normal   | Use wrappers for the GPU buffer copy/allocations                                  | Artem Zhmurov | 01/23/2020 12:01 PM | 2021-refactoring |
| 3317 | GROMACS | Task    | Resolved    | Normal   | Improve testing of the GPU code   | Artem Zhmurov | 10/06/2020 12:15 PM | 2021-refactoring |
| 3315 | GROMACS | Task    | Resolved    | Normal   | Platform agnostic DeviceContext   | Artem Zhmurov | 03/11/2020 04:15 PM | 2021-refactoring |
| 3314 | GROMACS | Task    | Resolved    | Normal   | Platform agnostic DeviceStream  | Artem Zhmurov | 03/20/2020 09:55 AM | 2021-refactoring |

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|------|---------|---------|-----------------|----------|---|---------------------|---------------------|----------------------------|
| 3290 | GROMACS | Task    | Resolved        | Normal   | Require CMake >= 3.12   |                     | 04/14/2020 02:45 PM | 2021-refactoring           |
| 2896 | GROMACS | Feature | Feedback wanted | Normal   | Python packaging  |                     | 01/16/2020 07:11 PM | 2021-refactoring           |
| 3266 | GROMACS | Bug     | New             | High     | gmx density show wrong symmetrize density profile using -symm?                                  | Super duper         | 02/28/2020 08:24 AM | 2020.2                     |
| 3334 | GROMACS | Bug     | New             | Normal   | Check for DD when increasing rlist is broken  | Berk Hess           | 02/25/2020 03:28 PM | 2020.2                     |
| 2958 | GROMACS | Bug     | New             | Normal   | Compiling master (to become 2020) using CUDA 9.0  |                     | 03/02/2020 03:57 PM | 2020.2                     |
| 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                     |
| 3050 | GROMACS | Bug     | New             | Low      | Fix tests on Solaris  | Vedran Miletic      | 02/27/2020 11:05 AM | 2020.2                     |
| 3361 | GROMACS | Task    | New             | Normal   | Gitlab source archive contains files from build directory                                       | Paul Bauer          | 02/25/2020 10:13 AM | 2020.2                     |
| 3294 | GROMACS | Bug     | New             | Normal   | multiple tests fail on fedora 31  | Paul Bauer          | 02/28/2020 03:12 PM | 2020.2                     |
| 2974 | GROMACS | Bug     | New             | Normal   | position-restraints regressiontest fails on intel GPU with OpenCL                               |                     | 02/25/2020 03:52 PM | 2020.2                     |
| 2667 | GROMACS | Feature | New             | Normal   | Suggested steps for calculating entropy in solution and binding                                 | David van der Spoel | 03/01/2020 01:35 PM | 2020.2                     |
| 2723 | GROMACS | Task    | New             | Normal   | Update mdrun-performance.rst to clearly express the nature of task                              | Joe Jordan          | 02/27/2020 11:07 AM | 2020.2                     |
| 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                     |
| 3408 | GROMACS | Bug     | Fix uploaded    | Normal   | Gmxapi* tests segfault in rpmbuild  | Eric Irrgang        | 03/23/2020 01:27 PM | 2020.2                     |
| 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                     |
| 3441 | GROMACS | Bug     | Resolved        | Normal   | Ewald surface-epsilon is incorrect  | Berk Hess           | 03/18/2020 11:15 PM | 2020.2                     |
| 3380 | GROMACS | Bug     | Resolved        | Low      | IBM VSX checks fail with gcc-10   | Erik Lindahl        | 04/30/2020 01:30 PM | 2020.2                     |
| 3125 | GROMACS | Bug     | Resolved        | Normal   | OpenCL on Volta and Turing broken   |                     | 02/27/2020 11:01 AM | 2020.2                     |
| 3021 | GROMACS | Feature | Feedback wanted | Normal   | Completion of docs for GPU developments   |                     | 03/02/2020 03:58 PM | 2020.2                     |
| 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 |
| 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 |
| 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 |
| 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 |
| 3264 | GROMACS | Task    | New             | Normal   | Break up MdrunMpiTests  | Paul Bauer          | 12/23/2019 11:44 AM | 2021-infrastructure-stable |
| 3379 | GROMACS | Feature | New             | Normal   | C++ API for simulation input and output   |                     | 02/28/2020 10:38 AM | 2021-infrastructure-stable |
| 3220 | GROMACS | Task    | New             | Normal   | change rolling pruning scheduling with GPU update   |                     | 02/25/2020 03:41 PM | 2021-infrastructure-stable |
| 3402 | GROMACS | Feature | New             | Normal   | Clarify distinction between public API documentation and developer docs.                        |                     | 02/26/2020 04:16 PM | 2021-infrastructure-stable |

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|------|---------|---------|--------|----------|--|-----------------|---------------------|----------------------------|
| 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 gmx_fatal   |                 | 09/06/2019 02:34 PM | 2021-infrastructure-stable |
| 2994 | GROMACS | Feature | New    | Normal   | Data flow topology in gmxapi 2020  |                 | 12/11/2019 11:33 AM | 2021-infrastructure-stable |
| 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 |
| 3275 | GROMACS | Task    | New    | Normal   | Document Gitlab CI instead of Jenkins and releng   | Paul Bauer      | 03/09/2020 05:55 PM | 2021-infrastructure-stable |
| 3013 | GROMACS | Task    | New    | Normal   | Extend logging levels in MDLogger  |                 | 09/06/2019 02:34 PM | 2021-infrastructure-stable |
| 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 |
| 3150 | GROMACS | Bug     | New    | Normal   | gmxapi data type annotations are confusing and inadequate  | Eric Irrgang    | 10/22/2019 03:08 PM | 2021-infrastructure-stable |
| 3141 | GROMACS | Bug     | New    | Normal   | gmxapi File placeholders missing from beta release   | Eric Irrgang    | 12/10/2019 02:02 PM | 2021-infrastructure-stable |
| 3273 | GROMACS | Bug     | New    | Normal   | gmxapi setup.py complains too much   |                 | 12/27/2019 06:42 PM | 2021-infrastructure-stable |
| 3147 | GROMACS | Feature | New    | Normal   | gmxapi workflow checkpointing  | Eric Irrgang    | 10/15/2019 06:18 PM | 2021-infrastructure-stable |
| 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 |
| 3136 | GROMACS | Bug     | New    | Normal   | gmxapi.operation data flow topology unclear or incomplete  | Eric Irrgang    | 12/11/2019 11:25 AM | 2021-infrastructure-stable |
| 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 |
| 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 |
| 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 |

