

## Issues

| #    | Project | Tracker | Status       | Priority | Subject  | Assignee         | Updated             | Target version             |
|------|---------|---------|--------------|----------|--|------------------|---------------------|----------------------------|
| 3403 | GROMACS | Bug     | Resolved     | Normal   | solvation free energy with couple-intramol set to no                                     |                  | 12/10/2020 02:45 PM |                            |
| 2628 | GROMACS | Bug     | Resolved     | Normal   | GMXRC removes trailing colon from existing MANPATH                                       |                  | 11/02/2020 11:45 AM |                            |
| 3219 | GROMACS | Bug     | Resolved     | Normal   | MANPATH setting is fragile   |                  | 11/02/2020 11:45 AM |                            |
| 2254 | GROMACS | Feature | Resolved     | Normal   | GPU extensions for Google Tests  |                  | 10/06/2020 12:15 PM |                            |
| 3317 | GROMACS | Task    | Resolved     | Normal   | Improve testing of the GPU code  | Artem Zhmurov    | 10/06/2020 12:15 PM | 2021-refactoring           |
| 3422 | GROMACS | Task    | Resolved     | Normal   | Implement modular checkpointing for modular simulator                                    | Pascal Merz      | 09/16/2020 09:45 AM | 2021-infrastructure-stable |
| 2859 | GROMACS | Task    | Resolved     | Normal   | Change ArrayRef iterator type from pointer to std::iterator                              |                  | 06/26/2020 06:15 PM |                            |
| 3041 | GROMACS | Task    | Resolved     | Normal   | Remove workaround for gcc bug 58265  |                  | 06/19/2020 04:45 PM |                            |
| 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                     |
| 3380 | GROMACS | Bug     | Resolved     | Low      | IBM VSX checks fail with gcc-10  | Erik Lindahl     | 04/30/2020 01:30 PM | 2020.2                     |
| 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 |
| 3290 | GROMACS | Task    | Resolved     | Normal   | Require CMake >= 3.12  |                  | 04/14/2020 02:45 PM | 2021-refactoring           |
| 3271 | GROMACS | Task    | Resolved     | Normal   | Adopt PEP-518 for Python package build system configuration.                             |                  | 04/09/2020 10:15 PM | 2021-infrastructure-stable |
| 3154 | GROMACS | Task    | Resolved     | Low      | Update use of Python subprocess for >=3.5  |                  | 04/09/2020 10:15 PM |                            |
| 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 |                            |
| 3440 | GROMACS | Bug     | New          | Normal   | Multi-nodes run exits with error with openmpi/4.0.0                                      |                  | 03/23/2020 02:10 PM |                            |
| 3408 | GROMACS | Bug     | Fix uploaded | Normal   | Gmxapi* tests segfault in rpmbuild   | Eric Irrgang     | 03/23/2020 01:27 PM | 2020.2                     |
| 3415 | GROMACS | Task    | New          | Normal   | Port Pre-submit matrix to Gitlab CI  | Szilárd Páll     | 03/23/2020 10:09 AM | 2021-refactoring           |
| 3417 | GROMACS | Feature | New          | Normal   | Make modular simulator feature-complete  | Pascal Merz      | 03/23/2020 03:57 AM | 2021-infrastructure-stable |
| 3314 | GROMACS | Task    | Resolved     | Normal   | Platform agnostic DeviceStream   | Artem Zhmurov    | 03/20/2020 09:55 AM | 2021-refactoring           |
| 3311 | GROMACS | Feature | In Progress  | Normal   | GPU infrastructure development   |                  | 03/20/2020 09:54 AM | 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           |
| 3446 | GROMACS | Task    | New          | Normal   | apply maintainability updates across all GPU kernels                                     | Jonathan Vincent | 03/19/2020 03:31 PM |                            |
| 3441 | GROMACS | Bug     | Resolved     | Normal   | Ewald surface-epsilon is incorrect   | Berk Hess        | 03/18/2020 11:15 PM | 2020.2                     |
| 2792 | GROMACS | Task    | New          | High     | Improvement of PME gather and spread CUDA kernels  |                  | 03/18/2020 03:57 PM |                            |
| 3445 | GROMACS | Task    | New          | Normal   | create heuristic for c_skipNeutralAtoms  | Jonathan Vincent | 03/17/2020 12:12 PM |                            |
| 3416 | GROMACS | Task    | New          | Normal   | Port post-submit matrix to Gitlab CI   | Joe Jordan       | 03/16/2020 05:50 PM | 2021-refactoring           |

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|------|---------|---------|-----------------|----------|--|---------------|---------------------|----------------------------|
| 3395 | GROMACS | Feature | Feedback wanted | Normal   | Consider scripted composition of Dockerfiles   |               | 03/16/2020 12:16 PM |                            |
| 3443 | GROMACS | Bug     | New             | Normal   | Bonded GPU kernel performance regression with 2020                                     |               | 03/15/2020 08:15 PM |                            |
| 3442 | GROMACS | Bug     | Accepted        | Normal   | continuing mdrun with -deffnm and pulling does not work                                |               | 03/15/2020 08:33 AM |                            |
| 3413 | GROMACS | Bug     | Feedback wanted | Normal   | COMM Removal Failure in GROMACS 2020.1   |               | 03/12/2020 02:31 PM |                            |
| 3392 | GROMACS | Task    | New             | Low      | Unify box correction for modular simulator   | Pascal Merz   | 03/11/2020 05:20 PM | 2021-infrastructure-stable |
| 2522 | GROMACS | Task    | Resolved        | Normal   | OpenCL context duplication   |               | 03/11/2020 04:15 PM | future                     |
| 3315 | GROMACS | Task    | Resolved        | Normal   | Platform agnostic DeviceContext  | Artem Zhmurov | 03/11/2020 04:15 PM | 2021-refactoring           |
| 3426 | GROMACS | Feature | New             | Normal   | Support acceleration in modular simulator  | Pascal Merz   | 03/11/2020 04:09 PM | 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 |
| 3439 | GROMACS | Feature | New             | Normal   | Optimize successive simulation segments  |               | 03/11/2020 01:42 PM |                            |
| 3437 | GROMACS | Task    | New             | Normal   | Use builders to prepare modules  | Pascal Merz   | 03/11/2020 07:05 AM | 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 |
| 3436 | GROMACS | Feature | New             | Normal   | Implement AWH for modular simulator  | Pascal Merz   | 03/11/2020 06:32 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 |
| 3434 | GROMACS | Feature | New             | Normal   | Support box deformation in modular simulator   | Pascal Merz   | 03/11/2020 12:50 AM | 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 |
| 3431 | GROMACS | Feature | New             | Normal   | Implement virtual sites for modular simulator  | Pascal Merz   | 03/11/2020 12:33 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 |
| 3428 | GROMACS | Feature | New             | Normal   | Implement SIMD version of modular simulator propagators                                | Pascal Merz   | 03/11/2020 12:12 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 |
| 3425 | GROMACS | Feature | New             | Normal   | Implement rerun for the modular simulator  | Pascal Merz   | 03/10/2020 11:57 PM | 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 |
| 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 |
| 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 |
| 3418 | GROMACS | Task    | New             | Normal   | Infrastructure improvements for modular simulator                                      | Pascal Merz   | 03/10/2020 10:24 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 |
| 3275 | GROMACS | Task    | New             | Normal   | Document Gitlab CI instead of Jenkins and releng                                       | Paul Bauer    | 03/09/2020 05:55 PM | 2021-infrastructure-stable |
| 3412 | GROMACS | Bug     | New             | Normal   | Domain decomposition problems with Gromacs >2018                                       |               | 03/06/2020 04:10 PM |                            |
| 3411 | GROMACS | Bug     | New             | Normal   | Nightly master release build failure   |               | 03/06/2020 11:44 AM | 2021-infrastructure-stable |

