

## Issues

| #    | Project | Tracker | Status   | Priority | Subject                                                                                  | Assignee         | Updated             | Target version             |
|------|---------|---------|----------|----------|------------------------------------------------------------------------------------------|------------------|---------------------|----------------------------|
| 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 |                            |
| 3446 | GROMACS | Task    | New      | Normal   | apply maintainability updates across all GPU kernels                                     | Jonathan Vincent | 03/19/2020 03:31 PM |                            |
| 3445 | GROMACS | Task    | New      | Normal   | create heuristic for c_skipNeutralAtoms                                                  | Jonathan Vincent | 03/17/2020 12:12 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                     |
| 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 |                            |
| 3441 | GROMACS | Bug     | Resolved | Normal   | Ewald surface-epsilon is incorrect                                                       | Berk Hess        | 03/18/2020 11:15 PM | 2020.2                     |
| 3440 | GROMACS | Bug     | New      | Normal   | Multi-nodes run exits with error with openmpi/4.0.0                                      |                  | 03/23/2020 02:10 PM |                            |
| 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 |
| 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 |
| 3433 | GROMACS | Feature | New      | Normal   | Decide how to handle multisim with modular simulator                                     | Pascal Merz      | 03/11/2020 06:42 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 |
| 3426 | GROMACS | Feature | New      | Normal   | Support acceleration in modular simulator                                                | Pascal Merz      | 03/11/2020 04:09 PM | 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 |
| 3422 | GROMACS | Task    | Resolved | Normal   | Implement modular checkpointing for modular simulator                                    | Pascal Merz      | 09/16/2020 09:45 AM | 2021-infrastructure-stable |
| 3421 | GROMACS | Task    | New      | Normal   | Implement client system for global reduction                                             | Pascal Merz      | 03/11/2020 03:31 PM | 2021-infrastructure-stable |
| 3420 | GROMACS | Task    | New      | Normal   | Unify force and shellfc elements for modular simulator                                   | Pascal Merz      | 03/10/2020 09:50 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 |

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|------|---------|---------|-----------------|----------|--------------------------------------------------------------------------------------------------------------------|-----------------|---------------------|----------------------------|
| 3417 | GROMACS | Feature | New             | Normal   | Make modular simulator feature-complete                                                                            | Pascal Merz     | 03/23/2020 03:57 AM | 2021-infrastructure-stable |
| 3416 | GROMACS | Task    | New             | Normal   | Port post-submit matrix to Gitlab CI                                                                               | Joe Jordan      | 03/16/2020 05:50 PM | 2021-refactoring           |
| 3415 | GROMACS | Task    | New             | Normal   | Port Pre-submit matrix to Gitlab CI                                                                                | Szilárd Páll    | 03/23/2020 10:09 AM | 2021-refactoring           |
| 3413 | GROMACS | Bug     | Feedback wanted | Normal   | COMM Removal Failure in GROMACS 2020.1                                                                             |                 | 03/12/2020 02:31 PM |                            |
| 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 |
| 3410 | GROMACS | Feature | New             | Normal   | Random Acceleration Molecular Dynamics (RAMD)                                                                      | Bernd Doser     | 03/05/2020 03:22 PM | 2021                       |
| 3408 | GROMACS | Bug     | Fix uploaded    | Normal   | Gmxapi* tests segfault in rpmbuild                                                                                 | Eric Irrgang    | 03/23/2020 01:27 PM | 2020.2                     |
| 3405 | GROMACS | Bug     | Accepted        | Normal   | intermittent OpenCL regressiontest failures                                                                        |                 | 03/02/2020 11:01 AM |                            |
| 3403 | GROMACS | Bug     | Resolved        | Normal   | solvation free energy with couple-intramol set to no                                                               |                 | 04/17/2020 04:00 PM |                            |
| 3402 | GROMACS | Feature | New             | Normal   | Clarify distinction between public API documentation and developer docs.                                           |                 | 02/26/2020 04:16 PM | 2021-infrastructure-stable |
| 3401 | GROMACS | Feature | New             | Normal   | Policy and procedure for installed headers (public API)                                                            |                 | 02/26/2020 04:17 PM | 2021-infrastructure-stable |
| 3398 | GROMACS | Bug     | New             | Normal   | Intermittent failure of non-bonded kernels when run using nvprof                                                   |                 | 02/25/2020 12:14 PM |                            |
| 3395 | GROMACS | Feature | Feedback wanted | Normal   | Consider scripted composition of Dockerfiles                                                                       |                 | 03/16/2020 12:16 PM |                            |
| 3394 | GROMACS | Feature | New             | Normal   | improve gmxapi error handling                                                                                      | Eric Irrgang    | 02/24/2020 11:45 AM | 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 |
| 3392 | GROMACS | Task    | New             | Low      | Unify box correction for modular simulator                                                                         | Pascal Merz     | 03/11/2020 05:20 PM | 2021-infrastructure-stable |
| 3387 | GROMACS | Bug     | New             | Normal   | Death test bug                                                                                                     |                 | 02/20/2020 05:39 PM |                            |
| 3385 | GROMACS | Bug     | New             | Normal   | FindLibStdCpp.cmake - wrong sanity check for clang                                                                 |                 | 03/04/2020 06:59 PM |                            |
| 3382 | GROMACS | Task    | Accepted        | Normal   | Split up t_inputrec                                                                                                |                 | 02/17/2020 05:28 PM |                            |
| 3380 | GROMACS | Bug     | Resolved        | Low      | IBM VSX checks fail with gcc-10                                                                                    | Erik Lindahl    | 04/30/2020 01:30 PM | 2020.2                     |
| 3379 | GROMACS | Feature | New             | Normal   | C++ API for simulation input and output                                                                            |                 | 02/28/2020 10:38 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 |                            |
| 3374 | GROMACS | Feature | New             | Normal   | SimulationInput abstraction                                                                                        |                 | 03/03/2020 05:32 PM | 2021-refactoring           |
| 3371 | GROMACS | Feature | New             | Normal   | Control FEP using AWH                                                                                              | Magnus Lundborg | 02/06/2020 02:20 PM | 2021                       |
| 3370 | GROMACS | Task    | New             | High     | Further improvements to GPU Buffer Ops and Comms                                                                   |                 | 03/04/2020 01:38 PM |                            |
| 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                     |
| 3366 | GROMACS | Task    | New             | Normal   | Enforce compability of MdModules                                                                                   |                 | 02/28/2020 11:20 AM |                            |

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|------|---------|---------|----------|----------|------------------------------------------------------------------------------------------------------|------------------|---------------------|----------------------------|
| 3365 | GROMACS | Task    | New      | Low      | consider making GPU bonded work independent from nonbonded                                           |                  | 03/01/2020 01:11 PM |                            |
| 3363 | GROMACS | Feature | New      | Normal   | Improve FEP testing                                                                                  | Pascal Merz      | 03/01/2020 03:22 PM | 2021-infrastructure-stable |
| 3362 | GROMACS | Feature | New      | Normal   | gmx traj: add an option to plot each component in a separate file                                    |                  | 01/29/2020 06:18 PM |                            |
| 3361 | GROMACS | Task    | New      | Normal   | Gitlab source archive contains files from build directory                                            | Paul Bauer       | 02/25/2020 10:13 AM | 2020.2                     |
| 3360 | GROMACS | Task    | New      | Normal   | investigate the future of DD dynamic load balancing with GPU offload                                 |                  | 01/29/2020 11:23 AM |                            |
| 3357 | GROMACS | Task    | New      | Normal   | Make sure "colvars" interoperates stably and smoothly with gromacs                                   |                  | 03/04/2020 11:25 AM |                            |
| 3356 | GROMACS | Task    | New      | Normal   | Expose setting of random seed to API                                                                 |                  | 01/29/2020 06:16 PM | 2021                       |
| 3355 | GROMACS | Feature | Accepted | Normal   | New PME parallel (GPU) scheme                                                                        | Jonathan Vincent | 02/12/2020 11:58 AM |                            |
| 3353 | GROMACS | Task    | New      | Normal   | Document gmx densmap output                                                                          |                  | 01/23/2020 12:52 PM |                            |
| 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                       |
| 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 |