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|------|---------|---------|--------|----------|---|----------------|---------------------|----------------------------|
| 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 |
| 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 |
| 3432 | GROMACS | Feature | New    | Normal   | Implement essential dynamics for modular simulator  | Pascal Merz    | 03/11/2020 12:38 AM | 2021-infrastructure-stable |
| 3430 | GROMACS | Feature | New    | Normal   | Implement NMR restraints for modular simulator  | Pascal Merz    | 03/11/2020 12:28 AM | 2021-infrastructure-stable |
| 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 |
| 3428 | GROMACS | Feature | New    | Normal   | Implement SIMD version of modular simulator propagators                                   | Pascal Merz    | 03/11/2020 12:12 AM | 2021-infrastructure-stable |
| 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 |
| 3363 | GROMACS | Feature | New    | Normal   | Improve FEP testing   | Pascal Merz    | 03/01/2020 03:22 PM | 2021-infrastructure-stable |
| 3394 | GROMACS | Feature | New    | Normal   | improve gmxapi error handling   | Eric Irrgang   | 02/24/2020 11:45 AM | 2021-infrastructure-stable |
| 3038 | GROMACS | Feature | New    | Normal   | Improvements to MD plugin development environment   | Eric Irrgang   | 12/10/2019 01:58 PM | 2021-infrastructure-stable |
| 2795 | GROMACS | Task    | New    | Normal   | Incorporate regressiontests into core gromacs   |                | 12/02/2019 01:44 PM | 2021-infrastructure-stable |
| 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 |
| 3130 | GROMACS | Task    | New    | Normal   | Interim handling of gmxapi data references.   | Eric Irrgang   | 12/11/2019 11:26 AM | 2021-infrastructure-stable |
| 3260 | GROMACS | Task    | New    | Low      | keep up to with mdspan reference implementation   | Christian Blau | 12/20/2019 01:16 PM | 2021-infrastructure-stable |
| 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 |
| 3417 | GROMACS | Feature | New    | Normal   | Make modular simulator feature-complete   | Pascal Merz    | 03/23/2020 03:57 AM | 2021-infrastructure-stable |
| 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 |
| 3229 | GROMACS | Task    | New    | Normal   | Move checkpointing to the beginning of the MD step  |                | 01/16/2020 04:31 PM | 2021-infrastructure-stable |
| 3096 | GROMACS | Task    | New    | Normal   | Multiple time-stepping: correct coupling algorithms, virial calculation and energy output | Christian Blau | 09/18/2019 02:18 PM | 2021-infrastructure-stable |
| 3411 | GROMACS | Bug     | New    | Normal   | Nightly master release build failure  |                | 03/06/2020 11:44 AM | 2021-infrastructure-stable |
| 3401 | GROMACS | Feature | New    | Normal   | Policy and procedure for installed headers (public API)                                   |                | 02/26/2020 04:17 PM | 2021-infrastructure-stable |
| 3272 | GROMACS | Task    | New    | Normal   | Port complete CI testing to Gitlab  | Paul Bauer     | 02/27/2020 11:04 AM | 2021-infrastructure-stable |
| 3035 | GROMACS | Task    | New    | Normal   | Provide central logger in wrapper binary  | Paul Bauer     | 09/06/2019 02:34 PM | 2021-infrastructure-stable |
| 3419 | GROMACS | Task    | New    | Normal   | Reduce / remove use of legacy t_state objects throughout modular simulator                | Pascal Merz    | 03/10/2020 10:24 PM | 2021-infrastructure-stable |
| 2396 | GROMACS | Task    | New    | Normal   | Refactor trajectoryanalysis module to allow handling of trajectory frame manipulation     | Paul Bauer     | 12/02/2019 01:24 PM | 2021-infrastructure-stable |