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|------|---------|---------|--------------------|----------|---|---------------------|---------------------|----------------------------|
| 3410 | GROMACS | Feature | New                | Normal   | Random Acceleration Molecular Dynamics (RAMD)   | Bernd Doser         | 03/05/2020 03:22 PM | 2021                       |
| 3385 | GROMACS | Bug     | New                | Normal   | FindLibStdCpp.cmake - wrong sanity check for clang  |                     | 03/04/2020 06:59 PM |                            |
| 3370 | GROMACS | Task    | New                | High     | Further improvements to GPU Buffer Ops and Comms  |                     | 03/04/2020 01:38 PM |                            |
| 3357 | GROMACS | Task    | New                | Normal   | Make sure "colvars" interoperates stably and smoothly with gromacs                              |                     | 03/04/2020 11:25 AM |                            |
| 1852 | GROMACS | Task    | New                | Normal   | Remove group scheme   |                     | 03/03/2020 09:03 PM | future                     |
| 3374 | GROMACS | Feature | New                | Normal   | SimulationInput abstraction   |                     | 03/03/2020 05:32 PM | 2021-refactoring           |
| 3021 | GROMACS | Feature | Feedback wanted    | Normal   | Completion of docs for GPU developments   |                     | 03/02/2020 03:58 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                     |
| 3279 | GROMACS | Task    | New                | Low      | Provide more advice for building client software  |                     | 03/02/2020 11:54 AM |                            |
| 3405 | GROMACS | Bug     | Accepted           | Normal   | intermitted OpenCL regressiontest failures  |                     | 03/02/2020 11:01 AM |                            |
| 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                     |
| 3363 | GROMACS | Feature | New                | Normal   | Improve FEP testing   | Pascal Merz         | 03/01/2020 03:22 PM | 2021-infrastructure-stable |
| 3252 | GROMACS | Task    | New                | Normal   | Remove support for 32 bit architectures   |                     | 03/01/2020 02:05 PM |                            |
| 3242 | GROMACS | Feature | New                | Normal   | Please do not remove the -nsteps flag   |                     | 03/01/2020 01:59 PM |                            |
| 3298 | GROMACS | Feature | New                | Normal   | start early PP work for first dimension of halo exchange  |                     | 03/01/2020 01:36 PM |                            |
| 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                     |
| 3283 | GROMACS | Feature | Resolved           | Normal   | Support for the string method with swarms of trajectories in GROMACS                            |                     | 03/01/2020 01:16 PM | 2021                       |
| 3365 | GROMACS | Task    | New                | Low      | consider making GPU bonded work independent from nonbonded                                      |                     | 03/01/2020 01:11 PM |                            |
| 3294 | GROMACS | Bug     | New                | Normal   | multiple tests fail on fedora 31  | Paul Bauer          | 02/28/2020 03:12 PM | 2020.2                     |
| 3366 | GROMACS | Task    | New                | Normal   | Enforce compability of MdModules  |                     | 02/28/2020 11:20 AM |                            |
| 3379 | GROMACS | Feature | New                | Normal   | C++ API for simulation input and output   |                     | 02/28/2020 10:38 AM | 2021-infrastructure-stable |
| 3266 | GROMACS | Bug     | New                | High     | gmx density show wrong symmetrize density profile using -symm?                                  | Super duper         | 02/28/2020 08:24 AM | 2020.2                     |
| 3285 | GROMACS | Feature | Resolved           | Normal   | Run simulations from the same tpr file with different random seeds                              |                     | 02/27/2020 11:22 PM | future                     |
| 3310 | GROMACS | Bug     | Blocked, need info | Low      | Thread affinity on Mac OS   |                     | 02/27/2020 11:10 PM |                            |
| 3331 | GROMACS | Task    | New                | Low      | Run physical validation tests in Gitlab   | Paul Bauer          | 02/27/2020 11:09 PM | future                     |
| 3309 | GROMACS | Bug     | New                | Normal   | -reprod: checkpoint reading bug and general considerations                                      |                     | 02/27/2020 10:45 PM |                            |
| 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                     |
| 3050 | GROMACS | Bug     | New                | Low      | Fix tests on Solaris  | Vedran Miletic      | 02/27/2020 11:05 AM | 2020.2                     |
| 3272 | GROMACS | Task    | New                | Normal   | Port complete CI testing to Gitlab  | Paul Bauer          | 02/27/2020 11:04 AM | 2021-infrastructure-stable |

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|------|---------|---------|-----------------|----------|--|------------------|---------------------|----------------------------|
| 3125 | GROMACS | Bug     | Resolved        | Normal   | OpenCL on Volta and Turing borken  |                  | 02/27/2020 11:01 AM | 2020.2                     |
| 3249 | GROMACS | Bug     | In Progress     | Low      | cmake bad tests for avx512 on AMD  | Erik Lindahl     | 02/26/2020 05:00 PM |                            |
| 3401 | GROMACS | Feature | New             | Normal   | Policy and procedure for installed headers (public API)                            |                  | 02/26/2020 04:17 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 |
| 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 |
| 3393 | GROMACS | Feature | Resolved        | Normal   | Allow gmxapi.commandline_operation to use STDIN                                    | Eric Irrgang     | 02/25/2020 05:15 PM | 2021-infrastructure-stable |
| 2974 | GROMACS | Bug     | New             | Normal   | position-restraints regressiontest fails on intel GPU with OpenCL                  |                  | 02/25/2020 03:52 PM | 2020.2                     |
| 3220 | GROMACS | Task    | New             | Normal   | change rolling pruning scheduling with GPU update                                  |                  | 02/25/2020 03:41 PM | 2021-infrastructure-stable |
| 3071 | GROMACS | Bug     | Accepted        | Normal   | complex.nbnxn-ljpme-LB-geometric failing with OpenCL timing debug mode assertions  | Szilárd Páll     | 02/25/2020 03:39 PM | 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                     |
| 3398 | GROMACS | Bug     | New             | Normal   | Intermittent failure of non-bonded kernels when run using nvprof                   |                  | 02/25/2020 12:14 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 |
| 3361 | GROMACS | Task    | New             | Normal   | Gitlab source archive contains files from build directory                          | Paul Bauer       | 02/25/2020 10:13 AM | 2020.2                     |
| 3394 | GROMACS | Feature | New             | Normal   | improve gmxapi error handling  | Eric Irrgang     | 02/24/2020 11:45 AM | 2021-infrastructure-stable |
| 3387 | GROMACS | Bug     | New             | Normal   | Death test bug   |                  | 02/20/2020 05:39 PM |                            |
| 3047 | GROMACS | Task    | Feedback wanted | Normal   | Set required versions for GROMACS 2021   |                  | 02/20/2020 11:42 AM |                            |
| 3382 | GROMACS | Task    | Accepted        | Normal   | Split up t_inputrec  |                  | 02/17/2020 05:28 PM |                            |
| 3117 | GROMACS | Feature | New             | Normal   | Coulomb FEP PME on GPU   | Magnus Lundborg  | 02/17/2020 03:58 PM | 2021-infrastructure-stable |
| 2915 | GROMACS | Feature | In Progress     | High     | GPU direct communications  |                  | 02/14/2020 12:48 PM |                            |
| 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 |
| 2890 | GROMACS | Feature | In Progress     | Normal   | GPU Halo Exchange  |                  | 02/14/2020 12:41 PM | 2021                       |
| 2891 | GROMACS | Feature | In Progress     | Normal   | PME/PP GPU communications  |                  | 02/14/2020 12:40 PM |                            |
| 2965 | GROMACS | Task    | In Progress     | Normal   | Performance of GPU direct communications   |                  | 02/14/2020 12:38 PM | 2021                       |
| 3093 | GROMACS | Task    | In Progress     | High     | rework GPU direct halo-exchange related force reduction complexities               |                  | 02/14/2020 11:35 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 |
| 3378 | GROMACS | Feature | New             | Normal   | genion usage without stdin (facilitates use in gmx python api)                     |                  | 02/13/2020 12:04 PM |                            |
| 2675 | GROMACS | Task    | In Progress     | Normal   | bonded CUDA offload task   |                  | 02/12/2020 05:54 PM | 2021                       |
| 3355 | GROMACS | Feature | Accepted        | Normal   | New PME parallel (GPU) scheme  | Jonathan Vincent | 02/12/2020 11:58 AM |                            |

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| 3114 | GROMACS | Feature | New         | Normal   | Improve GPU update-constraints module  | Artem Zhmurov       | 02/10/2020 04:30 PM | 2021                       |
| 2601 | GROMACS | Feature | New         | Normal   | Free energy calculations, soft-core potential  | Vytautas Gapsys     | 02/10/2020 11:29 AM | future                     |
| 1166 | GROMACS | Bug     | New         | Low      | g_order is incorrect for unsaturated carbons   | David van der Spoel | 02/06/2020 02:32 PM | future                     |
| 3371 | GROMACS | Feature | New         | Normal   | Control FEP using AWH  | Magnus Lundborg     | 02/06/2020 02:20 PM | 2021                       |
| 3369 | GROMACS | Feature | New         | Normal   | Add quote about "the truth"  |                     | 02/05/2020 05:08 PM |                            |
| 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                     |
| 2936 | GROMACS | Task    | New         | Normal   | introduce check that CPU-GPU transfers/assignments are made between compatible types                               |                     | 02/05/2020 03:57 PM | 2021                       |
| 3362 | GROMACS | Feature | New         | Normal   | gmx traj: add an option to plot each component in a separate file  |                     | 01/29/2020 06:18 PM |                            |
| 3356 | GROMACS | Task    | New         | Normal   | Expose setting of random seed to API   |                     | 01/29/2020 06:16 PM | 2021                       |
| 3325 | GROMACS | Task    | New         | Normal   | Allow complete re-initialization of a simulation   |                     | 01/29/2020 05:13 PM | 2021-refactoring           |
| 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 |
| 2045 | GROMACS | Task    | New         | Normal   | API design and language bindings   | Peter Kasson        | 01/29/2020 03:59 PM |                            |
| 2698 | GROMACS | Task    | In Progress | Normal   | gmxapi documentation integration   |                     | 01/29/2020 03:59 PM | 2021-infrastructure-stable |
| 3360 | GROMACS | Task    | New         | Normal   | investigate the future of DD dynamic load balancing with GPU offload   |                     | 01/29/2020 11:23 AM |                            |
| 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                       |
| 3287 | GROMACS | Task    | New         | Normal   | Deprecate make_ndx, use select instead   |                     | 01/23/2020 01:16 PM |                            |
| 3353 | GROMACS | Task    | New         | Normal   | Document gmx densmap output  |                     | 01/23/2020 12:52 PM |                            |
| 2967 | GROMACS | Feature | New         | Normal   | GPU reallocateDeviceBuffer improvements  |                     | 01/23/2020 12:15 PM | 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           |
| 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           |
| 3352 | GROMACS | Feature | New         | Normal   | GPU update-constraints feature support   | Artem Zhmurov       | 01/23/2020 11:59 AM | 2021                       |
| 3351 | GROMACS | Feature | New         | Normal   | GPU update-constraints code organization and integration   | 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                       |

