

## Issues

#	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
2896	GROMACS	Feature	Feedback wanted	Normal	Python packaging		01/16/2020 07:11 PM	2021-refactoring
2967	GROMACS	Feature	New	Normal	GPU reallocateDeviceBuffer improvements		01/23/2020 12:15 PM	2021-refactoring
3033	GROMACS	Task	In Progress	Normal	Clean up and modernize googletest bundling and usage		01/16/2020 04:50 PM	2021-refactoring
3290	GROMACS	Task	Resolved	Normal	Require CMake >= 3.12		04/14/2020 02:45 PM	2021-refactoring
3307	GROMACS	Feature	New	Normal	General interface for communication between simulation ranks		01/22/2020 03:22 PM	2021-refactoring
3311	GROMACS	Feature	In Progress	Normal	GPU infrastructure development		03/20/2020 09:54 AM	2021-refactoring
3324	GROMACS	Task	New	Normal	Rework CMake handling of GPU code		01/22/2020 09:52 AM	2021-refactoring
3325	GROMACS	Task	New	Normal	Allow complete re-initialization of a simulation		01/29/2020 05:13 PM	2021-refactoring
3326	GROMACS	Task	New	Normal	Allow changing task assignment		01/22/2020 09:44 AM	2021-refactoring
3327	GROMACS	Task	New	Normal	Refactor workload flags		01/22/2020 09:45 AM	2021-refactoring
3328	GROMACS	Feature	New	Normal	Testing framework for task assignment		01/22/2020 09:48 AM	2021-refactoring
3329	GROMACS	Task	New	Normal	Extend energy comparison testing framework		01/22/2020 09:51 AM	2021-refactoring
3330	GROMACS	Task	New	Normal	Compile list of codepaths for testing task assignment		01/22/2020 10:03 AM	2021-refactoring
3374	GROMACS	Feature	New	Normal	SimulationInput abstraction		03/03/2020 05:32 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
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
3314	GROMACS	Task	Resolved	Normal	Platform agnostic DeviceStream	Artem Zhmurov	03/20/2020 09:55 AM	2021-refactoring
3315	GROMACS	Task	Resolved	Normal	Platform agnostic DeviceContext	Artem Zhmurov	03/11/2020 04:15 PM	2021-refactoring
3316	GROMACS	Task	Accepted	Normal	Context and Stream manager	Artem Zhmurov	01/22/2020 09:49 AM	2021-refactoring
3317	GROMACS	Task	Resolved	Normal	Improve testing of the GPU code	Artem Zhmurov	10/06/2020 12:15 PM	2021-refactoring
3318	GROMACS	Feature	In Progress	Normal	Use wrappers for the GPU buffer copy/allocations	Artem Zhmurov	01/23/2020 12:01 PM	2021-refactoring
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
3320	GROMACS	Task	In Progress	Normal	Remove duplicating D2H/H2D wrappers in NBNXM	Artem Zhmurov	01/22/2020 09:50 AM	2021-refactoring

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3321	GROMACS	Task	Accepted	Normal	Add D2D wrapper	Artem Zhmurov	01/22/2020 09:50 AM	2021-refactoring
3322	GROMACS	Task	Accepted	Normal	Add reallocate(...) function that does not care about the contents of the buffer	Artem Zhmurov	01/22/2020 09:50 AM	2021-refactoring
3323	GROMACS	Task	In Progress	Normal	Rework the StatePropagatorDataGpu	Artem Zhmurov	01/22/2020 09:50 AM	2021-refactoring
3145	GROMACS	Task	New	Normal	gmxapi.mdrun needs improved (and public) interface for attaching an MD extension.	Eric Irrgang	01/16/2020 04:31 PM	2021-refactoring
3295	GROMACS	Feature	New	Normal	Expand gmxapi.modify_input use cases.	Eric Irrgang	01/16/2020 05:13 PM	2021-refactoring
3416	GROMACS	Task	New	Normal	Port post-submit matrix to Gitlab CI	Joe Jordan	03/16/2020 05:50 PM	2021-refactoring
3415	GROMACS	Task	New	Normal	Port Pre-submit matrix to Gitlab CI	Szilárd Páll	03/23/2020 10:09 AM	2021-refactoring
2958	GROMACS	Bug	New	Normal	Compiling master (to become 2020) using CUDA 9.0		03/02/2020 03:57 PM	2020.2
2974	GROMACS	Bug	New	Normal	position-restraints regressiontest fails on intel GPU with OpenCL		02/25/2020 03:52 PM	2020.2
3021	GROMACS	Feature	Feedback wanted	Normal	Completion of docs for GPU developments		03/02/2020 03:58 PM	2020.2
3125	GROMACS	Bug	Resolved	Normal	OpenCL on Volta and Turing broken		02/27/2020 11:01 AM	2020.2
3334	GROMACS	Bug	New	Normal	Check for DD when increasing rlist is broken	Berk Hess	02/25/2020 03:28 PM	2020.2
3441	GROMACS	Bug	Resolved	Normal	Ewald surface-epsilon is incorrect	Berk Hess	03/18/2020 11:15 PM	2020.2
3444	GROMACS	Bug	Resolved	Normal	do_dssp does not work(gmx 2020 and 2020.1)	Christian Blau	06/10/2020 02:45 PM	2020.2
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
3408	GROMACS	Bug	Fix uploaded	Normal	Gmxapi* tests segfault in rpmbuild	Eric Irrgang	03/23/2020 01:27 PM	2020.2
3380	GROMACS	Bug	Resolved	Low	IBM VSX checks fail with gcc-10	Erik Lindahl	04/30/2020 01:30 PM	2020.2
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
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
3294	GROMACS	Bug	New	Normal	multiple tests fail on fedora 31	Paul Bauer	02/28/2020 03:12 PM	2020.2
3361	GROMACS	Task	New	Normal	Gitlab source archive contains files from build directory	Paul Bauer	02/25/2020 10:13 AM	2020.2
3266	GROMACS	Bug	New	High	gmx density show wrong symmetrize density profile using -symm?	Super duper	02/28/2020 08:24 AM	2020.2
3071	GROMACS	Bug	Accepted	Normal	complex.nbnxn-ljme-LB-geometric failing with OpenCL timing debug mode assertions	Szilárd Páll	02/25/2020 03:39 PM	2020.2
3050	GROMACS	Bug	New	Low	Fix tests on Solaris	Vedran Miletic	02/27/2020 11:05 AM	2020.2
2481	GROMACS	Task	New	Low	Update gmx report-methods to write more method information		12/02/2019 01:22 PM	2021-infrastructure-stable
2698	GROMACS	Task	In Progress	Normal	gmxapi documentation integration		01/29/2020 03:59 PM	2021-infrastructure-stable
2699	GROMACS	Task	New	Normal	Test POWER9		12/04/2019 03:29 PM	2021-infrastructure-stable