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| 3274 | GROMACS | Bug     | New         | Normal   | Remove ARM NEON SIMD  |                | 12/28/2019 07:53 AM | 2021-infrastructure-stable |
| 3180 | GROMACS | Task    | New         | Normal   | Remove extra D2H and H2D copies of coordinates when the COM motion is compensated.                    | Artem Zhmurov  | 02/14/2020 12:45 PM | 2021-infrastructure-stable |
| 3197 | GROMACS | Bug     | New         | Normal   | Rework usage of gitattributes and filter in source code formatting scripts                            |                | 11/04/2019 12:50 PM | 2021-infrastructure-stable |
| 3148 | GROMACS | Feature | New         | Normal   | Roadmap for gmxapi filesystem interactions.   | Eric Irrgang   | 10/15/2019 06:23 PM | 2021-infrastructure-stable |
| 3235 | GROMACS | Task    | New         | Normal   | Run mdrun-test in parallel and make sure they tests test critical quantities like energy conservation | Christian Blau | 12/12/2019 03:46 PM | 2021-infrastructure-stable |
| 3171 | GROMACS | Task    | New         | Normal   | schedule CPU H2D force contribution in separate stream  |                | 12/20/2019 08:33 AM | 2021-infrastructure-stable |
| 3076 | GROMACS | Task    | New         | Normal   | Selectively activate MdModules during simulation instead of instantiating all of them                 | Christian Blau | 01/17/2020 02:40 PM | 2021-infrastructure-stable |
| 3426 | GROMACS | Feature | New         | Normal   | Support acceleration in modular simulator   | Pascal Merz    | 03/11/2020 04:09 PM | 2021-infrastructure-stable |
| 3434 | GROMACS | Feature | New         | Normal   | Support box deformation in modular simulator  | Pascal Merz    | 03/11/2020 12:50 AM | 2021-infrastructure-stable |
| 3131 | GROMACS | Task    | New         | Normal   | support ccache with clang-tidy  | Mark Abraham   | 12/20/2019 08:20 AM | 2021-infrastructure-stable |
| 3427 | GROMACS | Feature | New         | Normal   | Support freeze groups in modular simulator  | Pascal Merz    | 03/11/2020 12:07 AM | 2021-infrastructure-stable |
| 2699 | GROMACS | Task    | New         | Normal   | Test POWER9   |                | 12/04/2019 03:29 PM | 2021-infrastructure-stable |
| 3392 | GROMACS | Task    | New         | Low      | Unify box correction for modular simulator  | Pascal Merz    | 03/11/2020 05:20 PM | 2021-infrastructure-stable |
| 3420 | GROMACS | Task    | New         | Normal   | Unify force and shellfc elements for modular simulator  | Pascal Merz    | 03/10/2020 09:50 PM | 2021-infrastructure-stable |
| 2481 | GROMACS | Task    | New         | Low      | Update gmx report-methods to write more method information  |                | 12/02/2019 01:22 PM | 2021-infrastructure-stable |
| 2833 | GROMACS | Task    | New         | Normal   | Update topology datastructures  | Paul Bauer     | 12/02/2019 01:43 PM | 2021-infrastructure-stable |
| 3288 | GROMACS | Feature | New         | Normal   | Use build system infrastructure instead of custom scripts to manage API levels.                       |                | 02/26/2020 04:16 PM | 2021-infrastructure-stable |
| 3437 | GROMACS | Task    | New         | Normal   | Use builders to prepare modules   | Pascal Merz    | 03/11/2020 07:05 AM | 2021-infrastructure-stable |
| 3072 | GROMACS | Task    | New         | Normal   | Use gmx::index for indexing instead of int  | Christian Blau | 09/03/2019 04:23 PM | 2021-infrastructure-stable |
| 3113 | GROMACS | Bug     | New         | Low      | Use of read_tps_conf is depeccated  | Paul Bauer     | 10/01/2019 11:36 AM | 2021-infrastructure-stable |
| 3183 | GROMACS | Task    | Accepted    | Normal   | enable bonded interactions on GPU   |                | 12/20/2019 08:32 AM | 2021-infrastructure-stable |
| 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 |
| 2706 | GROMACS | Task    | Accepted    | Normal   | Rework classic QM/MM interface  |                | 12/02/2019 01:45 PM | 2021-infrastructure-stable |
| 2875 | GROMACS | Task    | Accepted    | Normal   | SIMD version of the free-energy kernel  | Berk Hess      | 12/02/2019 01:44 PM | 2021-infrastructure-stable |
| 3203 | GROMACS | Task    | Accepted    | Normal   | Tools should check that input is valid when first using it  | Paul Bauer     | 12/03/2019 05:26 PM | 2021-infrastructure-stable |
| 3155 | GROMACS | Task    | Accepted    | Normal   | Unify DD and CPU-GPU gather & scatter   | Artem Zhmurov  | 10/17/2019 03:50 PM | 2021-infrastructure-stable |
| 2395 | GROMACS | Task    | In Progress | Normal   | break up commrec  | Mark Abraham   | 12/15/2019 11:51 AM | 2021-infrastructure-stable |
| 3133 | GROMACS | Task    | In Progress | Normal   | Cookiecutter for sample_restraint   | Eric Irrgang   | 12/10/2019 01:59 PM | 2021-infrastructure-stable |
| 2698 | GROMACS | Task    | In Progress | Normal   | gmxapi documentation integration  |                | 01/29/2020 03:59 PM | 2021-infrastructure-stable |

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| 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 |
| 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 |
| 3093 | GROMACS | Task    | In Progress     | High     | rework GPU direct halo-exchange related force reduction complexities              |                  | 02/14/2020 11:35 AM | 2021-infrastructure-stable |
| 3010 | GROMACS | Task    | In Progress     | Normal   | upgrade OpenCL stack on bs-gpu01  |                  | 12/20/2019 08:25 AM | 2021-infrastructure-stable |
| 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 |
| 3271 | GROMACS | Task    | Resolved        | Normal   | Adopt PEP-518 for Python package build system configuration.                      |                  | 04/09/2020 10:15 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 |
| 3422 | GROMACS | Task    | Resolved        | Normal   | Implement modular checkpointing for modular simulator                             | Pascal Merz      | 09/16/2020 09:45 AM | 2021-infrastructure-stable |
| 3297 | GROMACS | Task    | Resolved        | Normal   | Require gcc > 5   |                  | 04/30/2020 11:00 AM | 2021-infrastructure-stable |
| 2998 | GROMACS | Task    | Resolved        | Normal   | Update Python detection   |                  | 04/23/2020 04:45 PM | 2021-infrastructure-stable |
| 3032 | GROMACS | Feature | Feedback wanted | Normal   | Clean up dev-manual structure   |                  | 12/11/2019 11:27 AM | 2021-infrastructure-stable |
| 3224 | GROMACS | Task    | New             | Normal   | add regression test case large enough to miscalculated GPU grid launch cases      |                  | 12/20/2019 01:18 PM | 2021                       |
| 3064 | GROMACS | Task    | New             | Normal   | add test for perturbed bonded forces  |                  | 12/27/2019 04:22 PM | 2021                       |
| 2686 | GROMACS | Task    | New             | Normal   | add tests for gpu bonded interactions   |                  | 12/27/2019 04:40 PM | 2021                       |
| 3062 | GROMACS | Task    | New             | Normal   | add twin cut-off mdrun test   |                  | 12/27/2019 04:22 PM | 2021                       |
| 3277 | GROMACS | Feature | New             | Normal   | Allow testing feature that is partly implemented                                  |                  | 12/31/2019 12:44 PM | 2021                       |
| 2987 | GROMACS | Bug     | New             | Normal   | assess the bonded GPU task assignment default                                     |                  | 12/20/2019 01:06 PM | 2021                       |
| 2976 | GROMACS | Task    | New             | Normal   | Basic math for Multidimensional arrays  |                  | 12/27/2019 04:37 PM | 2021                       |
| 2695 | GROMACS | Task    | New             | Low      | bonded GPU module timing  |                  | 12/27/2019 04:40 PM | 2021                       |
| 2770 | GROMACS | Task    | New             | Normal   | change branch maintenance policy  |                  | 01/16/2020 05:09 PM | 2021                       |
| 3119 | GROMACS | Task    | New             | Normal   | clang-tidy coverage of parallelizaton codepaths                                   |                  | 12/27/2019 04:20 PM | 2021                       |
| 3371 | GROMACS | Feature | New             | Normal   | Control FEP using AWH   | Magnus Lundborg  | 02/06/2020 02:20 PM | 2021                       |
| 3031 | GROMACS | Task    | New             | Normal   | evaluate the impact of particle order on PME                                      |                  | 12/27/2019 04:29 PM | 2021                       |
| 3001 | GROMACS | Task    | New             | Normal   | explore simplifying virial and shift force reduction                              |                  | 12/27/2019 04:30 PM | 2021                       |
| 3356 | GROMACS | Task    | New             | Normal   | Expose setting of random seed to API  |                  | 01/29/2020 06:16 PM | 2021                       |
| 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                       |
| 3104 | GROMACS | Task    | New             | Normal   | implement GPU DD cycle counting   |                  | 12/27/2019 04:21 PM | 2021                       |