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| 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 |
| 3334 | GROMACS | Bug     | New         | Normal   | Check for DD when increasing rlist is broken                                     | Berk Hess     | 02/25/2020 03:28 PM | 2020.2                     |
| 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 |
| 3332 | GROMACS | Feature | New         | Normal   | gmx helixorient doesn't have a -tu option to change time unit                    |               | 01/22/2020 11:57 AM |                            |
| 3331 | GROMACS | Task    | New         | Low      | Run physical validation tests in Gitlab                                          | Paul Bauer    | 02/27/2020 11:09 PM | future                     |
| 3330 | GROMACS | Task    | New         | Normal   | Compile list of codepaths for testing task assignment                            |               | 01/22/2020 10:03 AM | 2021-refactoring           |
| 3329 | GROMACS | Task    | New         | Normal   | Extend energy comparison testing framework                                       |               | 01/22/2020 09:51 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           |
| 3325 | GROMACS | Task    | New         | Normal   | Allow complete re-initialization of a simulation                                 |               | 01/29/2020 05:13 PM | 2021-refactoring           |
| 3324 | GROMACS | Task    | New         | Normal   | Rework CMake handling of GPU code                                                |               | 01/22/2020 09:52 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           |
| 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           |
| 3318 | GROMACS | Feature | In Progress | Normal   | Use wrappers for the GPU buffer copy/allocations                                 | Artem Zhmurov | 01/23/2020 12:01 PM | 2021-refactoring           |
| 3317 | GROMACS | Task    | Resolved    | Normal   | Improve testing of the GPU code                                                  | Artem Zhmurov | 10/06/2020 12:15 PM | 2021-refactoring           |
| 3316 | GROMACS | Task    | Accepted    | Normal   | Context and Stream manager                                                       | Artem Zhmurov | 01/22/2020 09:49 AM | 2021-refactoring           |
| 3315 | GROMACS | Task    | Resolved    | Normal   | Platform agnostic DeviceContext                                                  | Artem Zhmurov | 03/11/2020 04:15 PM | 2021-refactoring           |
| 3314 | GROMACS | Task    | Resolved    | Normal   | Platform agnostic DeviceStream                                                   | Artem Zhmurov | 03/20/2020 09:55 AM | 2021-refactoring           |
| 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           |
| 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           |
| 3311 | GROMACS | Feature | In Progress | Normal   | GPU infrastructure development                                                   |               | 03/20/2020 09:54 AM | 2021-refactoring           |

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|------|---------|---------|-----------------------|----------|-------------------------------------------------------------------------------------------------|----------------|---------------------|----------------------------|
| 3310 | GROMACS | Bug     | Blocked,<br>need info | Low      | Thread affinity on Mac OS                                                                       |                | 02/27/2020 11:10 PM |                            |
| 3309 | GROMACS | Bug     | New                   | Normal   | -reprod: checkpoint reading bug and general considerations                                      |                | 02/27/2020 10:45 PM |                            |
| 3308 | GROMACS | Task    | New                   | Normal   | GPU update-constraints: Cycle counting for GPU launches                                         |                | 01/23/2020 11:54 AM | 2021-infrastructure-stable |
| 3307 | GROMACS | Feature | New                   | Normal   | General interface for communication between simulation ranks                                    |                | 01/22/2020 03:22 PM | 2021-refactoring           |
| 3306 | GROMACS | Task    | New                   | Normal   | Document gmx dos tool more clearly                                                              | Christian Blau | 01/20/2020 02:31 PM | future                     |
| 3305 | GROMACS | Bug     | New                   | Normal   | Case gives FPE with Debug build when GPU update is enabled                                      |                | 01/21/2020 05:44 PM |                            |
| 3304 | GROMACS | Bug     | New                   | Normal   | Failure in Log Output for Expanded Ensemble Weights using Simulated Tempering in GROMACS 2019.5 | Michael Shirts | 03/01/2020 03:23 PM | 2020.2                     |
| 3301 | GROMACS | Bug     | New                   | Normal   | pdb2gmx adding hydrogen                                                                         |                | 01/15/2020 10:17 PM |                            |
| 3300 | GROMACS | Task    | New                   | Normal   | Abandon docs/OpenCLTODOList.txt?                                                                |                | 01/15/2020 02:46 PM |                            |
| 3298 | GROMACS | Feature | New                   | Normal   | start early PP work for first dimension of halo exchange                                        |                | 03/01/2020 01:36 PM |                            |
| 3297 | GROMACS | Task    | Resolved              | Normal   | Require gcc > 5                                                                                 |                | 04/30/2020 11:00 AM | 2021-infrastructure-stable |
| 3295 | GROMACS | Feature | New                   | Normal   | Expand gmxapi.modify_input use cases.                                                           | Eric Irrgang   | 01/16/2020 05:13 PM | 2021-refactoring           |
| 3294 | GROMACS | Bug     | New                   | Normal   | multiple tests fail on fedora 31                                                                | Paul Bauer     | 02/28/2020 03:12 PM | 2020.2                     |
| 3290 | GROMACS | Task    | Resolved              | Normal   | Require CMake >= 3.12                                                                           |                | 04/14/2020 02:45 PM | 2021-refactoring           |
| 3289 | GROMACS | Task    | New                   | Normal   | Distinguish identifying and non-identifying inputs to API operations.                           | Eric Irrgang   | 01/10/2020 11:30 AM |                            |
| 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 |
| 3287 | GROMACS | Task    | New                   | Normal   | Deprecate make_ndx, use select instead                                                          |                | 01/23/2020 01:16 PM |                            |
| 3285 | GROMACS | Feature | Resolved              | Normal   | Run simulations from the same tpr file with different random seeds                              |                | 02/27/2020 11:22 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 |
| 3283 | GROMACS | Feature | Resolved              | Normal   | Support for the string method with swarms of trajectories in GROMACS                            |                | 03/01/2020 01:16 PM | 2021                       |
| 3281 | GROMACS | Bug     | New                   | Normal   | Test data directory GMX_RELEASE_ASSERT triggers                                                 |                | 01/06/2020 08:07 PM |                            |
| 3279 | GROMACS | Task    | New                   | Low      | Provide more advice for building client software                                                |                | 03/02/2020 11:54 AM |                            |
| 3277 | GROMACS | Feature | New                   | Normal   | Allow testing feature that is partly implemented                                                |                | 12/31/2019 12:44 PM | 2021                       |
| 3275 | GROMACS | Task    | New                   | Normal   | Document Gitlab CI instead of Jenkins and releng                                                | Paul Bauer     | 03/09/2020 05:55 PM | 2021-infrastructure-stable |
| 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 |
| 3272 | GROMACS | Task    | New                   | Normal   | Port complete CI testing to Gitlab                                                              | Paul Bauer     | 02/27/2020 11:04 AM | 2021-infrastructure-stable |
| 3271 | GROMACS | Task    | Resolved              | Normal   | Adopt PEP-518 for Python package build system configuration.                                    |                | 04/09/2020 10:15 PM | 2021-infrastructure-stable |
| 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                     |

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| 3266 | GROMACS | Bug     | New                   | High     | gmx density show wrong symmetrize density profile using -symm?                                        | Super duper    | 02/28/2020 08:24 AM | 2020.2                     |
| 3265 | GROMACS | Bug     | Blocked,<br>need info | Low      | regressiontests/complex fails on ppc64le                                                              | Erik Lindahl   | 01/09/2020 05:00 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 |                            |
| 3260 | GROMACS | Task    | New                   | Low      | keep up to with mdspan reference implementation                                                       | Christian Blau | 12/20/2019 01:16 PM | 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 |
| 3256 | GROMACS | Task    | New                   | Normal   | Remove -nsteps option from mdrun                                                                      |                | 12/19/2019 12:12 PM |                            |
| 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 |                            |
| 3252 | GROMACS | Task    | New                   | Normal   | Remove support for 32 bit architectures                                                               |                | 03/01/2020 02:05 PM |                            |
| 3249 | GROMACS | Bug     | In Progress           | Low      | cmake bad tests for avx512 on AMD                                                                     | Erik Lindahl   | 02/26/2020 05:00 PM |                            |
| 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 |
| 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 |                            |
| 3242 | GROMACS | Feature | New                   | Normal   | Please do not remove the -nsteps flag                                                                 |                | 03/01/2020 01:59 PM |                            |
| 3240 | GROMACS | Bug     | New                   | Normal   | segv with GPU DD direct communication with GPU update and -dlb off                                    |                | 01/15/2020 06:16 PM |                            |
| 3239 | GROMACS | Bug     | New                   | Normal   | GPU DD direct communication with GPU update error with RF                                             |                | 12/14/2019 05:15 PM |                            |
| 3236 | GROMACS | Task    | New                   | Normal   | GPU update-constraints: Pulling support                                                               | Artem Zhmurov  | 01/23/2020 11:53 AM | 2021-infrastructure-stable |
| 3235 | GROMACS | Task    | New                   | Normal   | Run mdrun-test in parallel and make sure they tests test critical quantities like energy conservation | Christian Blau | 12/12/2019 03:46 PM | 2021-infrastructure-stable |
| 3234 | GROMACS | Bug     | Accepted              | Normal   | Signal: Floating point exception Signal code: Floating point divide-by-zero                           | Erik Lindahl   | 12/16/2019 03:40 PM |                            |
| 3233 | GROMACS | Bug     | New                   | Normal   | clang-format incorrectly aligning altered function arguments                                          |                | 12/13/2019 12:41 PM |                            |
| 3229 | GROMACS | Task    | New                   | Normal   | Move checkpointing to the beginning of the MD step                                                    |                | 01/16/2020 04:31 PM | 2021-infrastructure-stable |
| 3228 | GROMACS | Bug     | New                   | Normal   | gmxapi.commandline_operation should gracefully handle input/output file arguments                     | Eric Irrgang   | 12/04/2019 03:27 PM | 2021-infrastructure-stable |
| 3227 | GROMACS | Bug     | New                   | Normal   | solvate does not check return status of gmx_file_rename                                               |                | 12/04/2019 01:43 PM |                            |
| 3224 | GROMACS | Task    | New                   | Normal   | add regression test case large enough to miscalculated GPU grid launch cases                          |                | 12/20/2019 01:18 PM | 2021                       |