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| 3348 | GROMACS | Task    | New         | Normal   | GPU LINCS and SETTLE: unify virial reduction   | Artem Zhmurov | 01/23/2020 11:58 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 |
| 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 |
| 3344 | GROMACS | Task    | New         | Normal   | GPU update-constraints: Better virial reduction.   | Artem Zhmurov | 01/23/2020 11:57 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 |
| 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 |
| 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 |
| 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 |
| 3339 | GROMACS | Task    | New         | Normal   | GPU LINCS: Warp-level synchronization for coupled constraints  | Artem Zhmurov | 01/23/2020 11:55 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 |
| 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 |
| 3308 | GROMACS | Task    | New         | Normal   | GPU update-constraints: Cycle counting for GPU launches  |               | 01/23/2020 11:54 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 |
| 3236 | GROMACS | Task    | New         | Normal   | GPU update-constraints: Pulling support  | Artem Zhmurov | 01/23/2020 11:53 AM | 2021-infrastructure-stable |
| 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 |
| 3307 | GROMACS | Feature | New         | Normal   | General interface for communication between simulation ranks   |               | 01/22/2020 03:22 PM | 2021-refactoring           |
| 3332 | GROMACS | Feature | New         | Normal   | gmx helixorient doesn't have a -tu option to change time unit  |               | 01/22/2020 11:57 AM |                            |
| 3330 | GROMACS | Task    | New         | Normal   | Compile list of codepaths for testing task assignment  |               | 01/22/2020 10:03 AM | 2021-refactoring           |
| 3324 | GROMACS | Task    | New         | Normal   | Rework CMake handling of GPU code  |               | 01/22/2020 09:52 AM | 2021-refactoring           |
| 3329 | GROMACS | Task    | New         | Normal   | Extend energy comparison testing framework   |               | 01/22/2020 09:51 AM | 2021-refactoring           |
| 3323 | GROMACS | Task    | In Progress | Normal   | Rework the StatePropagatorDataGpu  | 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           |

| #    | Project | Tracker | Status             | Priority | Subject   | Assignee       | Updated             | Target version             |
|------|---------|---------|--------------------|----------|---|----------------|---------------------|----------------------------|
| 3321 | GROMACS | Task    | Accepted           | Normal   | Add D2D wrapper   | Artem Zhmurov  | 01/22/2020 09:50 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           |
| 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           |
| 3316 | GROMACS | Task    | Accepted           | Normal   | Context and Stream manager  | Artem Zhmurov  | 01/22/2020 09:49 AM | 2021-refactoring           |
| 3328 | GROMACS | Feature | New                | Normal   | Testing framework for task assignment   |                | 01/22/2020 09:48 AM | 2021-refactoring           |
| 3327 | GROMACS | Task    | New                | Normal   | Refactor workload flags   |                | 01/22/2020 09:45 AM | 2021-refactoring           |
| 3326 | GROMACS | Task    | New                | Normal   | Allow changing task assignment  |                | 01/22/2020 09:44 AM | 2021-refactoring           |
| 3305 | GROMACS | Bug     | New                | Normal   | Case gives FPE with Debug build when GPU update is enabled                            |                | 01/21/2020 05:44 PM |                            |
| 3306 | GROMACS | Task    | New                | Normal   | Document gmx dos tool more clearly  | Christian Blau | 01/20/2020 02:31 PM | future                     |
| 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 |
| 3172 | GROMACS | Feature | New                | Normal   | QM/MM Interface with CP2K   | Dmitry Morozov | 01/17/2020 12:18 PM | future                     |
| 2733 | GROMACS | Bug     | Blocked, need info | Normal   | MdrunUtilityMpiUnitTests timesout on i686 and armv7hl with OpenMPI 2.1.5              | Paul Bauer     | 01/17/2020 08:40 AM |                            |
| 2896 | GROMACS | Feature | Feedback wanted    | Normal   | Python packaging  |                | 01/16/2020 07:11 PM | 2021-refactoring           |
| 3295 | GROMACS | Feature | New                | Normal   | Expand gmxapi.modify_input use cases.   | Eric Irrgang   | 01/16/2020 05:13 PM | 2021-refactoring           |
| 2756 | GROMACS | Task    | In Progress        | Normal   | gmxapi integration testing  |                | 01/16/2020 05:12 PM | 2021-refactoring           |
| 2839 | GROMACS | Task    | New                | Normal   | make module and file naming consistent  |                | 01/16/2020 05:11 PM | 2021                       |
| 2770 | GROMACS | Task    | New                | Normal   | change branch maintenance policy  |                | 01/16/2020 05:09 PM | 2021                       |
| 3033 | GROMACS | Task    | In Progress        | Normal   | Clean up and modernize googletest bundling and usage                                  |                | 01/16/2020 04:50 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           |
| 3229 | GROMACS | Task    | New                | Normal   | Move checkpointing to the beginning of the MD step                                    |                | 01/16/2020 04:31 PM | 2021-infrastructure-stable |
| 3301 | GROMACS | Bug     | New                | Normal   | pdb2gmx adding hydrogen   |                | 01/15/2020 10:17 PM |                            |
| 3240 | GROMACS | Bug     | New                | Normal   | segv with GPU DD direct communication with GPU update and -dlb off                    |                | 01/15/2020 06:16 PM |                            |
| 3300 | GROMACS | Task    | New                | Normal   | Abandon docs/OpenCLTODOList.txt?  |                | 01/15/2020 02:46 PM |                            |
| 2855 | GROMACS | Task    | New                | Normal   | Allow compiling GROMACS without C compiler  |                | 01/10/2020 12:06 PM |                            |
| 3289 | GROMACS | Task    | New                | Normal   | Distinguish identifying and non-identifying inputs to API operations.                 | Eric Irrgang   | 01/10/2020 11:30 AM |                            |
| 3152 | GROMACS | Feature | New                | Normal   | Infrastructure and patterns for expressing public interfaces                          |                | 01/09/2020 05:19 PM | 2021-infrastructure-stable |