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2706	GROMACS	Task	Accepted	Normal	Rework classic QM/MM interface		12/02/2019 01:45 PM	2021-infrastructure-stable
2795	GROMACS	Task	New	Normal	Incorporate regressiontests into core gromacs		12/02/2019 01:44 PM	2021-infrastructure-stable
2994	GROMACS	Feature	New	Normal	Data flow topology in gmxapi 2020		12/11/2019 11:33 AM	2021-infrastructure-stable
2998	GROMACS	Task	Resolved	Normal	Update Python detection		04/23/2020 04:45 PM	2021-infrastructure-stable
2999	GROMACS	Task	New	Normal	Move all logging in core library and tools to use MDLogger		09/06/2019 02:36 PM	2021-infrastructure-stable
3010	GROMACS	Task	In Progress	Normal	upgrade OpenCL stack on bs-gpu01		12/20/2019 08:25 AM	2021-infrastructure-stable
3013	GROMACS	Task	New	Normal	Extend logging levels in MDLogger		09/06/2019 02:34 PM	2021-infrastructure-stable
3014	GROMACS	Task	In Progress	Normal	gmxapi example Python scripts		01/03/2020 11:00 AM	2021-infrastructure-stable
3015	GROMACS	Task	New	Normal	Create central log handle for calls to gmx_fatal		09/06/2019 02:34 PM	2021-infrastructure-stable
3032	GROMACS	Feature	Feedback wanted	Normal	Clean up dev-manual structure		12/11/2019 11:27 AM	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
3152	GROMACS	Feature	New	Normal	Infrastructure and patterns for expressing public interfaces		01/09/2020 05:19 PM	2021-infrastructure-stable
3153	GROMACS	Task	New	Low	Let CMake process module directories earlier to support more modern CMake idioms.		10/17/2019 10:40 AM	2021-infrastructure-stable
3171	GROMACS	Task	New	Normal	schedule CPU H2D force contribution in separate stream		12/20/2019 08:33 AM	2021-infrastructure-stable
3183	GROMACS	Task	Accepted	Normal	enable bonded interactions on GPU		12/20/2019 08:32 AM	2021-infrastructure-stable
3197	GROMACS	Bug	New	Normal	Rework usage of gitattributes and filter in source code formatting scripts		11/04/2019 12:50 PM	2021-infrastructure-stable
3220	GROMACS	Task	New	Normal	change rolling pruning scheduling with GPU update		02/25/2020 03:41 PM	2021-infrastructure-stable
3229	GROMACS	Task	New	Normal	Move checkpointing to the beginning of the MD step		01/16/2020 04:31 PM	2021-infrastructure-stable
3271	GROMACS	Task	Resolved	Normal	Adopt PEP-518 for Python package build system configuration.		04/09/2020 10:15 PM	2021-infrastructure-stable
3273	GROMACS	Bug	New	Normal	gmxapi setup.py complains too much		12/27/2019 06:42 PM	2021-infrastructure-stable
3274	GROMACS	Bug	New	Normal	Remove ARM NEON SIMD		12/28/2019 07:53 AM	2021-infrastructure-stable
3288	GROMACS	Feature	New	Normal	Use build system infrastructure instead of custom scripts to manage API levels.		02/26/2020 04:16 PM	2021-infrastructure-stable
3297	GROMACS	Task	Resolved	Normal	Require gcc > 5		04/30/2020 11:00 AM	2021-infrastructure-stable
3308	GROMACS	Task	New	Normal	GPU update-constraints: Cycle counting for GPU launches		01/23/2020 11:54 AM	2021-infrastructure-stable
3379	GROMACS	Feature	New	Normal	C++ API for simulation input and output		02/28/2020 10:38 AM	2021-infrastructure-stable
3401	GROMACS	Feature	New	Normal	Policy and procedure for installed headers (public API)		02/26/2020 04:17 PM	2021-infrastructure-stable
3402	GROMACS	Feature	New	Normal	Clarify distinction between public API documentation and developer docs.		02/26/2020 04:16 PM	2021-infrastructure-stable
3411	GROMACS	Bug	New	Normal	Nightly master release build failure		03/06/2020 11:44 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

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3155	GROMACS	Task	Accepted	Normal	Unify DD and CPU-GPU gather & scatter	Artem Zhmurov	10/17/2019 03:50 PM	2021-infrastructure-stable
3162	GROMACS	Task	New	Normal	Add virtual site support to GPU version of update-constraints.	Artem Zhmurov	01/23/2020 11:52 AM	2021-infrastructure-stable
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
3236	GROMACS	Task	New	Normal	GPU update-constraints: Pulling support	Artem Zhmurov	01/23/2020 11:53 AM	2021-infrastructure-stable
3246	GROMACS	Bug	Accepted	Normal	GPU code misses settle error check, simulation crashes with segfault without any further output	Artem Zhmurov	12/20/2019 09:52 AM	2021-infrastructure-stable
3258	GROMACS	Task	New	Normal	GPU update-constraints: Enable free energy perturbation	Artem Zhmurov	01/23/2020 11:54 AM	2021-infrastructure-stable
3337	GROMACS	Task	New	Normal	GPU update-constraints: Merge Leap-Frog, LINCS and SETTLE kernels.	Artem Zhmurov	01/23/2020 11:55 AM	2021-infrastructure-stable
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
3339	GROMACS	Task	New	Normal	GPU LINCS: Warp-level synchronization for coupled constraints	Artem Zhmurov	01/23/2020 11:55 AM	2021-infrastructure-stable
3340	GROMACS	Task	New	Normal	GPU LINCS: Move more data to local/shared memory	Artem Zhmurov	01/23/2020 11:56 AM	2021-infrastructure-stable
3341	GROMACS	Task	New	Normal	GPU LINCS: Use analytical solution for the matrix A inversion.	Artem Zhmurov	01/23/2020 11:56 AM	2021-infrastructure-stable
3342	GROMACS	Task	New	Normal	GPU SETTLE: Read only one index per water molecule.	Artem Zhmurov	01/23/2020 11:56 AM	2021-infrastructure-stable
3343	GROMACS	Task	New	Normal	GPU SETTLE: Use different ordering for matrices.	Artem Zhmurov	01/23/2020 11:57 AM	2021-infrastructure-stable
3344	GROMACS	Task	New	Normal	GPU update-constraints: Better virial reduction.	Artem Zhmurov	01/23/2020 11:57 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
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
3348	GROMACS	Task	New	Normal	GPU LINCS and SETTLE: unify virial reduction	Artem Zhmurov	01/23/2020 11:58 AM	2021-infrastructure-stable
2875	GROMACS	Task	Accepted	Normal	SIMD version of the free-energy kernel	Berk Hess	12/02/2019 01:44 PM	2021-infrastructure-stable
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
3072	GROMACS	Task	New	Normal	Use gm::index for indexing instead of int	Christian Blau	09/03/2019 04:23 PM	2021-infrastructure-stable
3076	GROMACS	Task	New	Normal	Selectively activate MdModules during simulation instead of instantiating all of them	Christian Blau	01/17/2020 02:40 PM	2021-infrastructure-stable