| #    | Project | Tracker | Status          | Priority | Subject                                                                                                                                       | Assignee         | Updated             | Target version             |
|------|---------|---------|-----------------|----------|-----------------------------------------------------------------------------------------------------------------------------------------------|------------------|---------------------|----------------------------|
| 3223 | GROMACS | Bug     | New             | Normal   | unit test failures give verify -1                                                                                                             |                  | 12/02/2019 11:58 AM |                            |
| 3220 | GROMACS | Task    | New             | Normal   | change rolling pruning scheduling with GPU update                                                                                             |                  | 02/25/2020 03:41 PM | 2021-infrastructure-stable |
| 3219 | GROMACS | Bug     | New             | Normal   | MANPATH setting is fragile                                                                                                                    |                  | 11/29/2019 12:44 PM |                            |
| 3216 | GROMACS | Task    | New             | Normal   | improve CPU force reductions                                                                                                                  | Szilárd Páll     | 12/04/2019 09:24 PM |                            |
| 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 |                            |
| 3210 | GROMACS | Bug     | New             | High     | rerun does not reproduce dVcoul/dl                                                                                                            |                  | 12/27/2019 10:45 AM |                            |
| 3209 | GROMACS | Bug     | New             | Normal   | Interactive molecular dynamics with VMD becomes stuttering after reconnecting                                                                 |                  | 11/19/2019 11:36 AM |                            |
| 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 |
| 3202 | GROMACS | Bug     | New             | Low      | gmx solvate fails to overwrite topology file                                                                                                  |                  | 11/13/2019 02:44 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 |                            |
| 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 |
| 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 |                            |
| 3183 | GROMACS | Task    | Accepted        | Normal   | enable bonded interactions on GPU                                                                                                             |                  | 12/20/2019 08:32 AM | 2021-infrastructure-stable |
| 3181 | GROMACS | Task    | New             | Normal   | consolidate task assignment and workload data initialization                                                                                  |                  | 10/28/2019 02:53 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 |
| 3179 | GROMACS | Feature | New             | Normal   | Clarify access to parallel data outputs                                                                                                       | Eric Irrgang     | 10/26/2019 12:23 PM |                            |
| 3177 | GROMACS | Feature | New             | Normal   | Spack package management support                                                                                                              |                  | 11/06/2019 06:37 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 |                            |

| #    | Project | Tracker | Status          | Priority | Subject                                                                           | Assignee       | Updated             | Target version             |
|------|---------|---------|-----------------|----------|-----------------------------------------------------------------------------------|----------------|---------------------|----------------------------|
| 3172 | GROMACS | Feature | New             | Normal   | QM/MM Interface with CP2K                                                         | Dmitry Morozov | 01/17/2020 12:18 PM | future                     |
| 3171 | GROMACS | Task    | New             | Normal   | schedule CPU H2D force contribution in separate stream                            |                | 12/20/2019 08:33 AM | 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 |                            |
| 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 |
| 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 |
| 3155 | GROMACS | Task    | Accepted        | Normal   | Unify DD and CPU-GPU gather & scatter                                             | Artem Zhmurov  | 10/17/2019 03:50 PM | 2021-infrastructure-stable |
| 3154 | GROMACS | Task    | Resolved        | Low      | Update use of Python subprocess for >=3.5                                         |                | 04/09/2020 10:15 PM |                            |
| 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 |
| 3152 | GROMACS | Feature | New             | Normal   | Infrastructure and patterns for expressing public interfaces                      |                | 01/09/2020 05:19 PM | 2021-infrastructure-stable |
| 3150 | GROMACS | Bug     | New             | Normal   | gmxapi data type annotations are confusing and inadequate                         | Eric Irrgang   | 10/22/2019 03:08 PM | 2021-infrastructure-stable |
| 3149 | GROMACS | Feature | New             | Normal   | Python user interface for obtaining simulation artifacts as files.                | Eric Irrgang   | 10/15/2019 06:21 PM |                            |
| 3148 | GROMACS | Feature | New             | Normal   | Roadmap for gmxapi filesystem interactions.                                       | Eric Irrgang   | 10/15/2019 06:23 PM | 2021-infrastructure-stable |
| 3147 | GROMACS | Feature | New             | Normal   | gmxapi workflow checkpointing                                                     | Eric Irrgang   | 10/15/2019 06:18 PM | 2021-infrastructure-stable |
| 3145 | GROMACS | Task    | New             | Normal   | gmxapi.mdrun needs improved (and public) interface for attaching an MD extension. | Eric Irrgang   | 01/16/2020 04:31 PM | 2021-refactoring           |
| 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                       |
| 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 |
| 3139 | GROMACS | Task    | New             | Normal   | gmxapi Futures should be subscribable                                             | Eric Irrgang   | 10/15/2019 03:56 PM |                            |
| 3138 | GROMACS | Feature | New             | Normal   | Improve ensemble support in Context specification.                                |                | 10/15/2019 03:56 PM |                            |
| 3136 | GROMACS | Bug     | New             | Normal   | gmxapi.operation data flow topology unclear or incomplete                         | Eric Irrgang   | 12/11/2019 11:25 AM | 2021-infrastructure-stable |
| 3135 | GROMACS | Feature | New             | Normal   | Make GPU traits into 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 |                            |
| 3133 | GROMACS | Task    | In Progress     | Normal   | Cookiecutter for sample_restraint                                                 | Eric Irrgang   | 12/10/2019 01:59 PM | 2021-infrastructure-stable |
| 3132 | GROMACS | Task    | New             | Normal   | gmxapi testing support tools                                                      |                | 10/31/2019 03:35 PM |                            |
| 3131 | GROMACS | Task    | New             | Normal   | support ccache with clang-tidy                                                    | Mark Abraham   | 12/20/2019 08:20 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 |



| #    | Project | Tracker | Status             | Priority | Subject                                                                                       | Assignee        | Updated             | Target version             |
|------|---------|---------|--------------------|----------|-----------------------------------------------------------------------------------------------|-----------------|---------------------|----------------------------|
| 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 |                            |
| 3125 | GROMACS | Bug     | Resolved           | Normal   | OpenCL on Volta and Turing broken                                                             |                 | 02/27/2020 11:01 AM | 2020.2                     |
| 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                       |
| 3123 | GROMACS | Task    | New                | Normal   | address sanitizer coverage of parallelization code-paths                                      |                 | 10/05/2019 12:32 AM |                            |
| 3119 | GROMACS | Task    | New                | Normal   | clang-tidy coverage of parallelization codepaths                                              |                 | 12/27/2019 04:20 PM | 2021                       |
| 3117 | GROMACS | Feature | New                | Normal   | Coulomb FEP PME on GPU                                                                        | Magnus Lundborg | 02/17/2020 03:58 PM | 2021-infrastructure-stable |
| 3116 | GROMACS | Bug     | New                | Normal   | regressiontests/freeenergy 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 |                            |
| 3114 | GROMACS | Feature | New                | Normal   | Improve GPU update-constraints module                                                         | Artem Zhmurov   | 02/10/2020 04:30 PM | 2021                       |
| 3113 | GROMACS | Bug     | New                | Low      | Use of read_tps_conf is deprecated                                                            | Paul Bauer      | 10/01/2019 11:36 AM | 2021-infrastructure-stable |
| 3105 | GROMACS | Task    | New                | Normal   | implement GPU PME/PP comm cycle counting                                                      |                 | 12/27/2019 04:20 PM | 2021                       |
| 3104 | GROMACS | Task    | New                | Normal   | implement GPU DD cycle counting                                                               |                 | 12/27/2019 04:21 PM | 2021                       |
| 3101 | GROMACS | Bug     | Blocked, need info | Normal   | detect compilation failed                                                                     | Erik Lindahl    | 12/27/2019 10:52 AM |                            |
| 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 |
| 3093 | GROMACS | Task    | In Progress        | High     | rework GPU direct halo-exchange related force reduction complexities                          |                 | 02/14/2020 11:35 AM | 2021-infrastructure-stable |
| 3088 | GROMACS | Bug     | New                | Normal   | Reference to theory needed for cylindrical pull geometry                                      |                 | 09/13/2019 11:26 AM |                            |
| 3086 | GROMACS | Bug     | New                | Normal   | gmxapi fails with MPI build of GROMACS 2020                                                   |                 | 09/25/2019 04:18 PM |                            |
| 3083 | GROMACS | Bug     | New                | Normal   | Listed forces tests failing on ICC19 with AVX2_256 nightly build                              |                 | 09/10/2019 11:56 AM |                            |
| 3082 | GROMACS | Task    | New                | High     | move launch/synchronization points to clarify task dependencies                               |                 | 12/27/2019 04:21 PM | 2021                       |
| 3078 | GROMACS | Task    | New                | Normal   | Allow MD modules to register energy output fields themselves                                  |                 | 09/06/2019 11:36 AM |                            |
| 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 |                            |
| 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 |
| 3075 | GROMACS | Bug     | New                | Normal   | Frozen atoms are moving                                                                       | Erik Lindahl    | 12/27/2019 10:51 AM |                            |
| 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 gmx::index for indexing instead of int                                                    | Christian Blau  | 09/03/2019 04:23 PM | 2021-infrastructure-stable |