| #    | Project | Tracker | Status                | Priority | Subject   | Assignee       | Updated             | Target version             |
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| 3265 | GROMACS | Bug     | Blocked,<br>need info | Low      | regressiontests/complex fails on ppc64le                                | Erik Lindahl   | 01/09/2020 05:00 PM |                            |
| 1347 | GROMACS | Feature | New                   | Normal   | future of tables  | Berk Hess      | 01/09/2020 02:37 PM | future                     |
| 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 |
| 3281 | GROMACS | Bug     | New                   | Normal   | Test data directory GMX_RELEASE_ASSERT triggers                         |                | 01/06/2020 08:07 PM |                            |
| 2070 | GROMACS | Feature | In Progress           | Normal   | Physical validation testing   | Michael Shirts | 01/03/2020 09:36 PM | future                     |
| 3014 | GROMACS | Task    | In Progress           | Normal   | gmxapi example Python scripts   |                | 01/03/2020 11:00 AM | 2021-infrastructure-stable |
| 3277 | GROMACS | Feature | New                   | Normal   | Allow testing feature that is partly implemented                        |                | 12/31/2019 12:44 PM | 2021                       |
| 1925 | GROMACS | Task    | In Progress           | Normal   | remove concept of unilateral global communication                       |                | 12/29/2019 10:35 AM | 2021                       |
| 2834 | GROMACS | Task    | In Progress           | Normal   | C++ matrix classes  | Christian Blau | 12/29/2019 10:32 AM | 2021                       |
| 2169 | GROMACS | Task    | New                   | Normal   | remove 'continuation' mdp option  |                | 12/29/2019 10:31 AM | 2021                       |
| 2660 | GROMACS | Task    | New                   | Low      | rework OpenCL nbxn kernel constants                                     | Szilárd Páll   | 12/28/2019 10:53 AM | future                     |
| 2771 | GROMACS | Task    | New                   | Normal   | Size independent Hessian for normal mode analysis                       |                | 12/28/2019 10:50 AM | future                     |
| 2832 | GROMACS | Bug     | New                   | Low      | PaddedVector move operations broken                                     | Mark Abraham   | 12/28/2019 10:40 AM | 2021                       |
| 2495 | GROMACS | Task    | Accepted              | Normal   | replace -noconfout with mdp option                                      | Mark Abraham   | 12/28/2019 10:39 AM | 2021                       |
| 3274 | GROMACS | Bug     | New                   | Normal   | Remove ARM NEON SIMD  |                | 12/28/2019 07:53 AM | 2021-infrastructure-stable |
| 3273 | GROMACS | Bug     | New                   | Normal   | gmxapi setup.py complains too much                                      |                | 12/27/2019 06:42 PM | 2021-infrastructure-stable |
| 2059 | GROMACS | Task    | In Progress           | Normal   | Separate different types of data in t_state                             |                | 12/27/2019 04:42 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                       |
| 2697 | GROMACS | Task    | New                   | Normal   | improve FFT library flavor/version reporting                            |                | 12/27/2019 04:40 PM | future                     |
| 2695 | GROMACS | Task    | New                   | Low      | bonded GPU module timing  |                | 12/27/2019 04:40 PM | 2021                       |
| 2686 | GROMACS | Task    | New                   | Normal   | add tests for gpu bonded interactions                                   |                | 12/27/2019 04:40 PM | 2021                       |
| 2889 | GROMACS | Task    | New                   | Normal   | update grompp warnings for brevity, usefulness and actionability        | Mark Abraham   | 12/27/2019 04:38 PM | future                     |
| 2976 | GROMACS | Task    | New                   | Normal   | Basic math for Multidimensional arrays                                  |                | 12/27/2019 04:37 PM | 2021                       |
| 2988 | GROMACS | Task    | In Progress           | Low      | clean up and refactor code to modern standards                          |                | 12/27/2019 04:37 PM | future                     |
| 2992 | GROMACS | Task    | New                   | Normal   | Split hw_opt in const user options and dynamic settings                 |                | 12/27/2019 04:31 PM | future                     |
| 2997 | GROMACS | Task    | New                   | Normal   | improve performance of alchemical free energy calculations              |                | 12/27/2019 04:31 PM | 2021                       |
| 3001 | GROMACS | Task    | New                   | Normal   | explore simplifying virial and shift force reduction                    |                | 12/27/2019 04:30 PM | 2021                       |
| 3008 | GROMACS | Task    | New                   | Normal   | verify block size choice of CUDA bonded kernel                          |                | 12/27/2019 04:30 PM | 2021                       |
| 3031 | GROMACS | Task    | New                   | Normal   | evaluate the impact of particle order on PME                            |                | 12/27/2019 04:29 PM | 2021                       |



| #    | Project | Tracker | Status             | Priority | Subject  | Assignee            | Updated             | Target version             |
|------|---------|---------|--------------------|----------|--|---------------------|---------------------|----------------------------|
| 3057 | GROMACS | Task    | New                | Normal   | re-enable fusion on Power8/9   | Szilárd Páll        | 12/27/2019 04:22 PM | 2021                       |
| 3062 | GROMACS | Task    | New                | Normal   | add twin cut-off mdrun test  |                     | 12/27/2019 04:22 PM | 2021                       |
| 3064 | GROMACS | Task    | New                | Normal   | add test for perturbed bonded forces   |                     | 12/27/2019 04:22 PM | 2021                       |
| 3082 | GROMACS | Task    | New                | High     | move launch/synchronization points to clarify task dependencies                |                     | 12/27/2019 04:21 PM | 2021                       |
| 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                       |
| 3119 | GROMACS | Task    | New                | Normal   | clang-tidy coverage of parallelization codepaths                               |                     | 12/27/2019 04:20 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                       |
| 2715 | GROMACS | Feature | New                | Normal   | Avoid requesting the user to recompile gromacs for Intel OpenCL support        |                     | 12/27/2019 04:06 PM | future                     |
| 2774 | GROMACS | Feature | New                | Normal   | Refactor shell code into its own integrator                                    | David van der Spoel | 12/27/2019 04:05 PM | 2021                       |
| 2944 | GROMACS | Feature | New                | Normal   | Roadmap for thermostats / barostats in new propagation/integration scheme      | Michael Shirts      | 12/27/2019 04:00 PM | 2021                       |
| 2806 | GROMACS | Feature | New                | Normal   | SIMD algorithms for ARM SVE // nonbonded cluster and others                    |                     | 12/27/2019 03:59 PM | 2021                       |
| 3101 | GROMACS | Bug     | Blocked, need info | Normal   | detect compilation failed  | Erik Lindahl        | 12/27/2019 10:52 AM |                            |
| 3075 | GROMACS | Bug     | New                | Normal   | Frozen atoms are moving  | Erik Lindahl        | 12/27/2019 10:51 AM |                            |
| 3210 | GROMACS | Bug     | New                | High     | rerun does not reproduce dVcoul/dl   |                     | 12/27/2019 10:45 AM |                            |
| 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                       |
| 3243 | GROMACS | Bug     | Feedback wanted    | Normal   | Convert GROMACS 1 OpenMP thread per rank fatal error into a warning            |                     | 12/27/2019 10:31 AM |                            |
| 3268 | GROMACS | Task    | New                | Normal   | add more Intel driver recommendations  |                     | 12/26/2019 04:39 PM |                            |
| 3267 | GROMACS | Task    | New                | Normal   | Document tools   |                     | 12/26/2019 03:20 PM | future                     |
| 1786 | GROMACS | Task    | New                | Normal   | Python style standards in developer docs                                       | Peter Kasson        | 12/26/2019 03:15 PM |                            |
| 3264 | GROMACS | Task    | New                | Normal   | Break up MdrunMpiTests   | Paul Bauer          | 12/23/2019 11:44 AM | 2021-infrastructure-stable |
| 3262 | GROMACS | Task    | New                | High     | Trjconv - dimer protein-ligand   |                     | 12/20/2019 09:26 PM |                            |
| 2766 | GROMACS | Task    | In Progress        | Normal   | Improve hardware option selection  | Kevin Boyd          | 12/20/2019 02:34 PM | 2021                       |
| 2877 | GROMACS | Task    | New                | Normal   | use gmx::Options more  | Mark Abraham        | 12/20/2019 01:22 PM | 2021                       |
| 3224 | GROMACS | Task    | New                | Normal   | add regression test case large enough to miscalculated GPU grid launch cases   |                     | 12/20/2019 01:18 PM | 2021                       |
| 2671 | GROMACS | Task    | New                | Normal   | replace constants like M_PI  |                     | 12/20/2019 01:17 PM | future                     |
| 3260 | GROMACS | Task    | New                | Low      | keep up to with mdspan reference implementation                                | Christian Blau      | 12/20/2019 01:16 PM | 2021-infrastructure-stable |

| #    | Project | Tracker | Status          | Priority | Subject   | Assignee        | Updated             | Target version             |
|------|---------|---------|-----------------|----------|---|-----------------|---------------------|----------------------------|
| 2773 | GROMACS | Task    | New             | Normal   | improve GPU error handling and make such handling uniform across modules                                |                 | 12/20/2019 01:09 PM | 2021                       |
| 2987 | GROMACS | Bug     | New             | Normal   | assess the bonded GPU task assignment default   |                 | 12/20/2019 01:06 PM | 2021                       |
| 2053 | GROMACS | Task    | New             | Normal   | refine notation in GPU code   |                 | 12/20/2019 01:04 PM | 2021                       |
| 2581 | GROMACS | Feature | Accepted        | Normal   | User interface for hybrid Monte Carlo   |                 | 12/20/2019 12:24 PM | future                     |
| 2537 | GROMACS | Task    | New             | Normal   | Simplify PME solve reduction  | Aleksei lupinov | 12/20/2019 12:21 PM | future                     |
| 2524 | GROMACS | Task    | New             | Normal   | struct alignment/packing for OpenCL host & device code  |                 | 12/20/2019 12:20 PM | future                     |
| 2518 | GROMACS | Task    | New             | Normal   | redesign task-assignment code for OpenCL  |                 | 12/20/2019 12:19 PM | future                     |
| 2054 | GROMACS | Feature | Accepted        | High     | PME on GPU  | Aleksei lupinov | 12/20/2019 12:18 PM | future                     |
| 2453 | GROMACS | Task    | Resolved        | High     | PME OpenCL porting effort   | Aleksei lupinov | 12/20/2019 12:18 PM | 2021                       |
| 2498 | GROMACS | Task    | New             | Normal   | OpenCL memory pinning/mapping   |                 | 12/20/2019 12:18 PM | future                     |
| 2480 | GROMACS | Bug     | New             | Normal   | pdb2gmx does not protonate correctly for united-atom Gromos   | Mark Abraham    | 12/20/2019 12:17 PM | 2021                       |
| 2475 | GROMACS | Task    | New             | Normal   | make OpenCL 1st class-citizen in the build system   |                 | 12/20/2019 12:14 PM | 2021                       |
| 2425 | GROMACS | Task    | New             | Normal   | testing multisim with multiple ranks per simulation   | Mark Abraham    | 12/20/2019 12:13 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                       |
| 2353 | GROMACS | Task    | New             | Normal   | improve on relative tolerance for constructing tables   |                 | 12/20/2019 12:12 PM | 2021                       |
| 2224 | GROMACS | Feature | New             | Normal   | Proposed feature: conditional stop  | Vedran Miletic  | 12/20/2019 12:11 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                       |
| 1985 | GROMACS | Bug     | Fix uploaded    | Low      | CUDA build system refactoring awaiting review   |                 | 12/20/2019 12:07 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                       |
| 1826 | GROMACS | Task    | New             | Normal   | investigate non-optimal results with CPU-GPU balancing on AMD   | Szilárd Páll    | 12/20/2019 12:04 PM | future                     |
| 1781 | GROMACS | Task    | Accepted        | Normal   | re-design benchmarking functionality  | Mark Abraham    | 12/20/2019 12:03 PM | future                     |
| 1587 | GROMACS | Task    | New             | Normal   | improve the configurability of regression tests   |                 | 12/20/2019 12:02 PM | 2021                       |
| 1165 | GROMACS | Feature | Accepted        | Low      | Multi-SIMD binaries   |                 | 12/20/2019 12:00 PM | future                     |
| 868  | GROMACS | Feature | In Progress     | Normal   | Implement parallelization support to analysis framework   | Kevin Boyd      | 12/20/2019 11:59 AM | 2021                       |
| 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 |
| 3171 | GROMACS | Task    | New             | Normal   | schedule CPU H2D force contribution in separate stream  |                 | 12/20/2019 08:33 AM | 2021-infrastructure-stable |