| #    | Project | Tracker | Status   | Priority | Subject   | Assignee            | Updated             | Target version |
|------|---------|---------|----------|----------|---|---------------------|---------------------|----------------|
| 3105 | GROMACS | Task    | New      | Normal   | implement GPU PME/PP comm cycle counting  |                     | 12/27/2019 04:20 PM | 2021           |
| 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           |
| 2353 | GROMACS | Task    | New      | Normal   | improve on relative tolerance for constructing tables   |                     | 12/20/2019 12:12 PM | 2021           |
| 2997 | GROMACS | Task    | New      | Normal   | improve performance of alchemical free energy calculations  |                     | 12/27/2019 04:31 PM | 2021           |
| 1587 | GROMACS | Task    | New      | Normal   | improve the configurability of regression tests   |                     | 12/20/2019 12:02 PM | 2021           |
| 2936 | GROMACS | Task    | New      | Normal   | introduce check that CPU-GPU transfers/assignments are made between compatible types                    |                     | 02/05/2020 03:57 PM | 2021           |
| 2839 | GROMACS | Task    | New      | Normal   | make module and file naming consistent  |                     | 01/16/2020 05:11 PM | 2021           |
| 2475 | GROMACS | Task    | New      | Normal   | make OpenCL 1st class-citizen in the build system   |                     | 12/20/2019 12:14 PM | 2021           |
| 3082 | GROMACS | Task    | New      | High     | move launch/synchronization points to clarify task dependencies   |                     | 12/27/2019 04:21 PM | 2021           |
| 3143 | GROMACS | Task    | New      | Normal   | move the non-force accumulation/accounting tasks out of the GPU wait functions                          | Szilárd Páll        | 12/27/2019 04:16 PM | 2021           |
| 2832 | GROMACS | Bug     | New      | Low      | PaddedVector move operations broken   | Mark Abraham        | 12/28/2019 10:40 AM | 2021           |
| 2480 | GROMACS | Bug     | New      | Normal   | pdb2gmx does not protonate correctly for united-atom Gromos   | Mark Abraham        | 12/20/2019 12:17 PM | 2021           |
| 2224 | GROMACS | Feature | New      | Normal   | Proposed feature: conditional stop  | Vedran Miletic      | 12/20/2019 12:11 PM | 2021           |
| 3410 | GROMACS | Feature | New      | Normal   | Random Acceleration Molecular Dynamics (RAMD)   | Bernd Doser         | 03/05/2020 03:22 PM | 2021           |
| 3057 | GROMACS | Task    | New      | Normal   | re-enable fusion on Power8/9  | Szilárd Páll        | 12/27/2019 04:22 PM | 2021           |
| 2774 | GROMACS | Feature | New      | Normal   | Refactor shell code into its own integrator   | David van der Spoel | 12/27/2019 04:05 PM | 2021           |
| 2053 | GROMACS | Task    | New      | Normal   | refine notation in GPU code   |                     | 12/20/2019 01:04 PM | 2021           |
| 2169 | GROMACS | Task    | New      | Normal   | remove 'continuation' mdp option  |                     | 12/29/2019 10:31 AM | 2021           |
| 2944 | GROMACS | Feature | New      | Normal   | Roadmap for thermostats / barostats in new propagation/integration scheme                               | Michael Shirts      | 12/27/2019 04:00 PM | 2021           |
| 2710 | GROMACS | Feature | New      | Normal   | Separate dvdI for each molecule (of couple-moltype) when running FEP                                    |                     | 12/27/2019 04:41 PM | 2021           |
| 3124 | GROMACS | Bug     | New      | Normal   | significant performance loss due to DLB auto-off when PP/PME load >1                                    |                     | 01/28/2020 02:44 PM | 2021           |
| 2806 | GROMACS | Feature | New      | Normal   | SIMD algorithms for ARM SVE // nobbonded cluster and others   |                     | 12/27/2019 03:59 PM | 2021           |
| 2425 | GROMACS | Task    | New      | Normal   | testing multisim with multiple ranks per simulation   | Mark Abraham        | 12/20/2019 12:13 PM | 2021           |
| 2877 | GROMACS | Task    | New      | Normal   | use gmX::Options more   | Mark Abraham        | 12/20/2019 01:22 PM | 2021           |
| 3008 | GROMACS | Task    | New      | Normal   | verify block size choice of CUDA bonded kernel  |                     | 12/27/2019 04:30 PM | 2021           |
| 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           |
| 1943 | GROMACS | Task    | Accepted | Low      | make sure releases are submitted early for Debian Experimental  | Szilárd Páll        | 12/20/2019 12:05 PM | 2021           |