| #    | Project | Tracker | Status          | Priority | Subject                                                                                                                                                       | Assignee            | Updated             | Target version             |
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| 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                     |
| 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                     |
| 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 |                            |
| 3064 | GROMACS | Task    | New             | Normal   | add test for perturbed bonded forces                                                                                                                          |                     | 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                       |
| 3058 | GROMACS | Bug     | Feedback wanted | Normal   | Error when using a large PME grid on a GPU                                                                                                                    |                     | 09/04/2019 07:26 PM |                            |
| 3057 | GROMACS | Task    | New             | Normal   | re-enable fusion on Power8/9                                                                                                                                  | Szilárd Páll        | 12/27/2019 04:22 PM | 2021                       |
| 3055 | GROMACS | Bug     | Feedback wanted | Normal   | Error in gmx xpm2ps                                                                                                                                           |                     | 08/22/2019 03:27 PM |                            |
| 3054 | GROMACS | Bug     | New             | Normal   | Missing dihedral define                                                                                                                                       |                     | 08/02/2019 05:47 PM |                            |
| 3050 | GROMACS | Bug     | New             | Low      | Fix tests on Solaris                                                                                                                                          | Vedran Miletic      | 02/27/2020 11:05 AM | 2020.2                     |
| 3049 | GROMACS | Bug     | New             | Low      | gmx nmeig should plot a real infrared spectrum                                                                                                                | David van der Spoel | 09/24/2019 03:25 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 |                            |
| 3047 | GROMACS | Task    | Feedback wanted | Normal   | Set required versions for GROMACS 2021                                                                                                                        |                     | 02/20/2020 11:42 AM |                            |
| 3045 | GROMACS | Feature | New             | Low      | Option to remove v-sites in trjconv?                                                                                                                          |                     | 07/19/2019 04:42 PM |                            |
| 3042 | GROMACS | Bug     | New             | Normal   | core dump error in grompp command                                                                                                                             |                     | 10/09/2019 07:30 PM |                            |
| 3041 | GROMACS | Task    | Resolved        | Normal   | Remove workaround for gcc bug 58265                                                                                                                           |                     | 06/19/2020 04:45 PM |                            |
| 3040 | GROMACS | Task    | New             | Normal   | Refactor Restraint module                                                                                                                                     |                     | 07/18/2019 03:59 PM |                            |
| 3038 | GROMACS | Feature | New             | Normal   | Improvements to MD plugin development environment                                                                                                             | Eric Irrgang        | 12/10/2019 01:58 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 |
| 3033 | GROMACS | Task    | In Progress     | Normal   | Clean up and modernize googletest bundling and usage                                                                                                          |                     | 01/16/2020 04:50 PM | 2021-refactoring           |
| 3032 | GROMACS | Feature | Feedback wanted | Normal   | Clean up dev-manual structure                                                                                                                                 |                     | 12/11/2019 11:27 AM | 2021-infrastructure-stable |
| 3031 | GROMACS | Task    | New             | Normal   | evaluate the impact of particle order on PME                                                                                                                  |                     | 12/27/2019 04:29 PM | 2021                       |
| 3030 | GROMACS | Feature | New             | Normal   | RST style guidelines                                                                                                                                          |                     | 07/09/2019 03:38 PM |                            |
| 3028 | GROMACS | Bug     | Feedback wanted | Normal   | install fail on Centos 6                                                                                                                                      |                     | 07/15/2019 12:32 PM |                            |
| 3021 | GROMACS | Feature | Feedback wanted | Normal   | Completion of docs for GPU developments                                                                                                                       |                     | 03/02/2020 03:58 PM | 2020.2                     |

| #    | Project | Tracker | Status      | Priority | Subject                                                                           | Assignee      | Updated             | Target version             |
|------|---------|---------|-------------|----------|-----------------------------------------------------------------------------------|---------------|---------------------|----------------------------|
| 3020 | GROMACS | Feature | New         | Low      | modernize DeviceBuffer and GPU memory management                                  |               | 08/13/2019 06:01 PM |                            |
| 3016 | GROMACS | Task    | New         | Normal   | intermittent failure of essentialdynamics test                                    |               | 07/18/2019 05:23 PM |                            |
| 3015 | GROMACS | Task    | New         | Normal   | Create central log handle for calls to gmxfatal                                   |               | 09/06/2019 02:34 PM | 2021-infrastructure-stable |
| 3014 | GROMACS | Task    | In Progress | Normal   | gmxfapi example Python scripts                                                    |               | 01/03/2020 11:00 AM | 2021-infrastructure-stable |
| 3013 | GROMACS | Task    | New         | Normal   | Extend logging levels in MDLogger                                                 |               | 09/06/2019 02:34 PM | 2021-infrastructure-stable |
| 3010 | GROMACS | Task    | In Progress | Normal   | upgrade OpenCL stack on bs-gpu01                                                  |               | 12/20/2019 08:25 AM | 2021-infrastructure-stable |
| 3008 | GROMACS | Task    | New         | Normal   | verify block size choice of CUDA bonded kernel                                    |               | 12/27/2019 04:30 PM | 2021                       |
| 3005 | GROMACS | Task    | New         | Normal   | Move logging in gmxf 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 |                            |
| 3001 | GROMACS | Task    | New         | Normal   | explore simplifying virial and shift force reduction                              |               | 12/27/2019 04:30 PM | 2021                       |
| 3000 | GROMACS | Bug     | New         | Normal   | CMake "webpage" target does not fail when it should                               |               | 06/25/2019 02:43 PM |                            |
| 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 |
| 2998 | GROMACS | Task    | Resolved    | Normal   | Update Python detection                                                           |               | 04/23/2020 04:45 PM | 2021-infrastructure-stable |
| 2997 | GROMACS | Task    | New         | Normal   | improve performance of alchemical free energy calculations                        |               | 12/27/2019 04:31 PM | 2021                       |
| 2996 | GROMACS | Feature | In Progress | Normal   | gmxfapi execution model                                                           | Eric Irrgang  | 12/10/2019 01:57 PM | 2021-infrastructure-stable |
| 2994 | GROMACS | Feature | New         | Normal   | Data flow topology in gmxfapi 2020                                                |               | 12/11/2019 11:33 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 |                            |
| 2992 | GROMACS | Task    | New         | Normal   | Split hw_opt in const user options and dynamic settings                           |               | 12/27/2019 04:31 PM | future                     |
| 2988 | GROMACS | Task    | In Progress | Low      | clean up and refactor code to modern standards                                    |               | 12/27/2019 04:37 PM | future                     |
| 2987 | GROMACS | Bug     | New         | Normal   | assess the bonded GPU task assignment default                                     |               | 12/20/2019 01:06 PM | 2021                       |
| 2984 | GROMACS | Feature | New         | Normal   | More Extensive Selections Examples                                                | Dallas Warren | 06/18/2019 11:50 PM |                            |
| 2983 | GROMACS | Task    | New         | Normal   | better suited data-types for bonded GPU kernels                                   |               | 07/11/2019 04:32 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 |                            |
| 2978 | GROMACS | Bug     | New         | Normal   | Some suggestions about the gmxf current tool                                      |               | 06/13/2019 12:41 PM |                            |
| 2977 | GROMACS | Feature | New         | Normal   | print DD load balancing improvement                                               |               | 06/13/2019 10:56 AM |                            |
| 2976 | GROMACS | Task    | New         | Normal   | Basic math for Multidimensional arrays                                            |               | 12/27/2019 04:37 PM | 2021                       |
| 2975 | GROMACS | Feature | New         | Normal   | LJ PME calculations on GPUs                                                       |               | 06/12/2019 01:17 PM |                            |
| 2974 | GROMACS | Bug     | New         | Normal   | position-restraints regressiontest fails on intel GPU with OpenCL                 |               | 02/25/2020 03:52 PM | 2020.2                     |
| 2967 | GROMACS | Feature | New         | Normal   | GPU reallocateDeviceBuffer improvements                                           |               | 01/23/2020 12:15 PM | 2021-refactoring           |