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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
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
3260	GROMACS	Task	New	Low	keep up to with mdspan reference implementation	Christian Blau	12/20/2019 01:16 PM	2021-infrastructure-stable
3284	GROMACS	Bug	New	Normal	gmx msd cannot output two xvg files as suggested by command line option	Christian Blau	01/08/2020 04:50 PM	2021-infrastructure-stable
2996	GROMACS	Feature	In Progress	Normal	gmxapi execution model	Eric Irgang	12/10/2019 01:57 PM	2021-infrastructure-stable
3038	GROMACS	Feature	New	Normal	Improvements to MD plugin development environment	Eric Irgang	12/10/2019 01:58 PM	2021-infrastructure-stable
3130	GROMACS	Task	New	Normal	Interim handling of gmxapi data references.	Eric Irgang	12/11/2019 11:26 AM	2021-infrastructure-stable
3133	GROMACS	Task	In Progress	Normal	Cookiecutter for sample_restraint	Eric Irgang	12/10/2019 01:59 PM	2021-infrastructure-stable
3136	GROMACS	Bug	New	Normal	gmxapi.operation data flow topology unclear or incomplete	Eric Irgang	12/11/2019 11:25 AM	2021-infrastructure-stable
3140	GROMACS	Feature	New	Normal	Allow explicit input definition for gmxapi.operation function wrapper	Eric Irgang	12/10/2019 02:00 PM	2021-infrastructure-stable
3141	GROMACS	Bug	New	Normal	gmxapi File placeholders missing from beta release	Eric Irgang	12/10/2019 02:02 PM	2021-infrastructure-stable
3147	GROMACS	Feature	New	Normal	gmxapi workflow checkpointing	Eric Irgang	10/15/2019 06:18 PM	2021-infrastructure-stable
3148	GROMACS	Feature	New	Normal	Roadmap for gmxapi filesystem interactions.	Eric Irgang	10/15/2019 06:23 PM	2021-infrastructure-stable
3150	GROMACS	Bug	New	Normal	gmxapi data type annotations are confusing and inadequate	Eric Irgang	10/22/2019 03:08 PM	2021-infrastructure-stable
3228	GROMACS	Bug	New	Normal	gmxapi.commandline_operation should gracefully handle input/output file arguments	Eric Irgang	12/04/2019 03:27 PM	2021-infrastructure-stable
3393	GROMACS	Feature	Resolved	Normal	Allow gmxapi.commandline_operation to use STDIN	Eric Irgang	02/25/2020 05:15 PM	2021-infrastructure-stable
3394	GROMACS	Feature	New	Normal	improve gmxapi error handling	Eric Irgang	02/24/2020 11:45 AM	2021-infrastructure-stable
3189	GROMACS	Task	In Progress	High	implement heuristics for switching between different spread/gather kernel layouts	Jonathan Vincent	01/29/2020 04:18 PM	2021-infrastructure-stable
3117	GROMACS	Feature	New	Normal	Coulomb FEP PME on GPU	Magnus Lundborg	02/17/2020 03:58 PM	2021-infrastructure-stable
2395	GROMACS	Task	In Progress	Normal	break up commrec	Mark Abraham	12/15/2019 11:51 AM	2021-infrastructure-stable
3131	GROMACS	Task	New	Normal	support ccache with clang-tidy	Mark Abraham	12/20/2019 08:20 AM	2021-infrastructure-stable
3363	GROMACS	Feature	New	Normal	Improve FEP testing	Pascal Merz	03/01/2020 03:22 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
3417	GROMACS	Feature	New	Normal	Make modular simulator feature-complete	Pascal Merz	03/23/2020 03:57 AM	2021-infrastructure-stable
3418	GROMACS	Task	New	Normal	Infrastructure improvements for modular simulator	Pascal Merz	03/10/2020 10:24 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
3420	GROMACS	Task	New	Normal	Unify force and shellfc elements for modular simulator	Pascal Merz	03/10/2020 09:50 PM	2021-infrastructure-stable

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3421	GROMACS	Task	New	Normal	Implement client system for global reduction	Pascal Merz	03/11/2020 03:31 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
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
3424	GROMACS	Feature	New	Normal	Implement stochastic dynamics / langevin integrator in modular simulator	Pascal Merz	03/10/2020 11:48 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
3426	GROMACS	Feature	New	Normal	Support acceleration in modular simulator	Pascal Merz	03/11/2020 04:09 PM	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
3428	GROMACS	Feature	New	Normal	Implement SIMD version of modular simulator propagators	Pascal Merz	03/11/2020 12:12 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
3431	GROMACS	Feature	New	Normal	Implement virtual sites for modular simulator	Pascal Merz	03/11/2020 12:33 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
3433	GROMACS	Feature	New	Normal	Decide how to handle multisim with modular simulator	Pascal Merz	03/11/2020 06:42 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
3435	GROMACS	Feature	New	Normal	Implement pull for modular simulator	Pascal Merz	03/11/2020 06:31 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
3437	GROMACS	Task	New	Normal	Use builders to prepare modules	Pascal Merz	03/11/2020 07:05 AM	2021-infrastructure-stable
2396	GROMACS	Task	New	Normal	Refactor trajectoryanalysis module to allow handling of trajectory frame manipulation	Paul Bauer	12/02/2019 01:24 PM	2021-infrastructure-stable
2833	GROMACS	Task	New	Normal	Update topology datastructures	Paul Bauer	12/02/2019 01:43 PM	2021-infrastructure-stable
2916	GROMACS	Task	New	Normal	Decide future of symtab	Paul Bauer	09/06/2019 02:35 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
3113	GROMACS	Bug	New	Low	Use of read_tps_conf is deprecated	Paul Bauer	10/01/2019 11:36 AM	2021-infrastructure-stable
3203	GROMACS	Task	Accepted	Normal	Tools should check that input is valid when first using it	Paul Bauer	12/03/2019 05:26 PM	2021-infrastructure-stable
3264	GROMACS	Task	New	Normal	Break up MdrunMpiTests	Paul Bauer	12/23/2019 11:44 AM	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
3275	GROMACS	Task	New	Normal	Document Gitlab CI instead of Jenkins and releng	Paul Bauer	03/09/2020 05:55 PM	2021-infrastructure-stable
3333	GROMACS	Bug	New	Normal	Assertion failure when trying to get unit test help	Paul Bauer	02/25/2020 10:16 AM	2021-infrastructure-stable
1587	GROMACS	Task	New	Normal	improve the configurability of regression tests		12/20/2019 12:02 PM	2021
1925	GROMACS	Task	In Progress	Normal	remove concept of unilateral global communication		12/29/2019 10:35 AM	2021
1985	GROMACS	Bug	Fix uploaded	Low	CUDA build system refactoring awaiting review		12/20/2019 12:07 PM	2021
2053	GROMACS	Task	New	Normal	refine notation in GPU code		12/20/2019 01:04 PM	2021
2059	GROMACS	Task	In Progress	Normal	Separate different types of data in t_state		12/27/2019 04:42 PM	2021