| #    | Project           | Tracker | Status          | Priority | Subject  | Assignee        | Updated             | Target version |
|------|-------------------|---------|-----------------|----------|--|-----------------|---------------------|----------------|
| 2495 | GROMACS           | Task    | Accepted        | Normal   | replace -noconfout with mdp option   | Mark Abraham    | 12/28/2019 10:39 AM | 2021           |
| 2675 | GROMACS           | Task    | In Progress     | Normal   | bonded CUDA offload task   |                 | 02/12/2020 05:54 PM | 2021           |
| 2834 | GROMACS           | Task    | In Progress     | Normal   | C++ matrix classes   | Christian Blau  | 12/29/2019 10:32 AM | 2021           |
| 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           |
| 2890 | GROMACS           | Feature | In Progress     | Normal   | GPU Halo Exchange  |                 | 02/14/2020 12:41 PM | 2021           |
| 868  | GROMACS           | Feature | In Progress     | Normal   | Implement parallelization support to analysis framework                      | Kevin Boyd      | 12/20/2019 11:59 AM | 2021           |
| 2766 | GROMACS           | Task    | In Progress     | Normal   | Improve hardware option selection  | Kevin Boyd      | 12/20/2019 02:34 PM | 2021           |
| 2965 | GROMACS           | Task    | In Progress     | Normal   | Performance of GPU direct communications                                     |                 | 02/14/2020 12:38 PM | 2021           |
| 1925 | GROMACS           | Task    | In Progress     | Normal   | remove concept of unilateral global communication                            |                 | 12/29/2019 10:35 AM | 2021           |
| 2059 | GROMACS           | Task    | In Progress     | Normal   | Separate different types of data in t_state                                  |                 | 12/27/2019 04:42 PM | 2021           |
| 1985 | GROMACS           | Bug     | Fix uploaded    | Low      | CUDA build system refactoring awaiting review                                |                 | 12/20/2019 12:07 PM | 2021           |
| 2453 | GROMACS           | Task    | Resolved        | High     | PME OpenCL porting effort  | Aleksei lupinov | 12/20/2019 12:18 PM | 2021           |
| 3283 | GROMACS           | Feature | Resolved        | Normal   | Support for the string method with swarms of trajectories in GROMACS         |                 | 03/01/2020 01:16 PM | 2021           |
| 2390 | GROMACS           | Bug     | Feedback wanted | Normal   | GROMACS build system should check for valid nvcc flags before use            |                 | 12/20/2019 12:13 PM | 2021           |
| 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 |                |
| 3300 | GROMACS           | Task    | New             | Normal   | Abandon docs/OpenCLTODOList.txt?   |                 | 01/15/2020 02:46 PM |                |
| 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 |                |
| 2928 | GROMACS           | Feature | New             | Normal   | Add ability to use expression "count of ATOM_EXPR" in selection statements.  |                 | 04/16/2019 04:52 PM |                |
| 687  | Support Platforms | Feature | New             | Normal   | Add content on the front page  |                 | 09/02/2019 01:08 PM |                |
| 2185 | GROMACS           | Task    | New             | Normal   | add docs on MPI + CUDA w/wo MPS  |                 | 05/24/2017 05:17 PM |                |
| 2080 | GROMACS           | Feature | New             | Normal   | add grompp warning for suitability for domain decomposition                  |                 | 11/23/2016 03:03 PM |                |
| 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 nbxn tests   | Mark Abraham    | 06/09/2014 08:36 PM |                |
| 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 |                |
| 2429 | GROMACS           | Feature | New             | Normal   | Add option of periodic chain topology to pdb2gmx                             |                 | 03/10/2018 01:01 PM |                |



| #    | Project | Tracker | Status | Priority | Subject  | Assignee         | Updated             | Target version |
|------|---------|---------|--------|----------|--|------------------|---------------------|----------------|
| 3369 | GROMACS | Feature | New    | Normal   | Add quote about "the truth"  |                  | 02/05/2020 05:08 PM |                |
| 1641 | GROMACS | Feature | New    | Normal   | Add toolchain file for Cray systems  |                  | 06/06/2015 11:24 PM |                |
| 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 |                |
| 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 |                |
| 2855 | GROMACS | Task    | New    | Normal   | Allow compiling GROMACS without C compiler   |                  | 01/10/2020 12:06 PM |                |
| 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 |                |
| 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 |                |
| 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 |                |
| 2478 | GROMACS | Task    | New    | Low      | avoid use of getenv in static initialization   |                  | 04/13/2018 11:57 AM |                |
| 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 |                |
| 2657 | GROMACS | Bug     | New    | Normal   | Biphasic tutorial  |                  | 09/28/2018 10:02 AM |                |
| 3443 | GROMACS | Bug     | New    | Normal   | Bonded GPU kernel performance regression with 2020   |                  | 03/15/2020 08:15 PM |                |
| 1634 | GROMACS | Feature | New    | Normal   | Boxed Molecular Dynamics   |                  | 11/04/2014 04:40 PM |                |
| 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 |                |
| 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 |                |

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|------|---------|---------|--------|----------|---|---------------------|---------------------|----------------|
| 3233 | GROMACS | Bug     | New    | Normal   | clang-format incorrectly aligning altered function arguments  |                     | 12/13/2019 12:41 PM |                |
| 3179 | GROMACS | Feature | New    | Normal   | Clarify access to parallel data outputs   | Eric Irrgang        | 10/26/2019 12:23 PM |                |
| 2375 | GROMACS | Task    | New    | Normal   | Clarify execution phases for MD simulation  |                     | 04/30/2019 12:59 PM |                |
| 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 |                |
| 3000 | GROMACS | Bug     | New    | Normal   | CMake "webpage" target does not fail when it should   |                     | 06/25/2019 02:43 PM |                |
| 2949 | GROMACS | Bug     | New    | Normal   | cmake fails when building mdrun only  |                     | 07/08/2019 10:04 AM |                |
| 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 |                |
| 3166 | GROMACS | Bug     | New    | Normal   | Compilation failing on Ubuntu 19.04 with Cuda 10.1  |                     | 10/19/2019 09:13 PM |                |
| 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 |                |
| 3002 | GROMACS | Task    | New    | Normal   | consider splitting bonded work into local/nonlocal  |                     | 06/25/2019 04:06 PM |                |
| 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 |                |
| 2060 | GROMACS | Feature | New    | Normal   | Convert enum to enum class  |                     | 10/17/2016 05:27 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 |                |
| 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 |                |

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|------|---------|---------|--------|----------|---|---------------------|---------------------|----------------|
| 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 |                |
| 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 |                |
| 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 |                |
| 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 |                |
| 3287 | GROMACS | Task    | New    | Normal   | Deprecate make_ndx, use select instead  |                     | 01/23/2020 01:16 PM |                |
| 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 |                |
| 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 |                |
| 3353 | GROMACS | Task    | New    | Normal   | Document gmx densmap output   |                     | 01/23/2020 12:52 PM |                |
| 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 |                |
| 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 |                |
| 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 |                |
| 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 |                |