| #    | Project                | Tracker | Status      | Priority | Subject                                                                                    | Assignee       | Updated             | Target version             |
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| 2965 | GROMACS                | Task    | In Progress | Normal   | Performance of GPU direct communications                                                   |                | 02/14/2020 12:38 PM | 2021                       |
| 2961 | GROMACS                | Feature | New         | Normal   | How should Python package find GROMACS resources under various circumstances?              |                | 12/09/2019 10:47 AM |                            |
| 2958 | GROMACS                | Bug     | New         | Normal   | Compiling master (to become 2020) using CUDA 9.0                                           |                | 03/02/2020 03:57 PM | 2020.2                     |
| 2956 | GROMACS                | Feature | New         | Normal   | SAXS resolution                                                                            |                | 05/17/2019 09:58 AM |                            |
| 2954 | GROMACS                | Bug     | New         | Normal   | genion changes residue numbering                                                           |                | 05/26/2019 12:08 AM |                            |
| 2949 | GROMACS                | Bug     | New         | Normal   | cmake fails when building mdrun only                                                       |                | 07/08/2019 10:04 AM |                            |
| 2948 | GROMACS                | Bug     | New         | Normal   | SIMD support detected as none on AMD R5 2500U                                              |                | 05/21/2019 12:58 PM |                            |
| 2947 | GROMACS                | Task    | Accepted    | Normal   | make an end to end test for membed                                                         |                | 09/24/2019 03:22 PM | future                     |
| 2944 | GROMACS                | Feature | New         | Normal   | Roadmap for thermostats / barostats in new propagation/integration scheme                  | Michael Shirts | 12/27/2019 04:00 PM | 2021                       |
| 2937 | TNG trajectory library | Bug     | New         | Normal   | tng_num_frames_get reports incorrect num frames                                            |                | 04/29/2019 11:30 AM |                            |
| 2936 | GROMACS                | Task    | New         | Normal   | introduce check that CPU-GPU transfers/assignments are made between compatible types       |                | 02/05/2020 03:57 PM | 2021                       |
| 2935 | Support Platforms      | Bug     | New         | High     | redmine issue updates about gerrit uploads stopped working                                 |                | 06/11/2019 01:42 PM | current                    |
| 2933 | GROMACS                | Task    | New         | Normal   | Convert walls to a ForceProvider                                                           |                | 04/25/2019 02:43 PM |                            |
| 2931 | GROMACS                | Feature | New         | Normal   | Tables in Verlet kernels                                                                   |                | 04/29/2019 12:01 PM |                            |
| 2930 | GROMACS                | Feature | New         | Normal   | Limited range for reference group detection in cylinder pulling                            |                | 04/26/2019 05:17 PM |                            |
| 2928 | GROMACS                | Feature | New         | Normal   | Add ability to use expression "count of ATOM_EXPR" in selection statements.                |                | 04/16/2019 04:52 PM |                            |
| 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 |
| 2924 | GROMACS                | Bug     | New         | Normal   | Failing version check when reading new tpr file with older gromacs version                 |                | 04/12/2019 10:52 AM |                            |
| 2919 | GROMACS                | Task    | New         | Normal   | C++ style guidelines for namespace use                                                     |                | 04/15/2019 01:21 PM |                            |
| 2916 | GROMACS                | Task    | New         | Normal   | Decide future of symtab                                                                    | Paul Bauer     | 09/06/2019 02:35 PM | 2021-infrastructure-stable |
| 2915 | GROMACS                | Feature | In Progress | High     | GPU direct communications                                                                  |                | 02/14/2020 12:48 PM |                            |
| 2910 | GROMACS                | Feature | New         | Normal   | Mixed scaling for 1-4 interactions                                                         |                | 04/10/2019 10:13 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 |                            |
| 2908 | GROMACS                | Task    | New         | Normal   | Renaming things in nbxnm                                                                   | Berk Hess      | 03/28/2019 10:10 AM |                            |
| 2907 | GROMACS                | Bug     | New         | Normal   | Gromacs autocompletion appears to be broken with ZSH                                       |                | 07/16/2019 04:46 AM |                            |
| 2905 | GROMACS                | Task    | New         | Normal   | Add a Jenkins configuration with std library assert                                        |                | 08/24/2019 05:22 PM |                            |
| 2902 | GROMACS                | Bug     | New         | Normal   | 2019.1 equilibration issue? (Intel 2018u3)                                                 |                | 04/30/2019 08:17 AM |                            |
| 2898 | GROMACS                | Task    | New         | Low      | Naming common variables                                                                    |                | 03/26/2019 11:46 PM |                            |

| #    | Project           | Tracker | Status          | Priority | Subject                                                                    | Assignee            | Updated             | Target version             |
|------|-------------------|---------|-----------------|----------|----------------------------------------------------------------------------|---------------------|---------------------|----------------------------|
| 2897 | GROMACS           | Bug     | New             | Normal   | rotation/flex2 can still fail on cpu-only run on OpenCL build              |                     | 04/04/2019 06:24 PM |                            |
| 2896 | GROMACS           | Feature | Feedback wanted | Normal   | Python packaging                                                           |                     | 01/16/2020 07:11 PM | 2021-refactoring           |
| 2891 | GROMACS           | Feature | In Progress     | Normal   | PME/PP GPU communications                                                  |                     | 02/14/2020 12:40 PM |                            |
| 2890 | GROMACS           | Feature | In Progress     | Normal   | GPU Halo Exchange                                                          |                     | 02/14/2020 12:41 PM | 2021                       |
| 2889 | GROMACS           | Task    | New             | Normal   | update grompp warnings for brevity, usefulness and actionability           | Mark Abraham        | 12/27/2019 04:38 PM | future                     |
| 2883 | GROMACS           | Bug     | New             | Normal   | essentialdynamics fail with Intel MPI                                      |                     | 03/08/2019 03:10 AM |                            |
| 2882 | GROMACS           | Task    | New             | Normal   | evaluate different storage layouts for GPU coordinates/changes/forces      | Szilárd Páll        | 03/07/2019 06:21 PM |                            |
| 2877 | GROMACS           | Task    | New             | Normal   | use gm::Options more                                                       | Mark Abraham        | 12/20/2019 01:22 PM | 2021                       |
| 2876 | GROMACS           | Bug     | New             | Normal   | 2019.1 make check fails on AVX and AVX2 (Intel 2018u3)                     | Erik Lindahl        | 03/08/2019 10:32 AM |                            |
| 2875 | GROMACS           | Task    | Accepted        | Normal   | SIMD version of the free-energy kernel                                     | Berk Hess           | 12/02/2019 01:44 PM | 2021-infrastructure-stable |
| 2874 | GROMACS           | Task    | New             | Normal   | Refactor Gromacs (cluster) neighborlist into separate module               | Erik Lindahl        | 02/28/2019 11:36 AM |                            |
| 2873 | GROMACS           | Bug     | New             | Normal   | Simple way to get last frame from trajectory                               |                     | 02/28/2019 11:14 PM |                            |
| 2872 | GROMACS           | Bug     | New             | Normal   | gmx solvate and genion topology update                                     |                     | 02/27/2019 10:18 AM |                            |
| 2870 | GROMACS           | Bug     | New             | Normal   | GPU detection error message missing from the output                        |                     | 03/05/2019 03:55 PM |                            |
| 2869 | GROMACS           | Bug     | New             | Normal   | GPU detection error only issued as a note to the log                       |                     | 03/05/2019 04:09 PM |                            |
| 2866 | GROMACS           | Feature | New             | Normal   | Alternative non-bonded potentials                                          | David van der Spoel | 03/05/2019 03:50 PM | future                     |
| 2864 | GROMACS           | Task    | New             | Normal   | Building incompatibilities                                                 | Benson Muite        | 02/19/2019 02:00 PM |                            |
| 2863 | GROMACS           | Task    | New             | Normal   | improve PBC handling                                                       |                     | 03/11/2019 04:28 PM |                            |
| 2860 | GROMACS           | Feature | New             | Normal   | Option for outputting min/max coordinates in gm traj                       |                     | 02/08/2019 12:35 AM |                            |
| 2859 | GROMACS           | Task    | Resolved        | Normal   | Change ArrayRef iterator type from pointer to std::iterator                |                     | 06/26/2020 06:15 PM |                            |
| 2857 | GROMACS           | Task    | New             | Normal   | Clarify recommended function specifies (constexpr, noexcept, pure)         |                     | 02/04/2019 04:48 AM |                            |
| 2855 | GROMACS           | Task    | New             | Normal   | Allow compiling GROMACS without C compiler                                 |                     | 01/10/2020 12:06 PM |                            |
| 2854 | GROMACS           | Bug     | New             | Normal   | OnlineHelpUnitTests segfaults on s390x with gcc-9.0.1                      | Paul Bauer          | 02/04/2019 11:17 AM |                            |
| 2853 | GROMACS           | Bug     | New             | Normal   | EwaldUnitTests segfault on armv7hl with gcc-9.0.1                          | Paul Bauer          | 02/04/2019 05:34 PM |                            |
| 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 |                            |
| 2850 | GROMACS           | Task    | In Progress     | Normal   | assess Raptor Talos for testing                                            | Szilárd Páll        | 02/12/2019 01:14 PM |                            |
| 2848 | GROMACS           | Bug     | New             | Normal   | gm make_ndx ignores last residue in case only CA's are present in GRO file |                     | 01/30/2019 06:16 AM |                            |