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2169	GROMACS	Task	New	Normal	remove 'continuation' mdp option		12/29/2019 10:31 AM	2021
2353	GROMACS	Task	New	Normal	improve on relative tolerance for constructing tables		12/20/2019 12:12 PM	2021
2390	GROMACS	Bug	Feedback wanted	Normal	GROMACS build system should check for valid nvcc flags before use		12/20/2019 12:13 PM	2021
2475	GROMACS	Task	New	Normal	make OpenCL 1st class-citizen in the build system		12/20/2019 12:14 PM	2021
2675	GROMACS	Task	In Progress	Normal	bonded CUDA offload task		02/12/2020 05:54 PM	2021
2686	GROMACS	Task	New	Normal	add tests for gpu bonded interactions		12/27/2019 04:40 PM	2021
2695	GROMACS	Task	New	Low	bonded GPU module timing		12/27/2019 04:40 PM	2021
2710	GROMACS	Feature	New	Normal	Separate dvdI for each molecule (of couple-moltype) when running FEP		12/27/2019 04:41 PM	2021
2770	GROMACS	Task	New	Normal	change branch maintenance policy		01/16/2020 05:09 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
2806	GROMACS	Feature	New	Normal	SIMD algorithms for ARM SVE // nobbonded cluster and others		12/27/2019 03:59 PM	2021
2839	GROMACS	Task	New	Normal	make module and file naming consistent		01/16/2020 05:11 PM	2021
2890	GROMACS	Feature	In Progress	Normal	GPU Halo Exchange		02/14/2020 12:41 PM	2021
2936	GROMACS	Task	New	Normal	introduce check that CPU-GPU transfers/assignments are made between compatible types		02/05/2020 03:57 PM	2021
2965	GROMACS	Task	In Progress	Normal	Performance of GPU direct communications		02/14/2020 12:38 PM	2021
2976	GROMACS	Task	New	Normal	Basic math for Multidimensional arrays		12/27/2019 04:37 PM	2021
2987	GROMACS	Bug	New	Normal	assess the bonded GPU task assignment default		12/20/2019 01:06 PM	2021
2997	GROMACS	Task	New	Normal	improve performance of alchemical free energy calculations		12/27/2019 04:31 PM	2021
3001	GROMACS	Task	New	Normal	explore simplifying virial and shift force reduction		12/27/2019 04:30 PM	2021
3008	GROMACS	Task	New	Normal	verify block size choice of CUDA bonded kernel		12/27/2019 04:30 PM	2021
3031	GROMACS	Task	New	Normal	evaluate the impact of particle order on PME		12/27/2019 04:29 PM	2021
3062	GROMACS	Task	New	Normal	add twin cut-off mdrun test		12/27/2019 04:22 PM	2021
3064	GROMACS	Task	New	Normal	add test for perturbed bonded forces		12/27/2019 04:22 PM	2021
3082	GROMACS	Task	New	High	move launch/synchronization points to clarify task dependencies		12/27/2019 04:21 PM	2021
3104	GROMACS	Task	New	Normal	implement GPU DD cycle counting		12/27/2019 04:21 PM	2021
3105	GROMACS	Task	New	Normal	implement GPU PME/PP comm cycle counting		12/27/2019 04:20 PM	2021
3119	GROMACS	Task	New	Normal	clang-tidy coverage of parallelization codepaths		12/27/2019 04:20 PM	2021
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
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
3277	GROMACS	Feature	New	Normal	Allow testing feature that is partly implemented		12/31/2019 12:44 PM	2021
3283	GROMACS	Feature	Resolved	Normal	Support for the string method with swarms of trajectories in GROMACS		03/01/2020 01:16 PM	2021
3356	GROMACS	Task	New	Normal	Expose setting of random seed to API		01/29/2020 06:16 PM	2021
2453	GROMACS	Task	Resolved	High	PME OpenCL porting effort	Aleksei lupinov	12/20/2019 12:18 PM	2021
3114	GROMACS	Feature	New	Normal	Improve GPU update-constraints module	Artem Zhmurov	02/10/2020 04:30 PM	2021
3350	GROMACS	Feature	New	Normal	GPU update-constraints performance	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
3352	GROMACS	Feature	New	Normal	GPU update-constraints feature support	Artem Zhmurov	01/23/2020 11:59 AM	2021
2192	GROMACS	Bug	Accepted	Low	grompp should read floats (e.g charge) from data files to double, to avoid accumulating round-off error	Berk Hess	12/20/2019 12:11 PM	2021
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
3410	GROMACS	Feature	New	Normal	Random Acceleration Molecular Dynamics (RAMD)	Bernd Doser	03/05/2020 03:22 PM	2021
2834	GROMACS	Task	In Progress	Normal	C++ matrix classes	Christian Blau	12/29/2019 10:32 AM	2021
2774	GROMACS	Feature	New	Normal	Refactor shell code into its own integrator	David van der Spoel	12/27/2019 04:05 PM	2021
868	GROMACS	Feature	In Progress	Normal	Implement parallelization support to analysis framework	Kevin Boyd	12/20/2019 11:59 AM	2021
2766	GROMACS	Task	In Progress	Normal	Improve hardware option selection	Kevin Boyd	12/20/2019 02:34 PM	2021
3371	GROMACS	Feature	New	Normal	Control FEP using AWH	Magnus Lundborg	02/06/2020 02:20 PM	2021
2425	GROMACS	Task	New	Normal	testing multisim with multiple ranks per simulation	Mark Abraham	12/20/2019 12:13 PM	2021
2480	GROMACS	Bug	New	Normal	pdb2gmx does not protonate correctly for united-atom Gromos	Mark Abraham	12/20/2019 12:17 PM	2021
2495	GROMACS	Task	Accepted	Normal	replace -noconfout with mdp option	Mark Abraham	12/28/2019 10:39 AM	2021
2832	GROMACS	Bug	New	Low	PaddedVector move operations broken	Mark Abraham	12/28/2019 10:40 AM	2021
2877	GROMACS	Task	New	Normal	use gm::Options more	Mark Abraham	12/20/2019 01:22 PM	2021
2944	GROMACS	Feature	New	Normal	Roadmap for thermostats / barostats in new propagation/integration scheme	Michael Shirts	12/27/2019 04:00 PM	2021
1943	GROMACS	Task	Accepted	Low	make sure releases are submitted early for Debian Experimental	Szilárd Páll	12/20/2019 12:05 PM	2021



#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
3057	GROMACS	Task	New	Normal	re-enable fusion on Power8/9	Szilárd Páll	12/27/2019 04:22 PM	2021
3143	GROMACS	Task	New	Normal	move the non-force accumulation/accounting tasks out of the GPU wait functions	Szilárd Páll	12/27/2019 04:16 PM	2021
2224	GROMACS	Feature	New	Normal	Proposed feature: conditional stop	Vedran Miletic	12/20/2019 12:11 PM	2021
1105	Benchmark suite	Feature	New	Normal	produce a benchmark suite		09/13/2016 10:31 PM	
1106	Benchmark suite	Feature	New	Normal	publish benchmark numbers		06/19/2014 12:08 PM	
677	GROMACS	Task	New	Normal	Make sure manual uses consistent style throughout		06/19/2014 11:49 AM	
731	GROMACS	Feature	New	Normal	pdb2gmx should warn about missing residues when bonds are too long		06/22/2014 10:55 AM	
838	GROMACS	Task	New	Normal	Improve generic error reporting routines		07/11/2016 08:29 PM	
921	GROMACS	Feature	Blocked, need info	Normal	Default index groups and selections		07/11/2016 08:27 PM	
950	GROMACS	Feature	New	Normal	Path/directory/filename handling in Gromacs		07/11/2016 08:24 PM	
1017	GROMACS	Task	New	Normal	C++ Vector/Matrix classes		07/11/2016 08:23 PM	
1026	GROMACS	Feature	New	Low	request for gen_vel to work with multiple temperature coupling groups at different temperatures		11/17/2016 04:39 PM	
1028	GROMACS	Feature	New	Normal	Tool to calculate fraction of native contacts during simulation		11/01/2012 10:27 PM	
1083	GROMACS	Feature	In Progress	Normal	Improve collective error/warning/note handling in mdrun		07/11/2016 08:21 PM	
1102	GROMACS	Feature	New	Normal	Detect incompletely written itp files		06/19/2014 03:23 PM	
1139	GROMACS	Feature	New	Normal	Adding the possibility to arbitrarily evaluate different components in the energy/force term when the energy/force is calculated		07/11/2016 08:19 PM	
1140	GROMACS	Task	New	Normal	Class design for passing options and data		07/11/2016 08:19 PM	
1328	GROMACS	Feature	Accepted	Normal	Names for selection positions		07/11/2016 08:15 PM	
1489	GROMACS	Feature	New	Normal	Don't solely rely on filename extension		04/30/2014 05:23 AM	
1511	GROMACS	Feature	Accepted	Normal	add PDBx (ie mmcif) support		10/05/2018 07:14 PM	
1523	GROMACS	Task	New	Normal	add missing code-paths to CUDA emulation kernel		07/11/2016 08:09 PM	
1530	GROMACS	Task	New	Low	Offer binary downloads		06/29/2014 02:58 PM	
1568	GROMACS	Bug	New	Low	inconsistent/incorrect threading checks and reporting in mdrun		05/25/2016 02:01 AM	
1583	GROMACS	Bug	New	Normal	gmx msd with mol flag requires excessive memory		12/18/2017 03:34 PM	
1602	GROMACS	Feature	New	Low	gmx order S per slice along all 3 axes		09/22/2014 07:25 AM	
1627	GROMACS	Feature	In Progress	Normal	DPD integrator		07/11/2016 08:08 PM	
1634	GROMACS	Feature	New	Normal	Boxed Molecular Dynamics		11/04/2014 04:40 PM	
1635	GROMACS	Feature	New	Normal	Proper Unicode support		06/18/2015 08:34 PM	
1641	GROMACS	Feature	New	Normal	Add toolchain file for Cray systems		06/06/2015 11:24 PM	