| #    | Project | Tracker | Status          | Priority | Subject   | Assignee       | Updated             | Target version             |
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| 3183 | GROMACS | Task    | Accepted        | Normal   | enable bonded interactions on GPU   |                | 12/20/2019 08:32 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 |
| 3131 | GROMACS | Task    | New             | Normal   | support ccache with clang-tidy  | Mark Abraham   | 12/20/2019 08:20 AM | 2021-infrastructure-stable |
| 3255 | GROMACS | Task    | New             | Normal   | Move benchmarking options from mdrun to a dedicated tool  |                | 12/19/2019 01:21 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 |                            |
| 3256 | GROMACS | Task    | New             | Normal   | Remove -nsteps option from mdrun  |                | 12/19/2019 12:12 PM |                            |
| 2822 | GROMACS | Task    | Accepted        | Normal   | Make nbxn a module  | Berk Hess      | 12/18/2019 10:49 AM | future                     |
| 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 |
| 3234 | GROMACS | Bug     | Accepted        | Normal   | Signal: Floating point exception Signal code: Floating point divide-by-zero                           | Erik Lindahl   | 12/16/2019 03:40 PM |                            |
| 2395 | GROMACS | Task    | In Progress     | Normal   | break up commrec  | Mark Abraham   | 12/15/2019 11:51 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 |                            |
| 3233 | GROMACS | Bug     | New             | Normal   | clang-format incorrectly aligning altered function arguments  |                | 12/13/2019 12:41 PM |                            |
| 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 |
| 2585 | GROMACS | Feature | Resolved        | Normal   | Infrastructure supporting external API  |                | 12/11/2019 12:39 PM |                            |
| 2994 | GROMACS | Feature | New             | Normal   | Data flow topology in gmxapi 2020   |                | 12/11/2019 11:33 AM | 2021-infrastructure-stable |
| 3032 | GROMACS | Feature | Feedback wanted | Normal   | Clean up dev-manual structure   |                | 12/11/2019 11:27 AM | 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 |
| 3136 | GROMACS | Bug     | New             | Normal   | gmxapi.operation data flow topology unclear or incomplete   | Eric Irrgang   | 12/11/2019 11:25 AM | 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                     |
| 3141 | GROMACS | Bug     | New             | Normal   | gmxapi File placeholders missing from beta release  | Eric Irrgang   | 12/10/2019 02:02 PM | 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 |
| 3133 | GROMACS | Task    | In Progress     | Normal   | Cookiecutter for sample_restraint   | Eric Irrgang   | 12/10/2019 01:59 PM | 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 |
| 2996 | GROMACS | Feature | In Progress     | Normal   | gmxapi execution model  | Eric Irrgang   | 12/10/2019 01:57 PM | 2021-infrastructure-stable |
| 2961 | GROMACS | Feature | New             | Normal   | How should Python package find GROMACS resources under various circumstances?                         |                | 12/09/2019 10:47 AM |                            |
| 3216 | GROMACS | Task    | New             | Normal   | improve CPU force reductions  | Szilárd Páll   | 12/04/2019 09:24 PM |                            |
| 2699 | GROMACS | Task    | New             | Normal   | Test POWER9   |                | 12/04/2019 03:29 PM | 2021-infrastructure-stable |

| #    | Project | Tracker | Status          | Priority | Subject   | Assignee     | Updated             | Target version             |
|------|---------|---------|-----------------|----------|---|--------------|---------------------|----------------------------|
| 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 |
| 3227 | GROMACS | Bug     | New             | Normal   | solvate does not check return status of gmx_file_rename   |              | 12/04/2019 01:43 PM |                            |
| 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 |
| 2706 | GROMACS | Task    | Accepted        | Normal   | Rework classic QM/MM interface  |              | 12/02/2019 01:45 PM | 2021-infrastructure-stable |
| 2795 | GROMACS | Task    | New             | Normal   | Incorporate regressiontests into core gromacs   |              | 12/02/2019 01:44 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 |
| 2833 | GROMACS | Task    | New             | Normal   | Update topology datastructures  | Paul Bauer   | 12/02/2019 01:43 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 |
| 2481 | GROMACS | Task    | New             | Low      | Update gmx report-methods to write more method information  |              | 12/02/2019 01:22 PM | 2021-infrastructure-stable |
| 3223 | GROMACS | Bug     | New             | Normal   | unit test failures give verify -1   |              | 12/02/2019 11:58 AM |                            |
| 3214 | GROMACS | Bug     | New             | Normal   | Out-of-bounds, overflow and incorrect outputs in gmx spatial  |              | 11/25/2019 04:11 PM |                            |
| 3213 | GROMACS | Bug     | New             | Normal   | Having a local residuetypes.dat for custom force field  |              | 11/21/2019 09:18 PM |                            |
| 3212 | GROMACS | Task    | New             | Normal   | Update regression tests for new kernel flavours   |              | 11/21/2019 11:50 AM |                            |
| 3209 | GROMACS | Bug     | New             | Normal   | Interactive molecular dynamics with VMD becomes stuttering after reconnecting   |              | 11/19/2019 11:36 AM |                            |
| 3202 | GROMACS | Bug     | New             | Low      | gmx solvate fails to overwrite topology file  |              | 11/13/2019 02:44 PM |                            |
| 3177 | GROMACS | Feature | New             | Normal   | Spack package management support  |              | 11/06/2019 06:37 PM |                            |
| 3201 | GROMACS | Task    | In Progress     | Normal   | Convert mdp parameters to key value tree  |              | 11/06/2019 06:06 PM |                            |
| 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 |                            |
| 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 |
| 3196 | GROMACS | Bug     | New             | Normal   | ExponentialMovingAverage.DeterminesCorrectlyIfIncreasing failing  |              | 11/01/2019 11:28 PM |                            |
| 3194 | GROMACS | Task    | New             | Normal   | consider passing GPU dependency list to both dependency producers and consumers   |              | 11/01/2019 07:10 PM |                            |
| 3077 | GROMACS | Task    | Feedback wanted | Normal   | PME/PP GPU Comms unique pointer deletion causes seg fault when CUDA calls exist in destructor   |              | 11/01/2019 06:56 PM |                            |
| 3132 | GROMACS | Task    | New             | Normal   | gmxapi testing support tools  |              | 10/31/2019 03:35 PM |                            |
| 3187 | GROMACS | Task    | New             | Normal   | Template updated PME kernels using threads per atom   |              | 10/30/2019 11:33 AM |                            |
| 3186 | GROMACS | Task    | In Progress     | Normal   | Update Constant/Variable naming in the PME GPU kernels.   |              | 10/30/2019 11:23 AM |                            |
| 3185 | GROMACS | Task    | New             | Normal   | Update PME CUDA kernels to allow a different number of threads per atom in the gather and spread kernels.                                     |              | 10/30/2019 11:18 AM |                            |
| 2126 | GROMACS | Feature | New             | Normal   | implement native CUDA support in CMake  |              | 10/29/2019 09:03 PM |                            |