| #    | Project | Tracker | Status             | Priority | Subject                                                                    | Assignee            | Updated             | Target version             |
|------|---------|---------|--------------------|----------|----------------------------------------------------------------------------|---------------------|---------------------|----------------------------|
| 2846 | GROMACS | Feature | New                | Low      | Set rpath in FindLibStdCpp.cmake                                           |                     | 02/02/2019 08:09 AM |                            |
| 2840 | GROMACS | Feature | New                | Normal   | Test that functionality does not compile that is not supposed to.          |                     | 01/25/2019 02:35 PM | future                     |
| 2839 | GROMACS | Task    | New                | Normal   | make module and file naming consistent                                     |                     | 01/16/2020 05:11 PM | 2021                       |
| 2835 | GROMACS | Task    | New                | Normal   | Matrix class constraint to upper or lower triangle                         |                     | 02/07/2019 02:44 PM |                            |
| 2834 | GROMACS | Task    | In Progress        | Normal   | C++ matrix classes                                                         | Christian Blau      | 12/29/2019 10:32 AM | 2021                       |
| 2833 | GROMACS | Task    | New                | Normal   | Update topology datastructures                                             | Paul Bauer          | 12/02/2019 01:43 PM | 2021-infrastructure-stable |
| 2832 | GROMACS | Bug     | New                | Low      | PaddedVector move operations broken                                        | Mark Abraham        | 12/28/2019 10:40 AM | 2021                       |
| 2828 | GROMACS | Bug     | Feedback wanted    | Normal   | Installation issue on Power 9 system with SIMD support                     |                     | 01/18/2019 11:54 AM |                            |
| 2822 | GROMACS | Task    | Accepted           | Normal   | Make nbxn a module                                                         | Berk Hess           | 12/18/2019 10:49 AM | future                     |
| 2818 | GROMACS | Task    | In Progress        | Normal   | bonded GPU kernel fusion                                                   | Magnus Lundborg     | 07/03/2019 09:01 PM |                            |
| 2806 | GROMACS | Feature | New                | Normal   | SIMD algorithms for ARM SVE // nobonded cluster and others                 |                     | 12/27/2019 03:59 PM | 2021                       |
| 2796 | GROMACS | Task    | New                | Low      | clarify what mdrun -cpt means                                              |                     | 01/03/2019 02:09 PM |                            |
| 2795 | GROMACS | Task    | New                | Normal   | Incorporate regressiontests into core gromacs                              |                     | 12/02/2019 01:44 PM | 2021-infrastructure-stable |
| 2792 | GROMACS | Task    | New                | High     | Improvement of PME gather and spread CUDA kernels                          |                     | 03/18/2020 03:57 PM |                            |
| 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                     |
| 2788 | GROMACS | Bug     | New                | Normal   | PME will not run on AMD GPU with NVidia GPU present                        |                     | 01/03/2019 02:24 PM |                            |
| 2787 | GROMACS | Task    | New                | Normal   | allow passing flags to allocateDeviceBuffer                                |                     | 12/03/2018 01:54 PM |                            |
| 2785 | GROMACS | Bug     | New                | Normal   | Inconsistent and erroneous behaviour of trjconv when writing a partial TNG |                     | 11/30/2018 02:36 PM |                            |
| 2774 | GROMACS | Feature | New                | Normal   | Refactor shell code into its own integrator                                | David van der Spoel | 12/27/2019 04:05 PM | 2021                       |
| 2773 | GROMACS | Task    | New                | Normal   | improve GPU error handling and make such handling uniform across modules   |                     | 12/20/2019 01:09 PM | 2021                       |
| 2771 | GROMACS | Task    | New                | Normal   | Size independent Hessian for normal mode analysis                          |                     | 12/28/2019 10:50 AM | future                     |
| 2770 | GROMACS | Task    | New                | Normal   | change branch maintenance policy                                           |                     | 01/16/2020 05:09 PM | 2021                       |
| 2766 | GROMACS | Task    | In Progress        | Normal   | Improve hardware option selection                                          | Kevin Boyd          | 12/20/2019 02:34 PM | 2021                       |
| 2764 | GROMACS | Task    | New                | Normal   | gmxapi version updates for post release-2019                               | Eric Irrgang        | 11/21/2018 12:53 PM |                            |
| 2763 | GROMACS | Bug     | New                | Normal   | GMXAPI layout / grouping in development docs "modules" page                |                     | 12/14/2018 12:49 PM | future                     |
| 2762 | GROMACS | Bug     | Blocked, need info | Normal   | incorrect results with Ubuntu 18.04 / glibc 2.27 (?) and >20 threads       |                     | 07/01/2019 11:26 PM |                            |
| 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                     |

| #    | Project | Tracker | Status             | Priority | Subject                                                                                        | Assignee            | Updated             | Target version             |
|------|---------|---------|--------------------|----------|------------------------------------------------------------------------------------------------|---------------------|---------------------|----------------------------|
| 2756 | GROMACS | Task    | In Progress        | Normal   | gmxapi integration testing                                                                     |                     | 01/16/2020 05:12 PM | 2021-refactoring           |
| 2755 | GROMACS | Feature | New                | Low      | md5 sums and sha256, sha512 hashes                                                             | Benson Muite        | 02/19/2019 11:00 PM |                            |
| 2754 | GROMACS | Bug     | New                | Normal   | Simulated Tempering seems to be broken                                                         | Michael Shirts      | 02/05/2019 03:58 PM |                            |
| 2740 | GROMACS | Bug     | New                | Normal   | mdrun reports incorrect error with -bonded gpu without gpu                                     | Mark Abraham        | 11/07/2018 01:59 PM |                            |
| 2739 | GROMACS | Feature | New                | Normal   | Parallel continuous tempering and enhanced sampling feature                                    |                     | 11/13/2018 11:36 PM |                            |
| 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                     |
| 2734 | GROMACS | Bug     | In Progress        | Normal   | regressiontests/kernel core dumps on ppc64le                                                   | Paul Bauer          | 06/15/2019 04:12 PM | future                     |
| 2733 | GROMACS | Bug     | Blocked, need info | Normal   | MdrunUtilityMpiUnitTests timeout on i686 and armv7hl with OpenMPI 2.1.5                        | Paul Bauer          | 01/17/2020 08:40 AM |                            |
| 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                     |
| 2715 | GROMACS | Feature | New                | Normal   | Avoid requesting the user to recompile gromacs for Intel OpenCL support                        |                     | 12/27/2019 04:06 PM | future                     |
| 2713 | GROMACS | Feature | New                | Normal   | Constant offset for external electric fields                                                   |                     | 10/28/2018 12:57 AM |                            |
| 2710 | GROMACS | Feature | New                | Normal   | Separate dvdI for each molecule (of couple-moltype) when running FEP                           |                     | 12/27/2019 04:41 PM | 2021                       |
| 2707 | GROMACS | Bug     | New                | Normal   | Installed OpenCL files include clh file from gpu_utils directory                               |                     | 10/30/2018 04:02 AM |                            |
| 2706 | GROMACS | Task    | Accepted           | Normal   | Rework classic QM/MM interface                                                                 |                     | 12/02/2019 01:45 PM | 2021-infrastructure-stable |
| 2702 | GROMACS | Bug     | Accepted           | Normal   | PME gather reduction race in OpenCL (and CUDA)                                                 |                     | 03/28/2019 03:14 PM |                            |
| 2699 | GROMACS | Task    | New                | Normal   | Test POWER9                                                                                    |                     | 12/04/2019 03:29 PM | 2021-infrastructure-stable |
| 2698 | GROMACS | Task    | In Progress        | Normal   | gmxapi documentation integration                                                               |                     | 01/29/2020 03:59 PM | 2021-infrastructure-stable |
| 2697 | GROMACS | Task    | New                | Normal   | improve FFT library flavor/version reporting                                                   |                     | 12/27/2019 04:40 PM | future                     |
| 2696 | GROMACS | Task    | In Progress        | Normal   | ensure PME queue is flushed                                                                    | Szilárd Páll        | 12/31/2018 11:21 AM | future                     |
| 2695 | GROMACS | Task    | New                | Low      | bonded GPU module timing                                                                       |                     | 12/27/2019 04:40 PM | 2021                       |
| 2693 | GROMACS | Bug     | New                | Normal   | Several memory leaks in mdrun                                                                  |                     | 12/18/2018 04:22 AM | future                     |
| 2686 | GROMACS | Task    | New                | Normal   | add tests for gpu bonded interactions                                                          |                     | 12/27/2019 04:40 PM | 2021                       |
| 2682 | GROMACS | Task    | New                | Normal   | Add MSAN configuration                                                                         |                     | 10/09/2018 06:28 PM |                            |
| 2675 | GROMACS | Task    | In Progress        | Normal   | bonded CUDA offload task                                                                       |                     | 02/12/2020 05:54 PM | 2021                       |
| 2674 | GROMACS | Task    | Accepted           | Normal   | Improve domain decomposition for bilayer systems                                               |                     | 12/07/2018 04:03 PM | future                     |
| 2672 | GROMACS | Task    | New                | Normal   | check & document execution width requirements in OpenCL                                        |                     | 12/31/2018 11:20 AM | future                     |
| 2671 | GROMACS | Task    | New                | Normal   | replace constants like M_PI                                                                    |                     | 12/20/2019 01:17 PM | future                     |
| 2670 | GROMACS | Task    | New                | Low      | remove old/backward compatibility OpenCL support from releng                                   |                     | 10/04/2018 06:06 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                     |