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
1655	GROMACS	Bug	New	Normal	g_membed and box type		12/09/2014 01:33 PM	
1670	GROMACS	Feature	New	Normal	create mdrun option checking mini-tool		06/23/2016 04:06 PM	
1688	GROMACS	Feature	New	Low	g_cluster "middle" is not exactly the same as the definition in the cited paper		04/01/2015 05:53 AM	
1745	GROMACS	Task	New	Normal	Moving to C++11 after Gromacs-5.1		06/01/2016 03:01 PM	
1770	GROMACS	Bug	New	Normal	segmentation fault with free energy changes and multiple GPU's		07/14/2015 03:24 AM	
1811	GROMACS	Bug	New	Normal	Extrae build issues		12/13/2017 03:43 AM	
1828	GROMACS	Task	New	Normal	Exception handling in mdrun		10/07/2015 11:36 AM	
1829	GROMACS	Task	New	Normal	Future of thread level parallelism		11/18/2016 05:29 PM	
1842	GROMACS	Feature	New	Normal	Replace XML with JSON		01/18/2018 05:12 PM	
1854	GROMACS	Feature	New	Normal	Remove all cyclic dependencies		05/25/2017 08:34 AM	
1855	GROMACS	Task	New	Normal	Convert preprocessor use so that symbols are always defined		06/28/2016 02:17 PM	
1862	GROMACS	Task	New	Normal	Fully replace t_topology by gmx_mtop_t		02/13/2019 04:53 PM	
1867	GROMACS	Feature	New	Normal	make coupling implementations reversible		12/02/2015 07:43 AM	
1885	GROMACS	Feature	New	Normal	DPD Thermostat		01/26/2016 10:17 AM	
1900	GROMACS	Feature	New	Normal	Implement some new errors in grompp		06/22/2016 05:20 PM	
1902	GROMACS	Feature	Accepted	Low	Add grompp check that non-excluded atoms are not too close to each other in the starting structure		02/15/2016 01:34 PM	
1907	GROMACS	Task	Accepted	Low	keeping compile- and run-time CPU/arch detection consistent		08/01/2016 10:09 PM	
1934	GROMACS	Bug	New	Normal	QMMM with ORCA: memory leaks, buffer overflows and much more		07/10/2016 09:26 AM	
1948	GROMACS	Feature	New	Low	add warning when non-identical GPUs are used		06/12/2017 08:45 PM	
1964	GROMACS	Feature	Accepted	Normal	"pull=no" should not produce warnings about "unknown" pull keywords		05/20/2016 02:37 PM	
1973	GROMACS	Task	New	Normal	OpenCL implementation wish list		05/27/2016 03:42 PM	
1974	GROMACS	Feature	New	Normal	Report atom numbers and types in the error message about missed parameters		05/30/2016 09:24 AM	
2001	GROMACS	Feature	New	Normal	add MPI info to the mdrun log header		07/06/2016 05:21 PM	
2003	GROMACS	Task	New	Normal	reconsider various simd flags		07/07/2016 11:23 PM	
2009	GROMACS	Task	New	Normal	improve command-line reporting of useful things		07/26/2016 12:54 PM	
2010	GROMACS	Task	New	Normal	Use size_t instead of int for indexing		07/01/2018 07:57 AM	
2015	GROMACS	Feature	New	Normal	Auto recovery from dd communication error		07/28/2016 03:17 PM	
2018	GROMACS	Feature	New	Normal	Pulling along a line between given points		07/27/2016 09:59 AM	
2039	GROMACS	Bug	New	Normal	mdrun -pinstride defaults are too confusing		12/13/2017 04:14 AM	
2048	GROMACS	Task	New	Normal	C++11: CUDA dependency on general headers		09/07/2016 10:30 PM	

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
2055	GROMACS	Task	New	Low	Wiki registration is broken		01/20/2017 11:31 AM	
2056	GROMACS	Feature	New	Low	rename "gmx select"		10/03/2016 08:24 PM	
2060	GROMACS	Feature	New	Normal	Convert enum to enum class		10/17/2016 05:27 PM	
2065	GROMACS	Bug	New	Normal	thread-MPI internal errors		11/08/2018 03:43 PM	
2069	GROMACS	Task	New	Low	Simple thread-parallelism inside routines		11/09/2016 06:06 PM	
2080	GROMACS	Feature	New	Normal	add grompp warning for suitability for domain decomposition		11/23/2016 03:03 PM	
2084	GROMACS	Task	New	Low	MPI and stderr/log output		11/28/2016 06:37 PM	
2089	GROMACS	Task	New	Normal	Encourage code review		01/10/2017 12:03 AM	
2094	GROMACS	Bug	New	Normal	Solvation Consistency with MARTINI forcefield water across GROMACS versions with user-specified VDW size		01/20/2017 04:56 PM	
2101	GROMACS	Feature	New	Low	warninp could print the offending line, as well as its number		01/20/2017 03:06 PM	
2111	GROMACS	Feature	In Progress	Normal	Implement Gaussian screening of electrostatics		02/23/2019 12:33 PM	
2113	GROMACS	Bug	New	Normal	Google tests and execution order		03/05/2018 02:05 PM	
2115	GROMACS	Task	New	Normal	trjconv does too many things, and combinations of them work poorly		10/02/2018 09:04 AM	
2118	GROMACS	Feature	New	Low	More verbose comments requested in header of gmx distance -oxyz		02/08/2017 05:46 AM	
2126	GROMACS	Feature	New	Normal	implement native CUDA support in CMake		10/29/2019 09:03 PM	
2133	GROMACS	Task	New	Low	gmx traj needs reform		03/07/2017 02:02 PM	
2139	GROMACS	Feature	New	Normal	More precise/explicit documentation conventions		01/07/2018 11:54 PM	
2147	GROMACS	Bug	Feedback wanted	Normal	Parrinello-Rahman barostat not properly working		06/06/2017 07:53 AM	
2158	GROMACS	Task	New	Normal	consider adding post-submit test that runs PME with 2xNN kernels		04/19/2017 08:04 PM	
2166	GROMACS	Task	Accepted	Normal	gmx trjconv functionality should check for mismatch between the tpr and the trajectory		05/05/2017 04:32 PM	
2178	GROMACS	Task	New	Normal	Move checks for specific warnings to source repo		05/12/2017 03:57 PM	
2182	GROMACS	Task	New	Low	de-duplicate code in densorder and hydorder		05/16/2017 11:29 AM	
2185	GROMACS	Task	New	Normal	add docs on MPI + CUDA w/wo MPS		05/24/2017 05:17 PM	
2194	GROMACS	Feature	Accepted	Low	xvg output requested as an output option in place of xpm files		05/31/2017 04:26 PM	
2207	GROMACS	Feature	New	Normal	solvent excluded volume of large molecule with periodic boundary condition		06/16/2017 10:37 AM	
2208	GROMACS	Bug	New	Normal	cuFFT linking		06/30/2017 01:58 PM	
2217	GROMACS	Bug	New	Low	GPU emulation and separate PME ranks doesn't work properly		12/12/2017 11:50 AM	
2218	GROMACS	Feature	Feedback wanted	Normal	A tiny feature: damping for umbrella pull		08/16/2017 07:20 PM	
2220	GROMACS	Feature	New	Normal	report relevant env var behaviour to console		07/31/2017 09:40 PM	
2221	GROMACS	Task	New	Normal	Avoid preprocessor for SIMD functions		02/21/2018 01:43 PM	