| #    | Project | Tracker | Status          | Priority | Subject  | Assignee            | Updated             | Target version             |
|------|---------|---------|-----------------|----------|--|---------------------|---------------------|----------------------------|
| 3181 | GROMACS | Task    | New             | Normal   | consolidate task assignment and workload data initialization                                     |                     | 10/28/2019 02:53 PM |                            |
| 3179 | GROMACS | Feature | New             | Normal   | Clarify access to parallel data outputs  | Eric Irrgang        | 10/26/2019 12:23 PM |                            |
| 3174 | GROMACS | Task    | Feedback wanted | Low      | Proposed gmxapi syntax update: "input" and "output" key word arguments -> "inputs" and "outputs" | Eric Irrgang        | 10/23/2019 06:34 PM |                            |
| 3150 | GROMACS | Bug     | New             | Normal   | gmxapi data type annotations are confusing and inadequate  | Eric Irrgang        | 10/22/2019 03:08 PM | 2021-infrastructure-stable |
| 3166 | GROMACS | Bug     | New             | Normal   | Compilation failing on Ubuntu 19.04 with Cuda 10.1   |                     | 10/19/2019 09:13 PM |                            |
| 3165 | GROMACS | Bug     | New             | Normal   | task assignment silent abort   |                     | 10/18/2019 07:46 PM |                            |
| 3155 | GROMACS | Task    | Accepted        | Normal   | Unify DD and CPU-GPU gather & scatter  | Artem Zhmurov       | 10/17/2019 03:50 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 |
| 2993 | GROMACS | Feature | New             | Normal   | Scalar and structured type expression and definitions for API                                    | Eric Irrgang        | 10/17/2019 09:55 AM |                            |
| 3148 | GROMACS | Feature | New             | Normal   | Roadmap for gmxapi filesystem interactions.  | Eric Irrgang        | 10/15/2019 06:23 PM | 2021-infrastructure-stable |
| 3149 | GROMACS | Feature | New             | Normal   | Python user interface for obtaining simulation artifacts as files.                               | Eric Irrgang        | 10/15/2019 06:21 PM |                            |
| 3147 | GROMACS | Feature | New             | Normal   | gmxapi workflow checkpointing  | Eric Irrgang        | 10/15/2019 06:18 PM | 2021-infrastructure-stable |
| 3138 | GROMACS | Feature | New             | Normal   | Improve ensemble support in Context specification.   |                     | 10/15/2019 03:56 PM |                            |
| 3139 | GROMACS | Task    | New             | Normal   | gmxapi Futures should be subscribable  | Eric Irrgang        | 10/15/2019 03:56 PM |                            |
| 3135 | GROMACS | Feature | New             | Normal   | Make GPU traits ino opaque types   |                     | 10/14/2019 10:24 AM |                            |
| 3134 | GROMACS | Feature | Feedback wanted | Normal   | gmxapi Python exception names may need improvement   | Eric Irrgang        | 10/13/2019 01:50 PM |                            |
| 3042 | GROMACS | Bug     | New             | Normal   | core dump error in grompp command  |                     | 10/09/2019 07:30 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 |                            |
| 3126 | GROMACS | Feature | New             | Normal   | State propagator GPU data manager  |                     | 10/09/2019 02:42 PM |                            |
| 3123 | GROMACS | Task    | New             | Normal   | address sanitizer coverage of parallelization code-paths   |                     | 10/05/2019 12:32 AM |                            |
| 3116 | GROMACS | Bug     | New             | Normal   | regressiontests/freenenergy core dumps on ppc64le  | Paul Bauer          | 10/04/2019 10:52 PM |                            |
| 3115 | GROMACS | Feature | New             | Normal   | Device stream manager  |                     | 10/04/2019 09:00 AM |                            |
| 3113 | GROMACS | Bug     | New             | Low      | Use of read_tps_conf is depeccated   | Paul Bauer          | 10/01/2019 11:36 AM | 2021-infrastructure-stable |
| 3086 | GROMACS | Bug     | New             | Normal   | gmxapi fails with MPI build of GROMACS 2020  |                     | 09/25/2019 04:18 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                     |
| 2947 | GROMACS | Task    | Accepted        | Normal   | make an end to end test for membed   |                     | 09/24/2019 03:22 PM | future                     |
| 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 |
| 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             |
|------|-------------------|---------|-----------------|----------|---|----------------|---------------------|----------------------------|
| 3088 | GROMACS           | Bug     | New             | Normal   | Reference to theory needed for cylindrical pull geometry  |                | 09/13/2019 11:26 AM |                            |
| 3083 | GROMACS           | Bug     | New             | Normal   | Listed forces tests failing on ICC19 with AVX2_256 nightly build  |                | 09/10/2019 11:56 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 |
| 2916 | GROMACS           | Task    | New             | Normal   | Decide future of symtab   | Paul Bauer     | 09/06/2019 02:35 PM | 2021-infrastructure-stable |
| 3013 | GROMACS           | Task    | New             | Normal   | Extend logging levels in MDLogger   |                | 09/06/2019 02:34 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 |
| 3035 | GROMACS           | Task    | New             | Normal   | Provide central logger in wrapper binary  | Paul Bauer     | 09/06/2019 02:34 PM | 2021-infrastructure-stable |
| 3078 | GROMACS           | Task    | New             | Normal   | Allow MD modules to register energy output fields themselves  |                | 09/06/2019 11:36 AM |                            |
| 3058 | GROMACS           | Bug     | Feedback wanted | Normal   | Error when using a large PME grid on a GPU  |                | 09/04/2019 07:26 PM |                            |
| 3073 | GROMACS           | Bug     | New             | Normal   | Total potential energy goes crazy, but I don't know why this happens.   |                | 09/04/2019 07:25 PM |                            |
| 3072 | GROMACS           | Task    | New             | Normal   | Use gm_x::index for indexing instead of int   | Christian Blau | 09/03/2019 04:23 PM | 2021-infrastructure-stable |
| 687  | Support Platforms | Feature | New             | Normal   | Add content on the front page   |                | 09/02/2019 01:08 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                     |
| 988  | GROMACS           | Task    | New             | Normal   | Definition of "public API"  |                | 08/28/2019 02:50 PM | future                     |
| 742  | GROMACS           | Feature | New             | Normal   | Enhancing the performance of the free energy code   |                | 08/26/2019 04:55 PM | future                     |
| 1500 | GROMACS           | Feature | New             | Normal   | Post-5.0 feature clean-up plan  | Mark Abraham   | 08/26/2019 03:47 PM |                            |
| 1665 | GROMACS           | Feature | New             | Normal   | improve free energy non-bonded kernel performance   |                | 08/26/2019 03:47 PM | future                     |
| 3068 | GROMACS           | Bug     | New             | Normal   | Misleading warning on rerun   |                | 08/26/2019 03:44 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 |                            |
| 2905 | GROMACS           | Task    | New             | Normal   | Add a Jenkins configuration with std library assert   |                | 08/24/2019 05:22 PM |                            |
| 3055 | GROMACS           | Bug     | Feedback wanted | Normal   | Error in gm_x xpm2ps  |                | 08/22/2019 03:27 PM |                            |
| 3020 | GROMACS           | Feature | New             | Low      | modernize DeviceBuffer and GPU memory management  |                | 08/13/2019 06:01 PM |                            |
| 3054 | GROMACS           | Bug     | New             | Normal   | Missing dihedral define   |                | 08/02/2019 05:47 PM |                            |
| 2341 | GROMACS           | Task    | New             | Low      | assess the state of building and using GROMACS on Windows   |                | 07/29/2019 11:09 PM | future                     |
| 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 |                            |
| 3045 | GROMACS           | Feature | New             | Low      | Option to remove v-sites in trjconv?  |                | 07/19/2019 04:42 PM |                            |
| 3016 | GROMACS           | Task    | New             | Normal   | intermittent failure of essentialdynamics test  |                | 07/18/2019 05:23 PM |                            |
| 3040 | GROMACS           | Task    | New             | Normal   | Refactor Restraint module   |                | 07/18/2019 03:59 PM |                            |