| #    | Project | Tracker | Status       | Priority | Subject                                                                                                             | Assignee          | Updated             | Target version |
|------|---------|---------|--------------|----------|---------------------------------------------------------------------------------------------------------------------|-------------------|---------------------|----------------|
| 2660 | GROMACS | Task    | New          | Low      | rework OpenCL nbxn kernel constants                                                                                 | Szilárd Páll      | 12/28/2019 10:53 AM | future         |
| 2658 | GROMACS | Task    | New          | Normal   | Secondary structure assignment via DSSP as native gromacs code                                                      | Christian Blau    | 10/09/2018 04:51 PM | future         |
| 2657 | GROMACS | Bug     | New          | Normal   | Biphasic tutorial                                                                                                   |                   | 09/28/2018 10:02 AM |                |
| 2650 | GROMACS | Task    | New          | Normal   | revise OpenCL stack recommendations                                                                                 |                   | 12/31/2018 11:19 AM | future         |
| 2649 | GROMACS | Bug     | New          | Normal   | Virial calculation necessary for correct energy calculation on GPU                                                  |                   | 12/17/2018 02:32 PM | future         |
| 2645 | GROMACS | Bug     | New          | Normal   | Security                                                                                                            |                   | 09/28/2018 01:16 PM |                |
| 2644 | GROMACS | Task    | New          | Normal   | Replace compute_globals                                                                                             | Mark Abraham      | 09/24/2018 05:51 PM | future         |
| 2643 | GROMACS | Feature | New          | Low      | mdp options and/or docs for anisotropic aspects of implementations                                                  |                   | 09/12/2018 02:23 PM |                |
| 2637 | GROMACS | Bug     | New          | High     | gmx solvate tears apart molecules                                                                                   |                   | 09/11/2018 07:43 PM |                |
| 2632 | GROMACS | Task    | New          | Low      | make sure cmake defines proper hwloc versionc with cross-compilation enabled                                        |                   | 12/03/2018 01:35 PM | future         |
| 2628 | GROMACS | Bug     | Fix uploaded | Normal   | GMXRC removes trailing colon from existing MANPATH                                                                  |                   | 08/28/2018 03:13 PM |                |
| 2624 | GROMACS | Bug     | New          | Normal   | GPU build system not robust enough                                                                                  |                   | 09/05/2018 02:00 AM |                |
| 2622 | GROMACS | Feature | New          | Low      | Reduce severity of Berendsen warning                                                                                |                   | 08/23/2018 11:16 PM | future         |
| 2621 | GROMACS | Task    | New          | Normal   | Fine-Grained API to Describe Force Calculation and Neighbourhood Search                                             | Prashanth Kanduri | 08/22/2018 11:36 AM | future         |
| 2616 | GROMACS | Task    | New          | Normal   | Model for MD state                                                                                                  |                   | 09/14/2018 05:12 PM |                |
| 2611 | GROMACS | Bug     | New          | Normal   | issues with gpu_utils-test with GMX_BUILD_UNITTESTS=OFF and on OSX                                                  |                   | 08/14/2018 07:03 PM |                |
| 2608 | GROMACS | Task    | New          | Normal   | Remove code duplication between OpenCL and CUDA                                                                     |                   | 09/24/2018 12:47 PM |                |
| 2607 | GROMACS | Bug     | New          | Normal   | Grompp becomes extremely slow when many pull groups are present                                                     |                   | 08/11/2018 08:54 AM |                |
| 2606 | GROMACS | Bug     | New          | Normal   | Free Energy Calculation -- Function type Fourier Dih. Not implemented in ip_pert                                    |                   | 08/10/2018 01:48 AM |                |
| 2603 | GROMACS | Task    | New          | Normal   | Add ability to properly check coordinate files during testing                                                       | Paul Bauer        | 10/15/2018 01:16 PM | future         |
| 2602 | GROMACS | Bug     | New          | Low      | build information gets outdated if build tree is reused                                                             |                   | 08/13/2018 09:04 PM |                |
| 2601 | GROMACS | Feature | New          | Normal   | Free energy calculations, soft-core potential                                                                       | Vytautas Gapsys   | 02/10/2020 11:29 AM | future         |
| 2600 | GROMACS | Bug     | New          | High     | coul-lambdas turns off all coulombic interactions in system instead of the molecule specified in the couple-moltype |                   | 08/07/2018 06:50 PM |                |
| 2598 | GROMACS | Bug     | New          | Normal   | Tools using read_next_x cannot read TNG files with sanitizers                                                       |                   | 10/15/2018 01:16 PM | future         |
| 2596 | GROMACS | Feature | New          | Normal   | Constant potential method                                                                                           | Benson Muite      | 05/10/2019 09:54 AM |                |
| 2595 | GROMACS | Task    | New          | Normal   | Reusable Utilities for Schedules                                                                                    | Prashanth Kanduri | 02/22/2019 03:48 PM | future         |



| #    | Project | Tracker | Status             | Priority | Subject                                                                                           | Assignee            | Updated             | Target version |
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| 2594 | GROMACS | Feature | New                | Normal   | Multi-level GMX API                                                                               | Prashanth Kanduri   | 02/22/2019 03:48 PM | future         |
| 2590 | GROMACS | Task    | New                | Normal   | Essential Dynamics as module providing forces                                                     | Christian Blau      | 08/22/2018 05:03 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 |                |
| 2585 | GROMACS | Feature | Resolved           | Normal   | Infrastructure supporting external API                                                            |                     | 12/11/2019 12:39 PM |                |
| 2582 | GROMACS | Bug     | Blocked, need info | Normal   | Compilation issues with CUDA V9.1.85 and both gcc5 and gcc6                                       | Szilárd Páll        | 07/23/2018 07:46 PM |                |
| 2581 | GROMACS | Feature | Accepted           | Normal   | User interface for hybrid Monte Carlo                                                             |                     | 12/20/2019 12:24 PM | future         |
| 2580 | GROMACS | Bug     | Feedback wanted    | High     | sc-coul option yields different free energy estimate on a ligand with zero partial charge         |                     | 09/11/2018 08:10 AM |                |
| 2579 | GROMACS | Feature | New                | Normal   | Add dimensionality option to gmx trjconv -center                                                  |                     | 07/19/2018 04:53 PM | future         |
| 2576 | GROMACS | Bug     | New                | Normal   | gmx potential -correct outputs the wrong potential                                                |                     | 07/25/2018 02:58 PM |                |
| 2574 | GROMACS | Feature | New                | Normal   | iForceSchedule Abstraction                                                                        | Prashanth Kanduri   | 03/29/2019 05:20 PM | future         |
| 2573 | GROMACS | Bug     | New                | High     | Different mdp files describing the same change yield different free energy on the same trajectory |                     | 07/19/2018 06:52 PM |                |
| 2570 | GROMACS | Feature | New                | Normal   | Better string formatting and printing                                                             |                     | 05/02/2019 12:20 PM |                |
| 2568 | GROMACS | Bug     | New                | Low      | gmx editconf -rotate does not rotate the box                                                      |                     | 07/10/2018 10:27 AM | future         |
| 2567 | GROMACS | Bug     | New                | Normal   | make check fails at test 23 SIMD errors                                                           |                     | 07/10/2018 09:35 AM |                |
| 2564 | GROMACS | Bug     | New                | Normal   | Result Summary Different For Jobs With Different Numbers of Nodes                                 |                     | 07/05/2018 02:39 PM |                |
| 2563 | GROMACS | Bug     | New                | Normal   | Windows 7 Compilation with GPU support                                                            |                     | 07/02/2018 09:58 AM |                |
| 2556 | GROMACS | Feature | New                | Normal   | make default selections suitable for DNA and RNA                                                  | Mark Abraham        | 06/20/2018 01:48 PM |                |
| 2555 | GROMACS | Bug     | New                | Low      | building GROMACS 2018.2                                                                           |                     | 07/03/2018 11:41 PM |                |
| 2547 | GROMACS | Feature | New                | Low      | Add option of averaging and obtaining error bars for AWH PMFs                                     | Viveca Lindahl      | 06/06/2018 11:31 AM | future         |
| 2546 | GROMACS | Task    | New                | Normal   | Add more assertions to AWH code                                                                   | Viveca Lindahl      | 06/06/2018 11:20 AM | future         |
| 2545 | GROMACS | Feature | New                | Normal   | Should grompp fix periodicity of input files?                                                     | David van der Spoel | 10/03/2018 11:32 PM | future         |
| 2544 | GROMACS | Bug     | New                | Normal   | gmx rmsf does not fix periodicity in reference structure                                          | David van der Spoel | 08/21/2018 10:36 AM | future         |
| 2538 | GROMACS | Task    | New                | Normal   | organize more of the PME GPU code along task-specific lines                                       | Mark Abraham        | 05/31/2018 05:41 PM |                |
| 2537 | GROMACS | Task    | New                | Normal   | Simplify PME solve reduction                                                                      | Aleksei Lupinov     | 12/20/2019 12:21 PM | future         |