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
2226	GROMACS	Feature	New	Normal	Harmonise commands for exit in make_ndx and distance		08/04/2017 12:24 PM	
2231	GROMACS	Bug	New	Normal	convert-tpz aborts when saving subset of the system		01/12/2018 03:52 PM	
2232	GROMACS	Bug	New	Normal	pdb2gmx can't form special bonds with terminal patched atoms		12/03/2017 01:35 PM	
2233	GROMACS	Bug	Accepted	Normal	replica exchange and -append bugged?		03/05/2018 01:38 PM	
2239	GROMACS	Feature	New	Normal	split libgromacs into base and full		01/07/2019 01:47 AM	
2240	GROMACS	Task	Accepted	Low	GPU emulation mode support for PME missing		09/16/2017 10:02 PM	
2241	GROMACS	Bug	New	Low	refdata can segfault when reading		09/07/2017 11:57 AM	
2248	GROMACS	Feature	New	Normal	Label all SIMD functions as pure/nodiscard		02/04/2019 04:49 AM	
2252	GROMACS	Bug	New	Low	Memory allocation failures with large page sizes during PME tuning		12/14/2017 04:27 AM	
2254	GROMACS	Feature	Resolved	Normal	GPU extensions for Google Tests		10/06/2020 12:15 PM	
2255	GROMACS	Bug	New	Normal	nstlist override stopped affecting the input parameter listing		12/17/2017 08:05 AM	
2288	GROMACS	Feature	Accepted	Low	gmx msd doesn't optimally handle missing input trajectory frames		11/10/2017 11:03 AM	
2289	GROMACS	Feature	New	Normal	gmx spatial add ability to perform over multiple reference structures		11/08/2017 12:31 AM	
2294	GROMACS	Task	New	Normal	Require identical hardware on nodes on parallel runs		11/19/2017 08:54 PM	
2373	GROMACS	Bug	New	Low	gmx -nice can't work		01/04/2018 11:17 AM	
2375	GROMACS	Task	New	Normal	Clarify execution phases for MD simulation		04/30/2019 12:59 PM	
2376	GROMACS	Task	New	Normal	max_mpi_ranks has wrong name		02/10/2018 11:03 AM	
2380	GROMACS	Bug	New	Low	cycle counter issues with separate PME rank + GPUs		01/16/2018 10:21 PM	
2382	GROMACS	Task	New	Normal	Simplify Doxygen guidelines		01/13/2018 12:40 AM	
2393	GROMACS	Bug	New	Normal	incorrect error message with omitted command line flag before its argument		01/24/2018 11:24 PM	
2412	GROMACS	Task	New	Normal	attempt to do better FFTW planning		03/15/2018 05:01 PM	
2422	GROMACS	Task	New	Normal	write C kernel for tables in Verlet scheme		02/26/2018 01:38 PM	
2427	GROMACS	Bug	New	Normal	gmx select gives syntax error for selection involving evaluating simple arithmetic expression		02/27/2018 05:15 PM	
2428	GROMACS	Feature	New	Normal	Add way of selecting interactive arguments of pdb2gmx by string rather than an index		02/27/2018 06:28 PM	
2429	GROMACS	Feature	New	Normal	Add option of periodic chain topology to pdb2gmx		03/10/2018 01:01 PM	
2435	GROMACS	Task	New	Normal	identify and note about/tune task offload in GPU-bound runs		03/02/2018 04:08 PM	
2445	GROMACS	Task	New	Normal	Decide if/how to check for incompatible user input to mdrun for bonds and vsites		03/13/2018 02:02 PM	
2448	GROMACS	Task	Accepted	Normal	should mdrun -multidir permit only one directory?		03/21/2018 12:10 PM	
2456	GROMACS	Task	New	Normal	Add a pull module external potential tests		03/15/2018 03:02 PM	
2460	GROMACS	Bug	New	Normal	Allow inclusion of user libraries through CMake cache variables		03/28/2018 08:47 PM	

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
2462	GROMACS	Task	New	Normal	consider adding STL misuse tests		03/23/2018 01:23 AM	
2463	GROMACS	Task	New	Low	PME GPU decomposition		03/26/2018 10:42 AM	
2464	GROMACS	Task	New	Normal	GPU performance goals overview		03/26/2018 10:42 AM	
2469	GROMACS	Task	New	Normal	implement GPU timer reduction for reporting		03/27/2018 05:08 PM	
2473	GROMACS	Bug	New	Normal	mdrun sometimes stalls due to large coordinates with no constraints		04/04/2018 10:15 PM	
2478	GROMACS	Task	New	Low	avoid use of getenv in static initialization		04/13/2018 11:57 AM	
2482	GROMACS	Bug	Feedback wanted	Normal	Atoms/molecules in freezegrps move and system crashes		05/18/2018 07:13 PM	
2488	GROMACS	Task	New	Normal	use MPI non-blocking collectives to overlap pull comm		04/25/2018 04:19 PM	
2496	GROMACS	Task	New	Low	find system xdr properly		05/02/2018 02:19 PM	
2519	GROMACS	Task	New	High	Improve/remove PME OpenCL kernel barriers		02/15/2019 06:34 PM	
2520	GROMACS	Task	New	Normal	Treat OpenCL kernel width more diligently		05/24/2018 06:21 PM	
2521	GROMACS	Task	New	Normal	Implement alternating PME/NB wait for OpenCL		10/15/2018 12:39 PM	
2526	GROMACS	Bug	New	Normal	Bug of gmx hbond		05/30/2018 03:12 PM	
2531	GROMACS	Task	New	Low	Consider optimizing tabulated data access on GPU		07/30/2018 12:31 PM	
2532	GROMACS	Task	New	Normal	enable queue priorities in OpenCL		05/29/2018 02:29 PM	
2535	GROMACS	Task	New	Normal	consider compiling opencl fft kernels once		05/31/2018 01:33 PM	
2555	GROMACS	Bug	New	Low	building GROMACS 2018.2		07/03/2018 11:41 PM	
2563	GROMACS	Bug	New	Normal	Windows 7 Compilation with GPU support		07/02/2018 09:58 AM	
2564	GROMACS	Bug	New	Normal	Result Summary Different For Jobs With Different Numbers of Nodes		07/05/2018 02:39 PM	
2567	GROMACS	Bug	New	Normal	make check fails at test 23 SIMD errors		07/10/2018 09:35 AM	
2570	GROMACS	Feature	New	Normal	Better string formatting and printing		05/02/2019 12:20 PM	
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	
2576	GROMACS	Bug	New	Normal	gmx potential -correct outputs the wrong potential		07/25/2018 02:58 PM	
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	
2585	GROMACS	Feature	Resolved	Normal	Infrastructure supporting external API		12/11/2019 12:39 PM	
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	
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	
2602	GROMACS	Bug	New	Low	build information gets outdated if build tree is reused		08/13/2018 09:04 PM	

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
2606	GROMACS	Bug	New	Normal	Free Energy Calculation -- Function type Fourier Dih. Not implemented in ip_pert		08/10/2018 01:48 AM	
2607	GROMACS	Bug	New	Normal	Grompp becomes extremely slow when many pull groups are present		08/11/2018 08:54 AM	
2608	GROMACS	Task	New	Normal	Remove code duplication between OpenCL and CUDA		09/24/2018 12:47 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	
2616	GROMACS	Task	New	Normal	Model for MD state		09/14/2018 05:12 PM	
2624	GROMACS	Bug	New	Normal	GPU build system not robust enough		09/05/2018 02:00 AM	
2628	GROMACS	Bug	Resolved	Normal	GMXRC removes trailing colon from existing MANPATH		11/02/2020 11:45 AM	
2637	GROMACS	Bug	New	High	gmx solvate tears apart molecules		09/11/2018 07:43 PM	
2643	GROMACS	Feature	New	Low	mdp options and/or docs for anisotropic aspects of implementations		09/12/2018 02:23 PM	
2645	GROMACS	Bug	New	Normal	Security		09/28/2018 01:16 PM	
2657	GROMACS	Bug	New	Normal	Biphasic tutorial		09/28/2018 10:02 AM	
2670	GROMACS	Task	New	Low	remove old/backward compatibility OpenCL support from releng		10/04/2018 06:06 PM	
2682	GROMACS	Task	New	Normal	Add MSAN configuration		10/09/2018 06:28 PM	
2702	GROMACS	Bug	Accepted	Normal	PME gather reduction race in OpenCL (and CUDA)		03/28/2019 03:14 PM	
2707	GROMACS	Bug	New	Normal	Installed OpenCL files include clh file from gpu_utils directory		10/30/2018 04:02 AM	
2713	GROMACS	Feature	New	Normal	Constant offset for external electric fields		10/28/2018 12:57 AM	
2739	GROMACS	Feature	New	Normal	Parallel continuous tempering and enhanced sampling feature		11/13/2018 11:36 PM	
2761	GROMACS	Feature	New	Low	lincs-order 4 is too conservative for some force fields		11/16/2018 09:55 AM	
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	
2785	GROMACS	Bug	New	Normal	Inconsistent and erroneous behaviour of trjconv when writing a partial TNG		11/30/2018 02:36 PM	
2787	GROMACS	Task	New	Normal	allow passing flags to allocateDeviceBuffer		12/03/2018 01:54 PM	
2788	GROMACS	Bug	New	Normal	PME will not run on AMD GPU with NVidia GPU present		01/03/2019 02:24 PM	
2792	GROMACS	Task	New	High	Improvement of PME gather and spread CUDA kernels		03/18/2020 03:57 PM	
2796	GROMACS	Task	New	Low	clarify what mdrun -cpt means		01/03/2019 02:09 PM	
2828	GROMACS	Bug	Feedback wanted	Normal	Installation issue on Power 9 system with SIMD support		01/18/2019 11:54 AM	
2835	GROMACS	Task	New	Normal	Matrix class constraint to upper or lower triangle		02/07/2019 02:44 PM	
2846	GROMACS	Feature	New	Low	Set rpath in FindLibStdCmake		02/02/2019 08:09 AM	
2848	GROMACS	Bug	New	Normal	gmx make_ndx ignores last residue in case only CA's are present in GRO file		01/30/2019 06:16 AM	