| #    | Project           | Tracker | Status             | Priority | Subject   | Assignee            | Updated             | Target version |
|------|-------------------|---------|--------------------|----------|---|---------------------|---------------------|----------------|
| 2907 | GROMACS           | Bug     | New                | Normal   | Gromacs autocompletion appears to be broken with ZSH                              |                     | 07/16/2019 04:46 AM |                |
| 3028 | GROMACS           | Bug     | Feedback wanted    | Normal   | install fail on Centos 6  |                     | 07/15/2019 12:32 PM |                |
| 2983 | GROMACS           | Task    | New                | Normal   | better suited data-types for bonded GPU kernels                                   |                     | 07/11/2019 04:32 PM |                |
| 3030 | GROMACS           | Feature | New                | Normal   | RST style guidelines  |                     | 07/09/2019 03:38 PM |                |
| 2949 | GROMACS           | Bug     | New                | Normal   | cmake fails when building mdrun only  |                     | 07/08/2019 10:04 AM |                |
| 2818 | GROMACS           | Task    | In Progress        | Normal   | bonded GPU kernel fusion  | Magnus Lundborg     | 07/03/2019 09:01 PM |                |
| 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 |                |
| 2034 | GROMACS           | Feature | New                | Normal   | Unit tests for bonded forces  | David van der Spoel | 06/29/2019 10:22 AM | future         |
| 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 |                |
| 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 |                |
| 3002 | GROMACS           | Task    | New                | Normal   | consider splitting bonded work into local/nonlocal                                |                     | 06/25/2019 04:06 PM |                |
| 3000 | GROMACS           | Bug     | New                | Normal   | CMake "webpage" target does not fail when it should                               |                     | 06/25/2019 02:43 PM |                |
| 2984 | GROMACS           | Feature | New                | Normal   | More Extensive Selections Examples  | Dallas Warren       | 06/18/2019 11:50 PM |                |
| 2981 | GROMACS           | Bug     | New                | Normal   | segfault in opencl build  |                     | 06/18/2019 03:30 AM |                |
| 2980 | GROMACS           | Bug     | New                | Normal   | taskassignment fails with unit tests when GPUs and custom number of ranks is used |                     | 06/17/2019 05:28 PM |                |
| 2734 | GROMACS           | Bug     | In Progress        | Normal   | regressiontests/kernel core dumps on ppc64le                                      | Paul Bauer          | 06/15/2019 04:12 PM | future         |
| 2978 | GROMACS           | Bug     | New                | Normal   | Some suggestions about the gmx current tool                                       |                     | 06/13/2019 12:41 PM |                |
| 2977 | GROMACS           | Feature | New                | Normal   | print DD load balancing improvement   |                     | 06/13/2019 10:56 AM |                |
| 2975 | GROMACS           | Feature | New                | Normal   | LJ PME calculations on GPUs   |                     | 06/12/2019 01:17 PM |                |
| 2935 | Support Platforms | Bug     | New                | High     | redmine issue updates about gerrit uploads stopped working                        |                     | 06/11/2019 01:42 PM | current        |
| 2516 | GROMACS           | Task    | New                | Low      | Support PME OpenCL execution width < 16   | Aleksei lupinov     | 06/05/2019 05:32 PM |                |
| 2954 | GROMACS           | Bug     | New                | Normal   | genion changes residue numbering  |                     | 05/26/2019 12:08 AM |                |
| 2948 | GROMACS           | Bug     | New                | Normal   | SIMD support detected as none on AMD R5 2500U                                     |                     | 05/21/2019 12:58 PM |                |
| 2956 | GROMACS           | Feature | New                | Normal   | SAXS resolution   |                     | 05/17/2019 09:58 AM |                |
| 2596 | GROMACS           | Feature | New                | Normal   | Constant potential method   | Benson Muite        | 05/10/2019 09:54 AM |                |
| 2570 | GROMACS           | Feature | New                | Normal   | Better string formatting and printing   |                     | 05/02/2019 12:20 PM |                |
| 2375 | GROMACS           | Task    | New                | Normal   | Clarify execution phases for MD simulation  |                     | 04/30/2019 12:59 PM |                |

| #    | Project                | Tracker | Status      | Priority | Subject  | Assignee            | Updated             | Target version |
|------|------------------------|---------|-------------|----------|--|---------------------|---------------------|----------------|
| 2902 | GROMACS                | Bug     | New         | Normal   | 2019.1 equilibration issue? (Intel 2018u3)   |                     | 04/30/2019 08:17 AM |                |
| 2931 | GROMACS                | Feature | New         | Normal   | Tables in Verlet kernels   |                     | 04/29/2019 12:01 PM |                |
| 2937 | TNG trajectory library | Bug     | New         | Normal   | tng_num_frames_get reports incorrect num frames  |                     | 04/29/2019 11:30 AM |                |
| 2930 | GROMACS                | Feature | New         | Normal   | Limited range for reference group detection in cylinder pulling                            |                     | 04/26/2019 05:17 PM |                |
| 2933 | GROMACS                | Task    | New         | Normal   | Convert walls to a ForceProvider   |                     | 04/25/2019 02:43 PM |                |
| 2928 | GROMACS                | Feature | New         | Normal   | Add ability to use expression "count of ATOM_EXPR" in selection statements.                |                     | 04/16/2019 04:52 PM |                |
| 2919 | GROMACS                | Task    | New         | Normal   | C++ style guidelines for namespace use   |                     | 04/15/2019 01:21 PM |                |
| 2924 | GROMACS                | Bug     | New         | Normal   | Failing version check when reading new tpr file with older gromacs version                 |                     | 04/12/2019 10:52 AM |                |
| 2910 | GROMACS                | Feature | New         | Normal   | Mixed scaling for 1-4 interactions   |                     | 04/10/2019 10:13 PM |                |
| 2897 | GROMACS                | Bug     | New         | Normal   | rotation/flex2 can still fail on cpu-only run on OpenCL build                              |                     | 04/04/2019 06:24 PM |                |
| 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 |                |
| 2574 | GROMACS                | Feature | New         | Normal   | iForceSchedule Abstraction   | Prashanth Kanduri   | 03/29/2019 05:20 PM | future         |
| 2702 | GROMACS                | Bug     | Accepted    | Normal   | PME gather reduction race in OpenCL (and CUDA)   |                     | 03/28/2019 03:14 PM |                |
| 2908 | GROMACS                | Task    | New         | Normal   | Renaming things in nbxnm   | Berk Hess           | 03/28/2019 10:10 AM |                |
| 2898 | GROMACS                | Task    | New         | Low      | Naming common variables  |                     | 03/26/2019 11:46 PM |                |
| 2282 | GROMACS                | Feature | New         | Normal   | Density map toolset  | Christian Blau      | 03/21/2019 06:08 PM | future         |
| 2863 | GROMACS                | Task    | New         | Normal   | improve PBC handling   |                     | 03/11/2019 04:28 PM |                |
| 2876 | GROMACS                | Bug     | New         | Normal   | 2019.1 make check fails on AVX and AVX2 (Intel 2018u3)                                     | Erik Lindahl        | 03/08/2019 10:32 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 |                |
| 2869 | GROMACS                | Bug     | New         | Normal   | GPU detection error only issued as a note to the log                                       |                     | 03/05/2019 04:09 PM |                |
| 2870 | GROMACS                | Bug     | New         | Normal   | GPU detection error message missing from the output  |                     | 03/05/2019 03:55 PM |                |
| 2866 | GROMACS                | Feature | New         | Normal   | Alternative non-bonded potentials  | David van der Spoel | 03/05/2019 03:50 PM | future         |
| 701  | GROMACS                | Task    | New         | Normal   | Add symbol visibility macros   |                     | 03/02/2019 01:46 AM | future         |
| 1625 | GROMACS                | Feature | New         | Normal   | Gromacs Python API   |                     | 03/02/2019 01:44 AM | future         |
| 2068 | GROMACS                | Feature | New         | Normal   | Access to low level classes  |                     | 03/02/2019 01:37 AM | 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         |
| 2873 | GROMACS                | Bug     | New         | Normal   | Simple way to get last frame from trajectory   |                     | 02/28/2019 11:14 PM |                |