| #    | Project | Tracker | Status          | Priority | Subject                                                                                 | Assignee        | Updated             | Target version             |
|------|---------|---------|-----------------|----------|-----------------------------------------------------------------------------------------|-----------------|---------------------|----------------------------|
| 2535 | GROMACS | Task    | New             | Normal   | consider compiling opencl fft kernels once                                              |                 | 05/31/2018 01:33 PM |                            |
| 2532 | GROMACS | Task    | New             | Normal   | enable queue priorities in OpenCL                                                       |                 | 05/29/2018 02:29 PM |                            |
| 2531 | GROMACS | Task    | New             | Low      | Consider optimizing tabulated data access on GPU                                        |                 | 07/30/2018 12:31 PM |                            |
| 2530 | GROMACS | Task    | New             | Normal   | consider using CUDA Driver API                                                          |                 | 09/23/2018 11:47 PM | future                     |
| 2528 | GROMACS | Task    | New             | Normal   | PME GPU tuning                                                                          |                 | 12/31/2018 11:18 AM | future                     |
| 2527 | GROMACS | Task    | New             | Normal   | Rename GpuEventSynchronizer to something more fitting (after mergin PME OpenCL)         |                 | 10/30/2018 04:06 AM | future                     |
| 2526 | GROMACS | Bug     | New             | Normal   | Bug of gmx hbond                                                                        |                 | 05/30/2018 03:12 PM |                            |
| 2524 | GROMACS | Task    | New             | Normal   | struct alignment/packing for OpenCL host & device code                                  |                 | 12/20/2019 12:20 PM | future                     |
| 2522 | GROMACS | Task    | Resolved        | Normal   | OpenCL context duplication                                                              |                 | 03/11/2020 04:15 PM | future                     |
| 2521 | GROMACS | Task    | New             | Normal   | Implement alternating PME/NB wait for OpenCL                                            |                 | 10/15/2018 12:39 PM |                            |
| 2520 | GROMACS | Task    | New             | Normal   | Treat OpenCL kernel width more diligently                                               |                 | 05/24/2018 06:21 PM |                            |
| 2519 | GROMACS | Task    | New             | High     | Improve/remove PME OpenCL kernel barriers                                               |                 | 02/15/2019 06:34 PM |                            |
| 2518 | GROMACS | Task    | New             | Normal   | redesign task-assignment code for OpenCL                                                |                 | 12/20/2019 12:19 PM | future                     |
| 2516 | GROMACS | Task    | New             | Low      | Support PME OpenCL execution width < 16                                                 | Aleksei lupinov | 06/05/2019 05:32 PM |                            |
| 2514 | GROMACS | Task    | New             | Normal   | PME OpenCL reductions with intrinsics                                                   |                 | 05/31/2018 12:27 AM | future                     |
| 2513 | GROMACS | Bug     | Feedback wanted | Normal   | ref_t and temperature incorrect with coulomb-type = user                                | Yu Du           | 05/31/2018 04:05 PM |                            |
| 2501 | GROMACS | Task    | New             | Normal   | Documentation section on log file contents                                              | Kevin Boyd      | 10/03/2018 09:48 PM | future                     |
| 2498 | GROMACS | Task    | New             | Normal   | OpenCL memory pinning/mapping                                                           |                 | 12/20/2019 12:18 PM | future                     |
| 2496 | GROMACS | Task    | New             | Low      | find system xdr properly                                                                |                 | 05/02/2018 02:19 PM |                            |
| 2495 | GROMACS | Task    | Accepted        | Normal   | replace -noconfout with mdp option                                                      | Mark Abraham    | 12/28/2019 10:39 AM | 2021                       |
| 2492 | GROMACS | Task    | New             | Normal   | implement force calculation via ForceProviders containing collections of IForceProvider | Mark Abraham    | 09/19/2018 03:13 PM | future                     |
| 2491 | GROMACS | Feature | New             | Low      | Allow constant bias AWH simulations                                                     | Viveca Lindahl  | 06/05/2018 10:38 PM | future                     |
| 2490 | GROMACS | Task    | New             | Normal   | evaluate two-step communicators                                                         | Szilárd Páll    | 10/03/2018 09:47 PM | future                     |
| 2488 | GROMACS | Task    | New             | Normal   | use MPI non-blocking collectives to overlap pull comm                                   |                 | 04/25/2018 04:19 PM |                            |
| 2483 | GROMACS | Bug     | New             | Low      | gmx dump writes mdp files that can not be parsed by grompp                              | Paul Bauer      | 10/08/2018 10:50 AM | future                     |
| 2482 | GROMACS | Bug     | Feedback wanted | Normal   | Atoms/molecules in freezegrps move and system crashes                                   |                 | 05/18/2018 07:13 PM |                            |
| 2481 | GROMACS | Task    | New             | Low      | Update gmx report-methods to write more method information                              |                 | 12/02/2019 01:22 PM | 2021-infrastructure-stable |
| 2480 | GROMACS | Bug     | New             | Normal   | pdb2gmx does not protonate correctly for united-atom Gromos                             | Mark Abraham    | 12/20/2019 12:17 PM | 2021                       |

| #    | Project | Tracker | Status      | Priority | Subject                                                             | Assignee            | Updated             | Target version |
|------|---------|---------|-------------|----------|---------------------------------------------------------------------|---------------------|---------------------|----------------|
| 2478 | GROMACS | Task    | New         | Low      | avoid use of getenv in static initialization                        |                     | 04/13/2018 11:57 AM |                |
| 2475 | GROMACS | Task    | New         | Normal   | make OpenCL 1st class-citizen in the build system                   |                     | 12/20/2019 12:14 PM | 2021           |
| 2473 | GROMACS | Bug     | New         | Normal   | mdrun sometimes stalls due to large coordinates with no constraints |                     | 04/04/2018 10:15 PM |                |
| 2469 | GROMACS | Task    | New         | Normal   | implement GPU timer reduction for reporting                         |                     | 03/27/2018 05:08 PM |                |
| 2468 | GROMACS | Bug     | New         | Low      | incorrect GPU timing reported with OpenCL and domain decomposition  |                     | 12/17/2018 01:28 PM | future         |
| 2464 | GROMACS | Task    | New         | Normal   | GPU performance goals overview                                      |                     | 03/26/2018 10:42 AM |                |
| 2463 | GROMACS | Task    | New         | Low      | PME GPU decomposition                                               |                     | 03/26/2018 10:42 AM |                |
| 2462 | GROMACS | Task    | New         | Normal   | consider adding STL misuse tests                                    |                     | 03/23/2018 01:23 AM |                |
| 2460 | GROMACS | Bug     | New         | Normal   | Allow inclusion of user libraries through CMake cache variables     |                     | 03/28/2018 08:47 PM |                |
| 2456 | GROMACS | Task    | New         | Normal   | Add a pull module external potential tests                          |                     | 03/15/2018 03:02 PM |                |
| 2453 | GROMACS | Task    | Resolved    | High     | PME OpenCL porting effort                                           | Aleksei lupinov     | 12/20/2019 12:18 PM | 2021           |
| 2452 | GROMACS | Task    | In Progress | Normal   | Reduce data dependencies in mdrun algorithms                        | Berk Hess           | 03/14/2018 08:47 PM |                |
| 2451 | GROMACS | Feature | Resolved    | Normal   | Linear virtual sites with fixed distance                            | David van der Spoel | 09/16/2019 01:15 PM |                |

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