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|------|-------------------|---------|--------|----------|---|------------------------|---------------------|----------------|
| 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 |                |
| 1849 | GROMACS           | Feature | New    | Normal   | expanded ensemble -- Adaptive Integration Method  | Christopher Mirabzadeh | 07/11/2016 08:01 PM |                |
| 1246 | GROMACS           | Task    | New    | Normal   | expanded ensemble .tpr cannot be rerun  | Michael Shirts         | 06/19/2015 01:56 PM |                |
| 3196 | GROMACS           | Bug     | New    | Normal   | ExponentialMovingAverage.DeterminesCorrectlyIfIncreasing failing  |                        | 11/01/2019 11:28 PM |                |
| 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 |                |
| 987  | Support Platforms | Feature | New    | Normal   | Feature wishlist should be moved to Redmine   |                        | 08/03/2012 12:22 PM |                |
| 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 |                |
| 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 |                |
| 3075 | GROMACS           | Bug     | New    | Normal   | Frozen atoms are moving   | Erik Lindahl           | 12/27/2019 10:51 AM |                |
| 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 |                |
| 1829 | GROMACS           | Task    | New    | Normal   | Future of thread level parallelism  |                        | 11/18/2016 05:29 PM |                |
| 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 |                |
| 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 |                |
| 2149 | Support Platforms | Bug     | New    | Normal   | gerrit server excessive CPU usage   |                        | 04/05/2017 07:25 PM |                |
| 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 |                |
| 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 |                |
| 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 |                |
| 1583 | GROMACS           | Bug     | New    | Normal   | gmx msd with mol flag requires excessive memory   |                        | 12/18/2017 03:34 PM |                |

| #    | Project | Tracker | Status | Priority | Subject  | Assignee            | Updated             | Target version |
|------|---------|---------|--------|----------|--|---------------------|---------------------|----------------|
| 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 |                |
| 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 |                |
| 3362 | GROMACS | Feature | New    | Normal   | gmx traj: add an option to plot each component in a separate file  |                     | 01/29/2020 06:18 PM |                |
| 3086 | GROMACS | Bug     | New    | Normal   | gmxapi fails with MPI build of GROMACS 2020  |                     | 09/25/2019 04:18 PM |                |
| 3139 | GROMACS | Task    | New    | Normal   | gmxapi Futures should be subscribable  | Eric Irrgang        | 10/15/2019 03:56 PM |                |
| 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 |                |
| 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 |                |
| 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 |                |
| 2217 | GROMACS | Bug     | New    | Low      | GPU emulation and separate PME ranks doesn't work properly   |                     | 12/12/2017 11:50 AM |                |
| 2464 | GROMACS | Task    | New    | Normal   | GPU performance goals overview   |                     | 03/26/2018 10:42 AM |                |
| 2907 | GROMACS | Bug     | New    | Normal   | Gromacs autocompletion appears to be broken with ZSH   |                     | 07/16/2019 04:46 AM |                |
| 2607 | GROMACS | Bug     | New    | Normal   | Grompp becomes extremely slow when many pull groups are present  |                     | 08/11/2018 08:54 AM |                |
| 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 |                |
| 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 |                |
| 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 |                |

| #    | Project | Tracker | Status | Priority | Subject  | Assignee       | Updated             | Target version |
|------|---------|---------|--------|----------|--|----------------|---------------------|----------------|
| 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 |                |
| 2435 | GROMACS | Task    | New    | Normal   | identify and note about/tune task offload in GPU-bound runs                              |                | 03/02/2018 04:08 PM |                |
| 2521 | GROMACS | Task    | New    | Normal   | Implement alternating PME/NB wait for OpenCL   |                | 10/15/2018 12:39 PM |                |
| 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 |                |
| 2126 | GROMACS | Feature | New    | Normal   | implement native CUDA support in CMake   |                | 10/29/2019 09:03 PM |                |
| 1900 | GROMACS | Feature | New    | Normal   | Implement some new errors in grompp  |                | 06/22/2016 05:20 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 |                |
| 3138 | GROMACS | Feature | New    | Normal   | Improve ensemble support in Context specification.                                       |                | 10/15/2019 03:56 PM |                |
| 838  | GROMACS | Task    | New    | Normal   | Improve generic error reporting routines   |                | 07/11/2016 08:29 PM |                |
| 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 |                |
| 2863 | GROMACS | Task    | New    | Normal   | improve PBC handling   |                | 03/11/2019 04:28 PM |                |
| 2519 | GROMACS | Task    | New    | High     | Improve/remove PME OpenCL kernel barriers  |                | 02/15/2019 06:34 PM |                |
| 2792 | GROMACS | Task    | New    | High     | Improvement of PME gather and spread CUDA kernels  |                | 03/18/2020 03:57 PM |                |
| 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 |                |
| 2393 | GROMACS | Bug     | New    | Normal   | incorrect error message with omitted command line flag before its argument               |                | 01/24/2018 11:24 PM |                |
| 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 |                |
| 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 |                |
| 1562 | GROMACS | Feature | New    | Normal   | introducing a Monte Carlo framework (first application: MC barostat)                     | Michael Shirts | 07/11/2016 08:08 PM |                |
| 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 |                |

| #    | Project           | Tracker | Status | Priority | Subject   | Assignee      | Updated             | Target version |
|------|-------------------|---------|--------|----------|---|---------------|---------------------|----------------|
| 1309 | Support Platforms | Task    | New    | Normal   | Jenkins verification improvements                                   |               | 06/01/2017 02:34 PM |                |
| 1214 | GROMACS           | Task    | New    | Normal   | Keep track of important changes for Changelog                       | Mark Abraham  | 06/26/2013 11:24 AM |                |
| 2248 | GROMACS           | Feature | New    | Normal   | Label all SIMD functions as pure/nodiscard                          |               | 02/04/2019 04:49 AM |                |
| 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 |                |
| 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 |                |
| 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 |                |
| 3357 | GROMACS           | Task    | New    | Normal   | Make sure "colvars" interoperates stably and smoothly with gromacs  |               | 03/04/2020 11:25 AM |                |
| 677  | GROMACS           | Task    | New    | Normal   | Make sure manual uses consistent style throughout                   |               | 06/19/2014 11:49 AM |                |
| 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 |                |
| 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 |                |
| 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 |                |
| 3020 | GROMACS           | Feature | New    | Low      | modernize DeviceBuffer and GPU memory management                    |               | 08/13/2019 06:01 PM |                |
| 2984 | GROMACS           | Feature | New    | Normal   | More Extensive Selections Examples                                  | Dallas Warren | 06/18/2019 11:50 PM |                |
| 2139 | GROMACS           | Feature | New    | Normal   | More precise/explicit documentation conventions                     |               | 01/07/2018 11:54 PM |                |