| #    | Project           | Tracker | Status          | Priority | Subject   | Assignee            | Updated             | Target version |
|------|-------------------|---------|-----------------|----------|---|---------------------|---------------------|----------------|
| 2874 | GROMACS           | Task    | New             | Normal   | Refactor Gromacs (cluster) neighborlist into separate module                      | Erik Lindahl        | 02/28/2019 11:36 AM |                |
| 2872 | GROMACS           | Bug     | New             | Normal   | gmx solvate and genion topology update  |                     | 02/27/2019 10:18 AM |                |
| 2111 | GROMACS           | Feature | In Progress     | Normal   | Implement Gaussian screening of electrostatics                                    |                     | 02/23/2019 12:33 PM |                |
| 2594 | GROMACS           | Feature | New             | Normal   | Multi-level GMX API   | Prashanth Kanduri   | 02/22/2019 03:48 PM | future         |
| 2595 | GROMACS           | Task    | New             | Normal   | Reusable Utilities for Schedules  | Prashanth Kanduri   | 02/22/2019 03:48 PM | future         |
| 2755 | GROMACS           | Feature | New             | Low      | md5 sums and sha256, sha512 hashes  | Benson Muite        | 02/19/2019 11:00 PM |                |
| 2864 | GROMACS           | Task    | New             | Normal   | Building incompatibilities  | Benson Muite        | 02/19/2019 02:00 PM |                |
| 2519 | GROMACS           | Task    | New             | High     | Improve/remove PME OpenCL kernel barriers   |                     | 02/15/2019 06:34 PM |                |
| 1862 | GROMACS           | Task    | New             | Normal   | Fully replace t_topology by gmx_mtop_t  |                     | 02/13/2019 04:53 PM |                |
| 2850 | GROMACS           | Task    | In Progress     | Normal   | assess Raptor Talos for testing   | Szilárd Páll        | 02/12/2019 01:14 PM |                |
| 2860 | GROMACS           | Feature | New             | Normal   | Option for outputting min/max coordinates in gmx traj                             |                     | 02/08/2019 12:35 AM |                |
| 2835 | GROMACS           | Task    | New             | Normal   | Matrix class constraint to upper or lower triangle                                |                     | 02/07/2019 02:44 PM |                |
| 2754 | GROMACS           | Bug     | New             | Normal   | Simulated Tempering seems to be broken  | Michael Shirts      | 02/05/2019 03:58 PM |                |
| 2853 | GROMACS           | Bug     | New             | Normal   | EwaldUnitTests segfault on armv7hl with gcc-9.0.1                                 | Paul Bauer          | 02/04/2019 05:34 PM |                |
| 2854 | GROMACS           | Bug     | New             | Normal   | OnlineHelpUnitTests segfaults on s390x with gcc-9.0.1                             | Paul Bauer          | 02/04/2019 11:17 AM |                |
| 2248 | GROMACS           | Feature | New             | Normal   | Label all SIMD functions as pure/nodiscard  |                     | 02/04/2019 04:49 AM |                |
| 2857 | GROMACS           | Task    | New             | Normal   | Clarify recommended function specifies (constexpr, noexcept, pure)                |                     | 02/04/2019 04:48 AM |                |
| 2846 | GROMACS           | Feature | New             | Low      | Set rpath in FindLibStdCpp.cmake  |                     | 02/02/2019 08:09 AM |                |
| 2852 | GROMACS           | Bug     | New             | Low      | the in-tree regressiontest download can get out of sync with code                 |                     | 01/30/2019 03:58 PM |                |
| 2851 | Support Platforms | Task    | New             | Normal   | uninstall redmine checklist plugin  |                     | 01/30/2019 03:33 PM |                |
| 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 |                |
| 2840 | GROMACS           | Feature | New             | Normal   | Test that functionality does not compile that is not supposed to.                 |                     | 01/25/2019 02:35 PM | future         |
| 2828 | GROMACS           | Bug     | Feedback wanted | Normal   | Installation issue on Power 9 system with SIMD support                            |                     | 01/18/2019 11:54 AM |                |
| 1354 | GROMACS           | Bug     | New             | Normal   | Constant acceleration NEMD is broken.   | David van der Spoel | 01/09/2019 04:42 PM |                |
| 951  | GROMACS           | Feature | New             | Normal   | Multiple versions of Gromacs (e.g., single and double) in the same library/binary |                     | 01/07/2019 02:10 AM | future         |
| 2239 | GROMACS           | Feature | New             | Normal   | split libgromacs into base and full   |                     | 01/07/2019 01:47 AM |                |
| 2788 | GROMACS           | Bug     | New             | Normal   | PME will not run on AMD GPU with NVidia GPU present                               |                     | 01/03/2019 02:24 PM |                |
| 2796 | GROMACS           | Task    | New             | Low      | clarify what mdrun -cpt means   |                     | 01/03/2019 02:09 PM |                |

| #    | Project | Tracker | Status      | Priority | Subject   | Assignee            | Updated             | Target version |
|------|---------|---------|-------------|----------|---|---------------------|---------------------|----------------|
| 1505 | GROMACS | Task    | New         | Normal   | improve handling of logging   | Mark Abraham        | 01/02/2019 06:06 PM |                |
| 2696 | GROMACS | Task    | In Progress | Normal   | ensure PME queue is flushed   | Szilárd Páll        | 12/31/2018 11:21 AM | future         |
| 2672 | GROMACS | Task    | New         | Normal   | check & document execution width requirements in OpenCL                                   |                     | 12/31/2018 11:20 AM | future         |
| 2650 | GROMACS | Task    | New         | Normal   | revise OpenCL stack recommendations   |                     | 12/31/2018 11:19 AM | future         |
| 2528 | GROMACS | Task    | New         | Normal   | PME GPU tuning  |                     | 12/31/2018 11:18 AM | future         |
| 2379 | GROMACS | Task    | New         | Normal   | check leftover FIXMEs in r2018  | Szilárd Páll        | 12/31/2018 11:16 AM | future         |
| 2693 | GROMACS | Bug     | New         | Normal   | Several memory leaks in mdrun   |                     | 12/18/2018 04:22 AM | future         |
| 2649 | GROMACS | Bug     | New         | Normal   | Virial calculation necessary for correct energy calculation on GPU                        |                     | 12/17/2018 02:32 PM | future         |
| 2468 | GROMACS | Bug     | New         | Low      | incorrect GPU timing reported with OpenCL and domain decomposition                        |                     | 12/17/2018 01:28 PM | future         |
| 2763 | GROMACS | Bug     | New         | Normal   | GMXAPI layout / grouping in development docs "modules" page                               |                     | 12/14/2018 12:49 PM | future         |
| 2674 | GROMACS | Task    | Accepted    | Normal   | Improve domain decomposition for bilayer systems  |                     | 12/07/2018 04:03 PM | future         |
| 1323 | GROMACS | Task    | New         | Normal   | determine future of existing tools for  | David van der Spoel | 12/04/2018 11:53 AM |                |
| 2787 | GROMACS | Task    | New         | Normal   | allow passing flags to allocateDeviceBuffer   |                     | 12/03/2018 01:54 PM |                |
| 2632 | GROMACS | Task    | New         | Low      | make sure cmake defines proper hwloc version with cross-compilation enabled               |                     | 12/03/2018 01:35 PM | future         |
| 1879 | GROMACS | Task    | In Progress | Low      | make the GROMACS OpenCL kernel work on Gallium  |                     | 11/30/2018 05:46 PM | future         |
| 2785 | GROMACS | Bug     | New         | Normal   | Inconsistent and erroneous behaviour of trjconv when writing a partial TNG                |                     | 11/30/2018 02:36 PM |                |
| 2186 | GROMACS | Feature | New         | Low      | Potential change for logical improvements: move control of constraints purely to the .mdp | Michael Shirts      | 11/27/2018 11:27 AM | future         |
| 2764 | GROMACS | Task    | New         | Normal   | gmxapi version updates for post release-2019  | Eric Irrgang        | 11/21/2018 12:53 PM |                |
| 2761 | GROMACS | Feature | New         | Low      | lincs-order 4 is too conservative for some force fields                                   |                     | 11/16/2018 09:55 AM |                |
| 2758 | GROMACS | Task    | New         | Low      | Modernize genconf   |                     | 11/15/2018 07:38 AM | future         |
| 2739 | GROMACS | Feature | New         | Normal   | Parallel continuous tempering and enhanced sampling feature                               |                     | 11/13/2018 11:36 PM |                |
| 2065 | GROMACS | Bug     | New         | Normal   | thread-MPI internal errors  |                     | 11/08/2018 03:43 PM |                |
| 2740 | GROMACS | Bug     | New         | Normal   | mdrun reports incorrect error with -bonded gpu without gpu                                | Mark Abraham        | 11/07/2018 01:59 PM |                |
| 2368 | GROMACS | Task    | In Progress | Normal   | update implementation of gmx msd  | Kevin Boyd          | 11/03/2018 07:43 PM | future         |
| 1793 | GROMACS | Task    | New         | Normal   | cleanup of integration loop   | Mark Abraham        | 10/31/2018 10:49 PM | future         |
| 2527 | GROMACS | Task    | New         | Normal   | Rename GpuEventSynchronizer to something more fitting (after merge in PME OpenCL)         |                     | 10/30/2018 04:06 AM | future         |
| 2707 | GROMACS | Bug     | New         | Normal   | Installed OpenCL files include clh file from gpu_utils directory                          |                     | 10/30/2018 04:02 AM |                |

| #    | Project | Tracker | Status      | Priority | Subject   | Assignee       | Updated             | Target version |
|------|---------|---------|-------------|----------|---|----------------|---------------------|----------------|
| 2713 | GROMACS | Feature | New         | Normal   | Constant offset for external electric fields  |                | 10/28/2018 12:57 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         |
| 1937 | GROMACS | Task    | New         | Low      | stop supporting changing CUDA host compiler   | Mark Abraham   | 10/15/2018 05:19 PM | future         |
| 2587 | GROMACS | Feature | In Progress | Normal   | Provide Context (e.g. to runner code) to manage client and runtime environment                    |                | 10/15/2018 03:34 PM |                |
| 2598 | GROMACS | Bug     | New         | Normal   | Tools using read_next_x cannot read TNG files with sanitizers                                     |                | 10/15/2018 01:16 PM | future         |
| 2603 | GROMACS | Task    | New         | Normal   | Add ability to properly check coordinate files during testing                                     | Paul Bauer     | 10/15/2018 01:16 PM | future         |
| 2521 | GROMACS | Task    | New         | Normal   | Implement alternating PME/NB wait for OpenCL  |                | 10/15/2018 12:39 PM |                |
| 1919 | GROMACS | Bug     | Accepted    | Normal   | static linking issues cause by hwloc support  |                | 10/12/2018 10:49 PM | future         |
| 2682 | GROMACS | Task    | New         | Normal   | Add MSAN configuration  |                | 10/09/2018 06:28 PM |                |
| 2658 | GROMACS | Task    | New         | Normal   | Secondary structure assignment via DSSP as native gromacs code                                    | Christian Blau | 10/09/2018 04:51 PM | future         |
| 1666 | GROMACS | Feature | New         | Normal   | new approach for Verlet-scheme kernel generation  | Erik Lindahl   | 10/08/2018 07:04 PM | future         |
| 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         |

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