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
2852	GROMACS	Bug	New	Low	the in-tree regressiontest download can get out of sync with code		01/30/2019 03:58 PM	
2855	GROMACS	Task	New	Normal	Allow compiling GROMACS without C compiler		01/10/2020 12:06 PM	
2857	GROMACS	Task	New	Normal	Clarify recommended function specifies (constexpr, noexcept, pure)		02/04/2019 04:48 AM	
2859	GROMACS	Task	Resolved	Normal	Change ArrayRef iterator type from pointer to std::iterator		06/26/2020 06:15 PM	
2860	GROMACS	Feature	New	Normal	Option for outputting min/max coordinates in gmx traj		02/08/2019 12:35 AM	
2863	GROMACS	Task	New	Normal	improve PBC handling		03/11/2019 04:28 PM	
2869	GROMACS	Bug	New	Normal	GPU detection error only issued as a note to the log		03/05/2019 04:09 PM	
2870	GROMACS	Bug	New	Normal	GPU detection error message missing from the output		03/05/2019 03:55 PM	
2872	GROMACS	Bug	New	Normal	gmx solvate and genion topology update		02/27/2019 10:18 AM	
2873	GROMACS	Bug	New	Normal	Simple way to get last frame from trajectory		02/28/2019 11:14 PM	
2883	GROMACS	Bug	New	Normal	essentialdynamics fail with Intel MPI		03/08/2019 03:10 AM	
2891	GROMACS	Feature	In Progress	Normal	PME/PP GPU communications		02/14/2020 12:40 PM	
2897	GROMACS	Bug	New	Normal	rotation/flex2 can still fail on cpu-only run on OpenCL build		04/04/2019 06:24 PM	
2898	GROMACS	Task	New	Low	Naming common variables		03/26/2019 11:46 PM	
2902	GROMACS	Bug	New	Normal	2019.1 equilibration issue? (Intel 2018u3)		04/30/2019 08:17 AM	
2905	GROMACS	Task	New	Normal	Add a Jenkins configuration with std library assert		08/24/2019 05:22 PM	
2907	GROMACS	Bug	New	Normal	Gromacs autocompletion appears to be broken with ZSH		07/16/2019 04:46 AM	
2909	GROMACS	Task	New	Normal	consider implementing mechanisms to ensure pair lists are not used past their max lifetime		04/03/2019 05:14 PM	
2910	GROMACS	Feature	New	Normal	Mixed scaling for 1-4 interactions		04/10/2019 10:13 PM	
2915	GROMACS	Feature	In Progress	High	GPU direct communications		02/14/2020 12:48 PM	
2919	GROMACS	Task	New	Normal	C++ style guidelines for namespace use		04/15/2019 01:21 PM	
2924	GROMACS	Bug	New	Normal	Failing version check when reading new tpr file with older gromacs version		04/12/2019 10:52 AM	
2928	GROMACS	Feature	New	Normal	Add ability to use expression "count of ATOM_EXPR" in selection statements.		04/16/2019 04:52 PM	
2930	GROMACS	Feature	New	Normal	Limited range for reference group detection in cylinder pulling		04/26/2019 05:17 PM	
2931	GROMACS	Feature	New	Normal	Tables in Verlet kernels		04/29/2019 12:01 PM	
2933	GROMACS	Task	New	Normal	Convert walls to a ForceProvider		04/25/2019 02:43 PM	
2948	GROMACS	Bug	New	Normal	SIMD support detected as none on AMD R5 2500U		05/21/2019 12:58 PM	
2949	GROMACS	Bug	New	Normal	cmake fails when building mdrun only		07/08/2019 10:04 AM	
2954	GROMACS	Bug	New	Normal	genion changes residue numbering		05/26/2019 12:08 AM	
2956	GROMACS	Feature	New	Normal	SAXS resolution		05/17/2019 09:58 AM	

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2961	GROMACS	Feature	New	Normal	How should Python package find GROMACS resources under various circumstances?		12/09/2019 10:47 AM	
2975	GROMACS	Feature	New	Normal	LJ PME calculations on GPUs		06/12/2019 01:17 PM	
2977	GROMACS	Feature	New	Normal	print DD load balancing improvement		06/13/2019 10:56 AM	
2978	GROMACS	Bug	New	Normal	Some suggestions about the gmx current tool		06/13/2019 12:41 PM	
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	
2981	GROMACS	Bug	New	Normal	segfault in openc1 build		06/18/2019 03:30 AM	
2983	GROMACS	Task	New	Normal	better suited data-types for bonded GPU kernels		07/11/2019 04:32 PM	
3000	GROMACS	Bug	New	Normal	CMake "webpage" target does not fail when it should		06/25/2019 02:43 PM	
3002	GROMACS	Task	New	Normal	consider splitting bonded work into local/nonlocal		06/25/2019 04:06 PM	
3003	GROMACS	Task	New	Normal	implement heuristic fallback to CPU when there is too little work for GPU offload		06/25/2019 04:10 PM	
3004	GROMACS	Task	New	Normal	Move trajectory analysis logging to MDLogger		06/26/2019 09:59 AM	
3005	GROMACS	Task	New	Normal	Move logging in gmx preprocess to MDLogger		06/26/2019 10:01 AM	
3016	GROMACS	Task	New	Normal	intermittent failure of essentialdynamics test		07/18/2019 05:23 PM	
3020	GROMACS	Feature	New	Low	modernize DeviceBuffer and GPU memory management		08/13/2019 06:01 PM	
3028	GROMACS	Bug	Feedback wanted	Normal	install fail on Centos 6		07/15/2019 12:32 PM	
3030	GROMACS	Feature	New	Normal	RST style guidelines		07/09/2019 03:38 PM	
3040	GROMACS	Task	New	Normal	Refactor Restraint module		07/18/2019 03:59 PM	
3041	GROMACS	Task	Resolved	Normal	Remove workaround for gcc bug 58265		06/19/2020 04:45 PM	
3042	GROMACS	Bug	New	Normal	core dump error in grompp command		10/09/2019 07:30 PM	
3045	GROMACS	Feature	New	Low	Option to remove v-sites in trjconv?		07/19/2019 04:42 PM	
3047	GROMACS	Task	Feedback wanted	Normal	Set required versions for GROMACS 2021		02/20/2020 11:42 AM	
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	
3054	GROMACS	Bug	New	Normal	Missing dihedral define		08/02/2019 05:47 PM	
3055	GROMACS	Bug	Feedback wanted	Normal	Error in gmx xpm2ps		08/22/2019 03:27 PM	
3058	GROMACS	Bug	Feedback wanted	Normal	Error when using a large PME grid on a GPU		09/04/2019 07:26 PM	
3068	GROMACS	Bug	New	Normal	Misleading warning on rerun		08/26/2019 03:44 PM	