| #    | Project | Tracker | Status | Priority | Subject   | Assignee     | Updated             | Target version |
|------|---------|---------|--------|----------|---|--------------|---------------------|----------------|
| 2118 | GROMACS | Feature | New    | Low      | More verbose comments requested in header of gmx distance -xyz  |              | 02/08/2017 05:46 AM |                |
| 3255 | GROMACS | Task    | New    | Normal   | Move benchmarking options from mdrun to a dedicated tool  |              | 12/19/2019 01:21 PM |                |
| 2178 | GROMACS | Task    | New    | Normal   | Move checks for specific warnings to source repo  |              | 05/12/2017 03:57 PM |                |
| 3005 | GROMACS | Task    | New    | Normal   | Move logging in gmx preprocess to MDLogger  |              | 06/26/2019 10:01 AM |                |
| 3004 | GROMACS | Task    | New    | Normal   | Move trajectory analysis logging to MDLogger  |              | 06/26/2019 09:59 AM |                |
| 1745 | GROMACS | Task    | New    | Normal   | Moving to C++11 after Gromacs-5.1   |              | 06/01/2016 03:01 PM |                |
| 2084 | GROMACS | Task    | New    | Low      | MPI and stderr/log output   |              | 11/28/2016 06:37 PM |                |
| 3440 | GROMACS | Bug     | New    | Normal   | Multi-nodes run exits with error with openmpi/4.0.0   |              | 03/23/2020 02:10 PM |                |
| 1448 | GROMACS | Bug     | New    | Normal   | multiple successive crashes during REMD can lead to .log files that do not represent the actual replica exchanges to match the .xtc files (complicating demultiplexing) | Mark Abraham | 06/23/2016 03:15 PM |                |
| 2898 | GROMACS | Task    | New    | Low      | Naming common variables   |              | 03/26/2019 11:46 PM |                |
| 2255 | GROMACS | Bug     | New    | Normal   | nstlist override stopped affecting the input parameter listing  |              | 12/17/2017 08:05 AM |                |
| 1530 | GROMACS | Task    | New    | Low      | Offer binary downloads  |              | 06/29/2014 02:58 PM |                |
| 2854 | GROMACS | Bug     | New    | Normal   | OnlineHelpUnitTests segfaults on s390x with gcc-9.0.1   | Paul Bauer   | 02/04/2019 11:17 AM |                |
| 1973 | GROMACS | Task    | New    | Normal   | OpenCL implementation wish list   |              | 05/27/2016 03:42 PM |                |
| 3439 | GROMACS | Feature | New    | Normal   | Optimize successive simulation segments   |              | 03/11/2020 01:42 PM |                |
| 2860 | GROMACS | Feature | New    | Normal   | Option for outputting min/max coordinates in gmx traj   |              | 02/08/2019 12:35 AM |                |
| 3045 | GROMACS | Feature | New    | Low      | Option to remove v-sites in trjconv?  |              | 07/19/2019 04:42 PM |                |
| 2538 | GROMACS | Task    | New    | Normal   | organize more of the PME GPU code along task-specific lines   | Mark Abraham | 05/31/2018 05:41 PM |                |
| 3214 | GROMACS | Bug     | New    | Normal   | Out-of-bounds, overflow and incorrect outputs in gmx spatial  |              | 11/25/2019 04:11 PM |                |
| 2739 | GROMACS | Feature | New    | Normal   | Parallel continuous tempering and enhanced sampling feature   |              | 11/13/2018 11:36 PM |                |
| 950  | GROMACS | Feature | New    | Normal   | Path/directory/filename handling in Gromacs   |              | 07/11/2016 08:24 PM |                |
| 3301 | GROMACS | Bug     | New    | Normal   | pdb2gmx adding hydrogen   |              | 01/15/2020 10:17 PM |                |
| 2232 | GROMACS | Bug     | New    | Normal   | pdb2gmx can't form special bonds with terminal patched atoms  |              | 12/03/2017 01:35 PM |                |
| 731  | GROMACS | Feature | New    | Normal   | pdb2gmx should warn about missing residues when bonds are too long  |              | 06/22/2014 10:55 AM |                |
| 3242 | GROMACS | Feature | New    | Normal   | Please do not remove the -nsteps flag   |              | 03/01/2020 01:59 PM |                |
| 2463 | GROMACS | Task    | New    | Low      | PME GPU decomposition   |              | 03/26/2018 10:42 AM |                |
| 2788 | GROMACS | Bug     | New    | Normal   | PME will not run on AMD GPU with NVidia GPU present   |              | 01/03/2019 02:24 PM |                |
| 2020 | GROMACS | Bug     | New    | Normal   | Possible issue with md-vv integrator  | Mark Abraham | 03/11/2017 08:30 AM |                |
| 1500 | GROMACS | Feature | New    | Normal   | Post-5.0 feature clean-up plan  | Mark Abraham | 08/26/2019 03:47 PM |                |
| 2977 | GROMACS | Feature | New    | Normal   | print DD load balancing improvement   |              | 06/13/2019 10:56 AM |                |



| #    | 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 |                |
| 1635 | GROMACS           | Feature | New    | Normal   | Proper Unicode support  |                | 06/18/2015 08:34 PM |                |
| 3279 | GROMACS           | Task    | New    | Low      | Provide more advice for building client software  |                | 03/02/2020 11:54 AM |                |
| 1106 | Benchmark suite   | Feature | New    | Normal   | publish benchmark numbers   |                | 06/19/2014 12:08 PM |                |
| 2018 | GROMACS           | Feature | New    | Normal   | Pulling along a line between given points   |                | 07/27/2016 09:59 AM |                |
| 1786 | GROMACS           | Task    | New    | Normal   | Python style standards in developer docs  | Peter Kasson   | 12/26/2019 03:15 PM |                |
| 3149 | GROMACS           | Feature | New    | Normal   | Python user interface for obtaining simulation artifacts as files.                              | Eric Irrgang   | 10/15/2019 06:21 PM |                |
| 1934 | GROMACS           | Bug     | New    | Normal   | QMMM with ORCA: memory leaks, buffer overflows and much more                                    |                | 07/10/2016 09:26 AM |                |
| 2003 | GROMACS           | Task    | New    | Normal   | reconsider various simd flags   |                | 07/07/2016 11:23 PM |                |
| 2090 | GROMACS           | Feature | New    | Normal   | redirecting stdout or stderr for testing  | Mark Abraham   | 12/15/2016 03:15 AM |                |
| 2096 | Support Platforms | Bug     | New    | Normal   | Redmine internal error with special characters  |                | 05/31/2017 08:48 PM |                |
| 1509 | GROMACS           | Task    | New    | Low      | Reduce the distance dependence of shifted potentials for free energies if possible              | Michael Shirts | 07/11/2016 08:10 PM |                |
| 2874 | GROMACS           | Task    | New    | Normal   | Refactor Gromacs (cluster) neighborlist into separate module                                    | Erik Lindahl   | 02/28/2019 11:36 AM |                |
| 3040 | GROMACS           | Task    | New    | Normal   | Refactor Restraint module   |                | 07/18/2019 03:59 PM |                |
| 2241 | GROMACS           | Bug     | New    | Low      | refdata can segfault when reading   |                | 09/07/2017 11:57 AM |                |
| 3088 | GROMACS           | Bug     | New    | Normal   | Reference to theory needed for cylindrical pull geometry  |                | 09/13/2019 11:26 AM |                |
| 3116 | GROMACS           | Bug     | New    | Normal   | regressiontests/freenenergy core dumps on ppc64le   | Paul Bauer     | 10/04/2019 10:52 PM |                |
| 3256 | GROMACS           | Task    | New    | Normal   | Remove -nsteps option from mdrun  |                | 12/19/2019 12:12 PM |                |
| 1854 | GROMACS           | Feature | New    | Normal   | Remove all cyclic dependencies  |                | 05/25/2017 08:34 AM |                |
| 2608 | GROMACS           | Task    | New    | Normal   | Remove code duplication between OpenCL and CUDA   |                | 09/24/2018 12:47 PM |                |
| 2670 | GROMACS           | Task    | New    | Low      | remove old/backward compatibility OpenCL support from releng                                    |                | 10/04/2018 06:06 PM |                |
| 3252 | GROMACS           | Task    | New    | Normal   | Remove support for 32 bit architectures   |                | 03/01/2020 02:05 PM |                |
| 3254 | GROMACS           | Task    | New    | Normal   | Remove support for generation of virtual sites to replace aromatic rings in standard residues   |                | 12/19/2019 12:13 PM |                |
| 1456 | GROMACS           | Task    | New    | Low      | remove the use of nbat->alloc/free pointers   | Szilárd Páll   | 06/20/2015 11:53 PM |                |
| 2056 | GROMACS           | Feature | New    | Low      | rename "gmx select"   |                | 10/03/2016 08:24 PM |                |
| 2908 | GROMACS           | Task    | New    | Normal   | Renaming things in nbxnm  | Berk Hess      | 03/28/2019 10:10 AM |                |
| 1842 | GROMACS           | Feature | New    | Normal   | Replace XML with JSON   |                | 01/18/2018 05:12 PM |                |
| 1974 | GROMACS           | Feature | New    | Normal   | Report atom numbers and types in the error message about missed parameters                      |                | 05/30/2016 09:24 AM |                |
| 2220 | GROMACS           | Feature | New    | Normal   | report relevant env var behaviour to console  |                | 07/31/2017 09:40 PM |                |
| 1026 | GROMACS           | Feature | New    | Low      | request for gen_vel to work with multiple temperature coupling groups at different temperatures |                | 11/17/2016 04:39 PM |                |

| #    | Project           | Tracker | Status | Priority | Subject   | Assignee     | Updated             | Target version |
|------|-------------------|---------|--------|----------|---|--------------|---------------------|----------------|
| 2294 | GROMACS           | Task    | New    | Normal   | Require identical hardware on nodes on parallel runs              |              | 11/19/2017 08:54 PM |                |
| 3210 | GROMACS           | Bug     | New    | High     | rerun does not reproduce dVcoul/dl                                |              | 12/27/2019 10:45 AM |                |
| 2564 | GROMACS           | Bug     | New    | Normal   | Result Summary Different For Jobs With Different Numbers of Nodes |              | 07/05/2018 02:39 PM |                |
| 1732 | Support Platforms | Bug     | New    | Normal   | review and extend jenkins tests setups, coverage                  |              | 05/03/2016 05:30 AM |                |
| 2897 | GROMACS           | Bug     | New    | Normal   | rotation/flex2 can still fail on cpu-only run on OpenCL build     |              | 04/04/2019 06:24 PM |                |
| 3030 | GROMACS           | Feature | New    | Normal   | RST style guidelines  |              | 07/09/2019 03:38 PM |                |
| 2956 | GROMACS           | Feature | New    | Normal   | SAXS resolution   |              | 05/17/2019 09:58 AM |                |
| 2993 | GROMACS           | Feature | New    | Normal   | Scalar and structured type expression and definitions for API     | Eric Irrgang | 10/17/2019 09:55 AM |                |
| 2645 | GROMACS           | Bug     | New    | Normal   | Security  |              | 09/28/2018 01:16 PM |                |
| 2981 | GROMACS           | Bug     | New    | Normal   | segfault in opencl build  |              | 06/18/2019 03:30 AM |                |
| 1770 | GROMACS           | Bug     | New    | Normal   | segmentation fault with free energy changes and multiple GPU's    |              | 07/14/2015 03:24 AM |                |

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