#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
3073	GROMACS	Bug	New	Normal	Total potential energy goes crazy, but I don't know why this happens.		09/04/2019 07:25 PM	
3077	GROMACS	Task	Feedback wanted	Normal	PME/PP GPU Comms unique pointer deletion causes seg fault when CUDA calls exist in destructor		11/01/2019 06:56 PM	
3078	GROMACS	Task	New	Normal	Allow MD modules to register energy output fields themselves		09/06/2019 11:36 AM	
3083	GROMACS	Bug	New	Normal	Listed forces tests failing on ICC19 with AVX2_256 nightly build		09/10/2019 11:56 AM	
3086	GROMACS	Bug	New	Normal	gmxapi fails with MPI build of GROMACS 2020		09/25/2019 04:18 PM	
3088	GROMACS	Bug	New	Normal	Reference to theory needed for cylindrical pull geometry		09/13/2019 11:26 AM	
3115	GROMACS	Feature	New	Normal	Device stream manager		10/04/2019 09:00 AM	
3123	GROMACS	Task	New	Normal	address sanitizer coverage of parallelization code-paths		10/05/2019 12:32 AM	
3126	GROMACS	Feature	New	Normal	State propagator GPU data manager		10/09/2019 02:42 PM	
3127	GROMACS	Bug	New	Normal	mdrun-mpi-test -ntmpi 2 runs out of memory with OpenCL on Nvidia		10/09/2019 05:33 PM	
3132	GROMACS	Task	New	Normal	gmxapi testing support tools		10/31/2019 03:35 PM	
3135	GROMACS	Feature	New	Normal	Make GPU traits ino opaque types		10/14/2019 10:24 AM	
3138	GROMACS	Feature	New	Normal	Improve ensemble support in Context specification.		10/15/2019 03:56 PM	
3154	GROMACS	Task	Resolved	Low	Update use of Python subprocess for >=3.5		04/09/2020 10:15 PM	
3165	GROMACS	Bug	New	Normal	task assignment silent abort		10/18/2019 07:46 PM	
3166	GROMACS	Bug	New	Normal	Compilation failing on Ubuntu 19.04 with Cuda 10.1		10/19/2019 09:13 PM	
3177	GROMACS	Feature	New	Normal	Spack package management support		11/06/2019 06:37 PM	
3181	GROMACS	Task	New	Normal	consolidate task assignment and workload data initialization		10/28/2019 02:53 PM	
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	
3186	GROMACS	Task	In Progress	Normal	Update Constant/Variable naming in the PME GPU kernels.		10/30/2019 11:23 AM	
3187	GROMACS	Task	New	Normal	Template updated PME kernels using threads per atom		10/30/2019 11:33 AM	
3194	GROMACS	Task	New	Normal	consider passing GPU dependency list to both dependency producers and consumers		11/01/2019 07:10 PM	
3196	GROMACS	Bug	New	Normal	ExponentialMovingAverage.DeterminesCorrectlyIfIncreasing failing		11/01/2019 11:28 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	
3201	GROMACS	Task	In Progress	Normal	Convert mdp parameters to key value tree		11/06/2019 06:06 PM	
3202	GROMACS	Bug	New	Low	gmx solvate fails to overwrite topology file		11/13/2019 02:44 PM	
3209	GROMACS	Bug	New	Normal	Interactive molecular dynamics with VMD becomes stuttering after reconnecting		11/19/2019 11:36 AM	
3210	GROMACS	Bug	New	High	rerun does not reproduce dVcoul/dl		12/27/2019 10:45 AM	

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
3212	GROMACS	Task	New	Normal	Update regression tests for new kernel flavours		11/21/2019 11:50 AM	
3213	GROMACS	Bug	New	Normal	Having a local residuetypes.dat for custom force field		11/21/2019 09:18 PM	
3214	GROMACS	Bug	New	Normal	Out-of-bounds, overflow and incorrect outputs in gmx spatial		11/25/2019 04:11 PM	
3219	GROMACS	Bug	Resolved	Normal	MANPATH setting is fragile		11/02/2020 11:45 AM	
3223	GROMACS	Bug	New	Normal	unit test failures give verify -1		12/02/2019 11:58 AM	
3227	GROMACS	Bug	New	Normal	solvate does not check return status of gmx_file_rename		12/04/2019 01:43 PM	
3233	GROMACS	Bug	New	Normal	clang-format incorrectly aligning altered function arguments		12/13/2019 12:41 PM	
3239	GROMACS	Bug	New	Normal	GPU DD direct communication with GPU update error with RF		12/14/2019 05:15 PM	
3240	GROMACS	Bug	New	Normal	segv with GPU DD direct communication with GPU update and -dlb off		01/15/2020 06:16 PM	
3242	GROMACS	Feature	New	Normal	Please do not remove the -nsteps flag		03/01/2020 01:59 PM	
3243	GROMACS	Bug	Feedback wanted	Normal	Convert GROMACS 1 OpenMP thread per rank fatal error into a warning		12/27/2019 10:31 AM	
3252	GROMACS	Task	New	Normal	Remove support for 32 bit architectures		03/01/2020 02:05 PM	
3254	GROMACS	Task	New	Normal	Remove support for generation of virtual sites to replace aromatic rings in standard residues		12/19/2019 12:13 PM	
3255	GROMACS	Task	New	Normal	Move benchmarking options from mdrun to a dedicated tool		12/19/2019 01:21 PM	
3256	GROMACS	Task	New	Normal	Remove -nsteps option from mdrun		12/19/2019 12:12 PM	
3262	GROMACS	Task	New	High	Trjconv - dimer protein-ligand		12/20/2019 09:26 PM	
3268	GROMACS	Task	New	Normal	add more Intel driver recommendations		12/26/2019 04:39 PM	
3279	GROMACS	Task	New	Low	Provide more advice for building client software		03/02/2020 11:54 AM	
3281	GROMACS	Bug	New	Normal	Test data directory GMX_RELEASE_ASSERT triggers		01/06/2020 08:07 PM	
3287	GROMACS	Task	New	Normal	Deprecate make_ndx, use select instead		01/23/2020 01:16 PM	
3298	GROMACS	Feature	New	Normal	start early PP work for first dimension of halo exchange		03/01/2020 01:36 PM	
3300	GROMACS	Task	New	Normal	Abandon docs/OpenCLTODOList.txt?		01/15/2020 02:46 PM	
3301	GROMACS	Bug	New	Normal	pdb2gmx adding hydrogen		01/15/2020 10:17 PM	
3305	GROMACS	Bug	New	Normal	Case gives FPE with Debug build when GPU update is enabled		01/21/2020 05:44 PM	
3309	GROMACS	Bug	New	Normal	-reprod: checkpoint reading bug and general considerations		02/27/2020 10:45 PM	
3310	GROMACS	Bug	Blocked, need info	Low	Thread affinity on Mac OS		02/27/2020 11:10 PM	
3332	GROMACS	Feature	New	Normal	gmx helixorient doesn't have a -tu option to change time unit		01/22/2020 11:57 AM	
3353	GROMACS	Task	New	Normal	Document gmx densmap output		01/23/2020 12:52 PM	
3357	GROMACS	Task	New	Normal	Make sure "colvars" interoperates stably and smoothly with gromacs		03/04/2020 11:25 AM	

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
3360	GROMACS	Task	New	Normal	investigate the future of DD dynamic load balancing with GPU offload		01/29/2020 11:23 AM	

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